

Book of Abstracts



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Welcome from Marián Slodička, Conference Chair

Dear participant,

First of all I wish to welcome you to the city of Ghent. We will have over one hundred talks during this week with participants from 29 countries!

This is already the sixth edition of the international conference on "Advanced COmputational Methods in ENgineering". Like the previous editions the conference themes are concentrated on mathematical modeling, simulation and numerical methods for solving scientific problems from various engineering disciplines. I would like to thank all of its participants because they turn every ACOMEN into an interesting, learning-full and pleasant event.

Another important factor of the success of ACOMEN are the highstanding invited main lectures given by world-wide recognized experts in their respective research fields: Gregoire Allaire (Ecole Polytechnique), Larisa Beilina (Chalmers University of Technology and Göteborgs universitet), Kai-Uwe Bletzinger (Technische Universität München), Oscar P. Bruno (California Institute of Technology), Axel Klawonn (Universität zu Köln), Youssef Marzouk (Massachusetts Institute of Technology), Andrew Stuart (The University of Warwick) and Enrique Zuazua (Basque Center for Applied Mathematics).

I also thank the session chairs and organizers of the mini symposia for their engagement; Marnix Van Daele, Florin Adrian Radu, Markus Bause, Andriy Sokolov, Jürgen Fuhrmann, Herbert De Gersem, Jens Förstner, Denis Constales, Sebastian Schöps, Erik Dick, Jan Vierendeels, Stefan Kurz, Stéphane Lanteri, Gert Van den Eynde, Hendrik Rogier, Tim Boonen and Stéphane Clenet.

Special thanks goes to the organizational team of this years edition, all technical staff working behind the scenes, and in particular Rob De Staelen, conference secretary.

Should you have any questions or specific needs during our meeting, we are more than glad to help you at the conference reception desk.

I hope you will enjoy your stay!

Kind regards, Marián Slodička



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Advanced COmputational Methods in ENgineering





Numerics for large-time horizon control of scalar conservation laws

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Abstract

In this lecture we will highlight the importance of employing proper discretization schemes when dealing with optimal control problems in long time horizons.

We focus on scalar conservation laws for which there is a clear dichotomy in what concerns their large time behavior. In the presence of viscosity, solutions behave like self-similar viscous nonlinear waves, while in the inviscid case they develop a N-wave like hyperbolic dynamics.

First, we discuss the various possible numerical solvers, and show that some of them fail to preserve the hyperbolic dynamics, due to the too large numerical diffusion introduced by the scheme. This allows classifying the schemes into two categories: those that preserve the large time dynamics and those that do not.

We then address an optimal control problem in a long time horizon, motivated by the problem of sonic-boom control of supersonic aircrafts ([2]). We show that when the problem is solved employing a numerical scheme that does not preserve the asymptotic dynamics, this often leads to a wrong minimizer, polluted by high frequency purely numerical spurious oscillations.

Our analytical results will be complemented with numerical simulations that confirm fully the predicted pathologies.

This presentation is based on earlier works in collaboration with C. Castro (Madrid), L. Ignat (Bucharest) and F. Palacios (Stanford).

Key words: Burgers equation, inverse problem, optimal control, optimization, large time.

1 Summary of the talk

Given a time T > 0 and a target function u^* we would like to minimize the following functional:

$$\mathcal{J}(u_0) = \frac{1}{2} \int_{\mathbb{R}} \left(u(x,T) - u^*(x) \right)^2 dx, \tag{1}$$

where u is the solution of the viscous Burgers equation

$$\begin{cases} \partial_t u + \partial_x \left(\frac{u^2}{2} \right) = v \partial_{xx} u, & x \in \mathbb{R}, t > 0, \\ u(x,0) = u_0(x), & x \in \mathbb{R}. \end{cases}$$
(2)

The control problem set in (1)-(2) can be viewed as a classical inverse problem, in the sense that for a given target function u^* , one can solve the equation backwards from datum u^* at time *T* to obtain the initial condition u_0 . But, of course, this may lead to a very unstable process due to the intrinsic ill-posedness of the problem under consideration.

The goal of this lecture is to discuss to which extent the numerical results developed to approximate the minimizers may lead to different results, depending on the numerical scheme one uses to approximate the nonlinear PDE under consideration. As we shall see, and it is expectable, some schemes approximate better the original dynamics in long time than others. But this difference can be dramatically enhanced when addressing the optimization problem above, a fact that could lead to catastrophic results.

At the analytical level it is well known that the solutions to the inviscid Burgers equation (v = 0) may develop shocks and that, if $u_0 \in L^1(\mathbb{R})$, they converge to the so-called N-wave (c.f. [9]). This behavior differs significantly for the viscous version (2), which is of parabolic nature (see [6]). Nevertheless, when v is sufficiently small and t is large (but not enough for the viscosity to be dominant), the behavior of the solutions is close to the hyperbolic case [8].

This phenomena needs to be handled carefully at the numerical level, when solving (2) with usual monotone conservative schemes ([5]). Indeed, in [7], the numerical parabolic-hyperbolic dichotomy is observed in the inviscid case. More precisely, it was shown that some numerical schemes when, in principle, designed to approximate the hyperbolic dynamics, may lead to viscous profiles in long time horizons.

In this talk, following [1], we will explain this issue and illustrate its possible consequences when addressing the optimization problem above. We shall mainly discuss the Engquist-Osher (EO) scheme, which is well behaved in what concerns the long time dynamics, and the modified Lax-Friedrichs (LFM) one which adds too much numerical viscosity destroying eventually the N-waves to generate viscous profiles. In Figure 1 we describe this fact.

To numerically approximate the minimizers of (1) we consider a simple quadrature rule:

$$\mathcal{J}_{\Delta}(u_{\Delta}^0) = \frac{\Delta x}{2} \sum_{\mathbb{Z}} (u_j^N - u_j^*)^2, \tag{3}$$

 u_i^k being the numerical solution achieved by means of a monotone scheme.

Let us choose T = 50 and the following target function:

$$u^{*}(x) = \begin{cases} \frac{3}{2000} \left(-e^{-(5\sqrt{20}+x)^{2}} + e^{-(2\sqrt{20}+x)^{2}} + \sqrt{\pi} x \left(\operatorname{erf}(5\sqrt{20}-x) + \operatorname{erf}(2\sqrt{20}+x) \right) \right), & |x-5| \le 25, \\ 0, & \text{elsewhere.} \end{cases}$$
(4)

Let us consider a space interval [-30, 50], which is large enough to avoid boundary effects. Regarding the time-step, we take it according to the CFL condition for LFM [5], that is

$$\frac{\Delta t}{\Delta x} \max_{j} |u_{j}^{0}| + v \frac{\Delta t}{\Delta x^{2}} \le \frac{1}{2}$$
(5)

Note that EO has a less restrictive CFL condition [3], but we take (5) as well in order to have the same Δt for both schemes.

We now apply a gradient descent method (GDM) from the function $u_0 = 0$ and perform 300 iterations of the GDM. For each of the numerical fluxes, we repeat the experiment using a mesh-size $\Delta x = 0.1, 0.2, 0.4, 0.8$.

[paper 1]





Figure 1: Plot of solutions of (2) from [1] with $v = 10^{-6}$ at t = 1, t = 100 and t = 5000, with $\Delta x = 0.2$ and numerical fluxes EO (dotted) and LFM (solid).

As we observe in Figure 2, using EO we are able to compute a quite satisfactory minimizer even for $\Delta x = 0.8$, which returns an optimal value below 10^{-6} . As Δx becomes smaller, the obtained result is even better (solid lines in Figure 4). This shows the robustness of the method, since the optimal solution is similar in the four cases.



Figure 2: [1]: Optimal solutions (dark) for (1)-(2) with $\nu = 10^{-4}$, obtained after 300 iterations of GDM+EO, and their corresponding state at time T = 50 (light) compared to the target (dotted). From left to right and top to bottom, $\Delta x = 0.8$, 0.4, 0.2 and 0.1 respectively.

Nevertheless, as we expected, the GDM did not perform so well when coupled with LFM. In fact, in Figure 3 we observe that a large enough mesh-size introduces spurious oscillations in the solution. Let us recall that LFM introduces numerical viscosity which is proportional to Δx^2 . Therefore, the dynamics of the numerical solution finds it complicated to preserve the negative part and, hence, it requires those oscillations in order to maintain the N-wave shape after large periods of time. Moreover, Figure 4 shows that the results obtained this way were always worse than the ones obtained using EO. Note that, despite the oscillations, the optimal solution approaches the one obtained using EO as Δx gets smaller. Thus, the method seems to be robust once the mesh-size is small enough.

The same experiments have been performed using the IPOPT optimization platform ([4], [10]) exhibiting a similar behavior but also an enhanced sensitivity with respect to the initialization chosen.





Figure 3: [1]: Optimal solutions (dark) for (1)-(2) with $\nu = 10^{-4}$, obtained after 300 iterations of GDM+LFM, and their corresponding state at time T = 50 (light) compared to the target (dotted). From left to right and top to bottom, $\Delta x = 0.8$, 0.4, 0.2 and 0.1 respectively.



Figure 4: [1]: Descent of the functional *J* after 300 iterations of the GDM coupled with EO (light) and LFM (dark), using $\Delta x = 0.8$, $\Delta x = 0.4$, $\Delta x = 0.2$ and $\Delta x = 0.1$ respectively, for the case $v = 10^{-4}$ and T = 50.

2 Conclusions and perspectives

The main conclusions that will be highlighted in this lecture are as follows:

- The optimization results obtained depend significantly on the discretization methods (EO or LFM) and, more precisely, on the way each discretization scheme alters the dynamics of the Burgers equation.
- The performance of LFM is not satisfactory. The initial data obtained are quite oscillatory in the vicinity of sharp slopes for large cell sizes. The spurious oscillations are due to the numerical viscosity inherent in the LFM method and they do not have any physical significance in relation with the dynamics of the true continuous Burgers equation.
- The numerical viscosity present in LFM is proportional to the square of the cell size $(\Delta x)^2$. The numerical viscosity is adjusted by the size of cells and hence the solution to the optimization problem depends on the mesh-size.
- The performance of EO is satisfactory. The obtained initial data is less sensitive to the choice of the cell size Δx and domain discretization. Furthermore, not only EO results



are less sensitive to the domain discretization, but also they are less sensitive to the initialization of the variables.

- The discretization scheme can alter the underlying continuous dynamics of the equation. For example, the oscillatory optimal initial datum obtained with LFM is not a best fit for the functional if the initial datum is evolved in time with EO scheme in forward mode, showing the unsuitability at the continuous level.
- The possibility of presence of multiple local minima in the functional landscape is excluded.

Acknowledgments

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A convergent mass conservative numerical scheme for two-phase flow in porous media by mixed finite elements

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Abstract

In this work we present a mass conservative numerical scheme for two-phase flow in porous media. The flow model consists of two fully coupled, nonlinear equations: a degenerate parabolic equation and an elliptic equation. The proposed numerical scheme is based on backward Euler for the temporal discretization and the mixed finite element method (MFEM) for the discretization in space. For each time step, the corresponding nonlinear system is solved by a robust linearization scheme, which does not involve any regularization step. The convergence of the linearization scheme is proved rigorously.

Key words: linearization, two-phase porous media flow, mixed finite element method, convergence analysis, linearization

1 Introduction

Two-phase flow in porous media is encountered is many real-life situations, such as water and soil pollution, oil recovery or nuclear waste management. These situations are of strong interest for the society and therefore a proper understanding of the two-phase flow in porous media is of high relevance. A crucial point in this sense is played by numerical simulations, based on accurate mathematical models and on appropriate numerical schemes.

2 Mathematical model and numerical scheme

In this work we concentrate on numerical schemes for two-phase flow through porous media. The fluids are assumed immiscible and incompressible and the solid matrix is assumed nondeformable. The formulation adopted here uses the global pressure and a complementary pressure (obtained by using the Kirchhoff transformation) as primary unknowns (see [2]). The system to be solved includes two coupled nonlinear partial differential equations, one degenerate elliptic - parabolic and one elliptic. for the the existence and uniqueness of a solution is we refer to [2].



Here we propose a mass conservative scheme based on MFEM and Euler implicit for solving numerically the system modeling the two-phase flow. For dealing with degenerate parabolic equations, whose solutions have typically low regularity, we use the lowest order Raviart-Thomas elements [1]. The nonlinear equations arising on each time step are solved by a robust linearization scheme. We emphasize that the new scheme does not involve any regularization step. The linearization scheme is a combination between a classical Picard method and the scheme presented in [3], and builds on the Lipschitz continuity of the saturation function with respect to the complimentary pressure. We show that the scheme is linearly convergent if the time step is small enough. Only a relative mild condition on the time step is required. Exactly this robustness is the main advantage of the scheme when compared to the quadratically, but locally convergent Newton method (see e.g. [4] for the convergence of the Newton method for the MFEM discretization of degenerate parabolic equations). One can use the proposed linearization scheme to increase the robustness of the Newton method by performing a few iterations at the begining of any Newton step. Moreover, the proposed scheme has a generic character and therefore can be applied also in connection with other discretization methods, like conformal finite elements or finite volumes.

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Coupling between Temperature, Solute Transport and Porosity Changes in a Geothermal Reservoir

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Abstract

Geochemistry has a substantial impact in exploiting geothermal systems. In a geothermal reservoir, the injected water and the in-situ brine have different temperatures and chemical compositions and flow through highly heterogeneous regions. Due to the varying chemical properties of the rocks, the temperature and the flow regimes can change significantly.

As a consequence of flow and geochemical reactions, composition of reservoir fluids as well as reservoir rock properties will develop dynamically with time. Minerals dissolving and precipitating onto the reservoir matrix, can change the porosity and hence the permeability of the system substantially. Mineral solubility can change by the cooling of the rock, or by the different ion content in the in-situ brine and in the injected water. The interaction between altering temperature, solute transport with mineral dissolution and precipitation, and fluid flow is highly coupled and challenging to model appropriately as the relevant physical processes jointly affect each other. The effect of changing porosity through the production period of the geothermal reservoir, may have severe impact on operating conditions, as pores may close and block flow paths, or new pores may open to create enhanced flow conditions.

When dealing with porosity changes, what happens at the pore scale is highly relevant. The pore size affects the reaction rates for the dissolution and precipitation process as the reactive surface area is changed, and the resulting permeability is affected by the pore geometry. To achieve expressions for both reaction rates and permeability that depend on the pore scale effects we start with a model at the pore scale, and derive the Darcy scale model by homogenization.

We propose an approach that models the three relevant processes; fluid flow, heat transport and reactive transport, on a relevant time scale. The considered mathematical and corresponding overall numerical solution strategy enables to investigate the coupling between flow, geochemical and thermal effects, as well as to develop tailored numerical approaches.

Key words: finite volume method, geothermal energy, homogenization, mineral precipitation/dissolution, porosity changes





Higher Order Variational Space-Time Discretizations of Mixed Transport Problems

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Abstract

In this contribution a family of variational space-time discretizations for transport problems in porous media is presented. The schemes are based on mixed finite element methods for the approximation of the spatial variables. Their convergence properties are studied by numerical experiments. Moreover, the schemes are applied to challenging and complex problems of practical interest in heterogeneous and anisotropic porous media.

Key words: Flow and transport, heterogeneous and anisotropic porous media, mixed finite element method, variational time discretization MSC 2010: 65M60, 80M10, 76M10

1 Introduction

Numerical simulations of time dependent flow and transport processes in heterogeneous porous media are desirable in several fields of natural sciences and in a large number of branches of technology. The accurate numerical approximation of such flow and transport phenomena continues to be a challenging task. The applicability and value of the mixed finite element method (MFEM) and its hybrid variant (MHFEM) have been demonstrated for a wide range of problems. While the discretization in space involves a significant set of complexities, temporal approximations for transient transport in porous media has received relatively little interest and has most often been limited to traditional non-adaptive low order methods.

The Galerkin method is a known approach to solve time dependent problems [1, 2]. So far, this variational approach has rarely been used in practice despite of its significant advantages like a uniform approach for numerical analyses, the natural construction of higher order methods, the applicability of a posteriori error estimation techniques (for instance, the dual weighted residual approach) and of well-known adaptive finite element techniques. One reason for this might be the high algorithmic complexity of the resulting algebraic systems.

In this contribution we present and analyze variational space-time approximations of a prototype convection-diffusion model problem. For the discretization in space mixed finite element methods of Raviart-Thomas type are used. The temporal variable is discretized by at least A-stable continuous Galerkin methods. Stability and error analyses of the schemes as well as implementational issues are addressed. Finally, their stability and accuracy properties and their potential for simulating complex transport phenomena are illustrated by numerical examples of practical interest; cf. Fig. 1.





Figure 1: Layered anisotropic medium and computed concentration profile and flux magnitude (l.t.r.) for diffusive transport.

2 Numerical approach

For a nonstationary diffusion problem written in mixed form, we consider and study the following continuous variant of our variational time discretization schemes:

Find $u_{\tau} \in \mathcal{X}^{r}(W)$ and $\mathbf{q}_{\tau} \in \mathcal{X}^{r}(\mathbf{V})$ such that $u(0) = u_{0}$ and

$$\int_0^T \langle \partial_t u_\tau + \nabla \cdot \mathbf{q}_\tau, w_\tau \rangle \, \mathrm{d}t = \int_0^T \langle f, w_\tau \rangle \, \mathrm{d}t \,, \quad \int_0^T \left\{ \langle \mathbf{D}^{-1} \mathbf{q}_\tau, \mathbf{v}_\tau \rangle - \langle u_\tau, \nabla \cdot \mathbf{v}_\tau \rangle \right\} \, \mathrm{d}t = 0$$

for all $w_{\tau} \in \mathcal{Y}^{r-1}(W)$, $\mathbf{v}_{\tau} \in \mathcal{Y}^{r-1}(\mathbf{V})$.

Here, $\langle \cdot, \cdot \rangle = \langle \cdot, \cdot \rangle_{L^2(\Omega)}$ and $X^r(X) := \left\{ u \in C(\overline{I}; X) \mid u|_{\overline{I}_n} \in \Pi_r(\overline{I}_n; X), \forall n \right\}, \mathcal{Y}^r(X) := \left\{ w \in L^2(I; X) \mid w|_{I_n} \in \Pi_r(I_n; X), \forall n \right\}$ with $\Pi_r(J; X) := \left\{ u(t) = \sum_{j=0}^r \xi_n^j t^j, \xi_n^j \in X, \forall j \right\}$ denote spaces of piecewiese polynomial functions in time.

The discontinuity of test functions $w_{\tau} \in \mathcal{Y}^{r-1}(W)$ and $\mathbf{v}_{\tau} \in \mathcal{Y}^{r-1}(\mathbf{V})$, respectively, then allows us by an appropriate choice of test basis functions to recast the variational problem as a time marching scheme. Further, we apply the Gaussian quadrature rule to the integration in time and solve the resulting variational problem in a finite dimensional LBB-stable pair of mixed finite element spaces $W_h \subset W$ and $\mathbf{V}_h \subset \mathbf{V}$. For instance, in the case r = 2 this yields a block matrix system of the following structure that has to be solved for the unknown coefficient vectors in each of the time intervals $I_n = (t_{n-1}, t_n], n = 1, \ldots, N$:

$$\begin{pmatrix} \mathbf{A} & \mathbf{0} & -\mathbf{B} & \mathbf{0} \\ \mathbf{0} & \mathbf{A} & \mathbf{0} & -\mathbf{B} \\ \frac{\tau_n}{2} \mathbf{B}^\top & \mathbf{0} & \hat{\alpha}_{1,1} \mathbf{G} & \hat{\alpha}_{1,2} \mathbf{G} \\ \mathbf{0} & \frac{\tau_n}{2} \mathbf{B}^\top & \hat{\alpha}_{2,1} \mathbf{G} & \hat{\alpha}_{2,2} \mathbf{G} \end{pmatrix} \begin{pmatrix} \mathbf{Q}_h^1 \\ \mathbf{Q}_h^2 \\ \mathbf{U}_h^1 \\ \mathbf{U}_h^2 \end{pmatrix} = \begin{pmatrix} \mathbf{0} \\ \mathbf{0} \\ \tilde{\mathbf{F}}^1 \\ \tilde{\mathbf{F}}^2 \end{pmatrix}.$$

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Pattern formation in morphogenesis on evolving biological surfaces: Theory, numerics and applications

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Abstract

In this talk, I will present our most recent results based on two finite element formulations: (i) the surface finite element and (ii) generalized projected finite element methods applied to solving partial differential equations of reaction-diffusion type on arbitrary stationary and evolving surfaces. Reaction-diffusion equations on evolving surfaces are formulated using the material transport formula, surface gradients and diffusive conservation laws. The evolution of the surface is defined by a material surface velocity. The generalized projected finite element method differs from the surface finite element method in that it provides a conforming finite element discretization which is "logically" rectangular. However, this property restricts the general applicability of the numerical method to arbitrarily evolving surfaces, a key advantage for the evolving surface finite element method. To demonstrate the capability, flexibility, versatility and generality of the numerical methodologies proposed, I will present various numerical results. This methodology provides a framework for solving partial differential systems on continuously evolving domains and surfaces with numerous applications in developmental biology, cancer research, wound healing, tissue regeneration, and cell motility among many others, where reaction-diffusion systems are routinely applied.





Modelling and Control of Blood Flow in an Automated Biomedical System

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Abstract

This paper describes the modelling of blood flow from a control system perspective, with an aim to automatically regulate the blood flow for medical applications. The modelling starts from the control forms, i.e. the end application, followed by substitution of the physical model of the blood flow into the control forms.

Key words: blood flow, control system, medical applications

1 Introduction

Blood is a biological substance in human body that contains a lot of information (Hackl et al., 2012). It has been widely used as a testing substance for health screening by the middle of 20th century (Morabia and Zhang, 2004), in static environment such as in health screening as well as in dynamic environment such as in an operation. Blood is also a biological substance in human body that transports most of vital substances, including nutrition, oxygen, and hormones. Likewise, the introduction of vital substances has been done in static environment such as through oral intake as well as in dynamic environment such as through injection. Understanding the blood stream with an aim to control is absolutely essential. In this paper, I present an analysis and development of blood stream model, starting from the control requirements and directed towards fluid mechanic analysis. In doing so, I introduce a flipped approach, where the starting point is at the downstream application and the end point is at the upstream theoretical analysis.

2 Modelling

For a control application, a system can be described in a transfer function form as follows:

$$G(s) = \frac{b_0 s^m + b_1 s^{m-1} + b_2 s^{m-2} + \dots + b_m}{a_0 s^n + a_1 s^{n-1} + a_2 s^{n-2} + \dots + a_n}$$
(1)

or in a state space form as follows:

$$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{B}\mathbf{u}$$

$$\mathbf{y} = \mathbf{C}\mathbf{x} + \mathbf{D}\mathbf{u}$$
(2)



where the transfer function can be obtained from the state space as follows:

$$G(s) = C(sI - A)^{-1}B + D$$
(3)

and where G(s) represents the system, *s* the frequency-domain of the time-domain state *x*, A the system matrix, B the input matrix, C the output matrix, D the feedthrough matrix and **u** the input.

Blood, being a relatively highly viscous fluid, is modelled as follows:

$$\upsilon = V \left(1 - \left(\frac{r}{R}\right)^2 \right) \tag{4}$$

$$-p + \mu \frac{\partial v}{\partial l} = 0 \tag{5}$$

where v is the velocity state of blood, V the maximum velocity, r the radial increment of the blood vessel, R the radius of the blood vessel, p the blood pressure, μ the viscosity modulus of the blood, and l the lateral increment of the blood vessel.

The objective of this paper is to express equation (4)-(5) into equation (1) or (2) such that it can be used to design a control law. Such transformation is done by taking v = x, i.e. taking the velocity as the state of the blood system.

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Numerical treatment of PDEs of evolving-in-time surfaces

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Abstract

Numerical simulation of PDEs on surfaces has become very important in the last years. A very wide range of corresponding biological applications exists, e.g., embryonic development, cancer tumor growth, dynamic of elastic lipid membranes, vasculogenesis and angiogenesis, protein-protein interaction, tissue development and immune responses. Processes in the scope are often described with continuum reaction-diffusionconvection models on deforming-in-time surfaces. The numerical simulation of such models is very challenging; and, modern numerical techniques are of predominant importance. In this talk, we discuss the construction of the FE level-set based technique for the reaction-diffusion-convection equations on evolving-in-time surfaces. High order FCT/TVD stabilization methods are used for the numerical treatment of arising convective/advective terms. Corresponding numerical tests for chemotaxis systems and for systems with the instability of the Turing type will be presented.

Key words: PDEs on evolving surfaces, level set, finite elements, flux corrected transport

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Domain decomposition methods - Towards extreme scalability using new nonlinear approaches and enhanced robustness using adaptive coarse spaces

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Abstract

The solution of nonlinear problems, e.g., in material science requires fast and highly scalable parallel solvers. FETI-DP (Finite Element Tearing and Interconnecting) domain decomposition (DD) methods are parallel solution methods for implicit problems discretized by finite elements. A common iterative DD approach for nonlinear problems is a Newton-Krylov-DD strategy where the nonlinear problem is linearized using a Newton method. Then, the linear system associated with the tangent stiffness matrix is solved with a preconditioned Krylov space method. The preconditioner is obtained by a domain decomposition method. In an efficient and parallel scalable domain decomposition method, local subdomain problems and a sufficiently small global problem have to be solved. The local problems are inherently parallel, the global problem is needed to obtain numerical and parallel scalability. FETI-DP domain decomposition methods have been shown to be parallel scalable for linearized elasticity problems on up to 65 536 cores of a BlueGene/P supercomputer (JUGENE, Jülich Supercomputing Center, Germany) in 2009. Recently, nonlinear versions of the well-known FETI-DP methods for linear problems have been introduced. Here, the nonlinear problem is decomposed directly before linearization. In these methods, in each iteration, local nonlinear problems are solved on the subdomains. The new approaches have the potential to reduce communication and to show a significantly improved performance, especially for problems with localized nonlinearities, compared to a standard Newton-Krylov-FETI-DP approach. Moreover, the coarse space of the nonlinear FETI-DP methods can be used to accelerate the Newton convergence. Another new approach can be viewed as a strategy to further localize computational work and to extend the parallel scalability of FETI-DP methods towards extreme-scale supercomputers. Here, a recent nonlinear FETI-DP method is combined with an approach that allows an inexact solution of the FETI-DP coarse problem. We combine the nonlinear FETI-DP domain decomposition method with an AMG (Algebraic Multigrid) method and obtain a hybrid nonlinear domain decomposition/multigrid method. We can show parallel scalability for up to 262 144 cores on the MIRA BlueGene/Q supercomputer (Argonne National Laboratory, USA) for our new implementation.

Robustness with respect to discontinuities in the coefficients of the partial differential equation is another important and desirable property of domain decomposition



methods. Adaptively computed coarse spaces can be used to obtain independence on the coefficient jumps for highly heterogeneous problems, even when coefficient jumps inside subdomains and across subdomain boundaries are present. In this talk, a construction of a coarse space for the FETI-DP domain decomposition method applied to highly heterogeneous problems is presented. The strategy is based on solving local generalized eigenvalue problems. For certain problems with highly varying coefficients, e.g., from multiscale simulations, the coefficient jump will appear in the condition number bound even if standard techniques as scaling and the weighting of constraints are used. The FETI-DP theory is revisited and two central estimates are identified where the dependency on the coefficient contrast can enter the condition number bound. The first is a Poincaré inequality and the second an extension theorem. These estimates are replaced by local eigenvalue problems. Enriching the FETI-DP coarse space by a few numerically computed eigenvectors yields independence of the contrast of the coefficients even in challenging situations.



On cost function transformations for the reduction of uncertain model parameters' impact towards the optimal solutions

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Abstract

Uncertainties affect the accuracy of nonlinear static or dynamic optimization and inverse problems. The propagation of uncertain model parameters towards the optimal problem solutions can be assessed in a deterministic or stochastic way using sensitivity analysis or Monte Carlo based techniques. This paper presents cost function transformations for reducing the impact of uncertain model parameters towards the optimal solutions. We assess the consistency of the methodology by determining the conditions on the cost function transformations.

Key words: cost function, optimization, robustness, uncertainty MSC 2010: 46N10, 47N10, 80M50, 90C31, 62G35

1 Introduction

Noise in measurement data and modeling errors lead to a deterioration of the optimal solutions' accuracy in optimal design problems and inverse problems. The impact of model parameters on the given static or dynamic model's outputs, can be assessed by performing e.g. a sensitivity or Monte Carlo analysis. Electromagnetic devices typically exhibit uncertainties toward uncertain material, geometrical or source parameters since they may contain parameter values that are difficult to determine or that their value is known to be situated within a certain range. Recently, techniques have been proposed that reduce the impact of uncertain model parameters in applications based on electromagnetic principles: reduction of the uncertain electrical conductivity parameter on electroencephalographic source reconstruction [1]; reduction of the uncertain geometrical parameters on the magnetic material identification of an electromagnetic inductor [2].

The work addresses the following specific class of problems: a sought vector $\mathbf{x} \in \Omega_x \subseteq \mathbb{R}^p$ needs to be estimated based on degraded data or objective $\mathbf{y} \in \Omega_y \subset \mathbb{R}^q$. Let $\mathbf{f} : \Omega_x \times \Omega_u \to \Omega_y$ denote the forward model that includes the physics of the system under study. Next to parameters \mathbf{x} to be estimated, \mathbf{f} depends on uncertain parameters $\mathbf{u} \in \Omega_u \subseteq \mathbb{R}^r$. This paper discusses the propagation of \mathbf{u} towards solutions in deterministic nonlinear least-squares problems.



2 Cost function transformations

In order to perform the analysis we have the following definitions. A least-squares formulation is often used to find a best parameter value $\mathbf{x}^* \in \Omega_x$ which is a minimum for $\gamma(\mathbf{x}, \mathbf{u}, \mathbf{y}) = \|\mathbf{f}(\mathbf{x}, \mathbf{u}) - \mathbf{y}\|_2^2$ over $\mathbf{x} \in \Omega_x$. A l_2 -norm formulation is used here for clarity.

Definition 1 Function $\mathbf{x}^* : \Omega_u \times \Omega_y \to \Omega_x$ is the propagation function of the uncertain model parameters towards the reconstructed parameters:

$$\mathbf{x}^{*}(\mathbf{u}, \mathbf{y}) = \arg\min_{\mathbf{x}\in\Omega_{x}} \gamma(\mathbf{x}, \mathbf{u}, \mathbf{y}).$$
(1)

Let us consider a transformation \mathcal{T} on the forward model, e.g. a first order transformation $\mathcal{T} \mathbf{f}(\mathbf{x}, \mathbf{u}) = \mathbf{f}(\mathbf{x}, \mathbf{u}) + (\mathbf{v}(\mathbf{x}, \mathbf{u}) \cdot \nabla_u)\mathbf{f}(\mathbf{x}, \mathbf{u})$ for a certain function $\mathbf{v}(\mathbf{x}, \mathbf{u}) : \Omega_x \times \Omega_u \to \Omega_v \subseteq \mathbb{R}^q$. In case, the function is specified as $\tilde{\mathbf{v}}(\mathbf{x}, \mathbf{u})$, the associated transformation becomes: $\mathcal{T} \mathbf{f}(\mathbf{x}, \mathbf{u}) = \mathbf{f}(\mathbf{x}, \mathbf{u}) + (\tilde{\mathbf{v}}(\mathbf{x}, \mathbf{u}) \cdot \nabla_u)\mathbf{f}(\mathbf{x}, \mathbf{u})$.

Definition 2 This transformation changes the cost function γ into $\tilde{\gamma}$ and thus the transformed propagation function: $\tilde{\mathbf{x}}^*(\mathbf{u}, \mathbf{y}) = \arg \min_{\mathbf{x} \in \Omega_x} \tilde{\gamma}(\mathbf{x}, \mathbf{u}, \mathbf{y}).$

Definition 3 Let the function $\tilde{\mathbf{v}}(\mathbf{x}, \mathbf{u})$ be defined as (case of l_2 -norm):

$$\widetilde{\mathbf{v}}(\mathbf{x},\mathbf{u}) = \arg\min_{\mathbf{v}\in\Omega_{ij}\subseteq\mathbb{R}^{q}} \|\mathbf{f}(\mathbf{x},\mathbf{u}) + (\mathbf{v}\cdot\nabla_{u})\mathbf{f}(\mathbf{x},\mathbf{u}) - \mathbf{y}\|_{2}^{2}.$$
(2)

We investigate whether a determined stationary point of the iteration coincides with the optimum of the model using actual uncertainty value \mathbf{u}_a . Not every $\tilde{\gamma}$ formulation is successful for having the algorithm to be consistent.

Lemma 1 We assume that if $\gamma(\mathbf{x}, \mathbf{u}_a, \mathbf{y})$ is locally convex at \mathbf{x}_a^* , than then $\gamma(\mathbf{x}, \mathbf{u}, \mathbf{y})$ is also locally convex at \mathbf{x}_a^* . We further assume that $\nabla_x(\mathbf{v}(\mathbf{x}_a^*, \mathbf{u}_a) \cdot \nabla_u)\mathbf{f}(\mathbf{x}_a^*, \mathbf{u}_a) = 0$. Any local minimizer $\gamma(\mathbf{x}, \mathbf{u}, \mathbf{y})$ for given measurement \mathbf{y} is a local minimizer of $\widetilde{\gamma}(\mathbf{x}, \mathbf{u}, \mathbf{y})$.

Assumption 1 (a) Function $\tilde{\mathbf{v}}$ is continuously differentiable towards \mathbf{x} , $\forall \mathbf{u} \in \Omega_u$. (b) Measurement or objective \mathbf{y} is reachable by the forward model \mathbf{f} . (c) $\mathbf{f}(\Omega_x, \Omega_u)$ is a differentiable manifold.

Theorem Let $\overline{\mathbf{x}}$ be the fixed point of the $\widetilde{\gamma}$ minimization and let $\gamma(\mathbf{x}, \mathbf{u}_a, \mathbf{y})$ for given measurement \mathbf{y} be locally convex at $\overline{\mathbf{x}}$, then the point $\overline{\mathbf{x}}$ is a local minimizer of $\gamma(\mathbf{x}, \mathbf{u}_a, \mathbf{y})$.

Proof. The sequence of $\widetilde{\mathbf{v}}$ -operators becomes in the limit: $\overline{\mathbf{v}}(\mathbf{x}, \mathbf{u}) = \arg \min_{\mathbf{v} \in \Omega_v \subseteq \mathbb{R}^q} \|\mathbf{f}(\overline{\mathbf{x}}, \mathbf{u}) + (\mathbf{v}(\overline{\mathbf{x}}, \mathbf{u}) \cdot \nabla_u)\mathbf{f}(\overline{\mathbf{x}}, \mathbf{u}) - \mathbf{y}\|_2^2$. Since $\mathbf{f}(\Omega_x, \Omega_u)$ is a differentiable manifold,

$$\overline{\mathbf{v}}(\overline{\mathbf{x}},\mathbf{u}) = \arg\min_{\mathbf{v}\in\Omega_{v}\subseteq\mathbb{R}^{q}} \|((\mathbf{u}-\mathbf{u}_{a})\cdot\nabla_{u})\mathbf{f}(\overline{\mathbf{x}},\mathbf{u})) - (\mathbf{v}(\overline{\mathbf{x}},\mathbf{u})\cdot\nabla_{u})\mathbf{f}(\overline{\mathbf{x}},\mathbf{u})\|_{2}^{2}$$

is equivalent. The \mathcal{T}_k operators in the *k*-th iteration converge therefore to $\overline{\mathcal{T}}$ with $\overline{\mathbf{v}}(\overline{\mathbf{x}}, \mathbf{u})$. This ends the proof.

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Bayesian estimates of thermodynamic uncertainties for flows governed by dense-gas equations of state

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Abstract

In recent years, dense gases have been studied extensively because of their interesting peculiar properties; specifically, dense gas flows have shown a potential for many engineering applications. Description of dense gas motion, e.g. through a Computational Fluid Dynamics (CFD) solver need a closure model to represent the thermodynamic behaviour of the fluid, i.e. an Equation of state (EOS). In spite of many improvements, EOS still suffer from a lack of knowledge about their mathematical form and closure parameters, thus it is necessary to evaluate the impact of this uncertainty on the code output. In this work, we use uncertainty quantification (UQ) techniques to: (*i*) propagate the uncertainty about EOS parameters through the dense gas solver and (*ii*) to calibrate EOS parameters thanks to some available data. The last step uses a Bayesian model update framework accounting for both parametric and model-form uncertainties. Bayesian calibration techniques are presented with focus on statistical modelling of model-form uncertainties, and their potential for robust CFD predictions of dense gas flows is shown up.

Key words: Uncertainty quantification, Bayesian inference, CFD, dense gas flow

Numerical simulations of dense gas flows can be extremely sensitive to the model used to describe the fluid thermodynamic behavior [1]. For many dense gases, accurate and comprehensive equations of state (EOS), i.e. thermodynamic laws designed to describe the fluid thermal and caloric behavior in the region of interest, are not available. As a consequence, reliable simulations of compressible flows with complex thermodynamic behavior require the quantification of thermodynamic modeling errors, especially for applications that look for improvements of the order of a few percents of the system performance.

EOS give raise to two kinds of uncertainties: the first one concerns the mathematical form of the EOS to be used for a given fluid; on the other hand, the material-dependent coefficients associated to the EOS are imperfectly known. Previous work [1] has shown that for some particularly complex gases the model-form uncertainty can be even overwhelming with respect to the parametric uncertainty.

In this work, we adopt a Bayesian approach to quantify EOS uncertainties associated to thermodynamic models used for dense gas flow simulations. Specific interest is put into the



stochastic representation of model-form uncertainties and their consequences on both calibration and prediction. Our aim is to develop a robust calibration allowing reliable predictions of configurations different from the calibration one.

The application case under study is the transonic flow of a silicon oil, namely cyclopentasiloxane (D5), past an airfoil, as in [1]. Numerical solutions of flow equations are generated by means of a finite volume code using a third-order accurate numerical scheme [2]. The code is supplemented with real-gas equations of state, namely the cubic Peng-Robinson-Stryjek-Vera [3] (PRSV) and Soave-Redlich-Kwong [4] (RKS) EOS, and the five-term virial Martin-Hou model [5] (MAH). Since no experimental data are available, synthetic calibration data are generated for this case by means of a reference EOS based on Helmholtz free energy [6].



Figure 1: Posterior expectancy of the wall pressure coefficient (-----), prior expectancy (- - -), experimental data (\blacksquare) and associated error bars.

Some preliminary results for model calibrations based on a multiplicative and correlated stochastic model are depicted in Figure 1.

The final paper will present results for different calibration strategies, and their assessment for the prediction of dense gas flows.

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Reduced Basis Methods for Time-Harmonic Maxwell's Equations with Stochastic Coefficients

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Abstract

The Reduced Basis Method generates low-order models of parametrized partial differential equations (PDEs) to allow for efficient evaluation of parametrized models in manyquery and real-time settings. We use the Reduced Basis model order reduction technique to generate a low order model of an electromagnetic system governed by time-harmonic Maxwell's equations. The reduced order model then makes it feasible to analyze the uncertainty by a Monte Carlo Simulation. Stochastic Collocation is employed as a second technique to estimate the statistics. In particular the combination of model order reduction and Stochastic Collocation allows low computation times.

Key words: Electromagnetic analysis, Maxwell equations, Reduced Basis Method, Reduced Order Systems, Uncertainty Quantification

1 Application Model

As an example model, we consider the coplanar waveguide, shown in Fig. 1. The model setup is contained in a shielded box with perfect electric conducting (PEC) boundary. We consider three perfectly conducting striplines as shown in the geometry. The system is excited at a discrete port and the output is taken at a discrete port on the opposite end of the middle stripline. These discrete ports are used to model input and output currents/voltages.

We are interested in parameter studies of the input-output behavior of electromagnetic models. Therefore, we need to compute the electromagnetic field induced by the applied current. We simulate Maxwell's equations in the second order timeharmonic formulation

$$\nabla \times \mu^{-1} \nabla \times E + j\omega \sigma E - \omega^2 \epsilon E = -j\omega J, \quad (1)$$

and solve for the electric field *E*. The equation is discretized with Nédélec finite ele-



ments (see [1]), over the entire shielded box Figure 1: Geometry of a coplanar waveguide. as the computational domain. The parameter vector is denoted by $v \in \mathcal{D} \subset \mathbb{R}^p$, such that E(v) is the parameter-dependent electric field solution.



2 Reduced Basis Model Reduction

Model Order Reduction (MOR) allows to significantly reduce the computational time required for parameter studies. MOR substitutes the large-scale model by a model of low order, which approximates the transfer behavior. The aim of the Reduced Basis Method (RBM) is to determine a low order space X_N of dimension N, which approximates the parametric manifold $M^{\nu} = \{E(\nu) | \nu \in \mathcal{D}\}$ well. Assuming sufficient smoothness of M^{ν} , a space X_N can be determined, such that projecting the variational form onto X_N gives good approximations $E_N(\nu)$ to $E(\nu)$. The space X_N is spanned by snapshots of the field solutions for a discrete set of parameter realizations. The snapshot locations are chosen in a greedy process using a rigorous error estimator. The error estimators $\Delta_N(\nu)$, which give rigorous bounds to the approximation error in the H(curl) norm:

$$||E(\nu) - E_N(\nu)||_{H(\operatorname{curl})} \le \Delta_N(\nu), \tag{2}$$

are used to certify the accuracy of the reduced order model. See [2] for more details.

3 Stochastic Collocation

Let $(\Omega, \mathcal{F}, \mathcal{P})$ denote a probability space. Given is a square integrable random variable $Y : \Omega \to \mathbb{R}$ with probability density function f and a function $g : \Gamma \to \mathbb{R}^d$, corresponding to a mapping of realizations of a random variable to the output of the electromagnetic system.

Stochastic collocation computes statistical quantities like the mean by a quadrature rule

$$\mathbb{E}(g(Y)) = \int_{\Gamma} g(x) f(x) dx \approx \sum_{i=1}^{n} g(\xi_i) w_i, \qquad (3)$$

where the realizations ξ_i are the sample points and the weights w_i are determined using the probability density function f. See [3] for more details.

In statistical analysis the expectation and variance of quantities of interest like the transfer behavior under uncertain parameters is computed. For this purpose, stochastic collocation uses a quadrature rule. To further enhance the computation speed of statistical quantities, stochastic collocation is combined with reduced basis model order reduction. This allows to quantify models of a much larger complexity.

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Time of Flight Estimation of Sparse Ultrasonic Reflections Using Reiterative Deconvolution Technique

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Abstract

Ultrasonic measurements are often based on the estimation of the time-of-flight of the waves through materials or structures. When signals are in close temporal proximity to the signal of interest, additional bias errors are introduced in ToF estimator. A novel optimization technique based on reiterative deconvolution is presented for accurate time of flight estimation for signals where reflections are sparse yet close to each other in the time domain.

Key words: Deconvolution, iterative algorithms, time measurements, time of arrival estimation, ultrasonic variable measurements. MSC 2010: 62M10, 60G35, 65F10, 68U20

1 Introduction

Many ultrasonic testing applications are based on the estimation of the time-of-flight (ToF) or time delay estimation (TDE): thickness, load [1, 2] and etc. meters all employ the ultrasound propagation time to extract the required properties of the test object. Usually correlation processing is used for signal-to-noise (SNR) improvement and the cross-correlation function (CCF) maximum location [3, 4] is assigned as ToF estimate. Automated CCF peak location and ToF estimation is complicated in case of multiple reflections presence in the signal. Our aim was to develop the technique for the reduction of the additional bias errors.

2 Reiterative deconvolution for TOF estimation

Iterative deconvolution has been suggested as simple technique to separate the reflections [5]. Once the position ToF_i of highest peak for subtraction is found then estimation of the multiplier A_i for reference signal to subtract is obtained using shifted reference signal ref_k and received signal s_k , the reference signal can be subtracted and the residual saved for next iteration i + 1:

$$s_{i+1,k} = s_{i,k} - A_i \cdot \operatorname{ref}_k. \tag{1}$$

If bias error is significantly reduced if interfering signal is removed by iterative deconvolution procedure then we suggest applying new reiterative deconvolution:



First iteration: ToF for largest reflection is obtained and this largest reflection subtracted using equations (1); ToF for second largest reflection is obtained from the remainder signal. This process is repeated until all reflections are subtracted.

Reiteration: re-estimation of the reflection position (ToF) and amplitude are obtained from the remainder after subtraction of other estimated reflections from the original signal. Second iteration is repeated until there is no significant bias errors reduction.

The results of the numerical simulation using the real signals confirm that time estimation error quickly diminishes when reiterative deconvolution is used.



Figure 1: (a) Example of detected simulated signals; (b) ToF errors vs. estimation technigues for rectangular pulse.

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A Fokker-Planck approach for probability distributions of species concentrations transported in heterogeneous media

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Abstract

Probability density functions (PDF) of random concentrations are modeled by Fokker-Planck equations. Numerical solutions for the joint concentration-position PDF are obtained by a global random walk (GRW). Drift and diffusion coefficients describing the PDF transport in physical space are provided by up-scaling procedures. Mixing models for concentration dynamics may be inferred from comparisons with Eulerian PDF equations or, alternatively, from measured or simulated concentration time series. The latter approach is used to construct a GRW-PDF numerical solution to a problem of contaminant transport in heterogeneous groundwater systems.

Key words: PDF methods, mixing, random walk MSC 2010: 60J60, 60G60, 86A05

1 Eulerian and Fokker-Planck PDF equations

Species concentrations $C(\mathbf{x}, t)$ linked through the reaction term S(C), with constant diffusion coefficient *D*, are transported in a random velocity field **V** according to

$$\partial_t C + \nabla(\mathbf{V}C) = D\nabla^2 C + S(C). \tag{1}$$

The Eulerian PDF $f(c; \mathbf{x}, t)$ of the random concentration *C* solving (1) verifies

$$\partial_t f + \nabla(\mathcal{V}f) = \nabla^2(\mathcal{D}f) - \nabla^2_c(Mf) - \nabla_c(Sf), \qquad (2)$$

where $\mathcal{V} = \langle \mathbf{V} \rangle - \nabla \mathcal{D}$ is the up-scaled drift and $\langle \mathbf{V} \rangle$ the mean velocity, $\mathcal{D} = D + \mathbf{D}^*$ is the diffusion coefficient up-scaled through the gradient-diffusion closure $\langle \mathbf{V} - \langle \mathbf{V} \rangle | \mathbf{C}(\mathbf{x}, t) = \mathbf{c} \rangle = -\mathbf{D}^* \nabla f$, ∇_c is the gradient in the concentration space, and $M = \langle D \nabla C \nabla C | C(\mathbf{x}, t) = c \rangle$ is the conditional dissipation rate which accounts for molecular mixing [1, Sect. 6.2]. The reaction



term *S* occurring in (2) is in a closed form, the same as in the concentration balance equation (1), which is the essential advantage of the PDF method [1]. A Fokker-Planck equation, formally the same as (2) but with a new mixing term $M = \langle D\nabla C\nabla C|C = c, X = x \rangle$, governs the joint concentration-position PDF $p(c, \mathbf{x}, t) = f(c; \mathbf{x}, t)\rho(\mathbf{x}, t)$, where $\rho(\mathbf{x}, t)$ is the position PDF (i.e. the ensemble mean concentration). The equivalent particle representation is given by the Itô equations

$$d\mathbf{X}(t) = \mathcal{V}(\mathbf{X}, t)dt + d\mathbf{W}(\mathbf{X}, t)$$

$$dC(\mathbf{X}(t)) = M(C(\mathbf{X}(t)))dt + S(C(\mathbf{X}(t))dt,$$
(3)

where **W** is a Wiener process with $E\{\mathbf{W}(\mathbf{X},t)\} = 0$ and $E\{\mathbf{W}^2(\mathbf{X},t)\} = 2\int_0^t \mathcal{D}(\mathbf{X},t')dt'$.

2 GRW solutions to modeled PDF equations

An efficient solution to (3) is obtained by a GRW algorithm consisting of a superposition of many weak Itô schemes projected on a regular lattice [3]. The GRW-PDF approach is illustrated for random concentrations integrated over the *y*-axis of a two dimensional aquifer model. The up-scaled coefficients \mathcal{V} and \mathcal{D} are estimated through a self-averaging first-order approximation [2]. The slope of the mean concentration at the plume center of mass models the mixing term *M*. The behavior of the PDF at the plume center of mass and a comparison of the cumulative probability distributions with the Monte Carlo results are shown in Figure 1.



(a) Transported PDF at the plume center of mass, $f(c; x, t), x = \mathcal{V}t$.



(b) GRW and Monte Carlo cumulative distribution functions $cdf(c; x, t), x = \mathcal{V}t, t = 0, 10, 30, 50, 100$ days (from right to left).

Figure 1: Concentration probability distributions.

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A numerical treatment of reactive flows in porous media

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Abstract

In this work we consider a model that describes the flow in a porous medium of a mobile species which precipitates into an immobile precipitate, leading to the formation/degradation of crystals inside a porous matrix. The flow is governed by a Darcy problem, where the permeability is changed according to the solute concentration. The dissolution rate is described by a set valued function. The problem has been solved numerically by a treatment of the discontinuity based on event-driven methods. We will present some analytical results about the model, and we will compare the results obtained by the application of event-driven methods against regularization methods, showing that our method captures the discontinuity more accurately.

Key words: reactive flow, porous media, event-driven, precipitation, dissolution model.

1 Introduction

A characteristic of reactive flow in porous media is sometimes the presence of phenomena that at the macroscale level are represented by a discontinuous reaction term, with a discontinuity that depends on the solution itself. This class of problems may be interpreted as differential inclusions, [1]. We follow here an approach, alternative to regularization, based on detecting when the solution reaches the discontinuity, and select its behavior according to Filippov theory [2]. This method may guarantee optimal convergence at a reasonable computational cost, and allows for the resolution of sliding motions, when the solution, after reaching the discontinuity surface, slides onto it.

2 Model problem

The adimensionalized equations for the concentrations of the mobile species u and the immobile precipitate v, complemented with suitable boundary conditions, are [3]:

$$\begin{cases} \frac{\partial}{\partial t}(u+v) - \nabla \cdot (\nabla u - \mathbf{q}u) = 0 & \text{in } \Omega^T, \\ u = u_0 & \text{in } \Omega & \text{for } t = 0, \end{cases} \qquad \begin{cases} \frac{\partial}{\partial t}v \in r(u) - H(v) & \text{in } \Omega^T \\ v = v_0 & \text{in } \Omega & \text{for } t = 0 \end{cases}$$
(1)

where **q** is the velocity vector field of the fluid. Here the production rate r(u) is a locally Lipschitz continuous function and the dissolution rate H(v) is described by the Heaviside distribution.



In this work the velocity field **q** is not a given function, but the solution of a Darcy problem where the scalar permeability k depends on the porosity. With the increase of the precipitate concentration there is a consequent reduction of porosity, an empirical law for the variation of porosity with varying precipitate concentration is given as $\frac{d\phi}{dt} = -\frac{dv}{dt}$. The permeability thus depends on the precipitate concentration as $k(\phi) = (\phi)^2 \rightarrow k(\phi(v)) = (1-v)^2$, to account for degradation/growth of the crystal.

The problem has been solved numerically by a treatment of the discontinuity based on event-driven methods [1]. We have applied it to a simple test case: the domain is a 2D square $\Omega := (0, 1) \times (0, 1)$, with a Dirichlet boundary $\Gamma_D := \{y : x = 0, y \in (0, 1)\}$ and $\Gamma_N := \partial \Omega \setminus \Gamma_D$. Moreover, the viscosity is set to $\mu = 1$ and precipitation is modeled as r(u) = u. An horizontal pressure gradient is imposed from left to right and, at the inflow boundary, we set u = 0. The initial conditions are $u_0 = 0$ everywhere, and $v_0 = 0.8$ only in $\Omega_v := \{(x, y) : 0.4 \le x \le 0.6, 0.4 \le y \le 0.6\}$, *i.e.* the precipitate is present only in a part of the domain.



Figure 1: Solute (*u*) and precipitate concentration (*v*). Streamlines and magnitude of the velocity field q.

The solution exhibits an attractive sliding motion in $\Omega \setminus \Omega_v$, where, as a consequence, the precipitate concentration v remains constant and equal to 0. It can be observed that the velocity **q** increases in Ω_v as the precipitate dissolves.

In this talk we will present some analytical results, as well as details on the numerical treatment, and we will compare the results obtained by the application of event-driven methods against regularization methods, showing that our method captures the discontinuity more accurately, obtaining sharper dissolution fronts.

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PDF Simulation of Surfactant Transport in Gas Phase and Adsorption in Reservoir Rocks Using the Stochastic -Lagrangian Particle Method

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Abstract

Surfactant transport and retention in the reservoir plays an important role in the effectiveness of a well stimulation procedure. For a given reservoir fluids-matrix-surfactant system, a limiting surfactant concentration may determine the technical/economic success or failure of the well intervention. Therefore, an accurate modeling and simulation of the coupled transport and retention mechanism are important for the surfactant deployment design. We propose a mathematical model of the surfactant transport in the reservoir, accounting for matrix adsorption and surfactant dissolution in liquid phases. An equivalent probability density function transport equation of the surfactant is used to describe the transport and retention of the scalar. The model predicts the evolution of surfactant distribution in the reservoir in matrix and soluble phases. Preliminary simulations indicate that the surfactant adsorption on the solid matrix is ca. 10-15%, depending on the physical-chemical properties of the stimulation fluid. The comparison of simulation results with experimental data indicates a maximum deviation of 5%. The model can be used for deployment optimization procedures in Gastim projects.

Key words: transport, adsorption, porous media, stochastic method.

1 Introduction

When chemical stimulating fluids are used for both, well remediation and stimulation operations and enhanced oil recovery processes, complex mass transfer, phase transitions and transport properties alteration [1] coupled physicochemical processes are present. Some processes are: surfactant advective, diffusive and dispersive transport, mixing and dissolution of surfactant with miscible phases, micro-emulsions generation, surfactant adsorption on matrix surface, surface and interfacial forces alteration, and others.

Recent developments in gas phase stimulation techniques (Gastim) [2, 3] indicate that the gas phase as carrier fluid enables a better transport and mobilization of the chemical agent in the reservoir. A full understanding of the underlying phenomena is of paramount importance



for designing and optimizing gas-based well - chemical stimulation procedures. As an initial approximation, we model the transport of a surfactant carried by a compressible fluid in a reservoir with gas-condensate blockage, following a state-of-the-art procedure [4].

2 Numerical solution

Flow equations are solved in cylindrical coordinates using the finite-volume method, and the resulting PDF equation is solved following a Lagrangian Monte-Carlo Method as described in [4]. The flow solver was calibrated with well-head pressure measured in a previous pilot and further scaled to bottom-hole flowing pressure. Results of the calibration are presented in Fig. 1(a). The model predicts the evolution of surfactant distribution in the reservoir in



(a) Bottom-hole flowing pressure. (symbol: measure- (b) Radial distribution of adsorbed surfactant on the ment; line: simulation) matrix and concentration front.

Figure 1: Preliminary results.

matrix and soluble phases. After 8 days of continuous surfactant injection in the gas phase, the adsorption in radial direction is presented in Fig. 1(b), as well as the total concentration front (i.e., mass of surfactant dissolved in gas, water and oil phases, and adsorbed per unit of porous volume).

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Some Hermite finite element methods for fluid and heat flow

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Abstract

In this work we study some Hermite finite element methods that can be used as advantageous alternatives to classical mixed methods, in the framework of heat or fluid flow simulations. More precisely we consider methods that are Hermite analogs of wellestablished mixed finite elements for flow in porous media or heat transfer, such as the lowest order Raviart-Thomas method [6] and its extensions to convection-diffusion problems proposed by Douglas and Roberts [2]. We also present results on the Zienkiewicz triangular plate element [8] as applied to represent the velocity in viscous incompressible flow.

Key words: Convection-diffusion, finite element, Hermite, incompressible flow, mixed

1 Introduction

Historically Hermite finite element methods were introduced to solve fourth order elliptic or parabolic equations, modeling a certain number of problems in Solid and Fluid Mechanics. Among well-known applications in this framework lie plate bending problems (cf. [3]) and the incompressible Navier-Stokes equations in terms of the stream function or the vector potential (cf. [5]). This is because this kind of methods using derivatives as degrees of freedom, seems quite natural to ensure an acceptable conforming representation of the solution. The fact that second order problems do not require this kind of approach to attain the same goal, is probably the reason why the use of Hermite finite element methods in this context had not been throughly exploited until very recently. Instead, whenever the direct representation of derivatives, fluxes or quantities alike is required, most authors consider the use of natural mixed formulations, in which the main unknown function and such related quantities are the multiple unknown fields of a system equivalent to the original equation. On the other hand sometimes the direct representation of derivatives is not essential. This is the case of incompressible viscous flow. However it turns out that the use of a Hermite velocity representation involving its first order derivatives can provide means to reduce the computational time in flow simulations. In this work we endeavour to illustrate the advantages of two types of Hermite finite elements as compared to mixed methods having either the same global amount of degrees of freedom or the same order.



2 Scope of the work

In the work's first part we consider Hermite analogs of the two extensions of the lowest order Raviart-Thomas mixed element [6] for flow in porous media proposed by Douglas and Roberts in [2] to treat convection-diffusion phenomena such as heat transfer. Complete convergence results are demonstrated for both new techniques including the one introduced in [7]. Our analysis shows that, in contrast to their mixed counterparts, the Hermite methods are second order convergent in L^2 , provided the Péclet number is not so high. Several numerical results for academic problems illustrate such convergence properties.

In the second part of our work we study an application of Hermite finite elements to the Stokes system in terms of the primitive variables in Galerkin formulation. More precisely the velocity is represented by the reduced cubic Zienkiewicz plate element, while the pressure is interpolated by means of standard continuos piecewise linear fucntions. Optimal second order convergence results obtained in [1] for the case of criss-cross meshes are extended to more general situations. The method is shown to perform better than the popular Taylor-Hood triangular element [4], which has the same order thanks to its velocity representation by means of Lagrange piecewise quadratic functions.

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Symmetry breaking in a bulk-surface reaction-diffusion model for signaling networks

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Abstract

Small GTPases are key regulators of membrane trafficking. The cycling of these GTPases between active and passive states and between cytosolic and membrane-bound states is essential for their function. The mathematical modeling of this scenario leads us to a coupled system of reaction-diffusion equations inside and on the membrane. For our numerical investigations, the membrane is implicitly treated in a diffuse-interface approach to study the influence of Turing-type mechanisms for the localization of act-ive/inactive GTPases. Furthermore, we use a phase field method in order to simulate a reaction-diffusion system which is coupled to the dynamics of the membrane.

Key words: Numerical simulations of reaction-diffusion systems, PDE's on surfaces, Reaction-diffusion systems, Turing instability MSC 2010: 92C37,35K57,35Q92

1 Introduction

In this contribution, we study a mathematical model for a GTPase cycle presented and analyzed in [3] and [4]. Thereby, we will represent the cytosolic volume and the membrane of a cell by a bounded, connected, open domain $B \subset \mathbb{R}^3$ in space and its two-dimensional boundary $\Gamma := \partial B$, respectively. We assume that Γ is given by a smooth, closed surface and denote by v the outer unit normal of B on Γ . Moreover, we fix a time interval $I := [0,T] \subset \mathbb{R}$ and consider smooth functions $V : \overline{B} \times I \to \mathbb{R}, u, v : \Gamma \times I \to \mathbb{R}$ (representing the cytosolic inactive, membrane-bound active, and membrane-bound inactive GTPase, respectively) that satisfy the coupled reaction–diffusion system (stated in a non-dimensional form)

$$\partial_t V = D\Delta V$$
 in $B \times I$, (1)

$$\partial_t u = \Delta_{\Gamma} u + \gamma f(u, v)$$
 on $\Gamma \times I$, (2)

$$\partial_t v = d\Delta_{\Gamma} v + \gamma (-f(u,v) + q(u,v,V))$$
 on $\Gamma \times I$, (3)

$$-D\nabla V \cdot v = \gamma q(u, v, V) \qquad \text{on} \quad \Gamma \times I \qquad (4)$$

on and inside Γ . Here *f* and *g* model the activation/inactivation processes and *q* describes attachment/detachment at the membrane. The non-dimensional parameter $\gamma > 0$ is related to the spatial scale of the cell. The coupling of bulk and surface equations in (1)–(4) is given by a Robin-type boundary condition. Furthermore, we assume initial conditions for the system at time *t* = 0.



2 Linear Stability Analysis

We present a linear stability analysis of the reaction-diffusion system (1)-(4). We study the stability of spatially homogeneous stationary states and find two possible scenarios for a diffusive instability. The first is similar to a classical Turing instability in the u, v variables and is only possible for large differences in lateral diffusion coefficients for u and v (i.e. for a coefficient $d \gg 1$). The second mechanism on the other hand does also occur for equal lateral diffusion constants (i.e. for d = 1) and is rather based on the different diffusion constants for u and V and therefore on the coupling of bulk and surface equations. As cytosolic diffusion is typically by a factor hundred faster than lateral diffusion, this scenario is much more realistic in the application to signaling networks. Moreover, we compare the stability of the full system (1)-(4) to its reduction in the formal limit $D \rightarrow \infty$. This reduction leads to a non-local two-variable system on the membrane that has been analyzed in [3]. The results of the stability analysis for the reduced model are similar to the results of the full system.

3 Numerical Treatment

We use a phase-field approach for the coupling of bulk and surface PDE's appearing in (1)–(4). We follow the diffuse interface descriptions for PDE's on surfaces [1, 5], in the bulk [2] and for the coupling [6, 7]. We will present numerical simulations for specific versions both of the full system and of the reduced system. The simulations confirm the instability criteria derived in the linear stability analysis and allow to investigate the time-evolution after the onset of heterogeneities and beyond the regime governed by the linearization. It turns out that even for simple choices of the constitutive relations f and q the system exhibits a rich behavior.

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A numerical method for simulation incompressible lipid membranes in viscous fluid.

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Abstract

A numerical method for simulating the dynamics of an incompressible elastic lipid membrane imbedded into viscous fluid is discussed. A new elliptic equation for the membranes tension implying local incompressibility of the membrane is introduced. Forces acting on the fluid from the membrane are implemented by the immersed boundary method.

Key words: incompressible lipid membranes, Willmore functional

1 Motivation and formulation of the problem

Mathematical modeling of lipid membranes and related mathematical problems as Willmore flow attracted much attention in last years. Lipid bio-membranes envelope cells and divide them into compartments. They also play a role in dynamic processes such as transport and signaling in cells. Direct micro-manipulation of artificial membranes is used to monitor biochemical enzyme reactions.

We consider here the Navier-Stokes equations as a model for incompressible viscous fluid with imbedded membrane Γ acting on the fluid with a force F concentrated on the smooth surface Γ :

$$\mathbf{F} = \mathbf{W} + 2\sigma H \mathbf{n} + \nabla_{\Gamma} \sigma + \theta \mathbf{n},\tag{1}$$

where $\mathbf{W} = \left[-2\kappa \left(\Delta_{\Gamma}H + 2H \left(H^2 - K\right)\right)\right] \mathbf{n}$, \mathbf{W} the bending force, and $2\sigma H\mathbf{n}$ the Young-Laplace force both acting in the normal direction \mathbf{n} . The elastic tension force $\nabla_{\Gamma}\sigma$ acts in the tangential direction along Γ .

The operator $\Delta_{\Gamma}H + 2H(H^2 - K)$ is the Euler-Lagrange operator of the Willmore functional $\int_{\Gamma} H^2 dS$. Here Δ_{Γ} is the Laplace-Beltrami operator, H and K are the mean an Gauss curvatures of Γ , κ is the bending modulus, σ is tension and θ is the osmotic pressure between the inside and the outside of Γ .

The coupling between the fluid and the membrane is approximated by the immersed boundary method with force $\delta_{\Gamma} \mathbf{F}$ where a smooth function δ_{Γ} approximates the delta function δ_{Γ} on the surface Γ :

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \mu \Delta \mathbf{u} + \widetilde{\delta}_{\Gamma} \mathbf{F}; \qquad \text{div } \mathbf{u} = 0$$



We use the notation V for the velocity of the membrane. Lipid membranes are kept locally incompressible by tension forces. This property implies a constrain on the in surface divergence: $\operatorname{div}_{\Gamma} V = 0$ of V. Membranes are nonpermeable and satisfy non-slip boundary conditions on Γ : V = u. The operator splitting is used to approximate solutions of the fluid equations together with the equations for the membrane. At each time step Δt the system of equations for the membrane velocity V and the mean curvature vector H is solved :

$$\frac{\partial \mathbf{V}}{\partial t} = \delta_0 \left(\left[-2k \left(\Delta_{\Gamma} H + 2H \left(H^2 - K \right) \right) \right] \mathbf{n} + 2\sigma \mathbf{H} + \nabla_{\Gamma} \sigma + \theta \mathbf{n} \right)$$
(2)
$$\frac{\partial \mathbf{H}}{\partial t} = \frac{1}{2} \Delta_{\Gamma} \mathbf{V}$$

for points on the surface Γ , and $\delta_0 = const$. We solve these equations in a semi-implicit fashion first with tension $\sigma = \sigma_n$ taken from the previous time step *n* and then with $\sigma_{n+1} = \sigma_n + \psi$ corrected to so that the corresponding velocity becomes divergence free on the surface. This constrain implies an elliptic equation for the tension corrector ψ :

$$\Delta_{\Gamma}\psi - 4\psi \left| \mathbf{H}^{(n+1)} \right|^{2} = -\left[\operatorname{div}_{\Gamma} \left(\mathbf{V}^{(n+1)} \right) \right] \left(\frac{1}{\delta_{0} \Delta t} \right)$$
(3)

The situation is similar to the one with incompressible Navier Stokes equation, where pressure corresponding to a divergence free velocity field must satisfy the Poisson equation. The exact volume conservation constrain for a closed not permeable membrane is implemented by adjusting at each time step the parameter θ in (2) together with σ .

2 Examples

The numerics is illustrated in Fig. 1 by two examples of the deformation and streamlines pictures: one with a nano-tube pulled out from an ellipsoidal membrane by external force and another one with the relaxation of initially ellipsoidal vesicle to the red blood cell form.



(a) Pulling out a nano-tube

(b) Relaxation to erythrocyte form





Adaptive Discontinuous Galerkin Finite Methods for advective Allen–Cahn equation

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Abstract

An adaptive space-time discontinuous Galerkin finite element method is studied for the advective Allen–Cahn equation. Time discretization is performed by Gauss-Radau discontinuous Galerkin finite elements, while symmetric interior penalty Galerkin method is used for space discretization. Numerical results for one and two dimensional droplet breakup models are presented to show the efficiency of the adaptive algorithm.

Key words: discontinuous Galerkin method, space-time adaptivity, Allen-Cahn equation

1 Introduction

We consider the advective Allen-Cahn equation [3] for a diffusive interface surface tension model

$$u_t + \nabla \cdot (u\mathbf{V}) + \epsilon \Delta u = \frac{1}{\epsilon} f(u) \tag{1}$$

with Ginzburg–Landau free energy $E(u) = \int_{\Omega} \left(\epsilon |\nabla u|^2 + \frac{1}{\epsilon} F(u) \right)$ and $F(u) = u^2 (1-u)^2$ is the bistable double–well potential that characterizes the two phases in which case f(u) = F'(u) = 2u(1-u)(1-2u) and **V** is prescribed velocity field. We assume no boundary flow condition, i.e. $\frac{\partial u}{\partial n} = 0$ on $\partial\Omega$.

The advective Allen–Cahn equation (1) represents surface tension of the droplet breakup phenomena under the influence flow field. The velocity field **V** is divergent free, when the the velocity field satisfies the Navier–Stokes equation. We consider droplet breakup phenomena under compressible flow. In this situation the velocity field **V** is not divergent free; it is expanding $\nabla \cdot \mathbf{V} > 0$ or contracting $\nabla \cdot \mathbf{V} < 0$.

The non-local Allen-Cahn equation is

$$u_t + \nabla \cdot (u\mathbf{V}) + \epsilon \Delta u = \frac{1}{\epsilon} f(u) + \lambda u$$
⁽²⁾

where the Lagrange multiplier λ is given by $\lambda = \frac{1}{\epsilon} \frac{1}{M} \int_{\Omega} f(u)$ so that $\int_{\Omega} u$ is a constant mass M.

The local (1) and nonlocal (2) Allen–Cahn equations are discretized in space by the symmetric interior point discontinuous Galerkin method (SIPG), due the flexibility an adaptive meshes and mass conservation. For time integration we use also discontinuous Galerkin Gauss–Radau method in time [1], which is strongly stable and preserves the energy decreasing property of the Allen–Cahn equation. Allen–Cahn equation evolves on two different time scales, the small surface time scale for small ϵ and convective time scale. The stiffness of Allen–Cahn equation is characteristic for sharp interface problems with small ϵ , whereas numerical schemes require that meshes have to locally refined. We apply modified version of space-time adaptive DG method linear diffusion-convection problems in [2] to resolve the features on small scales.

The disadvantage of the dG methods is the large coupled systems to be solved at each time step. We use iterative and sparse direct solvers for fast solution of the of the system of equations arising from space-time DG-FE discretizations. We prove that the Allen–Cahn model will not break up under certain circumstances due to a maximum principle. Simulations in one and two dimensions verify the theoretical results and provide more insight into the dynamics.

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Numerical Solving of a first order partial differential equation with a time delay and a retardation of a state variable

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Abstract

We construct a difference scheme for the numerical solution of a first order partial differential equation with a time delay and a retardation of a state variable. Coefficients in the equation are assumed to be dependent on state variable. Such equations are used to model the dynamic of structured cell populations when age and maturity level are taken into consideration. For the supplied difference schemes the order of approximation error, stability and convergency order are studied.

Key words: Difference scheme, Partial Delay Differential Equation MSC 2010: 65Q20, 65M06

1 Introduction. The problem

First order partial differential equations, also known as an advection equations, with distributed parameters arise in the modeling of dynamics of populations structured with respect to the cell size, the age of specimen, maturation level etc [1, 2].

Authors [2] note that the dynamics are not only dependent on the behavior of the cell population numbers some time in the past (time delayed effects), but also that the population behavior at a given maturation level is dependent on the behavior at a previous maturation level (nonlocal effects). Thus, this important biological problem leads, in a rather natural fashion, to an complex mathematical problem involving a delayed nonlocal dynamics described by a nonlinear advection equation.

Consider the following advection equation with after effect and retardation of state variable

$$\frac{\partial u}{\partial t} + a(x)\frac{\partial u}{\partial x} = f(x, t, u(x, t), u_t(\alpha x, \cdot)), \tag{1}$$

here $x \in [0; X]$ – space and $t \in [0; \theta]$ – time independent variables; u(x, t) – unknown function; $u_t(\alpha x, \cdot) = \{u(\alpha x, t + \xi), -\tau \le \xi < 0\}$ – prehistory-function of the unknown function to the moment t which also involves biasing in state variable, $\alpha \in (0, 1)$ – constant of the biasing, $a(x) > a_0 > 0$ – sufficiently smooth function.

Initial and boundary conditions are set:

 $u(t,x) = \varphi(x,t), x \in [0;X], t \in [-\tau;0], \text{ and } u(0,t) = g(t), t \in [0;\theta]$ (2)

Consensual conditions are satisfied $q(0) = \varphi(0,0)$.



2 Difference scheme

We follow technique elaborated in [3, 4]. Let *N* and *M* be the number of partition points for [0; X] and $[0; \theta]$ respectively. The uniform grid can be constructed $\{t_j, x_i\}_{j=0}^{M} \sum_{i=0}^{N} where t_j = j\Delta$, j = 0, ..., M, and $x_i = ih$, i = 0, ..., N. Let u_j^i denotes approximate solution $u(x_i, t_j)$ and $\varepsilon_j^i = u(x_i, t_j) - u_j^i$, i = 0, ..., N, j = 0, ..., M.

For $0 \le s \le 1$ we consider a family of difference schemes, j = 0, ..., M - 1,

$$\frac{u_{j+1}^{i}-u_{j}^{i}}{\Delta} + a\left(s\frac{-4u_{j+1}^{0}-2h/a(f_{j+1}^{0}-\dot{g}_{j+1})+4u_{j+1}^{1}}{2h} + (1-s)\frac{-4u_{j}^{0}-2h/a(f_{j}^{0}-\dot{g}_{j})+4u_{j}^{i}}{2h}\right) = f_{j}^{1},$$

$$\frac{u_{j+1}^{i}-u_{j}^{i}}{\Delta} + a\left(s\frac{u_{j+1}^{i-2}-4u_{j+1}^{i-1}+3u_{j+1}^{i}}{2h} + (1-s)\frac{u_{j}^{i-2}-4u_{j}^{i-1}+3u_{j}^{i}}{2h}\right) = f_{j}^{i}, \quad i = 2, ..., N.$$
(3)

Here f_j^i denotes the value of f in the node (i,j), $\dot{g}_j = dg(t)/dt \Big|_{t=j\Delta}$. Since f may depend on values of u between nodes, approximation is needed to evaluate functional f_i^i .

We say that the method converges with order $h^p + \Delta^q$, if there exists constant *C*, that $\|\varepsilon_i^i\| \leq C(h^p + \Delta^q)$ for all i = 0, ..., N and j = 0, ..., M.

Theorem Let the exact solution u(x,t) of the problem (1) thrice continuously differentiable by x and twice continuously differentiable by t, first derivative of the solution by x is continuously differentiable by t. Then if s > 0.5 the method (3) convergence with order $h^2 + \Delta$.

To test the proposed scheme we solved a model of cell dynamics - the system of two coupled advection equation with a time delay and a retardation of a state variable [2].

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Optimal location of green zones in metropolitan areas

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Abstract

In this paper we analyze and numerically solve a problem related to the optimal location of green zones in metropolitan areas in order to mitigate the urban heat island effect. So, we consider a microscale climate model and analyze the problem within the framework of optimal control theory of partial differential equations. Finally we compute its numerical solution using the finite element method, with the help of FreeFem++.

Key words: Parklands, Urban heat island, Optimal control, Partial differential equations

1 The environmental problem

We are interested in optimally locate two parklands (Γ_{p_1} and Γ_{p_2}) with a fixed total length M, whose vegetation is characterized by the leaf area density LAD : ($\Gamma_{p_1} \cup \Gamma_{p_2}$) × (0, z_p] $\rightarrow \mathbb{R}$ (with z_p the total height of the vegetation), in order to increase the comfort of the pedestrian on paved areas in a range of 1 to 2 meters (see Fig. 1) for a time interval I = (0, T).

2 Mathematical formulation and numerical resolution

From a mathematical viewpoint, we try to minimize the following cost function:

$$\min_{(p_1,p_2,l_1)\in\mathcal{U}_{ad}}\frac{1}{2T\operatorname{meas}(\Gamma_{s}\setminus(\Gamma_{p_1}\cup\Gamma_{p_2}))}\int_0^T\int_{(\Gamma_{s}\setminus(\Gamma_{p_1}\cup\Gamma_{p_2}))\times[1,2]}\theta(\mathbf{x},t)\,d\mathbf{x}\,dt,$$

where p_1 is the initial position of the first park, p_2 the initial position of the second one, and l_1 the length of the first one (that is, $\Gamma_{p_1} = [p_1, p_1 + l_1]$ and $\Gamma_{p_2} = [p_2, p_2 + l_2]$, with $l_2 = M - l_1$). The set of admissible controls $\mathcal{U}_{ad} = \{(p_1, p_2, l_1) \in \mathbb{R}^3 : a_1 \leq l_1 \leq b_1, p_1 + l_1 \leq p_2, and for <math>k = 1, 2, \Gamma_{p_k} \subset \Gamma_{s_i}$ for any $j = 1, \ldots, N\}$, with $0 < a_1 < b_1 < M$. The state variables in our study





Figure 1: Computational domain.

will be the velocity **u**, the pressure *p* and the temperature θ of wind, and the temperature θ_f of vegetation in both parklands $\Gamma_{p_1} \times (0, z_p]$ and $\Gamma_{p_2} \times (0, z_p]$:

())

$\left(\frac{\partial \theta}{\partial t} + \mathbf{u} \cdot \nabla \theta - \nabla \cdot (K_h \nabla \theta) \right)$
$= \chi_{(\Gamma_n \cup \Gamma_n) \times (0, z_n]} \text{LAD } J_{f,h} \text{ in } \Omega \times I$
$\theta = \theta_{ref} \text{ on } \Gamma_1 \times I$
$\nabla \theta \cdot \mathbf{n} = 0 \text{ on } \Gamma_3 \times I$
$\rho_{C_r} K_l \nabla \theta \cdot \mathbf{n} = v_1 (T^4 - \theta^4) \text{ on } (\Gamma_r \cup \Gamma_r) \times I$
$\int \rho c_p K_p \nabla \theta \cdot \mathbf{n} = \sigma_1 V_1 (T_p^4 - \theta^4) V_D$
$\int p c_p r_h \sqrt{c} n = O_1 \gamma_1 (r_r - c_r) \chi_{1_{p_1} \cup 1_{p_2}}$
$+\sigma_2\gamma_2(\theta_f- heta^4)\chi_{\Gamma_{p_1}\cup\Gamma_{p_2}}$
$+\gamma_1(T_r-\theta^4)(1-\chi_{\Gamma_{p_1}\cup\Gamma_{p_1}})$ on $\Gamma_s\times I$
$\theta(0) = \theta_{\text{ref}} \text{ in } \Omega$

with $\rho c_p J_{f,h} = \rho c_p \alpha r_a^{-1}(\theta_f - \theta) = \sigma_1 \gamma_1 (T_r^4 - \theta_f^4) + \sigma_2 \gamma_2 (\overline{\theta}_{|_{\Gamma_{p_1} \cup \Gamma_{p_2}}}^4 - \theta_f^4)$, where $\alpha = 1.1$, r_a is the aerodynamic resistance (depending on leaf geometry and wind velocity), γ_1 is the product of the Stefan-Boltzmann constant times the emisivity, γ_2 is the product of the Stefan-Boltzmann constant times the foliage and the boundary, T_r is the radiation temperature (computed from incident solar radiation), and $\sigma_1, \sigma_2 \in [0, 1]$ are attenuation coefficients related to vegetal mass density [1, 2].

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Drift-diffusion equation approach to the SEM charging problem

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Abstract

We investigate the applicability of the drift-diffusion model to the problem of sample charging in scanning electron microscopy (SEM). The drift-diffusion approach provides insight into the dynamics of the charging process and may be an interesting alternative to the currently prevalent Monte Carlo simulations.

Key words: Drift diffusion model, Scanning electron microscope, Secondary electrons

1 Introduction

Usually the SEM charging problem is studied by Monte Carlo (MC) techniques. The advantage of the MC approach is in the rigorous semi-classical account of the microscopic physics. However, the MC method suffers from the increase of the computational complexity in the case of long-range potentials. An alternative way to study such poorly conducting samples has been developed in semiconductor physics and makes use of the drift-diffusion equation.

2 The drift diffusion equation

The drift-diffusion model consists of a set of three coupled, nonlinear PDEs [1].





Figure 1: The considered geometry for the model

2.1 Boundary conditions

We assume a parallelepiped geometry denoted by Ω Figure 1.

$$n(\mathbf{x},t) = n_i, \quad p(\mathbf{x},t) = n_i, \quad V(\mathbf{x},t) = 0, \quad \text{on} \quad \partial \Omega_D \times (0,T]$$
$$\mathbf{J}_p \cdot \mathbf{v} = 0, \quad \text{on} \quad \partial \Omega_N \times (0,T].$$

2.2 Charge injection

The primary electrons penetrate the sample up to the maximum range $R(E_0)$ [2],

$$R(E_0) = 900\rho^{-0.8}E_0^{1.3}$$
 for $E_0 < 10$ keV, $R(E_0) = 450\rho^{-0.9}E_0^{1.7}$ for $E_0 > 10$ keV.

The secondary electrons and holes are created in parity as a Gaussian distribution with the maximum shifted by 0.3R from the surface into the sample [3],

$$g_{SE}(\mathbf{x}, E_0) = g_{SH}(\mathbf{x}, E_0) = \frac{1}{E_i} \frac{7.5C}{\pi R^2} e^{-\frac{7.5}{R^2} (\mathbf{x} - \mathbf{x}_0)^2},$$

For the material like silicon, silicon dioxide with the same backscattered rate ($\eta \approx 0.2$), *C* is calculated with the following formula $C(E_0) = 1.544 \frac{E_0}{R(E_0)}$.

Acknowledgements

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On New Techniques for Optimization over Polynomials

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Abstract

In this report two methods for optimization over polynomials is presented: Bernstein expantion and linear matrix inequalities approach.

Key words: Bernstein Expantion, Stability, Multivariable Polynomial, Linear Matrix Inequality.

MSC 2010: 15A15, 15A24, 93D30, 93D20.

1 Introduction

Numerous problems in control system theory (such as stability of linear and nonlinear systems, robust stability of uncertain systems, quadratic stability of system for perturbations, stabilization by linear feedback) involve optimization problems over multivariable polynomials. For example, the basic problem of establishing stability of an equilibrium point consists of determining a positive definite function such that its derivative along the trajectories of the system is negative. On the other hand the derivative of the state of the system and the candidate positive function are polynomials. Unfortunately optimization problems over polynomials are in general nonconvex and the corresponding minimization algorithms may get stuck in a local minimum.

In order to cope with this difficulty various methods have been proposed. In this report two such methods will be presented: Bernstein expansion of a multivariable polynomial and linear matrix inequality (LMI) approach (see [1, 2, 3]).

Given a multivariable polynomial the Bernstein expansion gives bounds for the range set over a box. In order to obtain convergent bounds for the range of a polynomial the initial box should be segmentially divided into two boxes. The Bernstein expansion is applied to the robust stability of different uncertain systems.

LMI techniques which mainly is based on sum of squares technique allow to obtain bounds to the sought solution by solving convex optimization problem.

In the report on the base of different examples from control theory a comparison of the Bernstein expansionand LMI approach has been given.



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Full discretization of a nonlinear parabolic integro-differential problem with an unknown Dirichlet boundary condition*

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Abstract

A nonlinear parabolic integro-differential problem containing an unknown solely time-dependent Dirichlet condition on a part of the boundary is considered. An additional integral measurement is used to recover the missing data. A full discretization method is designed to approximate the unique weak solution to this problem. Correpsonding error estimates are derived.

Key words: nonlinear parabolic integro-differential equation, unknown Dirichlet condition, full discretization, error estimates MSC 2010: 47J35, 65M12, 65M32

1 Introduction

Let $\Omega \subset \mathbb{R}^d$, $d \in \mathbb{N}$, be a bounded domain with a Lipschitz continuous boundary $\Gamma = \Gamma_1 \cup \Gamma_2$, with $\Gamma_1 \cap \Gamma_2 = \emptyset$ and $|\Gamma_2| > 0$. By ν we denote the outward unit normal vector on Γ . We consider the following nonlinear parabolic problem

$$\begin{cases} \partial_t g(u(t, \mathbf{x})) - \Delta u(t, \mathbf{x}) &= F(t, \mathbf{x}) + \int_0^t f(s, u(s, \mathbf{x})) \, ds & \text{in } (0, T) \times \Omega; \\ -\nabla u \cdot \mathbf{v} &= h(t, \mathbf{x}) & \text{on } (0, T) \times \Gamma_1; \\ u &= \alpha(t) & \text{on } (0, T) \times \Gamma_2; \\ u(0) &= u_0(\mathbf{x}) & \text{in } \Omega, \end{cases}$$
(1)

together with the additional integral measurement

$$\int_{\Omega} g(u(t, \mathbf{x})) \, \mathrm{d}\mathbf{x} = E(t) \quad \text{in } (0, T), \tag{2}$$

which is needed to recover the solely time-dependent Dirichlet boundary condition $\alpha(t)$. We assume that *f* and *q* are globally Lipschitz continuous functions in all variables.

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Such type of parabolic integro-differential equations have some applications in reactive contaminant transport in the saturated zone, cf. [1, Chap. 15]. The existence and uniqueness of a solution

$$\{u,\alpha\} \in \left(C\left([0,T],L_2(\Omega)\right) \cap L_{\infty}\left((0,T),H^1(\Omega)\right)\right) \times L_2\left(0,T\right)$$

to the problem (1)-(2), obeying $\partial_t u \in L_2((0,T), L_2(\Omega))$, and a numerical time-discrete approximation scheme have already been studied in [2] under appropriate assumptions on the data.

2 Full discretization

We use Rothe's method [3] with $n \in \mathbb{N}$ discretization intervals $[t_{i-1}, t_i]$, $t_i = i\tau$, i = 1, ..., n, for the time discretization. We work in a finite dimensional subspace V_h of V, with discretization parameter h. We introduce the notation $u_i^h \approx \pi_h u(t_i)$, $1 \le i \le n$, and for every other function z, we write

$$z_i^h = \pi_h z(t_i), \qquad \delta z_i^h = \frac{z_i^h - z_{i-1}^h}{\tau}, \quad 1 \le i \le n.$$

Now, let $\pi_h : C(\overline{\Omega}) \to V_h$ be the global interpolant on V_h . The recurrent approximation scheme for k = 1, ..., n reads as $(\forall \varphi \in V_h)$

$$\begin{split} \left(\delta g(u_k^h),\varphi\right) + \left(\nabla u_k^h,\nabla\varphi\right) &= (F_k,\varphi) - (h_k,\varphi)_{\Gamma_1} + \left(\sum_{j=0}^{k-1} f(t_j,u_j^h)\tau,\varphi\right) \\ &+ \varphi_{|\Gamma_2} \left[E'_k - (F_k,1) + (h_k,1)_{\Gamma_1} - \left(\sum_{j=0}^{k-1} f(t_j,u_j^h)\tau,1\right)\right], \\ &u_0^h &= \pi_h u_0. \end{split}$$

The existence of $u_i^h \in V_h$, $1 \le i \le n$, follows form the theory of monotone operators. We proved that, under appropriate conditions on the data, the approximation scheme satisfies the following error estimates $(1 \le j \le n)$

(i)
$$\sum_{i=1}^{j} \left\| u(t_{i}) - u_{i}^{h} \right\|^{2} \tau + \sum_{i=1}^{j} \left\| \nabla u(t_{i}) - \nabla u_{i}^{h} \right\|^{2} \tau^{2} + \left\| \sum_{i=1}^{j} \left(\nabla u(t_{i}) - \nabla u_{i}^{h} \right) \tau \right\|^{2} \\ \leqslant C \left(\tau + \sum_{i=1}^{n} \left\| \pi_{h} u(t_{i}) - u(t_{i}) \right\|_{H^{1}(\Omega)}^{2} \tau + \left\| \pi_{h} u_{0} - u_{0} \right\|^{2} \right),$$

(ii)
$$\left| \sum_{i=1}^{j} \left(\alpha(t_{i}) - \alpha_{i} \right) \tau \right|^{2} \leqslant C \left(\tau + \sum_{i=1}^{n} \left\| \pi_{h} u(t_{i}) - u(t_{i}) \right\|_{H^{1}(\Omega)}^{2} \tau + \left\| \pi_{h} u_{0} - u_{0} \right\|^{2} \right).$$

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Modelling of reactive nonisothermal mixture flow and its simulation in COMSOL Multiphysics

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Abstract

We investigate modelling and simulation of catalytic fluidized bed reactor producing H_2 and CO_2 gaseous mixture as catalytic decomposition of liquid formic acid in presence of solid catalyst. We derive, so called, Class II model of nonisothermal reactive mixture flow where we consider mixture of solid, liquid and gas distinguishing partial densities and velocities sharing one common thermal field. The reactions undergo Arrhenius kinetics producing gaseous bubbles whose flow in liquid/solid mixture is modelled as a flow in porous medium according to Darcy's law. We present simulations of such a model performed in COMSOL Multiphysics.

Key words: fluidized bed reactor, Class II mixture, Arrhenius kinetics, bubbly flow

1 Motivation

Hydrogen is often described as the fuel of the future due to its high energy content and a combustion pathway which produces only water as a by-product. However, conventional storage methods are disadvantageous due to significant energy requirements and inherent safety risks associated with hydrogen kept under extreme pressure. We study a system where hydrogen is stored chemically as formic acid, a non-hazardous liquid. In the presence of certain metal catalysts the decarboxylation, i.e. endothermic reaction $HCOOH \rightarrow H_2 + CO_2$, occurs where hydrogen is produced on demand which can be directly used in fuel cells.

2 Introduction

The reactor is considered as fluidized bed reactor of liquid formic acid with microscopic solid particles (diameter < $100\mu m$) producing gaseous mixture of H_2 and CO_2 . Physical model of the flow is kind of Class II model of nonisothermal reactive mixture. Here we distinguish more levels of description since for very small solid particles its mixture with liquid can be treated as a sol (colloid) and it can be sufficiently approximated as single non-Newtonian pseudo-incompressible continuous phase. Similarly, the gas mixture of H_2 and CO_2 can be without big loss of generality considered as single pseudo-compressible dispersed phase. The flow of continuous phase is mainly driven by thermal convection modelled by Boussinesq approximation influenced by bubbly flow of the gaseous product.



3 Model

Denote ρ_c the density of continuous phase and let u_d be its velocity. For ρ_d the density of dispersed phase we introduce mixture density as $\rho = \Phi_c \rho_d^{\text{mix}} + \Phi_d \rho_d^{\text{mix}}$ where Φ_d is volume fraction of dispersed phase; Φ_c is volume fraction of continuous phase and the volume additivity holds, i.e. $\Phi_d + \Phi_c = 1$. We introduce the continuity equation for volume fraction

$$\frac{\partial \Phi_d}{\partial t} + \operatorname{div}(\Phi_d u_d) = -\frac{r}{\rho_d} \tag{1}$$

where $r = \tilde{A}e^{-\frac{E_a}{RT}}$ is reaction rate modeled by Arrhenius law, for \tilde{A} being frequency factor, E_a activation energy for the reaction, T temperature and R the universal gas constant. We model a slip velocity u_{slip} according to Darcy's law or, so called, drag pressure balance

$$\frac{3}{4}\frac{C_d\rho_c}{d_d}|u_{\rm slip}|u_{\rm slip} = -\frac{\rho - \rho_d}{\rho}\nabla p \tag{2}$$

where d_d is the bubble diameter and we specify the coefficient C_d by convenient model due to the flow-regime and the size of the bubbles. In our case we can use common Hadamard Rybczynski model for spherical bubbles or Haidler-Levenspiel model for nonspherical bubbles where A, B, C, D are functions of the bubble-sphericity S_p and μ is viscousity of the mixture

$$C_d = \frac{24}{\text{Re}_p} (1 + A(S_p) \text{Re}_p^{B(S_p)}) + \frac{C(S_p)}{1 + D(S_p)/\text{Re}_p}, \quad \text{Re}_p = \frac{d_d \rho_c |u_{\text{slip}}|}{\mu}.$$

Consequently, we define mixture velocity as $u = u_d + c_c u_{slip}$ where $c_c = \frac{\Phi_c \rho_d^{mix}}{\rho}$ is concentration of continuous phase and $c_d = 1 - c_c = \frac{\Phi_d \rho_d^{mix}}{\rho}$. The momentum equations follows

$$\rho \frac{\partial u}{\partial t} + \rho(u \cdot \nabla)u = \operatorname{div} \mathbb{T} + \rho g + F - \operatorname{div} \left(\rho c_d c_c u_{\operatorname{slip}}^2\right)$$
(3a)

$$\mathbb{T} = -\nabla p + 2\mu \mathbb{D} \tag{3b}$$

$$(\rho_c - \rho_d) \operatorname{div} \left(\Phi_d c_c u_{\text{slip}} + \frac{r}{\rho_c} \right) + \rho_c \operatorname{div} u = 0$$
(3c)

and denoting C_p the heat capacity in constant pressure; k thermal coefficient and Q_r the heat of the reactions we finally close the model by heat equation for temperature T

$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p u \cdot \nabla T = \operatorname{div}(k \nabla T) + Q_r.$$
(4)

The simulations of such a model were performed in COMSOL Multiphysics and the results will be shown during the presentation.

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Recent advances in the level set method for shape and topology optimization of structures

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Abstract

We review some of our recent works concerning shape and topology optimization of structures. Their common feature is to rely on the level set algorithm. First, we discuss geometrical constraints and more precisely thickness constraints. Second, we present a linearized approach of worst-case design optimization in the presence of uncertainties. Third, we introduce a new algorithm for shape and topology optimization which features an exact mesh of the structure at each iteration of the optimization process.

Key words: level set method, shape optimization, topology optimization MSC 2010: 49Q10, 74P15, 74P20

1 Introduction

Since its inception [4], [5], [8], [9], [10], the level set method in structural optimization has gained an enormous popularity due to its versatility and the quality of the produced optimal shapes which always have a clear and well-defined boundary. Nevertheless, there are still progresses to be made and we report about three recent advances in this field. All examples are computed for a model of linearized elasticity.

2 Thickness constraints

In [3], [7] we consider structural optimization problems for which geometric constraints are imposed. More precisely we define a notion of thickness, based on the signed distance function to the shape. We formulate three global constraints using integral functionals and geometric notions as skeleton and offset set: a maximal thickness, a minimal thickness and a minimum members' distance. In the framework of Hadamard method we compute their shape derivatives which allows us to implement them in a standard constrained optimization algorithm. We discuss different strategies and possible approximations to handle the geometric constraints. As can be expected, the resulting optimized shapes are strongly dependent on the initial guesses and on the specific treatment of the constraints since, in particular, some topological changes may be forbidden by those constraints. On Figure 1 an example of minimum



thickness constraint is displayed for the classical test case of a force inverter (an horizontal load is applied at the middle of the left side which should produce an inverse displacement on the right side). The thin joints of the unconstrained optimal shape are thicken in the resulting optimal shape when the minimum thickness constraint is applied.



(a) Without constraint

(b) With a minimum thickness constraint

Figure 1: Force inverter (clamped at the two left corners).

3 Uncertainties and worst-case design

In [1], [6] we propose a deterministic method for optimizing a structure with respect to its worst possible behavior in the case when some of its features (loads, material properties, geometry) are plagued with "small" uncertainties. The main idea of the method is to linearize the considered cost function with respect to the uncertain parameters (which are assumed small), then to consider the supremum function of the obtained linear approximation, which can be rewritten as a more "classical" function of the design, owing to standard adjoint techniques from optimal control theory. The resulting linearized worst-case objective function turns out to be the sum of the initial cost function and of a norm of an adjoint state function, which is dual with respect to the considered norm over perturbations. This formal approach is very general, and can be justified in some special cases. In particular, it allows to address several problems of considerable importance in both parametric and shape optimization of elastic structures, in a unified framework. In Figure 2 is displayed an example, the so-called mast problem, for load uncertainties. There are given and known vertical loads at both ends of the upper rectangle in the domain design. On top of them, unknown (small) vertical forces can be applied anywhere in the shaded area on the lower side of this upper rectangle. The topology of the worst-case design turns out to be more complex (and actually more stable) than that of the original optimal design.

4 A level set based mesh evolution method

In [2], [6] we propose an approach to replace the standard "shape capturing" algorithm, based on the level set method, on a fixed computational mesh by a "shape tracking" algorithm for which the structure is exactly meshed at each iteration of the optimization process. The level





Figure 2: Optimal mast with uncertainties in the loads.

set method is still a key tool but now it plays a direct role in the meshing algorithm. The main ingredients of our method are two operators for switching from a meshed representation of a domain to an implicit one, and conversely. In particular, it requires an algorithm for generating the signed distance function to an arbitrary discrete domain and a mesh generation algorithm for implicitly-defined geometries. Of course, the gain is a more accurate mechanical analysis of the structure which is exactly meshed, a crucial feature for example when evaluating a Von Mises criterion. Furthermore, our approach retains the ability of the level set method to change the topology and to sustain large deformations of the structure. This is illustrated on Figure 3.



Figure 3: Optimal chair for multiple loadings.



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A finite volume approach to the numerical solution of Generalised Nernst-Planck Poisson systems

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Abstract

We present a novel finite volume based approach to the numerical solution of generalised Nernst-Planck-Poisson systems for ion transport in electrolytes.

Key words: Bikerman-Freise Model, Electrolytes, Finite Volume Methods, Nernst-Planck equations

MSC 2010: 65N08,78A57

Recent developments in electrochemical modeling have lead to an increased interest in numerical simulations of electrolytic systems which are able to resolve the polarization boundary layer. Classically, the problem is formulated based on the Nernst-Planck-Poisson system for ion transport in a self-consistent electrical field.



(a) negative ion concentration

(b) pressure (in case of the pressure correction model) and electrostatic potential

Figure 1: 500mV applied potential on ideally polarizable electrode in aqueous 1:1 aqueous electrolyte with mol/dm^3 bulk ion concentration. Numerical results for the classical Guoy-Chapman model (GC), the Guoy-Chapman-Stern model (GCS), the Bikerman-Freise model [3] (BF), the pressure correction model of [1] (PC), and the Fermi-Dirac model (FD). The physical limit of the concentration is $55.5mol/dm^3$.

Various model improvements are currently discussed in order to take into account the volume constraint for solute concentrations, see e.g. [1]. Several of these approaches are compared



in the talk. A reformulation of the problem avoids degenerating diffusion and cross-coupling of gradients [2].



(a) concentrations of singly and doubly charged negative ions

(b) electrostatic potential and pressure

Figure 2: Ternary electrolyte with settings similar to Fig. 1.

The talk reviews a successful finite volume discretization strategy from semiconductor analysis [4] and discusses its application in the context of electrolyte modeling. Special emphasis is made on the proper reflection of qualitative properties of the physical model at the discrete level [5] Along with calculation results for benchmark examples, the influence of various model improvements is demonstrated.

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Pulse current operation of alkaline gas diffusion electrodes

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Abstract

In this work, we investigate to what extend pulse current operation influences the species distribution in alkaline GDEs and determine parameters of possible pulse current applications of zinc-air-batteries. For this purpose a 1D-model of a GDE, containing partial differential equations for species concentrations and electrochemical equations, is applied and solved numerically with the finite-volume-method. *Key words:* 1D-model, alkaline gas diffusion electrode, FVM, PDE, pulse current

1 Introduction

Secondary zinc-air-batteries might be the upcoming alternative to state-of-the-art lithiumbased battery systems because of their higher theoretical energy density. However, dendrite formation and shape change of the zinc-electrode are currently the main drawbacks.

One strategy to avoid dendrite formation is to charge/discharge the battery with pulse currents [1]. However, pulse current response of the gas diffusion electrode (GDE) in zincair-batteries, has not been investigated in detail. Since, GDE flooding can significantly lower the overall performance of zinc-air-batteries due to blockage of transport paths for oxygen [2], it is a necessity to further elucidate the oxygen distribution within the GDE.

In this work, we investigate the species distribution in alkaline GDEs and determine parameters for useful pulse current operation of zinc-air-batteries. For this purpose a 1D-model of a GDE, containing partial differential equations for species concentrations and electrochemical equations, is applied and solved numerically with the finite-volume-method.

2 Model description

The GDE is composed of a gas-filled gas diffusion layer (GDL) part, a liquid-filled GDL part and a catalyst layer (CL). Within the model, the coupling of reactant transport, electrochemical reaction and electrode potential in liquid and solid phase is accounted for. The governing equations are adapted from Wang et al. [3] and are as follows:

$$\frac{\mathrm{d}\eta}{\mathrm{d}t} = -\frac{1}{C_{\mathrm{CL}}} \cdot \left(i_{\mathrm{cell}} - z \cdot \mathbf{F} \cdot \frac{r(t)}{A} \right) \tag{1}$$

$$\frac{\partial c_{\mathrm{O}_2}}{\partial t} = D_{\mathrm{O}_2}^{\mathrm{eff}} \cdot \frac{\partial^2 c_{\mathrm{O}_2}}{\partial x^2} - \frac{1}{2} \cdot \frac{r(t)}{V_{\mathrm{CL}}}$$
(2)

$$\frac{\partial c_{\rm OH^-}}{\partial t} = D_{\rm OH^-}^{\rm eff} \cdot \frac{\partial^2 c_{\rm OH^-}}{\partial x^2} + 2 \cdot \frac{r(t)}{V_{\rm CL}}$$
(3)



whereas r(t) is the reaction rate of the electrochemical reaction. Equation (1) describes the electrode over-potential, (2) represents the diffusion of oxygen and (3) the diffusion of hydroxide ions.

3 Results

Figure 1 shows one example of the simulations results for a 2 second pulse discharge at 100 mA/cm² and 6 seconds recovery time at 0 mA/cm². The set current is higher than the limiting current for GDEs with passive oxygen supply via diffusion. However, the recovery time of 6 seconds allows the system and the oxygen concentration directly at the CL to recover and the battery to withstand significantly higher current densities. This illustrates that GDEs can be applied in zinc-air-batteries operated with pulse current at a defined ratio of pulse current and recovery. For real technical applications, where e.g. constant power operation is needed, an equivalent amount of zinc-air-batteries is connected in series or parallel to compensate the fluctuating electrode potential.



Figure 1: Pulse operation for 2 seconds pulse time at 100 mA/cm² discharge current and 6 seconds recovery time at 0 mA/cm²; $p_{O_2} = 0.21$ atm, T=298 K, 6 M KOH as electrolyte.

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Efficient time-integration for discontinuous Galerkin time-domain calculations in nanophotonics

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Abstract

The discontinuous Galerkin time-domain (DGTD) approach has gained considerable attention as an efficient and accurate method for the simulation of nanophotonic systems. Its ability to combine explicit time integration with a higher-order spatial discretization on unstructured meshes makes it a very attractive method for complex nanophotonic structures. In order to match the accurate spatial discretization one also requires an efficient higher-order time integration method. In practice, explicit low-storage Runge-Kutta (LSRK) schemes were shown to offer an excellent compromise of accuracy, performance and memory consumption. Here, we present new low-storage Runge-Kutta methods of fifth order which significantly improve both the efficiency and the accuracy of DGTD simulations of Maxwell's equations.

 $Key \ words: \ discontinuous \ Galerkin \ time-domain \ (DGTD), \ low-storage \ Runge-Kutta, \ time \ integration$

1 Introduction

When simulating nanophotonic systems with discontinuous Galerkin time-domain (DGTD) method [1], an efficient and accurate time integration procedure is required. A variety of integrators are used in the literature, but probably the most common ones are either the leap-frog method or Runge-Kutta schemes. The leap-frog method is very memory efficient and allows large timesteps but has limited accuracy. On the other hand, classical Runge-Kutta schemes are known up to very high orders, but at the cost of an increased memory consumption. Low-storage Runge-Kutta (LSRK) methods offer a good compromise between accuracy and memory consumption and therefore are particularly attractive for practical purposes.

2 Low-storage Runge-Kutta schemes

While there are several ways to implement low-storage variations of the Runge-Kutta method, we focus on a formulation originally proposed by Williamson [2]. For a given number *s* of stages, this method has a total of 2s - 1 independent coefficients. For a sufficiently large number of stages, it is possible to generate schemes which are of order $p \le 4$ and also offer large stability regions [3, 4]. However, to the best of our knowledge, so far there are no schemes known in this formulation with orders p > 4.



To find fifth-order schemes with optimized stability regions, we first generate optimal stability coefficients for up to s = 22 stages, following an approach presented in [5]. With the stability coefficients at hand, we then employ the nonlinear optimization package **IPOPT** [6] to solve the nonlinear Runge-Kutta order conditions. As a result, we obtain coefficients for up to s = 22 stages which are accurate to fifth order. Moreover, for linear homogeneous problems our schemes are seventh-order accurate. To the best of our knowledge, our schemes are the first fifth-order low-storage Runge-Kutta schemes in Williamson formulation. They allow highly accurate time integration without increasing memory requirements.

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Reduced basis method for 3D electromagnetic scattering problems

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Abstract

In this contribution we will introduce the reduced basis method and demonstrate its performance for relevant, real-world metrology applications. Furthermore, we investigate advanced model parameterization schemes for complex 3D geometry models based on computer-aided design techniques.

Key words: CAD, computational metrology, FEM, nanophotonics, reduced basis method

1 Introduction

Efficient inverse lithography and computational metrology methods are becoming increasingly important for the semiconductor industry [1, 2]. With component feature sizes in the micro- and nanometer ranges these methods require solving nonlinear parameter identification problems based on rigorous solutions of Maxwell's equations.

The numerical costs required to solve such problems can easily be excessive for realworld applications in which modeled light field data is typically required in almost real time. Commonly, in such scenarious, solutions for parameters lying on a densely spaced parameter grid are pre-computed in a so-called 'offline phase'. Subsequently, during a 'online phase' (e.g. when parameters need to be identified based on measurements), a simple library search is performed to identify the best fitting parameter values. Such approaches suffer from two major drawbacks: Firstly, the number of pre-calculated solutions required increases exponentially with increasing number of parameters ('curse of dimensionality') and secondly, it is a priori not clear how dense the parameter space needs to be sampled. Oversampling will largely increase the 'offline phase' computational costs, whereas undersampling will lead to inaccurate or completely meaningless parameter estimates. In contrast, the reduced basis method (RBM) is capable of building an accurate low-order model given a predefined approximation accuracy facilitating low offline and online computational costs.



2 Reduced basis method

Given a parameterized model, the RBM determines self adaptively where exact, so-called snapshot solutions of the full problem are taken. These snapshot solutions form the reduced basis and are used to construct a reduced model in the offline phase. The reduced model is obtained by Galerkin projection, which could be characterized as physical interpolation: the solution for a given point in the parameter space is not obtained by data interpolation, but by solution of an electromagnetic scattering problem on the reduced basis space.

The reduced basis method is closely related to the finite element method (FEM). The snapshots included in the reduced basis are FEM solutions and the reduced model is a projection of the high dimensional finite element discretization onto the low dimensional reduced basis. Therefore, the reduced basis method inherits all of its unique features: exact modeling of complicated geometries with unstructured meshes, high-order ansatz functions, and low computational times for highly accurate solutions. Furthermore, methods from the well-developed area of a-posteriori error estimation of finite element solutions can be applied to the reduced basis setup. They are the key for self-adaptive algorithms which construct the reduced basis approximation and guarantee reliability of the reduced basis results.

In this contribution we will introduce the reduced basis method and demonstrate its performance for relevant, real-world metrology applications.

3 CAD based model parameterization

To date the RBM for Maxwell's equations has only been employed on rather simple 2D or 3D model geometries. Finding appropriate means of defining shape parameterizations for complex geometry models well suited for the RBM is subject of current research. Assuming that a parametric shape is given in the form of a triangulated bounded domain, pertubations of the shape parameters will lead to infinitesimal movements of the mesh nodes that can be described by a velocity field. To create an efficient inverse design environment based on the RBM, shape parameters need to be defined and related to the velocity field.

We investigate advanced model parameterization schemes within a history-based 3D geometry modelling environment. Our approach facilitates shape derivatives to be estimated in a fully automatic fashion for complex shapes constructed by the application of a sequence of solid modeling algorithms (sweeping, blending, boolean operations and so forth) and solid modification algorithms (e.g. draft, fillet, chamfer) on parameterized primitive shapes.

Acknowledgements

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Quasimodal analysis of periodic structures and discontinuous waveguides

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Abstract

In the present paper, the numerical determination of quasimodes (or quasi normal modes or leaky modes) of open electromagnetic structures is presented. The method is based on a finite element formulation completed with Perfectly Matched Layers (PMLs). These PMLs lead to non Hermitian matrices whose complex eigenvalues correspond to quasimode frequencies. Using Floquet-Bloch theory, a numerical model is set up that allows the spectral study of structures that are both open and periodic (*e.g.* diffraction gratings). With this model, we show that it is possible to use a periodic structure of disconnected elements (*e.g.* a line of rods) to guide electromagnetic waves, **in the direction of the periodicity**, on significant distances with very limited losses. Such structures would be more convenient to build than usual waveguides in the realm of nanophotonics.

Key words: quasimodes, PML, finite elements, waveguides, nanophotonics.

1 Quasimodes and discontinuous waveguides

Nowadays, the Finite Element (FE) method is an effective method to compute the behaviour of electromagnetic waves in photonic devices. It provides a tool that is extremely versatile and accurate at a reasonable computational cost. An important progress has been made by the introduction of Perfectly Matched Layers (PMLs) that are used for the reflectionless truncation of infinite domains. Using the PMLs, the spectral analysis of open electromagnetic structures (computing the eigenvalues of the FE matrices) gives very interesting information about their behaviour [1]. Open structures have to be analysed in terms of quasimodes (associated to complex frequencies) and the PMLs are crucial specially for the correct computation of the imaginary parts of the frequencies associated to losses and leakages. The role of the PMLs is to rotate the continuous spectrum in the complex plane in order to unveil the quasimodes (by providing a non-Hermitian extension of the operator associated to the initial problem). A practical way to design such PMLs is to consider Transformation Optics: PMLs may be

obtained by applying a complex-valued stretch to the coordinates and then computing the resulting equivalent materials[2].

Using Floquet-Bloch theory, a numerical model is set up that allows the spectral study of structures that are both open and periodic (*e.g.* diffraction gratings). In this paper, we consider periodic waveguides with waves travelling in the direction of the periodicity. With this model, we show that it is possible to use a periodic structure of disconnected elements (*e.g.* a chain of rods) to guide electromagnetic waves on significant distances with very limited losses. In a first step, the leaky mode dispersion diagram of a periodic structures is computed (involving one single elementary cell with PMLs for open directions and Floquet-Bloch conditions associated to a propagation constant for the periodic direction): given a propagation constant, some corresponding complex frequencies $\omega = \omega' + i\omega''$ are computed. In a second step, a frequency with a very small imaginary part is selected and the guiding proprety is checked using a finite chain of repeated elementary cells fed by a simple antenna.

We are particularly interested in the case where the structure if made of identical elements embedded in a bulk with some gap between them and we will call such a structure a *discontinuous waveguide*. As an example, we take chains of infinite cylinders with circular cross sections in order to keep the problem two-dimensional. Fig. 1 shows a realisation of such a waveguide: distance between centers of circular rods d = 500nm, radius of rods r = d/3, permittivity of rods $\varepsilon_r = 4$. Fig. 1(a) shows a branch of the dispersion diagram (frequency ω' versus propagation constant α) with the corresponding losses ($-\log(\omega''/\omega')$) on the vertical axis), the higher peaks corresponding to the lower losses. The third peak from the left is selected ($\omega' = 1.117 \, 10^{15} \, rad/s$, $\omega'' = 6.908 \, 10^8 \, rad/s$, $\omega''/\omega' = 6.184 \, 10^{-7}$). It corresponds to a free space wavelength $\lambda = 1686.18nm$ and the source is a monopole fed at the corresponding frequency and located at 853nm from the edge of the first rod. Fig. 1(b) shows a wave guided in a 21-rod structure.



(a) Dispersion diagram with losses.

(b) Wave guided with a finite chain of cells.

Figure 1: Guiding of an electromagnetic wave in a chain of circular rods.

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Curvilinear DGTD method for nanophotonics applications

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Abstract

Classical finite element methods rely on tessellations composed of straight-edged elements mapped linearly from a reference element, on domains which physical boundaries are indifferently straight or curved. This approximation represents serious hindrance for high-order methods, since they limit the precision of the spatial discretization to second order. Thus, exploiting an enhanced representation of the physical geometry of a considered problem is in agreement with the natural procedure of high-order methods, such as the discontinuous Galerkin method. In the latter framework, we propose and validate an implementation of a high-order mapping for tetrahedra, and then focus on specific nanophotonics setups to assess the gains of the method in terms of memory and performances.

Key words: Discontinuous Galerkin, curvilinear elements, Maxwell equations, nano-photonics

1 Curvilinear DGTD formulation

Classical discontinuous Galerkin time-domain (DGTD) methods rely on a linear mapping from a straight-edged reference element to each physical element of the mesh to evaluate the expressions of the finite-element matrices : this allows to save a lot in terms of computational efficiency and memory consumption. Indeed, in the linear case, the finite element matrices for the physical elements are simply multiples of the precalculated matrices of the reference element, since the Jacobian of the corresponding transformation is a constant. In a curvilinear setting, the reference element is mapped to the physical element *via* a quadratic form, thus allowing a quadratic representation of boundaries. Therefore, the Jacobian of this transformation is no longer a constant, and the matrices have to be evaluated by means of numerical integration, and stored for each physical curved tetrahedron. Efficient quadrature and cubature rules can be easily found up to sufficient order to our purposes.

A DGTD scheme accouting for curved elements was formulated and implemented in the framework of Maxwell's equations, using centered numerical fluxes. A validation step was conducted to verify the stability and accuracy of the method. Realistic situations related to the nanophotonics field will then be considered that demonstrate the potential of the approach, such as realistically-rounded metallic nanocubes described by a multipole dispersive model.



2 Validation

A spherical cavity of unit radius is considered, with PEC boundary conditions. A (0, 1, 1) mode is propagated inside it, which exact solution is known. Four different rectilinear meshes of increasing refinement were generated in order to check for *h*-convergence. \mathbb{P}_1 to \mathbb{P}_4 polynomial approximations were used. For each simulation, the L² error is calculated over the whole mesh, and the maximum error levels is retained. The obtained *h*-convergence results are displayed on table 1. As can be seen, the use of curvilinear tetrahedra restores quasi-optimal rates. Moreover, it allows to save a lot in terms of degrees of freedom, and therefore in CPU time. Indeed, the curvilinear M₁ solution is three times faster and occupies three times less memory than the linear M₂ solution, for a roughly similar error level. As an example, the \mathbb{P}_2 numerical solution on the M₁ and M₂ meshes are displayed on figure 2.

	5				^		,	
	Mı		M2		M3		M4	
	Rect.	Curv.	Rect.	Curv.	Rect.	Curv.	Rect.	Curv.
\mathbb{P}_1	-	-	1.62	-	1.25	-	1.16	-
\mathbb{P}_2	-	-	1.83	2.85	1.70	2.32	1.58	2.28
\mathbb{P}_3	-	-	1.75	3.84	1.66	3.53	1.55	3.41
\mathbb{P}_4	_	_	1.78	3.79	1.68	3.73	1.57	3.57

Table 1: Convergence rates of the spherical cavity case.



Figure 1: \mathbb{P}_2 numerical solution for the E_x field.

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Computational Bayesian Inversion

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Abstract

Many problems in the physical sciences require the determination of an unknown field from a finite set of indirect measurements. Examples include oceanography, oil recovery, water resource management and weather forecasting. The Bayesian approach to these problems is natural for many reasons, including the under-determined and ill-posed nature of the inversion, the noise in the data and the uncertainty in the differential equation models used to describe complex multiscale physics. The object of interest in the Bayesian approach is the posterior probability measure on the unknown field, given the data.

However the Bayesian approach presents a computationally formidable task as it results in the need to probe a probability measure on function space. The talk will describe three computational methods for this task, and their inter-relations. The first method is based on approximating the probability measure by a Dirac measure and computing the MAP estimator (maximum a posteriori estimator) for the point at which the measure is centered. It will be shown how to make sense of this idea in infinite dimensions, resulting in a problem from the calculus of variations [1]. The second method is based on approximation of the posterior measure by a Gaussian, looking for the closest Gaussian with respect to the Kullback-Leibler divergence. Again we show how to make sense of this in infinite dimensions, and again formulate the resulting problem in the calculus of variations [2]. The third method is to sample the posterior measure by means of MCMC methods, using the algorithmic approach described in [3], resulting in algorithms with rates of convergence which are independent of the mesh. Furthermore we show that use of the best Gaussian approximation from [2] within the MCMC method can lead to further beneficial computational speed-up.

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Nanophotonic simulations using the FDTD and DGTD methods

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Abstract

We present an overview of the application of the Finite Difference Time Domain (FDTD) and the Discontinuous Galerkin Time Domain (DGTD) electromagnetic simulation methods to several particular nanophotonic systems. We discuss the extension of the original methods with an emphasis on nonlinear, nonlocal and hydrodynamic material descriptions based on microscopic physical models.

Introduction Many natural materials exhibit an intensity dependence of their optical properties, i.e. a nonlinear optical behaviour. In the non-perturbative regime, i.e. beyond low intensities or for ultrafast/broadband excitation, time domain methods allow an immediate numerical treatment of the differential equations usually resulting from a physical modelling. However, these additional differential equations often introduce new requirements for a stable numerical evaluation even if the elecromagnetic coupling is simplified or completely neglected.

Semiconductor materials An important non-perturbative nonlinear material model is the quantum mechanical two-level system described by the Optical Bloch Equations, representing e.g. atoms, solid state quantum dots or other quantum oscillators. Even without electromagnetic backaction, for ultrafast optical excitation the numerical evaluation of these equations tend to become unstable with feasible time steps unless a higher order method is used. We show how the 4th order Runge Kutta integration technique (RK4) can be combined with the the FDTD method in the regions where nonlinear material exists, without the requirement to change the efficient FDTD central differences Yee update scheme anywhere else. For the intermediate values required by the multistep RK4 scheme, we compare different approaches like n-th order Lagrange extrapolation and a predictor scheme locally consistent with the FDTD update operation [1]. We show that significant numerical errors only occur for oth (constant) and 1st (linear) order Lagrange schemes.

Quantum mechanical models are intrinisically nonlocal as the wave function extends in space. This becomes relevant for larger coherent objects like quantum dots consisting of many atoms. We show that despite being smaller than the wavelength, field variations within the quantum dot occur. Further challenges for simulations are discussed, e.g. the different scales if a 30nm quantum dot is embedded in a 10000nm photonic crystal structure with a high-Q cavity, or if higher-dimensional semiconductors like quantum wells exhibiting a non-Lorentzian broadband response are present.





Figure 1: Simulated field pattern (left) and emission spectrum (right) of a quantum dot embedded in a 3d photonic crystal cavity (FDTD method).

Nonlinear metals Equally challenging is the physical modelling of metals beyond their linear properties. This is possible using a semiclassical hydrodynamical model which however tends to be highly surface sensitive and exhibits shock waves. Both is numerically difficult to handle, but recently a combination of the Discontinuous Garlerkin Time Domain method that allows local mesh refinement arround the interface regions with nonlinear filter techniques has lead to a successful description of the nonlinear optical properties like higher harmonic generation by arrays of metallic nanoparticles [2, 3].



Figure 2: Schematics (left) and calculated emission spectrum (right) showing second and third harmonic generation of a gold split ring resonator array (DGTD method).

Using the DGTD method we were also able to simulate the optical response of a complex bi-chiral interweaved metallic helix structure with tiny structural features but a large total extension [4]. While being very versatile and powerful the Achilles heel of DGTD currently is the mesh generation, as it is slow and most available mesh generation libraries only produce meshes optimized for frequency space methods like the FEM having different requirements.

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Runge-Kutta Based Local Time-Stepping Methods for Computational Electromagnetics

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Abstract

Starting from standard explicit Runge-Kutta (RK) methods, we propose high order explicit local time-stepping (LTS) methods for the simulation of electromagnetic wave phenomena. By using smaller time steps precisely where smaller elements in the mesh are located, these LTS methods overcome the bottleneck in explicit time integration caused by local mesh refinement, without sacrificing the explicitness, accuracy or efficiency of the original RK method.

Key words: Maxwell equations, high-order explicit time integration, local time-stepping, multirate methods

1 Introduction

We discretize the time-dependent Maxwell equations in space by using standard edge finite elements (FE) with mass lumping or a discontinuous Galerkin (DG) FE discretization, while leaving time continuous. Either discretization leads to a system of ordinary differential equations

$$\mathbf{y}'(t) = \mathbf{B}\mathbf{y}(t) + \mathbf{F}(t),\tag{1}$$

where the matrix **B** involves the inverse, M^{-1} , of the mass matrix **M**. Since **M** is essentially diagonal, its inverse is explicitly known, and so is **B**.

Standard explicit numerical methods for the time integration of (1) include explicit Runge-Kutta (RK) schemes and Adams-Bashforth (AB) methods, whose time-step, Δt , is dictated by the smallest elements in the mesh. In [1, 3, 4] multi-step based LTS methods were proposed, which alleviate that geometry induced stability restriction by using smaller time-steps, but only where the smallest elements in the mesh are located.

2 Runge-Kutta based LTS

Here we present explicit LTS methods of arbitrarily high accuracy based either on explicit classical or low-storage RK schemes [2]. In contrast to AB methods, RK methods are one-step





(a) Zoom on the refined mesh

(b) The solution at time t = 0.7.

Figure 1: A gaussian plane wave impinging upon a narrow gap.

methods; hence, they do not require a starting procedure and easily accommodate adaptivity in time. Starting from (1), we first split the vectors **y** and **F** as

$$y(t) = (I - P)y(t) + Py(t) = y^{[c]}(t) + y^{[f]}(t),$$

$$F(t) = (I - P)F(t) + PF(t) = F^{[c]}(t) + F^{[f]}(t).$$
(2)

Here the entries of the diagonal matrix **P**, equal to zero or one, identify the unknowns associated with the locally refined regions, $y^{[f]}$. Hence the exact solution of (1) is

$$\mathbf{y}(t_n + \xi \Delta t) = \mathbf{y}(t_n) + \int_{t_n}^{t_n + \xi \Delta t} \mathbf{B} \mathbf{y}^{[c]}(t) + \mathbf{F}^{[c]}(t) \, dt + \int_{t_n}^{t_n + \xi \Delta t} \mathbf{B} \mathbf{y}^{[f]}(t) + \mathbf{F}^{[f]}(t) \, dt \,.$$
(3)

To derive an LTS method, we now approximate the first integral in (3) by a sufficiently accurate quadrature formula, where the (unknown) values of $y^{[c]}$ at the quadrature points are approximated by Taylor expansion. Differentiation of the resulting expression then leads to a modified differential equation, which is solved numerically from t_n to $t_n + \Delta t$ by using a RK method with local time-step $\Delta \tau = \Delta t/p$; here, *p* denotes the coarse to fine aspect ratio. The resulting LTS-RK scheme has the same high rate of convergence as the original corresponding RK method.

In Fig. 1(b), we observe a time dependent wave impinging upon a narrow gap between to rectangular obstacles. During every time-step, Δt , the LTS-RK method takes p = 7 local steps of size $\Delta \tau = \Delta t/p$ inside the refined region, shown in Fig. 1(a).

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Validation of a Nonlinear, Cylindrical Finite Integration Technique for Active Optical Laser Cavities

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Abstract

A transient finite differences algorithm is used for the simulation of active optical cavities. Rotationally symmetric structures are treated using a 2.5-dimensional ρz -approach where the non-linearity of the gain material leads to a coupling of the azimuthal modes. Due to the complexity of the overall simulation process a thorough validation is required. An academic example is presented which is suited for such a validation, and a simulation of a sample VCSEL structure gives an outlook on the potential of such simulations.

Key words: laser simulation, FDTD, cylindrical mesh.

1 Introduction

The dynamics of active optical components such as lasing microcavities are simulated on the ultrafast timescale. The simulation approach is based on the Finite Integration Technique (FIT [1]) and the leapfrog time integration method, and thus closely related to corresponding Finite Difference Time Domain (FDTD) schemes. In order to cope for the highly nonlinear interplay between light and matter an extended material model for the active regions is used. Based on a two-level quantum mechanic ensemble, it can macroscopically be described by a rate equation and a Lorentz oscillator model for the polarization (e.g. [2]).

For structures with cylindrical symmetry a so-called 2.5-dimensional implementation is used. Based on a 2D computational mesh in ρz -coordinates, the fields are decomposed into azimuthal modes which – in the classical *linear* case – are treated separately. The active material, however, leads to a coupling between these modes, and they have to be integrated in time simultaneously. Nevertheless, due to the considerably reduced number of degrees of freedom in the two-dimensional mesh the overall numerical effort is within reasonable limits. The details of the method can be found in [3, 4], and an application example will be presented in the presentation.

The standard FIT procedure has been validated many times as a reliable and accurate tool for electromagnetic simulations. With the additional non-linear PDEs the situation becomes more complex, and some additional modeling assumptions have to be assessed. This includes the physical model itself (validity of the macroscopic non-linear description), numerical questions like the number of considered azimuthal modes, as well as implementation issues such



as the allocation of the additional quantity in the mesh. For a thorough validation of the overall simulation tool, however, it is not easy to find suitable benchmark problems with reference solutions.

2 Validation Example

The setup consists of a circular hollow waveguide with absorbing boundary conditions at both longitudinal terminations and a 30nm layer (one mesh step) of a non-linear material. The transversal field pattern of the TE_{11} waveguide mode is impressed on both sides of this layer, ensuring a longitudinally homogeneous field inside. For this case an analytical solution is available (see [4] and the references therein).



Figure 1: Validation setup: Rabi oscillation in a cylindrical waveguide.

The simulation results nicely reproduce the Rabi-type oscillation of the inversion density. Futheron, the setup allows to analyze the impact of several physical and simulation parameters such as the influence of the exciting field strength, the transversal mesh resolution and the number of considered azimuthal modes. There are small deviations to the reference solution which can be fully explained by the corresponding modeling steps.

The calculated signals further include all additionally generated spectral components as expected.

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Computational Plasmonics: Material Models for the Discontinuous Galerkin Time-Domain Method

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Abstract

Discontinuous Galerkin methods represent powerful approaches for computing the optical properties of nano-structured systems. Corresponding time-domain simulations for plasmonic systems require material models that are amenable to auxiliary differential equation techniques. In this work, suitable models for the magneto-optic properties of transition metals as well as for the nonlocal and nonlinear properties of ordinary metals are described and a number of the resulting effects and phenomena are investigated.

Key words: Plasmonics, Magneto-Optics, Discontinous Galerkin methods

1 Introduction

Over the past years, nodal Discontinous Galerkin Time-Domain (DGTD) approaches for the Maxwell equations [1, 2, 3, 4] have been advanced sufficiently far so as to facilitate real-world applications in several disciplines. This success stems from the combination of finite-element based high-order spatial discretization techniques on unstructured grids with very efficient explicit time-stepping schemes of comparable order.

For applications in nano-photonics it is highly desirable to model the complex behavior of a number of materials. Quite generally, this may include temporal and/or spatial dispersion as well as anisotropic and/or nonlinear material characteristics. Owing to the specifics of the DGTD approaches, notably the numerical flux that connects adjacent finite elements, it is typically preferred to include such complex material properties into the DGTD framework by way of auxiliary differential equation formulations.

Nano-structures containing metallic constituents, so-called plasmonic systems, represent a particular important class of structures where basically all the above material characteristics may play an important role.

2 Magneto-Plasmonics

The linear properties of traditional plasmonic materials such as aluminum, gold, or silver can be very well described through a Drude model combined with several Lorentz-poles. However, for transition metals this is not anymore the case. The strong electronic correlations in



these metals lead to an asymptotic ω^{-1} behavior of the imaginary part of the dielectric constant that is different from the ω^{-3} behavior of Drude-Lorentz models. In turn, this suggests that the Drude model has to be modified in order to accommodate the retarded response of the free electrons that experience these strong correlations [5].

In addition, this modified Drude model can be extended to account for the free electrons' response to an applied static magnetic field by incorporating the corresponding magnetic part of the Lorentz force [5]. A similar anisotropic extension can be applied to any number of Lorentz poles as well. The resulting anisotropic modified Drude + Lorentz model allows to treat the magnetooptic properties of nano-structured transition metal systems. In Fig. 1, the results of corresponding computations are compared with measurements of the magneto-optical Kerr rotation on a hexagonal array of pores in a nickel film [6].

3 Hydrodynamic model of conduction electrons

A description of the free electrons within a



Figure 1: Polar magneto-optical Kerr rotation from a hexagonal anti-dot array within a 100 nm thick nickel film that is deposited on an unstructured silicon substrate. The corresponding unit cell (see inset) is a regular hexagon with an edge length of 271.4 nm (corresponding to a lattice constant of 470 nm) with a cylindrical pore with radius 137.5 nm at the center. The experimental data are taken from [6] while the simulations for different incident polarizations (see inset) have been carried with the DGTD method using an anisotropic modified Drude + Lorentz model (see [5] for details).

metal as a plasma in confined geometry that is driven by the full Lorentz force constitutes a natural extension of the linear and (spatially) local Drude model to account for the metal's nonlocal and nonlinear properties. The defining feature of this model is the existence of bulk plasmon excitations that are are ignored in the standard Drude model that employs a constant electron density. For typical metals, these bulk plasmons have a natural wavelength of a few nanometers. In turn, this leads to stringent requirements on the spatial resolution that has to be employed for obtaining converged results. In particular, this applies to the resonance frequencies and field enhancements in typical nano-gap structures.

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High order predictor-corrector solver for the unsteady Navier-Stokes equations based on homotopy and perturbation techniques.

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Abstract

An efficient solver for the 2D unsteady Navier-Stokes equations is presented. We used a classic time stepping scheme combined with an high order predictor-corrector solver. This method combines an homotopy technique and the asymptotic numerical method (ANM). The main purpose is to gain CPU time during computations. The technique presented here reduces the number of factorization of the operators. A pseudo-residual criterion prevents the asymptotic numerical method to use more right hand side vectors than needed for a given accuracy. This specific technique is compared to the classical first order Newton-Raphson solver. We show that a significant number of factorization are avoided, keeping at the same time a good quality of the solution.

Key words: unsteady Navier-Stokes, perturbation method, homotopy technique MSC 2010: 76D05, 76M10, 74H10

1 Method and results

The Navier-Stokes equations are written in a discrete form as :

$$M\dot{\mathbf{U}} + L(\mathbf{U}) + Q(\mathbf{U}, \mathbf{U}) = \mathbf{F}$$
(1)

where **U** is a mixed unknown time dependent vector (*i.e.* $\mathbf{U} = {\mathbf{u}, p}$). The operators M, L and Q are respectively the mass matrix, the pressure and the diffusion terms and a quadratic operator with the convective term. To solve Eq.(1) we transformed it by applying a θ -scheme, and using an homotopy technique as in [1]:

$$\left[\frac{1}{\theta\Delta t}\mathbf{M} + \mathbf{L}_{t}^{\mathbf{U}_{s}}\right]\mathbf{V}_{t+1} + \varepsilon \mathbf{Q}\left(\mathbf{V}_{t+1}, \mathbf{V}_{t+1}\right) = \mathbf{F}_{\upsilon} + \frac{1}{\theta\Delta t}\mathbf{M}\left(\mathbf{V}_{t} + \dot{\mathbf{V}}_{t}(1-\theta)\Delta t\right)$$
(2)

where $\varepsilon \in [0,1]$ is a perturbation parameter. This latter permits to continuously transform the problem from a linear one with $\varepsilon = 0$ to the initial one when $\varepsilon = 1$. Finally Eq.(2) is



solved using the asymptotic numerical method. The unknown \mathbf{V}_{t+1} is sought as a polynomial approximation of order N:

$$\mathbf{U}_{t+1} = \mathbf{U}_s + \mathbf{V}_{t+1} \approx \mathbf{U}_s + \sum_{i=0}^{N} \varepsilon^i \mathbf{W}_{t+1}^{(i)}$$
(3)

The starting point U_s can be either a stationary solution [2], or a transient solution. The nonlinear system is now a set of linear systems with the same tangent operator at each order:

$$\left[\frac{1}{\theta\Delta t}M + L_t^{\mathbf{U}_s}\right]\mathbf{W}_{t+1}^{(k)} = -\sum_{i=0}^{k-1} \mathbf{Q}\left(\mathbf{W}_{t+1}^{(i)}, \mathbf{W}_{t+1}^{(k-1-i)}\right), \text{ with } 1 \le k \le N$$
(4)

Once the serie $\{\mathbf{W}\}_{t+1}$ is computed and if the solution is still valid (i.e. $\varepsilon \ge 1$), then a new time step is computed using the previous operators. Otherwise, new operators have to be factorized. During a time step, we proposed to check the validity of the solution at each order of Eq.(4) via a pseudo residual criterion. This latter allows monitoring the quality of the solution with no additional computations, and avoid a great number of useless orders.

Numerical results are obtained studying the flow around a cylinder. The flow is periodic in time for a Reynolds number greater than 50. Calculations start from a steady solution and reach a limit cycle (Fig.1). The classical 1st order solver leads to 6442 factorizations for a



required accuracy $\eta = 10^{-5}$. We compare this number with an equivalent number of factorization obtained with our proposed method (Tab.1). It shows a CPU gain with a good accuracy of the computed solutions.

η	#Fact.	#RHS CPU / Fact. CPU	CPU gain
1e-6	53	286.8	19
1e-5	1	421.3	15
1e-4	1	254.2	25

Table 1: CPU gain for 3 required accuracy η .

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An inverse source problem for a damped Dirichlet wave problem with memory

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Abstract

We investigate the well-posedness for an inverse problem of determining a spacewise dependent source in a hyperbolic Dirichlet problem with a memory term. The material coefficients appearing in the governing equations may depend both on space and time. The aim is to identify a space-wise dependent source from the usual initial and boundary conditions and the final-time over-determination.

1 Introduction

Inverse coefficient and source problems for partial differential equations represent a wellknown and established area of mathematical research in the last decades. They appear in various applied technologies (geophysics, optic, tomography, remote sensing, radar-location, etc.). Inverse source problems for hyperbolic settings have been intensively studied by many authors, e.g. [1–7].

We consider the following inverse problem (IP) with unknown functions u and f (the other data functions appearing in the problem setting are known and bounded in appropriate spaces)

$$u_{tt}(t) + g(u_t(t)) - \nabla \cdot (a(t)\nabla u(t)) + c(t)u(t) + (K * u)(t) = f + F(t),$$
(1)

where

$$(K * u)(t) = \int_0^t K(t - s)u(s) \,\mathrm{d}s.$$

This paper is devoted to the identification of a spatially distributed source f = f(x) from a given final-time over-determination

$$u(x,T) = \psi_T(x) \quad \text{for } x \in \Omega,$$
 (2)

where Ω is a bounded domain of \mathbb{R}^n , where $n \ge 1$, with Lipschitz boundary Γ . The solution u obeys the following boundary and initial conditions

$$u(x,0) = h_0(x) \quad \text{for } x \in \Omega$$

$$u_t(x,0) = h_1(x) \quad \text{for } x \in \Omega$$

$$u|_{\Gamma} = 0 \quad \text{for } t \in (0,T).$$
(3)

Nonlinear term is modelled by a monotonically increasing function g and memory is represented by the smooth time-convolution kernel K.

[paper 39]



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Residual Stress Reconstruction for Large-Eddy Simulation

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Abstract

A new modeling technique for Large-Eddy Simulation is presented, in which the residual-stress tensor is reconstructed by applying an optimal convolution operator to the resolved stresses. This convolution operator is defined as a Taylor-series expansion in which the coefficients are determined using a dynamic procedure. The method is evaluated for the 1D Burger's equation as proof of concept. Promising results are obtained.

Key words: Residual Stress Reconstruction, Optimal LES model, Large-Eddy Simulation, Turbulent flows.

1 Context

In Large-Eddy Simulation (LES) of turbulent flows, one may distinguish two categories of residual stress modeling for the effect of the unresolved turbulent scale-interactions onto the resolved flow[1]. First, functional models rely on the existence of a physical energy cascade in which the energy of largest resolved turbulent structures is transferred to subsequently smaller scales before it is dissipated at the filter cutoff. Traditional models, such as Smagorinsky's model, assume an eddy-viscosity representation which implies that the effect of the unresolved interactions is mainly dissipative and can be modeled through a turbulent shearthickening eddy-viscosity v_e in combination with a Laplacian operator, in analogy with the dissipative effect molecular diffusion. These popular and widely used models are limited by the Laplacian dissipator, which is known for its inaccurate differentiation of dissipation throughout the spectrum of turbulent scales. Indeed, the largest and medium resolved scales are often excessively damped whereas the cusped behaviour of the dissipation near the filter cutoff is insufficient. More advanced functional models attempt to remedy this deficiency by using high-order dissipative operators, either as an explicit source term, or implicitly as a dissipative discretization scheme. In contrast to functional models, structural models reconstruct the residual stress tensor by means of a deconvolution procedure of the resolved velocity field or a scale-similarity approach using a double-filtered velocity field. Structural models rely on mathematical series expansions assuming scale-similarity within the spectrum of turbulent scales. Although structural models, in general, give a good correlation with the true residual stresses, not seldomly a secondary artificial dissipation mechanism must be included because they do not guarantee absolute dissipation at all times. In the following, a new methodology for reconstructing the residual stress tensor is presented.



2 Residual Stress Reconstruction

The equations for Large-Eddy Simulation for homogeneous isotropic turbulence are obtained by applying the Fourier cutoff filter $\mathscr{H}(\mathbf{x},\kappa_c)$, to the Navier-Stokes equations. The Fourier filter allows to resolve all Fourier modes exactly up to the cutoff wavenumber κ_c , whereas all modes above the cutoff are entirely removed. The filtered momentum equations read

$$\frac{\partial \overline{u}_i}{\partial t} + \frac{\partial \overline{\overline{u}_i \overline{u}_j}}{\partial x_j} + \frac{\partial \overline{\tau}_{ij}}{\partial x_j} = -\frac{\partial \overline{p}}{\partial x_i} + v \frac{\partial^2 \overline{u}_i}{\partial x_i^2}, \tag{1}$$

where $\overline{u}(\mathbf{x},t)$ and $\overline{p}(\mathbf{x},t)$ denote the filtered velocity field and pressure field and $\overline{\tau}_{ij} = \overline{u_i u_j} - \overline{\overline{u_i u_j}}$ denotes the *residual-stress* tensor, representing the effect of the unresolved turbulent interactions.

We propose to reconstruct the positive and negative contributions of the residual stress tensor $\overline{\tau}_{ij} = \overline{\tau}_{ij}^+ + \overline{\tau}_{ij}^-$ by the convolution operation

$$\overline{\tau}_{ij}^{\pm} = \overline{\overline{u}_i \overline{u}_j}^{\pm} - \mathscr{G}_{ij} \left(x_1, \gamma \right) * \mathscr{G}_{ij} \left(x_2, \gamma \right) * \mathscr{G}_{ij} \left(x_3, \gamma \right) * \overline{\overline{u}_i \overline{u}_j}^{\pm}.$$
(2)

in which the fluxes $\overline{u}_i \overline{u}_j$ are split into positive and negative parts using a global Lax-Friederich method. This is similar to implicit LES methods, and guarantees global dissipation at all times. Then, we define the convolution kernel in the Cartesian direction x_m as the power series expansion

$$\mathscr{G}_{ij}\left(x_{m},\boldsymbol{\gamma}\right) = \mathscr{I} + \sum_{k=1}^{\infty} \gamma_{k,m} \Delta_{m}^{k} \frac{\partial^{k}}{\partial x_{m}^{k}} = \underbrace{\mathscr{I} + \sum_{k=1}^{\infty} \gamma_{2k,m} \Delta^{2k} \frac{\partial^{2k}}{\partial x_{m}^{2k}}}_{\text{Dispersion}} + \underbrace{\sum_{k=0}^{\infty} \gamma_{2k+1,m} \Delta_{m}^{2k+1} \frac{\partial^{2k+1}}{\partial x_{m}^{2k+1}}}_{\text{Dissipation}}.$$
 (3)

Working out expression (2), using Leibniz' rule, finally yields

$$\overline{\tau}_{ij}^{\pm} = \overline{\overline{u}_i \overline{u}_j}^{\pm} - \sum_{k,l,m,q,r,s=0}^{\infty} \alpha_{k,l,m,q,r,s} \Delta^{k+l+m+q+r+s} \frac{\partial^{k+l+m} \overline{u}_i'}{\partial x_1^k \partial x_2^l \partial x_3^m} \frac{\partial^{q+r+s} \overline{u}_j'}{\partial x_1^q \partial x_2^r \partial x_3^s}.$$
 (4)

By means of this series expansion of $\overline{\tau}_{ij}^{\pm}$, it is straightforward to observe the analogies with both structural and functional models, including Smagorinsky's model, hyperviscosity models, the tensor diffusivity model and even implicit LES. As indicated in (3), the odd terms in the convolution kernel provide dissipation in equation (1), conform the physics of the energy cascade, whereas the even terms lead to dispersion and thus accounting for the phase shift due to unresolved interactions. The crucial part of the residual stress reconstruction method is to determine the parameters $\gamma_{k,m}$ such that the resulting one-dimensional convolution operators provides an adequate amount of dissipation and dispersion in the corresponding Cartesian direction. For a finite number of terms in the series expansion, the parameters $\gamma_{k,m}$ are determined in a least-square sense by means of a dynamic procedure, leading to an optimal convolution operator based on scale-similarity assumptions.

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Accuracy verification for computed solutions in Cosserat elasticity

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Abstract

A class of a posteriori error estimates for solutions in the Cosserat elasticity theory is investigated. Using the so-called functional approach, theoretical and numerical results for plane problems are provided. Numerical justification of the approach is based on the implementation of the lowest order Arnold-Boffi-Falk approximation.

Key words: a posteriori error estimates, Cosserat elasticity, mixed approximations

1 Introduction

Cosserat continuum [2] is one of important generalizations of the classical elasticity theory. Such type of models takes into account an advanced spectrum of material properties and can more adequately describe materials with microstructure. For complete historical review of the subject, see, for instance, [3, 6] and the literature cited therein. The implemented approach to accuracy verification is based on functional grounds [7, 5]. A posteriori error estimates are reliable under quite general assumptions and are explicitly applicable not only to approximations possessing the Galerkin orthogonality property.

In contrast to the classical statement in linear elasticity with only displacements $u = (u_x, u_y)$ regarded as primary unknowns, Cosserat elasticity involves the microrotation ω_z as one additional independent degree of freedom. For any given approximate solution $(\tilde{u}, \tilde{\omega}_z)$ from the respective functional space, the deviation (error) is introduced as

 $\xi_x := u_x - \tilde{u}_x, \qquad \xi_y := u_y - \tilde{u}_y, \qquad \xi_z := \omega_z - \tilde{\omega}_z$

and the following a posteriori error estimate for the energy norm can be obtained:

$$\||(\xi_x,\xi_y,\xi_z)||^2 \le (1+\beta)D^2(\tilde{\tau}_1,\tilde{\tau}_2,\tilde{s}) + (1+\beta^{-1})C^2R^2(\tilde{\tau}_1,\tilde{\tau}_2,\tilde{s}), \quad \forall \beta > 0,$$
(1)

where D^2 represents the error in the constitutive relations, R^2 is a weighted sum of norms of residuals in the equilibrium equations for Cosserat continuum, C – is a mesh-independent constant, and $(\tilde{\tau}_1, \tilde{\tau}_2, \tilde{s})$ – is a triple of additional variables. This theoretical result generalizes the previous one obtained in [8]. The proof of the reliability of the class of estimates is provided in [4]. Additional variables have clear physical meaning – $\tilde{\tau} = (\tilde{\tau}_1, \tilde{\tau}_2)$ represents the true nonsymmetric stress tensor and \tilde{s} is an independent approximation of the non-zero components of the couple-stress tensor.



2 Numerical results

To implement the error estimate (1) one can use a suitable mixed finite element for vectorvalued fields. In this research, the element proposed in [1] is used. The respective space for it has the form $\mathcal{ABF}_0(\hat{\mathcal{K}}) = \mathcal{P}_{2,0}(\hat{\mathcal{K}}) \times \mathcal{P}_{0,2}(\hat{\mathcal{K}})$, where $\mathcal{P}_{i,j}(\hat{\mathcal{K}})$ – the space of polynomials over $\hat{\mathcal{K}}$ of power *i* or less on \hat{x}_1 and *j* – on \hat{x}_2 for the reference square $\hat{\mathcal{K}} = (-1,1) \times (-1,1)$, where \hat{x}_1 and \hat{x}_2 are local coordinates of the reference element. Results for one example of ten-

Table 1. Results of estimation by (1).								
Quantity	Mesh 1	Mesh 2	Mesh 3	Mesh 4	Ref. mesh			
DOF	336	1248	4800	18816	296448			
%	11.5	7.4	4.7	2.9				
$I_{\rm eff}$	1.85	1.72	1.70	1.77				
β	0.098	0.058	0.036	0.023				

Table 1: Results of estimation by (1).

sion of a square domain with a rotated square hole are collected in Table 1, where % denotes the relative error and I_{eff} is the efficiency index of estimates. It is seen that \mathcal{ABF}_0 -approximation yields good results and the proposed approach is reliable.

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Implementation of linear sensitivity analysis and uncertainty quantification procedures in the ALEPH burnup Monte Carlo code

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Abstract

Uncertainty propagation and sensitivity analysis for burnup codes are key topics in the nuclear field because of their huge involvement in safety-related problems. Consequently, a correct evaluation of given responses variations after propagating the system parameter uncertainties is a primary feature for any burnup code. In the previous version of the ALEPH Monte Carlo burnup code the uncertainty propagation was not handled, even though several uncertainties come into play when dealing with nuclear data. Variances or covariances are generally provided for neutron cross sections, decay data and neutron fission product yields by the general-purpose nuclear data libraries and they can have a major impact on the selected responses of the problem.

To cope with the presence of uncertainties in burnup calculations we implemented linear sensitivity analysis and uncertainty propagation options to the new version of the ALEPH Monte Carlo burnup code. We developed new linear Forward Sensitivity Analysis (FSA) and linear Adjoint Sensitivity Analysis (ASA) procedures to propagate nuclear data uncertainties throughout sequential burnup steps, and a Total Monte Carlo (TMC) uncertainty quantification routine for data comparison. In this work, we explained the methodology and compared the results of the uncertainty quantification of the different techniques on several major nuclear responses.

Key words: burnup, nuclear data, sensitivity analysis, uncertainty propagation.

1 Introduction

ALEPH [4] is a Monte Carlo burnup code that has been developed at SCK•CEN since 2004. It combines the potentialities of any version of the stochastic Monte Carlo N-Particle transport code MCNP(X) [7, 8] and of a deterministic numerical solver. The continuous work of improvement of the code brought to the recent release of its second version ALEPH-2 [6].

What was implemented in the frame of this work was a new ALEPH capability, that is, a full sensitivity analysis procedure for what concerns both parameter uncertainties coming from the evaluated libraries and perturbations introduced by the user. Consequently, we expanded this potentiality to a full uncertainty propagation. Furthermore, ALEPH provides a high flexibility having three different routines to propagate uncertainties, each of them with its own method: a linear Forward Sensitivity Analysis (FSA) procedure [1, 2], a linear Adjoint Sensitivity Analysis (ASA) procedure [3, 2] and a Total Monte Carlo (TMC) uncertainty quantification [5].



2 Results

Our purpose was to describe and evaluate the new uncertainty propagation features of the ALEPH code against several responses. We chose the fission pulse decay heat as one of the system responses for its relevance in several nuclear applications that involve safety-related problems. The ALEPH ASA procedure returned statistics comparable with the more performing TMC calculation. In addition, apart from processing the uncertainty propagation with accurate results, the ASA was computationally speaking superior to TMC as only one response function was evaluated. Moreover, ALEPH also made possible the determination of the sensitivity coefficients of those parameters that have a major impact on the uncertainty of the response.

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Multi-physics modelling for nuclear reactor transient analyses by codes coupling at Tractebel Engineering

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Abstract

The nuclear reactor transient analyses using best estimate codes provide a better understanding and more accurate modelling of the key physical phenomena, which allows a more realistic evaluation of the conservatism's and margins in the analyses performed for the Final Safety Analysis Report (FSAR). The use of the best estimate codes and methods is necessary to meet the increasing technical, licensing and regulatory requirements for major plant changes (e.g. steam generator replacement), power uprate, core design optimization (cycle extension), as well as Periodic Safety Review. This paper presents briefly the multi-physics capabilities currently in use at Tractebel Engineering, acting as owner's engineer for Electrabel who owns and operates all Belgian nuclear power plants.

Key words: nuclear engineering, PWR transient safety analysis, multi-physics, code coupling

1 Introduction

Tractebel Engineering (TE) has been working since 2000 on the application of advanced multiphysics code packages in order to perform high fidelity simulation of PWR reactor transients. The objective is to provide tools and methods for independent verification of the safety analyses performed for the Belgian plants. The TE code package was first used to develop a Main Steam Line Break in Hot Zero Power conditions (MSLB-HZP) accident analysis methodology [1]. This methodology has been accepted by the Belgian Safety Authorities for applications related to the power uprate and steam generator replacement project of the Doel 1 and Doel 2 plants, to the Tihange-3 FSAR re-analysis and to justify the cycle length extension of Doel 4 to 18 months. Those applications were extended to accident analysis methodologies at hot full power condition like the MSLB-HFP and the Feed Water Line Break (FWLB) accident.

Flow mixing in PWR's is an important phenomenon for the transient behaviour of asymmetric reactor accidents such as MSLB or FWLB. In such transients, the flow mixing is a key parameter because it will determine the temperature distribution at the core inlet which has a significant impact on the core power response. Recently, TE has demonstrated the potential of the Computational Fluid Dynamics (CFD) simulation to predict the mixing at the core inlet and to generate more realistic inlet coolant temperature maps for multi-physics simulation [2].

TE is currently developing a multi-physics methodology to evaluate the margins with respect to the revised safety criteria for the PWR Rod Ejection Accident (REA) [3].



2 Multi-physics modelling and transient analysis capabilities

The TE multi-physics code package (Fig. 1) is composed by the 3-dimensional neutronic code, PANTHER, coupled dynamically with the system thermal hydraulic code RELAP5 (via the TALINK coupler) and with the core thermal hydraulic code COBRA-3C_TE (using sockets). Built-in one-way links provide time-dependent high fidelity power histories and distributions for specific criteria evaluation, either with the sub-channel thermal hydraulic code COBRA-3C or with the fuel rod thermal-mechanical code FRAPTRAN.



Figure 1: The TE multi-physics code package.

PANTHER is a multi energy groups 3-D nodal diffusion code for both steady-state and transient core simulation. PANTHER has been developed by British Energy (BE) to perform a complete range of PWR reactor calculations for fuel management design safety parameters assessment, fault transient analysis and operational support.

The RELAP5 code is a 6 field equations (3 conservation's equations for the vapor and the liquid respectively) best estimate system thermal hydraulic transient analysis code, developed by the USNRC, to simulate the LWR plant response for different postulated accidents including loss of coolant and reactivity insertion accidents as well as operational transients.

COBRA-₃C_TE is a coupled version of the sub-channel thermal hydraulic code being developed by TE starting from the original COBRA₃C_MIT₂ code. The main new capabilities of the thermal-hydraulic core model, compared to the built-in PANTHER thermal-hydraulic module, are the modelling of channel cross flows and turbulent mixing (this effect will be more important for low flow cases) and the extension of the heat transfer correlation range to the very low flow region.

FRAPTRAN code is developed by Pacific Northwest National Laboratory (PNNL) for analysing the thermal-mechanical behaviour of a LWR fuel rod under transient and accident conditions such as LOCA and RIA. It is used on the basis of the steady-state fuel conditions calculated by the FRAPCON code.

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One-Block Method for Computing the Generalized Stress Intensity Factors for Laplace's Equation on Domains of L-shaped and Square with a Slit

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Abstract

A highly accurate approximation for the coefficients of the series expansion of the solution for Laplace's equation around the singular vertex, which are called the generalized stress intensity factors (GSIFs), is obtained by One-Block Method.

Key words: Keywords: Laplace equation, Corner singularity, Block method, Stress intensity factor, Convergence

MSC 2010: 65N12, 65N15, 65N22

1 Introduction

It is known that the behaviour of the solution u of the two dimensional Laplace equation in the vicinity of a singular point, when the boundaries sharing this point are not curved, is given by

$$u(r,\theta) = \sum_{j=0}^{\infty} a_j r^{\mu_j} f_j(\theta), \tag{1}$$

where (r, θ) are the polar coordinates, centered at the singular point, μ_j and $f_j(\theta)$ are determined by the geometry and the boundary conditions along the boundaries sharing the singular point. The unknown constants a_j are often called generalized stress intensivity factors (GSIFs) in which high approximations are very important in many engineering problems. Most of methods for the approximation of these coefficients can be divided into two groups: (i) the post-processing approach in the finite element or finite difference methods and (ii) directly calculated methods. It is obvious that if the goal of computation is the calculation of the GSIFs then the directly calculated methods become more preferable. If the local asymptotic expansion (1) converges over the entire solution domain, then by defining its N-th sum as an approximate solution of the boundary value problem, the boundary condition enforcement is necessary for the derivation of the unknown coefficients (see [1]). These approaches are called the boundary approximation methods (BAMs) and converge exponentialy with respect to N. However, the matrix of the algebraic system of equations for the unknowns a_j , j = 1, 2, ..., Ngets illconditioning (*cond.* > 10⁵) when N increases.

In this paper a one block method (see [2] for the approximation of a_0) is developed for a highly accurate approximation of any number of coefficients (GSIFs) in (1) for the problems in domains of L-shaped and a rectangle with a slit.



2 Boundary value problem on special polygons

Let *G* be an open simply connected polygon, γ_j , $1 \le j \le M$, be its sides, including the ends, enumerated counterclockwise, $\gamma = \gamma_1 \cup \cdots \cup \gamma_M$ be the boundary of *G*, and by $\gamma' = \gamma_2 \cup \cdots \cup \gamma_{M-1}$. Let $\alpha_j \pi$, $\alpha_j \in \left\{\frac{1}{2}, \frac{3}{2}, 2\right\}$, be the interior angle formed by the sides γ_{j-1} and γ_j , ($\gamma_0 = \gamma_M$), and let $\alpha_1 \in \left\{\frac{3}{2}, 2\right\}$. Denote by $A_j = \gamma_{j-1} \cap \gamma_j$ and let $\rho(x, y)$ be the distance from $(x, y) \in \gamma'$ to the vertex A_1 , and let $d_0 = \min_{\gamma'} \rho(x, y)$, $d_1 = \max_{\gamma'} \rho(x, y)$. It is assumed that $d_1 < 2d_0$. Let r, θ be a polar system of coordinates with pole in A_1 , where the angle θ is taken counterclockwise from the side γ_1 . Let ν_j be a prameter taking the values 0 or 1, and let $\overline{\nu_j} = 1 - \nu_j$.

We consider the boundary value problem

$$\Delta u = 0 \text{ on } G, v_j u + \overline{v}_j u_n^{(1)} = \varphi_j \text{ on } \gamma_j, \quad j = 1, 2, \dots, M,$$
(2)

where $\varphi_1 = \varphi_M = 0$, and $\varphi_j, j = 2, 3, \dots, M - 1$ are constants, $\nu_0 = \nu_M$ and $\nu_0 + \nu_1 \ge 1$.

Consider the sector $T^0 = T(r_0) = \{(r, \theta) : 0 < r < r_0, 0 < \theta < \alpha_1 \pi\}$, with the center at the vertex A_1 and with the radius r_0 , $(d_1 < r_0 < 2d_0)$. We harmonically extend the solution u of the problem (2) to the sector T^0 and represent it on $T^0 \supset G$ as

$$u(r,\theta) = \int_{0}^{\alpha_1 \pi} u(r_0,\eta) R_1(r,\theta,\eta) d\eta, \qquad (3)$$

where $R_1(r, \theta, \eta)$ is defined through the Poisson's kernel for unit circle.

Let *n* be a positive integer, $\beta = \frac{\alpha_1 \pi}{n}$, $\theta^m = (m - \frac{1}{2})\beta$ and consider the *n* points $z_m = r_0 e^{i\theta_m}$, m = 1, 2, ..., n, on the arc of the sector T^0 . By extension, there exists the point $P'_m \in G$ with coordinates $z'_m = r'e^{i\theta'_m}$, for each point z_m , m = 1, 2, ..., n, respectively, and from (3), by composite mid-point rule, we obtain a well conditioned system of algebraic equations for the approximate values u_m of $u(r_0, \eta)$ at the quadrature nodes z_m , m = 1, 2, ..., n. The GSIFs is approximated by using the following formula

$$\overline{a}_k = \frac{2}{\alpha_1 \pi} r_0^{-\mu_k} \frac{\alpha_1 \pi}{n} \sum_{m=1}^n u_m f_k\left(\left(m - \frac{1}{2}\right) \frac{\alpha_1 \pi}{n}\right), \quad k = 0, 1, \dots, N,$$

where μ_k and f_k are given in the series representation. It is proved that \overline{a}_k converges to a_k exponentially with respect to the number of quadrature nodes *n*.

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The interpolation of edge unknowns for constructing cell-centered diffusion schemes on skewed meshes

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Abstract

An algorithm is developed to interpolate edge unknowns from cell-centered ones for diffusion equations with discontinuities. It is applied to construct diffusion scheme with cell-centered unknowns only on skewed meshes. And the effectiveness of the scheme is demonstrated by numerical experiments.

Key words: cell-centered scheme, diffusion equations, discontinuity, finite volume methods, skewed meshes MSC 2010: 65M06

1 Introduction

Skewed or non-orthogonal meshes arise in various fields, e.g., grid generation on physical domains with complex geometry, and numerical solutions of diffusion problems in Lagrangian radiation hydrodynamics. In the construction of cell-centered finite volume schemes for diffusion problems, due to the skewness of the grids, auxiliary unknowns defined at the vertices or edges are often introduced in addition to the cell-centered unknowns. The auxiliary unknowns can also be treated as primary unknowns. However, such schemes lead to greater computational costs or more complex algorithms than those with cell-centered unknowns only, especially when the diffusion scheme needs to be coupled with a cell-centered hydrodynamic scheme. This disadvantage has motivated researchers to construct schemes with cell-centered unknowns only.

We develop an algorithm to interpolate the auxiliary unknowns defined at the edge points from those defined at the cell-centers. Then a diffusion scheme with cell-centered unknowns only is constructed. Our algorithm deals with discontinuities strictly. Numerical results show that the scheme is second order accurate for discontinuous problems on skewed meshes.

2 Approximation of edge unknowns

The diffusion problem under consideration is

$$-\nabla \cdot \mathbf{k} \,\nabla \mathbf{u} = f \quad \text{in } \Omega. \tag{1}$$



In [1], we obtain the approximation of node unknowns

$$u_{M_{r+1}} - u_{M_r} = \psi \left[\tau_{\sigma_1} \left(u_{C_j^R} - u_{C_i^L} \right) - \tau_{\sigma_2} \left(u_{C_j^L} - u_{C_i^R} \right) \right]$$
(2)

where

$$\begin{split} \psi &= \frac{1}{\tau_{\sigma_1} D_{\sigma_1} - \tau_{\sigma_2} D_{\sigma_2}}, \\ \tau_{\sigma_1} &= \frac{k_{C_i^L} k_{C_j^R}}{k_{C_i^L} h_{\delta_{r,r+1}}^{C_j^R} + k_{C_j^R} h_{\delta_{r,r+1}}^{C_i^L}}, \\ D_{\sigma_1} &= \frac{(x_{M_{r+1}} - x_{M_r})(x_{C_j^R} - x_{C_i^L}) + (y_{M_{r+1}} - y_{M_r})(y_{C_j^R} - y_{C_i^L})}{l_{r,r+1}^2}. \end{split}$$

As shown in Fig. 1, M_r and M_{r+1} are the nodes. C_i and C_j are the centers of the cells. With (2), we obtain the explicit expression for the auxiliary unknowns which can be defined at any point on the edge. Note that the interpolation method for the anisotropic problems can be found in [2].



Figure 1: Points used in the approximation of the node unknowns

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A Fast Algorithm for Sampling from the Moyal Distribution

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Abstract

It is shown that the Ziggurat algorithm designed for sampling for monotone decreasing and symmetric unimodal distributions can be utilized for asymmetric unimodal distributions with necessary modifications. An efficient random number generator (RNG) for sampling from the Moyal distribution implementing the modified version of the Ziggurat algorithm is presented.

Key words: Ziggurat algorithm, Moyal distribution, random number generation.

1 Introduction

Modeling and simulation of ionization of fluctuations plays an important role in nuclear physics research and in solving practical problems that arise in development of nuclear reactors. Fluctuation of energy loss by ionization of a charged particle in a thin layer of matter was theoretically described by Landay [2]. This description was presented in the form of an asymmetric probability density function (pdf).

The values of the pdf of the Landau distribution are calculated via numerical integration, which makes it very difficult to obtain random numbers from this distribution needed for Monte Carlo simulation of energy loss by ionization. Moyal proposed a good approximation to the Landau distribution called the Moyal distribution [3]. The values of its pdf are calculated via a simple formula

$$f(x) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2}(x + \exp(-x))\right).$$

However, despite the simplicity of the formula, efficient algorithms for sampling from the Moyal distribution have not been presented to date. In this article we show that a very fast Ziggurat algorithm [1] designed for sampling from a monotone decreasing probability distribution or a symmetric unimodal distribution extends to asymmetric unimodal distributions and therefore can be implemented for the Moyal distribution.

2 Description of the Modified Ziggurat Algorithm

The idea of the Ziggurat algorithm is covering the target density with a set of n equal-area regions, called layers, all of which except one are horizontal rectangles, then choosing one of them and sampling from it.



In the presented asymmetric unimodal (AU) version of the Ziggurat algorithm the layers L_i , $i = \overline{2, n}$ are horizontal rectangles which extend horizontally from l_i to r_i and vertically from y_i to y_{i+1} , $l_2 < l_3 < ... < l_n < 0$, $r_2 > r_3 > ... > r_n > 0$, $y_i = f(l_i)$, $2 \le i \le n$, $y_{n+1} = f(0)$. The first layer L_1 is a union of a rectangle which extends horizontally from l_2 to r_2 and vertically from $y_1 = 0$ to y_2 , and two infinite tails. The left tail is the set of all points (x, y) below the curve y = f(x) for which $x < l_2$ and the right tail is the set of all points below the curve for which $x > r_2$.

Let $p_i^* = d_{i+1}/d_i$, $p_i^{**} = (l_{i+1} - l_i)/d_i + p_i^*$, where $d_i = r_i - l_i$, $2 \le i \le n$, $l_{n+1} = d_{n+1} = 0$, and let $p_1^* = y_2/(y_3 - y_2)$, $d_1 = d_2$.

The setup stage includes the initialization of the tables for l_i, d_i, y_i, p_i^* and p_i^{**} , and the choice of auxiliary algorithms for generating from the tails. The main stage of the *AU* Ziggurat algorithm looks as follows

- 1. Generate U_0 uniformly distributed in [0, 1). Set $i = [U_0 \cdot n]$ and set $s = i U_0 \cdot n$.
- 2. If $s < p_i^*$, set $x = l_{i+1} + s \cdot d_i$ and return x.
- 3. If i = 1, generate a point *T* from one of the tails, set x = T and return *x*.
- 4. Generate U_1 uniformly distributed in [0, 1) and set $y = y_i + U_1 \cdot (y_{i+1} y_i)$.
- 5. If $U_0 < p_i^{**}$, set $x = l_i + (s p_i^*) \cdot d_i$; otherwise set $x = l_i + d_i \cdot s$.
- 6. Compute f(x). If y < f(x), return x.
- 7. Go to step 1.

3 Concluding Remark

A RNG for generating the Moyal random variable (rv) based on the presented algorithm has been developed and tested. The RNG proved to be very efficient, since the algorithm terminates at step 2, and therefore requires a uniform random number and only one comparison for a generated value of the Moyal rv with probability 0.97 at n = 64.

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An inexact semi-smooth Newton method for solving contact problems with friction: analysis and experiments

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Abstract

The contribution deals with the semi-smooth Newton method applied to the solution of contact problems with friction. The primal-dual algorithm is reformulated as the dual one. Its globally convergent variant based on computing a monotonously decreasing sequence is analyzed. Numerical experiments illustrate the performance of different implementations of the method.

Key words: contact, friction, semi-smooth Newton method, convergence rate MSC 2010: 65K10, 65N22, 49M29, 74M15

Problem description and main results

Finite element approximations of frictional contact problems of linear elasticity lead typically to non-smooth equations that are equivalent, in many cases, to a constrained minimization. Algorithms based on active sets belong to the most efficient iterative methods for solving such problems. There are at least two strategies how to introduce active set algorithms in context of contact problems. The first ones have been developed for dual contact problems given by the minimization of a strictly quadratic cost function subject to separable inequality constraints [4, 3, 6, 7] that is the case of the Tresca friction law. Here, the active set is the index subset of components, for which the constraints are satisfied by equalities in the current iteration. The conjugate gradient method (CGM) generates iterations with respect to remaining non-active components and, when the progress is not sufficient, the active set is changed by a gradient projection step. Thus, the algorithm seeks for the active set in the solution so that it generates monotonously decreasing iterations laying in the feasible set and enjoys the R-linear convergence rate [4, 3, 7].

Another class of active set algorithms arises from the use of the semi-smooth Newton method (SSNM). The starting point is the primal-dual formulation of contact problems, in which contact conditions are reformulated by non-smooth functions as proposed already in [1]. Later on, it was recognized that the SSNM may be interpreted as a primal-dual active set method [5]. This approach is widely used for solving contact problems in two (2D) as well as three (3D) space dimensions with different friction laws. The standard convergence analysis uses the slant differentiability concept [2, 5] leading to the local superlinear convergence



rate. This convergence result assumes exact solutions of inner linear systems that is, however, unrealistic for large-scale problems. Another drawback consists in the fact that an initial iteration "sufficiently close" to the solution is required. To overcome these difficulties one can modify the SSNM so that the resulting algorithm is globally convergent and, consequently, an appropriate initial iteration is known a-priori.

In the contribution, we analyze a relation between above-mentioned active set strategies. First, we show that the primal-dual active set algorithm of the SSNM is fully identical with a pure dual algorithm. We propose its heuristic implementation that accepts inexact solutions of inner subproblems computed by few CGM iterations terminated by an adaptive inner stopping criterion. Then we modify the algorithm so that a sequence of the cost function values is monotonously decreasing. The global R-linear convergence rate of the modified algorithm is proven using the decrease of the cost function along the projected gradient [4, 3, 7]. We will also observe a relation to the classical projected gradient methods. Results of numerical experiments will be reported including of an extended algorithm treating Coulomb friction for realistic engineering problems [8].

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Differentials of Eigenvalues and Eigenvectors in Undamped Discrete Systems

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Abstract

First- and second-order differentials of a (simple) eigenvalue and the associated eigenvector in an undamped discrete system are investigated. For the eigenvector, several normalizations have been considered in the literature; incidentally, we review them and clarify under what conditions they uniquely identify the eigenvector. Then we provide closed-form expressions for the differentials under the vector-component, orthogonal, mass and unit-length normalizations. The proposed formulas have no pretension to be computationally efficient in large systems, but may be useful for the interpretation of the results.

Key words: differentials, eigenvalues, eigenvectors, undamped systems

1 Introduction

In the analysis of free undamped vibration and structural stability, the following generalized eigenvalue problem is often considered:

$$(\mathbf{K} - \lambda \mathbf{M}) \, \mathbf{u} = \mathbf{0}$$

where λ is called *eigenvalue*, **u** (right) *eigenvector*, K *stiffness matrix*, and M *mass matrix*. An interesting problem that has received attention in the literature is the computation of the derivatives of the eigenvalues and of the eigenvectors of the problem with respect to a design variable. Here we choose to consider a strictly related but slightly different topic, namely the matrix differentials (see [2, 1]) of the eigenvalues and of the eigenvectors of this generalized eigenvalue problem.

2 Main Results

For the purposes of this short exposition, we just recall that the matrix differential of a matrix function is the part of the perturbation of the function in response to a perturbation of its argument that is linearly related to the variation of the argument itself.

Let

$$(\mathsf{K}_0 - \lambda_0 \mathsf{M}_0) \, \mathbf{u}_0 = \mathbf{0}$$



be the unperturbed problem. Here and in the following, the index 0 (such as in K_0 or M_0) indicates that the quantity is obtained before the perturbation is applied (e.g., λ_0).

Consider now two matrices M and K that are obtained as (first-order) perturbations of the matrices M_0 and K_0 , say $M = M_0 + dM$ and $K = K_0 + dK$ where dM and dK are matrix differentials. Our aim is to identify the matrix differentials $d\lambda$, $d^2\lambda$, du and d^2u in the developments:

$$\begin{split} \lambda &\simeq \lambda_0 + d\lambda + \frac{1}{2} d^2 \lambda, \\ \mathbf{u} &\simeq \mathbf{u}_0 + d\mathbf{u} + \frac{1}{2} d^2 \mathbf{u}. \end{split}$$

While the eigenvalue is identified without any need for normalizations, the eigenvector needs to be normalized in order to be univocally defined. The literature on this topic is quite complicated and not always very precise as concerns the assumptions. In passing by, we review it clarifying the conditions under which several normalizations can be applied.

The formula for $d\lambda$ is:¹

$$d\lambda = \frac{\mathbf{v}_0^{\mathsf{T}} (d\mathsf{K} - \lambda_0 d\mathsf{M}) \mathbf{u}_0}{\mathbf{v}_0^{\mathsf{T}} M_0 \mathbf{u}_0}$$
(1)

while the one for $d^2\lambda$ is:

$$d^{2}\lambda = -2d\lambda \cdot \frac{\mathbf{v}_{0}^{\mathsf{T}}dM\mathbf{u}_{0}}{\mathbf{v}_{0}^{\mathsf{T}}M_{0}\mathbf{u}_{0}} + \frac{2\mathbf{v}_{0}^{\mathsf{T}}\left(d\mathsf{K}-\lambda_{0}d\mathsf{M}-d\lambda\mathsf{M}_{0}\right)d\mathbf{u}}{\mathbf{v}_{0}^{\mathsf{T}}M_{0}\mathbf{u}_{0}}.$$

As concerns the eigenvector, we have:

$$\mathbf{d}\mathbf{u} = -(\mathbf{K}_0 - \lambda_0 \mathbf{M}_0)^+ (\mathbf{d}\mathbf{K} - \lambda_0 \mathbf{d}\mathbf{M} - \mathbf{d}\lambda \mathbf{M}_0) \mathbf{u}_0 + \delta_1 \mathbf{u}_0$$
(2)

$$d^{2}\mathbf{u} = (K_{0} - \lambda_{0}M_{0})^{+} (2d\lambda dM + d^{2}\lambda M_{0})\mathbf{u}_{0}$$

-2 (K_{0} - \lambda_{0}M_{0})^{+} (dK - \lambda_{0}dM - d\lambda M_{0}) d\mathbf{u} + \delta_{2}\mathbf{u}_{0} (3)

where δ_1 and δ_2 are determined according to the normalization.

3 Extensions

In the paper this result is extended to the case in which M and K are obtained as second-order perturbations of M_0 and K_0 . Moreover, it is applied to several normalizations presented in the literature, namely the vector-component, orthogonal, mass and unit-length normalizations. We also provide some applications of the previous result, namely to the simplification of formulas in the case of distinct eigenvalues, to the obtention of derivatives, and to the perturbation of eigenvalues and eigenvectors in systems with small hysteretic damping.

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 $^{^{1}}$ In the following, for a generic matrix X, X^T denotes the transpose. For a square matrix X, X⁺ is the Moore-Penrose pseudoinverse.



Wavelet characterization of directional regularity

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Abstract

Many images belong to classes of functions with various directional regularity behaviors. These behaviors are important for detection of edges. Standard isotropic multidimensional wavelets obtained as tensor product do not give a satisfactory algorithm to detect directional singularities. Using Triebel anisotropic wavelets, we obtain a criteria of directional regularity.

Key words: Images, contours, directional regularity, anisotropic Hölder regularity, anisotropic Triebel wavelet basis, anisotropic wavelet coefficients

1 Introduction

Many natural mathematical objects, as well as many multi-dimensional signals and images from real physical problems, need to distinguish local directional behaviors (for tracking contours in image processing for example), see for instance [1] and the references therein. A wide range of directional transform ideas have been proposed. Steerable Pyramids and Cortex Transforms were developed in the 1980s by vision researchers (Adelson, Freeman, Heeger, and Simoncelli [7] and Watson [9]) to offer increased directional representativeness. Extensions of wavelet bases which can be elongated in particular directions were considered. They include the ridgelets of Candes and Donoho, see [4], or the bandelets of Mallat, see [6], but are efficient with singularities along lines, along hyperplanes, etc, for which wavelets do not deal with efficiently.

For pointwise singularities, it is natural to define the Hölder regularity at a point y in a direction $e \in \mathbb{R}^m$ with |e| = 1 as the Hölder regularity at 0 of the one variable function $f_e : s \mapsto f(y + se)$. It seems that one cannot expect directional regularity to be characterized in terms of the size of the usual wavelet coefficients, because f_e is defined as the trace of f on a line, which is a set of vanishing measure and wavelets have a support of nonempty interior. Thus we should take into account the values of f around the line considered. Therefore the definition of directional smoothness should include such information. However, in the asymptotic of small scales, the values taken into account should be localized more and more sharply around this line. These considerations motivate an alternative definition by Jaffard [5] which can be seen as an extension of the notion of anisotropic regularity which was already introduced by Ben Slimane [2].

We will give a criterion of directional Hölder regularities [3] in terms of decay conditions of anisotropic Triebel wavelet coefficients [8].



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Convergence Properties and Iteration Accelerations of Nonlinear Schemes for Nonlinear Coupled Problem

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Abstract

In this work, some nonlinear fully implicit finite difference discrete schemes are studied for a two-dimensional nonlinear coupled system of parabolic and hyperbolic equations. These nonlinear schemes are proved to be absolutely stable and have $L^{\infty}(H^1)$ convergence. Efficient iteration algorithms are designed to accelerate the solution of these nonlinear schemes. Numerical tests are done to demonstrate the high accuracy and efficiency of these schemes and iterations.

Key words: nonlinear coupled problem, nonlinear fully implicit discrete scheme, convergence analysis, iteration acceleration MSC 2010: 65M06, 65M12, 65B99

1 Nonlinear coupled problem

Coupled systems of parabolic and hyperbolic equations often appear in the study of high temperature hydrodynamics and thermo-elasticity problems [1], [2], [3]. And their accurate and fast solution is of great importance in practice. In this paper, we consider the following nonlinear problem

$$\begin{aligned} u_t - \nabla \cdot (a(X, t, u, v) \nabla u) &= f(X, t, u, v, u_x, u_y, v_x, v_y), & X \in \Omega, t \in J, \\ v_{tt} - \nabla \cdot (b(X, t, u, v) \nabla v) &= g(X, t, u, v, u_x, u_y, v_x, v_y, v_t), & X \in \Omega, t \in J, \\ u(X, t) &= 0, & v(X, t) = 0, & X \in \partial\Omega, t \in J, \\ u(X, 0) &= u_0(X), v(X, 0) &= v_0(X), v_t(X, 0) = v_{t0}(X), & X \in \bar{\Omega}, \end{aligned}$$
(1)

where X = (x, y), Ω is an open rectangular domain in \mathbb{R}^2 with boundary $\partial \Omega$. J = (0, T], T is a positive constant. $a, b, f, g, u_0, v_0, v_{t0}$ are known functions.



2 Nonlinear discrete schemes and iteration accelerations

Two nonlinear discrete schemes are proposed to solve the problem. And Picard iteration and Newton iteration are respectively designed to solve those nonlinear schemes. For example, a basic three-level fully implicit finite difference scheme for (1) is given by finding U_{ij}^{n+1} , V_{ij}^{n+1} and W_{ij}^{n+1} such that

$$\frac{3}{2}d_{t}U_{ij}^{n+1} - \frac{1}{2}d_{t}U_{ij}^{n} - \delta(a^{n+1}(U,V)\delta U^{n+1})_{ij} = f_{ij}^{n+1}(U,V),$$

$$\frac{3}{2}d_{t}W_{ij}^{n+1} - \frac{1}{2}d_{t}W_{ij}^{n} - \delta(b^{n+1}(U,V)\delta V^{n+1})_{ij} = g_{ij}^{n+1}(U,V,W),$$

$$\frac{3}{2}d_{t}V_{ij}^{n+1} - \frac{1}{2}d_{t}V_{ij}^{n} = W_{ij}^{n+1},$$
(2)

with homogeneous Dirichlet boundary conditions and corresponding initial approximations, where $d_t \phi^{n+1} = \frac{\phi^{n+1} - \phi^n}{\tau}$ represents for the backward Euler time discretization for ϕ_t^{n+1} and $\delta(\psi(U, V)\delta\phi)_{ij}$ the central difference quotient approach for corresponding diffusion operator.

3 Theoretical analysis and numerical experiments

Discrete function analysis are applied to prove the convergence and stability of the nonlinear schemes. Especially their $L^{\infty}(H^1)$ convergence properties are obtained with introducing new inductive hypothesis reasoning techniques to overcome the difficulties caused by the nonlinearity and the coupling of different equation types. Using these convergence properties, the convergence accuracy of the iterations to the original problem and the convergent ratio of the iterations to the discrete schemes are attained. For example, theoretical analysis shows Scheme (2) is absolutely stable, has second order $L^{\infty}(H^1)$ accuracy in both spatial and temporal variants to the original problem, its Picard iteration and Newton iteration have the same order accuracy and yet a linear and quadratic convergent speed respectively. Amounts of numerical experiments verify the validity of the theoretical conclusions and demonstrate the superior performance (much higher accuracy and efficiency) of Newton iteration over Picard iteration, and the second order temporal accuracy scheme over its first order counterpoint.

Acknowledgements

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Error analysis in the kernel reconstruction in a semilinear parabolic problem with integral overdetermination

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Abstract

A semilinear parabolic problem of second order with an unknown solely time-dependent convolution kernel is considered. We already proved, based on a given global measurement, the existence of a unique weak solution. In this contribution, we perform an error analysis of the proposed numerical algorithm based on Rothe's method.

Key words: parabolic IBVP, convolution kernel, reconstruction, error analysis

1 Introduction

In [1], we determined the solution u and reconstructed a solely time-dependent convolution kernel K of the following nonlinear problem

$$\begin{cases} \partial_t u - \Delta u + K(t)h + (K * u)(t) = f(u, \nabla u), & \text{in } \Omega \times \Theta, \\ -\nabla u \cdot \mathbf{n} = g, & \text{on } \Gamma \times \Theta, \\ u(\mathbf{x}, 0) = u_0(\mathbf{x}), \end{cases}$$
(1)

where Ω is a Lipschitz domain in \mathbb{R}^N , $N \ge 1$, with $\partial \Omega = \Gamma$ and $\Theta = [0,T]$, T > 0, the time frame, when a global measurement

$$\int_{\Omega} u(\mathbf{x},t) \mathrm{d}\mathbf{x} = m(t)$$

is known. Such type of problems arise for example in the theory of reactive contaminant transport [2]. We proved the following [1]:

Theorem Suppose f is bounded and Lipschitz continuous in all variables, $g \in C^1(\Theta, L^2(\Gamma))$, $h \in C^0(\Theta, H^1(\Omega)) \cap C^1(\Theta, L^2(\Omega))$ and $\min_{t \in \Theta} |(h(t), 1)| \ge \omega > 0$, $m \in C^2(\Theta, \mathbb{R})$ and $u_0 \in H^2(\Omega)$. Then there exists a unique couple solutions $\langle u, K \rangle$ to (1), where $u \in C(\Theta, H^1(\Omega))$, $\partial_t u \in L^{\infty}(\Theta, L^2(\Omega))$ and $K \in C(\Theta)$, $K' \in L^2(\Theta)$.

In this contribution, we derive error estimates for the time discretized model.



2 Time discretization

We apply the Rothe method [3]. Consider an equidistant time-partitioning of the time frame Θ with a step $\tau = T/n$, for any $n \in \mathbb{N}$. We use the notation $t_i = i\tau$ and for any function z we write

$$z_i = z(t_i), \qquad \delta z_i = \frac{z_i - z_{i-1}}{\tau}.$$

Now, let us introduce the following piecewise linear function in time

$$u_n: \Theta \to \mathcal{L}^2(\Omega): t \mapsto \begin{cases} u_0 & t = 0\\ u_{i-1} + (t - t_{i-1})\delta u_i & t \in (t_{i-1}, t_i] \end{cases}, \quad 0 \le i \le n$$

and a step function

$$\bar{u}_n: \Theta \to L^2(\Omega): t \mapsto \begin{cases} u_0 & t = 0\\ u_i & t \in (t_{i-1}, t_i] \end{cases}, \quad 0 \le i \le n.$$

Similarly, we define \bar{K}_n , \bar{h}_n , \bar{g}_n , \bar{m}_n and $\overline{m'}_n$. At time t_i , we infer from the variational formulation of (1) the backward Euler scheme

$$(\delta u_i, \phi) - (\Delta u_i, \phi) + K_i(h_i, \phi) + \sum_{k=1}^i (K_k u_{i-k}\tau, \phi) = (f_{i-1}, \phi).$$
(2)

where $f_i = f(u_i, \nabla u_i)$ and where K_i is recovered from the integral overdetermination. Using Rothe's functions, we can write the discretized problem on the whole time frame as¹

$$(\partial_t u_n, \phi) + (\nabla \bar{u}_n, \nabla \phi) + (\bar{g}_n, \phi)_{\Gamma} + \bar{K}_n(\bar{h}_n, \phi) + \sum_{k=1}^{\lfloor t \rfloor_{\tau}} (\bar{K}_n(t_k)\bar{u}_n(t-t_k)\tau, \phi)$$
$$= (f(\bar{u}_n(t-\tau), \nabla \bar{u}_n(t-\tau)), \phi)$$

and alike for the measurement ($\phi = 1$). In this paper, we show that

$$\max_{t \in [0,T]} \|u_n(t) - u(t)\|_{L^2(\Omega)}^2 + \int_0^T \|\nabla u_n(t) - \nabla u(t)\|_{L^2(\Omega)}^2 \, \mathrm{d}t = O(\tau^2)$$

and

$$\int_0^T |\bar{K}_n(t) - K(t)|^2 \mathrm{d}t = O(\tau^2).$$

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¹ $\lfloor t \rfloor_{\tau} = i$ when $t \in (t_{i-1}, t_i]$



Fast spectral frequency- and time-domain PDE solvers for general engineering problems and structures

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Abstract

We present fast spectral solvers for Partial Differential Equations that address some of the main difficulties associated with simulation of realistic engineering systems in the frequency- and time-domains. Based on a novel Fourier-Continuation (FC) method for the resolution of the Gibbs phenomenon and fast high-order methods for evaluation of integral operators, these methodologies give rise to efficient frequency- and timedomain solvers for PDEs for general engineering problems and structures. Our integral algorithms can solve, with high-order accuracy, problems of electromagnetic and acoustic scattering for complex three-dimensional geometries as well as PDE eigenvalue problems in complex (singular) domains and with mixed boundary conditions (e.g. Dirichlet/Neumann); our FC-based differential solvers for time-dependent PDEs, in turn, give rise to essentially spectral time evolution, essentially free of pollution or dispersion errors, for general PDEs in the time domain. A variety of applications to linear and nonlinear PDE problems, including the Maxwell equations, the Navier-Stokes equations, the elastic wave equation, Laplace eigenvalue problems, etc., demonstrate the significant improvements the new algorithms can provide over the accuracy and speed resulting from other approaches.

Key words: Dispersionless solver, Fast integral-equation solver, Fast spectral PDE solver, Fourier Continuation method (FC), High-frequency problems

Description

This presentation concerns computational solvers for Partial Differential Equations (PDE), associated theoretical questions, and application in various areas of science and engineering including applied physics, electrical engineering, geophysics, photonics and remote sensing. An emphasis is placed on accurate, efficient and generally applicable algorithms; the associated theoretical discussions, in turn, seek to provide necessary background and performance guarantees. From a mathematical standpoint this presentation concerns two main areas, namely,

- I. Frequency-domain, time-harmonic acoustics and electromagnetism, and
- II. Time-domain Partial Differential Equations in general three-dimensional domains, including applications in acoustics and electromagnetism as well as elasticity and fluiddynamics.

The basic elements underlying the techniques and methodologies to be considered are not numerous, but they do have broad applicability. They include new types of high-order integral equation solvers [3, 5, 6, 7, 8, 10], novel rapidly-convergent Green functions for periodic media [2], and explicit as well as unconditionally stable general-geometry Fourier-based methods for time-evolution of PDE [1, 8, 9, 11]. The fast high-order integral equation solvers rely on efficient integration rules and use of certain "equivalent sources" and FFT acceleration. The new Green functions can be used at and around spectral anomalies (Wood anomalies) at which periodic Green functions used previously cease to exist. The time-domain algorithms, finally, are based on a novel concept of Fourier continuation for accurate Fourier-series approximation of non-periodic functions. A number of benefits arising from these approaches will be mentioned: accurate solution of frequency domain problems (see e.g. Figure 1 and its caption) as well as essentially dispersionless solutions of time-domain problems. Application in a range of challenging areas of present interest in science and technology will be presented—which validate and demonstrate the enabling character of the methodologies discussed.



Figure 1: Left: Zaremba (Dirichlet/Neumann) eigenfunction for Laplace's equation at high frequency in the unit circle, with homogeneous (singular!) Neumann and Dirichlet boundary conditions on the left ($|\theta - \pi| < \pi/2$) and right ($|\theta| < \pi/2$) halves of the circular boundary, respectively. Using a total of 1,024 boundary unknowns and a four minute computation in a single processor of a present day laptop computer, the eigenvalue $\lambda = 10,005.97295$ and corresponding eigenfunction (depicted) were obtained with 10-digit accuracy. Center and Right: Neumann-Laplace eigenfunctions on (singular!) domains of the type displayed on the lower-right image (which arise in connection with mode-matching shape optimization for certain types of antennas). The center and right eigensolutions were obtained in a computing time of four seconds each with ~ 0.1% error.

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Methods for the Quantification of Uncertainties in Nonlinear Material Laws in Electrical Engineering

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Abstract

This paper discusses efficient techniques for the uncertainty quantification of electrical engineering problems, in particular magnetoquasistatic and electroquasistatic systems. The main contribution is the stochastic modelling of nonlinear material curves in terms of discrete random variables by the Karhunen-Loève expansion.

1 Introduction

Electrical fields are used to accelerate particles, to transduce energy, in deep brain stimulation or in field grading materials of high-voltage insulators to avoid flashover voltages. The robust design of those devices is a complicated task and to avoid costly prototypes the design process relies on computer simulations based on Maxwell's equations. In particular the strong nonlinear behavior of materials due to magnetic saturation or microvaristors is a challenge. In practice, the underlying nonlinear curve is fitted according to measurement data that typically contain uncertainties and is finally affected by rather large variances due to imperfect manufacturing. The electromagnetic fields and thus any quantity of interest inherits this uncertainty.

2 Magnetoquasistatic example

The transient magnetoquasistatic problem is commonly formulated in terms of the magnetic vector potential. In 2D it is $\mathbf{A}^{\top} = (0, 0, A_z)$ with $A_z =: u$ being the longitudinal component transverse to the xy-plane and the curl operator $|\nabla \times (0, 0, A_z)| = |\nabla u|$. Let (Ω, Σ, μ) be a probability space then the stochastic problem reads

$$\begin{cases} \sigma \partial_t u(\omega) - \nabla \cdot \left(v(|\nabla u(\omega)|, \omega) \nabla u(\omega) \right) = J_z, & \text{ in } T \times D, \\ u(\omega) = u_0, & \text{ on } \{0\} \times D, \\ u(\omega) = 0, & \text{ on } T \times \Gamma_{\text{Dir}}, \end{cases}$$
(1)

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Figure 1: Eigenfunctions and Simulation results

with the conductivity σ , the time interval of interest $T = (0, t_{end})$ and the magnetic reluctivity ν (inverse permeability) that depends on the flux $B(\omega) := |\nabla u(\omega)|$. Furthermore, the potential $u(\omega)$ and the nonlinear material law depend on random outcomes $\omega \in \Omega$ due to imperfect manufacturing and measurement errors. Typically one is interested in the impact of the uncertainty on some quantities of interest, e.g. magnetic multipoles. The multipole expansion is given by the (stochastic) Fourier coefficients $\underline{c}_{p}(\omega)$ of A_{z} on the circular contour (r_{ref}, θ)

$$b_p(\omega) = -\operatorname{Re}\left\{\underline{c}_p(\omega)\right\} \frac{p}{r_{\operatorname{ref}}}, \quad a_p(\omega) = -\operatorname{Im}\left\{\underline{c}_p(\omega)\right\} \frac{p}{r_{\operatorname{ref}}}$$

where p is the pole-pair number, b_p and a_p are the normal and skew coefficients.

3 Karhunen-Loève expansion

We propose to use a Karhunen-Loève (KL) expansion instead of parametrized analytic curves, c.f. [1] to obtain a stochastic model of the nonlinear material relation in terms of discrete random random variables $X_i(\omega)$. It is obtained by solving an eigenvalue problem. Let (λ_i, φ_i) denote a sequence of the eigenpairs, see Fig. 1a), then the truncated Karhunen-Loève expansion reads

$$\nu(B,\omega)\approx \sum_{i=1}^M \sqrt{\lambda_i}\varphi_i(B)X_i(\omega).$$

By means of the KL-expansion (and the Doob-Dynkin Lemma) the stochastic problem (1) is transformed into a high-dimensional deterministic problem, with X_i as additional variables and standard discretization techniques can be applied. In particular we discretize by lowest order Whitney Elements and the implicit Euler method w.r.t. the "deterministic" variables $x \in D$ and $t \in T$, respectively. For the discretization w.r.t. the "stochastic variables" X_i we describe and compare the Monte Carlo, gPC and perturbation method, [2], see Fig. 1b).

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Residual a posteriori error estimation for a stochastic magnetostatic problem

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Abstract

In this work, we propose a residual error estimator for a stochastic magnetostatic problem. The reliability as well as the efficiency of the estimator are established, and a numerical test illustrates our theoretical predictions.

Key words: Stochastic a posteriori residual error estimator, finite element method, polynomial chaos expansion.

1 Setting of the problem

This work is devoted to a stochastic magnetostatic problem, consisting in determining the magnetic field H induced by a source H_s generated in a bounded domain $D \subset \mathbb{R}^3$. This field is given by $H = H_s - \nabla \Omega$, where Ω stands for the so-called magnetic scalar potential defined up to an additive constant by :

$$\begin{cases} \nabla \cdot (\mu(\mathbf{x},\boldsymbol{\zeta}) \,\nabla \Omega(\mathbf{x},\boldsymbol{\zeta})) &= \nabla \cdot (\mu(\mathbf{x},\boldsymbol{\zeta}) \,\mathbf{H}_{s}(\mathbf{x})) & \text{ in } D, \\ \\ \mu(\mathbf{x},\boldsymbol{\zeta}) \,(\nabla \Omega(\mathbf{x},\boldsymbol{\zeta}) - \mathbf{H}_{s}(\mathbf{x})) \cdot \mathbf{n} &= 0 & \text{ on } \partial D. \end{cases}$$

In the above system, **x** stands for the space variable, whereas $\zeta \in \mathbb{R}^M$ is a vector of random independent variables to account for the uncertainties on the material behavior law. The Stochastic Partial Differential Equations is solved by applying the Spectral Stochastic Finite Element Method (SSFEM, see [1]), and leads to the determination of the approximated solution $\Omega^{h,p}$ given by :

$$\Omega^{h,p}(\mathbf{x},\boldsymbol{\zeta}) = \sum_{1 \leq i \leq N} \sum_{\alpha \in K} \Omega_{i,\alpha} \Psi_{\alpha}(\boldsymbol{\zeta}) w_i(\mathbf{x}),$$

where Ψ_{α} are the elements of a finite dimensional set of polynomial chaos, and w_i are the usual nodal finite element basis functions in space.



2 A posteriori error estimation

We are interested in deriving a residual a posteriori error estimator η_{glo} for the control of the numerical error e_{glo} generated by the space and stochastic discretizations, defined for any ζ by:

$$e_{\rm glo}^2(\boldsymbol{\zeta}) = \int_D \left| \mu(\mathbf{x},\boldsymbol{\zeta})^{\frac{1}{2}} \nabla \left(\Omega^{h,p}(\mathbf{x},\boldsymbol{\zeta}) - \Omega(\mathbf{x},\boldsymbol{\zeta}) \right) \right|^2 \, d\mathbf{x},$$

so that $e_{\text{glo}}(\zeta) \leq C \eta_{\text{glo}}(\zeta)$, where *C* is a constant which does not depend on the discretization parameters involved and on the data, so that the reliability of the proposed estimator is established. The proof is based on a decomposition of the error, allowing to make appear the so-called stochastic error part. Indeed, we derive a stochastic estimator η_{sto} and a spatial one η_{spa} so that $\eta_{\text{glo}}^2 = \eta_{\text{sto}}^2 + \eta_{\text{spa}}^2$, and propose a result which is an extension of the deterministic case [2]. Moreover, some efficiency results are also derived so that the proposed estimator is equivalent to the error.

3 Numerical example

A numerical test is then proposed, in which some parts of the domain have some random relative permeabilities (namely μ_3 and μ_4 in Figure 1). The mean value of the proposed stochastic estimator η_{sto} is compared to the mean value of the stochastic error estimated by the use of a Monte-Carlo method, for different truncation orders of the polynomial chaos expansion. Then, the behaviors of the stochastic and spatial parts of the estimator are compared, refining the spatial mesh or the order of the polynomial chaos to illustrate their behaviors in different configurations.



Figure 1: Numerical test for the magnetostatic problem.

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A probabilistic model of the adhesive contact forces between rough surfaces in the MEMS stiction context

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Abstract

Stiction is a common failure mechanism in microelectromechanical systems (MEMS) in which two interacting bodies permanently adhere together. This problem is due to the comparability of adhesive surface forces (e.g. Van der Waals forces, capillary forces) and body forces in the MEMS context.

To predict the adhesive contact forces coupled with stiction phenomenon, the combination of the Nayak statistical approach with the asperity-based theories is a common solution. However, this method contains some limitations due to the underlying assumptions: infinite size of the interacting rough surfaces and negligibility of asperity interactions. Furthermore, the Nayak solution suffers from a considerable dependency on the choice of the minimum wave length considered in the surface representation, which remains difficult to select.

The main goal of our research is to propose an improved method (i) which accounts for the finite size of the interacting surfaces, (ii) accounts for the uncertainties related to these surface topologies, (iii) in which the minimum wave length selection is physically based, and (iv) in which the validity of the asperity-based theories is demonstrated.

From the topology measurements of MEMS samples, an analysis of the power spectral density function is carried out to determine the minimum relevant wave length for the problem of interest (here capillary stiction). We also show that at this scale of interest the asperity-based theories remain valid for polysilicon materials.

Moreover, instead of considering infinite surfaces as in the Nayak approach, a set of surfaces, whose sizes are representative of the MEMS structure, is generated based on the approximated power spectral density analysis and using the Monte Carlo method. From this description of the contacting surfaces, the adhesive contact forces can be evaluated by applying the asperity contact theories, leading to a probabilistic distribution of the adhesive contact forces.

In addition, as the contact forces are rooted from the micro-scale adhesive forces, while their consequence, stiction, happens at the macro-scale of the considered device,

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the multi-scale nature of the phenomenon is accounted for. To predict this macro-scale behavior in a probabilistic form, the uncertainty quantification process is coupled with a multiscale analysis.

Key words: Asperity contact, multiscale contact, random field, stiction, surface topography.

Acknowledgements

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Uncertainty Quantification of Field/Circuit coupled problems

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Abstract

Mathematical modeling of electric devices and nanoelectronics systems, involving parameters with uncertainty, results in stochastic coupled problems. In a multi-physical framework, such systems can be partitioned into subsidiary problems, and then solved numerically by co-simulation techniques. A key challenge in the formulation and implementation of stochastic, coupled problems is to facilitate the communication between subproblems at every iteration. Therefore, the proposed method first uses a Karhunen-Loève Expansion (KLE) in order to reduce the number of random variables and then, for such a reduced representation, each subproblem is solved by the Stochastic Collocation Method (SCM) in order to determine the coefficient of a Polynomial Chaos Expansion (PCE). Finally, we provide an example relevant to electronic engineering.

Key words: stochastic coupled problems, polynomial chaos, stochastic collocation method MSC 2010: 60G15, 60G60, 60H10, 60H15, 60H30

1 Problem settings and preliminary results

In today's applications, the modelling and simulation of coupled systems is necessary because of the progressive miniaturization and the increasing complexity of components in electronic systems. In such kind of systems, some parameters often exhibit uncertainties. In this paper, the PCE with the SCM [1] is used for the uncertainty propagation in the coupled problem consisting of DAEs and PDEs subproblems with uncertain geometrical/material parameters.

In a multi-physical framework, the Field/Circuit system, shown on Figure 1(a), can be easily partitioned into a set of coupled index-1 DAEs of subsystems [2] and then, taking into account that random variables $\xi, \zeta \in L^2(\Omega, \mathcal{F}, \mathbb{P})$ it can be written in the semi-explicit form as



$$\dot{\mathbf{y}}_i = \mathbf{f}_i(\mathbf{y}, \mathbf{z}, \boldsymbol{\xi}), \quad \mathbf{0} = \mathbf{g}_i(\mathbf{y}, \mathbf{z}, \boldsymbol{\zeta}), \quad i = 1, \dots, r,$$

where $\mathbf{f} = (\mathbf{f}_1, \dots, \mathbf{f}_r)^{\mathsf{T}}$, $\mathbf{g} = (\mathbf{g}_1, \dots, \mathbf{g}_r)^{\mathsf{T}}$ and $\partial \mathbf{g}_i / \partial \mathbf{z}_i$ is nonsingular. The first subsystem results from the application of FE analysis to the nonlinear curl-curl equation, equipped with a circuit coupling equation, while the second one comes from a modified nodal analysis [3].



(b) FEM model of a transformer [4].

Figure 1: Nonlinear Field/Circuit configuration.

The FEM model, shown Fig.1(b), is excited by $u(t) = 220 \sin(\omega t)$ V, where $\omega = 2\pi$ kHz. The only values that are taken subject to variations are R, C and the reluctivity $v: R(\xi_2) =$ $R_0[1+0.1\xi_2], C(\xi_3) = C_0[1+0.05\xi_3]$ and $v(\xi_1) = v_0[1+0.03\xi_1]$, where $\xi_j \in [-1,1]$ for j = 1, 2, 3are independent uniformly distributed random variables. In a more realistic situation for a large number of sources of uncertainty in the field model, a KLE will be required.



Figure 2: Results of deterministic and stochastic modeling.

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Accelerating the Alternating Projection Algorithm for the Construction of Packings in Real Projective Space

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Abstract

In [3] Tropp established a way to construct optimal packings in a metric space through alternating projection. While the method worked well, its main drawback was its slow convergence. In this paper we develop a method to accelerate the convergence of the method. *Key words: alternating projection, iterative method, projective spaces, quasi-Newton*

method

1 Introduction

Ways to construct optimal packings in a metric space have been widely studied for centuries. Applications can be found in a wide range of fields (see [2] and references therein). The existence of a solution to the optimal packing problem is guaranteed due to the use of a compact metric space and a continuous objective function. This does not mean however that the solution can be found easily as the problem is highly non-convex.

In [3] a method was developed that constructs packings in Grassmannian manifolds equipped with several different metrics using an alternating projection method, a method first mooted by von Neumann [4]. An alternating projection method between two closed, convex subsets of a Hilbert space is guaranteed to converge to a point in their intersection (if such a point exists) [1]. However, in the case of the optimal packing problem this hypotheses is not satisfied as only one of the spaces is convex, although both are compact. This means that convergence is not certain from a theoretical point of view.

While the packings that were obtained in [3] were very satisfactory, the authors indicated that one of its drawbacks was its slow convergence. In this paper we address that shortcoming. We do this by reformulating the original mathematical problem as a root-finding problem which can be solved with a quasi-Newton method of which we propose two variants, based on Broyden's method. Using this approach we note that two distinct convergence histories can occur for all three algorithms (the original one by Tropp [3] and our two quasi-Newton methods): either convergence is (nearly) monotonous, or after a number of iterations convergence stalls, by which we mean that the norm of the difference between two consecutive iterates stays (nearly) constant for a long time (sometimes even for more than a thousand



iterates).

When convergence is monotonous our algorithm required fewer iterations for convergence than the original algorithm, with typical reductions of 50 to 75%. When the convergence stalls, the modification does not help. Stalls seem entirely dependent on the initial (random) iterate that is generated using the method proposed by Tropp [3]. Encouraged by the possible gain, we allow the new algorithm to restart from a new initial iterate whenever a stall is detected. Numerical experiments confirm that this improves the overall performance of the algorithm. We illustrate this in figure 1 for a three-dimensional vector space.

2 Tables and Figures



Figure 1: Mean number of iterations needed for convergence of the three algorithms (the original one by Tropp and our two Broyden-based methods) as a function of the number of 1D subspaces (N) in a 3D vector space.

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An Approximate Mathematical Model for Global Convergence of a Coefficient Inverse Problem Related to Parabolic Equation

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Abstract

In this work an approximate mathematical model for global convergence of a Multidimensional Coefficient Inverse Problem (MCIP) is considered.

Key words: Global convergence, coefficient inverse problem, parabolic problem.

Introduction

In this work an approximate mathematical model for global convergence of a Multidimensional Coefficient Inverse Problem (MCIP) related to following parabolic problem

$$\begin{cases} u_t = D\Delta u - a(x)u \text{ in } \mathbb{R}^r \times (0, \infty), \quad D > 0; \\ u(x,0) = \delta(x - x_0) \text{ for } x \in \mathbb{R}^r, \quad r \in \{1,2,3\} \end{cases}$$
(1)

is considered. The unknown coefficient a(x) satisfies the following conditions: $0 \le a(x) \le b$, $x \in \mathbb{R}^r$; $a|_{\Omega^c} \equiv 0$. Thus, the MICP can be posed formally on $\Omega \subset \mathbb{R}^r$ as follows:

Suppose that the diffusion coefficient D = const. > 0 is known. Determine the coefficient $a(x), x \in \Omega$, assuming that the function g(x,t) is known for a fixed source position at $x_0 \notin \overline{\Omega}$:

$$u(x,t)=g(x,t), \; \forall (x,t)\in \partial\Omega\times (0,\infty).$$

As we see above the MCIP is studied with the data resulting from a single measurement situation. The most important property of the proposed approach is that we do not need any information about true solution inside the domain Ω . Because of this reason the numerical algorithm presented here is called approximately globally convergent. An important part of our technique is based on so called *tail functions* estimation. According to our approximate globally convergent theorem, the accuracy of the solution strongly depends from the accuracy of the reconstruction of the tail function. Here in order to estimate tail functions, we use asymptotic behavior of the laplace transformation of the solution of direct problem (1). Such techniques are frequently used in science for example we refer to the geometrical optics assumption. In the literature, it is well known that the globally convergent method for MCIP related to hyperbolic PDE with single measurement data is proposed in detail in [1]. Here the same method is considered for parabolic equation case.



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Solving low Mach number Riemann problems by momentum interpolation

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Abstract

Momentum interpolation methods for unsteady low Mach number flow calculations are re-examined to allow for solution of low Mach number Riemann problems.

Key words: Godunov-type schemes, Low Mach number, Momentum interpolation, Rhie-Chow interpolation

1 Introduction

Considering compressible flows calculation, accuracy and robustness of numerical methods with co-located arrangement of the unknowns depend heavily on the way of interpolation on the cell faces. Broadly speaking, there are two types of interpolation methods: (1) Godunov-type methods, which are derived from the characteristic equations ; (2) momentum interpolation methods, often associated with the pioneering work by Rhie and Chow [6], which are derived from the momentum equation. To the best of our knowledge, Godunov-type schemes only are used for solving shock-tube-like problems. Thus, our goal is to explore the possibility of adapting the momentum interpolation method to deal with this kind of problems. Several aspects of the relation between Godunov-type schemes and Rhie-Chow-like methods are investigated on this occasion.

2 Rhie-Chow-like interpolation method

A 1-D flow of air governed by the Euler equations is considered. First-order accurate finite volume formulation based on the Euler explicit time integration is used to discretize the equations. First, the existing variants of momentum interpolation suitable for unsteady calculations are recalled. They share the common feature that, if a steady state is reached, this solution does not depend on the time-step [3, 4, 5]. Their ability to properly capture smooth unsteady low Mach number solutions with acoustic waves was evidenced in [4]. Their ability to deal with flows exhibiting discontinuities is investigated in the present study.



3 Low Mach number Riemann problems with nearly incompressible initial conditions

As a first step, Riemann problems with jumps in density, velocity and pressure that are small with respect to the reference Mach number M_r of the flow, are considered. More precisely, the pressure and density jumps between the right and left states scale as M_r^2 , and the velocity jump scales as M_r . Such initial conditions are often referred to as "well-prepared" and correspond to nearly incompressible flow. The solutions of these Riemann problems were studied by low Mach number asymptotic analysis in [2], and the behaviour of Godunov-type schemes for these problems was studied in [1, 2].

First, the inability of the Rhie-Chow-like interpolation method to capture weak discontinuities is evidenced. Some paths of improvement are explored, which are based on the analysis of the possibility of transposition of Godunov-type methods recipes.

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Damage modeling of woven-fabric laminates with SAMCEF: validation at the coupon level

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Abstract

Inter and intra-laminar damages in laminated composites made up of woven fabric plies are considered. Simulation, carried out with the SAMCEF finite element code, is compared to experimental results and validations are done at the coupon level.

Key words: woven fabrics, damage models, laminar, SAMCEF

Inter and intra-laminar damage models for woven fabrics

Inter and intra-laminar damages in laminated composites made up of woven fabric plies are considered. Simulation, carried out with the SAMCEF finite element code, is compared to experimental results and validations are done at the coupon level. The material model for the intra-laminar damage is based on continuum damage mechanics [1, 2]. In the laminate made of homogenous plies, damage variables impacting the stiffness of each ply are associated to the different failure modes and represent the fiber breaking, matrix cracking and de-cohesion between fibers and matrix. A specific identification procedure is used to determine the values of the damage model parameters.

This procedure is based on test results at the coupon level. It allows determining not only the elastic properties but also the value of the parameters describing the non-linear behavior of the material, including non-linearity in the fiber direction, as well as damage and plasticity in the matrix. The material parameters are then validated by comparing test and simulation results on a stacking sequence not used for the identification. In Figure 1, the identification is done on a balanced [45]n laminate, while the validation is carried out on a [67.5]n laminate.

The cohesive elements approach is used for modeling the inter-laminar damage, that is delamination. A damage model is assigned to some interface elements inserted between plies





Figure 1: Left: identification on a [45]n; right: validation on a [67.5]n

to represent their possible de-cohesion and a fracture criterion is used to decide on the interlaminar crack propagation [3]. It is demonstrated here that, in general applications, modeling delamination alone is not enough, concluding that it is essential to model the damage inside the plies besides the damage at their interface. This is illustrated for the ENF (End Notched Flexure) test case, as depicted in Figure 2, in which simulation is compared to the test results. In Figure 2, the dashed line represents the constant slope characterizing the beam stiffness when only delamination is taken into account. In reality, the ply is also damaged during the loading. When the simulation takes this effect into account, there is a good agreement with the experimental results.



Figure 2: Left: DCB problem with 45° interfaces; right: ENF problem with 45° interfaces

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Multirate technique for explicit Nodal Discontinuous Galerkin computations of time domain Maxwell equations on complex geometries

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Abstract

Computing electromagnetic waves in complex geometries have to face the problem due to using of small size elements in the generated meshes. This affect convergence criteria of explicit numerical schemes. This paper presents a multirate technique to improve and optimize the time step of Runge-Kutta or Leap Frog numerical schemes. This technique is developed for accelerating explicit discontinuous Galerkin computations of time domain Maxwell equations. An application example is proposed to show efficiency of this technique to simulate wave propagation on human skull geometry.

Key words: Discontinuous Galerkin method, Explicit numerical schemes, Maxwell equations, Multirate technique

1 Introduction

Today due to increasing development of electromagnetic applications and devices, we need implementation of efficient tools to solve Maxwell equations in complex geometries. The meshes used for computation on complex geometries contain elements of small size that affect convergence properties and increase the computational cost of the classical numerical techniques such as finite difference method, finite element method or finite volume method. The discontinuous Galerkin methods are introduced to improve spatial discretization on small size elements thanks to the parametrization rules. These methods are suitable for parallel computing. Numerical schemes such as Leap Frog or Runge-Kutta are often implemented for explicit computations in time domain. Unfortunately the presence of small size mesh elements impose to reduce the time step. In this article a multirate approach is presented in order to optimize the time step of explicit schemes. This technique is recently proposed for accelerating computations of geophysical flows with a nodal discontinuous Galerkin method. An illustration example on a human skull geometry is presented. It consists on evaluating the specific absorption rate of a human skull when the incident field is a modulated gaussian pulse. It shows gain of computational cost on simulations in comparison of those performed with a classical CFL (Courant-Friedrichs-Lewy) condition.



2 Multirate approach on skull geometry

In this paper we will show results obtained for a 3D tetrahedral mesh with a 3rd order spatial discretization. Due to the gap between the smallest and largest acceptable explicit time step, classical singlerate time integration techniques are inefficient. The multirate strategy consists in gathering mesh elements in appropriate groups which are stable for a certain range of time steps. Bulk groups, were a classical explicit Runge-Kutta method is used, are separated by buffer groups that accommodate the transition between them by means of adapted methods to maintain important properties such as consistency, convergence, conservation, ... For high order spatial discretization we will use a third order multirate strategy originally developed by *Schlegel et. al* in [1] and adapted for the discontinuous Galerkin framework in [2]. Due to the high number of degrees of freedom it is required to use parallel computers. However, in a multirate strategy, mesh elements have a different workload depending on their multirate group. The challenge is to build a mesh partitioning such that the workload is well balanced at every stage of the multirate algorithm while the communication overheads are minimized [3].



(a) Skull geometry of a human body

(b) Surfacic distribution of electric field

Figure 1: Electric gaussian modulated pulse propagated on skull surface .

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Approximating the Bayesian Solution of Inverse Problems

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Abstract

Inverse problems arise from indirect observations of parameters of interest. The Bayesian approach to inverse problems formalizes the characterization of these parameters through exploration of the posterior distribution of parameters conditioned on data. This lecture will focus on two complementary efforts to make the Bayesian solution of inverse problems more computationally tractable. First, we will discuss principled approximations of the forward model or likelihood function, and the approximate (or in some cases exact) posterior distributions they induce. Then we will discuss dimension reduction schemes that lead to approximate factorizations of the posterior distribution, designed to improve the efficiency of posterior sampling in high dimensions.

Key words: Bayesian inference, inverse problems, approximation theory, model reduction, Markov chain Monte Carlo, dimension reduction, Rao-Blackwellization

Introduction

Predictive simulation of complex physical systems increasingly rests on the interplay of experimental observations with computational models. Inference from observational data has become an essential task in fields ranging from subsurface modeling to weather prediction. In this context, Bayesian statistics provides a natural framework for treating *inverse problems*— by quantifying uncertainty in parameter estimates and model predictions, fusing heterogeneous sources of information, and optimally planning experiments or selecting observations. Yet the computational expense associated with rigorous Bayesian methods presents significant bottlenecks in large-scale inverse problems.

This lecture will cover approximation methods designed to make the Bayesian solution of inverse problems more computationally tractable. We will address this challenge from two directions: first, by developing approximations of the forward model or likelihood function; and second, by understanding and exploiting the structure of the posterior distribution in high dimensions.

Approximating the forward model

Exploration of the Bayesian posterior distribution, whether using Markov chain Monte Carlo (MCMC) methods or other sampling schemes, requires repeated evaluations of the likelihood function and hence the *forward model* or parameter-to-observable map. An important

strategy for mitigating this cost is to recognize that the forward model may exhibit regularity in its dependence on the parameters of interest, such that the model outputs may be approximated with fewer samples than are needed to characterize the posterior via MCMC. Replacing the forward model with an approximation or "surrogate" *decouples* the required number of forward model evaluations from the length of the MCMC chain, and thus can vastly reduce the overall cost of inference.

We will begin by discussing sparse polynomial expansions [10, 11, 12] as well as projectionbased reduced order models [6] that are useful when the forward model comprises a large set of differential equations. Both yield surrogate posterior densities that can be evaluated at reduced online computational cost. Convergence results [14, 12] describe the error in the posterior distribution induced by error in the forward model approximation; alternatively, exact sampling of the posterior distribution can be achieved via multi-stage (e.g., delayed acceptance) MCMC schemes [2].

While it is natural to construct forward model approximations over the support of the prior distribution, more efficient approaches seek accuracy with respect to the posterior distribution, which typically concentrates on a small fraction of the prior support. In this setting, forward model approximations can be constructed iteratively, in conjunction with MCMC or importance sampling. We will present a method for constructing polynomial approximations with respect to a posterior-focused biasing distribution identified via a stochastic optimization procedure [9]. One specific instantiation finds a Gaussian approximation q of the posterior π , optimal in the sense of minimizing the right-sided Kullback-Leibler divergence $D_{\text{KL}}(\pi || q)$, then constructs a polynomial approximation of the nonlinear forward model with respect to q, yielding a surrogate posterior distribution that accurately captures the non-Gaussian features of π .

Finally, we will discuss a recently-developed framework that constructs local likelihood approximations *within* the Metropolis-Hastings kernel, borrowing ideas from derivative-free optimization and experimental design [3]. This work departs from previous work in surrogate-based inference by exploiting useful convergence characteristics of local approximations. We prove ergodicity of the resulting approximate Markov chain and show that it samples asymptotically from the *exact* posterior distribution of interest. Variations of the algorithm can employ either local polynomial approximations or local Gaussian process regression, thus spanning two widely used function approximation schemes.

Approximating the prior-to-posterior update

Approximating the forward model or likelihood may mitigate the cost of each sampling step, but generating high-quality posterior samples—particularly for the high-dimensional parameter spaces that result from discretizing an underlying *function* of space and/or time—requires that we understand the structure of the posterior distribution. The intrinsic dimensionality of an inverse problem is affected by prior information, the accuracy and number of observations, and the smoothing properties of the forward operator. From a Bayesian perspective, changes from the prior to the posterior are, in many problems, confined to a relatively lowdimensional subspace of the parameter space. In the second half of the lecture, we will discuss ways of characterizing and exploiting this kind of low-dimensional structure.

We first present some results in the linear-Gaussian setting, where the posterior covariance matrix can be approximated as a low-rank update of the prior covariance matrix [13]. We prove optimality of a particular update, based on the leading eigendirections of the matrix pencil defined by the Hessian of the log-likelihood and the prior precision, for a broad class of loss functions typified by the Förstner metric [8] for symmetric positive definite matrices. These loss functions emphasize directions where the *relative* reduction in variance, from prior to posterior, is greatest. They are naturally generalized to optimality statements between distributions, e.g., optimality in Kullback-Leibler divergence and Hellinger distance.

Next, we extend this idea to inversion with nonlinear forward models and Gaussian priors [6]. We present a dimension reduction approach that defines and identifies a "likelihoodinformed subspace" (LIS) by characterizing the relative influences of the prior and the likelihood over the support of the posterior distribution. This identification facilitates computationally useful decompositions of the posterior. In particular, we approximate the posterior distribution as the product of a lower-dimensional posterior defined on the LIS and the prior distribution marginalized onto the complementary subspace. Markov chain Monte Carlo sampling can then proceed in lower dimensions, with significant gains in computational efficiency. We also introduce a Rao-Blackwellization strategy that de-randomizes Monte Carlo estimates of posterior expectations for additional variance reduction.

Finally, we connect the notion of the likelihood-informed subspace to *exact* and dimensionindependent posterior sampling schemes first proposed in [4, 1]. We describe an MCMC scheme that separates the parameter space into a finite-dimensional LIS and its infinitedimensional complement [5]. The distribution on the infinite-dimensional complement is mainly determined by the Gaussian prior, and thus dimension-independent algorithms that rely on the prior covariance kernel in the proposal can mix quite effectively.

Numerical examples illustrating these techniques will range from X-ray tomography and atmospheric remote sensing to large-scale inverse problems involving partial differential equations, including an ocean general circulation model.

Topics covered in this lecture represent joint work with Patrick Conrad, Tiangang Cui, Patrick Heimbach, Kody Law, Jinglai Li, James Martin, Habib Najm, Natesh Pillai, Aaron Smith, Alessio Spantini, Antti Solonen, Luis Tenorio, Karen Willcox, and Dongbin Xiu.

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The effect of exponential fitting on the stability of numerical methods for solving first order IVPs

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Abstract

It will be shown that the stability of the EF methods for solving first order IVPs depends strongly on the choice of the fitting space. We will in particular focus on the fact that the traditional choice to include $\langle \exp(\omega x), \exp(-\omega x) \rangle$ with $\omega \in \mathbb{R}$ in the fitting space may drastically reduce the size of the stability region of the EF method in comparison with the original method.

Key words: Exponential fitting, Stability MSC 2010: 65L07

1 Introduction

Many numerical methods are available for the solution of initial value problems which take advantage of special properties of the solution. In particular much efforts have been concentrated on the development of techniques for problems with oscillatory and/or exponential solutions. These methods, relying on pioneering work by Gautschi [1] and nowaways commonly called Exponentially-Fitted (EF) methods (see [2] and references therein for an excellent overview), are designed to numerically integrate the problem up to machine accuracy whenever the solution is in a so-called fitting space S. An example of a frequently used fitting space is $S = \langle \cos(v x), \sin(v x), 1, x, \dots, x^{p-2} \rangle$. Various kinds of methods were constructed for different types of problems in the past years but they all have in common that both the trigonometric and the exponential case can be treated in one framework by replacing v by $\omega = i v$, i.e. the fitting space always contains $\langle \exp(\omega x), \exp(-\omega x) \rangle$ where ω is either real or purely imaginary. In fact, a unifying approach to cover both cases has been introducted by Ixaru (see e.g. [3]).

The purpose of the talk is to show that the linear stability properties of an EF method depend to a large extent on the choice of the fitting space S. In particular, we will show that the traditional choice to include $\langle \exp(\omega x), \exp(-\omega x) \rangle$, $\omega \in \mathbb{R}$ in S can be a very poor choice, as far as stability is concerned, especially for methods with a finite region of stability.



2 The linear stability of (*a*, *b*)-EF methods

We consider the more general class of EF methods for which the fitting space S contains $\langle \exp(\omega x), \exp(\theta x) \rangle$. Since we want to obtain real solutions when solving real linear problems, ω and θ are allowed to be both real or complex conjugate. For a classical method, the coefficients are constant. The coefficients of EF methods however depend upon the products $a = \omega h$ and $b = \theta h$ whereby h is the (constant) step size of the method; a and b are called the fitting parameters of the method. We will call a method that is fitted to a and b an (a,b)-EF method.

The application of an (a, b)-EF method to the test equation $y' = \lambda y$, y(0) = 1 with step size *h* results in a linear recursion relation for the numerical solution $\{y_n | n = 0, 1, ...\}$ whereby the coefficients depend upon *a*, *b* and $z = \lambda h$. The numerical solution will be stable iff all roots of the corresponding characteristic equation have modulus at most equal to 1 and if those of modulus 1 are simple. The region \mathcal{R} in the complex *z*-plane for which the stability condition is satisfied is called the region of stability of the method. Every (a, b)-EF method thus has its own region of stability $\mathcal{R}_{(a,b)}$. For well chosen combinations (a, b), the stability region $\mathcal{R}_{(a,b)}$ may become much larger and may even grow from a finite region to an infinite one, while for badly chosen combinations (a, b) the region $\mathcal{R}_{(a,b)}$ may shrink with respect to the original $\mathcal{R}_{(0,0)}$.

As an example, let us consider two kinds of (a, b)-EF variants of the well-known two-step Adams-Bashforth method: (a, b) = (a, -a) and (a, b) = (a, a), $a \in \mathbb{R}$. For both kinds, we have drawn the boundaries of stability regions $\mathcal{R}_{(a,b)}$ in Figure 1 for some values of a. The region of stability itself is the inner (bound) region of the corresponding curve. One notices that for the (a, -a)-EF versions the region shrinks as a increases, while for the (a, a)-EF versions, the stability region grows as a gets more negative.



Figure 1: Boundary of stability regions of the (a, b)-EF two-step Adams-Bashforth method with b = -a (left) and b = a (right) whereby a = -5, -3, -1 and 0.

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Exponentially Fitted Two Step Peer Methods

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Abstract

The peer methods for the numerical solution of Initial Value Problems (IVP) in ordinary differential systems were introduced by R. Weiner *et al* to solve different types of IVPs either in sequential or parallel computers. In this work, we study exponentially fitted two-stage and three-stage peer schemes that are able to fit spaces with dimension four and six respectively. Analysis of the stability on the real and imaginary axes is also given.

Key words: Explicit peer methods, Exponential fitting MSC 2010: 65L06, (65L20)

1 Introduction

We consider the numerical solution of IVPs for first order differential systems

$$\frac{\mathrm{d}}{\mathrm{d}t}y(t) = f(t, y(t)), \quad t \in [t_0, t_0 + T], \quad y(t_0) = y_0 \in \mathbb{R}^m, \tag{1}$$

with a sufficiently smooth vector field f(t, y) where some knowledge of the behaviour of their unique global solution is known in advance. In the case that the solution of (1) has an oscillatory behaviour and further we know an estimate of the frequency, some modified Runge-Kutta (RK) methods using this information, usually called trigonometrically fitted or more generally exponentially fitted methods [2, 3, 6], have been proposed to improve their accuracy and efficiency over standard RK methods that are based on a polynomial approximation of the local approximation at each point.

For explicit RK methods the stage order is limited to one and this implies serious restrictions in the dimensionality of the fitting space. On the other hand, linear multistep methods do not have such a limitation, as shown for example in the early paper of Gautschi [2]. In this case, with k steps, a method can be fitted to k + 1 dimensional spaces.

Here, we consider explicit two step peer methods introduced by R. Weiner, *et al* [4, 5] as an alternative to classical Runge–Kutta (RK) and multistep methods attempting to combine the advantages of these two classes of methods.



In this work fitted two-stage and three-stage peer methods based on the previous schemes given in [1] to some fitting spaces are constructed and also a study of the stability on the real and imaginary axes is also given.

Some numerical experiments are presented to show the performance of the above fitted methods for problems with oscillatory solutions. The proposed methods are compared to exponentially fitted Adams-Bashforth-Moulton methods with the same order.

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Error estimates for splitting methods based on AMF and Radau-IIA formulas for the time integration of advection diffusion reaction PDEs.

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Abstract

The convergence of a family of AMF-Radau methods for the time integration of evolutionary Partial Differential Equations (PDEs) of Advection Diffusion Reaction type semidiscretized in space is considered. The methods are based on very few inexact Newton Iterations of Aproximate Matrix Factorization type (AMF) applied to the two-stage Radau IIA method and allow a cheap implementation. Furthermore, they have given competitive results when compared with other methods in the literature. Uniform bounds for the global time-space errors on semi-linear PDEs when simultaneously the time step-size and the spatial grid resolution tend to zero are derived. Numerical illustrations supporting the theory are presented.

Key words: Evolutionary Advection-Diffusion-Reaction PDEs, Approximate Matrix Factorization, Runge-Kutta Radau IIA methods, Convergence.

1 AMF-Radau methods

Time integration schemes for Initial Value Problems in systems of ordinary differential equations (ODEs)

$$y'_{h}(t) = f_{h}(t, y_{h}(t)), \quad y_{h}(0) = u^{*}_{0,h}, \quad 0 \le t \le t^{*}, \quad y_{h}, f_{h} \in \mathbb{R}^{m(h)}, \quad h \to 0^{+},$$
(1)

are proposed. The system (1) is assumed to come from the spatial semidiscretization of an l-dimensional (typically $1 \le l \le 3$) Advection Diffusion Reaction problem in time dependent Partial Differential Equations (PDEs), with prescribed Boundary Conditions and an Initial Condition. A time-integration method combining the Approximate Matrix Factorization approach [2] and the Radau IIA method was proposed in [3], whereas a variable stepsize integrator based on this method was successfully tested in [1] on several non-academic 2D and 3D problems (e.g., 2D and 3D combustion model, a 2D radiation-diffusion problem and a 3D Burgers-type problem). By assuming that the Jacobian matrix J can be split as $J = \sum_{j=1}^{d} J_j$



(typically the matrices J_j possess a banded structure), we consider a more general family of methods of the form

Predictor:
$$Y_n^0 \equiv (Y_{n,i}^0)_{i=1}^2 = e \otimes y_n$$
,
q Iter.: $(I \otimes I - T_v \otimes \tau P)(Y_n^v - Y_n^{v-1}) = D_n^{v-1}, \quad 1 \le v \le q$, (2)
Corrector: $y_{n+1} = Y_{n,2}^q$.

where the matrices T_{ν} might change with the iterations, but sharing the same one-point spectrum. Above, *P* is certain matrix fulfilling $P - J = O(\tau)$ and $D^{\nu-1} = e \otimes y_n - Y_n^{\nu-1} + \tau (A \otimes I_m)F(t_ne + c\tau, Y_n^{\nu})$ is the residual defined by the two-stage Radau IIA formula. Moreover, the matrices T_{ν} can be selected in order to increase the order of convergence and for stability requirements.

2 Selected methods and error estimates

We consider a convergence analysis for AMF-Radau methods (2) on semi-linear problems $y'_h(t) = f_h(t, y_h) := J_h y_h(t) + g_h(t)$. The time-space global errors ϵ_n fulfil the recurrence $\epsilon_{n+1} := u_h(t_{n+1}) - y_{n+1} = R_q(\tau J_1, \dots, \tau J_d)\epsilon_n + l(t_n, \tau, h)$, where $l_n \equiv l(t_n, \tau, h) := u_h(t_{n+1}) - y_{met}(t_n, u_h(t_n), \tau)$ are the time-space local errors and $R_q(z_1, \dots, z_d)$ is the linear stability function of the method. For AMF-Radau methods (2) based on just q = 1 iteration we have that $l_n = \tau^2(e_2^T(A - T_1)c) \cdot (Ju'_h(t_n)) + O(\tau^3) + O(\tau h^r)$ and we consider an AMF-Radau-11 with matrix T_1 selected according to the conditions $(A - T_1)c = 0$, $\sigma[T_1] = \{\gamma\}$. The original method AMF-Radau-31t [3, 1] based on q = 3 iterations does not fulfil this latter condition since the matrices $T_1 = T_2 = T_3 = T$ where given by $e_2^T(I_2 - T^{-1}A) = 0^T$, $\sigma[T] = \{\sqrt{6}/6\}$. Furthermore, we select an AMF-Radau-21t method with matrices T_1 and T_2 as for AMF-Radau-11t and AMF-Radau-31t, respectively. The time-space global errors provided by an AMF-Radau-11t and then fulfil $\epsilon_{n+1} := u_h(t_{n+1}) - y_{n+1} = R_q(\tau J_1, \dots, \tau J_d)\epsilon_n + l(t_n, \tau, h)$ and realistic error estimates of the form $\epsilon_n = O(\tau^{p_1}) + O(h^r) + O(\tau^{p_2}h^{p_3})$, $\tau, h \to 0^+$, will be presented and numerically checked both for time-independent and time-dependent boundary conditions.

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MATSLISE 2.0: a Matlab toolbox for Sturm-Liouville computations

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Abstract

The MATSLISE 2.0 software package is a thorough revision of the successful Matlab package MATSLISE of 2005. The purpose of the package is to compute the eigenvalues and eigenfunctions of regular and singular Sturm-Liouville boundary value problems. The code uses some new or improved algorithms, offers some new features, and has an updated graphical user interface. We discuss the algorithms and illustrate that the code forms a powerful Matlab Sturm-Liouville solver for a very wide range of problems.

Key words: Sturm-Liouville Problems, Schrödinger equations, eigenvalues, shooting

1 Introduction

MATSLISE [1] is a graphical Matlab software package for the interactive numerical study of Sturm-Liouville problems (SLPs)

$$-(p(x)y'(x))' + q(x)y(x) = Ew(x)y(x) \quad x \in (a,b).$$
(1)

It allows the fast and accurate computation of the eigenvalues *E* and the visualization of the corresponding eigenfunctions *y* by making use of the power of high-order piecewise constant perturbation methods, also called the CP methods. Many researchers, in particular the ones from applied fields, prefer to use the user friendly problem solving environment MATSLISE over Fortran subroutines, like SLEDGE and SLEIGN₂, although these latter packages can deal with a larger range of singular problems.

The successor code MATSLISE 2.0 has now been developed to work for a broad class of singular problems. This is realized by including the recent extension of the CP algorithm from problems in Liouville normal form to the general Sturm-Liouville form (see [2]) and by using specially adapted algorithms in a narrow interval around the singularity. In addition, piecewise continuous coefficient functions are allowed and the calculation of the eigenfunctions has been improved in terms of numerical stability by rescaling the wave function variables in each CP step. A new feature is the option to evaluate these eigenfunctions in a set of user-specified points, which facilitates further manipulation.

The MATSLISE 2.0 package can be downloaded from http://sourceforge.net/projects/matslise/. The package contains a number of routines which the user can run from the Matlab command line or which can be invoked from user-written scripts or functions. Given the interest of researchers from various fields, a user-friendly graphical user interface is also provided. A broad set of test problems has been predefined.





Figure 1: Matslise 2.0 GUI

2 Some results

As an example of the use of MATSLISE 2.0, see Figure 1, we choose the Coffey-Evans equation. The triple well of the Coffey-Evans potential produces triplets of eigenvalues which can be made arbitrarely close by deepening the well. Here

$$-y'' + (-2\beta\cos 2x + \beta^2\sin^2 2x)y = Ey$$
 (2)

with $y(-\pi/2) = y(\pi/2) = 0$. The parameter β controls the depth of the well, we have used a value of $\beta = 30$, which may cause difficulties to SLP software.

In the presentation, also results for some singular problems will be shown. These results illustrate the large applicability range of MATSLISE 2.0 and the effectiveness and accuracy of the newly introduced algorithms for singular endpoints.

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Geometric Integrators in Population Balance Simulation

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Abstract

Geometric integration is the numerical integration of a differential equation, while preserving one or more of its "geometric" properties exactly (i.e. up to rounding errors). It is recognized that the preservation of geometric properties allows for a more accurate long-time integration than with general-purpose methods. We explain how to obtain a geometric integrator for the famous prey-predator Lotka-Volterra problem. We provide Matlab programs, user manual and some typical examples.

Key words: Conservative Lotka-Volterra system, Geometric Numerical Integrator, Hamiltonian system, integrator Matlab, prey-predator system.

Introduction In [1] it is shown that a conservative prey-predator Lotka-Volterra system is defined by the ordinary differential equation:

$$\dot{x}_i = x_i(r_i + \sum_{j=1}^n a_{ij}x_j), \qquad a_{ij} = -a_{ij}$$
 (1)

where i = 1, ..., n, and x_i represents the number of individuals of species *i*. The coefficients a_{ij} quantify the interaction between species. This system possesses at least an invariant, i.e., a conserved quantity along any solution of the differential equation. We observe however that invariants are rarely conserved by classical integrators (see for example figure 1a).

It is explained in [1] how they are related to Hamiltonian systems, an important part of geometric numerical theory. We explain this development and how to obtain a geometric integrator for (1) which has a satisfactory long-time behaviour. We study some examples of two-species models, before moving on to general population models for the interactions of n species. We focus on the invariants of these problems over long time.

Geometric integration Geometric numerical integration forms an important class of numerical integrators which have been well studied by many authors since the 1980s. One of the most important books about the subject is [2] by E. Hairer, C. Lubich and G. Wanner.

Geometric integrators are methods that exactly (i.e. up to rounding errors) conserve qualitative properties associated to the solutions of the system under study. A simple example of property is the total energy of a physical system which has to be conserved. As for Lotka-Volterra system, classical integrators are in general not able to preserve an invariant. Typically they show a linear drift as in figure 1(a).





Figure 1: (a): Error in the invariant of a two-dimensional Lotka-Volterra system: classical (ode45) and geometric integrator. (b): Maximum error in the invariant as a function of the CPU time for a three-dimensional food-chain system over an interval of length 200: classical integrators (ode45 and ode113) and several geometric solvers (The letter "G" refers to "Geometric" and the number that follows indicates the order of the corresponding method).

It turns out that the preservation of geometric properties (such as preservation of invariant, symplectic and Poisson structure, symmetries, time-reversal symmetry or phase-space volume) improves significantly the quality of the solution and allows for a more accurate long-time integration than with general-purpose methods.

Matlab implementation and numerical results We propose a Matlab implementation of several geometric integrators for Lotka-Volterra systems (1). With these solvers the conservation of the invariant is significantly improved as shown in Figure 1(a). We illustrate the use of our code with some typical examples of Lotka-Volterra systems. Figure 1b compare the relative performance between integrators of the Matlab ode suite and with our implementation for a three-dimensional food chain system.

The coding is close to the Matlab ODE suite (ode45, ode113, etc.) [3]. We discuss the implementation, e.g., step size adaptation, compensated summation in order to reduce the influence of round-off, solution of the nonlinear system for the implicit method.

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Random walks in Temporal Analysis of Products reactors

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Abstract

We present and discuss our C++/Python software package "tapwalk" for modelling by random walks the trajectories of individual gas molecules travelling under the Knudsen regime in a Temporal Analysis of Products reactor.

Key words: Temporal Analysis of Products, random walks, Knudsen diffusion

1 Introduction

Temporal Analysis of Products (TAP) is a catalyst investigation technique pioneered by [1] and based on a special research reactor, a cylindrical diffusion-only porous fixed-bed reactor consisting of longitudinal zones, typically three, packed either with inert quartz or with a porous active catalyst. This device is situated inside a high vacuum; a special valve is used to inject into one end of the reactor a tiny amount of gas molecules — tiny with respect to the number of active sites in the catalyst, so that the effect of a single pulse is insignificant — and the exit flux is monitored at the other end, which is kept open to the vacuum chamber, using a mass spectrometer. The temporal distribution of outlet gas fluxes of both reactants and products contains detailed information on the reactions occurring inside the catalyst, on the order in which the products are obtained, etc. In this basic configuration all has been designed to let the reactor be modelled very accurately as a one-dimensional diffusion-reaction system, see [2] for the general spatially one-dimensional theory of TAP reactors in the Laplace domain.

In recent years, researchers have also run TAP experiments in which the active zone is not purely as cylindrical slice, but is concentrated in a small particle, typically of spherical shape. If the particle is centred on de reactor's axis, the modelling can still be reduced to two dimensions (longitudinal and radial) but the formal elegance of the 1D theory is lost.

In order to study quantitatively the effects of running TAP experiments with a single particle, or maybe with several single particles at fixed positions inside the reactor, we have developed the present random walk simulation software.

2 Software design

Computational speed is of the essence in random walk simulation, so we have opted to implement the actual simulation software in C++, including the statistical analysis of the trajectories, and to make these accessible from dedicated Python objects that encapsulate the



C++ counterparts. With some extra wrapping code, the resulting Python script files are quite intuitive, e.g.,

```
import reactor
a = reactor.reactor(R=2.5e-3, L=25.4e-3, dx=0.005e-3, D=10e-3, seed=10000)
reactor.addball(a, x=0, y=0, z=12.7e-3 - 0.300e-3, r=0.250e-3, k=1e16)
reactor.addball(a, x=0, y=0, z=12.7e-3 + 0.300e-3, r=0.250e-3, k=1e16)
reactor.onebyone(a, 100000)
```

which creates the software representation of a TAP reactor 2.5 mm in radius and 25.4 mm in length, where the random walk steps will be of 0.005mm each, with diffusivity 0.01 m² / s, and with random number generator (which is gsl_rng_ranlxs2 from the Gnu Scientific Library) seed value 1000 for reproducibility. Then two particles (ball-shaped) are defined, both on the longitudinal axis (x = y = 0 mm), of radius 0.25 mm and with essentially infinite reaction rate constant $k = 10^{16}$ s⁻¹. The last line calls for 100000 random walks to be calculated, and for each to output the time (in s) at which the simulated gas molecule either exits the reactor (coded by L-1) or reacts with the first (coded D0) or the second (D1) particle. The initial output is then



and so on for 100000 lines; the corresponding cumulative exit and reaction probability distributions are plotted versus time in s alongside. The statistical descriptors (moments and cumulants) of the distributions are calculated by the C++ layer internally.

Acknowledgements

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Nonlinear Model Reduction of a Continuous Fluidized Bed Crystallizer

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Abstract

Proper Orthogonal Decomposition is applied to a nonlinear dynamic population balance model of a novel crystallization process. A strong reduction of the system order is achieved while the reduced model is in good agreement with the reference model. The reduction method is promising for a large class of chemical engineering processes.

Key words: crystallization, empirical interpolation, model reduction, proper orthogonal decomposition, population balance equations

Process and Reference Model

The separation of enantiomers (molecules that are mirror images of each other) is a challenging problem with high relevance especially in pharmaceutical industry. Recently, a new continuous process for enantiomer separation has been proposed [1], whose key element is a fluidized bed crystallizer as shown schematically in Figure 1. Supersaturated liquid solution flows through the crystallizer from bottom to top and causes seeding crystals to grow. Small crystals move with the liquid flow to the top, larger crystals sink to the bottom. They are broken into small fractions by a ultrasonic (US) attenuator and recycled back into the crystallizer. An outlet at the side of the crystallizer enables product removal.

The successful operation of this quite complex process requires the adjustment of various geometrical and operation parameters, like shape of the crystallizer tube, location of the product outlet, or liquid flow rates. A first model of the fluidized bed crystallizer was presented in [2]. It describes the number density function *n* of the particle phase by a population balance equation with the following structure:



Figure 1: Scheme of fluidized bed crystallizer

$$A(x)\frac{\partial n}{\partial t} = -A(x)G\frac{\partial n}{\partial L} - \frac{\partial}{\partial x}\left\{A(x)\upsilon(x,L,t)n(x,L,t) - DA(x)\frac{\partial n}{\partial x}\right\}$$
(1)



In (1), *t* is the time coordinate, *x* is an external (geometrical) coordinate in flow direction, *L* is an internal (property) coordinate, A(x) is the cross-sectional area, *G* is the growth rate of the crystals, *D* is a dispersion coefficient, and v(x,L,t) is the crystals' flow velocity that depends nonlinearly on the number density function *n*. The reference model is solved numerically using a finite volume method, resulting in a system of ordinary differential equations of the type

$$\frac{d\mathbf{n}}{dt} = \mathbf{M}\,\mathbf{n} + \mathbf{g}(\mathbf{n}) \tag{2}$$

The number of equations of the discretized system is in the order of 10^4 . This is quite inconvenient for process design and process control tasks and motivates the development of a reduced low order model.

Nonlinear Model Reduction

A reduced model is obtained by Proper Orthogonal Decomposition (POD). First a matrix of snapshots $\mathbf{N} = [\mathbf{n}(t_1), \mathbf{n}(t_2), \ldots]$ is generated from numerical solutions of the reference model (2). From a singular value decomposition of N, a reduced basis Ψ is constructed, and the state vector **n** is approximated by $\mathbf{n} \approx \Psi \varphi$, φ being the low order state vector of the reduced model. Galerkin projection gives the equations of the reduced order model as

$$\frac{d\boldsymbol{\varphi}}{dt} = \boldsymbol{\Psi}^T \mathbf{M} \boldsymbol{\Psi} \, \boldsymbol{\varphi} + \boldsymbol{\Psi}^T \mathbf{g} \left(\boldsymbol{\Psi} \, \boldsymbol{\varphi} \right) \tag{3}$$

Empirical interpolation [3] is applied to treat the nonlinear term in an efficient way, i.e. the nonlinearity is approximated by $\mathbf{g} \approx \Psi^g \boldsymbol{\varphi}^g$ with a basis Ψ^g and an additional set of algebraic linear equations to determine the coefficients $\boldsymbol{\varphi}^g$.

It is found that 50 basis functions, i.e. 50 ordinary differential equations, are sufficient for a satisfactory approximation of the reference model, which consists of 24000 equations after discretization.

The advantage of this reduction process compared to other approaches may be its applicability to a large class of systems in chemical engineering.

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Recent advances in kinetic Monte Carlo techniques for an improved understanding of polymerization processes

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Abstract

Two new kinetic Monte Carlo procedures to simulate polymerization processes in high detail are discussed. The first procedure starts from the premise that all necessary information on polymerization kinetics and polymer microstructure can be contained in a multivariate distribution with a finite number of variates, in which the stochastic variates are chosen *a priori*. The second procedure records every reaction event a growing polymer molecule undergoes, allowing the *a posteriori* calculation of the marginal distribution with respect to any desired variate (chain length, chemical composition, number of branches, monomer sequence, *etc.*)

Key words: chemical kinetics, mass transport, modeling, Monte Carlo, polymerization

1 Introduction

Polymerizations are an important class of chemical reactions for the industrial production of materials used in daily life and for high-tech applications. The application range is determined by chemical, rheological, mechanical and physical properties, which are influenced by the polymer microstructure. Microstructural characteristics include the chain length of the polymer molecule, its chemical composition, short chain branch number, *etc.* The stochastic nature of chemical reactions implies that polymer molecules are, hence, distributed with respect to these variables, *i.e.* a multivariate mathematical treatment is necessary. Such treatment requires the development of advanced stochastic numerical techniques to facilitate the tailored design of the polymer microstructure, including the effect of the polymerization technique, the monomer types, the reactor configuration and the operating conditions. In this contribution, two recently developed kinetic Monte Carlo (kMC) procedures are presented.

2 Composite binary trees based kinetic Monte Carlo procedure

The advent of computer cluster architectures, recent advances in compiler technology and improved algorithms have decreased the kMC computational time to simulate

polymerization processes by orders of magnitude, closing in on simulation times offered by commercial deterministic methods. In particular for the univariate chain length distribution (CLD) calculation in homopolymerization, Chaffey-Millar et al. [1] extended Gillespie's algorithm [2] with binary trees to accelerate the retrieval of chain lengths of reacting macromolecules. For polymerizations with branch formation or involving more than one monomer type, a fast kMC calculation method [3] has been recently reported by our research group, allowing a binary tree based calculation of the bivariate chemical composition—CLD (CC-CLD), in which the stochastic variables are chain length and branch/comonomer content. Hence, chains are contained in composite binary trees in which each leaf node of the main tree, which differentiates chains with respect to their length, serves as the root node of a sub-tree, which differentiates chains with respect to their length are composition/branching amount and, hence, contains conditional information, *i.e.* valid for the selected chain length in the main tree. For low maximum chain lengths of 10³, the improvement already results in a reduction of the kMC operations by a factor between 10³ and 10⁶.

3 Reaction event recording based kinetic Monte Carlo procedure

For the synthesis of well—tailored polymers, it does not suffice to only calculate the CLD or CC—CLD but the monomer sequence of individual macrospecies is also required, as recently highlighted by our research group [4]. In this work, a complete reaction event history is calculated allowing extraction of the desired information. This not only paves the way to define stochastic variables representing the molecular quality of polymer molecules, but also to the synthesis of polymer molecules with predefined monomer sequence. One example of a well-chosen stochastic variable is the recently introduced gradient deviation GD [4], reflecting deviations from desired gradient-like monomer sequences product specifications.

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Isogeometric analysis in contact mechanics and its industrial applications

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Abstract

The simulation of contact mechanics plays an important role in mechanical engineering and is necessary to ensure a cost- and time-efficient product development. Large sliding contacts involving curved surfaces appear for instance in gears, roller bearings, valves and pumps, but simulating these systems is a challenging task from a numerical point of view. In contrast to classical finite element methods, discretizing a structure with Isogeometric Analysis (IGA) results in a smooth surface representation and higher inter-element continuity. These are promising characteristics of IGA which could help to improve efficiency and robustness of contact mechanics simulations in the future. We will present an implementation of a 3D-contact algorithm based on IGA and give an overview of possible industrial applications.

Key words: contact mechanics, NURBS, isogeometric analysis

1 Introduction

Isogeometric analysis, presented by Hughes in 2005, promises to close the gap between computer aided design (CAD) and finite element analysis by using basis functions, such as B-Splines, NURBS, T-Splines or subdivision surfaces which describe the geometry exactly instead of C^0 -continuous Lagrange interpolatory polynomials to describe finite elements which approximate the initial geometry for analysis.

Isogeometric analysis has been an efficient approach for problems of fluid-solid interactions, extended finite element methods and electromagnetics [3]. We aim to apply isogeometric analysis to contact problems. In the original work which introduced isogeometric analysis, Hughes suggests that smooth, compactly-supported basis functions might improve the modelling of contact problems [1]. Some work in this direction has been done already. Temizer et al. [3] give an overview of this work and suggest a three-dimensional mortar-based frictional contact treatment in isogeometric analysis. The pieces of work done so far show the superiority of the NURBS discretization in terms of quality and robustness of the results when applied to contact computation.



2 FEM and IGA for contact problems

Results of contact computation are dependent on the contact discretization and on how contact is taken into account. There are several mathmatical methods for this purpose. Due to its simple implementation we will make use of the penalty method. This method adds a penalty term to the potential energy of the system, if contact occures. This term is defined using a penetration function. For normal contact the penetration function is

$$g_N = \begin{cases} (\mathbf{x}_2 - \overline{\mathbf{x}}_1) \cdot \overline{\mathbf{n}}_1 & \text{if } (\mathbf{x}_2 - \mathbf{x}_1) \cdot \overline{\mathbf{n}}_1 < 0\\ 0 & \text{otherwise} \end{cases},$$
(1)

where the master point $\overline{\mathbf{x}}_1$ is the orthogonal projection of the given slave point \mathbf{x}_2 and $\overline{\mathbf{n}}_1$ is the master-surface normal. In classical finite element contact computations described in [2] the normal vector \mathbf{n} is generally not continuous across element boundaries. This is due to the interpolation of the structural boundary as well as non-smooth ansatz functions and leads to incorrect results and convergence problems [3].



Figure 1: FE- (left) and NURBS-discretization (right) of a deformed quarter ring

However, using NURBS and IGA allows a continuous representation of **n** across the contact surface in all computation steps. In Figure 1 the situation is depicted. A deformed quarter ring is shown, the FEM discretization results in non-smooth normal vectors across the structural boundary.

3 Implementation and industrial applications

We will present a 3D frictionless contact formulation based on NURBS dicretization. Special attention is given to the evaluation of the penetration function. To emphasize the practical relevance of this research, some industrial applications will be shown.

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Isogeometric analysis using B-splines on triangulations

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Abstract

We discuss Powell-Sabin splines and their rational extension, the so-called NURPS surfaces, in the context of isogeometric analysis. NURPS are an interesting alternative for classical tensor-product NURBS, because they allow local refinement, while retaining a B-spline like representation and an exact description of conic sections.

Key words: Isogeometric analysis, local refinement, Powell-Sabin B-splines, NURPS

1 Introduction

Isogeometric Analysis (IgA) is a paradigm for numerical simulation which combines Finite Element Analysis (FEA) with Computer Aided Design (CAD) methods [1]. The CAD representations are used both to describe the geometry and to approximate the unknown solutions of differential equations. Tensor-product B-splines and Non-Uniform Rational B-Splines (NURBS) are common tools in CAD, and so they are in IgA.

Adaptive local refinement is an important ingredient for obtaining, in an efficient way, an accurate solution of differential problems. Unfortunately, the tensor-product structure of B-spline/NURBS spaces precludes a strictly localized refinement. This motivates the interest in alternative structures for IgA that permit local refinement. Here, we consider B-splines on triangulations, and in particular we focus on Powell-Sabin B-splines [7, 6].

2 Splines on triangulations: PS splines

Powell-Sabin (PS) splines are C^1 quadratic splines defined on a given triangulation with a particular macro-structure. Although often expressed in terms of a Hermite basis, they can be represented with basis functions possessing properties similar to the classical (tensor-product) B-splines [2]. These PS B-splines form a convex partition of unity, and the coefficients of this representation have a clear geometric meaning. A rational extension of PS splines, referred to as NURPS (Non-Uniform Rational PS) surfaces, can also be easily defined [5, 6]. NURPS surfaces allow an exact representation of quadrics, and their shape can be locally controlled by control points and weights in a geometrically intuitive way. Higher order B-splines can be defined as well on triangulations with this PS macro-structure [4].

Thanks to their structure based on triangulations, PS splines and their rational extension offer the flexibility of classical Finite Element Methods (FEM) with respect to local refinement. Moreover, they share with standard NURBS the increased smoothness, the B-spline like





Figure 1: NURPS solution for the Hemker problem on a locally refined triangulation.

basis, and the ability to exactly represent profiles of interest in engineering applications as conic sections. Therefore, they constitute a natural bridge between classical FEM and NURBS-based IgA.

We will discuss NURPS as reference functions for IgA, focussing both on their ability to represent conic sections and to their flexibility to perform local refinement. Fig. 1 illustrates the solution of the Hemker problem [3], discretized by the NURPS-based IgA approach. Further details on this example can be found in [7]. The ability of refining locally and the smoothness of the discretization space allow a very sharp detection of internal and boundary layers.

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Geometrically enhanced isogeometric segmentation of boundary-represented solids

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Abstract

The isogeometric segmentation problem is to decompose a boundary represented solid into a small number of topological hexahedra. We survey previous progress on the segmentation of contractible solids with convex and non-convex edges. We present ongoing work addressing challenging geometric problems which arise in this context: constructing a cutting loop, segmenting a face into two, constructing a cutting surface and producing special cutting surfaces as extensions of existing faces.

Key words: isogeometric analysis, isogeometric discretization, spline interpolation

Introduction We report our ongoing research, initiated in [1, 2], on the problem of segmenting a boundary-represented solid into a small number of topological hexahedra suitable for isogeometric analysis. We consider a boundary-represented contractible solid with a 3-vertex-connected edge graph. After a summary of the state of the art, we focus on recent research that addresses challenging geometric problems arising in this context.

State of the art The work in [2] sheds light on complications associated with *non-convex edges*. An edge **e** is non-convex if the two surfaces incident to **e** meet at a concave interior angle somewhere along **e**. In order for the resulting hexahedra to admit non-singular parameterizations, all non-convex edges need to be removed as part of the segmentation process.

One step of our procedure segments the solid into two solids with e.g. less non-convex edges or less vertices. Repeating the procedure results in base solids, e.g. topological tetrahedra, which can be decomposed in predefined ways into topological hexahedra. For solids with convex edges, the algorithm of [1] searches for a *cutting loop* consisting of existing or auxiliary edges, then interpolates the loop with a *cutting surface*. In [2] a novel version of the algorithm is developed for solids with non-convex edges. They are more difficult to deal with as the existence of a cutting surface requires geometric criteria to hold at the vertices.

Geometric challenges and recent progress We report our recent progress on three of the interesting challenges which arise in isogeometric segmentation. The first arises when we improve the method of [2] by allowing a more general type of cutting loop. The other two challenges appear when realizing cutting surfaces with splines (an important step which is not addressed in [1, 2]).



Figure 1: Complications arise when splitting a solid by extending a face.

(c)

(b)

(a)

Figure 2: Splitting a domain into two: finding a guiding curve and fitting it with a spline curve.

- Segmentation based on extension of an existing surface. In certain situations it is possible to segment a solid by extending a face. Fig. 1 shows some possible scenarios. Solid (a) was segmented into 31 topological hexahedra in [2] but can be segmented into just 4 by joining the two marked faces up as a first step. Extending the marked face in Solid (b) creates a solid that is not simply connected. Solid (c), which has an artificial edge, can be segmented into two hexahedra but it requires extending three faces and merging two of them.
- **Subdivision of a face based on an interior curve.** The creation of an edge splitting a face of a solid can be done by subdividing the parameter domain. We construct a *guiding curve* that splits the domain into two, then fit a spline to the guiding curve (see Figure 1). There are a variety of ways to construct the guiding curve, including pathfinding algorithms.
- **Construction of a cutting surface from a cutting loop.** Given a cutting loop, we construct a trimmed surface which can be used for the new faces of the two solids resulting from the segmentation. We choose a unit normal at each corner based on the tangent vectors of the incident edges. Then we interpolate the normals in a valid way along the edges, construct a domain and fit a surface using a least squares approach (see Figure 3).



Figure 3: (a) a cutting loop with normals defined at each corner; (b) interpolating the normals along the edges; (c) domain for the trimmed surface; (d) surface found by least squares fitting.

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Damage tolerance assessment directly from CAD: (extended) isogeometric boundary element methods (XIGABEM)

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Abstract

We develop in this work a procedure for obtaining the fatigue life of complex structures directly from Computer-Aided Design (CAD) data, without any mesh generation or regeneration as the cracks evolve. The method relies on a standard isogeometric boundary element method (BEM) where the same basis functions are used to both describe the geometry of the component and approximate the displacement and traction fields.

To capture the stress singularity around the crack tip in the framework of linear elastic fracture mechanics, two methods are proposed: (1) a graded knot insertion near crack tip; (2) partition of unity enrichment.

A well-established CAD algorithm [1] is adopted to generate a smooth crack surface as the crack grows. The M integral and J_k integral methods for the extraction of stress intensity factors are compared in terms of accuracy and efficiency. The numerical results are compared against closed-form solutions as well as other numerical methods, namely the collocation BEM with a Lagrangian basis, a symmetric Galerkin BEM and extended finite element methods. The crack growth paths and fatigue lives obtained by the proposed method are validated using experimental data.

Key words: Isogeometric analysis, partition of unity enrichment, linear elastic fracture, boundary element method, fatigue crack growth

The isogeometric analysis (IGA) based on finite element methods was proposed by [2]. The idea of IGA is to use the same shape functions to describe the known CAD geometry and the unknown field variables. However, CAD systems typically only provide the boundary of the domain [1] and do not provide any description of its interior. Hence, in its original form, as proposed in [2], IGA still requires an additional parametrization of the domain's interior, which has been the subject of much effort since the first inception of the method.

To resolve this issue, the isogeometric collocation BEM was developed and exercised in elastostatics by Simpson et al [3] to perform stress analysis directly from CAD and without

any meshing [4]. Implementation aspects of the method were provided in [5] and the method was extended to three-dimensional stress analysis of complex structures in [6].

In this work, we advance the concept we proposed in [3] to predict the fatigue life of engineering structures using a simple Paris law. In conventional fatigue simulations as performed industrially [7] using the finite element based methods, the key difficulty is the accurate computation of the crack driving force, namely the stress intensity factors (SIFs). The second difficulty is that the domain mesh used for stress analysis and hence for the detection of "sensitive" regions in the component, where initial flaws are introduced, is typically at least one order of magnitude too coarse to provide quality SIFs. The third difficulty lies in the geometrical complexity of the domain which, if the predicted fatigue life is deemed inadequate must be redesigned. For each new design, and for each crack configuration, a new mesh typically needs to be generated, not only to conform to the new chosen geometry, but also to properly resolve stresses in the vicinity of the crack tip. Even when enriched finite element methods are used, some level of remeshing is required [7].

Collocation BEM is an strong contender to attack fracture mechanics problems, because it requires only boundary discretization, simplifies the insertion of new crack segments during growth and offers superior accuracy for the computation of the SIFs for the same number of degrees of freedom compared to other methods. Since BEM requires only boundary discretization, it is also an ideal partner for IGA. We show that isogeometric dual BEM with or without partition of unity enrichment is a robust and accurate method to deal with for fracture simulations and that such simulations require no meshing nor remeshing in the conventional sense.

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High Order Isogeometric Simulation of Lorentz Detuning in Superconducting Accelerator Cavities

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Abstract

In this work we simulate the Lorentz detuning of an accelerating cavity, which is the change of the resonant frequency due to the mechanical deformation of the cavity wall induced by the electromagnetic pressure. The coupled electromagnetic-mechanical problem has been solved using Isogeometric Analysis, leading to an efficient full 3D simulation and to solutions which are substantially more accurate than standard finite element techniques.

Key words: Isogeometric Simulation, Lorentz detuning, Particle accelerators, Superconducting Devices

1 Introduction

The radiation pressure generated by the electromagnetic field in superconducting cavities causes a non-negligible deformation of the cavity walls. Lorentz detuning effect is the frequency shift of the accelerating eigenmode associated with this deformation of the geometry [1]. The coupled electromagnetic-mechanical problem to be solved is the following:

$$\nabla \times \left(\frac{1}{\mu_0} \nabla \times \mathbf{E}\right) = \omega^2 \epsilon_0 \mathbf{E} \quad \text{and} \quad \nabla \cdot \left(2\eta \nabla^{(S)} \mathbf{u} + \lambda \mathbf{I} \nabla \cdot \mathbf{u}\right) + f = 0.$$
(1)

The domain of the left equation of (1) is vacuum within the cavity, while the right equation is solved in the wall region. μ_0 and ϵ_0 are the permeability and permittivity of vacuum, ω is the angular eigenfrequency, **E** is the electric and $\mathbf{H} = \nabla \times \mathbf{E}/(i\omega\mu_0)$ the magnetic field, η and λ are the Lamé constants of niobium, **u** is the displacement of the wall and f is the force density. The coupling between the electromagnetic problem and the mechanical one takes the form of the radiation pressure on the common interface: $p = -1/2\epsilon_0 E_n E_n^* + 1/2\mu_0 \mathbf{H}_t \mathbf{H}_t^*$. Despite the relevance of the frequency shift, the displacements of the walls are very small with respect to the typical cavity dimensions. Therefore, it is necessary to represent the geometry and its deformation with the greatest accuracy. We propose to exploit the interesting features of Isogeometric Analysis (IGA) [3] to solve the coupled problem (1).





Figure 1: TESLA cavity [6]: undeformed geometry (green); deformed geometry (brown, amplified by a factor 400000); the solution has been replicated along the *z* axis to show an ideal 3-cell cavity. On the right: deformed accelerating cavity mode.

Table 1: Frequency shift values.

No. of subdivisions	shift
2 (7356 DoFs)	9.603630 Hz
3 (18768 DoFs)	9.232927 Hz
4 (38260 DoFs)	9.023365 Hz
5 (67922 DoFs)	8.951231 Hz

Isogeometric Analysis was introduced in [2] less than a decade ago with the aim of *bridging the gap between Computer Aided Design (CAD) and Finite Element Method (FEM)*. One can build the approximation spaces for the discrete solutions using the same basis functions (primarily B-Splines and NURBS) that describe the CAD geometry, leading to the so-called *isoparametric* approach. For the discretization of the mechanical problem (1) the isoparametric concept has been applied since with this choice, the new geometry is simply obtained by adding the solution vector to the control net of the original NURBS domain. On the other hand, for electromagnetic problems, it has proved more useful to use basis functions that have the advantage of generating a De Rham graph. In particular, the discretization of Maxwell's eigenproblem (1) is obtained using the scheme introduced in [4].

2 Results and conclusions

The simulation of the complete problem has been done using the free software GeoPDEs [5]. The values of the eigenfrequencies of the first accelerating modes of the TESLA cavity [6] obtained with the 3D IGA simulation were compared to the ones computed by a 2D lowest order FE simulation [1]. The results show that we were able to obtain a higher order of accuracy per-degree-of-freedom with respect to classical FEM (even when comparing 3D IGA with 2D FEM). The relevant accelerating mode is the first eigenmode and corresponds to a frequency value of approximately 1.3 GHz. In Fig. 1 the comparison between the starting geometry of the walls and the deformed one is shown along with the frequency shift values in Table 1. In conclusion, it has been shown that IGA is more than capable of competing with FEM for cavity simulation. We were, in fact, able to accurately represent both the reference geometry and its deformation, and to obtain smooth and accurate solutions. The calculated frequency shifts results are in very good agreement with results reported in literature.

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IGATOOLS: a new dimension-independent Isogeometric C++11 library

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Abstract

We present a novel mathematically faithful object oriented design for a general purpose isogeometric library and introduce a high quality C++11 open source implementation of it, igatools(www.igatools.org).

Key words: isogeometric analysis, software library, object oriented, dimension independent, CAD integration

MSC 2010: 65N30, 97N80, 97N40, 68N19, 65D07

Inspired by the desire to unify the fields of computer aided geometrical design (CAGD) and the finite element method (FEM), the visionary work [1] introduced a technique for the discretization of partial differential equations dubbed *isogeometric analysis* (IGA).

The mainly advertised feature of IGA has been the ability to describe exactly CAGD type geometries. This is so because the method proposes to use the same type of spaces to represent the geometry and the shape functions (mostly non uniform rational B-splines). In addition, the use of B-spline functions allows global smoothness beyond the classical C^0 continuity of standard finite elements: this permits the design of novel numerical schemes that would be extremely difficult to obtain with standard finite elements. Isogeometric methods have been summarized in a recent book [2] and intensively studied in the last years. They have been successfully used in applications such as fluid, structural mechanics, electromagnetism.

The similarity between IGA and FEM permits to enhance an existing finite elements solvers with isogeometric capability quite easily and without breaking the classical finite element assembling strategy: loop over the elements \rightarrow computation of the local (element-based) operators \rightarrow assembling of the global operators from the local one.



After a decade of research in the area, with many successes, some issues (that require further research) and many promising ideas, it is time –at least in the research community–to have an open source modernly designed isogeometric software library.

We present a novel mathematically faithful object oriented design for a general purpose isogeometric [2] library and introduce a high quality C++11 open source implementation of it, igatools (www.igatools.org).

igatools uses advanced programming techniques and supports dimension independent programming [4], and includes support for manifolds and isogeometric elements of the H-div and H-curl type [3].

All classes are designed in such a way that the space dimension, co-dimension and the tensorial range are selected as template parameters. The use of templates is very convenient for scientific computing, they allow to have a single code that is resolved at compile time generating optimized code as it was written for each instance of the dimension and with no run-time checks and without using virtual functions that would affect performance. This approach allows us to write an application code that is independent of dimension and range (provided that the mathematical problem can so be formulated). For example, let's say that a user writes the code for a 2D problem that can be mathematically formulated in any dimension (e.g. Poisson's equation). If this code is written with some minimal care, then the same code will run for the problem with the physical domain being 1D, 3D or a 2D manifold embedded in \mathbb{R}^4 and for the solution being scalar-, vector- or tensor-valued.

Moreover, the modularity of igatools let the user to easily integrate the built-in capabilities with external libraries (e.g. CAD routines) if needed, and its generality allows to use igatools in order to implement IGA methods into existing FEM codes.

We present the general design and some applications in order to show the potential and the flexibility of the library. In particular it is shown an application in which igatools is used in combination with an existing library for the finite element analysis of non-linear elastic solid deformations. A comparison between the proposed implementation and the plain finite element code is proposed on some test problems, revealing the superiority of the isogeometric approach.

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Identification of the Poincaré-Steklov Operator in Hybrid FE-BIE Formulations for the Analysis of Internal Resonances

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Abstract

The interest in combining the Finite Element (FE) method with the Boundary Integral Equation (BIE) method led to various hybrid FE-BIE formulations in literature. However, some formulations suffer from breakdown frequencies at which the solution is not uniquely defined, introducing errors due to internal resonances. The occurrence of these errors is investigated by identifying the Poincaré-Steklov operator, which relates the tangential electric field to the equivalent electric current on the boundary of a domain, in both the FE and BIE method. This identification provides new insight in internal resonances for both conformal and non-conformal formulations.

Key words: hybrid FE-BIE, internal resonances, Poincaré-Steklov operator

1 Introduction

The exact formulation for combining the Finite Element (FE) method with the Boundary Integral Equation (BIE) method appears to be very important in order to avoid so-called spurious solutions. Previous contributions demonstrated that formulations applying the Electric Field Integral Equation (EFIE) or the Magnetic Field Integral Equation (MFIE) as BIE method in combination with an FE method contain certain *forbidden frequencies* if the background medium is lossless [1]. At these frequencies, the EFIE and MFIE are not uniquely defined and the sourceless hybrid system contains non-trivial solutions that introduce errors to the result.

Here, these spurious solutions are investigated on an operator level thanks to the concept of the Poincaré-Steklov (PS) operator, which describes the relationship between the tangential electric field and the equivalent electric current on the boundary of a domain. In this way, different properties regarding internal resonances are easily derived for both conformal and non-conformal hybrid FE-BIE formulations [2].



2 Identifying the Poincaré-Steklov operator

In the FE domains, all interior unknowns are eliminated by reducing the system matrix to its Schur complement. This already provides a relationship between the tangential electric field and the equivalent electric current on the boundary of the FE domain: $SE^t = jk_0\eta_0 J$. Here, E^t and J are the tangential electric field and the equivalent electric current, respectively, S is the Schur complement, j is the imaginary unit, k_0 is the free space wave number and η_0 is the free space impedance. Hence, the PS operator is easily obtained by scaling this Schur complement with $jk_0\eta_0$.

In the BIE method, the PS operator is obtained from the Calderón projector. This reveals several interesting properties of the PS operator, such as its relation with the BIE integral operators \mathcal{T} and \mathcal{K} [2].

3 Internal resonances

The internal resonance problem originates from the non-uniqueness of the EFIE and the MFIE at certain frequencies. However, the spurious solutions of the sourceless EFIE and MFIE are different from each other. Hence no internal resonances occur when both the EFIE and the MFIE are satisfied. Therefore, the occurrence of internal resonances is investigated by verifying if a hybrid formulation satisfies both the FE wave equation, the EFIE and the MFIE at all frequencies. This verification can be done for both conformal hybrid formulations, where adjacent domains share the same discretisation, and non-conformal hybrid formulations, where all domains are allowed to have independent discretisations.

Thanks to the obtained properties of the PS operator, the breakdown frequencies of several hybrid formulations can be predicted for simple configurations. It can also be demonstrated that only induced resonance currents (or fields) radiate.

4 Conclusion

By identifying the PS operator in both the FE wave equation, the EFIE and the MFIE, it becomes possible to investigate the stability of several hybrid FE-BIE formulations on an operator level. Moreover, the internal resonances can be predicted for simple configurations.

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Local Multiple Traces Formulation for Scattering Problems: Extension to Spectral Elements

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Abstract

We discuss the so-called *Local Multiple Traces Formulation* recently introduced by Hiptmair & Jerez-Hanckes [2] for solving Helmholtz and Maxwell transmission problems for heterogeneous scatterers. Using integral boundary operators and local Dirichlet and Neumann traces per subdomain, the resulting Fredholm first-kind formulation is free from spurious resonances, easy to construct with standard schemes and though illconditioned, it is amenable to preconditioning via diagonal or Calderón-type techniques. We present new results for higher frequencies via conforming spectral discretizations.

Key words: Boundary integral equations; domain decomposition; Calderón preconditioning

1 Introduction

Consider the simplest setting for the Helmholtz case¹. Let $\Omega := \overline{\Omega}_1 \cup \overline{\Omega}_2$ be a heterogenous scatterer, composed of two bounded subdomains Ω_1, Ω_2 and set $\Omega_0 := \mathbb{R}^d \setminus \overline{\Omega}$ with interfaces $\Gamma_{ij} := \partial \Omega_i \cap \partial \Omega_j$. Helmholtz operators with constant wavenumbers $\kappa_i \in \mathbb{C} \setminus \mathbb{R}_-$ are to be satisfied in each subdomain Ω_i . With this, the local MTF hinges on the following ideas:

- 1. Every pair of Dirichlet/Neumann traces defined on subdomains Ω_i denoted by $\lambda^i := (\lambda_D^i, \lambda_N^i)$ are unknowns;
- 2. Transmission conditions across each interface Γ_{ij} are enforced weakly via local restriction and normal orientation operators;
- 3. Use integral representations in each subdomain to set up Calderón identities over boundaries $\partial \Omega_i$, such that

$$\boldsymbol{\lambda}^{i} = \left(\frac{1}{2}\operatorname{Id} + A_{i}\right)\boldsymbol{\lambda}^{i} = \left(\begin{array}{cc}\frac{1}{2}\operatorname{Id} - K_{i} & V_{i}\\W_{i} & \frac{1}{2}\operatorname{Id} + K_{i}'\right)\begin{pmatrix}\lambda_{D}^{i}\\\lambda_{N}^{i}\end{pmatrix}$$

where A_i contains the standard weakly singular, double layer, adjoint double layer and hypersingular integral operators, denoted V_i, K_i, K'_i and W_i , respectively, over $\partial \Omega_i$ for a wavenumber κ_i .

¹The general case can be found in [1, 2]





Figure 1: Dirichlet trace approximation for different harmonics used.

After defining *restriction-orientation-and-extension operators* \widetilde{X}_{ij} , which are no more than signed duality products, the local MTF system becomes

$$\left\langle \begin{pmatrix} \mathsf{A}_0 & -\frac{1}{2}\widetilde{\mathsf{X}}_{01} & -\frac{1}{2}\widetilde{\mathsf{X}}_{02} \\ -\frac{1}{2}\widetilde{\mathsf{X}}_{10} & \mathsf{A}_1 & -\frac{1}{2}\widetilde{\mathsf{X}}_{12} \\ -\frac{1}{2}\widetilde{\mathsf{X}}_{20} & -\frac{1}{2}\widetilde{\mathsf{X}}_{21} & \mathsf{A}_2 \end{pmatrix} \begin{pmatrix} \boldsymbol{\lambda}_0 \\ \boldsymbol{\lambda}_1 \\ \boldsymbol{\lambda}_2 \end{pmatrix}, \begin{pmatrix} \boldsymbol{\varphi}^0 \\ \boldsymbol{\varphi}^1 \\ \boldsymbol{\varphi}^2 \end{pmatrix} \right\rangle = \left\langle \begin{pmatrix} \mathbf{g}^0 \\ \mathbf{g}^1 \\ \mathbf{g}^2 \end{pmatrix}, \begin{pmatrix} \boldsymbol{\varphi}^0 \\ \boldsymbol{\varphi}^1 \\ \boldsymbol{\varphi}^2 \end{pmatrix} \right\rangle$$

which is ready for parallelization and whose variational form requires local test functions such that their restrictions to interfaces Γ_{ij} lie in $\tilde{H}^{1/2}(\Gamma_{ij}) \times \tilde{H}^{-1/2}(\Gamma_{ij})$.

Theorem ([2]) The local MTF system is uniquely solvable for all g in $H^{1/2}(\partial \Omega_i) \times H^{-1/2}(\partial \Omega_i)$.

2 Spectral approximation and Results

We prove the amenability of the MTF for spectral elements in 2D under the simple case of a circle divided in two halves. Particular choices over canonical parametrizations of the curves –circle for the subdomain boundary, segment [-1,1] for the interfaces– are

- Trial spaces: Fourier polynomials for both Dirichlet and Neumann unknowns;
- Test spaces per interface: weighted Tchebyshev polynomials of the first and second kind, i.e. wU_l for $\widetilde{H}^{1/2}(\Gamma_{ij})$ and $w^{-1}T_l$ for $\widetilde{H}^{-1/2}, (\Gamma_{ij})$, with $w = \sqrt{1 x^2}$.

The structure of test bases depends on the number of interfaces and number of harmonics. Computational results for this case show accurate convergence to Mie series (Figure 1).

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On the Application of the Calderon Relations for the Regularization of the Electromagnetic Surface Integral Equations

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Abstract

We propose a dual basis formalism based on the Poisson-Neumann functions for general polygonal surface cells. The basis functions possess the dual H(curl) and H(div) space properties needed for a stable discretization of the tangential fields and surface currents. The Calderon identities are reformulated in terms of an impedance and an admittance surface integral operator. The dual basis is applied to obtain a discrete representation of the Calderon identities. We discuss the accuracy of the Calderon relations and evaluate their spectral properties to regularize the ill-conditioned electric field integral operator.

Key words: Calderon identities, dual basis, Poisson-Neumann, regularization, integral equations

1 Introduction

The electric (EFIE) and magnetic (MFIE) surface integral equations are widely used for the solution of EM scattering problems at homogeneous and composite objects. In order to deal with the ill-conditioned electric field integral operator, so called Calderon pre-conditioning techniques have been proposed [1]. They rely on the Calderon identities to transform the first kind integral equations into a second-kind integral equation. For reasons of numerical stability and orthogonality, the Rao-Wilton-Glisson (RWG) functions are typically complemented with the Buffa-Christiansen (BC) functions [2] to obtain a dual basis for the discrete representation of the equivalent surface currents that show up as the unknowns in the surface integral equations. The RWG functions have triangular support while the BC functions are composed as a linear combination of smaller RWG's defined over the barycentric refined triangular mesh.

2 Poisson-Neumann dual basis formalism

In this paper, we propose a novel dual basis setup based on the Poisson-Neumann (PN) functions [3]. These functions are defined for general polygonal shaped support. We present the



PN functions for a primary mesh consisting of a general assembly of rectangular, triangular and quadrangular cells. The barycentric defined dual mesh consists of general polygonal shaped cells. By construction, the PN functions possess the proper dual H(curl) and H(div) space properties. The Poisson-Neumann dual basis setup is applied to obtain a discrete representation of the tangential fields and currents on the surface of a general simply connected volume. Figure 1 shows as example the vector plots of a primary and the corresponding dual edge Poisson-Neumann basis function. It is clearly visible that the dual edge basis function is almost orthogonal with the primary edge basis function.

3 Discrete Calderon identities

The Calderon relations are reformulated in terms of an impedance and an admittance operator. The impedance operator maps the electric surface current onto the tangential electric field. The admittance operator maps the magnetic surface current onto the tangential magnetic field. It is shown that the admittance operator discretized over the dual mesh regularizes the ill-conditioned impedance operator discretized over the primary mesh and vice versa. The accuracy of the discretized Calderon relations are evaluated for a number of generally shaped, simply connected volumes with general materials (dielectric and conducting). By computing the condition numbers of the discretize are demonstrated. As an example, figure 2. shows the condition number of the electric field impedance operator and the improved condition number of the pre-conditioned impedance matrix for the volume object of figure 1. Note that the scales of the plot are logarithmic. The electric field impedance operator exhibits a low-frequency break-down which scales with the inversed square of the frequency and flattens out at the machine precision of floating point numbers.



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Challenges in Developing Calderon Preconditioners for Penetrable Objects

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Abstract

Calderon preconditioning is an efficient technique for improving conditioning of ill-conditioned matrices arising from discretization of electromagnetic surface integral equations. In the case of penetrable objects the large variety of material parameters poses additional challenges in developing efficient preconditioners.

Key words: Calderon preconditioning, electromagnetic scattering, surface integral equations

1 Introduction

Surface integral equation method provides elegant solutions for time-harmonic electromagnetic scattering by homogeneous penetrable objects. Most often these methods are based on the Poggio-Miller-Chang-Harrington-Wu-Tsai (PMCHWT) [1] formulation. Discretization of the PMCHWT equations with conventional techniques, however, leads to a very illconditioned matrix equation. Recently Calderon preconditioning techniques, developed originally for perfectly conducting objects [2], have been extended for the PMCHWT formulation too [3]. In this contribution we discuss challenges in developing efficient Calderon preconditioning techniques for the PMCHWT formulation.

2 Calderon Preconditioned PMCHWT Formulation

Consider time-harmonic electromagnetic scattering by a homogeneous penetrable object in a homogeneous background medium. Let us formulate the problem with the PMCHWT equations. By discretizing these equations using Galerkin's method and Rao-Wilton-Glisson (RWG) functions gives a matrix equation [3]

$$\mathbf{P}_{ff}\mathbf{x}_f = \mathbf{b}_f. \tag{1}$$

Here f stands for an RWG function. A Calderon preconditioner for (1) reads

$$\mathbf{P}_{qq}\mathbf{G}^{-1}\mathbf{P}_{ff}\mathbf{x}_f = \mathbf{P}_{qq}\mathbf{G}^{-1}\mathbf{b}_f,\tag{2}$$

where P_{gg} is the PMCHWT operator discretized with the Buffa-Christiansen functions [4] and G is the Gram matrix linking the $n \times RWG$ and BC functions [3]. Here n is the unit normal vector of the boundary of the object pointing into the exterior.



3 Numerical Experiments

Consider planewave scattering by a sphere with kr = 1, where k is the wavenumber in vacuum and r is the radius of the sphere. Figure 1 shows the number of GMRES iterations required to obtain relative residual error of 10^{-4} and the magnitudes of the smallest and largest eigenvalues of the Calderon preconditioned PMCHWT formulation with respect to the permittivity of the sphere. We can make the following observations:

- 1. The number of iterations and the magnitude of the largest eigenvalue increase as the permittivity is increased.
- 2. At certain permittivities the number of iterations increase and the smallest eigenvalue decrease.
- 3. The number of iterations show a significant increase for negative permittivities.



4. The formulation becomes singular at $\varepsilon_r = 0$.

Figure 1: Number of GMRES iterations (left) and magnitudes of the eigenvalues (right).

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[paper 80]



Convergence of the Mixed MFIE in the Energy Norm

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Abstract

The convergence behavior of the solution of the mixed discretization of the magnetic field integral equation is investigated. It is proved that, when the scatterer is smooth and simply connected, the discretization achieves optimal convergence in the $H_{\text{div}}^{-\frac{1}{2}}$ or energy norm. This norm is as sensitive to the charge as to the current. Hence, this convergence result explains why the mixed discretization leads to much more accurate solutions than the standard discretization, for which only convergence in the L_2 norm has been proved. *Key words: MFIE, mixed discretization, convergence, energy norm.*

1 Introduction

The magnetic field integral equation (MFIE) models the scattering of electromagnetic waves by a perfectly conducting scatterer. When the scatterer occupies the domain Ω and has boundary Γ , the MFIE is given by

$$\lim_{\mathbf{r}' \to \mathbf{r}} \hat{\mathbf{n}}(\mathbf{r}) \times \left[\mathbf{h} \left[\mathbf{j} \right] (\mathbf{r}') + \mathbf{h}^{i}(\mathbf{r}') \right] = \mathbf{0}, \quad \forall \mathbf{r} \in \Gamma$$
(1)

where $\hat{\mathbf{n}}(\mathbf{r})$ is the exterior surface normal to Γ and $\mathbf{h}[\mathbf{j}](\mathbf{r})$ is the magnetic field in the point \mathbf{r} , generated by the surface current distribution $\mathbf{j}(\mathbf{r})$. For the modeling of the fields outside of Ω , the limit should be taken such that \mathbf{r} approaches the boundary Γ from the *inside* of the scatterer. In this case, equation (1) is sometimes called the external MFIE. Essentially, it states that the tangential magnetic field just inside of the PEC should be zero.

To solve the external (or similarly the internal) MFIE, its solution is usually approximated as a linear combination of Rao-Wilton-Glisson (RWG) basis functions. Subsequently, the equation is tested with the same functions. This leads to what will henceforth be called the 'standard MFIE'. However, the literature is rife with evidence that the standard MFIE yields results that are, in general, much less accurate than those obtained using the electric field integral equation (EFIE), given the same mesh density. In addition, a low-frequency breakdown can be identified [1] that leads to nonphysical solutions when the frequency gets too low.

Recently, a different testing scheme for the MFIE was proposed [2], dubbed the mixed discretization, using rotated Buffa-Christiansen (BC) functions. As shown in [3], this scheme

avoids the low-frequency breakdown of the standard MFIE for simply connected scatterers. Therefore, it is well understood why the mixed MFIE works at low frequencies, while the standard MFIE does not. However, numerical results also show that the mixed MFIE leads to much improved accuracy (over the standard MFIE), rivaling the EFIE for comparable mesh density. The reasons for this behavior are less well understood and cannot be fully explained based on the mechanism of the low-frequency breakdown.

2 Optimal Convergence for the Mixed MFIE

In this contribution, an at least partial explanation for this behavior will be provided. In particular, it will be shown that the solution of the mixed MFIE converges in the $H_{\text{div}}^{-\frac{1}{2}}$ norm, whereas the best known result for the standard MFIE is convergence in the L_2 norm. The surface of the scatterer will be assumed to be smooth, such that the integral operator $\mathbf{h}[\mathbf{j}](\mathbf{r'})$ becomes

$$\mathbf{h}[\mathbf{j}](\mathbf{r}) = \frac{1}{2}\mathbf{j}(\mathbf{r}) + \mathbf{C}[\mathbf{j}](\mathbf{r}), \qquad (2)$$

where C is a compact operator.

Using these assumptions, a discrete Inf-Sup condition for the mixed MFIE will be derived, based on the discrete Inf-Sup property of the RWG-BC dual finite element pair and the compactness of C:

$$\inf_{\mathbf{u}\in X_{h}}\sup_{\mathbf{v}\in B_{h}}\frac{|\langle \mathbf{n}\times\mathbf{v}(\mathbf{r}),\mathbf{h}[\mathbf{u}](\mathbf{r})\rangle|}{\|\mathbf{v}(\mathbf{r})\|_{H^{-\frac{1}{2}}_{\mathrm{div}}}\|\mathbf{u}(\mathbf{r})\|_{H^{-\frac{1}{2}}_{\mathrm{div}}}} \ge \beta > 0.$$
(3)

Here, X_h is the span of all RWGs defined on a given quasi-uniform mesh with maximal edge length h, while B_h is the span of all BC functions on the same mesh. The details of the derivation require that h is sufficiently small and that the frequency is not a resonance frequency of the scatterer's interior. Finally, the discrete Inf-Sup property (3) is used to prove optimal converge (up to constant factors) in the $H_{\text{div}}^{-\frac{1}{2}}$ norm.

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Stable Solutions of EM Integral Equation in the Entire Frequency Spectrum Without the Search for Global Loops

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Abstract

We introduce a novel combined field integral equation that does not suffer from internal resonances and solves several drawbacks of existing resonance-free formulations. The new equation is obtained by combining a regularized electric type operator with a new magnetic type operator that exhibits uniform frequency scaling when acting on, or being tested within, the harmonic Helmholtz subspace for surface currents. With an appropriate use of quasi-Helmholtz projectors, the equation is stable for arbitrarily low-frequencies. Numerical results confirm the theoretical developments and show the effectiveness of the scheme.

Key words: Calderon Preconditioning, Integral Equations

1 Introduction

All known integral equation techniques for simulating scattering and radiation from arbitrarily shaped, perfect electrically conducting objects suffer from one or more of the following shortcomings: (i) they give rise to ill-conditioned systems when the frequency is low (ii) and/or when the discretization density is high; (iii) their applicability is limited to the quasi-static regime; (iv) they require a search for global topological loops; (v) they suffer from numerical cancelations in the solution when the frequency is very low. A recent paper [1] presented a new integral operator of the electric type that does not suffer from any of the above drawbacks.

This contribution extends a recently developed electric type operator immune from (i)-(v) by developing a new magnetic type operator that can be used to construct a combined field operator that does not suffer from (i)-(v) and is immune from interior resonances, i.e. that is uniquely solvable for all frequencies. The new formulation is obtained starting from a Helmholtz decomposition of two discretizations of the electric field integral operator and from a suitably symmetrized mixed discretization of the magnetic field integral operator obtained by using RWGs and dual bases functions, respectively. The new decomposition does not





(a) Sphere: far field calculated when the (b) Sphere: condition number as a function of frequency. frequency equals 10^{-40} Hz.

Figure 1: Numerical results

leverage Loop and Star/Tree basis functions; rather, it employs projectors that derive from them and does not require the explicit detection of global topological loops. The theoretical developments will be corroborated by numerical results, confirming the effectiveness of the newly developed method.

2 A new combined field equation

The new combined field equation we propose reads

$$\left(\eta^{2}\left(\frac{I}{2}-\mathcal{K}_{ik}\right)\left(\frac{I}{2}+\mathcal{K}_{k}\right)(k)+\mathcal{T}_{ik}\mathcal{T}_{k}\right)(\mathbf{J})=\left(\frac{I}{2}-\mathcal{K}_{ik}\right)(\hat{\mathbf{n}}_{r}\times\mathbf{H})+\mathcal{T}_{ik}(\hat{\mathbf{n}}_{r}\times\mathbf{E})$$
(1)

The equation is discretized by adopting a mixed-discretization strategy (see references in [1]) where the magnetic operators are tested with Buffa-Christiansen (BC) basis functions. For the sake of brevity we consider a discretization for the case of simply connected structures; minor modifications are required for the non-simply connected case. The discretization reads:

$$\left(\eta^2 \mathbb{M} \left(\frac{\bar{\mathbf{G}}_{\min}^T}{2} - \bar{\mathbf{K}}_{\min}^{ik} \right) \left(\bar{\mathbf{G}}_{\min}^T \right)^{-1} \cdot \left(\frac{\bar{\mathbf{G}}_{\min}^T}{2} + \bar{\mathbf{K}}_{\min}^k \right) \bar{\mathbf{M}} + \mathbb{M} \bar{\mathbf{T}}_{BC}^{ik} \mathbb{M} \bar{\mathbf{G}}_{\min}^{-1} \bar{\mathbf{M}} \bar{\mathbf{T}}_{RWG}^k \bar{\mathbf{M}} \right) \bar{\mathbf{I}} =$$

$$\eta^2 \mathbb{M} \left(\frac{\bar{\mathbf{G}}_{\min}^T}{2} - \bar{\mathbf{K}}_{\min}^{ik} \right) \left(\bar{\mathbf{G}}_{\min}^T \right)^{-1} \bar{\mathbf{V}}_H + \mathbb{M} \bar{\mathbf{T}}_{BC}^{ik} \mathbb{M} \bar{\mathbf{G}}_{\min}^{-1} \bar{\mathbf{M}} \bar{\mathbf{N}}.$$

$$(2)$$

The definition of the matrices and in particular of the projectors \mathbb{M} and $\overline{\mathbf{M}}$ is omitted here for space limitations, but it can be found in [1] for low frequency simulations. The projectors are set equal to the identity, instead, for high frequency ones.

3 Numerical results

The numerical tests involve a sphere of unit radius that is excited by a plane wave. The fact that the new equation is immune from the very low frequency current cancelation is confirmed by Fig. 1(a) which show the far field calculated using the new equation at 10^{-40} Hz. From Fig. 1(a) it is clear that although a standard Calderón equation can provide a stable solution till relatively low frequencies, the new equation is immune from the very low frequency current cancelation and provides stable solutions even when the frequency is arbitrarily low. The resonance free behavior of the new equation is tested in Fig. 1(b) where the new formulation clearly shows to be resonance-free.

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Calderón preconditioning for the EFIE on junction containing geometries

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Abstract

The EFIE results upon application of the BEM in a systems that becomes increasingly ill-conditioned as the mesh parameter tends to zero. For structures that do not contain junctions, this problems has been mitigated by application of Calderón preconditioning [1]. Calderón preconditioning requires not only a divergence conforming finite element space such as the space of RWG/RT functions, but also a dual finite element space such that the discrete Helmholtz subspaces are of complementing dimensionality and such that the overlap matrix is well-conditioned, both with respect to the matrix and energy norms. These families have been described in [2] for both closed and open manifolds. In this contribution, a Calderón preconditioning scheme for the EFIE applied to scatterers containing junctions is introduced. This scheme is based of the per manifold preconditioning of the EFIE operator and an appropriate combination procedure. The scheme hinges on the correct generalisation of the functions described in [2]. In this contribution, the EFIE on junction structures [3] and the Calderon Preconditioned EFIE [1] is revisited, the dual finite element spaces are introduced and described, and numerical results are presented that corroborate the correctness and effectiveness of the method.

Key words: Calderón Preconditioning, Electromagnetic Scattering, Electric Field Integral Operator, Junctions, Frequency Domain Analysis

1 Introduction

To simplify the discussion, consider a geometry comprising three open sheets Γ_i with normals \mathbf{n}_i that meet at the curve γ . The structured is submerged in a background medium characterized by an impedance η and is illuminated by an incident electric field \mathbf{e} . The induced current \mathbf{j} on Γ is divergence conforming in the sense that at every curve in Γ (including the junction γ), the total incoming flux adds to zero. Moreover, the current is the solution to

$$\begin{split} t(\mathbf{n} \times \mathbf{k}, \mathbf{j}) &:= -\frac{1}{\mathrm{i}\,k} \iint_{\Gamma \times \Gamma} \operatorname{div} \mathbf{k}(\mathbf{r}) \operatorname{div} \mathbf{j}(\mathbf{r}') \frac{e^{-\mathrm{i}\,k \,|\mathbf{r} - \mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|} \,\mathrm{d}\,\mathbf{r}\,\mathrm{d}\,\mathbf{r}' \\ &- \mathrm{i}\,k \iint_{\Gamma \times \Gamma} \mathbf{k}(\mathbf{r}) \cdot \mathbf{j}(\mathbf{r}') \frac{e^{-\mathrm{i}\,k \,|\mathbf{r} - \mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|} \,\mathrm{d}\,\mathbf{r}\,\mathrm{d}\,\mathbf{r}' \\ &= \frac{1}{\eta} \langle \mathbf{k}, \mathbf{e} \rangle_{\Gamma}, \end{split}$$
(1)

for all **k** that are divergence conforming. This equation is most commonly discretized using the set of Raviart-Thomas/Rao-Wilton-Glisson (RT/RWG) basis functions \mathbf{f}_n on a triangular mesh of Γ , which is a subset of the larger set of basis functions $\tilde{\mathbf{f}}_n$ whose normal components are not constraint at γ . The set of the divergence conforming functions can be written as the range of a recombination matrix P such that $\mathbf{f}_n = \sum_m P_{m,n} \tilde{\mathbf{f}}_n$. The expansion coefficient w.r.t $\tilde{\mathbf{f}}$ of the induced currents are then the solution to P'TPy = P'e, where T is the matrix constructed by substituting $\tilde{\mathbf{f}}_n$ for **k** and **j**. The expansion coefficients w.r.t \mathbf{f}_n are $\mathbf{x} = P\mathbf{y}$. The regularized discrete equation is

$$Q'G'^{-1}SG^{-1}TPy = Q'G'^{-1}SG^{-1}e.$$
 (2)

Here S is the discretization of (1) w.r.t a dual set of basis functions \tilde{g}_n to the set \hat{f}_n , and Q is the recombination matrix for the dual set of basis functions. The correct dual set of divergence conforming basis functions is a generalization of the set introduced in [2]. In [2], three families of basis functions were introduced such that the dimensions of the kernel and images of the surface curl and divergence yields the same Betti numbers as found by studying the homology group. The functions introduced here generalize this to the homology relative to the subset of the boundary that coincides with the junction. In particular, the Helmholtz structure is such that the square of the hyper-singular contribution vanishes, thus suppressing the norm and condition number of the preconditioned system matrix.



Figure 1: The basis functions introduced here are generalisations of those introduced in [2]: there are basis functions that are attached to edges on the junction, there are basis functions whose support touches the junction or both the junction and the structure's boundary.

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Two-stage numerical procedure for the solution of hyperbolic coefficient inverse problem

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Abstract

We briefly present two-stage numerical procedure of [1] for the solution of hyperbolic coefficient inverse problem. On the first stage an approximate globally convergent algorithm of [1] rigorously guarantee obtaining at least one point in a small neighborhood of the exact solution without any advanced knowledge of that neighborhood. On the second stage an adaptive finite element method of [3] refines the solution obtained on the first stage.

We demonstrate numerical verification of the two-stage procedure, presented in [2, 5, 4] and implemented in the software package WavES [6], on the reconstruction of refractive indices and shapes of inclusions from backscattered experimental data provided by the Optoelectronics and Optical Communications Center of University of North Carolina at Charlotte, Charlotte, USA.

Key words: coefficient inverse problems, approximate global convergence, adaptive finite element method

MSC 2010: 65N15, 65N30, 35J25

1 Introduction

We consider the problem of reconstruction of refractive indices, shapes and locations of objects placed in the air from blind backscattered time-dependent experimental data using twostage numerical procedure presented in our recent works [1, 2, 5, 4]. In these works only targets located in air are considered. The work on real data for the case when targets are buried under the ground is ongoing. Experimental data were collected using a microwave scattering facility which was built at the University of North Carolina at Charlotte, USA. A potential application of our work is in imaging of explosives. Our experimental data are generated using a single location of the source. The backscattered signal is measured on a part of a plane, see [2, 5] for the description of the data collection procedure. Two-stage numerical procedure means that we combine two different methods to solve our Coefficient Inverse Problem (CIP). On the first stage the approximately globally convergent method of [1] is applied in order to obtain a good first approximation for the exact solution. We have presented results of reconstruction on this stage in our recent publications [2, 5]. Only refractive indices $n(\mathbf{x}) = \sqrt{\varepsilon_r(\mathbf{x})}$, $\mathbf{x} = (x, y, z) \in \mathbb{R}^3$, and locations were accurately reconstructed in [2, 5].

On the second stage the local adaptive finite element method of [3] is applied by taking the solution of the first stage obtained in [2, 5] as the starting point in the Tikhonov minimization functional in order to obtain better approximations of refractive indices and shapes of objects on the locally adaptively refined meshes. In our recent publication [4] is shown that we can simultaneously reconstruct three components of interest of targets: their refractive indices, shapes and locations.



Figure 1: Results of the reconstruction on the second stage from [4]. (a) xy-projection, (b) xz-projection, and (c) yz-projection of the three times refined (optimal) mesh; (d) Computed image of the blind heterogeneous target (doll, air inside) on that mesh. Thin lines indicate correct shape.

2 Statement of Forward and Inverse Problems

On the first stage we have considered in [2, 5] the problem of the reconstruction of the spatially distributed dielectric constant $\varepsilon_r(\mathbf{x}), \mathbf{x} \in \mathbb{R}^3$, from blind experimental data which was the unknown coefficient in a wave-like PDE

$$\varepsilon_r(\mathbf{x})\frac{\partial^2 E_2}{\partial t^2} = \Delta E_2. \tag{1}$$

To reconstruct $\varepsilon_r(\mathbf{x})$, we have used the approximately globally convergent algorithm of [1]. The notion of the approximate global convergence was introduced in [1]. It is well known that conventional least squares cost functionals for CIPs are non convex and typically have many local minima. Hence, given a CIP, the first question to address in its numerical treatment is: *How to obtain a good approximation for the exact solution without any a priori knowledge of a small neighborhood of this solution*? Since it is difficult to address that question a certain reasonable approximation was made in [1]. Because of this approximation a room is left





Figure 2: Results of the reconstruction on the second stage from [4]. Three views and zooms of the reconstructed blind heterogeneous target of Figure 1. Thin lines indicate correct shape.

for a refinement of results. Thus, a locally convergent numerical method can be used for a refinement of the solution obtained on the first stage.

In [4] we use an adaptive finite element method of [3] in order to improve images obtained on a first stage. Let $\Omega \subset \mathbb{R}^3$ be a convex bounded domain. In [4] we model the electromagnetic wave propagation in an isotropic non-magnetic space with $\mu = 1$ in \mathbb{R}^3 with the dimensionless coefficient $\varepsilon_r(\mathbf{x})$, which describes the spatially distributed dielectric constant of the medium. We consider the following Cauchy problem for the electric field *E*:

$$\varepsilon_r \frac{\partial^2 \mathbf{E}}{\partial t^2} + \nabla \times (\nabla \times \mathbf{E}) = (0, \delta(z - z_0) f(t), 0), \text{ in } \mathbb{R}^3 \times (0, T),$$

$$\mathbf{E}(\mathbf{x}, 0) = \mathbf{0}, \quad \mathbf{E}_t(\mathbf{x}, 0) = \mathbf{0} \text{ in } \mathbb{R}^3,$$
(2)

where $f(t) \neq 0$ is the time-dependent amplitude of the component E_2 of the incident plane wave, which is originated at the plane $\{z = z_0\}$ and propagates along the *z*-axis. The function $\mathbf{E}(\mathbf{x},t)$ in (2) represents the voltage of the electric field $\mathbf{E}(\mathbf{x},t) = (E_1, E_2, E_3)(\mathbf{x}, t)$. In our experiment the component E_2 corresponds to the electromagnetic pulse which is sent into the medium. Thus, in (2) and in our computer simulations of [4] the incident field has only one non-zero component $E_2(\mathbf{x},t)$. This component propagates along the *z*-axis until it reaches the target, where it is scattered.

We impose the following conditions on the function $\varepsilon_r(\mathbf{x})$

$$\varepsilon_r(\mathbf{x}) \in C^{\alpha}\left(\mathbb{R}^3\right), \ \varepsilon_r(\mathbf{x}) \in [1,d], \ \varepsilon_r(\mathbf{x}) = 1 \text{ for } \mathbf{x} \in \mathbb{R}^3 \setminus \Omega,$$
(3)

where d = const. > 1. We *a priori* assume the knowledge of the constant *d*. This means the knowledge of the set of admissible coefficients in (3). However, we do not impose small-value assumptions on the unknown coefficient $\varepsilon_r(\mathbf{x})$. Here $C^{\alpha}, \alpha \in (0, 1)$ is the Hölder space. Let $\Gamma \subset \partial \Omega$ be a part of the boundary $\partial \Omega$ and also Γ be a part of a plane.

Coefficient Inverse Problem (CIP). Suppose that the coefficient $\varepsilon_r(\mathbf{x})$ satisfies conditions (3) and that $\overline{\Omega} \cap \{z = z_0\} = \emptyset$. Determine the function $\varepsilon_r(\mathbf{x})$ for $\mathbf{x} \in \Omega$, assuming that the following function $\mathbf{g}(\mathbf{x},t)$ is known for a single incident plane wave

$$\mathbf{E}(\mathbf{x},t) = \mathbf{g}(\mathbf{x},t), \ \forall (\mathbf{x},t) \in \Gamma \times (0,\infty).$$
(4)

3 Reconstruction

Figures 1–2 display 3-D images of reconstruction as well as corresponding adaptively locally refined meshes of the heterogeneous object (doll, air inside) of [4]. Heterogeneous targets present models for explosive devices in which explosive materials are masked by dielectrics. These figures also show estimates of sizes of our object in the *z*-direction. In all reconstruction cases of [4] we have obtained a significant improvement of the image quality after the application of the adaptivity technique on the second stage compared with the results of the first stage.

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Some inverse problems in parabolic partial differential equations

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Abstract

An inverse problem (IP) can be seen as a system consisting of a governing partial differential equation (PDE) and an additional measurement. The last one can be eliminated by applying the measurement operator to the PDE. Afterwards a suitable variational formulation in appropriate function spaces can be derived. In this way the existence and uniqueness of a solution to the IP can be addressed.

Key words: inverse source problem, parabolic PDE MSC 2010: 65M32, 65M20

1 Introduction

Inverse problems are typically ill-posed in the sense of Hadamard i.e. there is either no classical solution, or there are more ones, or a solution might not depend continuously on the data. To prove global in time existence and uniqueness of a solution turn out to be a difficult task. Another important goal in IPs is to find a constructive algorithm for finding a solution. The usual techniques for IPs are based on a suitable parametrization tacitly assuming continuous dependence of a parametrized solution on the parameter. A error/cost functional describing the difference between the parametrized and the exact solution at a given measurement place is minimized. The typical feature is lack of convexity of the cost functional, which leads to multiple local minima's. One can try to regularize the minimization problem by adding a suitable term to the functional in order to enforce its convexity, cf. [1]. Then the existence of a unique solution to the minimization problem can be obtained by means of the theory of monotone operators [2]. This later task can be solved numerically by adequate approximation techniques, such as the steepest descend, Ritz or Newton or Levenberg-Marquardt method.

We describe an another technique for IPs. We see the IP as a system consisting of a PDE and a measurement. We eliminate the measurement and derive a corresponding variational formulation. We apply the semi-discretization in time to address the existence and uniqueness of a solution to the IP. We demonstrate this approach on the following two settings.



2 Problem 1

We study an identification problem of a solely time-dependent source in a multi-dimensional heat equation accompanied with mixed (Dirichlet and nonlinear evolutionary) BCs. We consider a bounded domain $\Omega \subset \mathbb{R}^n$, $n \ge 1$ with sufficiently smooth boundary Γ , which is split into two non-overlapping complementary parts Γ_D and Γ_N . The inverse source problem consists of finding (u(x,t), h(t)) obeying

$$\begin{aligned} \partial_t u(x,t) &- \Delta u(x,t) &= h(t) f(x) & \text{ in } \Omega \times (0,T), \\ -\nabla u(x,t) \cdot v &= \partial_t u(x,t) + \sigma(u(x,t)) & \text{ on } \Gamma_N \times (0,T), \\ u(x,t) &= 0 & \text{ on } \Gamma_D \times (0,T), \\ u(x,0) &= u_0(x) & \text{ for } x \in \Omega, \end{aligned}$$
 (1)

The symbol ν denotes the outer normal vector associated with Γ . The unknown time-dependent function h(t) will be determined from the following additional measurement

$$m(t) = \int_{\Omega} u(x,t) \mathrm{d}x, \qquad t \in [0,T].$$
⁽²⁾

3 Problem 2

Find the unknown couple (u, h) obeying

$$\begin{cases} u_t(x,t) - \Delta u(x,t) &= h(t)f(x) + \alpha(u(x,t)) + \beta(x,t) & \text{ in } \Omega \times (0,T), \\ \nabla u(x,t) \cdot \boldsymbol{\nu} &= 0 & \text{ on } \Gamma \times (0,T), \\ u(x,0) &= u_0(x) & \text{ for } x \in \Omega, \end{cases}$$
(3)

where $\Omega \subset \mathbb{R}^n$, $n \ge 1$ is a bounded domain with a sufficiently smooth boundary Γ .

The data functions u_0, f, α, β are given. The unknown purely time-dependent source term h(t) will be recovered from the following measurement on the boundary

$$m(t) = \int_{\Gamma} u(x,t) \mathrm{d}x, \qquad t \in [0,T].$$
(4)

Acknowledgements

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Creating optimal form by vertex morphing and sensitivity filtering

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Abstract

The proper parameterization of structural shape which is suitable for creating structural form and shape optimal design is a great challenge. The demand for large design spaces with large and very large numbers of design parameters is in conflict with the robustness of the numerical model. There is a need for regularization. The currently most successful techniques which overcome those burdens and, simultaneously, are most intuitive and easy to be used are so-called filter techniques. They directly use the coordinates of the discretization nodes as design parameters. Filters are applied to smooth the shape sensitivity fields as the generator of the design update towards the optimum. However, the filters are much more than mathematical means to prevent numerical problems such as mesh distortion or checker board patterns. Even more important, from the point of view of shape design they deal as a design tool to controlling the local and global shape properties. The actual presentation will show that filtering is equivalent to the implicit definition of standard spline models. Impressive applications in the fields of CSD and CFD with problem sizes up to 3.5 million design parameters can easily be handled by this technique.

Key words: Shape optimization, sensitivity filtering, morphing, structural optimization, CFD optimization

1 Introduction

Sensitivity filtering is a well-established and very successful procedure in discrete topology and shape optimization. It is used to regularize the optimization problem by introducing an additional filter length scale which is independent of the discretization. The filter is both, a design tool controlling local shape or density distribution and a mean to prevent numerical problems such as mesh distortion or checker board patterns. Together with adjoint sensitivity analysis to determine the discretized shape gradient, the filter technique is a most powerful optimization procedure and successively applied to the largest optimization problems known. Filtering is the key technology for using the vertices of even the finest discretization mesh directly as design handles for discrete shape optimization. In contrast to standard shape morphing techniques and CAD methodologies no other design handles are used.



Among those techniques which do not use CAD parameters to parameterize shape there are meshfree and node-based or parameter-free methods which means "free of CAGD parameters" (Le et al. 2011; Scherer et al. 2010; Hojjat et al. 2014), the traction method (Azegami and Takeuchi 2006), for CFD problems (Pironneau 1984; Jameson 1995, 2000, 2003; Mohammadi and Pironneau 2000, 2004; Stück and Rung 2011).

2 Continuous Shape control by using filters

We start by introducing an additional field p. This serves as the control which steers the evolution of shape. In analogy to splines the control field can be identified as the continuous equivalent to the convex hull which is discretized by control nodes. As with splines where the coordinates of the control nodes are the design variables, now, the control field represents the design degrees of freedom which drive the shape.

The considered shape optimization problem states as:

$$\min_{p} f(x, z(x, p), u(x, z(x, p)))$$

s.t.: $\mathbf{R}(x, z(x, p), u(x, z(x, p))) = \mathbf{0}$
 $g_{j}(x, z(x, p), u(x, z(x, p))) \le 0; \quad j = 1, \dots, m$ (1)

where f and g_j are the objective function and constraints and **R** are the state equations which may be non-linear. There are four fields describing the state u, the surface coordinate x, the geometry z as well as the design control field, p, see Fig. 1. For the sake of simplicity, (1) is formulated in 1D geometric space. As a consequence, the geometry z is a function of the one spatial surface coordinate x and the design control p. Extended to 3D, (1) represents the classical view at a surface controlled shape optimization problem following the ideas of Hadamard. Then, the shape relevant modifications of geometry z are identified as in the normal direction to the surface spanned by surface coordinates x_1 and x_2 .

The geometry *z* at x_0 is generated from the design control field p(x) by a filter operation as integration over the surface Γ with filter function F_0 of radius *r* and center at x_0 :

$$z(x_0) = \int_{\Gamma} F_0 p \, d\Gamma = \int_{x_0-r}^{x_0+r} F(x, x_0, r) \, p(x) \, dx \; ; \quad \frac{dz|_{x_0}}{dp|_{x_1}} = F(x_1, x_0, r) \tag{2}$$

where
$$\int_{x_0-r}^{x_0+r} F_0 \, dx = 1$$
 and $F_0 = 0$ if $x < x_0 - r$ or $x > x_0 + r$ (3)

Applying the chain rule of differentiation the derivative of a response function f with respect to the design control p at x_1 is given as

$$\frac{\mathrm{d}f}{\mathrm{d}p}\Big|_{x=x_1} = \int_{\Gamma} \frac{\mathrm{d}f}{\mathrm{d}z} \frac{\mathrm{d}z}{\mathrm{d}p}\Big|_{x_1} \,\mathrm{d}\Gamma = \int_{\Gamma} \frac{\mathrm{d}f}{\mathrm{d}z} F(x_1, x, r) \,\mathrm{d}\Gamma = \int_{\Gamma} \frac{\mathrm{d}f}{\mathrm{d}z} A_1 \,\mathrm{d}\Gamma \tag{4}$$

The geometry gradient $\frac{df}{dz}$ is filtered by the adjoint filter function A_1 where the center coordinate x_1 and the free coordinate x are exchanged compared to F_1 .



3 Shape discretization and discrete sensitivity filtering

The design control field and the geometry derivative are discretized using shape functions N_j related to design and geometry parameters p_j and z_i , respectively:

$$p = N_j p_j = N_j (x) p_j$$

$$\frac{df}{dz} = N_i \frac{df}{dz_i}$$
(5)

The discrete versions of (2) and (4) are:

$$z_{i} = \int_{\Gamma} F_{i} N_{j} p_{j} \, d\Gamma = B_{ij} p_{j}$$

$$\frac{df}{dp_{j}} = \int_{\Gamma} \frac{df}{dz_{i}} N_{i} A_{j} \, d\Gamma = \int_{\Gamma} F_{i} N_{j} \, d\Gamma \frac{df}{dz_{i}} = B_{ij} \frac{df}{dz_{i}}$$
(6)

On regular grids together with symmetric filter functions $F_i = A_i$ the filter operator matrix B_{ij} is symmetric as well.



Figure 1: Shape optimization of the side mirrors for drag reduction of the complete car referring to the center column of Fig. 26. Longitudinal section of the mirror body. The shape is morphed whilst the displayed feature lines are maintained. The shape of the mirror itself (left straight line) has been constrained to guarantee the usability. Therefore, the optimizer was prevented to simply remove the mirrors to reduce drag.

4 Choice of filters and shape functions, relations to splines

Linear hat functions are the simplest choice for filter and shape functions F and N. Filtering a linear shape function by a linear filter results in a cubic geometry. As a matter of fact the control field is the continuous equivalent of spline control polygons. For the special case of regular grids, linear hat functions for F = N a cubic B-spline geometry is derived from a piecewise linear control field. The filter technique is equivalent with the subdivision spline



technique sharing important properties with general splines.

As the filter modifies the gradient vector the filtering effect can be exploited best by first order gradient methods. Those methods converge to that local minimum which is characterized by a shape mode wave length that is not smaller than the filter radius or the variance in case of Gaussian filters. The filter shape is not important at all. That allows to using any kind of filter for the sensitivity filtering as long as B_{ij} remains non-singular. In turn, we can conclude that every simple gradient method with sensitivity filtering will converge to a solution of the original, unmodified problem. For non-convex problems, the choice of filter will affect which local optimum will finally be found. This is the intended effect which helps to efficiently explore the design space.

5 Selected Example

The technique is successfully applied to all kind of structural and fluid shape optimization problems. As a representative example the shape optimization of the VW Passat side mirrors is presented which was done in close cooperation with Volkswagen and others partners of the EU-project FLOWHEAD, Fig. 1. The goal was to reduce the drag of the complete car by shape modifications of the mirrors only. That gives 32,000 design parameters for each mirror, i.e. 64,000 in total. A complete model of the car had to be simulated in an appropriate numerical wind tunnel using OpenFoam for CFD simulation, an adjoint solver provided by project partners, and CARAT++ for optimization which is the own optimization and structural simulation code. In further applications, the complete car body had been optimized which comes together with up to 3.5 Mio shape parameters.

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Understanding Population Balances Involving Aggregation and Breakage Through Homotopy Approaches

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Abstract

Key words: Population balance equation, Aggregation, Breakage, homotopy, asymptotic An area of considerable industrial concern is the phenomenon of particulate aggregation and breakage in chemical and biochemical process systems such as crystallization [1], fluidization [2] and activated sludge flocculation [3]. Population balance equations (PBEs) are widely used to describe the evolution of the particle size distribution (PSD) in the above mentioned processes [1, 3]. These PBEs are integro-partial differential equations which seldom have analytical solutions. This study details several homotopy approaches namely, the Homotopy Perturbation Method (HPM), the Optimal Homotopy Asymptotic Method (OHAM) and the Homotopy Analysis Transform Method (HATM) to obtain approximate analytical solutions for the Population Balance Equation (PBE) involving particulate aggregation and breakage. Using symbolic computation several case studies have been considered and the numerical results have been compared with the analytical solutions obtained from the literature.

The most common approximate solutions for differential equations in the literature involve various asymptotic expansions. There are, however, practical problems associated with this. Instead of trying to develop the asymptotic solutions of a differential equations, it is often more convenient to find an integral expression for the solution and then seek an asymptotic expansion afterwards. This thought gives rise to some novel methods such as Homotopy Perturbation method (HPM) [5] and more recent frequently used variants such as Optimal Homotopy Asymptotic method (OHAM) [6] and Homotopy analysis transform method (HATM) [7], which are based on the same homotopy theory.



We consider a problem with simultaneous aggregation and breakage for which analytical solution is available [4]. As can be seen in Figure 1, solutions provided by all the methods match reasonably well with the analytical solution. In Figure 1, it can be observed that a comparatively better match with the analytical solution is obtained via OHAM. This is because OHAM additionally uses the best approximation (or optimal error) mechanism which is obtained by optimizing the residual to determine fabricated parameters. OHAM may be used for other more complex realistic physical problems in the future.



Figure 1: The solution are given for S = 0.25 at t = 1.

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Parametric Analysis of Windowed Poligonal Tubes Under Dynamic Impact Loading

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Abstract

The present paper aims to evaluate the impact absorption characteristics of polygonal cross sections tubes under a dynamic axial compression loading through a numerical comparison. The original tubes behaviour are compared to tubes with patterned windows on their flat walls. The windowed tubes shows a significant weight reduction and a decrease in the initial peak load while keeping a similar specific energy absorption.

Key words: Energy absorption, Finite Element Analysis, Progressive Buckling

1 Introduction

Thin-walled tubes show high capability to absorb impact energy, specially when one keeps in mind the more or less straightforward manufacturing process. The dissipation characteristics of thin-walled tubes are commonly related to the progressive folding mechanism and where-fore it is fundamental to guarantee local buckling leading to a maximal energy absorbed.

For thin-walled tubes, the addition of patterned windows in the side walls influence the mechanism of deformation and the absorbed energy as shown in [2]. Therefore, the present paper deals with the behaviour of square and hexagonal windowed tubes under an axial compression, comparing the initial peak load as well as the specific energy absorption to the original geometries.

2 Progressive Buckling Analysis

The buckling modes of square tubes are described by [3], where three distinct dissipation regions are defined. In the same way, [1] presented a study concerning the dissipation energy and the mode of failures of polygonal thin-walled tubes under compression describing the total amount of energy for one fold formation as

$$W_i = W_1 + W_2 + W_3 = 2M_p \left[\pi (h + 8c) + \frac{h^2}{r} \right],$$
(1)

where W_1 , W_2 and W_3 are respectively the energies dissipated by: the stationary horizontal hinge lines; the flattening of the initial corners of shell; the travelling vertical hinges. M_p is the plastic bending moment, h is the fold height and c is the side length.





Figure 1: Different polygonal models subject to axial compression load.

Fig.1 shows the deformed finite element models for the original and windowed square and hexagonal tubes when subjected to a 500kg mass at 5m/s. The numerical analysis have been developed in LS-Dyna 9.71 and consider a strain rate sensitive material via the Cowper-Simonds constitutive equation. The simulation results are presented in Tab. 1, where the peak load is the maximum force applied on the structure before progressive buckling starts.

Table 1: Numerical Results.								
Model	Peak Load (kN)	Energy Absorbed (kJ)	SEA (kJ/kg)					
Original Square	200	5.09	15.05					
Windowed Square	138	4.85	18.29					
Original Hexagon	132	4.47	8.27					
Windowed Hexagon	94	3.57	7.56					

SEA - Specific Energy Absorption

For booth geometries the initial peak load decreases for the windowed tubes, owing to the reduction of the cross section area and consequently of the yielding resistance. However the efficiency of the windowed tubes is specially highlighted in the square tubes where the travelling hinges plays an important hole in the absorption capacity.

There is a lost of efficiency for the hexagonal windowed tubes due to the stability loss when the first fold is complete. To improve the efficiency of the hexagonal tubes the position of the windows cuts request further studies to take into account the deformation mechanism of the structure to guarantee stability during the crushing.

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Phaseless coefficient inverse problems

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Abstract

In some applications one can measure only the magnitude of the scattered wave field but cannot measure the phase. In this case one deals with the problem of the reconstruction of an unknown coefficient of a wave-like PDE from the modulus of the scattered wave measured on a frequency interval outside of the scatterer. Recently the author has proven some uniqueness theorems for these inverse problems and they will be presented on the talk.

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Heat transfer study in an enclosed rotor-stator system

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Abstract

A numerical study was performed to determine the turbulent heat transfer in the air-gap of an enclosed rotor-stator system. Rotor-stator interaction has been modeled using sliding mesh (SM) and multiple reference frame techniques (MRF). With taking into account rotational Reynolds number $\text{Re} = \Omega R^2 / v$ and air-gap ratio G = s/R, the heat transfer rate and the flow characteristics in the gap between the disks were calculated. A new cooling solution was then investigated. In fact, the presence of holes in the rotor has been examined and it was found that the addition of the holes in the rotor is advantageous for the heat transfer as air is allowed to enter into the air-gap through the holes, resulting in a net radial flow in the gap region between the rotor and the stator. For the case investigated, the maximum increase in the heat transfer was up to 23% with an increase in the rotor torque equal to 18%.

Key words: Heat Transfer, Holes, Multiple References Frame, Rotor-Stator, Sliding Mesh

1 Introduction

Heat transfer in discoidal systems is crucial in many fields of engineering especially in disc type electrical machines [1, 2]. In an effort to avoid damage of components arising from local high temperature due to electromagnetic losses, the designers must take into account the effect of heat transfer, and pay essential attention to the shape, rotational speed and gap size between rotor and stator. In particular, the magnets should be sufficiently below the critical temperature $T_c = 150^{\circ}$ C to avoid demagnetization. To the best of our knowledge, no study has been reported regarding the presence of holes in the rotor disk. So, this paper presents a numerical study of the local heat transfer on the rotor surface in the air-gap of a discoidal rotor-stator system, in which air is allowed to pass through the holes into the air-gap.

2 Problem setup

Figure 1 shows the problem configuration where the left disk is the rotor and the right one is the stator. The SST $k - \omega$ model has been used for turbulence modeling. The surface temperature of the rotor, the stator and the cover are kept at 100°C, 120°C and 50°C, respectively. The



boundary layers around the solid walls were designed to obtain a y+ value below 5. The aim of this study is to exam the thermal performance of the discoidal system with and without the presence of holes in the rotor. Rotor-stator interaction has been modeled using multiple reference frame and sliding mesh approaches where the latter case takes into account the effect of the changing position of the holes during rotation. The air-gap size is determined by the air-gap ratio, G = s/R, with R equal to the radius of the rotor.



Figure 1: Problem configuration.

Figure 2: Velocity vectors inside the hole for Re = 7.16×10^4 and G = 0.02.

Results and conclusion 3

Table 1 indicates that the addition of the holes in the rotor is advantageous for the heat transfer. To give more insight about the flow pattern inside the hole, the velocity vector for SM method in a meridional plane of the rotor has been shown in the figure 2.

Fable 1: H	eat transfer r	ates (W) for Re =	$= 7.16 \times$	10^4 and	IG = 0.0
		Without Holes	With Holes		
			MRF	SM	
	Rotor Wall	16.0	21.0	21.1	
	Stator Wall	24.6	31.9	31.0	
	Cover Wall	-40.6	-52.9	-52.1	

2.

With the presence of holes in the rotor, the heat transfer rate could be enhanced for this specific rotor-stator combination. Further optimization is under investigation.

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Bottom-up multiscale modelling of microstructural response in a P91 martensitic steel

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Abstract

In this study, we have developed a multiscale finite element (FE) modelling framework to explicitly account for the polycrystalline microstructure and sub-micron precipitate structure for a P91 tempered martensitic steel. A dislocation-mechanics based and length-scale dependent crystal plasticity model has been used to represent slip based inelastic deformation in the material. Homogenisation analysis is performed to connect FE models at different length scales, indicating a strong effect of the sub-micron geometries on dislocation accumulations. Softening effects with respect to precipitate and lath coarsening are identified and quantified at the macroscopic scale. The results can be further used to implement a component level constitutive law which phenomenologically takes the microstructural effects into account. The present multiscale FE simulations have been validated through the use of uniaxial tensile test data at room temperature.

Key words: Multiscale modelling; Precipitate hardening; Strain gradient crystal plasticity; Dislocation accumulations; Tempered martensitic steels

1 Introduction

Tempered martensitic steels containing 9-12% Cr are widely used as structural materials in critical power plant components operating at elevated temperatures. To fulfil the current and future needs for safety, efficiency and flexibility of fossil fuel fired power plants, there is a requirement for rigorous and accurate structural integrity assessment procedures, taking into account recent advances in multi-scale computational and experimental techniques for a better understanding of inelastic deformation and failure mechanisms (operating at the micron and sub-micron scale). Tempered martensitic steels have a complex microstructure exhibiting a hierarchical arrangement consisting of prior austenite grains, packets, blocks, laths and



precipitates. The strengthening/hardening contributions of the hierarchical microstructure in tempered martensitic steels have not yet been fully understood. The present study addresses a multiscale modelling method to quantify precipitate hardening in a P91 martensitic steel by means of crystal plasticity based finite element (FE) analysis [1, 2].

2 Bottom-up multiscale model for martensitic steels

Figure 1 shows the multiscale FE model developed for a P91 martensitic steel. A bottom-up strategy has been used to connect the FE models at different length scales such that micro-structural effects on the mechanical performance of the material/component can be examined.



Figure 1: Illustration of microstructure and multiscale FE model for P91.

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Wavelet-based parameterization of control variables in diffuse optical tomography

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Abstract

The present paper deals with the use of wavelet theory in the ill-posed inverse problem of diffuse optical tomography. The rationale behind this choice is to exploit the filtering potential of wavelets to the noisy cost function gradient, the latter being an essential ingredient in the optical properties reconstruction process. The proposed algorithm is based on the Broyden-Fletcher-Goldfarb-Shanno (BFGS) method with an inexact linesearch method, where the continuous cost function gradient is computed with the adjoint state method. After decomposition of this gradient with the discrete wavelet transform, filtering is performed through a thresholding rule on the detail coefficient vectors.

Key words: BFGS, filtering, inverse problem, parameterization, wavelet MSC 2010: 78M50, 65T60, 35Q93

1 Introduction

The Optical Tomography (OT) consists in reconstructing optical property maps of heterogeneous semi-transparent media from radiative measurements obtained with the help of sources and sensors located on the edges of the medium. Two mathematical descriptions are commonly used to predict the propagation of optical radiation through the participating medium, namely the Radiative Transfer Equation (RTE) based model and the Diffuse Approximation (DA) model. The DA model, which is considered in this paper, assumes that the media is poorly absorbing and highly diffusing. Applications of the OT with the DA model typically concern the detection of cancerous tumors in tissues such as the breast. It is also planned to use such method to characterize radiative properties of materials such as metallic open-cell foam, allowing the systematic design of materials in thermal and energetics engineering.

The forward model associated to the diffuse optical tomography problem is given by [1]:

$$-\nabla \cdot \left(\left[n(\kappa + \sigma) \right]^{-1} \nabla \varphi \right) + \left(\kappa + \frac{2i\pi \nu}{c} \right) \varphi = 0 \quad \text{in } \mathcal{D}$$
 (1)

$$\varphi + \frac{A}{2\gamma} \left[n(\kappa + \sigma) \right]^{-1} \nabla \varphi \cdot \boldsymbol{n} = \frac{I}{\gamma} \mathbb{1}_{\left[\zeta \in \partial \mathcal{D}_{S} \right]} \quad \text{on } \partial \mathcal{D}$$
(2)



with $\varphi : \mathcal{D} \to \mathbb{C}$ is the photon density, κ and σ are, respectively, the absorption and reduced scattering coefficients, and *I* denotes the prescribed radiative intensity on $\partial \mathcal{D}_s$. Parameters γ , which only depends on the dimension of \mathcal{D} , *n*, and *A*, which characterizes the reflection at the boundary, are given. Finally, ν is the source modulation frequency and *c* is the velocity of the light. The difference, in the least squares sense, on sensor locations between the state φ and experimental measurements is integrated to a cost function *j* to be minimized. Thus, the solution of the inverse problem reads: "*Find the functions* κ^* and σ^* such that $j(\kappa^*, \sigma^*) < v$ ", where *v* integrates variances of errors for all measurements.

2 Optimization

The minimization of the cost function is carried out by the Broyden-Fletcher-Goldfarb-Shanno algorithm associated to a fast inexact line-search. This algorithm relies on the gradient computed through the solution of the additional adjoint problem. In [2], the cost function gradient are written in a continuous way before being discretized choosing a finite element basis for the parameterization of the optical properties. These continuous gradients are given by:

$$\nabla^{\kappa} j(\mathbf{x}) = \Re \left(\varphi(\mathbf{x}) \varphi^{*}(\mathbf{x}) - n \left[n(\kappa + \sigma) \right]^{-2} \nabla \varphi(\mathbf{x}) \cdot \nabla \varphi^{*}(\mathbf{x}) \right)$$
(3)

$$\nabla^{\sigma} j(\mathbf{x}) = -n \left[n(\kappa + \sigma) \right]^{-2} \Re \left(\nabla \varphi(\mathbf{x}) \cdot \nabla \varphi^{*}(\mathbf{x}) \right)$$
(4)

3 Filtering

In reality, the computed gradients present high frequency fluctuations due to the noise coming from measurements and propagating through the adjoint variable. So far, regularization strategies concerned: (i) parameterization based on a coarser mesh, performed using projection of the state and adjoint variables on the coarse mesh, and (ii) the use of Sobolev inner products when extracting the cost function gradient. The strategy implemented in this paper is based on the wavelet decomposition of functions $f \in L^2(\mathbb{R}^n)$ applied to the cost function gradients. Concretely, the gradient maps are discretized with 2^{nJ} values. Then, the dyadic wavelet transform [3] is computed for scales 2^j , $j = 1, \ldots, J$. A thresholding rule is finally considered on the detail coefficient vectors before reconstructing the filtered gradient. The study concerning the selection of the wavelet and thresholding method is in progress.

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Efficient index-1 time stepping for magnetoquasistatic models with voltage-driven stranded conductors

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Abstract

A standard field-circuit coupled magnetoquasistatic model with n voltage-driven coils corresponds to an index-2 system for which straightforward time integration may lead to increasing errors for decreasing time steps. An index-1 reformulation brings up a dense system. The solution thereof becomes feasible when applying the Woodbury formula for rank-n corrected matrices.

Key words: field-circuit coupling, electromagnetic field simulation, time stepping, numerical stability

1 Introduction

Field-circuit coupled models are extensively used in electrotechnical and electronic design procedures. After finite-element (FE) discretisation, the field-circuit coupled magnetoquasi-static formulation in terms of the magnetic vector potential (MVP) reads

$$\begin{bmatrix} s\mathbf{M}_{\sigma} + \mathbf{K}_{\nu} & -\mathbf{X}_{\text{str}} \\ s\mathbf{X}_{\text{str}}^{T} & \mathbf{R}_{\text{str}} \end{bmatrix} \begin{bmatrix} \widehat{\mathbf{a}} \\ \mathbf{i}_{\text{str}} \end{bmatrix} = \begin{bmatrix} 0 \\ \mathbf{u}_{\text{str}} \end{bmatrix} , \qquad (1)$$

where K_{ν} and M_{σ} are the FE reluctance-loop and conductance matrices, *s* denotes the (discrete) time derivative, X_{str} distributes the currents i_{str} applied to the *n* coils to the computational grid, \hat{a} collects the degrees of freedom (DoFs) for the MVP, R_{str} is an *n*-by-*n* diagonal matrix of the coil resistances and u_{str} are the voltages applied to the coils. Typically (1) is solved for given currents

$$(s\mathbf{M}_{\sigma} + \mathbf{K}_{\nu})\widehat{\mathbf{a}} = \mathbf{X}_{\rm str}\mathbf{i}_{\rm str}$$
(2)

and the voltages are obtained by postprocessing. In [2, 3], it is shown that (1) for given currents i_{str} is an index-2 problem and leads to unacceptably large errors when standard time integrators (e.g. implicit Euler) are used with too small time steps.

The favourable index-1 property is guaranteed by the alternative formulation

$$\left(\mathbf{K}_{\nu} + s(\mathbf{M}_{\text{str}} + \mathbf{M}_{\sigma})\right)\widehat{\mathbf{a}} = \mathbf{X}_{\text{str}}\mathbf{R}_{\text{str}}^{-1}\mathbf{u}_{\text{str}} \quad , \tag{3}$$



Figure 1: Small inductor with voltage-driven coil; solution for voltage and current.

where $\mathbf{M}_{\text{str}} = \mathbf{X}_{\text{str}} \mathbf{R}_{\text{str}}^{-1} \mathbf{X}_{\text{str}}^{T}$ is considered as an *n*-rank correction to $\mathbf{K}_{\nu} + s\mathbf{M}_{\sigma}$. The additional term spoils the sparsity of $\mathbf{K}_{\nu} + s\mathbf{M}_{\sigma}$. This seriously diminishes the computational efficiency of the field-circuit coupled formulation. For that reason, (2) is favoured over (3), despite of the disastrous time-integration error.

2 Dedicated System Solution

At every time step, a system of the form (3) has to be solved. The Woodbury formula allows to reorganise this procedure into the application of

$$\left(\mathbf{I} - \mathbf{W}_{\text{str}} \mathbf{Z}_{\text{str}}^{-1} \mathbf{s} \mathbf{X}_{\text{str}}^{T}\right) \left(\mathbf{K}_{\nu} + \mathbf{s} \mathbf{M}_{\sigma}\right)^{-1}$$
(4)

to a vector. Here, $\mathbf{W}_{\text{str}} = (\mathbf{K}_{\nu} + s\mathbf{M}_{\sigma})^{-1} \mathbf{X}_{\text{str}}$ is a precomputed set of unit discrete field fluxes (fluxes arising from unit currents in the coils), $\mathbf{L}_{\text{str}} = \mathbf{X}_{\text{str}}^T \mathbf{W}_{\text{str}}$ is the inductance matrix and $\mathbf{Z}_{\text{str}} = \mathbf{R}_{\text{str}} + s\mathbf{L}_{\text{str}}$ is the system's impedance. Compared to the application of $(\mathbf{K}_{\nu} + s\mathbf{M}_{\sigma})^{-1}$, the application of (4) only requires 2n additional vector-vector operations and the solution of an *n*-by-*n* system. Hence, it is only marginally more expensive than solving (1). Moreover, a standard multigrid algorithm for $(\mathbf{K}_{\nu} + s\mathbf{M}_{\sigma})^{-1}$ remains applicable. The proposed approach, however, requires the precomputation of \mathbf{W}_{str} , which amounts to solving *n* systems with matrix $\mathbf{K}_{\nu} + s\mathbf{M}_{\sigma}$ on beforehand. This is feasible as long as *n* is substantially smaller than the number of time steps and $\mathbf{K}_{\nu} + s\mathbf{M}_{\sigma}$ does not change over time, e.g. due to nonlinearities. The approach is illustrated for an inductor example (Fig. 1).

Acknowledgements

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Double Sweep Preconditioners for propagation problems solved by Optimized Schwarz Methods

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Abstract

We present a parallel version of the otherwise sequential double sweep preconditioner, used to accelerate the convergence of an optimized Schwarz domain decomposition method. The method is based on the same sweeping strategy, yet applied on a shorter scale and in parallel, on distinct groups of subdomains. The modified algorithm, unlike the original one designed for layered decompositions, has the advantage of being directly applicable to cyclic decompositions as well. The whole method is described in terms of combinations of transport operators and is therefore suitable to both Helmholtz and frequency-domain Maxwell problems.

Key words: Domain Decomposition, Preconditioner, Propagation, High Frequency.

1 Introduction

The idea of sweeping for the solution of wave propagation problems in the frequency domain, of the form $(\Delta + k^2)\mathbf{u} = 0$, is quite natural, since it somehow mimics the physical phenomenon of a wave propagating inside a medium. It is therefore not surprising that techniques inspired by this observation have proved successful [1, 2]. In the slightly different context of Domain Decomposition solvers for these problems, we have recently proposed the double sweep preconditioner for the non-overlapping optimized Schwarz algorithm [3]. A limitation of the method is the sequential nature of the sweeping process that makes the iterative part of the solution less scalable on parallel architectures—the factorization of the subproblems remaining fully parallel. This paper addresses that issue, by proposing a modification of the algorithm to partially restore its parallelism.

2 Algorithms

The double sweep preconditioner was originally designed as the inverse of the iteration operator in the particular case of a layered decomposition, supposing that perfectly non-reflecting operators are used as transmission condition. In that case, the matrix that represents the iteration operator is easy to invert. Since it is, like its inverse, made of transport operators that involve the solution of subproblems, we give it an interpretation in terms of a combination of such subproblems. It is a double sequence of solves, that we call the forward and backward sweeps. That inverse is then used to precondition more complex problems [3].



Unlike the standard algorithm, the application of the preconditioner is sequential and exploits no more than 2 CPUs simultaneously, which is a very suboptimal use of the resources if more CPUs are available. By performing the sweeps independently and concurrently over smaller groups of domains, we still benefit of the long range sharing of information provided by the sweeps, while reducing the idleness of the CPUs (Figure 1). Introducing a cut in a cyclic decomposition makes it topologically equivalent to a layered one, making the preconditioner readily applicable.



Figure 1: Timelines of the double sweep preconditioner application without cuts (left) and with 2 cuts (right). The white diamonds indicate solves performed in the iteration operator; the black circles and squares indicate solves in the forward and backward sweeps, respectively.

Table 1 shows the number of iterations and an estimation of the normalized time required to attain convergence $(||r||/||r_0|| < 10^{-4})$ for the solution of a Maxwell problem in the challenging COBRA cavity benchmark. The standard algorithm (np) failed to converge, while the (wall-clock) time to solution with the preconditioned algorithm (ds) decreases when cuts are added, though too many cuts are detrimental (the reported times do not include subproblem factorization).

#CPU	2	4	6	8	14	22		
N _c	0	1	2	3	6	10		
$N_{ m it}^{ m (ds)}$	44	74	105	135	230	354		
$T_{\rm sol}^{\rm (ds)}$	2024	1702	1680	1485	1610	1416		
$N_{\rm it}^{\rm (np)}$	> 1000							
$T_{\rm sol}^{(\rm np)}$	> 16016	> 8008	> 5339	> 4004	> 2288	> 1456		

Table 1: COBRA test case for Maxwell with 32 subdomains (N_c cuts) at k = 314.16.

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Coupled Boundary Conditions for Co-simulation of Power System Dynamics

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Abstract

Co-simulation of power system dynamics requires the choice of proper boundary conditions at the interface between the subdomains, which greatly influences the rate of convergence of the co-simulation relaxation iterations. In this paper, Dirichlet boundary conditions are compared to disjoint and coupled impedance boundary conditions in terms of the mean number of relaxation iterations. The study is illustrated by a test case in which the power system under study is divided into two subdomains, connected through three connection busses. The subdomains are represented with different modeling assumptions, simplified and full-transient models respectively.

Key words: Co-simulation, Boundary Conditions, Power Systems

1 Co-Simulation of Power System Dynamics

Power systems dynamic models are generally classified in two categories depending on the time-scale of the phenomena under study: Phasor-Mode (PM) models and ElectroMagnetic Transients (EMT) ones. In PM models, the three-phase system is represented with a single-phase equivalent and the dynamics are approximated by a succession of sinusoidal regimes (phasors with time-varying amplitude and phase). The EMT models take into consideration virtually any fast transient phenomenon. Both models are represented by sets of Differential Algebraic Equations (DAEs). Co-simulation combines the speed of PM models with the details of EMT ones [1]. Improvements in accuracy [2] and convergence [3] still require research.

2 Coupled Boundary Conditions

Fig. 1 represents the test-case power system. It was subdivided into two subdomains, connected through N = 3 boundary busses 4041, 4044 and 4042. The expression $\mathbf{\bar{I}} = \mathbf{Y}_0 \mathbf{\bar{V}} + \mathbf{\bar{I}}_0$ is the impedance boundary condition that links the boundary current vector $\mathbf{\bar{I}}$ with the vector of boundary voltages $\mathbf{\bar{V}}$. If coupled boundary conditions are considered, \mathbf{Y}_0 is an NxN full matrix that can be either predetermined or calculated on-the-fly.



Figure 1: Boundary conditions for PM and EMT subdomains.

Fig. 2 shows the number of relaxation iterations obtained on a single-bus connection test case when varying the ratio between the estimated admittance \hat{y}_{emt} and the true value y_{emt}^* .



Figure 2: Relaxation iterations sensitivity to the value of the boundary admittance.

In the full paper the convergence will be assessed when either disjoint or coupled boundary conditions are used, the latter being predetermined or calculated on-the-fly.

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Anisotropic and Feature Sensitive Triangular Remeshing using Normal Lifting

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Abstract

This work describes an automatic method to anisotropically remesh an input bad quality mesh while preserving sharp features. We extend the method of [1], based on the lifting of the input mesh in a 6D space (position and normal), and the optimization of a restricted Voronoï diagram in that space. The main advantage of this method is that it does not require any parameterization of the input geometry: the remeshing is performed globally, and triangles can overlap several input charts. We improve this work by modifying the objective function minimized in the optimization process, in order to take into account sharp features. This new formulation is a generalization the work of [2], which does not require any explicit tagging of the sharp features. We provide efficient formulas to compute the gradient of our objective function, thus allowing us to use a quasi-Newton solver [3] to perform the minimization.

Key words: geometry, mesh generation, restricted Voronoï diagram

1 Introduction

In this work, we focus on the problem of *triangular surface remeshing*. Our approach is based on the optimization of restricted Voronoï diagrams, which is a generalization of Lloyd's algorithm for the sampling of surfaces. The remeshing is performed in two steps. First a regular sampling of the input surface is generated using an optimization procedure on the sample positions. Then the samples are connected with triangles to form the output mesh using the restricted Delaunay triangulation of the samples. [1] embed the input mesh in 6D space by appending the normal coordinates to the vertex coordinates. An isotropic remeshing in this 6D space is performed and then projected as an anisotropic remeshing in 3D space. We propose an improvement of this approach, preserving the sharp features of the input mesh.

2 Contributions

[2] manage to take sharp features into account in the case of a remeshing in 3D space. Their formulation however relies on the normal of the input mesh, and is therefore not applicable in the context of a mesh embedded in 6D space, where triangles have a *normal space* rather than





Figure 1: Parameters of our algorithm: the density controls how small the elements get in regions where the normal varies, the anisotropy how thin the elements become in these regions, and the feature sensitivity controls the influence of the sharp features. For comparison, [1] provide anisotropy and density, while [2] provide feature sensitivity.



Figure 2: Remeshing a CAD model. The input is the raw mesh used to render the object (36k vertices). The meshes of the various patches do not match on boundaries and cracks appear. The remeshing is done in 75 seconds for 20k vertices.

a simple normal. We provide a new formulation based on the *tangent space* of a triangle, thus generalizing their method for meshes embedded into any higher dimensional space. We also provide new formulas for the gradient of the minimized objective function, using Reynold's transport theorem. Our final algorithm has three major parameters summarized on section 2, controlling the feature preservation, and both the anisotropy and the density of the elements in curved regions of the input mesh. As shown on Figure 2, our method successfully handles bad quality input meshes with cracks and very stretched triangles. We neither use a parameterization of the input mesh, nor require any manual or third party tagging of sharp features.

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Optimizing the geometrical accuracy of 2D curvilinear finite element meshes

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Abstract

We present a procedure for optimizing curved two-dimensional finite element meshes, which aims at minimizing the distance between the mesh and the underlying CAD model. The method allows both to ensure mesh validity and geometrical accuracy.

Key words: geometry, mesh generation, curved meshes, high-order methods

1 Introduction

The development of high-order numerical technologies for engineering analysis has been underway for many years now. For example, Discontinuous Galerkin methods have been largely studied in the literature, initially in a theoretical context, and now from the application point of view. In many contributions, it is shown that the accuracy of the method strongly depends on the accuracy of the geometrical discretization.

The aim of this paper is to present a method that enables to build geometrically accurate curvilinear meshes.

2 Geometrical accuracy

Consider a model entity G and the mesh entity M that is supposed to discretize G. The first questions to address are the following ones: how do we define a proper distance d(G, M) between G and M and how do we compute this distance efficiently? Two principal definitions for such distances have been proosed in the computational geometry literature, namely the Fréchet distance and the Hausdorff distance [3, 4]. In this paper, we present a way to accurately compute such distances between a curvilinear finite element mesh and its underlying CAD.

The next step is to minimize d(G, M) in order to obtain a valid [1] and accurate high order mesh. Figure 1 shows different meshes of a NACA0012 wing where the optimization procedure [2] was able to reduce the CAD-to-mesh distance by two orders of magnitude.









(b) unoptimized quadratic mesh with invalid elements



(c) valid quadratic mesh without geometrical accuracy optimization [1]

(d) geometrically optimized valid quadratic mesh



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Parallel Finite Element Assembly of High Order Whitney Forms

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Abstract

This paper presents an efficient method for the finite element assembly of high order Whitney elements. We start by highlighting the most time consuming parts of the classical assembly technique. This approach can be reformulated into a computationally efficient matrix-matrix product. We conclude by presenting numerical results.

Key words: finite element, high order, high performance computing, Whitney elements

1 Introduction

There is a growing consensus that state of the art finite element (FE) technology requires, and will continue to require, too extensive computational resources to provide the necessary resolution for complex high-frequency electromagnetic compatibility simulations, even at the rate of computational power increase. This leads us to consider methods with a higher order of grid convergence than the classical second order.

2 Classic finite element assembly

By applying the classical Galerkin FE scheme with a curl-conforming basis, the solution of the time harmonic propagation of an electrical wave is computed using elementary integrals $\mathcal{T}_{i,j}^{e}$, as developed in [2]. Each $\mathcal{T}_{i,j}^{e}$ is giving the contribution of the degrees of freedom (DOF) *i* and *j* of the mesh element *e*.

The classical FE assembly algorithm computes the $\mathcal{T}_{i,j}^{e}$ terms for every pair of DOF *i* and *j* on every element *e* of the mesh. It is worth noticing that increasing the basis order will have two impacts on the computation time: each element will have more DOFs and the numerical quadrature will require more points. These two phenomena will substantially increase the assembly time, as shown in Figure 1.

3 Efficient assembly

The key idea of a fast assembly procedure is to compute all the $\mathcal{T}_{i,j}^{e}$ terms using matrix-matrix products, as proposed by [3, 4] for standard nodal Lagrange finite elements. Indeed, this operation has an excellent cache reuse and highly optimized implementations can be found.



The $\mathcal{T}_{i,j}^{e}$ terms can be computed by the product of two matrices. The first matrix will be composed of the Jacobian matrices and non linear terms. The second matrix will be composed only of the basis functions defined over the reference element.

It is worth noticing that depending on the mesh elements orientation, the curl-conforming basis functions cannot simply be reordered, as for classical H^1 Lagrange bases. This situation may be overcome by considering more than one reference element, as proposed by [1].

4 Numerical results

Figure 1 presents the assembly times of the classical and efficient assembly procedures for an increasing basis order. The FE matrix is assembled for a propagation problem into a wave guide, meshed with 8579 curved tetrahedra. The tests were done on a Intel Core i7 960 and by using the OpenBLAS implementation of the matrix-matrix product with 4 threads. It is worth mentioning that the classical implementation also uses 4 threads for the assembly.



Figure 1: Assembly time and speedup for the classical and fast procedures

It can be seen from Figure 1 that the matrix procedure is much faster than the classical one for high order interpolations. For instance, the speedup on an order 6 problem, with more than 900.000 unknowns, is around 20.

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A limit on the stability of volume-of-fluid methods in quiescent two-phase flow simulations

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Abstract

The simulation of quiescant water with volume-of-fluid methods gives rise to spurious velocities. From a certain treshold on time step, these velocities grow in unstable modes. The mechanism for the instability is identified and a quantitative upper bound for a stable time step is given. Theoretical results are checked against simulated cases.

Key words: CFD, volume of fluid, two-phase flow, stability, time step restriction MSC 2010: 35Q30, 65M12, 76T10

1 Introduction

This paper presents the result of a study on the appearance of unstable modes in the twophase flow solver interFoam. InterFoam is a part of the open-source OpenFOAM library for Computational Fluid Dynamics [1], and solves the Navier-Stokes equations together with a transport equation for the Volume of Fluid (VoF).

The appearance of unstable modes is already obvious when trying to find a solution for the hydrostatic case (the "bucket of water"), using orthogonal meshes, aligned with gravity. Once the solution is initialized, one does not expect anything to happen. However, it appears that the solution is unstable for time steps much smaller than the stable time step predicted by the CFL-criterion. We were able to identify the mechanism for the instability, which is explained below.

2 Governing Equations

In order to identify the source of the instability, subsequently, terms in the original equations were elimated. As such, we arrived at a stripped system of a constant density flow, with a buoyancy force, proportional to the gradient of the volume fraction:

$$\frac{\partial \alpha}{\partial t} + \nabla \cdot (u\alpha) = 0 \tag{1}$$

$$\frac{\partial u}{\partial t} = -\nabla p_{rgh} - gh\nabla\alpha \tag{2}$$

$$7 \cdot u = 0, \tag{3}$$



with a similar behaviour concerning the spurious velocities as the original solver. α is the VoF function, *u* the velocity, p_{rgh} a modified pressure, *g* the gravitational acceleration and *h* the local heigth (vertical coordinate). The system is solved as follows. First, the equation for α (1) is progressed in time, using an explicit step. Next, the velocity is predicted from the momentum equation (2), disregarding the effect of pressure and buoyancy. The velocity is corrected after solving an equation for pressure, following from combination of (2) and (3).

3 Derivation of an upper bound for the time step restriction

The above system proves unstable for high time steps. Indeed: after the solving the pressure equation, a correction is added to the face volume flux:

$$u^{n+1} = u^* + \dots - \Delta t g h \nabla \alpha \tag{4}$$

Taking the derivative of the above equation with respect to time and making use of the explicit VoF equation (with u evaluated at the phase), we can destillate an amplification factor G for the stripped algorithm:

$$\frac{\partial u^{n+1}}{\partial t} = \frac{\partial u^*}{\partial t} + \dots + \Delta t g h \nabla \left(\nabla \cdot (u\alpha) \right), \tag{5}$$

$$G = 2 \frac{(\Delta t)^2}{(\Delta x)^2} gh\alpha \le 2 \frac{(\Delta t)^2}{(\Delta x)^2} gh.$$
(6)

A stable solution is obtained when G < 1:

$$\Delta t < \frac{\Delta x}{\sqrt{2gh}}.\tag{7}$$

The time step restriction is only applicable in multi-dimensional simulations, as in 1D, the pressure perfectly counterbalances the buoyuancy force. In multi-D, the pressure equation is only a weak formulation of this counterbalancing effect, and hence the rotational component of $gh\nabla\alpha$ is a trigger for instability. As such, after some manipulation a better estimate of the time step restriction (7) can be determined:

$$\Delta t < \frac{\Delta x}{\sqrt{g\Delta x}}.\tag{8}$$

As an example, the above restrictions were evaluated on a mesh with grid cell size $0.1m \times 0.1m$. By virtue of (8) a stable time step of 0.1 seconds is predicted. During simualtion, an unstable solution was obtained from $\Delta t = 0.3s$ onwards, where a growing diffusivity of the interface was seen to aid in the stability of the entire solution.

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A geometric multigrid solver for the free-surface equation in environmental models featuring irregular coastlines

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Abstract

A recently developed multigrid method [Botto, CPC 184, 1033–1044] has been tested for the inversion of the Helmholz-type equation for the free surface in the environmental public domain code COHERENS. Using standard multigrid, convergence issues might arise in cases where coarse grid cells are agglomerated from both dry and wet cells at irregular coastlines. We show that by modifying the prolongation operator and the coarse grid discretization, better convergence is obtained. Several test cases from literature support this conclusion.

Key words: multigrid, Helmholz equation, shallow water flow, stair-case boundary MSC 2010: 35J05, 35Q35, 65M08, 65M55

1 Problem statement and method description

The present paper is a continuation of the work, presented in [6], where the 3D hydrostatic free surface flow solver COHERENS [4] was modified into a semi-implicit solver for acceleration of the code. As a result of this operation, an elliptic equation for the free surface ζ needs inversion:

$$\frac{\partial\zeta}{\partial t} - \frac{\partial}{\partial x} \left(gH\Delta t \frac{\partial\zeta}{\partial x} \right) - \frac{\partial}{\partial y} \left(gH\Delta t \frac{\partial\zeta}{\partial y} \right) = -\frac{\partial U^*}{\partial x} - \frac{\partial V^*}{\partial y}.$$
 (1)

The present contribution involves the implementation of a geometric multigrid solver, to achieve further acceleration. We use Gauss-Seidel Red-Black iterations as a smoother, standard averaging for the restriction and bilinear prolongation in a multigrid W-cycle on the staggered mesh configuration. The code typically uses meshes that are not aligned with the boundaries, resulting in a stair-case representation of e.g. coastlines (Fig. 1a). This has particular repercussions on the multigrid scheme, since coarse cells can be made out of both wet and dry cells on the finer level. Recent progress on how to deal with these circumstances is reported in [1, 2, 3, 5]. We follow the approach of [2], introducing a cell volume fraction β , indicating the amount of fine grid wet cells in one coarse cell. This parameter is then introduced in the time derivative term of eq. (1) and in the prolongation operator.



The method shows good convergence on the Rhône-estuary test case presented (Fig. 1b). In case no β -weighting is used, the method converges more slowly, confirming the results of [3]. In contrast to the findings of [5], we did not encounter any instabilities because of insufficient error smoothing the boundaries.

In the full paper, more details on the method, convergence tests and a series of challenging test problems, including obstacles of different shapes, are presented.



Figure 1: Results from test-case Rhône, featuring stair-case boundaries.

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An immersed-boundary lattice Boltzmann method using local mesh refinements for simulation of flows around multiple moving objects

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Abstract

Relevant to a large number of industrial applications, moving boundary problems have been routinely simulated using different computational fluid dynamics approaches. As a novel strategy, this study is aimed at enhancing the variant immersed-boundary lattice Boltzmann method (IB-LBM) by more seamlessly connecting the feedback model with local mesh refinement techniques, so that an enlarged class of moving boundary problems, including the interactions between flowing fluids and moving objects of engineering interests, can be numerically investigated. Owing to the utilization of both explicit and implicit schemes in the present approach, the advantages resulting from this hybrid method, such as simple principle, easy implementation, and inherent satisfaction of no-slip boundary condition for solid surfaces, are fully exhibited. The local mesh refinement procedure employed in the present approach relies on the bubble function, which requests only the spatial interpolation but no temporal interpolation. Ranging from the flows around a single cylinder of both stationary and mobile natures to the flow around bi-cylinders in motion with respect to each other, a variety of test cases performed in this study has demonstrated the accuracy of the present IB-LBM approach when compared to the results obtained by using other numerical methods. Moreover, the IB-LBM is also employed to simulate a more challenging flow associated with a flapping wing as moving object, the analysis is fully provided on the influences of the Reynolds number, flapping amplitude, and phase difference between the translation and rotation motions on the aerodynamic performance in this case, and the usefulness and effectiveness of this new approach are further revealed.

Key words: Lattice Boltzmann method, Immersed boundary method, Feedback model, Mesh refinement, Moving boundary

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Numerical Integration of Lattice Systems with a Lyapunov Function

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Abstract

In this contribution we implement and assess numerical methods for gradient systems, i.e. dynamical systems that possess a Lyapunov function, and consequently are stable. In particular, we claim that discrete gradient methods are well suited to so-called lattice systems, i.e. systems of ordinary differential equations that can reach high dimensionality. For these systems, reproducing the stable qualitative behaviour is more important than achieving an overly accurate quantitative approximation. The presented results show that discrete gradient methods outperform conventional Runge-Kutta methods, since these latter algorithms destroy the stability of the original system.

Key words: Gradient Systems, Geometric Numerical Integration, Lyapunov Function, Discrete Gradient, Lattice Systems MSC 2010: 34D20, 65P40

1 Introduction

The main aim of this paper is to analyse the performance of numerical methods specifically designed to preserve the Lyapunov function of a stable dynamical system. In particular, we deal with higher-dimensional systems of Ordinary Differential Equations (ODEs), which can be regarded as abstract models of lattice systems arising in a wide variety of fields of physics, biology and engineering, e.g. the Ising model in statistical mechanics, and the Toda lattice in crystallography. Although some of these systems present a cyclic behaviour, it is often the case that the system converges towards a stable state while, at the same time, the energy diminishes.

From a mathematical point of view, the energy-diminishing feature amounts to proving that the system possesses a Lyapunov function, which in turn is a proof for the asymptotic stability of fixed points (see e.g. [3] for references and background). In other words, the distinguishing characteristic of a Lyapunov function is that it decreases along the system trajectories and the main goal of this work is to reproduce this behaviour under discretization by a numerical method. ODEs with a Lyapunov function V receive the name of *gradient systems* because they can be rewritten as

$$\frac{d\mathbf{y}}{dt} = L(\mathbf{y})\,\nabla V(\mathbf{y})\tag{1}$$



where $\nabla V(y)$ is the gradient of *V* and *L* is a negative definite matrix.

Within the framework of Geometric Numeric Integration [1], many methods for ODEs have been designed to preserve qualitative features. However, most of these proposals are related to symplectic methods, i.e. methods for Hamiltonian systems. In contrast, numerical methods for gradient systems are scarce. In this regard, because of its conceptual simplicity, discrete gradient methods [4] are appealing, but there is still limited experience as to their relative strengths and limitations. This paper aims at exploring a discrete gradient method, by undertaking its implementation and application to a particular class of lattice systems.

2 Discrete gradient methods for Hopfield neural networks

Discrete gradient methods consist in approximating (1) by the iteration

$$\frac{\mathbf{y}_{n+1} - \mathbf{y}_n}{h} = \widetilde{L}(\mathbf{y}_n, \mathbf{y}_{n+1}, h) \ \overline{\nabla} V(\mathbf{y}_n, \mathbf{y}_{n+1}),$$

where \widetilde{L} and $\overline{\nabla}V$ are discretizations of L and ∇V , respectively, which must fulfil the consistency conditions $\widetilde{L}(\mathbf{y}, \mathbf{y}, \mathbf{0}) = L(\mathbf{y})$ and $\overline{\nabla}V(\mathbf{y}, \mathbf{y}) = \nabla V(\mathbf{y})$. Besides, the discrete gradient is defined by the requirement $\overline{\nabla}V(\mathbf{y}_n, \mathbf{y}_{n+1}) \cdot (\mathbf{y}_{n+1} - \mathbf{y}_n) = V(\mathbf{y}_{n+1}) - V(\mathbf{y}_n)$. It is worth emphasizing that there is considerable freedom in the choice of \widetilde{L} and $\overline{\nabla}V$, so one of the contributions of this work is to determine which values of these design parameters result in more favourable solutions. We have implemented the *coordinate increment discrete gradient*, whereas the matrix \widetilde{L} is assumed to be identical to L. It turns out that this choice allows for obtaining an explicit method for particular cases of ODEs.

Continuous Hopfield neural networks [2] were proposed as a model of biological neurons, given by the system of ODEs:

$$\frac{du_i}{dt} = \sum_{j=1}^n w_{ij} y_j - b_i, \quad y_i = \tanh u_i, \quad 1 \le i \le n.$$

These networks may be defined for a high dimension n, and they possess a multilinear Lyapunov function $V(\mathbf{y}) = -\frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} y_i y_j + \sum_{i=1}^{n} b_i y_i$. After eliminating the internal variables u_i , this model can be cast into the gradient form of (1). The numerical experiments that have been performed show that the discrete gradient method preserves the energydiminishing feature of Hopfield networks, whereas the Euler rule and other conventional Runge-Kutta methods fail to reproduce the expected stable behaviour. Also, the implemented discrete gradient method is computationally favourable, since it can be written in explicit form.

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Kernel reconstruction in a semilinear parabolic problem with integral overdetermination

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Abstract

A semilinear parabolic problem of second order with an unknown solely time-dependent convolution kernel is considered. The missing kernel is recovered from an additional integral measurement. The existence, uniqueness and regularity of a weak solution is addressed. We design a numerical algorithm based on Rothe's method, derive a priori estimates and prove convergence of iterates towards the exact solution.

Key words: parabolic IBVP, convolution kernel, reconstruction, convergence, a priori estimates

1 Introduction

We want to determine the solution u and reconstructed a solely time-dependent convolution kernel K of the following nonlinear problem

$$\begin{cases} \partial_t u - \Delta u + K(t)h + (K * u)(t) = f(u, \nabla u), & \text{in } \Omega \times \Theta, \\ -\nabla u \cdot \mathbf{n} = g, & \text{on } \Gamma \times \Theta, \\ u(\mathbf{x}, 0) = u_0(\mathbf{x}), \end{cases}$$
(1)

where Ω is a Lipschitz domain in \mathbb{R}^N , $N \ge 1$, with $\partial \Omega = \Gamma$ and $\Theta = [0,T]$, T > 0, the time frame, when a global measurement

$$\int_{\Omega} u(\mathbf{x},t) \mathrm{d}\mathbf{x} = m(t)$$

is known.

Such type of integro-differential problems arise for example elastoplasticity (cf. [1]) or in the theory of reactive contaminant transport. In [2] one considers the following differential equation

$$\partial_t C + \nabla \cdot (\mathbf{V}C) - \Delta C = \frac{-\rho_b}{n} \partial_t S$$

for the aqueous concentration C and sorbed concentration per unit mass of solid S with mass transformation rate in first order kinetics form of

$$\partial_t S = K_r (K_d C - S)$$



with desorption rate K_r and equilibrium distribution coefficient K_d . This is indeed a problem of type (1) for u = C with

$$K(t) = -\frac{\rho_b}{n} K_r^2 K_d e^{-K_r t}, \quad h(t) = -\frac{S_0}{K_r K_d} \quad \text{and} \quad f(x, \mathbf{r}) = \frac{-\rho_b}{n} K_r K_d x - \mathbf{V} \cdot \mathbf{r}.$$

We will prove the following existence and uniqueness result.

Theorem Suppose f is bounded and Lipschitz continuous in all variables, $g \in C^1(\Theta, L^2(\Gamma))$, $h \in C^0(\Theta, H^1(\Omega)) \cap C^1(\Theta, L^2(\Omega))$ and $\min_{t \in \Theta} |(h(t), 1)| \ge \omega > 0$, $m \in C^2(\Theta, \mathbb{R})$ and $u_0 \in H^2(\Omega)$. Then there exists a unique couple solutions $\langle u, K \rangle$ to (1), where $u \in C(\Theta, H^1(\Omega))$, $\partial_t u \in L^{\infty}(\Theta, L^2(\Omega))$ and $K \in C(\Theta)$, $K' \in L^2(\Theta)$.

Moreover we construct a numerical model to solve this problem based on the variational formulation and Rothe's functions [3].

Algorithm: numerical scheme in pseudo code
input : $T > 0, n \in \mathbb{N}$ and functions f, g, h, m and u_0
output : kernel <i>K</i> and solution <i>u</i> at discrete time steps
$\tau \leftarrow T/n;$
$2 \ \theta \leftarrow [0:\tau:T];$
$_{3} \text{ K} \leftarrow \text{zeros}(n+1);$
$_{4}$ u \leftarrow eval $(u_{0}, \theta);$
₅ K[0] ← $\frac{1}{(h_0, 1)}$ ((f(u_0, ∇u_0), 1) − m'_0 − (g_0, 1)_Γ);
6 for $i = 1$ to n do
7 $K[i] \leftarrow \frac{1}{(h_i, 1) + m_0 \tau} \left((f_{i-1}, 1) - (g_i, 1)_{\Gamma} - \sum_{k=1}^{i-1} K_k m_{i-k} \tau - m'_i \right);$
8 $\lfloor u[i] \leftarrow solveEP(B(u_i,\phi) = F_i(\phi));$

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