University of Basel

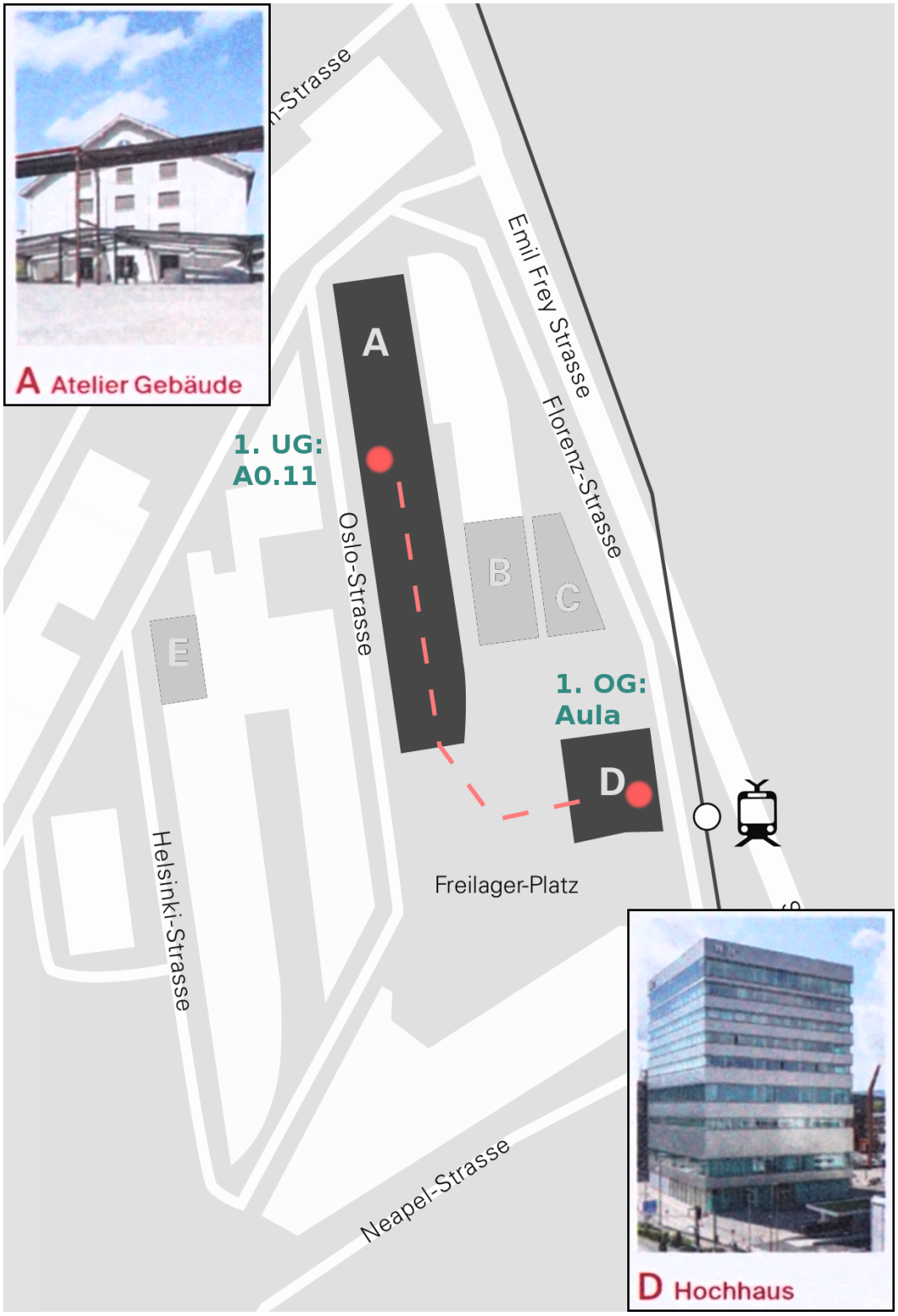
Department of
Mathematics and Computer Science

Swiss Numerical Analysis Day 2017

Program

Schedule

09:00 - 10:00	Welcome Coffee	
10:00 - 11:10	Opening and First Plenary Talk Patrick Joly	
	Hochhaus D	**Ateliergebäude A**
11:20 - 11:40	Lukas Herrmann	Carlos Parés Pulido
11:40 - 12:00	Michele Pisaroni	Luc Grosheintz-Laval
12:00 - 12:20	Roman Fuchs	Davide Torlo
12:30 - 13:30	Lunch	
	Hochhaus D	**Ateliergebäude A**
13:40 - 14:00	Stefano Massei	Lucas D. Wittwer
14:00 - 14:20	Marcel Schweitzer	Anna Stopka
14:20 - 14:40	Bo Song	Simone Pezzuto
14:50 - 15:30	Poster Session and Coffee Break	
15:30 - 16:40	Second Plenary Talk and Closing Barbara Wohlmuth	
	Hochhaus D	**Ateliergebäude A**
16:50 - 17:10	Alessio Quaglino	Andrea Di Blasio
17:10 - 17:30	Aymen Laadhari	Simon Lemaire
17:30 - 17:50	Alberto Paganini	Denis Devaud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Freilager-Platz
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D Hochhaus

Speakers

Patrick Joly	ENSTA ParisTech
Barbara Wohlmuth	TU Munich
Denis Devaud	ETH Zurich (SAM)
Andrea Di Blasio	EPF Lausanne (ANMC)
Roman Fuchs	HSR Rapperswil (IET)
Luc Grosheintz-Laval	ETH Zurich (SAM)
Lukas Herrmann	ETH Zurich (SAM)
Aymen Laadhari	ETH Zurich (CVL)
Simon Lemaire	EPF Lausanne
Stefano Massei	EPF Lausanne
Alberto Paganini	University of Oxford
Carlos Parés Pulido	ETH Zurich (SAM)
Simone Pezzuto	Università della Svizzera Italiana
Michele Pisaroni	EPF Lausanne
Alessio Quaglino	Università della Svizzera Italiana
Marcel Schweitzer	EPF Lausanne
Bo Song	University of Geneva
Anna Stopka	ETH Zurich (D-BSSE)
Davide Torlo	University of Zurich
Lucas D. Wittwer	ETH Zurich (D-BSSE)

Talks

Using potentials in linear elastodynamics: a challenge for finite element methods?

Joly Patrick, ENSTA ParisTech

In this work, we revisit the classical question of solving 2D time domain elastodynamics equations in piecewise homogeneous media from a new point of view. We wish to exploit the decomposition of the displacement field into potentials in homogeneous media, which allows us to decouple locally pressure and shear waves. Even though our initial motivation was academic, such a technique has a potential interest for applications for nearly incompressible media (such as soft tissues). In the particular case of a homogeneous medium, the main issueis the treatment of boundary conditions: clamped boundary conditions (Dirichlet) or free boundary conditions (Neumann). This raises unusual difficulties, especially for the Neumann case. In this talk, I will describe the approach that we propose to overcome these difficulties and present some theoretical and numerical results that support the mathematical soundness of this approach.

Domain decomposition for complexity reduction in large scale simulation

Barbara Wohlmuth, TU Munich

We discuss classical tearing and interconnecting strategies in combination with reduced order modeling, adaptive strategies and large scale multigrid solvers. The concepts of overlapping domain decomposition techniques are applied to eigenvalue problems in structural mechanics. A greedy algorithm is used to set up a reduced basis for rather large multi-storey timber construction. Material parameters enter by the wall type and elastomer. The abstract framework of non-overlapping Dirichlet-Neumann or Dirichlet-Dirichlet components is used in combination with over-balancing techniques to design fault robust multigrid solver. The reconnecting step is controlled by an hierarchical error estimator accounting for the algebraic error and a residual type one for the discretization error.

Exponential convergence in $H^{1/2}$ of hp-approximation for parabolic equations

Denis Devaud, ETH Zurich (SAM)

We introduce and analyze a continuous hp-finite element approximation for linear parabolic evolution problems considering a novel framework based on Sobolev spaces of fractional order for the time variable. First, the well-posedness of the equations is discussed. In particular, the bilinear form associated to the problem is inf-sup stable and we can construct explicitly elements satisfying this property. Then we define an interpolation operator and present bounds in the L^2 and $H^{1/2}$ norms which are fully explicit in the meshwidth and the polynomial degree. Based on this, we state an exponential convergence result for the space-time approximation. We conclude the presentation by showing numerical results in accordance with the developed theory.

Solving elliptic multiscale inverse problems using Bayesian techniques and numerical homogenization

Andrea Di Blasio, EPF Lausanne (ANMC)

We introduce a new Bayesian numerical homogenization method for the solution of elliptic multiscale inverse problem. From measurements at the boundary of the full multiscale problem, we aim at recovering a macroscopic description of the conductivity by means of numerical homogenization [1, 2]. A rigorous Bayesian formulation of the problem is given (well-posedness of the effective posterior measure). Moreover we establish a link between the effective posterior and the one associated to the fine scale model in terms of Hellinger distance by means of G-convergence [3]. Numerical results illustrating our theoretical findings will be presented.

References

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[2] A. Abdulle and A. Di Blasio. Numerical homogenization and model order reduction for multiscale inverse problems. Submitted to publication, 2016.

[3] A. Abdulle and A. Di Blasio. A Bayesian numerical homogenization method for elliptic multiscale inverse problems. Preprint, 2017.

Uncertainty quantification in multibanded P1 radiation model

Roman Fuchs, HSR Rapperswil (IET)

Thermal plasma simulations require appropriate modelling of the radiative heat flux to obtain an accurate and computationally tractable model. Despite that the absorption coef-

ficient can be calculated arbitrary accurately, the computational complexity of the multi-banded grey P1-model allows only for a low number of intervals to cover the spectral domain. A mean absorption coefficient is calculated for each interval or band. Therefore, the solution of an electric arc simulation depends on averaging method as well as on the uncertainties in the raw absorption data and the judicious selection of band boundaries. We systematically quantify the modelling errors in a wall-stabilized electric arc due to the band-averaged absorption coefficient with a spectrally finely resolved reference solution. For small band numbers, the Rosseland average overestimates the arc center temperature while the Planck average leads to lower temperatures, and they converge to the reference solution as the number of bands is increased. Furthermore, we present a sensitivity analysis of the arc voltage on the uncertainties in the mean absorption coefficient. The variations almost coincide with explicit parameter studies and the relative change in the arc voltage is proportional to the spectral bandwidth. The linearized model has much lower computational costs, so that this new methodology is applicable also very fine resolved spectral datasets.

Tyr, a well-balanced FVM on a 3D icosahedral grid

Luc Grosheintz-Laval, ETH Zurich (SAM)

We present a multi-GPU, well-balanced, explicit Finite Volume code for Euler equations on a spherical shell. Our horizontal grid is an icosahedral grid and therefore avoids singularities at the poles. Well demonstrate that the scheme preserves hydrostatic equilibrium with arbitrary thermal stratification exactly (up to machine precision) and resolves perturbations there from very accurately. Moreover, it generalizes to general equations of state, including tabulated. Well show that the scheme preserves a notion of radial symmetry exactly, despite the unstructured horizontal grid.

MLQMC with product weights for elliptic PDEs with lognormal coefficients parametrized in multiresolution representations

Lukas Herrmann, ETH Zurich (SAM)

Co-author: Christoph Schwab

Parametric diffusions are considered with lognormal coefficients that are given by multiresolution representations. Approximations by quasi-Monte Carlo (QMC) with randomly shifted lattice rules for first order are analyzed with dimension independent convergence rates. The local support structure in the multiresolution expansion are known to allow product weights for QMC rules, cp. [Herrmann, Schwab, SAM-report 2016-39]. Product weights allow for linear scaling in the dimension of integration in the cost to create QMC rules by the CBC construction, cp. [Nuyens, Cools, Math. Comp. 2006]. Multilevel QMC quadratures are considered to reduce the work of the QMC approximation in general polyhedral spatial domains, cp. [Herrmann, Schwab, SAM-report MLQMC 2017-(in preparation) and SAM-report 2017-04]. Analogous results hold for affine-parametric operator equations, cp. [Gantner, Herrmann, Schwab, SAM-reports 2016-32 and 2016-54]. This research is supported in part by the Swiss National Science Foundation (SNSF) under grant SNF 159940.

Eulerian fluid-structure interaction method for the modeling of thin elastic structures in an incompressible fluid

Aymen Laadhari, ETH Zurich (CVL)

The modeling of the large deformations of a thin elastic structure immersed in an incompressible Newtonian flow remains a tremendously challenging topic within the field of computational fluid-structure interaction (FSI). This problem is of significant interest in many real life and industrial applications, including e.g. the dynamics of heart valves and red blood cells in small capillaries. Recently, an increasing number of contributions have been made in the fields of scientific computing and numerical methods applied to the study of such a problem. The standard Arbitrary Lagrangian Eulerian methods have been successfully employed only for problems with relatively small structural deformations. In contrast, the fully Eulerian approaches represent a promising alternative to model the large structural deformations [1,2]. Additional numerical difficulties are encountered when solving FSI problems involving extremely thin structure with low mass (or massless) and incompressible fluid. A well-known problem is the artificial added mass effect [3].
We propose a new framework based on the use of the Newton and level set methods and tailored for the simulation of highly deformable and thin elastic structures in an incompressible flow. A purely Eulerian framework is established and enables to use a unique fluid solver for both fluid and membrane problems on a fixed mesh. To circumvent the instability issues due to the added mass effect, a partitioned strongly coupled strategy is devised [4]. We present a number of examples to address in detail the main features of the numerical method. Convergence studies and comparisons with benchmark results depict the efficiency and robustness of the approach.

Keywords: Elastic membrane; Imcompressible flow; Finite element method; Newton; Partitioned algorithm; Numerical stability.

References:

[1] A. Laadhari, R. Ruiz-Baier and A. Quarteroni. Fully Eulerian finite element approximation of a fluid-structure interaction problem in cardiac cells. International Journal for Numerical Methods in Engineering, 96(11): 712–738, 2013.

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A new paradigm for the numerical approximation of elliptic problems with sign-changing coefficients

Simon Lemaire, EPF Lausanne

We consider a diffusion problem with a conductivity coefficient that changes sign in the domain. This kind of problem arises, e.g., in the modeling of the interface between a dielectric and a (negative) metamaterial. Applications for such settings are abundant, ranging from superlensing to cloaking. The numerical approximation of sign-changing equations has been investigated in [1] but the approach therein is based on restrictive meshing assumptions (symmetries with respect to the interface), and does not apply to all interesting practical cases (including some cloaking devices). We introduce a new paradigm for the approximation of sign-changing problems, that is based on a reformulation of the original problem as a transmission problem, and on an optimization strategy. Our approach [2] does not rely on any assumption on the meshes (except that the latter are compliant with the interface) and applies without a priori limitations.

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[2] A. Abdulle, M. E. Huber, and S. Lemaire. An optimization-based numerical method for diffusion problems with sign-changing coefficients. C. R. Acad. Sci. Paris, Série I, to appear, 2017. DOI: 10.1016/j.crma.2017.02.010.

Computations with semi-infinite quasi-Toeplitz matrices

Stefano Massei, EPF Lausanne

Denote by $\mathscr{W}_1$ the set of complex valued functions of the form $a(z) = \sum_{i\in\mathbb{Z}} a_i z^i$ which are continuous on the unit circle, and such that $\sum_{i\in\mathbb{Z}} |ia_i| < \infty$. We call CQT matrix a quasi-Toeplitz matrix A, associated with a continuous symbol $a(z) \in \mathscr{W}_1$, of the form $A = T(a) + E$, where $T(a) = (t_{i,j})_{i,j\in\mathbb{Z}^+}$ is the semi-infinite Toeplitz matrix such that $t_{i,j} = a_{j-i}$, for $i, j \in \mathbb{Z}^+$, and $E = (e_{i,j})_{i,j\in\mathbb{Z}^+}$ is a semi-infinite matrix such that $\sum_{i.j} |e_{i,j}|$ is finite. We prove that the class of CQT matrices is a Banach algebra with a suitable sub-multiplicative matrix norm. We introduce a finite representation of CQT matrices together with algorithms which implement elementary matrix operations. Applications to the solution of matrix equations and to the computation of matrix functions are discussed.

Higher-order mesh-moving methods for PDE-constrained shape optimization

Alberto Paganini, University of Oxford

PDE-constrained shape optimization problems are characterized by target functionals that depend both on the shape of a domain (the control) and on the solution of a boundary value problem formulated on that domain (the state).

Such optimization problems are commonly solved with mesh-moving methods. First, an initial mesh is constructed. Then, a (first order) finite element approximation of the state is computed and used to evaluate the misfit functional and its shape derivative. Finally, the coordinates of the mesh nodes are update. This procedure is repeated until convergence. We describe a higher-order mesh-moving method based on deformation diffeomorphisms. This approach supports naturally the use of higher-order finite element approximations of the state.

Arbitrarily high order WENO finite difference schemes for incompressible flows on staggered meshes

Carlos Parés Pulido, ETH Zurich (SAM)

The talk is based on work, jointly with K. Pressel, T. Schneider (Climate Dynamics Group, Caltech) and S. Mishra (MATH, ETH Zurich).

We will present recently derived arbitrary high-order accurate (essentially) non-oscillatory finite difference schemes for the incompressible and anelastic Euler equations in both two and three space dimensions.
These equations are the fundamental governing equations for atmospheric flows and their numerical approximation is an essential component of all modern climate dynamics codes. Most of these codes use very high-order finite difference schemes, based on central stencils to solve these equations cite[1],[2] and references therein. However, these central schemes suffer from several defects; namely, they can produce spurious oscillations when the solution contains sharp gradients, such as in shear layers. Consequently, combining these schemes with sub-grid scale models for atmospheric turbulence leads to large numerical errors. Moreover, some of these schemes are only second-order accurate. Finally, the behavior of these schemes on problems with long time scales is inadequate on account of dispersive errors.
Given these defects, WENO schemes have been recently proposed as the suitable simulation framework for some atmospheric flows, see [3]. These schemes have been developed and integrated into the PYCLES simulation code. Although these schemes have many desirable properties, one can show that they are necessarily limited to only second order accuracy, even though arbitrary high order piecewise polynomial functions may be used in the WENO interpolation step.
We propose a variant of the scheme of [3] where the interpolations, based on ENO stencils, are used to augment WENO finite differences for approximating cross-terms in the momentum equations. The resulting scheme is provably arbitrarily high order accurate and non-oscillatory. We present many numerical experiments to illustrate the behavior of the scheme.

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Space–discretization error analysis and stabilization schemes for conduction velocity in cardiac electrophysiology

Simone Pezzuto, Università della Svizzera Italiana

The bidomain equation is the most commonly used model to describe in detail the spatial and temporal electric activity of the heart. The solution are often travelling waves characterised by a very steep front, about 0.1 mm thick. This yields a considerable computational effort on patient-specific human geometries. The aim of this work is to analyse in detail the effect of specific discretisations in space on traveling wave solutions of the bistable (or Nagumo) equation, which is a simple but mathematically reasonable approximation of the dynamics at the front of the wave. We show how specific discretisation schemes (FD, FE, DG), and the choice of a coarse grid, can affect the solution, leading so to possibly erroneous physiological conclusions. In this talk we provide several error estimates of the conduction velocity for different numerical schemes, by performing a perturbation analysis of the discrete problem associated to the discrete traveling wave. We also analyse the impact of mass lumping, adopted by several authors in relation with operator splitting schemes. Secondly, we exploit the error estimates to design a robust numerical scheme for the problem of interest. We propose and analyse two different schemes: the first one is a forth-order (in space) scheme obtained by a weighted average of the finite difference and the finite element method. The second one is a "stabilised" finite element scheme, where we introduce a numerical conductivity to consistently adjust the conduction velocity. These novel schemes show very good approximation properties of the conduction velocity. Finally, we test the methodology on realistic ionic models and geometries. The results are in excellent agreement with our analytical results based on the bistable model, thus showing the validity of the approach.

A Multi Level Monte Carlo Algorithm for Uncertainty Quantification and Robust Design Optimization in Aerodynamics

Michele Pisaroni, EPF Lausanne

Optimization has always been an integral part in aeronautic design. Nowadays the ever-increasing demand for aircrafts with better performance, higher reliability and robustness at lower cost requires optimization techniques seeking optimality under uncertain conditions that may arise during design, manufacture and operation of the vehicle. Indeed, the geometrical and operational parameters, that characterize aerodynamic systems, are naturally affected by aleatory uncertainties due to the intrinsic variability of the manufacturing processes and the surrounding environment. For this reason designs obtained with traditional deterministic optimization techniques seeking only optimality in a specific set of conditions may have very poor off-design performances or may even be unreliable. In this work we present a novel technique based on the combination of Evolutionary Algorithms (EAs) and a Continuation Multi Level Monte Carlo (C-MLMC) methodology to

estimate robust designs, without relying on derivatives and meta-models. Detailed numerical studies are presented for a 2D transonic airfoil design affected by geometrical and operational uncertainties. The performance of a robust optimal designs is compared to the deterministic optimal solution to underline the improvement in robustness that can be achieved.

Quasi-quadratic elements for nonlinear compressible and incompressible elasticity

Alessio Quaglino, Università della Svizzera Italiana

Elasticity problems involving incompressible materials or large strains are both notoriously difficult, for which several specialized techniques have been developed. For the former, the displacement-pressure (u, p) formulation is studied in the incompressible limit, as the Poisson ratio ν tends to $1/2$. The main challenge is to provide an approximation that does not exhibit locking, i.e. which converges uniformly with respect to ν. For the latter, the difficulty is to ensure a good approximation already on coarse meshes, which often yield an overly stiff solution. This is particularly undesirable in engineering, unless expensive higher-order elements are employed.
This work deals with the development of novel 2D and 3D elements for the solution of the Saint Venant-Kirchhoff nonlinear elasticity equations. While it is well-known that standard linear and quadratic elements perform, respectively, poorly and accurately in this context, their cost is also very different. Here, we address the question of finding an approximation that falls in-between these two cases, which we will refer to as quasi-quadratic. More precisely, we seek to satisfy the following: (i) absence of locking and pressure oscillations in the incompressible limit, (ii) an exact equivalence to quadratic elements on linear problems, and (iii) a computational cost comparable to linear elements on nonlinear problems. Our construction is formally based on the Hellinger-Reissner mixed principle, where strains and displacement are interpolated linearly on nested meshes, but it can be easily recast in a pure displacement form via static condensation.
We show that properties (i) and (ii) are fulfilled via numerical studies on a series of benchmarks and analyze the cost of quadrature in order to show property (iii). Finally, we show that in 1D the good accuracy properties of our element can be interpreted as stemming from an approximate quadrature rule of the elastic energy of fully-quadratic elements.

Bounds for the decay of the entries in inverses and Cauchy–Stieltjes functions of sparse, normal matrices

Marcel Schweitzer, EPF Lausanne

It is known that in many functions of banded (or more generally, sparse) Hermitian positive definite matrices, the entries exhibit a rapid decay away from the main diagonal (or the sparsity pattern). This is in particular true for the inverse, and based on results for the inverse, bounds for Cauchy–Stieltjes functions of Hermitian positive definite matrices have recently been obtained. We add to the known results by considering the more general case of normal matrices, for which fewer and typically less satisfactory results

exist so far. Starting from a very general estimate based on approximation properties of Chebyshev polynomials on ellipses, we obtain as special cases insightful decay bounds for various classes of normal matrices, including (shifted) skew-Hermitian and Hermitian indefinite matrices. In addition, some of our results improve over known bounds when applied to the Hermitian positive definite case.

New coarse spaces for the Additive Schwarz method

Bo Song, University of Geneva

The Additive Schwarz method (AS) does not converge in general when used as a stationary iterative method, it can only be used as a preconditioner for a Krylov method. In the two level variant of AS, a coarse grid correction is added to make the method scalable. We propose new coarse space components which allow the two level method to become convergent when used as a stationary iterative method, and show that a suitable choice makes the method even nilpotent, i.e. it converges in two iterations, independently of the overlap and the number of subdomains. One of the coarse spaces we obtain is optimal, which means it is of smallest dimension possible for the method to become nilpotent. We also consider a harmonic enrichment with the eigenvectors corresponding to the eigenvalue problem along each interface to approximate the optimal coarse space, which reduces the number of basis functions needed for good performance. We derive the convergence factor of our new method in the two subdomain case in two spatial dimensions. We also compare our approximate coarse spaces with GenEO recently proposed by Spillane, Dolean, Hauret, Nataf, Pechstein, and Scheichl. We finally illustrate our theoretical results with numerical experiments.

Performing cell-based tissue simulations to explore the impact of cell mechanics on tissue dynamics

Anna Stopka, ETH Zurich (D-BSSE)

Complementary to experimental approaches computational models are important to take full advantage of reported results in developmental biology. To this end, we investigate growing tissues using a 2D cell-based simulation framework (LBIBCell) that is being developed in our group [1]. LBIBCell models the fluid-structure interaction within a biological tissue by combining the Lattice Boltzmann (LB) and Immersed Boundary (IB) method. Cells are represented as finely resolved polygons according to the IB method interacting with their neighbors via spring-like cell-cell junctions. The fluid movement inside and outside of the cells is described by the LB equations. Performing simulations of growing tissue in LBIBCell, we explore the impact of cell-based events, such as cell division and cell-cell-interactions, on various core mechanisms of animal organogenesis. For instance, we study the effect of biased cell division orientation on anisotropic tissue expansion.

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Asymptotic Preserving Deferred Correction Residual Distribution schemes

Davide Torlo, University of Zurich

Joint work with Prof. Remi Abgral

In many models, such as kinetic models, multiphase flows, viscoelasticity or relaxing gas flows, hyperbolic systems with relaxation can occur. Stiff relaxation terms in these situations may produce spurious unphysical results. To deal with such small scale parameter we should classically refine our discretization depending on relaxation parameter, and this is not always feasible. We present a scheme that can be used over the complete range of the relaxation parameter and, moreover, that can preserve the asymptotic limit of the physical model.
To deal with stiff terms, it is natural to use an implicit or semi-implicit formulation. In order to get a high order scheme, we need a special treatment of the off-diagonal mass matrices. To avoid the inversion of these matrices, we recur to a (DeC) Deferred Correction approach. This consists in two methods coupled together. The first one can be a first order model (with easily invertible mass matrix) that we will use implicitly, in our context, while the second one, can be higher order and we will always use it in a completely explicit way. The coupling of this two models allows to reach the high order through a few intermediate steps. Thanks to this, we can produce a scheme which is fast and reliable.
The low order and the high order schemes, that we have used, come from the Residual Distribution (RD) framework. In this context, we compute residuals for each cell of the discretized domain, then we distribute each residual to vertices of the cell. For the first order scheme we used an only-flux residual distribution scheme, while for the higher order scheme we used a full space-time residual distribution scheme.
We have tested some example with different schemes, reaching the asymptotic preserving properties and the correct order of convergence.

Acknowledgments: This research is funded by the ITN ModCompShock.

Phase-Field Based Simulations of Embryonic Branching

Lucas D. Wittwer, ETH Zurich (D-BSSE)

The mechanism that controls embryonic branching is not fully understood. Of all proposed mechanism, only a Turing pattern-based model succeeds in predicting the location of newly emerging branches during lung and kidney branching morphogenesis. Turing models are based on at least two coupled non-linear reaction-diffusion equations. In case of the lung model, the two components (ligands and receptors) are produced in two different tissue layers. Thus the ligand is produced in the outer mesenchymal layer and the receptor is produced in the inner, branching epithelial layer; the diffusion of receptors is restricted to this epithelial layer. So far, numerical instabilities due to highly complex mesh deformations limit the maximal rounds of branching that can be simulated in an ALE-based framework. I will present our new Phase-Field-based framework for simulating embryonic lung morphogenesis and how we coupled the reaction-diffusion equations to the implicit domain.

Participants

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