Colloque Numérique Suisse / Schweizer Numerik Kolloquium

David Cohen, Marcus Grote, and Olaf Schenk

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Talks

Numerical methods for multiscale problems: stability and averaging

Assyr Abdulle[1],

[1]Ecole Polytechnique Fédérale de Lausanne

Abstract: Numerous methods have been recently developed for (ordinary, partial or stochastic) differential equations with multiple scales. For ordinary differential equations, a class of problems with multiple scales (so-called stiff problems) has been studied for many years and several efficient numerical methods are available for these problems. The efficiency of such methods rely on favorable stability (or damping) properties. For some problems, damping the fast scales may not lead to capture the correct effective behavior of the dynamics and methods based on averaging are more appropriate.

In this talk we will discuss some methods recently developed for stiff/multiscale stochastic problems based on stability or averaging concepts. We will see that the framework based on averaging used to construct numerical methods for time dependent multiscale differential equations can serve to construct finite element or finite difference methods for multiscale partial differential equations and we will also briefly discuss such methods.

Massively Parallel PDE Solvers for Flow Simulation

Ulrich Rüde[1],

[1]University of Erlangen-Nuremberg

Abstract: Large scale numerical simulation requires that we exploit parallelism on all levels. High performance computers will continue to be built as parallel systems with physically distributed memory, but each node will be have processors, each of which contains many cores. Additionally each core may rely on vectorization. Such systems can provide enormous compute power, but they may require a special programming and a new design of the algorithms. The multigrid finite element solvers HHG developed at Erlangen have been run on up to tenthousand processor cores, solving systems with three hundred billion unknowns. As a second example, the talk will report on the Walberla software framework that is being developed for parallel computational fluid dynamics using on the Lattice Boltzmann method.

Sparse adaptive Tensor FEM for elliptic sPDEs

Ch. Schwab

Abstract: We consider the Finite Element Solution of second order elliptic problems in a physical domain $D \subset \mathbb{R}^d$ with spatially inhomogeneous random coefficients.

We present convergence rates and complexity estimates for sparse Galerkin semidiscretization in the probability domain of the random solution. It is parametric in the first M Karhúnen-Loève (KL) variables of the input data [1].

Two cases are distinguished:

[1] Exponential decay of the input's KL expansion based on [2]

[2] algebraic decay of the input's KL expansion.

In (i), a "polynomial chaos" type Galerkin discretization is shown to yield spectral convergence rates in terms of N_Ω, the number of deterministic elliptic problems to be solved. In (ii), first approximation rates in terms of N_Ω are available.

Finally, ongoing work [3, 4, 5] on the total complexity vs. accuracy of (adaptive) tensor Galerkin discretizations in both, stochastic as well as in the deterministic domain D will be addressed.

Sufficient conditions on the joint pdf's of the random field input to ensure better complexity than with (Quasi) Monte Carlo in the probability domain and with Galerkin discretization in D will be identified and implementational issues will be addressed in each case.

[1] Ch. Schwab and R.A. Todor, Karhúnen-Loève Approximation of Random Fields by Generalized Fast Multipole Methods. Journal of Computational Physics **217** (2006), 100-122

[2] R.A. Todor and Ch. Schwab, Convergence Rates of Sparse Chaos Approximations of Elliptic Problems with stochastic coefficients. IMA Journ. Numer. Anal. (2007)

[3] M. Bieri and Ch. Schwab, Sparse high order FEM for elliptic sPDEs (in press in Comp. Meth. Appl. Mech. Engg. 2009)

[4] M. Bieri, R. Andreev and Ch. Schwab, Sparse Tensor Galerkin FEM for elliptic sPDEs (in review 2008)

[5] A. Cohen, R. DeVore and Ch. Schwab (in preparation 2009)

Exponential Convergence of hp-DGFEM for Linear Second-Order Elliptic Problems in 3-d Polyhedra

Thomas P. Wihler[1],

[1] Universität Bern, Mathematisches Institut,
(wihler@math.unibe.ch)

Abstract: In this talk we will present and analyze hp-type interior penalty discontinuous Galerkin discretizations for the numerical approximation of linear second-order elliptic PDE in polyhedral domains in 3-d. Particularly, the well-posedness of hp-DGFEM and the exponential convergence in terms of the number N of degrees of freedom of hp-DGFEM shall be established. Here, due to the presence of edge singularities in the exact solution, anisotropic geometric mesh refinements and anisotropic polynomial degree distributions are necessary to achieve exponential convergence rates for hp-DGFEM. To account for the anisotropic regularity of solutions in different (local) coordinate directions, our analysis will be based upon possibly irregular hexahedral meshes. For this type of mesh, hp-DG methods constitute a particularly practical choice.

Joint work with D. Schötzau (UBC) and Ch. Schwab (ETH Zürich).

An algebraic optimized Schwarz method that converges in finitely many steps

Felix Kwok[1] and Martin J. Gander[1]

[1] Section de mathématiques, Université de Genève,
(Felix.Kwok / Martin.Gander@unige.ch)

Abstract: Recent advances in the design of optimized transmission conditions in domain decomposition methods (DDMs) have improved the convergence rate of such methods significantly. These efficient transmission conditions are usually local approximations of the nonlocal Calderon-Seeley operators, which are known to lead to DDMs that converge in a finite number of iterations. Unfortunately, these Calderon-Seeley operators may not be available in the many-subdomain case, and even when they do exist, they need to be derived separately for each PDE. In this talk, we present an algebraic, Schur complement based approach for deriving nonlocal boundary operators that lead to convergence in finitely many steps. This approach is applicable as long as the subdomain problems are well posed and the subdomains are connected. We will also comment on how these operators can be approximated cheaply by solving recurrence relations.

Scale-Induced Closure for Approximations of Kinetic Equations

Peter Kauf[1], Manuel Torrilhon[1]

[1] Seminar for Applied Mathematics, ETH Zurich,
(peter.kauf@sam.math.ethz.ch / matorril@sam.math.ethz.ch)

Abstract: The order-of-magnitude method proposed by Struchtrup [1] is a new closure procedure for the infinte moment hierarchy in kinetic theory of gases, taking into account the scaling of the moments. The scaling parameter is the Knudsen number Kn, which is the mean free path of a particle divided by the system size.

In this talk we generalize the order-of-magnitude method and derive a formal theory of scale-induced closures on the level of the kinetic equation [2]. Generally, different orders of magnitude appear through balancing the stiff production term of order $1/Kn$ with the advection part of the kinetic equation. A cascade of scales is then induced by different powers of Kn.

The new closure produces a moment distribution function that respects the scaling of a Chapman-Enskog expansion. The collision operator induces a foliation of the non-equilibrium part of the distribution function in terms of the Knudsen number.

The new closure can be shown to be of second-order in Kn for specific cases, to be L^2-stable and to possess an entropy law. In principle the derivation of higher order approximations is also possible. We illustrate the features of this approach in the framework of a 16 discrete velocities model.

[1] Struch2H. Struchtrup, *Stable transport equations for rarefied gases at high orders in the Knudsen number*, Phys. Fluids **16**(11), (2004) p.3921-3934

[2] ScalIndProcM. Torrilhon, P. Kauf, C.D. Levermore, and M. Junk *Scale-Induced Closure for Approximations of Kinetic Equations*, in Rarefied Gas Dynamics, Proc. 26th Symposium on Rarefied Gas Dynamics in Kyoto, Japan 2008, ed. by T. Abe, AIP Conference Proceedings vol. 1084, p.123-128.

Simulating viscoplastic avalanches

M. Rentschler[1], C. Ancey[1], S .Wiederseiner[1], N. Andreini[1] and Steve Cochard[2]

[1] Laboratoire d'Hydrolique Environnemental , EPFL,
(martin.rentsschler@epfl.ch / chistophe.ancey@epfl.ch)
[2] Complex Fluids Laboratory , University of British Coloumbia
(scochard@math.ubc.ca)

Abstract: Avalanches and mudflows threat in Switzerland major infrastructure and a considerable number of homes and goods. To improve protection and prediction of those hazards, understanding of the physics involved in these flows is necessary. Comparison between experiments at laboratory scale and numerical simulations represent an important tool on this way, as they allow to control a variety of parameters, giving insight into the interplay between different processes involved in these flows.

In this talk we present a comparison between dam-break experiments of a non-Newtonian fluid on an inclined plane and a continuum based numerical simulation using a non-Newtonian two phase solver. This solver is based on a semi implicit projection scheme with a level-set representation of the interface between the non-Newtonian liquid on one side and the air on the other side. A modified Herschel-Bulkley model is used to represent the rheology of the fluid, using parameters that have been determined independently with a rheometer.

Numerical simulation of the dynamics of a glacier.

Guillaume Jouvet[1], Marco Picasso[1], Jacques Rappaz[1],
Matthias Huss[2] and Heinz Blatter[3]

[1] Institut d'Analyse et Calcul Scientifique, EPFL, Lausanne, Switzerland
(guillaume.jouvet@epfl.ch / marco.picasso@epfl.ch / jacques.rappaz@epfl.ch)
[2] Laboratory of Hydraulics, Hydrology and Glaciology, ETHZ, Zurich, Switzerland
(mhuss@vaw.baug.ethz.ch)
[3] Institute for Atmospheric and Climate Science, ETHZ, Zurich, Switzerland
(heinz.blatter@env.ethz.ch)

Abstract: An Eulerian formulation is presented in order to compute the dynamics of a glacier during centuries. Ice is modelled as an incompressible non-Newtonian fluid. The top surface of the glacier is obtained by solving a transport equation for the Volume Of Fluid function (VOF) [1]. Climatic effects (accumulation of ice on the top of the glacier and ablation on the tongue) are taken into account by adding a source term in the transport equation. Two different fixed meshes are used. An unstructured mesh with standard stabilized finite elements is used to solve the non linear Stokes problem. The VOF function is computed on a structured grid with high resolution. The first application consists in reconstructing the Rhône glacier (Wallis, Switzerland) during the past century. Three climatic scenarios are investigated in order to predict the shape of Rhône glacier until 2100 [2]. The second application focuses on steady state shape of glaciers (when internal motion, ice accumulation and ice ablation equilibrate). Numerical experiments suggest the existence of a unique steady shape. Mathematical existence is proved for a simplified model.

[1] *A new algorithm to simulate the dynamics of a glacier: theory and applications*. G. Jouvet, M. Picasso, J. Rappaz, H. Blatter. Journal of Glaciology, Volume 54(188), 2008.

[2] *Numerical simulation of Rhonegletscher from 1874 to 2100*. G. Jouvet, M. Huss, M. Picasso, J. Rappaz, H. Blatter. Submitted to Journal of Computational Physics.

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

Hadi Hajibeygi[1] and Patrick Jenny[1]

[1] Institute of Fluid Dynamics,
(hajibeygi@ifd.mavt.ethz.ch)

Abstract: The Multiscale Finite Volume (MSFV) method [Jenny et al., 2003 & 2006, JCP] was originally developed to overcome the computational complexity of elliptic problems arising from incompressible multiphase flow in highly heterogeneous porous media. Recently, an iterative MSFV (i-MSFV) method [Hajibeygi et al., 2008, JCP] for elliptic problems, which converges to the fine-scale reference solution, was devised. At each iteration, the MSFV solution is smoothed by applying a small number of fine-scale solver (smoother) iterations. The smoothed solution is then used to improve the localization condition (boundary condition of the local problems) for the next iteration step. It is an important property of the i-MSFV method that a locally conservative velocity field can be reconstructed after every iteration step. More recently, Hajibeygi and Jenny [ECMOR XI, Norway, 2008] proposed a new MSFV method for compressible multiphase flow in porous media, which resolves peculiarities that exist in the solutions of previously introduced MSFV methods [Lunati and Jenny, JCP, 2006; Zhou and Tchelepi, SPE, 2008; Lee et al. Comput. Geosci., 2008]. In this work, we extend the MSFV method for compressible multiphase flow by introducing an i-MSFV method for parabolic problems arising from compressible multiphase flow in porous media. Convergence studies of the scheme are presented for many challenging test cases including applications for multiphase flow in porous media. We show that only a few iterations per time step are sufficient in order to obtain results which are in excellent agreement with fine-scale reference; even for highly anisotropic heterogeneous problems. In any case, however, the resulting solution honors mass balance at the fine scale.

Bio simulation of the normal pressure hydrocephalus (NPH): influence of the inhomogeneity and anisotropy in permeability and elasticity

Kamal Shahim[1], Jean-Marie Drezet[1], Jean-François Molinari[2], Shahan Momjian[3] and Ralph Sinkus[4]

[1] Departement of Material, Ecole Polytechnique Fédérale de Lausanne, (kamal.shahim / Jean-marie.drezet@epfl.ch)
[2] Departement of Civil, Ecole Polytechnique Fédérale de Lausanne, (jean-francois.molinari@epfl.ch)
[3] Hôpitaux Universitaires de Genève, (Shahan.Momjian@hcuge.ch)
[4] Ecole Supérieure de Physique Chimie Industrielle (ESPCI), (ralph.sinkus@espci.fr)

Abstract: In hydrocephalus, brain ventricles enlarge and compress the brain parenchyma towards the skull. The aim of the present work is to study a particular form of hydrocephalus, the so-called NPH. A slice model (quasi 2D) of one given brain is built in a finite element software. The geometries of ventricles and skull are obtained by Magnetic Resonance Imaging (MRI). The brain itself is a complex material. Due to the existence of bundles of neurons, it can show locally anisotropic behaviour. Indeed, permeability and elasticity stiffness are higher along the fibre tracts (white matter). Other regions called grey matter are much more isotropic. The brain parenchyma is modelled as a porous medium fully saturated by the Cerebrospinal Fluid (CSF) using the Biot's theory of consolidation. Tracts directions are determined by Diffusion Tensor Imaging (DTI) to establish the reference coordinate systems in each voxel together with the permeability coefficients in each direction. Magnetic Resonance Elastography (MRE) is used to provide us with the shear properties in the same reference frame. Using MRI, DTI and MRE, the geometry, permeability and elasticity are obtained. To find out the influence of anisotropy and inhomogeneity; isotropic, isotropic in elasticity but anisotropic and inhomogeneous in permeability and finally anisotropic and inhomogeneous in elasticity and permeability models are tested. Results such as pressure distribution, void ratio, total displacement magnitude, CSF flow and ventricles dilatation and stresses, are presented and discussed.

Massive Scale-out of Parallel Graph Partitioning: A Case in Human Bone Simulations

C. Bekas[1], A. Curioni[1] P. Arbenz[2], C. Flaig[2], R. Müller[3], G. H. van Lenthe[3] and A. Wirth[3]

[1] IBM, Zurich Researh Laboratory,
(bek / cur @zurich.ibm.com)
[2] Computer Science Department, ETH Zurich
(arbenz / cflaig @inf.ethz.ch)
[3] Institute of Biomechanics, ETH Zurich
(ram / vanlenthe / wirth @ethz.ch)

Abstract: High-resolution in vivo peripheral quantitative computed tomography provides detailed information on bone structure. The analysis of bone density (using other, more commonly available technology) is today's approach of predicting bone strength and fracture risk in diseases like osteoporosis that is, according to the WHO, second only to cardiovascular disease as a leading health care problem.

Coupling recent imaging capabilities with microstructural finite element analysis offers a powerful means to determine bone stiffness and strength. The intricate microarchitectural structure of bone entails that these micro-FE models possess a very large number of degrees of freedom. We predict that this setting will appear ever more frequently in the coming years. We will need to develop methods and software in order to simulate physical phenomena on highly irregular topologies, using tens of billions, or more, of degrees of freedom and efficiently utilizing tens of thousands of computing elements.

It is clear that parallel graph partitioning becomes of imperative importance in the new petaflop era. We will show that the major bottleneck in extreme scale-out of large scale human bone simulations (and micro-FE applications in general) is in graph repartitioning: a) The intricate structure of bone causes significantly imbalanced partitions that have a strong negative effect when thousands of processors are used. b) The scalability of parallel graph partitioning tools (such as ParMETIS, Zoltan and others) on tens of thousands of processors appears to be a formidable task. These problems will be further amplified in the case of dynamic simulations, in which we seek to simulate the non-linear behavior of bone and of fracture formation. In this case, we will need to repeatedly and adaptively repartition huge irregular meshes.

Clearly, with the advent of the petaflop machines, efficient mapping of applications with irregular topologies on millions of processing elements will require next generation algorithms and efficient mapping models.

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Graphical modeling of mixed-logical dynamical systems for model-predictive control

Jan Poland[1] and Sebastian Gaulocher[1]

[1] ABB Switzerland Ltd, Corporate Research,
(jan.poland / sebastian.gaulocher@ch.abb.com)

Abstract: Model-predictive control (MPC) is an optimal control method which is increasingly used for controlling industrial processes appearing in various industries. Traditionally, MPC has been used for rather slow processes, e.g. in the chemical industry. But currently it is expanding into areas requiring faster execution times, such as power electronics.

The rationale behind MPC is to solve a constrained optimization problem that covers a finite horizon of time. At every sampling time, only the first move of the computed sequence of control actions is executed ("receding horizon"). The main ingredients are a dynamical model of the system, the knowledge of its current state, a revenue function, and constraints. Given real-time requirements, solving the resulting optimization problems (LP/QP in simple cases, MILP/MIQP if discrete variables are involved, or NLP/MINLP in general) is often a non-trivial task.

Building models is the typically the most expensive and challenging part of designing a model predictive controller. We present a graphical modeling engine [2] which builds on Mixed Logic Dynamical (MLD) models [1,3]. The graphical environment allows to combine basic MLD blocks and thus build complex models in a hierarchical way. This facilitates in particular first principles modeling of a plant by describing each of its components. The method is also appropriate for other types of models (black-box, gray-box, etc.).

This type of graphical modeling offers very nice tools for rapid controller prototyping and closed-loop simulation. In addition, we will demonstrate the advantages with some real-world applications: Control of a cement kiln, optimization of a flotation plant, and water pump scheduling.

[1] A. Bemporad and M. Morari: Control of systems integrating logic, dynamics, and constraints, Automatica 35(3) (1999), 407–427.

[2] E. Gallestey, D. Castagnoli, and A. Stothert: Method of generating optimal control problems for industrial processes, European Patent EP1607809 (2006).

[3] F.D. Torrisi and A. Bemporad: HYSDEL — A tool for generating computational hybrid models for analysis and synthesis problems. IEEE Transactions on Control Systems Technology 12(2) (2004), 235-249.

Parametric Free-Form Shape Design with PDEs Models and Reduced Basis Method

Gianluigi Rozza and Toni Lassila

Modelling and Scientific Computing, Institute of Analysis and Scientific Computing,
École Polytechnique Fédérale de Lausanne
(gianluigi.rozza / toni.lassila@epfl.ch)

Abstract: We combine free-form deformations [1] and reduced basis methods [2] for geometrically parameterized partial-differential equations in shape optimization problems. Free-form deformations are used to obtain flexible low-order shape parameterizations that are completely independent on the reference geometry. Reduced basis methods can then be used to solve effectively and in "real-time" the parametric partial differential equations for many different system configurations. An empirical interpolation method [3] is used to recover an important affine parameterization property, leading to truly efficient, reliable and accurate reduced order model computations. Some test cases dealing with airfoil shape optimization in potential flows and advection-diffusion (thermal) problems are presented.

[1] T.W. Sederberg and S.R. Parry: Free-form deformation of solid geometric models, Comput. Graph., no. 20(4) (1986).

[2] G. Rozza, D.B.P. Huynh, and A.T. Patera: Reduced basis approximation and a posteriori error estimation for affinely parametrized elliptic coercive partial differential equations, Arch. Comput. Methods Engrg., no. 15 (2008), 229-275.

[3] M. Barrault, Y. Maday, N.C. Nguyen, and A.T. Patera: An empirical interpolation method: application to efficient reduced-basis discretization of partial differential equations, C. R. Math. Acad. Sci. Paris, no. 339(9) (2004), 667-672.

Finite-difference high-order implementation of the immersed-boundary technique for the incompressible Navier-Stokes equations

Giuseppe Bonfigli[1],

[1] Institute of Fluid Dynamics, ETH Zurich,
(bonfigli@ifd.mavt.ethz.ch)

Abstract: A novel implementation of the immersed-boundary technique is proposed for the solution of the incompressible Navier-Stokes equations in primitive variables. The standard formulation with direct imposition of the discrete continuity equation and Dirichlet boundary conditions at solid walls for the velocity is used [1]. Fourth-order finite differences on Cartesian staggered grids[1] are considered for spatial discretization, whereby adapted stencils including intersection points between grid lines and immersed boundary are introduced for derivation and interpolation at boundary-near points. Explicit schemes are considered for time integration (standard Runge-Kutta).

Consistency and accuracy tests have been carried out solving the Navier-Stokes equations in the 2-d rectangular domain $[-1,1]\times[-1,1]$ with exclusion of the circular region $\{\underline{x} : |\underline{x}| < 0.2\}$. Non-homogeneous boundary conditions have been imposed on $|\underline{x}| = 0.2$ according to the immersed boundary technique and an unsteady volume-force has been added to the right-hand side of the momentum equation, so that

$$\begin{aligned} u_1 &= \frac{\pi}{4}(1-\cos(\pi x_1))\sin(\pi x_2)\sin(\omega t) \\ u_1 &= -\frac{\pi}{4}\sin(\pi x_1)(1-\cos(\pi x_2))\sin(\omega t) \\ p &= \cos(\pi x_1)\cos(\pi x_2)\sin(\omega t) \end{aligned}$$

was known to be the exact solution of the problem. Consistency with the accuracy of the used time-integration and spatial discretization schemes was observed.

[1] Harlow and Welch: First paper, J. Comp. Phys., no. 8 (1965), 2182–2189.

Numerical Simulation of Periodic Structure Problems

Matthias Ehrhardt[1] and Chunxiong Zheng[2]

[1] Weierstraß–Institut für Angewandte Analysis und Stochastik, Mohrenstr. 39, 10117 Berlin, Germany,
(ehrhardt@wias-berlin.de)
[2] Department of Mathematical Sciences, Tsinghua University, Beijing 100084, P.R. China,
(czheng@math.tsinghua.edu.cn)

Abstract: In order to numerically solve periodic structure problems (like photonic crystals (PC) structures, meta materials, etc.) efficiently one usually confines the spatial domain to a bounded computational domain (in a neighborhood of the region of physical interest).

The usual strategy is to introduce so-called artificial boundaries and impose adequate boundary conditions [1]. For wave-like equations, the ideal boundary conditions should not only lead to well-posed problems, but also mimic the perfect absorption of waves traveling out of the computational domain through the artificial boundaries.

We will review results of a series of papers [2,3,4] on solving partial differential equations (PDEs) with periodic coefficients and/or periodic geometries and present a novel analytical impedance expression for general second order ODE problems with periodic coefficients and a new numerical technique containing a fast evaluation of the Robin-to-Robin operator for periodic array problems.

[1] X. Antoine, A. Arnold, C. Besse, M. Ehrhardt and A. Schädle: A Review of Transparent and Artificial Boundary Conditions Techniques for Linear and Nonlinear Schrödinger Equations, Commun. Comput. Phys. Vol. 4, Number 4, (2008), 729–796. (open-access article)

[2] M. Ehrhardt and C. Zheng: Exact artificial boundary conditions for problems with periodic structures, J. Comput. Phys. Vol. 227, Issue 14, (2008), 6877–6894.

[3] M. Ehrhardt, H. Han and C. Zheng: Numerical simulation of waves in periodic structures, Commun. Comput. Phys. Vol. 5, Number 5, (2009), 849–872.

[4] M. Ehrhardt, J. Sun and C. Zheng: Evaluation of exact boundary mappings for one-dimensional semi-infinite periodic arrays, to appear: Communications in Mathematical Sciences, 2009.

Approximation by plane waves

Andrea Moiola[1] and Ralf Hiptmair[1]

[1] Seminar for Applied Mathematics, ETH Zürich
(andrea.moiola / ralf.hiptmair@sam.math.ethz.ch)

Abstract: The analysis of the plane wave discontinuous Galerkin method (PWDG) for the homogeneous Helmholtz equation, introduced in [1], can be generalized both to the three dimensional setting and to a p-version of the method. One of the main step in the convergence analysis is the proof of a best approximation estimate for a space of plane wave functions: given a solution $u \in H^{k+1}(D)$ of the Helmholtz equation $\Delta u + \omega^2 u = 0$ in D, we prove an estimate like

$$\inf_{\alpha \in \mathbb{C}^p} \left\| u - \sum_{k=1}^{p} \alpha_k e^{i\omega d_k \cdot x} \right\|_{H^j(D)} \leq C\, \epsilon(p) \left(\operatorname{diam}(D) \right)^{k+1-j} \|u\|_{H^{k+1}(D)}, \qquad 0 \leq j \leq k,$$

where d_k are fixed directions in S^{N-1}, $\epsilon(p) \to 0$ for $p \to \infty$.

We are able to give an estimate with algebraic convergence in p in two dimensions, while in three dimensions we can prove the convergence only with respect to $\operatorname{diam}(D)$.

The main tool used in the proof is the Vekua theory for two-dimensional elliptic PDEs: this allows to reduce part of the problem to the approximation of an harmonic function by harmonic polynomials in the same domain. In the particular case of the Helmholtz equation the Vekua operator can be generalized to every dimension.

[1] C. Gittelson, R. Hiptmair, and I. Perugia: Plane Wave Discontinuous Galerkin Methods: analysis of the h-version, Mathematical Modelling and Numerical Analysis, in press, (2009).

Rapid Solution of Exterior Wave Problems.

Stefan A. Sauter[1]

[1] Institut für Mathematik, Universität Zürich
(Stefan A. Sauter)

Abstract: In our talk we will present and analyse a new fast method for the numerical solution of the time domain boundary integral formulations of the wave equation. We employ Lubich's convolution quadrature method for the time discretization and a Galerkin boundary element method for the spatial discretization. The coefficient matrix of the arising system of linear equations is a triangular block Töplitz matrix. Our fast solution method combines the advantages of two existing approaches – a) solution of the Töplitz system in the Fourier domain. b) Applying cutoff and panel-clustering strategies in the time domain. The idea is to transform first the discrete convolution (related to the block Töplitz system) to the (discrete) Fourier image and, then, to apply a new panel-clustering method to the transformed system. This requires efficient ($\mathcal{H}$- and $\mathcal{H}^2$- matrix) representations of integral operators related to Helmholtz-type equations for a large range of complex wave numbers.

The Theodorus spiral: An exercise in functional equations, summation of series integration of analytic functions, and asymptotics

Jörg Waldvogel[1],

[1]ETH, Seminar für Angewandte Mathematik

Abstract: The remarkable classical pattern of the discrete Theodorus spiral, or square root spiral, can intuitively be supplemented by a closely related *inner* spiral asymptotic to it. A "nice" interpolating analytic curve was constructed by Philip J. Davis (1993) as an infinite product satisfying the same functional equation as the discrete points. We show that the analytic continuation of the Davis solution to a different sheet of its Riemann surface interpolates the points of the inner spiral.

This intriguing pattern opens a wide field for applying concepts and algorithms of numerical mathematics, such as functional equations, summation of slowly converging series, integration of analytic functions, and asymptotic expansions. We will present and discuss a few of these topics.

[1] Philip J. Davis (1993): Spirals: From Theodorus to Chaos. A. K. Peters, 220 pp.

Posters

Modeling and simulation of cardiovascular flows: medical applications

J. Bonnemain[1], P. Crosetto[1], S. Deparis[1], G. Fourestey[1], and A. Quarteroni[1].

[1] Chaire de Modélisation et Calcul Scientifique, IACS,EPFL, 1015 Lausanne,
(jean.bonnemain@epfl.ch / paolo.crosetto@epfl.ch / simone.deparis@epfl.ch / gilles.fourestey@epfl.ch / alfio.quarteroni@epfl.ch)

Abstract: The results presented here aim at applying mathematical models and numerical simulations to cardiovascular medicine. The results obtained can lead to a better understanding of physiological and pathological processes and help physicians in clinical decision making and treatment.

For the physiological state, a simulation of blood flow and its interaction with the vascular wall is performed with aorta and carotid artery models. Then, to understand the complex flow patterns in pathological states, the simulation of an idealized Fontan procedure and of an aneurysm of the internal carotid is executed.

An efficient method of fundamental solutions for Stokes flow problems

Francesco Boselli, Dominik Obrist and Leonhard Kleiser

Institute of Fluid Dynamics, ETH Zurich,
(boselli / obrist / kleiser@ifd.mavt.ethz.ch)

Abstract: The method of fundamental solutions (MFS) is a mesh free method for boundary value problems. In MFS, the solution is approximated by a superposition of fundamental solutions (FS) with singularities located outside the domain. The weights of the FS are determined by imposing the boundary conditions. MFS was recently identified as an efficient and accurate method for the solution of Stokes flow problems [1]. The accuracy and the stability of MFS are strongly related to the location of the singularities. Usually several attempts are required to find a good location for the singularities which yields the desired accuracy and does not lead to numerical instabilities. Alternatively, an optimization algorithm for the location of the singularities can be used to avoid instability problems. However, such algorithms can lead to prohibitively high computational costs. We will present an efficient adaptive MFS approach which improves the stability of MFS and increases the computational cost only moderately.

[1] D. L. Young, S. J. Jane, C. M. Fan, K. Murugesan, and C. C. Tsai: The method of fundamental solutions for 2D and 3D Stokes problems, J. Comp. Phys., no. 211(1) (2006), 1–8.

Explicit ions influence on titration curves of flexible polyelectrolytes by Monte Carlo simulations

Fabrice Carnal[1] and Serge Stoll[1]

[1] F.-A. Forel Institute, University of Geneva,
(fabrice.carnal / serge.stoll@unige.ch)

Abstract: The complexation of polyelectrolyte chains with oppositely charged nanoparticles has recently attracted much attention, because of their important potential applications in nanoscience, environmental chemistry and biology. In the vicinity of polyelectrolytes, small charged mobile ions interact strongly leading to a rich chemical and structural behavior. In the case of weak (or annealed) polyelectrolytes, the amount of charged sites may vary with the pH leading to configurational and ion condensation changes. In order to investigate the influence of parameters such as the monomer radius, chain length, ionic concentration, ion charge and pH on the chain ionization degree, titration curves are calculated. A common way to simulate such systems consists in performing Monte Carlo simulations according to the Metropolis algorithm using an electrostatic Coulomb potential with explicit objects (only the solvent is taken into account implicitly through its dielectric constant). It is shown that the explicit presence of ions in solution significantly influences the polyelectrolyte chains behavior.

Scalable Stencil Computations on Modern Chip-Multithreading Architectures

Matthias Christen and Olaf Schenk

High Performance and Web Computing Group, Department of Computer Science, University of Basel,
(m.christen@unibas.ch / olaf.schenk@unibas.ch)

Abstract: Novel micro-architectures such as the Cell Broadband Engine Architecture (Sony, Toshiba, IBM) and general purpose graphics processing units are just two examples for the hardware diversity found in nowadays high performance computing landscape. Modern micro-architectures are typically inherently highly parallel and therefore offer fantastic peak performances, which make them attractive platforms for compute-intensive simulations.

Partial differential equation (PDE) solvers constitute a large fraction of scientific applications in such diverse areas as heat diffusion, astrophysics, biomechanics, electromagnetics, and fluid dynamics. These applications are often implemented using iterative finite-difference or finite-volume techniques that sweep over a spatial grid, performing nearest neighbor computations called *stencils*. In a stencil operation, each point in a multidimensional grid is updated with weighted contributions from a subset of its neighbors in both time and space — thereby representing the coefficients of the PDE for that grid point. These operations are then used to build solvers that range from simple Jacobi iterations to complex multigrid and adaptive mesh refinement methods. Stencil calculations perform global sweeps through data structures that are typically much larger than the capacity of the available data caches. In addition, the amount of data reuse is limited to the number of points in a stencil, which is typically small. As a result, these computations generally achieve a low fraction of theoretical peak performance, since data from main memory cannot be transferred fast enough to avoid stalling the computational units on modern microprocessors. Reorganizing these stencil calculations to take full advantage of memory hierarchies has been the subject of much investigation over the years. These have principally focused on tiling optimizations that attempt to exploit locality by performing operations on cache-sized blocks of data before moving on to the next block [2, 3, 5, 6].

On this poster we give an architectural overview over the Cell processor and NVIDIA GPUs and show some performance numbers that were obtained for a stencil code used in the simulation of thermal behavior of the human body during

biomedical hyperthermia cancer treatment. Hyperthermia is a promising treatment modality for various types of cancer. The technique involves heating the tumour with electromagnetic fields, generally using antenna arrays to focus the energy. In planning the therapy, the therapeutically optimal antenna parameters for the applicator have to be determined for each patient individually given the patient's geometry. The temperature distribution is predicted by solving the 3D Pennes bio-heat transfer equation. Although this can be a demanding task, a planning and simulation tool can greatly help clinical researchers to model and simulate the medical treatment [4]. We are addressing the practical concerns of fitting into a clinician's standard work-flow, and the question of how to use optimal algorithms and relevant HPC architectures to maximize a biomedical application performance.

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Asymptotic analysis around a thin wire in the case of self-similar tips

Xavier Claeys[1], Monique Dauge[2]

[1] Seminar fr Angewandte Mathematik, ETH Zrich,
(xavier.claeys@sam.math.ethz.ch)
[2] IRMAR, Université de Rennes 1,
(Monique.Dauge@univ-rennes1.fr)

Abstract: The asymptotic analysis for thin wire models has been the subject of several works such as [1,2]. In these articles, the authors considered the Laplace problem posed around a wire-shaped obstacle, and derived an expansion of the solution with respect to the thickness of this wire. Whereas one would naturally consider a self-similar shape for the tip of a thin wire, the current mathematical state of the art only allows to take into account wires whose tips shrink ellipsoidally as the thickness goes to 0. We present a work aiming at studying the scattering by thin wires whose tips are genuinely self-similar, formulating some hypothesis on the symetry of the problem. We use the multiscale expansion technique with three boundary layers: a central cylindrical one, and two others with spherical shape localised at both ends of the wire. Such an approach is closely related to the study of elliptic problems in domains with a cuspidal corner on their boundary.

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Modeling and simulation of cardiovascular flows: mathematical methods

P. Crosetto[1], J. Bonnemain[1], S. Deparis[1], G. Fourestey[1], and A. Quarteroni[1].

[1] Chaire de Modélisation et Calcul Scientifique, IACS,EPFL, 1015 Lausanne,
(jean.bonnemain@epfl.ch / paolo.crosetto@epfl.ch / simone.deparis@epfl.ch / gilles.fourestey@epfl.ch / alfio.quarteroni@epfl.ch)

Abstract: The results presented here aim at describing different possible strategies for the solution of 3D Navier-Stokes and Fluid-Structure Interaction problems in a parallel framework with focus on hemodynamics applications. In particular we present a comparison between modular and non modular FSI procedures. We stress the importance of the preconditioner choice for the resulting linear system. We also explain how these methods are implemented in our finite elements library LifeV.

Atomistic Materials Modeling

Andreas Elsener, Christian Brandl, Peter Derlet and Helena Van Swygenhoven

Materials Science and Simulations, ASQ/NUM, Paul Scherrer Institut
(Andreas.Elsener@PSI.ch)

Abstract: Large scale molecular dynamics (MD) computer simulations are of great help in understanding the structural and mechanical behaviour of nanostructured (nc) materials. Although it is very well known that this technique suffers from limitations in length and time scales, and thus inappropriate for determining rate limiting processes, it is however an excellent tool to investigate the atomistic details of deformation mechanisms that result from an interplay between microstructure at the atomic level and applied mechanical stress. As examples, MD computer simulation of structural and mechanical properties of nanocrystalline metals under uniaxial deformation as well as the simulation of Oxygen impurities will be shown. Last but not least the interplay of MD with other simulation techniques such as density functional theory in materials research will be presented.

Interfacing Single Column Lake and Atmospheric Models: Application over Lake Geneva for Observed and Climate Warming Scenario

Stéphane Goyette[1], Marjorie Perroud[1]

[1] Climate Change & Climate impacts, University of Geneva,
(stephane.goyette@unige.ch / marjorie.perroud@unige.ch)

Abstract: A single-column atmospheric model has been coupled to a single-column lake model to simulate present-day as well as future lake temperature profiles following global climate warming conditions. Results of multi-year climate simulations are shown for the case of the deep station SHL2 (309 m) of Lake Geneva, Switzerland. The atmospheric model termed FIZC, is a column version of a limited-area model developed for regional climate modelling based on an off-line downscaling of GCM simulations. It is a physically-based model and it requires outputs from a previous GCM integration. The issues of local lake climate is addressed by combining precomputed atmospheric large-scale transports of momentum, heat, and moisture, called "the Dynamics", and recomputed subgrid-scale parameterized effect (solar and infrared radiation fluxes, and latent and sensible heat fluxes), called "the Physics", with the explicit numerical computations of the evolving lower boundary conditions provided by the lake model. The lake model, called k-epsilon (k-e), combines a buoyancy-extended k-e model with a seiche excitation and damping model to predict the diffusivity below the surface mixed layer. In this model, the vertical turbulent diffusivities are determined from the turbulent kinetic energy and energy dissipation. Details of the atmospheric-lake interface module, and a sensitivity analysis of the simulated thermal profiles to this coupler parameters are presented. Finally statistics of the change in the lake thermal profiles is also shown for the case of an equilibrium 2xCO_2 global climate warming scenario.

Anisotropic finite element adaptation for compressible flows around aircrafts

Wissam Hassan[1], Marco Picasso[1], Frédéric Alauzet[2] and Yves Bourgault[3]

[1] Institut d'Analyse et Calcul Scientifique, Ecole Polytechnique Fédérale de Lausanne,
(wissam.hassan / marco.picasso@epfl.ch)
[2] INRIA, Paris-Rocquencourt, France,
[3] Department of Mathematics and Statistics, University of Ottawa

Abstract: A 3D adaptive finite element algorithm is proposed to solve compressible flows around bodies. Tetrahedrons with large aspect ratio are used, with goal of reducing the number of vertices without increasing error. The refinement and coarsening criterion is based on an a posteriori error estimator justified for elliptic and parabolic problems.
Numerical simulations using Euler and Navier-Stokes calculations were carried out for a supersonic flow around an aircraft and for a transonic flow around a wing profile. The main problem lies in the capture of various physical phenomena involved, as the shock waves or the boundary layer.
This project is supported by Dassault Aviation.

Semi-Lagrangian Galerkin methods for Discrete Differential Forms

Holger Heumann[1], Ralf Hiptmair[1], and Jinchao Xu[2]

[1] Seminar for Applied Mathematics, ETH Zürich,
(Holger.Heumann / Ralf.Hiptmair@sam.math.ethz.ch)
[2] Department of Mathematics, Pennsylvania State University,
(xu@math.psu.edu)

Abstract: When solving non-stationary convection diffusion problems stability is a major issue. In cases where the diffusive part is very small, only implicit schemes can guarantee this stability. In contrast to other implicit methods Semi-Lagrangian methods treat only the elliptic part of the problem implicitly, hence the resulting symmetric algebraic system can be solved efficiently [4]. We will present two different types of Semi-Lagrangian formulations for general transport problems stated in the discrete differential forms formalism [1]. Using the notion of exterior derivative d, Lie derivative $L_{\boldsymbol{\beta}}$ and Hodge operator $*$ the time dependent convection diffusion problem of a differential form ω reads as

$$-d * d\omega(\cdot,t) + *\partial_t\omega(\cdot,t) + *L_{\boldsymbol{\beta}}\omega(\cdot,t) = \varphi \quad \text{in } \Omega \subset \mathbb{R}^n.$$

We show further that the two different types are adequate for either the $\mathbf{H}$- or the $\mathbf{A}$-formulation of the eddy-current model in moving media [5]. A welcome side effect is the automatic preservation of the divergence-free constraint in either a weak or a strong fashion [3].

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Scientific Computing for Aluminum Production

Thomas Hofer[1] and Gilles Steiner[1]

[1] Institut d'analyse et de calcul scientifique, EPFL,
(thomas.hofer / gilles.steiner@epfl.ch)

Abstract: The goal of this poster is to present some aspect around the numerical simulation of the industrial aluminum electrolysis process. In a first part the magnetohydrodynamics equations that rule the multi-fluid flow in a cell are presented. In a second step we model the dissolution of alumina particles and the evolution of the concentration field of liquid alumina in the electrolyte. Numerical solutions for these two problems are computed using Stabilized Finite Element Method and some significant results are presented.

Interior-Point Optimization for Inverse Wave Propagation in Heterogeneous Media

†Marcus Grote, †Johannes Huber, ‡Olaf Schenk

†Department of Mathematics and ‡Computer Science Department,
University of Basel, CH-4051 Basel
(johannes.huber@unibas.ch)

Abstract: Many engineering and science problems — in such diverse areas as wave propagation, atmospheric sciences, image registration, medicine, structural-fluid interactions, and chemical process industry — can be expressed in the form of a PDE-constrained problem. The common difficulty is that the PDE solution is just a subproblem associated with the optimization problem. Moreover, the inverse problem is often ill-posed despite the well-posedness of the forward problem, and the inverse problem can have numerous local solutions. For these reasons the optimization problem is often significantly more difficult to solve than the simulation problem. The size, complexity, and infinite-dimensional nature of PDE-constrained optimization problems present significant challenges for general-purpose optimization algorithms, and Tikhonov regularization, iterative solvers, preconditioning, inexactness, and parallel implementations are typically necessary to cope with the numerical challenges. In this work we formulate an inverse problem of the Helmholtz equation in heterogeneous media [1] as a PDE-constrained optimization problem and will use inexact primal-dual interior point optimization methods [2].

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Boundary hybrid Galerkin method for elliptic problems in 3-D over flat planar structures

C. Jerez-Hanckes[1], J.-C. Nédélec[2], S. Nicaise[3]

[1] Seminar für Angewandte Mathematik, ETH Zurich
(cjerez@sam.math.ethz.ch)
[2] CMAP, École Polytechnique, France
(nedelec@cmap.polytechnique.fr)
[3] LAMAV, Université de Valenciennes, France
(serge.nicaise@univ-valenciennes.fr)

Abstract: We present a boundary element method for modeling elliptic problems in 3-D with Dirichlet conditions imposed over flat surfaces having very large aspect ratios. Via an integral representation of the field over Ω, the entire problem is condensed to solving a first-kind Fredholm integral equation on the screen Γ_m. However, even for a smooth boundary $\partial\Gamma_m$, solutions are known to portray singularities [1,2], and if Lipschitz, corner singularities may also show up. To handle this,

our numerical scheme uses tensor products between weighted Tchebychev polynomials and polynomial functions are used to describe "edge"-like areas while triangular mesh refinement is carried out in "corner"-like areas over which first-order polynomials are employed. Finally, we attempt to convey a convergence analysis and show some results for the Laplacian in an industrial setting [3].

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Enhanced graph-based dimensionality reduction with repulsion Laplaceans

Effrosyni Kokiopoulou[1], Yousef Saad[2]

[1] Seminar for Applied Mathematics, ETH.
(effrosyni.kokiopoulou@sam.math.ethz.ch)
[2] Computer Science & Engineering Department, University of Minnesota.
(saad@cs.umn.edu)

Abstract: The goal of dimensionality reduction is to map a set of high dimensional data samples to a lower dimensional space such that certain properties of the initial data are preserved. Graph-based methods for linear dimensionality reduction have recently attracted much attention and research efforts. The main goal of these methods is to preserve the properties of a graph representing the affinity between data points in the input high dimensional space. It has been observed that, in general, supervised graph-methods outperform their unsupervised peers in various classification tasks. Supervised graphs are typically constructed by allowing two nodes to be adjacent only if they are of the same class. However, such graphs are oblivious to the proximity of data from different classes and this can lead to potential misclassification. To alleviate this problem, we propose a novel methodology which builds on 'repulsion graphs', i.e., graphs that model undesirable proximity between points. The main idea is to repel points from different classes that are close by in the input high dimensional space. The proposed methodology is generic and can be combined with any graph-based method for linear dimensionality reduction. We provide ample experimental evidence in the context of face recognition, which shows that the proposed methodology (i) offers significant performance improvement to various graph-based methods and (ii) outperforms existing solutions relying on repulsion forces.

Decomposition Techniques for Strongly Non-linear and Heterogeneous Problems

Rolf Krause[1], Thomas Dickopf[2], Konstantin Fackeldey, Christian Groß[2], Dorian Krause[1], Christina Mohr[1], and Johannes Steiner[2]

[1] Institute for Computational Science, University of Lugano,
({dorian.krause,rolf.krause,christina.mohr}@unisi.ch)
[2] Institute for Numerical Simulation, University of Bonn,
({dickopf,gross,jsteiner}@ins.uni-bonn.de)

Abstract: The mathematical modeling of complex (bio)mechanical models often gives rise to heterogeneous and strongly non-linear models, whose numerical treatment is far from trivial. We present several decomposition based approaches, which can be applied to, e.g., problems with large deformations and strongly non-linear materials as well as to constrained minimization problems. Efficiency and flexibility of our solution methods is obtained by using scale dependent models in a multiscale setting. Within this multiscale context, we furthermore derive a new coupling approach between different models as atomistic models and models from continuum mechanics, which shows excellent stability properties. This new approach is based on ideas from non-conforming domain decomposition methods; Interestingly, based on similar ideas, we are able to construct stable transfer operators between different finite elements discretizations, which are applicable to contact problems involving realistic geometries in (bio)mechanics. Numerical examples in 3D are given.

A novel parallel QR algorithm for hybrid distributed memory HPC systems

Daniel Kressner[1], Robert Granat[2] and Bo Kågström[2]

[1] Seminar for Applied Mathematics, ETH Zurich, Switzerland
(kressner@math.ethz.ch)
[2] Department of Computer Science, Umeå University, Sweden,
(granat / bokg @cs.umu.se)

Abstract: A novel variant of the parallel QR algorithm for solving dense nonsymmetric eigenvalue problems on hybrid distributed high performance computing systems is presented. For this purpose, we introduce the concept of multi-window bulge chain chasing and parallelize aggressive early deflation. The multi-window approach ensures that most computations when chasing chains of bulges are performed in level 3 BLAS operations, while the aim of aggressive early deflation is to speed up the convergence of the QR algorithm. Mixed MPI-OpenMP coding techniques are utilized for porting the codes to distributed memory platforms with multithreaded nodes, such as multicore processors. Numerous numerical experiments confirm the superior performance of our parallel QR algorithm in comparison with the existing ScaLAPACK code, leading to an implementation that is 10 to 60 times faster for sufficiently large problems.

Simulating the fragmentation of large heterogeneous structures with the Discontinuous Galerkin Method

S. Levy[1], A. Seagraves[2], J.F. Molinari[1] and R. Radovitzky[2]

[1] LSMS-IS-ENAC, Ecole Polytechnique Federale de Lausanne
(sarah.levy@epfl.ch)
[2] Department of aeronautics, Massachussetts Institue of Technology

Abstract: Submitted to an intense loading, brittle materials break into many fragments. The description of the phenomenon involves both the micro and the macro scales: the distribution of the microscopic defects conduct the numerous fracture initiations, while stress wave propagations and interactions characterize the macroscopic behavior. Due to the complexity of the process, understanding intuitively and deriving an analytical prediction remain challenging issues.

As a result, numerical simulations, which are able to address the communication between the two scales and the non-linear macroscopic response, are a suitable tool to characterize accurately fragmentation. Moreover, a further challenge consists in simulating the fragmentation of large scale structures while keeping an explicit description of the resulting fragment characteristics (mass, velocity, shape).
Thereby, we are using the Discontinuous Galerkin method [1] to model the elastic expansion of the body, and a cohesive approach [2] to handle the fracture initiation and propagation. This original framework makes possible parallel simulations to deal with large heterogeneous structures and to determine explicitly the temporal and spatial evolution of the damage.

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Explicit local time-stepping for transient electromagnetic waves

Marcus Grote[1] and Teodora Mitkova[1]

[1] Departement Mathematik, Universität Basel,
(Marcus.Grote / Teodora.Mitkova@unibas.ch)

Abstract: The accurate and reliable simulation of electromagnetic wave phenomena is of fundamental importance in a wide range of engineering applications. For the numerical simulation of time dependent electromagnetic waves, we consider Maxwell's equations in second-order form. The problem is discretized in space by the symmetric interior penalty (IP) discontinuous Galerkin (DG) method, which yields a block-diagonal mass matrix with fixed block size determined by the number of degrees of freedom per element only. Hence, when combined with explicit time integration, the resulting time marching scheme is truly explicit. To overcome the standard stability restriction of explicit time-stepping schemes due to the smallest elements in the mesh, we develop local time-stepping methods of second-order of accuracy that allow smaller time-steps precisely where the smallest elements in the mesh are located, while remaining fully explicit. Numerical experiments illustrate the efficiency of the proposed time integration and validate the theory.

A short and versatile finite element multiscale code for homogenization problems

Assyr Abdulle[1] and Achim Nonnenmacher[1]

[1] Mathematics Section, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne
(assyr.abdulle@epfl.ch / achim.nonnenmacher@epfl.ch)

Abstract: We describe a multiscale finite element (FE) solver for elliptic problems with highly oscillating coefficients. Based on recent developments of the so-called heterogeneous multiscale methods (HMM), the algorithm relies on coupled macro and micro solvers. The framework of the HMM allows to design a code whose structure follows the classical finite elements implementation at the macro level. To account for the fine scales of the problem, elementwise numerical integration is replaced by micro FE methods on sampling domains.

We present a short and flexible FE implementation of the multiscale algorithm, which can accommodate simplicial or quadrilateral FE and various coupling conditions for the constrained micro simulations. Numerical examples illustrate the capabilities and versatility of the proposed implementation.

CSCS, the Swiss National Supercomputing Centre

Jean-Guillaume Piccinali[1], Neil Stringfellow[1]

[1] High Performance Scientific Computing Group, CSCS

Abstract: To remain internationally competitive, scientists and engineers must be provided with leadership-class supercomputer systems. Supercomputers are indispensable tools for solving the most challenging and complex scientific and technological problems through simulations. In order to better serve the needs of Swiss science community, the Swiss National Supercomputing Centre is currently upgrading its main computing system to a CRAY XT5 system named Rosa that will deliver a total of 141 TFlop/s in June 2009 and a total of 212 TFlop/s in November 2009. Significant improvements in terms of software environment including new programming models will be available in addition to existing paradigms. This poster will present the CSCS, focusing on its current status, HPC infrastructures and future directions.

Parallel Scalable PDE-Constrained Optimization: Antenna Identification in Hyperthermia Cancer Treatment Planning

Olaf Schenk[1], Murat Manguoglu[2], Ahmed Sameh[2], Matthias Christen[1], and Madan Sathe[1]

[1]Department of Computer Science, University of Basel, Switzerland
(olaf.schenk@unibas.ch / m.christen@unibas.ch / madan.sathe@unibas.ch)
[2]Computer Sciences, University of Purdue
(mmanguog@cs.purdue.edu, sameh@cs.purdue.edu)

Abstract: We present a PDE-constrained optimization algorithm which is designed for parallel scalability on distributed-memory architectures with thousands of cores. The method is based on a line-search interior-point algorithm for large-scale continuous optimization, it is matrix-free in that it does not require the factorization of derivative matrices. Instead, it uses a new parallel and robust iterative linear solver on distributed-memory architectures. We will show almost linear parallel scalability results for the complete optimization problem, which is a new emerging important biomedical application and is related to antenna identification in hyperthermia cancer treatment planning.

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Krylov subspace methods for linear systems with tensor product structure

Christine Tobler and Daniel Kressner

Seminar für angewandte Mathematik, ETH Zürich
christine.tobler@sam.math.ethz.ch / daniel.kressner@sam.math.ethz.ch

Abstract: The numerical solution of linear systems with certain tensor product structures is considered. Such structures arise, for example, from the discretization of a linear PDE on a d-dimensional hypercube. These systems can be regarded as linear matrix equations for $d = 2$ and appear to be their most natural extension for $d > 2$. A standard Krylov subspace method applied to such a linear system suffers from the curse of dimensionality and has a computational cost that grows exponentially with d. The key to breaking the curse is to note that the solution can often be very well approximated by a vector of low tensor rank. We propose a new class of methods, so called *tensor Krylov subspace methods*, which exploit this fact and attain a computational cost that grows linearly with d.

Neutrino transport in 3D simulations of core-collapse supernovae

Stuart C. Whitehouse[1] and Matthias Liebendörfer[1]

[1] Department of Physics, University of Basel,
(s.whitehouse / matthias.liebendoerfer@unibas.ch)

Abstract: The mechanism which causes a core-collapse supernova to explode is presently not fully understood. Simulations can model the collapse and bounce phases, but the shock expansion stalls around a few hundred kilometres. The majority of the energy from a supernova is radiated away as neutrinos, and it has been suggested that some of these neutrinos heat the matter behind the stalled accretion shock and revive the explosion.

We present preliminary results of some of the first 3D simulations of spectral neutrino transport in MHD supernova models. These models use the isotropic diffusion source approximation to efficiently perform the neutrino transport. This involves splitting the distribution function of the neutrinos into two components based on whether the particles are trapped in the matter or not, and evolving them separately using appropriate approximations for each. This algorithm means that a simulation can be performed in a reasonable amount of parallel supercomputer time.

Optimized domain decomposition methods applied to the one-dimensional heat equation and diffusive systems

Yves Courvoisier[1]

[1] Departement of Mathematics, University of Geneva,
(yves.courvoisier@unige.ch)

Abstract: Domain Decomposition Methods (DDM) were first introduced by Schwarz in 1869 for proving the *Dirichlet Principle*. After a century of latency, Lions revived Schwarz's theory with innovative convergence proofs, and since then these methods have shown themselves to be very convincing parallel algorithms.

This poster provides a short introduction to DDM, followed by a discussion of Optimized DDMs with Robin transmission conditions applied to the one-dimensional heat equation. In particular, we emphasize the surprising influence of the length of the time interval on the convergence rate. Finally, the DDM with Robin transmission conditions is applied to diffusive systems and, in a very simple situation, we provide the optimal parameter of the algorithm.

Improvement of the Effective Mass Approximation for Silicon Nanowires

Aniello Esposito[1] and Martin Frey[1] Andreas Schenk[1]

[1] Integrated Systems Laboratory, ETH Zurich, Gloriastrasse 35, CH-8092, Switzerland,
(esposito@iis.ee.ethz.ch / mfrey@iis.ee.ethz.ch / schenk@iis.ee.ethz.ch)

Abstract: This work investigates the impact of a weak external perturbation on a silicon nanowire and addresses the difficulties of the effective mass approximation (EMA) [1] in reproducing the energy of the lowest unoccupied molecular orbital (LUMO). The Hamiltonian of the nanostructure surrounded by hydrogen passivated surfaces is expressed within an empirical pseudopotential (EP) [2] framework and expanded in terms of plane waves. Initially, no perturbations are taken into consideration. In this case the LUMO energy obtained by using the EMA is found to be considerably larger than the energy computed via the EP method. This result is a consequence of the EMAs key ingredient, i.e. the parabolic approximation of the crystals bandstructure. For an increasing wire width the discrepancy between the EMA and the EP method diminishes as the parabolic approximation becomes more realistic. In a second step a weak harmonic perturbation is added to the pseudopotential and both the EMA and EP calculations are repeated for the same set of wire widths. The energy overestimation caused by the EMA is found to be close to the one of the free case addressed above. Therefore, by adding the energy shifts from the free case to the EMA Hamiltonian an improvement concerning the prediction of LUMO energies of nanowires subjected to harmonic-like perturbation can be expected. Such an improvement is particularly interesting for quantum transport simulations of small nanowires, where the simplicity of the EMA considerably reduces the computational burden and a precise knowledge of the energies becomes crucial for the reliable prediction of currents.

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Simulations of the ChI a fluorescence rise (OJIP), do they imply that the QA-based model of variable ChI a fluorescence emission is wrong?

Gert Schansker

Laboratory of Bioenergetics, University of Geneva,
(Gert.Schansker@unige.ch)

Abstract: ChI *a* fluorescence induction phenomena are known since the 1930s. However, the whole transient (OJIP) shown on a logarithmic timescale with its well-defined intermediate steps was only published in the nineties. It has provided a quite popular simulation-target. Nearly all of these simulations assume that variable ChI *a* fluorescence is determined mainly by changes in the redox state of QA as proposed by Duysens and Sweers [1]. Simulations can be a good test for this postulate. Looking at the published simulations, the fluorescence rise calculated on the basis of a Q_A-based model (with $P680^+$ and presumed PQ-pool quenching) is at least a factor 10 too fast. For the most sophisticated models that have been published the maximum fluorescence intensity is reached after approximately 20 ms; experimentally measured this is approx. 200 ms.

In this contribution the assumptions made in these models are discussed. It is proposed that the failure to get a correct simulation despite a wealth of available kinetic information is a strong indication that the postulate of Duysens and Sweers [1] is incorrect.

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Transmission conditions by asymptotic expansion versus thin sheet bases

Kersten Schmidt[1] and Sébastien Tordeux[2]

[1] Group POEMS, INRIA Paris-Rocquencourt,
(kersten.schmidt@inria.fr)
[2] Institut de Mathématiques de Toulouse, Université de Toulouse,
(sebastien.tordeux@insa-toulouse.fr)

Abstract: Sensitive measurement and control equipment is protected from disturbing electromagnetic fields by thin shielding sheets [1]. We will compare two frameworks for their modelling, both derived for higher orders:

- transmission conditions derived by asymptotic expansion in the sheet thickness [3],
- incorporating thin basis functions which are adapted to the shielding behaviour [2].

The asymptotic expansion providing a Taylor expansion of the solution w.r.t. the sheet thickness ε provides Leontovich-type transmission conditions. For the terms of the asymptotic expansion derived for any order for smooth sheets and show regularity, stability and convergence in ε.

The approach with thin sheet basis functions accommodates the different behaviour of the solution in thickness direction and along the sheets and is also applicable for high frequencies. We will show that the convergence to any order in ε can be reached by increasing the number N of functions, whereas the error also decreases for a particular thickness.

We will compare the benefits, efficiency and limits of the two frameworks within FEM discretisations.

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Solving Bi-Objective Many-Constraint Bin Packing Problems in Automobile Sheet Metal Forming Processes

Madan Sathe[1], Olaf Schenk[1]

[1]Department of Computer Science, University of Basel, Switzerland
(madan.sathe@unibas.ch)

Abstract: The solution of bi-objective bin packing problems with many constraints is of fundamental importance for a wide range of engineering applications such as wireless communication, logistics, or automobile sheet metal forming processes. When the bi-objective bin packing problem is single-constrained, state-of-the-art multi-objective genetic algorithms such as NSGA-II combined with standard constraint handling techniques can be used. In the case of many-constraint bin packing problems, problems with thousand of additional constraints, it is not easy to solve this kind of problem accurately and fast with classical methods. Our approach relies on two key ingredients, NSGA-II and a clustering algorithm in order to generate always feasible solutions independent of the number of constraints. The method allows to tackle bi-objective many-constraint bin packing problems. We will present results for challenging artificial bin packing problems which model typical bi-objective bin packing problems with many constraints arising in the automobile industry.

Perfectly Matched Layers for the Transient Wave Equation

Marcus J. Grote[1] and Imbo Sim[1]

[1] Department of Mathematics, University of Basel
(Marcus.Grote@unibas.ch / Imbo.Sim@unibas.ch)

Abstract: In the last decade, the perfectly matched layer (PML) approach [2] has proved a flexible and accurate method for the simulation of waves in unbounded media. Standard PML formulations, however, usually require wave equations stated in their standard second-order form to be reformulated as first-order systems, thereby introducing many additional unknowns. To circumvent this cumbersome and somewhat expensive step we propose instead a simple PML formulation directly for the transient wave equations in its second-order form [4]. Our formulation requires fewer auxiliary unknowns than previous formulations [1, 3] and is easily coupled with standard finite difference or finite element methods. Our computational experiments verify its accuracy, simplicity and efficiency.

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Finite Element Heterogeneous Multiscale Method for the Wave Equation

Assyr Abdulle[1], Marcus J. Grote[2] and Christian Stohrer[2]

[1] Institute of Analysis and Scientific Computing, EPFL,
(assyr.abdulle@epfl.ch)
[2] Departement of Mathematics, University of Basel,
(marcus.grote / christian.stohrer@unibas.ch)

Abstract: The simulation of time dependent waves propagating through a medium with rapidly varying propagation speed can be prohibitively expensive with a standard finite element (FE) approach, because it requires a resolution down to the finest scales of the medium. We propose a FE-scheme within the framework of the heterogeneous multiscale method (HMM), which overcomes these problems. The HMM has been presented by E and Enquist [1] as a general methodology for the computation of multiscale problems. Numerous applications for elliptic and parabolic problems have been developed using this methodology [2,3,4]. Here, we adapt the method described by Abdulle [5] to the time dependent wave equation, derive error estimates and illustrate our results by numerical experiments.

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