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Abstracts Plenary Sessions

Sustained petaflop/s computing: an application developer's perspective
By Thomas C. Schulthess

Peta-scale computers are monstrous (literally speaking) compared to the workstations or clusters most scientists use when developing models, methods and codes. Yet, several applications that sustain a petaflop/s under production condition on general-purpose supercomputers have emerged within months of the existence of systems that could sustain a petaflop/s on the Linpack benchmark. In this presentation we will review the developments that lead to the much faster than expected advent of "sustained petaflop/s computing". The experience of integrated teams that unify domain knowledge, applied mathematics and computer science, as well as the challenge to develop applications to solve models of complex systems call for a nimble programming environment. We will discuss the use of generic libraries and the concept of just in time abstraction that enable several of today's sustained petaflop/s applications.

Robust high-order finite volume schemes for multi-dimensional ideal MHD equations
by Siddhartha Mishra

Many macroscopic plasma models, arising in astrophysics, solar physics, electrical and aerospace engineering are modeled with the equations of ideal Magneto-HydroDynamics (MHD).

These constitute a non-linear system of conservation laws in several space dimensions, augmented with the divergence constraint. Efficient numerical simulation for the MHD equations is quite complicated on account
of the lack of strict hyperbolicity or convexity of the equations and due to the divergence constraint. We design robust finite volume schemes for an equivalent Godunov-Powell form of the MHD equations, based on HLL type
approximate Riemann solvers for computing numerical fluxes. The Godunov-Powell source term is discretized in an upwind manner using the local wave structure. Positivity preserving non-oscillatory high-order reconstructions are also proposed. The resulting schemes are tested on a large number of benchmark numerical experiments in two and three space dimensions. The talk is based on joint work with F. Fuchs, A. D. McMurry, N. H. Risebro (CMA, Univ. of Oslo, Norway) and K. Waagan (CSCAMM, Univ. of Maryland, U.S.A).

Second-Order EllipticPDE with discontinuous boundary conditions

Thomas Wihler

Abstract

We will consider the weak formulation of linear elliptic PDE with discontinuous Dirichlet boundary conditions. Since such problems are typically not well-defined in the standard $H^1 - H^1$ setting, we will introduce a suitable saddle point formulation in terms of weighted Sobolev spaces. Furthermore, we will discuss the numerical solution of such problems. Specifically, we employ an hp–discontinuous Galerkin method and derive an L^2-norm a posteriori error estimate. Numerical experiments demonstrate the effectiveness of the proposed error indicator in both the h– and hp–version setting. Indeed, in the latter case exponential convergence of the error is attained as the mesh is adaptively refined.

Time domain Maxwell equations and Schwarz Waveform Relaxation methods

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A short historical introduction to Schwarz Waveform Relaxation (SWR) method and its optimized versions will be presented. Those will then be applied to the time domain Maxwell equations. We present and study optimized transmission conditions for Maxwell's equations, and show some analogies between the Maxwell equations and the wave equation. We first recall a result stating that the wave equation solved with the SWR method converges in a finite number of steps depending on the time window and the overlap, and show that the same is true for Maxwell's equations. Then we emphasize the strong link between the wave equation and the time domain Maxwell equations, and use this link to show how one can obtain optimized local transmission conditions from the previously defined optimal transmission conditions. This effort emphasizes the wave behavior of solutions of Maxwell's equation and uses results for the wave equation in order to simplify the analysis.

Modeling boundary conditions for solving stationary Schrödinger equations

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Abstract

In this talk we present some novel absorbing boundary conditions (ABCs) for modeling the solution of linear and nonlinear variable potentials one-dimensional stationary Schrödinger equations. Using pseudodifferential calculus and factorization theorems we construct a hierarchy of novel ABCs and generalize the well-known quantum transmitting boundary condition of Kirk and Lentner to the case of space-dependent potential. Moreover, we propose a rapidly converging iterative method based on finite elements suitable for computing scattering solutions and bound states. The accuracy of our new absorbing boundary conditions is investigated numerically for two different situations. The first problem is related to the computation of linear scattering problems. The second application concerns the computation of energies and ground-states for linear and nonlinear Schrödinger equations. It turns out that these absorbing boundary conditions and their variants lead to a higher accuracy than the usual Dirichlet boundary condition. Finally, our approach also offers the possibility to construct ABCs for higher dimensional problems.

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HIGH-ORDER EXPLICIT LOCAL TIME-STEPPING FOR DAMPED WAVE EQUATIONS

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The accurate and reliable simulation of wave phenomena is of fundamental importance in a wide range of engineering applications. In the presence of complex geometry, adaptivity and mesh refinement are certainly key for the efficient numerical solution of the damped wave equation. Locally refined meshes, however, impose severe stability constraints on explicit time-stepping schemes due to the smallest elements in the mesh. When mesh refinement is restricted to a small region, the use of implicit methods, or a very small time step in the entire computational domain, are very high a price to pay. To overcome that stability restriction, local time-stepping methods are developed, which allow arbitrarily small time-steps precisely where small elements in the mesh are located. When combined with a finite element discretization in space with an essentially diagonal mass matrix, the resulting discrete numerical scheme is fully explicit. Starting from the standard leap-frog scheme, explicit second-order local time-stepping integrators for transient wave motion have been derived [**?**, **?**]. In the absence of damping these time-stepping schemes, when combined with the modified equation approach [**?**], yield methods of arbitrarily high (even) order. In the presence of damping, however, this approach cannot be used effectively. Therefore, we derive explicit local time-stepping schemes of arbitrarily high accuracy starting insted from explicit multi-step Adams-Bashforth methods. Numerical experiments validate the theoretical results and illustrate the efficiency of the proposed time integration schemes.

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Analysis and numerical analysis of a nonlinear Stokes problem arising in glaciology

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In this talk, a three dimensional problem describing the motion of glaciers is addressed. An ice flow model that accounts for shearing and sliding is coupled with a complex mass balance model accounting for climate. This allows a numerical simulation of Aletsch glacier over the last 120 years to be performed, see the figure. Simulations over the coming century can be investigated according to several climatic scenarios [1].

At each time step, the velocity of ice is obtained by solving a stationary non-linear Stokes problem with mixed Dirichlet and non-linear Robin condition along the bedrock-ice interface. The well-posedness of the weak formulation is proved [2]. A finite element discretization based on stable inf-sup spaces for velocity and pressure is proposed and *a priori* error estimates are established by using a quasi-norm technique [3]. Several schemes are proposed to solve the non-linearity and are proved to be convergent.

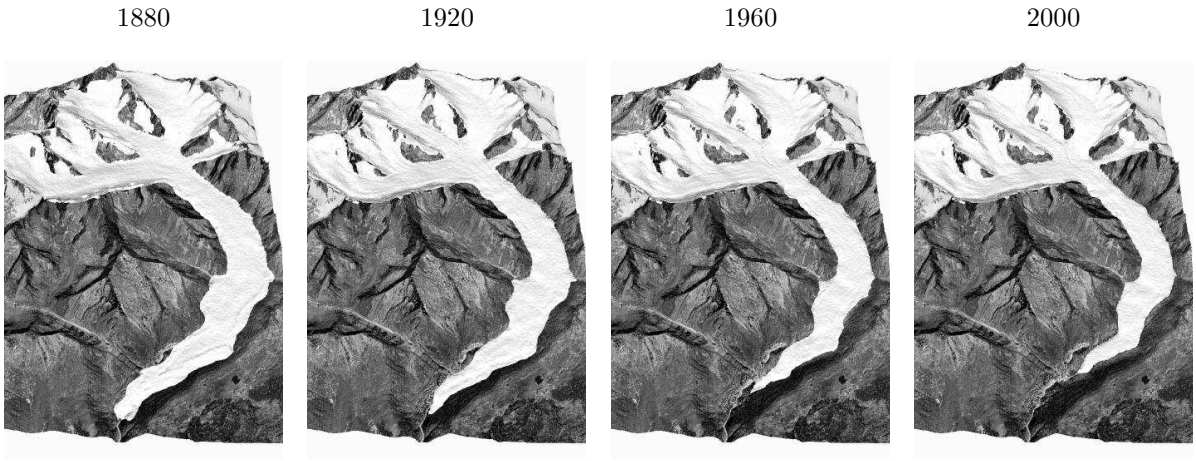

Figure 1: Simulation of Aletsch glacier over the period 1880-2000.

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Space-time wavelet FEM for parabolic equations

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For the model linear parabolic equation we propose a wavelet finite element space-time discretization motivated by [**?**]. The problem is reduced to a finite, overdetermined linear system of equations. We show that the corresponding normal equations are well-conditioned if appropriate Riesz bases are employed, and that the solution is quasi-optimal in the natural solution space for the original equation. The presented numerical examples confirm the theory. These results are part of a PhD thesis under the supervision of Prof. Ch. Schwab, supported by SNF Grant No. PDFMP2-127034/1.

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MODEL ORDER REDUCTION BY REDUCED BASIS METHODS FOR FLOW SIMULATION AND SHAPE OPTIMIZATION IN HAEMODYNAMICS

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Computational fluid dynamics provides models and methods to describe, simulate and control blood flows in cardiovascular districts, aiming at the analysis of blood circulation and prevention of cardiovascular diseases. Hence, a detailed understanding of local haemodynamics phenomena and the effect of vascular wall modication on flow patterns can have useful clinical applications especially in surgical procedures. The evaluation of wall shear stresses in a stenosed vessel or the minimization of vorticity in a cardio-vascular bypass anastomosis [**?**, **?**] are just two examples of problems in which we are interested considering flows which are highly dependent on vessels configuration combined with shape optimization of graftings.
These problems usually imply big computational efforts, basically due to fluid dynamics phenomena and geometrical complexity. Moreover, we need to face with many query problems, due to multiple evaluations of outputs depending on field variables during an optimization procedure, or to repetitive simulations on different geometries in a patient-dependent framework in view of a real-time solution. For these reasons, looking for computational efficiency in numerical methods and algorithms is mandatory, making the interplay between scientific computing and new reduction strategies a crucial topic. For an efficient model order reduction, reduced basis (RB) methods [**?**, **?**], built upon a high-fidelity "truth" finite element (FE) approximation, combined with free-form deformations (FFD) techniques for efficient shape parametrization are introduced [**?**, **?**], decreasing both the computational effort and the geometrical complexity. A parametrized RB approach can provide rapid and reliable results in real-time and many-query contexts; reliability is ensured by rigorous a posteriori error bounds, while rapid response is ensured by a suitable Offline–Online computational strategy [**?**]. Free-form deformations are built upon a low-dimensional parametrization and enable global shape deformations by acting on a small set of control parameters, resulting in a flexible, versatile and accurate tool [**?**]. Some results for haemodynamics applications are presented, dealing with shape optimization of parametrized configurations and real-time simulation of complex flows, discussing computational advantages and efficiency, obtained by geometrical and computational model order reduction.

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Numerical Methods for Complex Crystalline Materials

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Atomistic models are essential in many applications of solid mechanics, such as modeling cracks, structural defects, or nanoelectromechanical systems (NEMS), but full atomistic simulations are prohibitively expensive. Among the efficient methods based on atomistic models, the quasicontinuum (QC) method, introduced by Tadmor, Ortiz, and Phillips, has attracted growing interest in recent years. Originally, the QC method was developed for materials with simple crystalline structure. In the present work we propose an extension of the QC method to complex crystalline materials based on numerical homogenization. We first discuss discrete homogenization, and then formulate and analyze a macro-micro method capable of capturing the effective behavior of the complex material. Numerical examples illustrating the performance of our method will be presented.

Iterative Multiscale Finite Volume Method for Multiphase Flow in Heterogeneous Fractured Porous Media

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The Multiscale Finite Volume (MSFV) method is an efficient numerical method for the solution of heterogeneous elliptic and parabolic problems when approximate, but locally conservative solutions are required. Conservative solutions are important for the accurate solutions of transport problems. These requirements are common in oil reservoir simulations, where the classical numerical schemes become too expensive, since the size of the domain is much bigger than the resolution of the data provided by the geoscientists. It has been shown that the MSFV results match very well with those obtained from a classical numerical scheme at fine-scale. However, the level of error introduced by the method is problem dependent and is not bounded for highly anisotropic heterogeneous problems. To resolve this problem, a convergent iterative MSFV (i-MSFV) method is proposed. The i-MSFV method can be used as an iterative linear solver; however, its main advantage lies on the fact that a conservative solution field can be reconstructed after any iteration level. Therefore, it is shown that only few iterations are required in order to obtain good results even for very tough problems. Moreover, the i-MSFV iterations can be employed adaptively for a small sub-domain where the MSFV solutions are not acceptable.

In this work, the i-MSFV method is extended to include multiphase flow in heterogeneous fractured porous media. The n dimensional (nD) continuum medium (matrix) is loosely coupled with $(n-1)D$ fractures through a Darcy type coupling term. Local fracture functions are introduced to capture the fractures at the coarse scale accurately. Convergence study of the method is presented for many test cases. With the proposed loosely coupling strategy, it is very convenient to apply different type of physical modeling for the fracture and matrix media. This strategy also results in a much smaller system of equations to be solved for the matrix. In addition, independent grids are employed for the matrix and the fractures. Neither local grid refinement nor grid alinement are necessary in the proposed model. The numerical results show that the i-MSFV method is an efficient multiscale method for simulation of multiphase flow in heterogeneous fractured porous media.

Simulation of alumina dissolution in aluminium electrolysis

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Abstract: Aluminium is produced by electrolysis. Alumina (Al_2O_3) is added to an electrolyte, and by electrolysis it is reduced to aluminium. During the process, alumina has to be added periodically. We are going to present a model which simulates the injection of alumina powder, the transport of the particles, their dissolution, the movement of the appearing concentration and it's consumption by the electrolysis. In such a numerical simulation, the accuracy of mass conservation is of high importance. Our model involves convection-diffusion equations, where the velocity field is incompressible. In the talk we will focus on methods which ensure mass conservation when the velocity field is not exactly incompressible.

Nonlinear spectral problems with applications to photonic crystals

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1 Introduction

Dielectric and metallic photonic crystals are promising materials for controlling and manipulating electromagnetic waves [1]. For frequency independent material models considerable mathematical progress has been made [2]. In the frequency dependent case, however, the nonlinearity of the spectral problem complicates the analysis. We study the spectrum of a scalar operator-valued function with periodic coefficients, which after application of the Floquet transform become a family of spectral problems on the torus. The frequency dependence of the material parameters lead to spectral analysis of a family of holomorphic operator-valued functions.

2 Results

We show that the spectrum for a passive material model consists of isolated eigenvalues of finite geometrical multiplicity. These eigenvalues depend continuously on the quasi momentum and all non-zero eigenvalues have a non-zero imaginary part whenever losses (absorption) occur [3].

Lorentz permittivity model, which is a common model for solid materials, lead to a rational eigenvalue problem. We study both the self-adjoint case and the non-self-adjoint case. Moreover, a high-order discontinuous Galerkin method is used to discretize the operator-valued function, and the resulting matrix problem is transformed into a linear eigenvalue problem [4]. Finally, we use an implicitly restarted Arnoldi method to compute approximate eigenpairs of the sparse matrix problem.

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A Multiscale FEM for 2D Photonic Crystal Bands

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Abstract

A Multiscale Finite Element Method (MSFEM) for wave propagation in locally periodic media, e.g., Photonic Crystals (PhC), will be presented [1]. We consider wave propagation at wavelengths of the size of the local periodicity. In this case homogenisation techniques are not applicable. The MSFEM uses two-scale basis functions inside the PhC. As micro functions we use Bloch modes, which are computed as FEM solutions for a fully periodic PhC [7]. The macro functions are piecewise polynomials of degree p^{mac} which are supported over many periods of the crystal. We will numerically show that such a multiscale basis is very efficient as only a constant number of these functions are needed to simulate arbitrary large, finite PhCs with a constant L_2-error. In contrast, for standard discretisation schemes like FD, PWM, h- or p-FEM more and more basis functions are required when the number of scatterers increases inside the computational domain. We will explain how to use this multiscale basis to construct a conforming FEM which is coupled to a discretisation of the exterior domain. In particular, we will show how to numerically integrate the highly oscillatory two-scale functions with constant computational effort. We will verify the properties of the MSFEM by numerical experiments for PhC bands (see Fig. 1), an infinite band of locally-periodic dielectric scatterers in 2D.

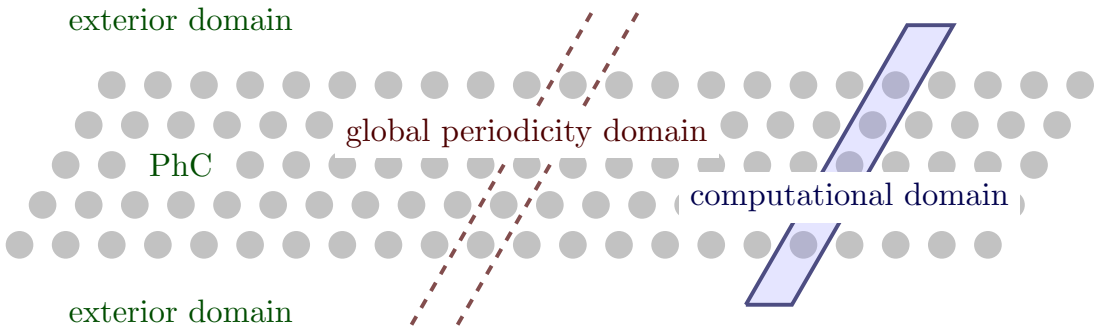

Figure 1: An example Photonic Crystal band

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GPU and multi-core accelerated simulations of bluff body flows using vortex methods

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Abstract

We present a "full on-GPU" solver and a "multi-core/GPU-assisted" solver for simulating bluff body flows using a remeshed vortex particle method. The efficiency of the method relies on fast and accurate particle-grid interpolations on GPUs for the remeshing of the particles and the computation of the field operators. The full on-GPU implementation uses hardware framebuffer operations to perform efficient particle-grid operations and a CUFFT-based solver for the Poisson Equation with unbounded boundary conditions. The accuracy and performance of the full on-GPU simulations and their relative advantages/drawbacks over CPU based computations are reported in simulations of flows past an impulsively started circular cylinder from Reynolds numbers between 40 and 9,500. The results indicate up to two orders of magnitude speed up of the GPU implementations over the respective CPU implementation. The accuracy of the GPU computations depends on the Re number of the flow. For Re up to 1000 there is little difference between the full on-GPU and CPU calculations but this agreement deteriorates (albeit remaining to within 5% in drag calculations) for higher Re numbers as the single precision of the GPU adversely affects the accuracy of the simulations.

Space-Time Wavelet adapted Grids on Multicore Architectures for the Simulation of Shock-Bubble Interactions

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Abstract

We present a wavelet-based space-time adaptive solver for single- and multi-phase compressible flows that couples average interpolating wavelets with high-order finite volume schemes. The solver is able to handle high resolution jumps (2 or more) and benefits from a straightforward technique for fast local time stepping schemes in the context of multicore computing. Wavelet based adaptivity is inherently sequential and in this work we demonstrate that these numerical methods can be implemented in software that exploits the capabilities of multicore machines while maintaining their computational efficiency. This is achieved by exploiting task-based parallelism, a new multithreading technology, and the concept of wavelet blocks. We verify our computational method on standard tests and the simulation of shock-bubble interaction at different Mach numbers that demonstrate the accuracy of our method and performance of the solver.

in-situ Visualization

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1 Introduction

The availability of high-performance computing resources enables the exploration of scientific phenomena and engineering design problems with numerical simulations of unprecedent quality and size. Scientific visualization contributes to converting the raw numerical output to mental images, yet it is more and more hindered by the overwhelming data I/O from disks. Similarly, numerical simulations often cannot archive all their results to disk files, because of the sheer sizes involved, and because I/O to disks is the slowest operation overall, imposing a huge bottleneck on the whole process. As we reach exascale computing, the conventional post-processing model *compute-store-analyze* can no longer cope with this data deluge. At that scale, it would take a visualization platform almost as powerful as the supercomputing running the simulation to read and analyse the data.

In-situ visualization is a process whereby visualization computations are done simultaneously with the simulation. It is attractive, because all relevant data about the simulation is available in memory; it can greatly contribute to the overall efficiency by limiting the data archived to disk files; it is a way of achieving run-time monitoring or even steering of a simulation. A couple of open-source solutions for data analysis tools enabling *in-situ* visualization are now emerging.

However, some refactoring of the simulation code is most likely required to enable live monitoring. In this talk, we wish to describe the generic parallel execution model proposed by VisIt[1], the leading *in-situ* visualization software. Simulation codes need to make room for a control interface to accept connections and receive commands from the remote visualization program and to provide a callback mechanism by which to return or share data. Beyond command and data transfers, both the simulation and the visualization must be able to continue their own processing independently. We will describe how the restructured execution models will enable this in a totally application-independent manner, for all common grid types.

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Numerical tools for the simulation of core-collapse supernovae

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1 Abstract

Core-collapse supernovae herald the spectacular death of massive stars by an energetic explosion. The gravitational collapse of the innermost stellar core leads to the transport of a tremendeous amount of neutrinos through hot accumulated stellar layers. The complexity of the arising fluid instabilities in multiple dimensions can only be tackled by numerical means. The physical system can be described by the equations of radiation- magnetohydrodynamics which form a non-linear system of conservation laws with source terms. We will outline the solution methods of this non-linear set of PDEs with the focus on our contribution to the algorithms. The magnetohydrodynamic equations are solved with a Riemann solver free central method, where the magnetic field is guaranteed to be solenoidal by a dimensionally split constrained transport method and a newly developed general method for the treatment of balance laws near steady states [**?**]. The spectral radiation transport is handled by the newly developed isotropic diffusion source approximation (IDSA) method [**?**], which efficiently captures the asymptotic limits of diffusive and transparent regimes. Further we detail on our parallelisation strategies of the algorithm for distributed and shared memory architectures.

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A thin HDF5 interface for parallel in-situ visualization within ParaView

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Abstract

As simulation codes become more powerful and more interactive, it is desirable to monitor the simulation *in-situ*, performing not only visualization, but analysis of the incoming data as it is generated - so that the simulation may be stopped, or modified, thereby conserving CPU resources. This talk describes an implementation of an in-situ framework which has been integrated into the ParaView visualization package alongside existing analysis modules.

The architecture is intended to address three principal objectives: Require little or no modification to the simulation code in order to allow a live visualization. Allow the simulation to be run on one parallel machine whilst the visualization is run on a separate (or the same) parallel machine. Provide good performance to ensure that massive simulations may be handled as easily as small test cases.

The interface developed is built around the HDF5 file IO library used commonly in HPC applications and a thin Xdmf layer [1]. The HDF5 API allows the derivation of custom *virtual file drivers* (VFDs) which may be instantiated at run-time on a per file basis to control how data is written to the file system. We have made use of this facility to create a specialized MPI based VFD which allows the simulation to write data in parallel to a file, but which is actually redirected over the network to a visualization cluster where the data is stored in a Distributed Shared Memory (DSM) buffer - in effect a (remote) virtual file system. The ParaView application acts as a server/host for this DSM and can read the file contents directly using the HDF5 API as if reading from disk. The transfer of data between simulation and visualization machines may be done using either an MPI based communicator shared between the applications, or using a socket based communication. The management of both ends of the network transfer is transparently handled by the DSM VFD layer, meaning that an application using HDF5 can make use of in-situ visualization without any code changes. It is only necessary to re-link the application against a modified version of the HDF library which contains our driver. However, the complexity of HDF5 is such that many different data layouts are possible and it is not feasible to read all HDF5 files using a single common standard reader. To mitigate this problem, we support several readers/formats within our ParaView plugin, including the H5Part particle format and the Xdmf format for other arbitrary HDF5 data. The user may provide a light XML template which is used to generate Xdmf description files automatically. Once data has been loaded, all existing ParaView filters and display methods are available and the user may setup an analysis workflow which is updated automatically as new data is received.

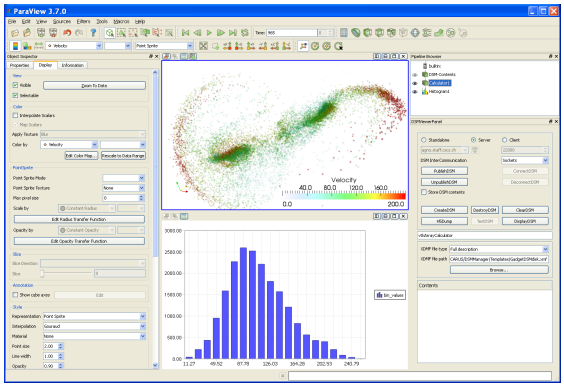

Figure 1: In-Situ Visualization of Gadget2 results in ParaView

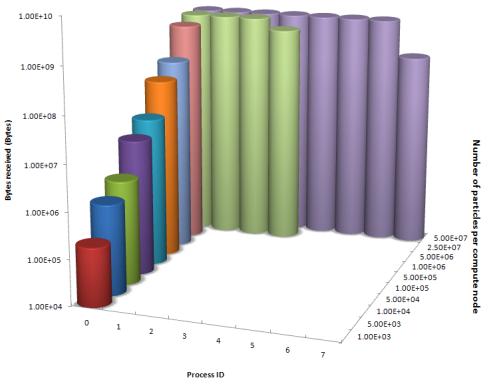

Figure 2: Distribution of data to parallel DSM nodes for fixed (10GB) DSM size

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Nonlinear Control and Estimation for Industrial Processes

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1 Abstract

We present a framework for online nonlinear dynamical modeling and optimization. This allows, in particular, to formulate and directly solve control problems, state estimation problems, and parameter estimation problems for relatively slow industrial processes. Although formulating these problems is straightforward, care has to be taken to enable the solver (in our case IpOpt [**?**]) to deliver robust and efficient solutions. The highlights of the presentation are the following:

- We show how the way the optimization problems are formulated affects the speed and robustness of the solution [**?**]. In particular, the importance of variable elimination is pointed out.
- When parameter estimation is used together with non-zero state noise, a problem of biasedness of the estimators arises. We discuss how to deal with this, based on [**?**].
- A case study of state and parameter estimation of a coal mill for a coal fired power plant is presented.
- A case study of model predictive control of the coal mills in a coal fired power plant is presented, taking into account online condition monitoring of the mills' status and according optimal load scheduling to the mills.

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Spatial Asymptotic Behavior in PDE and its Application in Finite Element Method

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1 Introduction

Many problems in PDE are naturally given in relatively big domains but usually we are interested only in the solution in a sub-domain. So it is natural to study the behavior of the solution in a sub-domain as the size of the whole domain grows.

A very practical problem in this direction is when we want the finite element approximation of the solution in a sub-domain. Then it is natural to triangulate the domain a priori finer in this region of interest and to coarsen the triangulation by getting far from this region of interest.

In this talk we present an iteration technique to obtain estimates that suggest the local behavior of the solution and also the a priori mesh adaptation for the region of interest.

2 Results

We bring two cases of asymptotic behavior estimates. First, we state the local behavior of the solution to an elliptic variational inequality with constraint on the gradient. Second, we bring estimates which suggest the appropriate a priori mesh adaptation for the region of interest in finite element calculations.

2.1 Elliptic Variational Inequality

Let us consider the domain $\omega \subset \mathbb{R}^{d-1}$ and the cylinder $\Omega_\ell = (-\ell, \ell) \times \omega \subset \mathbb{R}^d$. Let us consider in $\mathbb{R}^d$ the norm $|x|_p^p = |x_1|^p + \ldots + |x_d|^p$ and for $g \in H^1(\Omega_\ell)$ such that $g = 0$ on the lateral boundary $(-\ell, \ell) \times \partial\omega$ let us define the closed convex set

$$K_g = \left\{ v \in H^1(\Omega_\ell) \;\middle|\; v - g \in H_0^1(\Omega_\ell),\ |Dv|_p \leq 1 \text{ a.e in } \Omega_\ell \right\}$$

then for $f \in H^{-1}(\Omega_\ell)$ we may consider the variational inequality

$$\begin{cases} \displaystyle\int_{\Omega_\ell} Du \cdot D(u - v) \leq \langle f, u - v \rangle\,, \quad \forall v \in K_g \\ u \in K_g \end{cases}$$

As an example let us consider the case when $d = 2$, $\omega = (0, 1)$, $f = 0$ and $g(x_1, x_2) = \frac{1}{2} - |x_2 - \frac{1}{2}|$ then the solution to the variational inequality for $p = 2$ is depicted in figure **??** for $\ell = 1$ and in figure **??** for $\ell = 1.25$. As the figures suggest the solution converges to 0 in the middle of the cylinder as the length

(a)(b)
$\ell =$ $\ell =$
1 1.25

Figure 1: Solution of Variational Inequality with $p = 2$.

of the cylinder grows. For a harmonic function with the same boundary values this convergence is well known.

For the case $1 < p \leq \infty$ in the talk we present an estimate which when $f = 0$ is

$$\int_{\Omega_{\ell_1}} |Du|^2 \leq Ce^{-\alpha(\ell_2-\ell_1)} \int_{\Omega_{\ell_2}} |Du|^2$$

where C and α are positive constant depending on p. Here α converges to 0 as p converges to 1. The proof is based on an iteration technique.

2.2 A Priori Mesh Adaptation for Region of Interest

Let us consider the polygonal domain $\Omega \in \mathbb{R}^d$ and the problem

$$\begin{cases} -\triangle u + u = f \text{ in } \Omega \\ \dfrac{\partial u}{\partial \nu} = 0 \text{ on } \partial\Omega \end{cases}$$

let us assume that one is interested in the solution only in a polygonal sub-domain $\Omega' \subset \Omega$, such that $\text{dist}(\partial\Omega, \Omega') >> 1$. To compute the solution by finite element method it is natural to have the finest refinement of the triangulation in the domain Ω' and gradually the triangulation to get coarse away from this region of interest, in this way one tries to obtain less error in the region of interest with the same number of total bases.

Let us fix a sequence of growing polygonal domains

$$\Omega' = \Omega_1 \subset \Omega_2 \subset \cdots \subset \Omega_\ell = \Omega$$

such that

$$d_i = \text{dist}(\Omega_{i-1}, \Omega \backslash \Omega_i) > 0$$

Now let us consider a triangulation of the domain Ω which is compatible with the domains Ω_i in the sense that each Ω_i is a union of triangles in this triangulation. Let us consider the P_1 finite element method.

With similar iteration technique as the problem in the previous subsection was dealt with, we obtain the following local error estimate for the region of interest. There exists constants $\alpha, C > 0$ which depend on the regularity of the triangulation such that denoting by $\hat{u}$ the finite element solution, for any w in our finite element subspace we have the following local error estimate

$$\|u - \hat{u}\|^2_{H^1(\Omega_1)} \leq C\Big(e^{-\alpha \sum_{k=1}^{\ell} \tilde{d}_k} \|u - \hat{u}\|^2_{H^1(\Omega)} + \sum_{i=1}^{\ell} \Big\{ \sum_{j=i}^{\ell} e^{-\alpha \sum_{k=1}^{j} \tilde{d}_k} \Big\} \|u - w\|^2_{H^1(\Omega_i \backslash \Omega_{i-1})}\Big)$$

here $\tilde{d}_k = \min(1, d_k)$. We will show that this estimate suggests an appropriate a priori mesh adaptation to achieve less error with a fixed number of bases.

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Hybrid rational Krylov methods for matrix functions

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Matrix functions appear in exact solutions of various algebraic or differential equations. For example, the solution of a first-order linear ODE is given in terms of a matrix exponential, or in solutions of second-order linear ODEs trigonometric functions arise. It is not surprising that this has increased the interest in fast methods to evaluate matrix functions. Rational Krylov methods are among such methods. We present a novel hybrid rational Krylov method, which is particularly useful for approximating the action of a matrix function onto many different vectors. This method is a combination of the widely used Rayleigh–Ritz method and a more recent method, the PAIN method (which stands for poles and interpolation nodes, cf. [**?**]), both of which are implicitly based on rational interpolation. We combine the excellent ability of the Rayleigh–Ritz method to obtain near-optimal interpolation nodes, and use these nodes as input parameters for the PAIN method. The latter method requires less iteration work and storage need, which makes it possible to run multiple instances of this method on a parallel computer.

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Condition number estimates for the nonoverlapping optimized Schwarz method and the 2-Lagrange multiplier method for general domains and cross points

Sébastien Loisel

March 16, 2010

Abstract

The optimized Schwarz method and the closely related 2-Lagrange multiplier method are domain decomposition methods which can be used to parallelize the solution of partial differential equations. Although these methods are known to work well in special cases (e.g., when the domain is a square and the two subdomains are rectangles), the problem has never been systematically stated nor analyzed for general domains with general subdomains. The problem of cross points (when three or more subdomains meet at a single vertex) has been particularly vexing. We introduce a 2-Lagrange multiplier method for domain decompositions with cross points, and describe its relationship with the nonoverlapping optimized Schwarz method. We estimate the condition number of the iteration and provide an optimized Robin parameter for general domains. We hope that this new systematic theory will allow broader utilization of optimized Schwarz and 2-Lagrange multiplier preconditioners.

A Posteriori Modelling Error Estimates for the Stationary Diffusion Equation with Complicated Diffusion Matrix

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1 Introduction

In this talk a new computable a posteriori error majorant for hierarchically simplified models of the stationary diffusion equation with a complicated diffusion coefficient is presented. The original problem is considered with homogeneous Dirichlet boundary conditions and without any specific assumptions on the domain geometry and the right-hand sides.

2 Results

Functional a posteriori estimates focused on numerical approximation errors were extended to estimate the modelling errors in a reliably way. Based on the local behavior of the error majorant an adaptive strategy was developed, which includes the local enrichment of the finite element space and the hierarchically adapted "models". The numerical tests indicate the efficiency of the estimator and its ability to represent the error distribution needed for an adaptive improvement of the simplified models.

Joint work with S. Sauter (Universität Zürich) and S. I. Repin (PDMI St.-Petersburg)

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A stabilized finite volume element method for the Stokes' problem

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Abstract

We will devote ourselves to the study of a particular stabilized finite volume element (FVE) method constructed on the basis of a conforming finite element formulation for the Stokes equations, where the velocity and pressure fields are approximated by linear piecewise polynomials. Among the wide class of stabilized finite element formulations available from the literature, such as Streamline-Upwind/Petrov-Galerkin (SUPG), Galerkin-Least-Squares (GLS) and other methods, in this contribution we include a stabilization technique similar to the one introduced by Araya *et al.* [**?**], in which a Petrov-Galerkin approach is used to enrich the trial space with bubble functions being solutions to a local problem involving the residual of the momentum equation, which can be solved analytically. By enriching the velocity space using a *multiscale* approach combined with static condensation, the resulting FE method includes the classical GLS additional terms at the element level and a suitable jump term on the normal derivative of the velocity field at the element boundaries. Then, the essential point is to appropriately connect the finite element and FVE formulations. We also carry out a superconvergence analysis of the approximate solution. The main goal is to improve the current accuracy of the approximation by applying a postprocessing technique constructed on the basis of a projection method presented in [**?**, **?**]. The technique consists in projecting the FVE space to another approximation space (possibly of higher order) related to a coarser mesh. Finally, some numerical experiments that confirm the predicted behavior of the method are provided.

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Numerical Solution of Non-Smooth Diffusion Problems: Application to Sand Mechanics

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Abstract

We present a simple model for the simulation of deposition processes in sand mechanics, and the formation of sand piles on non-flat surfaces. The sand height is modeled by a time-dependent diffusion equation involving a fast/slow non-smooth diffusion operator, that is reminiscent of the infinite Laplacian operator. The diffusion operator contains a point-wise inequality constraint on the gradient of the solution that models the internal friction in the sand. Piecewise linear finite elements and an implicit scheme are used for the discretization in space and time respectively. We introduce an augmented Lagrangian method for the approximation of the fast/slow non-smooth diffusion operator. The inequality constraints on the solution and its gradient are treated either by projection methods or penalization approaches with local Newton methods. The introduction of an advection operator, together with a splitting algorithm, allows to address the simulation of sediment deposition in riverbeds. Numerical experiments illustrate the efficiency of the algorithm, for the simulation of sand piles and the deposition of sediment. This is a joint work with Prof. Roland Glowinski (University of Houston).

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Conservative FEM-simulation of the Einstein-Dirac system in spherically symmetric spacetime

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Abstract

Our work considers the massive spherically symmetric Einstein–Dirac system obtained from the relativistic two–fermion singlet state. First, we reviewed classical construction of the Einstein–Dirac equations in a general globally hyperbolic spacetime, with additional help of recent results by A. N. Bernal and M. Sànchez about smoothness of spacelike slicing. Some new analytical results have been found for the spherically symmetric case, e.g. an estimate of total ADM–mass against spatial Sobolev norms of the Dirac fields. In particular, we introduced a probably well posed initial value formulation for massive spherically symmetric Einstein–Dirac system in Schwarzschild coordinates. Further, we developed a spatial Galerkin method, suitable for finding numerical solutions of this initial value problem. The discretization scheme features exact conservation of the total electric charge, and allows for spatial mesh adaption based on physical arclength. We also derived error estimates and conditions that imply L^2–convergence of numerical solution to exact solution along lattice refinements. Based on these algorithms we realized a new platform independent and highly optimized UNIX commandline simulation software implemented in C++. In particular, our software allows for computations of static configurations as well as time evolutions obtained from suitable initial configurations w.r.t. the same discretization scheme and data structures. Numerical experiments and convergence tests due to Richardson's extrapolation confirm excellent robustness and convergence properties of our approach. Finally, we applied our software in order to confirm and significantly extend recent results about critical behaviour near the black hole threshold as well as structure and stability of static solutions.

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High order transmission conditions for conductive thin sheets – asymptotic expansion versus optimal basis

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Sensitive measurement and control equipment is protected from disturbing electromagnetic fields by thin shielding sheets (see Fig. 1). Such thin shielding layers would lead due to their smallness in one direction to a huge number of elements in a usual FE discretisation. We are interested in impedance transmission conditions modelling the behaviour of the conducting sheet. Within the first approach those transmission conditions are derived by asymptotic expansions up to third order, showing the stability and convergence of the mixed variational formulation [1–3].

The second approach [1,4] relies in an enrichment of the FE scheme with optimal thin sheet bases – that are basis functions suggested by the asymptotic behaviour of the solution. This leads to intrinsically stable transmission conditions which depend on the skin-effect and the curvature. These conditions distinguish by additional interface variables and can be easily written for any order.

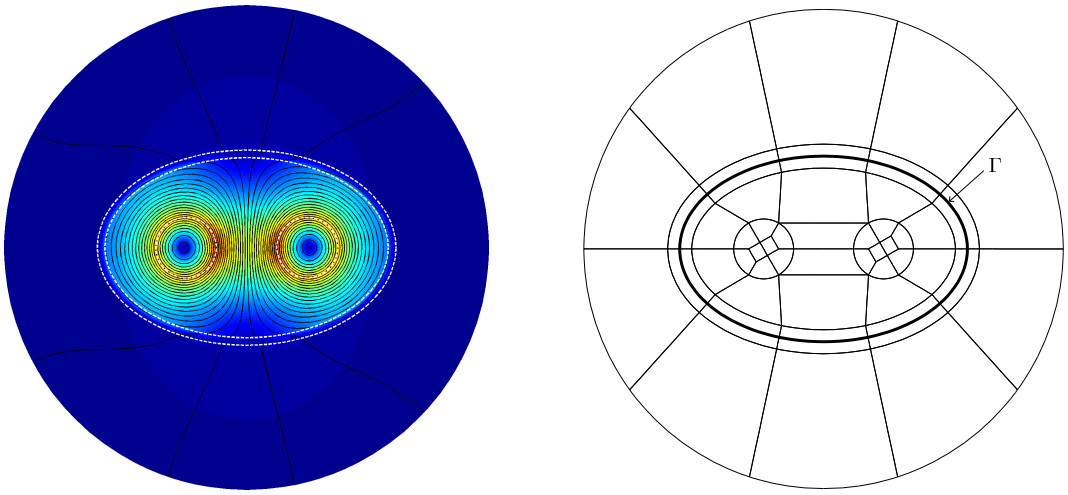

Figure 1: Magnetic field around two live wires protected by a thin shielding layer (*left*) and the mesh for transmission conditions (*right*).

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