Schweizer Numerik Kolloquium
Colloque numérique suisse 2008

April 25, 2008

Université de Fribourg, Campus Pérolles

Book of Abstracts

Invited lectures

The technique of hierarchical matrices

Wolfgang Hackbusch

Max-Planck-Institute for Mathematics in the Sciences,
Inselstr. 22-26, D-04103 Leipzig,
Wolfgang.Hackbusch@mis.mpg.de

Abstract: Matrices of large size arise in particular from elliptic partial differential equations and integral equations. In the former case one make use of the sparsity, in the latter case a standard treatment of the matrices leads already to storage problems. The technique of hierarchical matrices allows to organise the storage as well as all matrix operations (including inversion) with almost linear complexity. The hierarchical matrix operations yield only approximations, but the arising error can be made at least as small as the discretisation error.

The lecture explains the matrix representation, the organisation of the operations and underlines the black-box character of the method. Furthermore, applications are described which are usually considered to be impossible for large scale matrices: computation of functions of matrices and solution of matrix equations (of Lyapunov, Sylvester, Riccati, etc.).

New challenges for stochastic simulations: theoretical and numerical issues

Denis Talay

Projet TOSCA, INRIA Sophia Antipolis,
2004 route des Lucioles, BP 93, F-06902 Sophia Antipolis,
denis.talay@sophia.inria.fr

Abstract: The lecture is aimed to present some recent results and some fascinating theoretical and/or numerical questions related to stochastic modelling and stochastic simulations. The presentation does not suppose any prerequisite in stochastic calculus. It will provide intuitive explanations of the difficulties to overcome and of relevant techniques which combine PDE analysis and probability theory.

Contributed oral presentations

Problems in cylinders: when and what to compute in lower dimensions?

Michel Chipot

Angewandte Mathematik, Universität Zürich,
m.m.chipot@math.unizh.ch

Abstract: We show on some examples why some problems set in large cylinders can be solved numerically by reducing the computations to the section.

Simple Simplex Sampling: Exploring the Solution Space of Degenerate Problems in High Dimensions

Jonathan Coles

Institut für Theoretische Physik, Universität Zürich,
jonathan@physik.uzh.ch

Abstract: I will present a method of sampling the solution space of matrix inversion problems. When the space is bounded by linear equations the space forms a convex polytope called a simplex. For many applications, one is interested not just in a single solution, as would be given by a standard matrix inversion technique, but a range of solutions which explore the degeneracies of a problem. This new method can sample arbitrarily shaped simplexes in N dimensions, is metric insensitive, and does not show projection biases as N increases. It has been used in several astrophysical contexts and, in particular, has been instrumental in estimating the age of the universe by way of gravitational lens modeling.

Plane wave discontinuous Galerkin methods

C.J. Gittelson[1], R. Hiptmair[1] and I. Perugia[2]

[1] Seminar für Angewandte Mathematik, ETH Zürich
claude.gittelson@sam.math.ethz.ch

[2] Dipartimento di Matematica, Universitá di Pavia, Italy

Abstract: Nonconforming Galerkin methods with discontinuous trial and test spaces allow a great deal of flexibility in the choice of local basis functions. For homogeneous boundary value problems, these can be chosen in the kernel of the differential operator, resulting in a problem-adapted Trefftz-type discretization. We persue this approach for the Helmholtz equation with plane waves as local basis functions [1,2]. This generalizes the ultra-weak variational formulation of O. Cessenat and B. Deprés and embeds it in a discontinuous Galerkin setting. Uniform plane wave basis functions already lead to significant improvements in efficiency as compared to classical finite elements. First numerical experiments indicate that the use of plane wave spaces adapted to locally dominant propagation directions is rewarded by a further gain in accuracy.

[1] C.J. Gittelson, R. Hiptmair and I. Perugia, *Plane wave discontinuous Galerkin methods*, Preprint NI07088-HOP, Isaac Newton Institute Cambride, Cambridge, UK, December 2007. http://www.newton.cam.ac.uk/preprints/NI07088.pdf. Submitted to M2AN.

[2] C.J. Gittelson, *Plane wave discontinuous Galerkin methods*, Master's Thesis, Depertment of Mathematics, ETH Zürich, January 2008.

Discretization of generalized convection diffusion equations

Holger Heumann

Seminar for Applied Mathematics, ETH Zürich
Holger.Heumann@sam.math.ethz.ch

Abstract: Upwinding and SUPG-like Methods [1] are well established methods to obtain stable discretizations of the scalar convection-diffusion equations in the case of singular perturbation. This talk will focus on the discretization of the generalization of the convective terms. The generalization is based on the notion of the Lie derivative [2] and includes for example magnetic convection $\mathbf{v}\times\mathrm{curl}\mathbf{A}$. Starting with the scalar case we show that in a variational setting the discrete Lie derivative is identical to a Galerkin method using some inexact first order upwind quadrature. We even generalize this to higher order. Since there is very little reported experience with the stability of convection in the vector case, we will then present several conceivable discretizations, including the Lie derivative approach and a SUPG-like method and a few first numerical results.

[1] A.N. Brooks and T.J.R. Hughes: Streamline-upwind/Petrov-Galerkin formulations for convection dominated flows with particular emphasis on the incompressible Navier-Stokes equations, Comput. Meth. Appl. Mech. Engrg., 32 (1982), pp. 199–259.

[2] A. Bossavit: Extrusion, contraction: their discretization via Whitney forms, COMPEL, 22 (2003) , pp. 470–480.

Coupling atomistic and continuum descriptions using dynamic control

Evangelos Kotsalis and Petros Koumoutsakos

CSE Lab, ETH Zürich,
kotsalie@inf.ethz.ch petros@inf.ethz.ch

Abstract: Molecular Dynamics (MD) simulations are often used to model atomistic effects such as those from surface modifications to the properties of the boundary. MD models can not be extended to larger systems due to their computational cost. In turn, mesoscale and macroscale descriptions are employed in order to simulate systems of larger size and for times that would be relevant for engineering applications. In the past hybrid, atomistic/continuum techniques have been presented for monatomic molecules such as argon. The inclusion of polar multi-atom molecules, such as water, introduces a number of computational challenges, such as the handling of electrostatic effects. A potential of mean force is developed through a novel control algorithm that aims to reduce spurious density fluctuations associated with the coupling of atomistic and continuum descriptions.

Optimization-constrained differential equations with discontinuities: application to air quality modeling

Chantal Landry[1], Alexandre Caboussat[2] and Ernst Hairer[3]

[1] Institute of Analysis and Scientific Computing, EPFL,
chantal.landry@epfl.ch

[2] Department of Mathematics, University of Houston,
caboussat@math.uh.edu

[3] Section de mathématiques, Université de Genève,
Ernst.Hairer@math.unige.ch

Abstract: A numerical method for the resolution of a system of ordinary differential equations coupled with a mixed constrained minimization problem is presented. Such coupling appears for instance in computational chemistry when a system at equilibrium exchanges mass with a surrounding media ([1]). Discontinuities of some variables are induced when inequality constraints are activated or deactivated. The ordinary differential equations are combined with the first order optimality conditions of the optimization problem. The resulting differential-algebraic system is solved between the discontinuities with the implicit Runge-Kutta method of order 5 (RADAU5, [2]). The main difficulty consists in the characterization of the discontinuity points via minimization problems and not by an explicit switching (or event) function. An algorithm for the detection of discontinuities is developed, that relies on continuation techniques for the determination of local minima and dense output formulas. Numerical results applied to atmospheric particles are proposed to show the efficiency of this approach.

[1] N. R. Amundson, A. Caboussat, J.W. He, C. Landry and J. Seinfeld: A Dynamic Optimization Problem Related to Organic Aerosols, C. R. Acad. Sci. Paris, 344 (2007), 519–522.

[2] E. Hairer and G. Wanner: Solving Ordinary Differential Equations II. Stiff and Differential-Algebraic Problems, Springer-Verlag, Berlin, Heidelberg, New York, 2nd edition, 1996.

Explicit energy conserving local time stepping for acoustic and electromagnetic wave propagation

Julien Diaz[1], Marcus Grote[2] and Teodora Mitkova[2]

[1] Magique 3D, INRIA Futurs,
Julien.Diaz@inria.fr

[2] Departement Mathematik, Universität Basel,
Marcus.Grote@unibas.ch Teodora.Mitkova@unibas.ch

Abstract: The numerical solution of the wave equation and of Maxwell's equations in second-order form is of fundamental importance to the simulation of time dependent acoustic and electromagnetic phenomena. To adress the wide range of difficulties involved, the model equations are discretized in space by symmetric interior penalty discontinuous Galerkin methods, which yield an essentially diagonal mass matrix.

In the presence of complex geometry, adaptivity and mesh refinement are certainly key for the efficient numerical solution of partial differential equations. However, locally refined meshes impose severe stability constraints on explicit time-stepping schemes, where the maximal time-step allowed by a CFL condition is dictated by 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 the stability restriction, we propose local time-stepping schemes, which allow arbitrarily small time steps where small

elements in the mesh are located. When combined with the discretization in space, the resulting fully discrete scheme is explicit and exactly conserves a discrete energy. Numerical experiments illustrate the efficiency of these methods and validate the theory.

A Tensor Framework for Multidimensional Signal Processing

Oleksii Morozov, Patrick Hunziker

Physics in Medicine Group, University Hospital of Basel,
MorozovA@uhbs.ch HunzikerP@uhbs.ch

Abstract: Based on the dimensionality of physical space, signal processing often involves multidimensional data. While preservation of the multidimensional structure in the problem formulation might seem desirable at first sight, currently, the standard way of treating such problems is their reduction to a matrix representation through matricizing or vectorizing of the terms in the problem formulation. We propose instead a natural tensor based approach which preserves the geometry and transformational properties of a multidimensional system under consideration. We describe a definition of tensors and their basic operators specifically suited for handling multidimensional problems arising from signal processing and other engineering fields. We introduce the notion of a multilinear system of equations and discuss questions related to its solution in a natural way using tensors, without conversion to matrix representation. We show that proposed theoretical ideas have direct relation to generation of elegant and efficient computational algorithms which explicitly exploit geometrical structure and physical coherence of multidimensional data.

Complex multiphase flow simulation using immersed surfaces and local mesh refinement methods

C. Narayanan, D. Caviezel, and D. Lakehal

ASCOMP GmbH, Technoparkstrasse 1, 8005 Zurich
chidu@ascomp.ch

Abstract: Multiphase flow is by nature a multi-scale problem due to the presence of interfaces separating the phases. We present a new integrated immersed surfaces approach for multiphase flow simulation (including multiple solid and fluid phases), in combination with a block–based local mesh refinement (BMR) technique. The formulation is such that it accounts for conjugate heat transfer between the solid and the fluid phase in a natural way. The fluid–fluid interface is captured using interface tracking methods such as Level Set or Volume of Fluid methods. The immersed surfaces technique (IST) allows for rapid mesh generation with locally refined grids. Complex multiphase flow problems with (conjugate) heat and mass transfer can be set up with minimum effort. Several examples of such flow simulations of interest to particular industry sectors will be presented.

A Stochastic-Lagrangian Modeling Framework for Multiphase Flow in Porous Media

Manav Tyagi and Patrick Jenny

Institute of Fluid Dynamics, ETHZ,
tyagi@ifd.mavt.ethz.ch

Abstract: CO_2 storage in subsurface formations involves many complex physical processes that are well understood at the pore scale. However, in a real scenarios, it is not feasible to perform pore scale simulations, and one needs a large scale model. Unfortunately, the Darcy based large scale models for multiphase flow and transport are questionable, particularly in the context of CO_2 storage. One of the main assumptions in these models is the concept of relative permeability and capillary pressure, which are expressed as functions of saturation. Moreover, these quantities are typically measured under equilibrium conditions and scale independence is assumed. However, under unstable conditions these assumptions may not be valid. We proposed [1] an alternative modeling approach based on the Lagrangian movement of stochastic particles, which represent infinitesimal fluid phase volumes and evolve such that their statistics represent the statistics of the actual fluid volumes. Each particle is labeled by a fluid phase, has its individual velocity, a position in physical space and possibly other properties, e.g. CO_2 concentration. As a particle moves in physical space, its properties change according to the stochastic processes such that the specified Lagrangian statistics is honored. The goal of this work is to model these stochastic processes based on the pore scale physics. For the illustration purpose a simplified 3D pore-network consisting of spherical pores and cylindrical throats is considered. The flow through the network is described by simple rules for the fluid movement in the throats and for the pore filling [2]. First, flow with self-similar average saturation profiles are investigated. These cases correspond to multiphase Darcy flow, where the relative permeabilities are uniquely determined by the saturation values. More interesting are those scenarios, where no self-similar profile can observed and classical multiphase Darcy model fails. For such cases non-equilibrium phenomena at the pore scale play an important role and we demonstrate how these can be modeled in our stochastic particle framework. With the help of pore-network simulations first the non-equilibrium pore scale dynamics has been studied. Then, based on the extracted Lagrangian statistics, comparative simulations with stochastic particle method have been performed.

[1] M. Tyagi, P. Jenny, I. Lunati, H.A. Tchelepi: Multiscale method for multiphase flow in porous media using stochastic particles, CMWR XVI , 19-22 June 2006, Copenhagen, Denmark.

[2] R. Lenormand, E. Touboul, and C. Zarcone: Numerical models and experiments on immiscible displacements in porous media, J. Fluid Mech. 189 (1988), 165–187.

Efficient approaches to quantum dynamics based on semiclassical dynamics and the imaginary-time path integral

Jiří Vaníček

Laboratory of theoretical physical chemistry, EPFL Lausanne,
jiri.vanicek@epfl.ch

Abstract: In the case of chemical kinetics, quantum-instanton approximation can be used to transform the dynamical problem of computing a rate constant of a reaction at finite temperature to a quantum thermodynamical problem. As such, it can be numerically solved by a discretized

imaginary-time path integral techniques (Monte Carlo or Molecular Dynamics). In both cases, the central part of the calculation is how the statistical error of a computed quantity (an estimator) scales with the number P of imaginary time slices of the path integral as we approach the quantum limit. We develop a method to compute kinetic isotope effects and we show that the simplest estimators have errors growing linearly with P and therefore the computational time grows with P^2. Finally, we derive alternative, efficient estimators for the same quantities, for which the error and therefore the computational time is approximately independent of P.

High-order numerical integrators based on modified differential equations

Philippe Chartier[1], Ernst Hairer[2] and Gilles Vilmart[1,2]

[1] INRIA Rennes, France
[2] Section de mathématiques, Université de Genève, Switzerland
http://www.unige.ch/~vilmart

Abstract: Inspired by the theory of modified differential equations (backward error analysis for ordinary differential equations), we present a general procedure for the construction of high-order numerical integrators that preserve geometric properties of the exact flow (e.g. symmetry, symplecticity, conservation of first integrals).

For the special case of the equations of motion of the free rigid body, this approach yields efficient high-order integrators that exactly preserve all first integrals. We also study the propagation of round-off errors in rigid body dynamics, for an accurate integration over long times.

[1] P. Chartier, E. Hairer, and G. Vilmart, Modified differential equations. *ESAIM Proceedings*, Vol 21 (2007) 16–20.

[2] P. Chartier, E. Hairer, and G. Vilmart, Numerical integrators based on modified differential equations. *Math. Comp.* 76 (2007) 1941-1953.

[3] E. Hairer and G. Vilmart, Preprocessed Discrete Moser–Veselov algorithm for the full dynamics of the rigid body. *J. Phys. A: Math. Gen.* 39 (2006) 13225-13235.

[4] G. Vilmart, Reducing round-off errors in rigid body dynamics. *submitted*.

Contributed posters

Stochastic Modeling of Evaporating Turbulent Sprays

Gaurav Anand and Patrick Jenny

Institute of Fluid Dynamics, ETH Zürich,
anand@ifd.mavt.ethz.ch

Abstract: Polydispersed turbulent evaporating and reacting flows are complex two-phase flow phenomena occuring in many industrial processes. This phenomena is characterised by liquid fuel droplets dispersion, their evaporation, and the fuel vapour reaction with the oxidizer, all occuring interactively at the same time. Thus signifying the need for accurate prediction of the fuel droplets dispersion and their evaporation. In the present study, a framework for modeling two-phase evaporating flow is presented.

This framework employs an Eulerian-Lagrangian-Lagrangian approach [1] . For the continuous phase, a joint velocity-composition probability density function (PDF) method is used [2]. Opposed to other approaches, such PDF methods require no modeling for turbulent convection and chemical source terms. For the dispersed phase, the mass density function (MDF, density-weighted PDF) $\mathcal{F}_p\ (x, V_p, D_p, \psi_p, V_s, \psi_s; t)$ of velocity, diameter, temperature, seen gas velocity and seen gas composition is calculated. This provides a unified formulation, which allows to consistently address the different modeling issues associated with such a system. Because of the high dimensionality, particle methods are employed to solve the PDF transport equations.

The above framework has been used to simulate the experimental results obtained by Sommerfeld and Qiu [3] for the evaporating iso-propyl alcohol spray. The figure below shows the preliminary comparison between the mean droplet diameter profiles obtained from the experiment and simulation. A good overall agreement is observed.

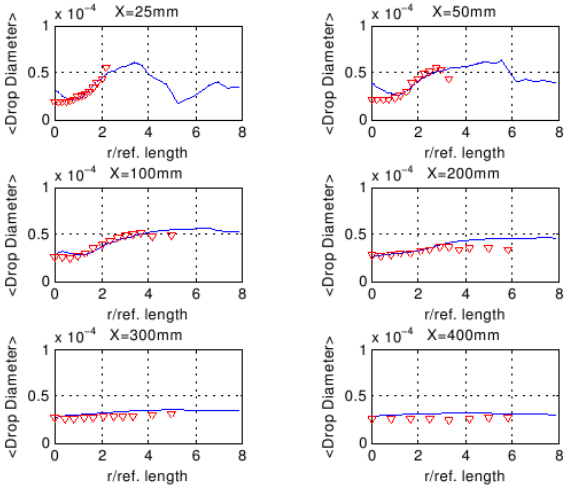

Figure: Experimental ($\bigtriangledown$) and simulation ($-$) result for the evaporating spray.

[1] B. Naud, PhD Thesis, Delft University of Technology, (2003).

[2] P. Jenny and S. B. Pope, J. Comp. Physics 166(2), 218 (2001).

[3] M. Sommerfeld and H. H. Qiu, Int. J. of Heat and Fluid Flow 19, 10 (1998).

A boundary integral method for time dependent problems

Lehel Banjai and Stefan Sauter

Institute of Mathematics, University of Zurich,
lehelb@math.unizh.ch stas@math.unizh.ch

Abstract: Recently, see [1], a highly efficient method for the numerical solution of the wave equation in unbounded domains has been introduced by the authors. A retarded potential formulation is discretised by convolution quadrature in time and a boundary element method (BEM) in space. By means of a discrete Fourier transform, the method arrives at a decoupled system of Helmholtz problems with complex frequencies, which can then be solved in parallel by the BEM. Due to the complex frequencies many of the boundary-element matrices are sparse and the remaining dense parts can be approximated by data sparse techniques.

In this poster, we describe the basic method and the choice of parameters and present a number of numerical experiments which demonstrate the efficiency and stability at long times of the method. We concentrate on the wave equation but also indicate that to solve a number of other interesting time-dependent partial differential equations a one-line change of the computer code is sufficient.

[1] L. Banjai and S. Sauter: Rapid solution of the wave equation in unbounded domains, Preprint 10-2007, University of Zurich (2007).

ROOT: a Data Storage and Analysis Framework

Bertrand Bellenot

PH/SFT Departement, CERN, Genève
bertrand.bellenot@cern.ch

Abstract: The Large Hadron Collider (LHC) is a particle accelerator being installed in a tunnel 27 km in circumference located near Geneva, between the Jura and the Lake Leman. The LHC will produce head-on collisions between two beams of particles, either protons or lead ions.

When the LHC begins operations, it will produce roughly 15 petabytes (15 million gigabytes) of data annually, enough to fill 100 000 DVDs a year.

This poster shows an overview of the Data Storage and Analysis using ROOT, an Object-Oriented Data Analysis Framework (`http://root.cern.ch`).

Numerical solution of the incompressible Navier-Stokes equations with the immersed-boundary technique

Giuseppe Bonfigli and Patrick Jenny

Institute of Fluid Dynamics, ETH Zurich,
bonfigli@ifd.mavt.ethz.ch jenny@ifd.mavt.ethz.ch

Abstract: A numerical procedure for the simulation of flows in complex geometries is being developed relying on the immersed boundary technique. The incompressible Navier-Stokes equations are formulated in primitive variables [1] and boundary conditions are imposed exactly by adaption of the discretization stencils at grid nodes close to the boundary. The Multi-Scale-Finite-Volume method [2], originally developed for the solution of elliptic problems governing flows in porous

media, is used to solve the pressure Poisson equation. Solid bodies are easily accounted for by introducing regions with zero permeability.

Ongoing work aims to enhance the order of accuracy of the numerical procedure, whereby consistence and accuracy are verified by means of numerical tests. Future work will be focused on the implementation of moving walls.

[1] Harlow and Welch: Numerical calculation of time-dependent viscous incompressible flow of fluid with free surface, J. Comp. Phys, vol. 8 (1965), 2182-2189.

[2] P. Jenny, S. H. Lee and H. A. Tchelepi: Multi-scale finite-volume method for elliptic problems in subsurface flow simulation, J. Comp. Phys., vol. 187 (2003), 47-67.

Compact Third Order Limiter Functions for Non-Linear Hyperbolic Conservation Laws

Miroslav Čada and Manuel Torrilhon

Seminar für Angewandte Mathematik, ETH Zürich,
miroslav.cada@math.ethz.ch manuel.torrilhon@math.ethz.ch

Abstract: In this study, we employ and generalize the idea of double-logarithmic reconstruction for the numerical solution of hyperbolic equations, as proposed recently by Artebrandt and Schroll. The result is a class of efficient third-order schemes with a compact three-point-stencil and a single limiter.

An identification of the basic properties of the double-logarithmic reconstruction led to conditions for the construction of new non-oscillatory third-order limiter functions. These functions were optimized for simplicity and efficiency. The resulting methods handle discontinuities as well as local extrema within the standard semi-discrete MUSCL algorithm using only a single limiter function.

In order to match the spatial discretization we adjust the time integration scheme to be third-order accurate as well. A stability analysis of third-order Runge-Kutta schemes applied to the new spatial operator shows an improved CFL condition such that simulations with CFL < 1.5 are stable.

We will illustrate the performance of this scheme with several numerical experiments, including gas dynamic and MHD flows.

Simulating cosmological galaxy formation with N-body/SPH

Simone Callegari[1], Lucio Mayer[1,2] and Elena D'Onghia[1]

[1] Istitute for Theoretical Physics, University of Zurich
callegar@physik.uzh.ch lucio@physik.uzh.ch elena@physik.uzh.ch

[2] Institute of Astronomy, ETH Zurich - Hönggerberg
lucio@phys.ethz.ch

Abstract: Modelling the formation of galaxies in cosmological simulations is an unsolved problem which spans a broad range in physical conditions; both the large-scale structure of the Universe and the (relatively) small-scale physics of star formation need to be accounted for with sufficient accuracy. I will describe the standard approach [1] to multiscale cosmological simulations, and in particular the algorithms employed by one of the most succesful [2] codes in this field: GASOLINE [3], an N-body tree-code with Smoothed Particle Hydrodynamics. Star formation and its feedback on environment are treated with sub-resolution, phenomenological prescriptions [4] which allow to tackle the problem on modern supercomputers.

[1] E. Bertschinger: Multiscale Gaussian Random Fields and their application to cosmological simulations, The Astrophysical Journal Supplement Series, Vol. 137 Issue 1 (2001), 1–20

[2] F. Governato, B. Willman, L. Mayer, A. Brooks, G. Stinson, O. Valenzuela, J.W. Wadsley, T. Quinn: Forming disc galaxies in ΛCDM simulations, Monthly Notices of the Royal Astronomical Society, Vol. 374 Issue 4 (2007), 1479–1494

[3] J.W. Wadsley, J. Stadel, T. Quinn: Gasoline: a flexible, parallel implementation of TreeSPH, New Astronomy, Vol. 9 Issue 2 (2004), 137–158

[4] G. Stinson, A. Seth, N. Katz, J.W. Wadsley, F. Governato, T. Quinn: Star formation and feedback in Smoothed Particle Hydrodynamic simulations - I. Isolated Galaxies, Monthly Notices of the Royal Astronomical Society, Vol. 373 Issue 3 (2006), 1074–1090

Chemical kinetics with delays in the R-leaping stochastic simulation algorithm

André Leier, Philippe Chatelain and Petros Koumoutsakos

Computational Science and Engineering Laboratory, ETH Zurich,
andre.leier@inf.ethz.ch philippe.chatelain@inf.ethz.ch petros@inf.ethz.ch

Abstract: In recent years, stochastic simulation algorithms for chemical kinetics have seen important advances, most notably the introduction of approximate accelerated schemes such as τ-leaping[1], binomial τ-leaping[2] and R-leaping[3]. The recently introduced R-leaping algorithm proceeds by triggering a pre-determined number of reaction firings. This approach has proved efficient in the case of large systems with disparate rates.

Gene expression and regulation problems can be modeled more accurately through the introduction of delayed firings, e.g. for the mRNA translocation and transcription processes[4]. We present the implementation of delayed reaction firings into the R-leaping framework and assess its performance.

[1] D.T. Gillespie: Approximate accelerated stochastic simulation of chemically reacting systems, Journal of Chemical Physics, 115 (2001), 1716.

[2] T. Tian and K. Burrage: Binomial leap methods for simulating stochastic chemical kinetics, Journal of Chemical Physics, 121 (2004), 10356.

[3] A. Auger and P. Chatelain and P. Koumoutsakos: R-leaping: accelerating the stochastic simulation algorithm by reaction leaps, Journal of Chemical Physics, 125 (2006), 84103.

[4] A. Leier and T.T. Marquez-Lago and K. Burrage: Generalized Binomial τ-leap method for biochemical kinetics incorporating both delay and intrinsic noise, Journal of Chemical Physics, submitted.

Large-Scale PDE-constrained Optimization in Hyperthermia Cancer Treatment Planning

Matthias Christen, Olaf Schenk and Helmar Burkhart

High Performance and Web Computing Group, Departement of Computer Science, University of Basel,
m.christen@unibas.ch olaf.schenk@unibas.ch helmar.burkhart@unibas.ch

Abstract: Hyperthermia treatment is a promising option in oncology. By heating the tumor using electro-magnetic energy, it is made more susceptible to an accompanying radio or chemo therapy. The problem addressed in this project is a large-scale optimal control problem for finding the therapeutical optimal antenna parameters given the patient geometry. The temperature distribution is modeled by Penne's steady-state bioheat equation (a Helmholtz equation). An FD method is used for discretization. The goal is optimization in real-time using HPC hardware so that the physician could react to patient feedback during treatment. We are using primal-dual interior point methods as the most efficient methods for solving these nonlinear nonconvex programming problems [1,2]. These resulting optimization problems are computationally demanding and require special algorithmic solution schemes that are addressed in the research project.

[1] O. Schenk, A. Wächter, and M. Weiser: Inertia Revealing Preconditioning, For Large-Scale Nonconvex Constrained Optimization, Technical Report CS-2007-12 (2007), Computer Science Department, University of Basel, Switzerland. Submitted.

[2] A. Wächter and L. T. Biegler: On the implementation of a primal-dual interior point filter line search algorithm for large-scale nonlinear programming, Mathematical Programming, 106 (2006), pp. 25–57.

SfePy: finite element analysis software in Python

Robert Cimrman, Eduard Rohan, Vladimír Lukeš

Department of Mechanics & New Technologies Research Centre
University of West Bohemia, Plzeň, Czech Republic
cimrman3@ntc.zcu.cz rohan@kme.zcu.cz lukes@kme.zcu.cz

Abstract: SfePy is an open source finite element analysis software written primarily in Python programming language, cf. [1]. It was designed to provide a flexible general finite element modeling tool which is easily adaptable to solve problems defined in terms of PDEs systems. A variety of problems treated by SfePy is demonstrated in several examples. In the first one an application concerning shape optimization of closed channels is presented where a criterion is aimed at improving the velocity profile of the Newtonian liquid flow, see [2]. Then a multiscale modeling example follows, originating from the description of a strongly heterogeneous porous medium (e.g. bone) by the theory of homogenization, cf. [3]. In the final example we present some results on modeling so-called phononic materials, elastic periodic structures featured by strong heterogeneities in the elasticity; in the homogenized medium, negative eigenvalues of an effective mass tensor appear for certain frequency ranges, leading to so-called band gaps in acoustic wave propagation, see [4]. The examples are interleaved with general information on SfePy; the choice of the Python is discussed as well as other tools required to install or use the software.

[1] R. Cimrman et al.: SfePy home page, http://sfepy.kme.zcu.cz, 2008.

[2] R. Cimrman and E. Rohan: On shape optimization of conduits with incompressible flow, Applied and Computational Mechanics, no. 2 (2007), 393–400.

[3] G. Griso and E. Rohan. On the homogenization of a diffusion-deformation problem in strongly heterogeneous media. Ricerche di Matematica, 56, No. 2, (2007), 161–188.

[4] A. Ávila and G. Griso and B. Miara and E. Rohan, Multi-scale modelling of elastic waves – theoretical justification and numerical simulation of band gaps, Accepted for publication in MMS (Multiscale Modeling and Simulation), SIAM, (2007).

Error estimates for optimized domain decomposition methods applied to the one-dimensional heat equation

Yves Courvoisier

Section de mathématiques, Université de Genève,
yves.courvoisier@math.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 very innovative convergence proofs, and Dryja and Widlund studied Schwarz methods in a discrete setting for parallel computing purposes. Later, optimized Schwarz methods were introduced, based on an optimization of the communication between the subdomains. These methods are of interest because of their fast convergence rates.

This presentation provides a short introduction to DDM, followed by a discussion of Optimized DDMs with Robin transmission conditions applied to the one-dimensional heat equation. The efficiency of the Robin transmission conditions will be emphasized. We present existing results for these algorithms, and a very recent performance analysis for short time intervals.

Numerical investigation of eye lens proteins stability: a colloidal approach

N. Dorsaz[1], G. Foffi[1], A. Stradner[2], G. Thurston[3] and P. Schurtenberger[2]

[1] IRRMA and ITP, Ecole Polytechnique Federale de Lausanne,
nicolas.dorsaz@epfl.ch giuseppe.foffi@epfl.ch

[2] Physics Department and Fribourg Center for Nanomaterials, University of Fribourg
anna.stradner@unifr.ch peter.schurtenberger@unifr.ch

[3] Physics Department, Rochester Institute of Technology (NY)
george.thurston@rit.edu

Abstract: Understanding interparticle interactions in protein solutions is of central importance to gain insight into the origin of protein condensation diseases. We developped a coarse-grained model to study mixtures of eye lens proteins and we simulated it by molecular dynamics. Validation of the model came by small-angle neutron scattering experiments. We demonstrated that transparency of eye lens crystallin mixtures is greatly enhanced by a weak, short-range attraction between α and γ-crystallin, two of the proteins involved in cataract disease. Provided it is not too strong, such mutual attraction considerably decreases the critical temperature and corresponding opacity due to light scattering, and it is consequently essential for eye lens transparency [1]. The thermodynamic stability of the binary α-γ model mixture was then investigated via Barker-Henderson perturbation theory. The instability boundary of these crystallin mixtures was found to depend on the α-γ attraction in a manner that is both extremely sensitive and non-monotonic, in excellent agreement with the experimental and numerical results [2].

[1] A. Stradner, G. Foffi, N. Dorsaz, G. Thurston and P. Schurtenberger, Phys. Rev. Lett., 99 (2007), 198103

[2] N. Dorsaz, A. Stradner, G. Thurston, P. Schurtenberger and G. Foffi (to be submitted)

Adaptive time series filters obtained by minimisation of the Kullback-Leibler divergence criterion

Jean-François Emmenegger[1], and Elena L'vovna Pervukhina[2]

[1] Department of Quantitative Economics, University of Fribourg,
jean-francois.emmenegger@unifr.ch

[2] Sevastopol National Technical University, Ukraine,
elena@pervuh.sebastopol.ua

Abstract: This study presents an extension of the Kalman filter techniques used in state space time series filtering and proposes adaptive filters, based on the minimisation of the Kullback-Leibler divergence criterion, measuring the difference between two distributions of random variables. The paper discusses algorithms working under conditions of deficient information concerning the knowledge of the distribution of the error terms of the system described in state space form.

Limitations of the Effective Mass Approximation: A Specific Example

Aniello Esposito[1] and Andreas Schenk[1,2]

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

[2] Synopsys LLC., Affolterstrasse 52, CH-8050 Zurich, Switzerland

Abstract: A suitable Schrödinger problem is solved by exact diagonalization (ED) and the result is compared to the one obtained via the effective mass approximation (EMA) [1]. The problem consists of an optical lattice embedded in a variable external potential (EP). By decreasing the EP width from ≈5nm down to ≈1nm the EMA is found to increasingly overestimate the ground state energy (GSE) as expected. For the largest EP width considered in this example the EMA reproduces the GSE up to ≈1 meV. The matrices resulting from the plane wave expansion used for the EMA as well as for the ED are typically of the order of ≈70000. On a CRAY XT3 machine the ScaLAPACK is used in order to compute the corresponding eigensystems. The framework is compared to an alternative diagonalization algorithm [2] being suitable for the present problem which yields a considerable speed up as well as a smaller memory consumption.

[1] J.M. Luttinger and W. Kohn: Motion of Electrons and Holes in Perturbed Periodic Fields Phys. Rev., no. 97 (1954), 869–883.

[2] D.M. Wood and A. Zunger: A new method for diagonalizing large matrices, J. Phys. A: Math. Gen., no. 18 (1985), 1343–1359.

Fully convective giant planets: fluid dynamics through a density-stratification

Martha Evonuk[1], and Gary Glatzmaier[2]

[1] Institut fuer Geophysik, ETH,
mevonuk@erdw.ethz.ch

[2] Earth and Planetary Science, University of California, Santa Cruz,
glatz@pmc.ucsc.edu

Abstract: Modeling giant planets without cores is relevant for extrasolar giant planets as well as for Jupiter. We present three-dimensional numerical simulations of thermal convection in a fully convective (without a solid core), non-magnetic, rotating, density-stratified, spherical fluid body. Discontinuous axially aligned vortices spiral prograde, eastward, momentum away from the axis of rotation as a result of vorticity generated by fluid flowing through the density-stratification. The convergence of this nonlinear Reynolds stress maintains a banded pattern of differential rotation with a strong prograde jet at the equator, without the classical vortex stretching of convective columns. Moreover this flow structure preferentially transports heat to high latitudes, which could explain the nearly latitudinally independent surface heat flux on Jupiter given the greater solar insolation at low latitude.

Atomistic simulation of the disordered, incommensurate phase of *p*-azoxydiphenetol

Eric Germaneau, Kurt Schenk and Gervais Chapuis

Laboratoire de Cristallographie (LCr), EPFL
eric.germaneau@epfl.ch

Abstract: The aim of this work was to simulate the behaviour of an incommensurate molecular crystal using Monte Carlo (MC) and molecular dynamics (MD) technics. Incommensurate crystals are part of the more general class of aperiodic materials. In addition to diffraction methods, atomistic methods can be applied in order to afford complementary information on the mechanisms leading to the aperiodicity of crystalline structures. Incommensurate crystals exhibit sometimes characteristics of disorder which should also be included in the modelling. An MC program has been developed in order to simulate the disorder, whereas MD calculations where performed with the parallel code ddgmq [1]. The system is *p*-azoxyphenetol [2]. This compound exhibits two distinct crystalline phases from melting down to 100K. Phase I, stable above 356 K is described by a triclinic space group. Phase II is incommensurately modulated. The disorder is due to the distribution of the oxygen of the azoxy group on two possible sites. A model of disorder based on four molecular orientations has been investigated to determine the appropriate sequence of the oxygen positions using an ad hoc developed code based on the Metropolis algorithm. Subsequently, the resulting structure was relaxed by the molecular dynamic simulations. It has been shown that these combined simulations give rise to diffuse scattering which is very similar to that found in the observed diffraction patterns.

[1] D. Brown, H. Minoux and B. Maigret: Comp. Phys. Comm., no. 103 (1997),170–186.

[2] C.B. Pinheiro, M. Gardon, P. Pattison and G. Chapuis, Ferroelectrics, no. 305 (2004), 83–87.

Anisotropic finite element adaptation for compressible flows around aircrafts

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

[1] Department of Mathematics and Statistics, University of Ottawa
[2] Institut d'Analyse et Calcul Scientifique, Ecole Polytechnique Fédérale de Lausanne,
wissam.hassan@epfl.ch marco.picasso@epfl.ch

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. Preliminary results for viscous flows call be presented. 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 and is a collaboration with the GAMMA project, INRIA Rocquencourt.

Simulation of the dissolution of alumina particles in an electrolyte

Thomas Hofer

Chaire d'Analyse et Simulation Numérique, EPFL
thomas.hofer@epfl.ch

Abstract: The last part of the aluminium production is the transformation of alumina (Al_2O^3) to aluminium, which is done by electrolysis. We model the dissolution of alumina particles and the evolution of the concentration field of liquid alumina in the electrolyte. This results in coupled convection-diffusion and convection equations which are solved with stabilized Galerkin methods.

Optimal design of electromagnets for homogeneous high-intensity magnetic fields

Aleš Janka[1] and Christophe Trophime[2]

[1] Département de mathématiques, Université de Fribourg,
ales.janka@unifr.ch

[2] Laboratoire des Champs Magnétiques Intenses, CNRS, Grenoble,
christophe.trophime@grenoble.cnrs.fr

Abstract: We present a preliminary study of a shape optimization technique applied to optimal design of high-power electromagnets for the Grenoble High Magnetic Field Laboratory of CNRS. The aim of the shape optimization is twofold: i) to improve the homogeneity of high-intensity magnetic fields, and ii) to produce, in a small test-chamber, constant magnetic fields of the highest possible intensity (up to 30 Tesla).

We use a gradient-free deterministic optimization algorithm, with a mesh-independent parameterization inspired by the Free Form Deformation technique [1].

The point i) requires a fast numerical solution of non-linear PDE's of thermo-electro-statics (the thermistor problem) and magneto-statics (Biot-Savart integral), in each new shape of the domain. The limiting factor for a successful approach is the accuracy of the underlying numerical schemes [2].

For each optimization step of the point ii), a whole series of thermo-magnetostatics simulations are required, for different values of boundary values. The main limit is the simulation time. We test the computational feasibility of the project.

[1] Michele Andreoli, Aleš Janka and Jean-Antoine Désidéri: Free-form-deformation parameterization for multilevel 3D shape optimization in aerodynamics, INRIA research report no. RR-5019, November 2003, `http://www.inria.fr/rrrt/rr-5019.html`

[2] Claire Chauvin, Pierre Saramito and Christophe Trophime: Convergence properties and numerical simulation by an adaptive FEM for the thermistor problem, submitted to Computer Meth. in Appl. Mech. and Engineering.

Numerical simulation of the dynamics of a glacier

Guillaume Jouvet

Institut d'Analyse et Calcul Scientifique, EPFL
CH-1015 Lausanne, Switzerland
guillaume.jouvet@epfl.ch

Abstract: An Eulerian method is proposed ([1]) to compute the changes of a glacier geometry for given mass balances. The surface of the glacier is obtained by solving a transport equation for the Volume Of Fluid (VOF) function. The surface mass balance is taken into account by adding an interfacial term in the transport equation. Two different 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. A simulation of the evolution of the Rhône glacier is shown from 1874 to 2100 using a realistic mass balance distribution ([2]).

[1] G. Jouvet, M. Picasso, J. Rappaz and H. Blatter: A new algorithm to simulate the dynamics of a glacier: theory and applications, submitted to Journal of Glaciology.

[2] M. Huss, D. Farinotti, A. Bauder and M. Funk: Modelling runoff from highly glacierized alpine drainage basins in a changing climate, submitted to Hydrological Processes.

Parametric analysis of rotating surface flow

Yalin Kaptan, Ali Ecder, Kunt Atalik and Hakki Karaman

Department of Mechanical Engineering, Bogazici University,
yalin.kaptan@boun.edu.tr ecder@boun.edu.tr atalik@boun.edu.tr hakkikaraman@hotmail.com

Abstract: Flow due to rotating surfaces in a cylindrical enclosure is commonly used in rheometry applications and has drawn scientists' attention for many years. The main objective of this study is to develop a robust, efficient, parallelizable and preconditioned algorithm. Codes in this study were developed by using PETSc [1] which is a computational tool for the parallel solution of scientific problems. Variants of Newton's Method as well as different linear solvers, preconditioning techniques and also number of processors are tested for performance. Additionally, the effects of Reynolds number, aspect ratio, change of rotating surface on the flow and grid dependence for the problem are investigated. Some of the results are compared with the data in literature.

[1] S. Balay, K. Buschelman, W.D. Gropp, D. Kaushik, M.G. Knepley, L.C. McInnes, B.F. Smith and H. Zhang: PETSc web page, http://www.mcs.anl.gov/petsc, 2001.

Ordering-based approaches for improving solver efficiency in reservoir simulation

Felix Kwok

Section de mathématiques, Université de Genève,
Felix.Kwok@math.unige.ch

Abstract: Nonlinear conservation laws that govern fluid flow in oil reservoirs generally use implicit time discretizations for stability reasons. However, implicit methods require the solution of a very large system ($\sim 10^6$ unknowns) of nonlinear algebraic equations at every time step, and these nonlinear solves can often take up to 80% of the total simulation time. To increase solver efficiency, we propose an ordering of equations and unknowns based on the hydrostatic potential of each fluid phase. By exploiting flow direction information, this ordering leads to a more robust nonlinear solver that can circumvent the convergence difficulties experienced by Newton's method when large time steps are used. The ordering also benefits the linear iterative solver by improving the quality of the Constrained Pressure Residual (CPR) preconditioner and reduces its sensitivity to flow configurations.

Accelerated stochastic simulation of chemical kinetics with delays: Bτ - DSSA

André Leier[1], Tatiana T. Marquez-Lago[2] and Kevin Burrage[3]

[1]Computational Science and Engineering Laboratory, ETH Zürich,
andre.leier@inf.ethz.ch

[2]Computational Systems Biology, ETH Zürich,
tatiana.marquez@inf.ethz.ch

[3]ComLab, Oxford University,
kevin.burrage@comlab.ox.ac.uk

Abstract: In recent years stochastic modeling and simulation of chemical kinetics has become an important tool for studying the role of intrinsic noise in genetic regulatory networks and cellular processes. Since simulations can become computationally highly expensive for large biological systems, leap-methods (e.g. [1,2]) have been suggested for temporally coarse-graining the simulation, leading to a significant improvement of efficiency while ensuring a high accuracy.

In order to account for delays that are often associated with more complex biological processes such as transcription and translation, the stochastic simulation method has to be adjusted. In the case of the basic SSA this has been done by introducing the delay-SSA (DSSA) [3]. Here, we present the implementation of a leaping scheme for chemical kinetics with delays, the Binomial τ-leap DSSA (Bτ-DSSA) [4-6], and assess its performance on sample biochemical systems.

[1] D.T. Gillespie: Approximate accelerated stochastic simulation of chemically reacting systems, Journal of Chemical Physics, 115 (2001), 1716.

[2] T. Tian and K. Burrage: Binomial leap methods for simulating stochastic chemical kinetics, Journal of Chemical Physics, 121 (2004), 10356.

[3] M. Barrio, K. Burrage, A. Leier and T. Tian: Oscillatory regulation of Hes1: Discrete stochastic delay modelling and simulation, PLoS Computational Biology 2(9) (2006), e117.

[4] A. Leier, T.T. Marquez-Lago and K. Burrage: Generalized Binomial-leap method for biochemical kinetics incorporating both delay and intrinsic noise, Journal of Chemical Physics, submitted.

[5] A. Leier, T.T. Marquez-Lago, K. Burrage and P. Burrage: Modeling intrinsic noise and delays in chemical kinetics of coupled auto-regulated oscillating cells, International Journal for Multiscale Computational Engineering, 6(1) (2008).

[6] K. Burrage, P. Burrage, A. Leier and T.T. Marquez-Lago: Stochastic delay models for molecular clocks and somite formation. In Proceedings of SPIE. Complex Systems II. Abbott, D. et al. (Eds.), 68020Z, 6802 (2008).

Investigation of a fast algorithm for spherical transforms

Kuan Li

Institut für Geophysik, ETHZ
kuan.li@erdw.ethz.ch

Abstract: Due to the high accuracy and elimination of the 'pole problem', the Spherical Fourier transform method, involving Spherical Harmonics $\left\{Y_l^m(\theta,\phi) = P_l^m(\theta)e^{im\phi}\right\}$ where P_l^m is called an associated Legendre functions, is widely used in geomagnetism, global seismology, meteorology and also in medical tomography and crystallography.

The traditional spherical transform algorithm is stable but computationally expensive (using Gauss Legendre quadrature rule in θ direction and ordinary Fast Fourier transform 'FFT' in ϕ direction), due to the slow Legendre transform. It costs asymptotically L_{max}^3 operations but the ordinary 2D 'FFT' only costs $2L_{max}^2 ln\left(L_{max}\right)$ operations, where L_{max} is the highest spectrum degree. Therefore to find a fast and stable spherical transform is of great interest.

Daniel Potts and his colleagues [1,2,3] published a fast spherical transform algorithm on arbitrary sampling sets and developed a toolbox **'NFFT'** [4], which allows the computation using a variety of different quadrature rules. We have carried out an initial study of the numerical stability and computational efficiency of this fast spherical transform algorithm, using the **'NFFT'** toolbox and compared its performance to the traditional algorithm.

[1] D. Potts, G. Steidl and M. Tasche: Fast and stable algorithms for discrete spherical Fourier transforms, Linear Algebra Appl. 275 (1998), 433–450.

[2] S. Kunis and D. Potts: Fast spherical Fourier algorithms., J. Comput. Appl. Math. 161 (2003), 75–98.

[3] J. Keiner, D. Potts: Fast spherical Fourier algorithms, Preprint 2006-6, Universitat zu Lübeck (2006).

[4] http://www-user.tu-chemnitz.de/~potts/nfft/

Equalizer: Parallel OpenGL Application Framework

Stefan Eilemann[1] and Maxim Makhinya[2]

[1] Eyescale Software GmbH
eilemann@gmail.com

[2] Visualization and MultiMedia Lab. Department of Informatics. University of Zürich
makhinya@ifi.uzh.ch

Abstract: Interactive visualization of large data sets is one of the interesting and challenging topics for computer graphics scientists nowadays. Constantly increasing computational power and parallelism of modern CPUs, and therefore increasing number and abilities of high performance cluster solutions, as well as widely available storage lead to the generation of gigabytes of scientific data, which has to be visualized in a real time. Often this data is so vast that even using modern algorithms for data reduction it seems to be impossible to achieve high rendering speed on a single machine. In that case, parallel rendering becomes vitally important. However, it is non-trivial to develop non-application specific but generic parallel rendering software. Providing a scalable parallel rendering environment, which can cope with various types of multi-pipe graphics clusters and at the same time is generic enough to be easily used by different kinds of visualization software, seems to be the ha

In this talk we introduce a novel system, a toolkit for scalable parallel rendering software development, called Equalizer. Applications, written using Equalizer, are able to work on a wide range of graphics hardware, from laptops and single-pipe home PCs to multi-pipe workstations and high performance visualization clusters. Equalizer has several advantages over other solutions, which we are going to discuss, and first of all its amazingly flexible configurability: it can combine multiple data decomposition modes as well as heterogeneous hardware in a single configuration. Moreover, the OpenGL-based Equalizer system provides a minimally invasive application programming interface (API), making application porting as easy as possible while delivering maximum performance.

Maxwell Stresses On The Inner Core

Philippe Marti and Andrew Jackson

Earth and Planetary Magnetism Group, Institute of Geophysics, ETH Zürich,
philippe.marti@erdw.ethz.ch andrew.jackson@erdw.ethz.ch

Abstract: The Earth's inner core is elastically anisotropic. Seismic waves travel faster along the Earth's rotation axis than in the equatorial plane and display complex variations with depth. It has been proposed that this is caused by a preferred orientation of iron alloy crystals, for example due to Maxwell stresses, originating from magnetic forces, on the inner core. The Maxwell stresses and the resulting pattern of crystal alignment have been computed for simple magnetic fields. In future work, the Maxwell stresses caused by more realistic magnetic fields produced by numerical geodynamo models will be studied. For this study, a simulation based on an expansion in spherical harmonics and Jacobi polynomials is under development.

Simulation of the plasma arc in a thermal spray gun

Felix A. Muggli

Ass. Head Fluid Technology
Sulzer Innotec 1554
Sulzer Markets and Technology Ltd.
felix.muggli@sulzer.com

Abstract: The use of computation fluid dynamics (CFD) to model the operation of thermal spray processes has gained interest in the thermal spray community; able to provide an understanding as to how a process functions, and better yet how to make a process work more effectively. Advancements to the science of modeling now permits the ability to create a comprehensive model of a plasma gun that not only simulates the dynamics of the gas but also the mechanics of arcs, thermodynamics, and entrained particulates to form a nearly complete model of a working thermal spray process. The arc model includes the magnetic field (Lorentz forces), the interaction of the energy flow in the formation of plasma, and the electrical field potential that determines the arc path in the gas stream. Work presented includes the methods and procedures used to validate the model to a plasma spray gun of Sulzer Metco and exploration of the operating regime to give an in depth and insightful look into the physics behind the operation of such a gun.

Concentration Profiles Determination for Chemical Reactions using Multivariate Curve Resolution-Alternating Least Square (MCR-ALS) and Hard-Modeling

Olivier Naef[1] and Claude Daul[2]

[1] Section of Chemistry, Ecole d'Ingenieurs et d'Architectes de Fribourg,
olivier.naef@hefr.ch

[2] Departement of Chemistry, University of Fribourg,
claude.daul@unifr.ch

Abstract: A methodology for the determination of concentration profiles of chemical reactions is proposed. Online infrared spectra and standard chemical variables (temperature, pH, mass, and so on) collected during a chemical reaction are used to calculate the concentration pro-files. The used chemometric method is the Multivariate Curve Resolution-Alternating Least Square (MCR-ALS). The first imposed constraint is the pure infrared spectra of the different species present in the mixture. This spectral information comes from a direct measure of the pure components, from a database, or from computational chemistry calculation. The second constraint is an approximation of the concentration profiles itself build with a knowledge model (hard-modeling). This methodology, will be used in a batch to batch optimization process, doesn't required calibration curves and will be seen as a complementary tool for chemical development.

The methodology is illustrated for (i) a simulated reaction (anhydride acetic hydrolysis) with only one irreversible reaction, and (ii) the corresponding real reaction. The reaction is isothermal and semi-batch (one reactant is introduced during a given time). A comparison is made with the isothermal batch mode. For each system, a knowledge model (hard-modeling) is build to approximate the concentration profiles. The quality of the constraints given by the pure infrared spectrum species for the Multivariate Curve Resolution-Alternating Least Square (MCR-ALS) is evaluated.

For the simulation the best model is obtained by excluding the solvent from the re-searched species and by fixing the start and the end concentrations (constraints in the MCR-ALS procedure).

[1] C.A. Mendez, J. Cerda, I.E. Grossmann, Iiro Harjunkoski and Marco Fahl: State-of-the-art review of optimization methods for short-term scheduling of batch processes, Computers & Chemical Engineering, 30, Issues 6-7, (2006), 913–946.

[2] A. Zogg: A Combined Approach using Calorimetry and IR-ATR Spectroscopy for the Determination of Kinetic and Thermodynamic Reaction Parameters: Diss. ETH No. 15086 (2003).

[3] Erdal Din: Linear regression analysis and its application to the multivariate spectral calibrations for the multiresolution of a ternary mixture of caffeine, paracetamol and metamizol in tablets, Journal of Pharmaceutical and Biomedical Analysis, 33, Issue 4 , (2003), 605–615.

[4] G. Corminboeuf, M. Amrhein and O. Naef: Automatic detection of reaction start/endpoints in chemical and biotechnological reaction systems, Chemometrics and Intelligent Laboratory Systems, 86, Issue 2, (2007), 168–178.

Simulation of the flow in the inner ear with the method of fundamental solutions

Dominik Obrist, Francesco Boselli and Leonhard Kleiser

Institute of Fluid Dynamics, ETH Zürich,
obrist@ifd.mavt.ethz.ch boselli@ifd.mavt.ethz.ch kleiser@ifd.mavt.ethz.ch

Abstract: The semicircular canals which are located in the inner ear are the primary human sensors for angular motion. Movement of the head induces a flow of the endolymph inside the semicircular canals. This flow deflects a gelatinous structure called cupula which triggers nerve signals leading to the perception of angular motion.

We present early results from a numerical simulation of the transient endolymph flow in a two-dimensional representation of a semicircular canal. The temporal dynamics of the elastic cupula is captured by an explicit time-integration scheme. At each time-step we solve the quasi-steady Stokes equations for the endolymph with the method of fundamental solutions (MFS) [1,2]. The transient movement of the head leads to time-dependent boundary conditions for the flow field. This numerical scheme is examined for its accuracy, robustness and computational efficiency. In particular, we will discuss a numerical instability in MFS and will derive an upper bound to characterize this instability.

[1] M. Golberg and C. Chen: The method of fundamental solutions for potential, Helmholtz and diffusion problems, in: Boundary Integral Methods: Numerical and Mathematical Aspects, (WIT Press, 1999).

[2] 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. Comput. Phys., no. 211 (2006), 1-8.

Spatio-angular model for the formation of oriented patches in chondrocytes cultures

Viviana Palumberi[1], Andrea Barbero[2], Barbara Wagner[3], Marcus J. Grote[1] and Ivan Martin[2]

[1] Departement of Mathematics, University Basel,
Viviana.Palumberi@unibas.ch abarbero@uhbs.ch

[2] ICFS, University Hospital Basel,

[3] WIAS, Berlin

Abstract: We seek a mathematical model to understand the growth dynamics of chondrocytes (cartilage cells) cultured on two-dimensional plates with growth factors. Since in this environment chondrocytes loose their original spherical shape in favor of an elongated, fibroblast-like morphology (3), we opt for the model used by Edelstein Keshet (4), which allows cells to change their orientation and position not only randomly, but also in response to neighboring cells.
We adapt this model to our particular biological system, coupling it with logistic growth, and also prove the existence of a smooth solution. Furthermore we study parameter regimes that lead to the formation of one or more patterns and compare the simulations to experiments. To do so, we discretize the three dimensional time-dependent integro-partial differential equation using Chebychev methods, finite differences and trapezoidal quadrature rule. These studies are expected to identify possible relationships between the spatial patterns displayed by chondrocytes during monolayer culture and their growth dynamics.

[1] A. Barbero, S.P. Grogan, D. Schäfer, M. Heberer, P. Mainil-Varlet, I. Martin (2004), *Age related changes in human articular chondrocyte yield, proliferation and post-expansion chondrogenic capacity*, Osteoarthritis Cartilage, 12(6):476-84.

[2] A. Barbero, V. Palumberi, B. Wagner, R. Sader, M. J. Grote and I. Martin (2005), *Experimental and Mathematical Study of the Influence of Growth Factors on the Growth Kinetics of Adult Human Articular Chondrocytes*. Journal of Cellular Physiology, 204:830-838.

[3] M. Jakob, O. Dematreau, D. Schäfer, B. Hintermann, W. Dick, M. Heberer, I. Martin (2001) *Specific Growth Factor during the expansion and redifferentiation of adult human articular chondrocytes enhance chondrogenesis and cartilaginous tissue formation in vitro*, Journal of Cellular Biochemistry, 81:368-377.

[4] A. Mogilner, L. Edelstein-Keshet (1996) *Spatio-angular order in populations of self-aligning objects: formation of oriented patches.* Physica D 89, 346-367.

An anisotropic error estimator for the Crank-Nicolson method: application to a parabolic problem

Alexei Lozinski[1], Marco Picasso[2] and Virabouth Prachittham[2]

[1] Laboratoire MIP, Université de Toulouse,
alexei.lozinski@math.univ-toulouse.fr

[2] EPFL-SB-IACS-ASN, Ecole Polytechnique Fédérale de Lausanne
marco.picasso@epfl.ch virabouth.prachittham@epfl.ch

Abstract: In this work we derive two *a posteriori* upper bounds for the heat equation [1]. A continuous, piecewise linear finite element discretization in space and the Crank-Nicolson method for the time discretization are used. The error due to the space discretization is derived using anisotropic interpolation estimates and a post-processing procedure. The error due to the time

discretization is obtained using two different continuous, piecewise quadratic time reconstructions. The first reconstruction is developed following [2], while the second one is new. An adaptive algorithm is developed. Numerical studies are reported for several test cases and show that the second error estimator is more efficient than the first one. In particular, the second error indicator is of optimal order with respect to both the mesh size and the time step when using our adaptive algorithm.

[1] A. Lozinski, M. Picasso and V. Prachittham, *An anisotropic error estimator for the Crank-Nicolson method: Application to parabolic problem*, submitted to SIAM J. Scientific Computing, 2008.

[2] G. Akrivis, C. Makridakis and R. H. Nochetto, *A posteriori error estimates for the Crank-Nicolson method for parabolic equations*, Math. Comp., 75(254):511-531 (electronic), 2006.

Simulating viscoplastic flows

Martin Rentschler, Sébastien Wiederseiner, Nicolas Andreini and Christophe Ancey

Laboratory of environmental hydraulics, EPFL
martin.rentschler@epfl.ch sebastien.wiederseiner@epfl.ch
nicolas.andreini@epfl.ch christophe.ancey@epfl.ch

Abstract: Many geophysical flows are far from equilibrium. One typical example are snow-avalanches or mud-flows, which consists of a multi-phase flow of granular media. Rheologically these materials are characterized by the presence of a yield stress, a threshold which defines the minimal stress required to shear the material.

In this contribution we compare experimental and numerical results. In our experiments, we released a fixed volume of a viscoplastic fluid (a polymeric gel) on the top of an inclined plane and tracked the free surface using a three-dimensional camera [1]. The rheological properties of the fluid were measured using a Bohlin CVOR rheometer. As a first approximation, the rheological properties could be described using a *Herschel-Bulkley* model.

For the numerical simulations, we used a finite-volume approach. We extended a two-phase *Navier-Stokes* solver developed by Griebel and coworkers [2] to cope with nonlinear rheologies. For this purpose, we considered a shear-rate dependent viscosity, the crux being the behaviour at low shear rates, where viscosity diverges. A *level-set* function captured the position of the air/fluid interface, which avoided to explicitly solve the boundary conditions at the free surface. This also made it possible to solve the governing equations in a fixed Cartesian grid. A semi-implicit *Chorin's projection scheme* in combination with a *bi-conjugate gradient* method was used to solve this resulting equations. The comparison shows fairly good agreement between experimental and numerical results.

[1] S. Cochard and C. Ancey: Tracking the free surface of time-dependent flows: Image processing for the dam-break problem, Experiments in Fluids 44 (2008) 59–71.

[2] R. Crocce, M. Griebel, and M.A. Schweitzer, A Parallel Level-Set Approach for Two-Phase Flow Problems with Surface Tension in Three Space Dimensions, Universitt Bonn, Sonderforschungsbereich 611, Bonn, 2004.

Vortex Methods for Flow Simulations on the GPU

Diego Rossinelli and Petros Koumoutsakos

CSE Lab, ETH Zürich,
diegor@inf.ethz.ch petros@inf.ethz.ch

Abstract: In this work we present Vortex Particle Methods for incompressible flow simulations in GPUs. The present work demonstrates that, contrary to common practice in particle simulations, it is necessary to remesh the (vortex) particle locations in order to solve accurately the equations they discretize. The particle locations are reinitialized periodically on a regular grid and it is shown that remeshing does not burden the accuracy of the method. In addition a grid is used in order to solve for the Poisson equation required in order to recover the velocity field from the vorticity field. In the present implementation of particle methods on the GPU the remeshing and the solution of the Poisson equation rely on fast and efficient fast mesh-particle interpolation operators. The remeshing step introduces minimal artificial dissipation while it allows for an order of magnitude increase in computational speed for the discretization of differential operators on particles over grid-free techniques. This increase in speed is complemented by the efficient implementation of vortex methods on the GPU. The present method leads to unprecedented, accurate and efficient simulations of incompressible vortical flows on GPUs.

Multiple zonal jets and drifting in rotating thermal convection

Jon Rotvig

Institut für Geophysik, ETH Zürich,
rotvig@erdw.ethz.ch

Abstract: The magnetic main field of the Earth is maintained by the geodynamo. This dynamo acts in the outer liquid iron core and is driven by thermal and compositional convection. In Boussinesq models of reversing dynamos, where the buoyancy sources are most efficient at the inner boundary, the magnetic Lorentz force only has a weak influence on the flow. This highlights the importance of studies on non-magnetic rapidly rotating thermal convection when seeking to understand the geodynamo.

We present a new type of multjet zonal flow obtained in a rapidly rotating spherical shell [1]. The numerical model is a parallel quasi-spectral implementation using spherical harmonics and radial Chebyshev polynomials. The convection is maintained by heating from below. The rigid outer boundary slows down the zonal flow, but it also enables multijet formation outside the tangent cylinder defined as the imaginary cylinder along the rotation axis that touches the inner boundary. The alternating jets are drifting towards the tangent cylinder. In a simplified 2D model we have shown that the jet drift in the 3D model is due to the strong curvature of the outer boundary. Assuming that the effects of the Lorentz force are small, these radially moving jets suggest a time-periodic dynamo efficiency that would be detectable outside the shell.

[1] J. Rotvig, Multiple zonal jets and drifting: Thermal convection in a rapidly rotating spherical shell compared to a quasigeostrophic model, Phys. Rev. E **76**, 046306 (2007).

Mixed integer optimization in automobile sheet metal forming processes

Madan Sathe, Olaf Schenk and Helmar Burkhart

High Performance and Web Computing Group, Department of Computer Science, University of Basel,
madan.sathe / olaf.schenk / helmar.burkhart@unibas.ch

Abstract: The reliable solution of hard linear and mixed integer programs is one of the key technologies for the implementation of optimization modules. On the one hand, the mixed integer programs to be solved get larger and larger, also because of improvements in hardware. On the other hand, ever new areas of optimization are covered, which leads to new requirements on the solution software.

In this research project we focus on new mixed integer modeling arising in the automobile industry. In automobile sheet metal forming processes the blank sheet has to be processed on some stages of a press to be at the end of the process a formed and manufactured sheet. Each press has installed a special die type which processed the features of a sheet. The geometry analyzer of the sheet metal forming analyzes the sheet to find several features such as rounded holes or flanges. Each feature can be manufactured by different processing sequences such as punching with a cam on one of the given presses (operations).

Obtaining a solution with minimal costs requires an optimal assignment of processing units of detected features to operations with respect to minimize the time consumption at each operation. The challenging task is to solve this assignment, scheduling and combinatorial problem with suitable discrete optimization algorithms while ensuring full cost transparency and result reproducibility.

High-order numerical modeling of highly conductive thin sheets

Kersten Schmidt[1] and Sébastien Tordeux[2]

[1] Seminar for Applied Mathematics, ETH Zrich,
kersten.schmidt@sam.math.ethz.ch

[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]. Alternatively to discretisation of the sheets, the electromagnetic fields are modeled only in the surrounding of the layer taking them into account with transmisson conditions [2], [3].

We study the shielding effect by means of the model problem of a diffusion equation with additional dissipation in the curved thin sheet. We propose asymptotic expansion [4] models with transmission conditions for arbitrary order in the thickness ε. These models allow for highly accurate modeling of the shielding effect on meshes without cells at the scale of ε.

To numerically compute the modeling error we discretised both, the asymptotic expansion models on the limit mesh and the original problem on meshes with cells in the sheet of thickness ε. Thereby we used high-order finite elements [5] on curved cells to diminish the effect of discretisation errors.

[1] Arnulf Kost. *Numerische Methoden in der Berechnung elektromagnetischer Felder*. Springer, Berlin, 1994.

[2] L. Krähenbühl and D. Muller. Thin layers in electrical engineering. example of shell models in analysing eddy-currents by boundary and finite element methods. *IEEE Trans. on Mag.*, 29:1450–1455, 1993.

[3] H. Igarashi, A. Kost, and T. Homma. Impedance boundary condition for vector potentials on thin layers and its application to integral equations. *Eur. Phys. J. AP*, 1:103–109, 1998.

[4] A. Bendali, and K. Lemrabet. The effect of a thin coating on the scattering of a time-harmonic wave for the Helmholtz equation. *SIAM J. Appl. Math.*, 6:1664–1693, 1996.

[5] Concepts Development Team. Webpage of Numerical C++ Library Concepts 2. `http://www.concepts.math.ethz.ch`, 2008.

Network Partitioning by Efficient Modularity Optimisation with Multi-Step Greedy Algorithm and Vertex Mover Refinement

Philipp Schütz and Amedeo Caflisch

Department of Biochemistry, University of Zurich,
schutz@bioc.uzh.ch caflisch@bioc.uzh.ch

Abstract: Identifying strongly connected substructures in large networks provides insight in their coarse-grained organization. Several approaches based on the optimization of a quality function, e.g. the modularity, have been proposed. We present a multi-step extension of the greedy algorithm (MSG) that allows the merging of more than one pair of communities at each iteration step. Upon convergence of the MSG a simple refinement procedure called "Vertex Mover" (VM) is used for reassigning vertices to neighboring communities to improve the final modularity value. With an appropriate choice of the step-width, the combined MSG&VM algorithm is able to find solutions of higher modularity than those reported previously. The MSG&VM approach has the same complexity as the greedy algorithm which is the fastest available optimization procedure for a generic network.

Local Nonreflecting Boundary Condition for Time-Dependent Multiple Scattering

Imbo Sim and Marcus J. Grote

Department of Mathematics, University of Basel
Rheinsprung 21, CH-4051 Basel
Imbo.Sim@unibas.ch Marcus.Grote@unibas.ch

Abstract: In [2] a nonreflecting boundary condition(NBC) for time-dependent multiple scattering was derived, which is local in time but nonlocal in space. Here, based on a high-order *local* nonreflecting boundary condition (NBC) for single scattering [1], we seek a local NBC for time-dependent multiple scattering, which is completely *local both in space and time*. To do so, we first develop a high order representation formula for a purely outgoing wave field, given its values and those of certain auxiliary functions needed for the artificial boundary condition. By combining that representation formula with a decomposition of the total scattered field into purely outgoing contributions, we obtain the first exact, completely local, NBC for time-dependent multiple scattering. The accuracy and stability of this local NBC is evaluated by coupling it to standard finite element and finite difference methods.

[1] T. Hagstrom, S.I. Hariharan: A formulation of asymptotic and exact boundary conditions using local operators, Appl. Numer. Math. 27, no. 4, (1998), 403–416.

[2] M.J. Grote, C. Kirsch: Nonreflecting boundary conditions for time-dependent multiple Scattering, J. Comp. Phys, 221, no 1, (2007), 41–62.

[3] M.J. Grote, I. Sim: Local Nonreflecting Boundary Condition for Time-Dependent Multiple Scattering., Proc. of 8th Intern. Conf. on Math. and Numerical Aspects of Wave Propagation (WAVES 2007), 283–285.

hp-Optimal discontinuous Galerkin methods for linear elliptic problems

Benjamin Stamm[1] and Thomas P. Wihler[2]

[1]Institute of Analysis and Scientific Computing, EPFL
benjamin.stamm@epfl.ch

[2]Department of Mathematics & Statistics, McGill University,
wihler@math.mcgill.ca

Abstract: In this talk we present an *hp*-optimal discontinuous Galerkin (DG) method for linear elliptic problems. We will present the key features for a priori estimates to overcome the well-known lack of *p*-optimality for such problems which leads to estimates that are optimal with respect to both the local element sizes and polynomial degrees. The theoretical explanations will be followed by some numerical illustrations.

[1] B. Stamm and T.P. Wihler: *hp*-Optimal discontinuous Galerkin methods for linear elliptic problems, EPFL-IACS report 07.2007, (2007).

Numerical simulation of magnetohydrodynamics phenomena applied to the electrolysis of aluminum

Gilles Steiner, Christophe Laurent, Michel Flück, Marco Picasso and Jacques Rappaz

[1] Departement of Mathematics, Swiss Federal Institute of Technology of Lausanne,
gilles.steiner / michel.flueck / marco.picasso / jacques.rappaz@epfl.ch

This work is financially supported by Alcan-Pechiney

Abstract: Electrolysis is a chemical technique used to split molecules by exploiting the energy of an electric current between two electrodes. A major application for this method is the industrial production of aluminum (Al) from alumina (Al_2O_3).
The extreme conditions around an electrolytic aluminum cell (temperature, current, magnetic induction) do not allow many physical observations. In this context, numerical simulation has proved to be very useful.
The goal of this poster is to present a numerical approach ([1], [2]) used to solve the magnetohydrodynamics (MHD) equations with a computer. We are particularly interested in the resolution of Maxwell equations for the magnetic induction field $\vec{B}$. On this topic we present an efficient Schwarz domain decomposition technique ([3]).

[1] J-F. Gerbeau, T. Lelièvre, C. Le Bris: Simulations of MHD flows with moving interfaces, Journal of computational Physics 184, 1 (2003), 163–191.

[2] J. Descloux, M. Flueck, M. V. Romerio: A modelling of the stability of aluminum electrolysis cells, Nonlinear partial differential equations and their applications, Collège de France Seminars, Vol XIII. D. Cioranescu and J.L. Lions editors, Pitman Research Notes in Mathematics Series 391. Addison Wesley Longman 1998, 117–133

[3] J. Rappaz, G. Steiner: On a domain decomposition method for numerically solving a magnetic induction problem. Scientific report in Analysis and Numerical Analysis, EPFL. To appear.

Efficent Algorithms for Radiative Transfer

Gisela Widmer

Seminar für Angewandte Mathematik, ETHZ
gisela.widmer@math.ethz.ch

Abstract: The stationary monochromatic radiation equation is stated in five dimensions, with the intensity depending on space and direction.

In order to reduce the computational costs due to the high dimensionality of the problem, we propose a sparse tensor product ansatz based on a multilevel decomposition of finite element spaces in space and solid angle. This reduces the number of degrees of freedom in the discretization to the number of degrees of freedom in space only (up to logarithmic terms). Combined with subspace correction preconditioning techniques, this approach can break the 'curse of dimension' of the discrete ordinates method under the condition that the solution is sufficiently smooth.

A homogeneous fluid approach to model yellow dung fly sperm flow

Christian Wüst

Institut für Mathematik, Universität Zürich,
christian.wuest@math.uzh.ch

Abstract: One of the most contested questions in sexual selection research concerns the adaptive significance of female reproductive traits that cause sexual selection in males. Are these traits adaptations that improve female indirect fitness (e.g., via good-genes sexual selection) or direct fitness (e.g., via inter-sexual conflict). These hypotheses can only be adequately evaluated through detailed study of the mechanisms by which female traits impose sexual selection. We study this question by exploring the mechanisms underlying sperm transfer and storage in the yellow dung fly (Scathophaga stercoraria) . In this species, females can partly sort sperm into multiple sperm storage organs, perhaps assisted by the curvature and roughness (microvillosity) of spermathecal ducts. We employed computational mathematics to model the fluid dynamics of sperm flow to determine which traits might increase the females control over sperm movement. We determined the influence of the geometric parameters spermathecal duct length, diameter, curvature, and surface roughness (microvillosity) on the flow rate of seminal fluid. Of the two presumed adaptations of the female duct, curvature had only a small influence on the flow rate (effect size 1.6%), whereas microvillosity had a much greater impact on sperm flow (effect size up to 50%). We also found slight evidence of interactions between microvillosity and curvature, such that in the presence of rough spermathecal walls the influence of curvature was slightly higher (1.7%).

Numerical Solution of the Atomic Kohn-Sham Equation - XATOM

Claude Daul[1], Matija Zlatar[1,2] and Florian Senn[1]

[1] Departement of Chemistry, University of Fribourg, Switzerland,
claude.daul / matija.zlatar / florian.senn@unifr.ch

[2] Center for Chemistry, IHTM, University of Belgrade, Serbia

Abstract: In chemistry, Density Functional Theory (DFT) has become a powerful tool for the study of molecular properties. The basic notion in DFT, that the energy of an electronic system can be expressed in terms of its density, is based on works of Hohenberg, Kohn and Sham [1], which emerged from Slater's idea [2]. From a set of one-electron Kohn-Sham (KS) equations, in principle, when correct functional would be known, one could obtain the exact electron density and thus the total energy. As the functional depends on the density, these second order differential equations with eigenvalue problem have to be solved iteratively.

For atoms, because of symmetry, we can separate angular and radial part of KS equations. A MATLAB [3] script, XATOM, for calculating the radial part of KS equation using a grid [4] developed in our group, has been written. Design of the script allows several extensions for calculations of, in chemistry interesting, properties.

[1] P. Hohenberg and W. Kohn: Inhomogeneous electron gas, Physical Review, 136 (1964), B864–B871. b) W. Kohn and L. J. Sham: Self-Consistent Equations Including Exchange and Correlation Effects, Physical Review, 140 (1965) A1133–A1138.

[2] J. C. Slater: International Series in Pure and Applied Physics, Vol. 4: The Self-Consistent Field for Molecules and Solids. Quantum Theory., McGraw-Hill, New York, 1974.

[3] MATLAB® (The MathWorks, Inc., Natick, MA), http://www.mathworks.com

[4] V. Weber, C. Daul and R. Baltensperger: Radial Numerical Integrations Based on the sinc Function, Computer Physics Communications , 163(3) (2004), 133–142.