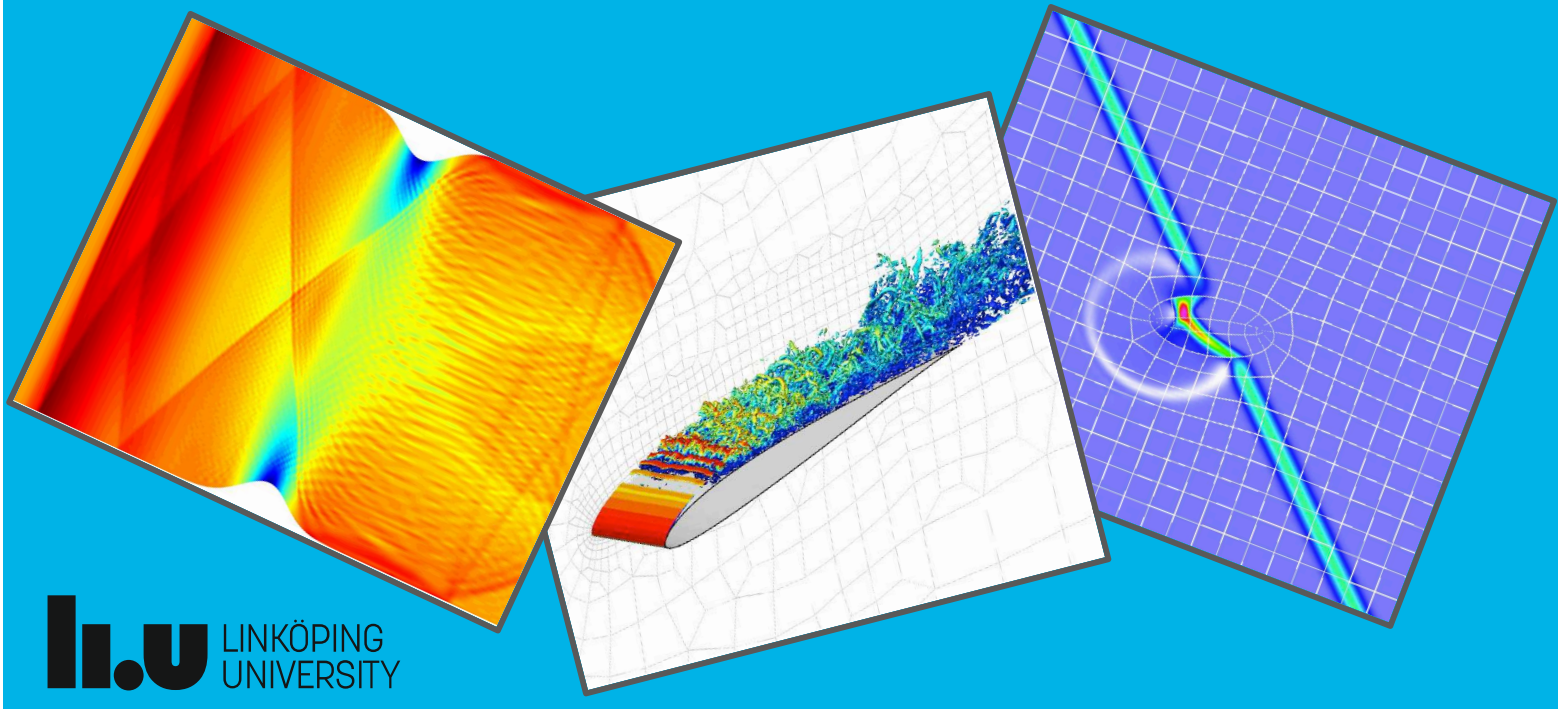
3rd Workshop on Scientific Computing in Sweden

SWEDCOMP20

Schedule and Book of Abstracts

16 - 18 September



LINKÖPING UNIVERSITY

3rd Workshop on Scientific Computing in Sweden

Schedule and Book of Abstracts

September 16 - 18, 2020

Schedule

Presentations during each session are 25 minutes long with an additional 5 minutes for questions.

Wednesday September 16

Time	Activity	Presenter
12.00 – 13.00	Lunch	
13.00 – 13.30	Welcome and opening remarks	Jan and Andrew
13.30 – 15.00	**Afternoon session 1**	**Chair: Gunilla Kriess**
13.30 – 14.00	Flexural wave propagation in floating ice	Jonatan Werpers
14.00 – 14.30	High-order trapezoidal rule-based quadrature for non-parametrised boundary integral methods	Federico Izzo
14.30 – 15.00	The number of boundary conditions for initial boundary value problems	Jan Nordström
15.00 – 15.30	Coffee break	
15.30 – 17.00	**Afternoon session 2**	**Chair: Jan Nordström**
15.30 – 16.00	A residual-based artificial viscosity finite difference method for scalar conservation laws	Vidar Stiernström
16.00 – 16.30	Inverses of SBP-SAT finite difference operators approximating the first and second derivative	Sofia Eriksson
16.30 – 17.00	Learning to differentiate	Oskar Ålund
17.00 – 18.30	**Time for discussion between participants**	
19.00	**Dinner**	

Thursday September 17

Time	Activity	Presenter
7.00 – 8.30	Breakfast	
8.30 – 10.00	**Morning session 1**	**Chair: Olof Runborg**
8.30 – 9.00	—	—
9.00 – 9.30	A joint use of pooling and imputation for SNP genotyping	Camille Clouard
9.30 – 10.00	Stability analysis of finite element methods for the second order wave equation	Benjamin Weber
10.00 – 10.30	Coffee break	
10.30 – 12.00	**Morning session 2**	**Chair: Sofia Eriksson**
10.30 – 11.00	Multiscale computations for elliptic problems and time averaged waves	Olof Runborg
11.00 – 11.30	Homogenization and numerics for the Landau-Lifshitz equation with highly oscillatory coefficient	Lena Leitenmaier
11.30 – 12.00	Patient specific modeling and simulation of mitral valve disease	Frida Svelander

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12.00 – 13.00	Lunch	
13.00 – 14.30	**Afternoon session 1**	**Chair: Andrew Winters**
13.00 – 13.30	A linearisation technique for nonlinear eigenproblems with eigenvector nonlinearities	Parikshit Upadhyaya
13.30 – 14.00	A time adaptive multirate Dirichlet–Neumann waveform relaxation method for heterogeneous coupled heat equations	Peter Meisrimel
14.00 – 14.30	Randomized schemes for the approximation of nonlinear evolution equations	Monika Eisenmann
14.30 – 15.00	Coffee break	
15.00 – 16.30	**Afternoon session 2**	**Chair: Philipp Birken**
15.00 – 15.30	Structure preserving iterative methods in CFD	Viktor Linders
15.30 – 16.00	Space-time multigrid preconditioners — local Fourier analysis	Lea Miko Versbach
16.00 – 16.30	Spectral properties of the incompressible Navier-Stokes equations	Fredrik Laurén
16:30 – 18:30	Break	
18:30	**Dinner**	

Friday September 18

Time	Activity	Presenter
7.00 – 8.30	Breakfast	
8.30 – 10.00	**Morning session 1**	**Chair: Fredrik Laurén**
8.30 – 9.00	A new master program in computational science	Philipp Birken
9.00 – 9.30	Solely hyperbolic numerical approximations of elliptic equations	Andrew Winters
9.30 – 10.00	Closing remarks	Jan and Andrew
10.00 – 10.30	Coffee break	
10.30 – 12.00	**Final discussions and hotel checkout**	—
12.00 – 13.00	Lunch	

Book of abstracts

Note, the underlined name in each abstract indicates the speaker.

Wednesday afternoon session 1

Session chair: Gunilla Kriess

13.30 – 14.00 **Flexural wave propagation in floating ice**

Speaker: Jonatan Werpers

14.00 – 14.30 **High-order trapezoidal rule-based quadrature for non-parametrised boundary integral methods**

Speaker: Federico Izzo

14.30 – 15.00 **The number of boundary conditions for initial boundary value problems**

Speaker: Jan Nordström

FLEXURAL WAVE PROPAGATION IN FLOATING ICE

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Flexural gravity waves in ice sheets can arise when very long wave length ocean waves interact with large floating ice sheets in the antarctic. This causes bending and stressing of the ice and may speed up breaking. The interaction could play a large role in climate models. It is therefore important to understand how the ice behaves and derive models for how flexural waves propagate.

The waves propagate through interaction between stiff ice and the water beneath the ice. Because of the size of these ice sheets they can be modeled as thin plates and one example of a model for such a system is

$$\varepsilon\phi_{tt} = \nabla^2\phi, \quad \bar{x} \in \Omega_{\text{water}},$$
$$aw_{tt} + \nabla^2 b\nabla^2 w + w + \gamma\phi_t = 0, \quad \bar{x} \in \Gamma_{\text{ice}},$$
$$\hat{n}\cdot\nabla\phi = w_t, \quad \bar{x} \in \Gamma_{\text{ice}},$$

where ϕ is a velocity potential of the water, w is the height of the ice and ε, a, b and γ are dimensionality parameters.

Due to changing requirements and continuing exploration of models for the ice-water system, we require the numerical methods we derive for this problem to be highly robust and flexible. Being a wave propagation problem we also demand high order of accuracy. Using the summation by parts framework for both space and time dimensions we are able to derive higher order schemes that meet these requirements, including robust coupling of the ice and water equations using simultaneous approximation terms.

We will present methods for deriving such schemes. We will also verify the robustness and accuracy as well as show example solutions.

HIGH-ORDER TRAPEZOIDAL RULE-BASED QUADRATURE FOR NON-PARAMETRISED BOUNDARY INTEGRAL METHODS

FEDERICO IZZO* **OLOF RUNBORG*** **AND RICHARD TSAI***

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Boundary integrals methods are well renowned for their usefulness with homogeneous elliptic equations such as Laplace or with the Helmholtz equation, especially in unbounded domains. With these methods, the solution is built by solving a boundary integral equation (BIE). The integrands are singular in a point, but there are many techniques to accurately discretise the integrals using the explicit parametrisation of the surface.

Instead of using an explicit parameterisation, we consider the case where the surface is described by a closest point mapping, or equivalently a distance function. Avoiding explicit parametrisation can be advantageous when dealing with surfaces with complicated shapes or available in the form of point cloud data.

Using the technique from [1], we rewrite the surface integral as an integral over a small volume encompassing the surface using the closest-point mapping to the surface, without explicit parametrisation. The integrands in the non-parametrised version of the BIEs are singular not in a point but along a line, and few methods have been developed to accurately evaluate these integrals.

In this work, we present new quadrature methods based on corrections to trapezoidal rule, which accurately integrate functions singular along straight lines in 3D. The methods developed are specific for the kind of singularities encountered in the Single-Layer and Double-Layer potentials for Laplace and Helmholtz boundary integral formulations in the non-parametric setting.

REFERENCES

[1] Catherine Kublik and Richard Tsai, “Integration over curves and surfaces defined by the closest point mapping.” *Research in the Mathematical Sciences* (3)1:3, (2016).

THE NUMBER OF BOUNDARY CONDITIONS FOR INITIAL BOUNDARY VALUE PROBLEMS

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Both the energy method and the Laplace transform method are frequently used for determining the number of boundary conditions required for a well posed initial boundary value problem. The energy method builds on integration-by-parts. One obtains an expression for the energy rate that involves boundary terms. The number of boundary conditions is given by the minimal number that limits these boundary terms.

The Laplace transform method is different, and employs an expansion of the solution in modes that turn the initial boundary value problem into a one-dimensional boundary value problem. The number of boundary conditions is given by the number of conditions required to determine these modes.

We show that these two distinctly different methods yield the same results [1].

REFERENCES

[1] J. Nordström and T. Hagstrom, "The Number of Boundary Conditions for Initial Boundary Value Problems." *SIAM J. Numerical Analysis* accepted, (2020).

Wednesday afternoon session 2

Session chair: Jan Nordström

15.30 – 16.00 **A residual-based artificial viscosity finite difference method for scalar conservation laws**

Speaker: Vidar Stiernström

16.00 – 16.30 **Inverses of SBP-SAT finite difference operators approximating the first and second derivative**

Speaker: Sofia Eriksson

16.30 – 17.00 **Learning to differentiate**

Speaker: Oskar Ålund

A RESIDUAL-BASED ARTIFICIAL VISCOSITY FINITE DIFFERENCE METHOD FOR SCALAR CONSERVATION LAWS

VIDAR STIERSTRÖM[*], **LUKAS LUNDGREN**[*], **MURTAZO NAZAROV**[*] **AND KEN MATTSSON**[*]

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We present an accurate, stable and robust shock-capturing finite difference method for solving scalar non-linear conservation laws. The spatial discretization uses high-order accurate upwind summation-by-parts finite difference operators combined with weakly imposed boundary conditions via simultaneous-approximation-terms. The method is an extension of the residual-based artificial viscosity methods developed in the finite- and spectral element communities to the finite difference setting. The three main ingredients of the proposed method are: (i) shock detection provided by a residual-based error estimator; (ii) first-order upwind applied in regions with strong discontinuities; (iii) additional dampening of spurious oscillations provided by high-order dissipation from the upwind finite difference operators. The method is validated against a set of benchmark problems in 2D, covering both convex and non-convex fluxes.

INVERSES OF SBP-SAT FINITE DIFFERENCE OPERATORS APPROXIMATING THE FIRST AND SECOND DERIVATIVE

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The scalar, one-dimensional advection equation and heat equation are considered. These equations are discretized in space, using a finite difference method satisfying summation-by-parts (SBP) properties. To impose the boundary conditions, we use a penalty method called simultaneous approximation term (SAT). Together, this gives rise to two semi-discrete schemes where the discretization matrices approximate the first and the second derivative operators, respectively. The discretization matrices depend on free parameters from the SAT treatment.

We derive the inverses of the discretization matrices, interpreting them as discrete Green's functions. In this direct way, we also find out precisely which choices of SAT parameters that make the discretization matrices singular. In the second derivative case, it is shown that if the penalty parameters are chosen such that the semi-discrete scheme is dual consistent, the discretization matrix can become singular even when the scheme is energy stable.

The inverse formulas hold for SBP-SAT operators of arbitrary order of accuracy. For second and fourth order accurate operators, the inverses are provided explicitly.

LEARNING TO DIFFERENTIATE

OSKAR ÅLUND[†] **AND JAN NORDSTRÖM**[†,∗]

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Artificial neural networks together with associated computational libraries provide a powerful framework for constructing both classification and regression algorithms. In this paper we use neural networks to design linear and non-linear discrete differential operators. We show that neural network based operators can be used to construct stable discretizations of initial boundary-value problems by ensuring that the operators satisfy a discrete analogue of integration-by-parts known as summation-by-parts. Our neural network approach with linear activation functions is compared and contrasted with a more traditional linear algebra approach. An application to overlapping grids is explored. The strategy developed in this work opens the door for constructing stable differential operators on general meshes.

Thursday morning session 1

Session chair: Olof Runborg

8.30 – 9.00 —

Speaker: —

9.00 – 9.30 **A joint use of pooling and imputation for SNP genotyping**

Speaker: Camille Clourad

9.30 – 10.00 **Stability analysis of finite element methods for the second order wave equation**

Speaker: Benjamin Weber

A JOINT USE OF POOLING AND IMPUTATION FOR SNP GENOTYPING

CAMILLE CLOUARD[*], **CARL NATTELBLAD**[*] **AND KRISTIINA AUSMEES**[*]

[*] Department of Information Technology, Uppsala University, Uppsala, Sweden.
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The latest decades development biotechnologies have substantially cut the costs of DNA sequencing. Nevertheless, when performing for example genotyping on large data sets, i.e., with thousands of individuals in a cost-sensitive context, whole-genome or targeted sequencing can remain expensive. In particular, genotyping variants with low minor allele frequency (MAF) is a challenge because of the sparsity of the rare allele carriers in the population, which requires very large sampling for ensuring sufficient statistical power in further testing. Investigating such rare variants is meaningful and informative in association studies and plant breeding. Using techniques from the field of group testing theory has been suggested even when single-marker PCR genotyping was performed in the 1990s. By implementing pooling strategies, several studies have shown it is an effective and accurate means for reducing DNA processing costs and optimizing rare variants detection. However, few works specifically consider pooling samples on SNP-arrays for genotyping purposes.

The cost reduction achieved with combinatorial group testing has a drawback as pooling individuals results in a loss of information about genotypes at the individual level when analyzing the arrays, and the uncertainty introduced by pooling appears as missing individual genotypes in the data set. Computational methods for genotype imputation have been widely used for dealing with missing genotypes. In many cases, they implement iterative procedures in a Bayesian statistical framework for determining the most likely genotypes at unassayed markers. Traditionally, imputation is used to infer additional markers states in a study population genotyped at low density by using a reference population with similar genetic structure which was genotyped at high density.

We present tentatively promising results for combining a pooling scheme for SNP genotyping with computational genotype imputation in humans as well as important foodcrop species, and compare our process to the results of a classical high-density genotyping from a low-density genotyped panel. We also suggest how modelling the possible outcomes for uncertain genotypes from pooling can inform the imputation algorithms further in order to fully and accurately reconstruct the genotypes of all individuals within each pool, while using less than half the number of assays needed for non-pooled genotyping of each individual.

STABILITY ANALYSIS OF FINITE ELEMENT METHODS FOR THE SECOND ORDER WAVE EQUATION

BENJAMIN WEBER[*], **GUNILLA KREISS**[*] **AND MURTAZO NAZAROV**[*]

[*] Department of Information Technology, Uppsala University, Uppsala, Sweden.
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Time-step restrictions of standard or Lagrange finite element methods (LFEM), the Hermite finite element method (HFEM) and discontinuous Galerkin methods using the symmetric interior penalty (DG-SIM) for the wave equation are analysed. We implement a matrix Fourier transform to analyse periodic block tridiagonal matrices and use it to calculate stability limits for a simple explicit time-stepping method when using higher order finite elements on a uniform grid in one dimension. HFEM is shown to have a more relaxed time-step limit than LFEMs of the same order, and DG-SIMs of the same order are shown to share a common stability limit. We evaluate time-step restrictions for the methods considered in 1D and observe agreement with the derived relationships. We test the evaluated time-step limits in 1D with both continuous and discontinuous initial data and validate the previous calculations.

Thursday morning session 2

Session chair: Sofia Eriksson

10.30 – 11.00 **Multiscale computations for elliptic problems and time averaged waves**

Speaker: Olof Runborg

11.00 – 11.30 **Homogenization and numerics for the Landau-Lifshitz equation with highly oscillatory coefficient**

Speaker: Lena Leitenmaier

11.30 – 12.00 **Patient specific modeling and simulation of mitral valve disease**

Speaker: Frida Svelander

MULTISCALE COMPUTATIONS FOR ELLIPTIC PROBLEMS AND TIME AVERAGED WAVES

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Elliptic problems with rapidly varying coefficients are computationally costly to solve by traditional techniques because the smallest scales must be represented over a domain determined by the largest scales of the problem. We discuss different numerical multiscale methods for such problems, which can find the solution significantly faster than traditional techniques, including HMM and LOD. In particular we will show how efficient, localized, basis functions for generalized FEM can be obtained by averaging short time solutions of the wave equations.

HOMOGENIZATION AND NUMERICS FOR THE LANDAU-LIFSHITZ EQUATION WITH HIGHLY OSCILLATORY COEFFICIENT

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We use a simplified version of the Landau-Lifshitz equations, to study a composite ferromagnetic object that consists of magnetic materials with different interaction behavior. In the model this is represented by a rapidly varying material coefficient a^ε, $\varepsilon \ll 1$. More precisely, we study

$$\partial_t \mathbf{m} = -\mathbf{m} \times \mathbf{H} - \alpha \mathbf{m} \times \mathbf{m} \times \mathbf{H}, \tag{1}$$

where

$$\mathbf{H} = \boldsymbol{\nabla} \cdot (a^\varepsilon \boldsymbol{\nabla} \mathbf{m}) .$$

Direct numerical simulation of the problem is expensive as the small ε-scale must be resolved; however, the small scale cannot be ignored either, since it has a significant influence on the magnetization behavior on the coarse scale. We aim to design an efficient numerical method for this case using the framework of heterogeneous multiscale methods (HMM).

In order to understand which behavior to expect from the solution and to obtain a good reference solution, we derive a homogenized equation where $\mathbf{H}$ in (1) is replaced by $\bar{\mathbf{H}} = \boldsymbol{\nabla} \cdot (A \boldsymbol{\nabla} \mathbf{m})$ with a constant matrix A. We also derive equations for higher order correction terms to the homogenized solution $\mathbf{m}_0$. We show estimates for the difference $\mathbf{m}_0 - \mathbf{m}^\varepsilon$ in terms of ε. Investigating the correction terms, we find that there is a rapidly oscillating contribution that dominates the short-term behavior but decays exponentially with time t/ε^2. This is expecially important in the context of HMM where we average over short time intervals in order to approximate the effective long time behavior.

We use these results to analyze an HMM method and also show numerical results that confirm the accuracy of the method.

PATIENT SPECIFIC MODELING AND SIMULATION OF MITRAL VALVE DISEASE

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Diagnosis and treatment of heart disease is of major interest on as well societal as individual level, being one of the major causes of death worldwide. In our joint work, we focus on modeling and simulation of valve disease from a computational and clinical perspective, and we present a general framework for patient specific simulation of mitral valve disease. The blood flow in the left ventricle of the human heart is modeled by the incompressible Navier-Stokes equations in an already existing high performance finite element framework (FEniCS-HPC). Due to instrumental limitations and high complexity in capturing the anatomy and the rapidly changing valvular dynamics, and the computational cost of resolving a very fine geometry, the computational framework is in a first study extended with a simple two dimensional model of the mitral valve (MV), built upon 4D-TTE ultrasound images of the projection of the valve on the left ventricle endocardium, and a parametric model of the dynamics of the valve leaflets. A parametric study of the MV dynamics is performed to model different grades of mitral stenosis, a severe valve disorder. Preliminary results show that the level of modeled stenosis is directly related to a stronger blood flow jet and a higher pressure in the ventricle; symptoms that in the long run can cause for example mechanical damage on the heart. More studies are planned to validate the model, and the development and implementation of a 3D MV model in the computational framework is planned.

Thursday afternoon session 1

Session chair: Andrew Winters

13.00 – 13.30 **A linearisation technique for nonlinear eigenproblems with eigenvector nonlinearities**

Speaker: Parikshit Upadhyaya

13.30 – 14.00 **A time adaptive multirate Dirichlet–Neumann waveform relaxation method for heterogeneous coupled heat equations**

Speaker: Peter Meisrimel

14.00 – 14.30 **Randomized schemes for the approximation of nonlinear evolution equations**

Speaker: Monika Eisenmann

A LINEARISATION TECHNIQUE FOR NONLINEAR EIGENPROBLEMS WITH EIGENVECTOR NONLINEARITIES

PARIKSHIT UPADHYAYA[*], **ELIAS JARLEBRING**[*], **ROB CLAES**[†] **AND KARL MEERBERGEN**[†]

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We consider a nonlinear eigenproblem with eigenvector nonlinearities that appear as a ratio of two linear functions. The goal is to find $\lambda \in \mathbb{C}$ and $x \in \mathbb{C}^n$ such that

$$(A + \lambda B + f_1(x)C_1 + \cdots + f_m(x)C_m)x)0 \tag{1}$$

with $A, B \in \mathbb{C}^{n\times n}$, $C_i \in \mathbb{C}^{n\times n}$

$$f_i(x) = \frac{r_i^T x}{s_i^T x}, \quad r_i \in \mathbb{C}^n, \quad s_i \in \mathbb{C}^n \tag{2}$$

for $i = 1, \ldots, m$. Solutions to (1) and related equations are required in a wide range of applications, from the Gross-Pitaevskii equation in quantum physics [1] to spectral clustering [2] in machine learning.

The most widely used approach for solving (1) is the self-consistent field (SCF) algorithm combined with an acceleration scheme; see e.g. [3] and references therein. This involves solving a linear eigenvalue problem in each iteration. In contrast to this, we introduce a novel technique that converts (1) into an equivalent multiparameter eigenvalue problem (MEP) [4] with $m + 1$ parameters. The resulting MEP and the associated operator determinants have a specific structure. This allows us to adapt several existing algorithms for solving MEPs by exploiting this structure. In particular, we propose a new adapted version of the residual inverse iteration [5] and the inverse iteration for the operator determinants. Results from the numerical experiments show that our technique provides an efficient way to compute solutions to problems arising in (1).

REFERENCES

[1] W. Bao and Q. Du, "Computing the ground state solution of Bose-Einstein condensates by a normailzed gradient flow." *SIAM J. Scientific Computing*, 25(5):1674–1697, (2004).

[2] T. Bühler and M. Hein, "Spectral clustering based on the graph p-Laplacian." *Proceedings of the 26th International Conference on Machine Learning*, 81–88, (2009).

[3] X. Liu, X. Wang, Z. Wen and Y. Yuan, "On the convergence of the self-consistent field iteration in Kohn-Sham density functional theory." *SIAM J. Matrix Analysis and Applications*, 35(2):546–558, (2014)

[4] F. V. Atkinson, Multiparameter eigenvalue problems. *Academic Press, New York*, 1972.

[5] B. Plestenjak, "Numerical methods for nonlinear two-parameter eigenvalue problems." *BIT Numerical Mathematics*, 56:241–262, (2016).

A TIME ADAPTIVE MULTIRATE DIRICHLET–NEUMANN WAVEFORM RELAXATION METHOD FOR HETEROGENEOUS COUPLED HEAT EQUATIONS

PETER MEISRIMEL[†], **AZAHAR MONGE**[†], **PHILIPP BIRKEN**[†]

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Efficient simulation of dynamical thermal interaction between fluids and structures is important in many industrial applications such as heat treatment of metal work-pieces (gas-quenching), thermal anti-icing systems of airplanes or even the cooling of rocket thrust chambers.

One models dynamical thermal fluid structure interaction using two PDEs, describing fluid and structure, coupled via a shared interface. The principle spatial coupling is based on a Dirichlet-Neumann (DN) iteration, in which the PDEs use a Dirichlet resp. Neumann boundary condition on the shared interface with boundary data provided by the other problem. Our work focuses on efficiently resolving the dynamical aspects of this coupling, for two coupled heterogeneous heat equations.

We consider so called Waveform-Relaxation methods, in which the Dirichlet-Neumann iteration is done on (discrete) functions in time, rather than time-points in each timestep. Combined with suitable interpolation techniques, this enables the use of distinct and adaptive time-grids for each problem, without loss of order.

We present a second order, multirate, resp. adaptive Dirichlet-Neumann Waveform Relaxation method. We calculate the analytical optimal relaxation parameter for 1D, implicit Euler and fixed Δt. This relaxation parameter is then used in the 2D case with adaptive time-integration. Numerical results show that our method is very robust, yielding fast convergence rates. In particular, it is more robust than the related Neumann-Neumann Waveform Relaxation method.

RANDOMIZED SCHEMES FOR THE APPROXIMATION OF NONLINEAR EVOLUTION EQUATIONS

MONIKA EISENMANN†

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In this talk, we will focus on the numerical approximation of nonlinear, nonautonomous evolution equations with nonsmooth temporal coefficients. A common method for the approximation of the integral of an irregular function is a Monte Carlo type quadrature rule. We use a similar approach to approximate the solution of a nonautonomous evolution equation. First, we show how randomized point evaluations can be used to obtain error bounds when the data is merely integrable and the solution is Hölder continuous. A further randomization can be applied to generalize the regularity assumptions. After introducing a randomly shifted grid, it is possible to allow for a solution in a fractional Sobolev space and obtain error bounds of a possibly higher order.

Thursday afternoon session 2

Session chair: Philipp Birken

15.00 – 15.30 **Structure preserving iterative methods in CFD**
Speaker: Viktor Linders

15.30 – 16.00 **Space-time multigrid preconditioners — local Fourier analysis**
Speaker: Lea Miko Versbach

16.00 – 16.30 **Spectral properties of the incompressible Navier-Stokes equations**
Speaker: Fredrik Laurén

STRUCTURE PRESERVING ITERATIVE METHODS IN CFD

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The discrete preservation of linear and nonlinear physical invariants, such as conservation of mass, energy and entropy, form the backbone of robust high order methods in CFD. For stiff problems, e.g. wall-bounded flows, these methods are necessarily implicit, resulting in large systems of nonlinear equations. Solutions to these systems are typically approximated using iterative methods. However, since iterative methods in practice are truncated well before asymptotic convergence is reached, the approximate solution may violate physical invariants.

In this talk, we explore the possibility of preserving certain invariants with iterative methods for linear and nonlinear problems. We discuss the conservation of mass for the most ubiquitous iterative methods, noting that common methods such as Jacobi and Gauss-Seidel are not conservative. Concerning the energy stability for linear problems, linear multigrid is analyzed and a condition for the stability of the coarse grid correction is presented. For a nonlinear problem it is demonstrated that Newton?s method violates entropy conservation. A variety of approaches towards a remedy is discussed.

SPACE-TIME MULTIGRID PRECONDITIONERS — LOCAL FOURIER ANALYSIS

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Our main interest is to construct cheap and efficient implicit high order solvers for compressible turbulent flow problems, which arise, for example, in the design of next generation jet engines, air frames, wind turbines or star formation. A suitable high order discretisation for these problems are space-time discontinuous Galerkin (DG) methods, which provide an implicit solver of variable order in the spatial and temporal directions.

An efficient solver for the resulting large nonlinear systems has to be chosen carefully with respect to storage and computational time. We use a preconditioned Jacobian-free Newton-Krylov method and construct the preconditioner using multigrid (MG) methods. We base these on lower order replacement operator, as suggested in [2].

In order to analyse these preconditioners, a Local Fourier Analysis (LFA) can be applied. The aim of this analysis is to study the efficiency of the smoother as well as of a two-grid procedure for a given multigrid method. We present a new space-time multigrid algorithm for solving a model problem, similar to [1]. We consider the linear advection equation, which we discretise with a finite volume in space and a DG method in time. With the LFA, smoothing and convergence factors can be calculated using so-called Fourier symbol. These are of smaller size than the original system and make the calculations feasible. From this analysis we obtain asymptotic two-grid convergence factors as well as smoothing factors, which are the basis to construct efficient multigrid preconditioners for space-time DG solvers. We explain some basic ideas of the LFA we performed and show numerical results.

REFERENCES

[1] M. Gander and M. Nermüller, “Analysis of a new space-time parallel multigrid algorithm for parabolic problems.” *SIAM J. Scientific Computing* 38:A2173–A2208, (2016).

[2] P. Birken, G. J. Gassner and L. M. Versbach, “Subcell finite volume multigrid preconditioning for high-order discontinuous Galerkin methods.” *International Journal of Computational Fluid Dynamics* (33)9:353–361, (2019).

SPECTRAL PROPERTIES OF THE INCOMPRESSIBLE NAVIER-STOKES EQUATIONS

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The influence of different boundary conditions on the spectral properties of the incompressible Navier-Stokes equations is investigated. By using the Fourier-Laplace transform technique, we determine the spectra, extract the decay rate in time, and investigate the dispersion relation. In contrast to an infinite domain, where only diffusion affects the convergence, we show that also the propagation speed influence the rate of convergence to steady state for a bounded domain. Once the continuous equations are analyzed, we discretize using high-order finite-difference operators on summation-by-parts form and demonstrate that the continuous analysis carries over to the discrete setting. The theoretical results are verified by numerical experiments, where we highlight the necessity of high accuracy for a correct description of time-dependent phenomena.

Friday morning session 1

Session chair: Fredrik Laurén

8.30 – 9.00 **A new master program in computational science**
Speaker: Philipp Birken

9.00 – 9.30 **Solely hyperbolic numerical approximations of elliptic equations**
Speaker: Andrew Winters

9.30 – 10.00 **Closing remarks**

A NEW MASTER PROGRAM IN COMPUTATIONAL SCIENCE

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The faculty of Science at Lund University has over the last year taken a critical evaluation of the education in computational Science on the Bachelor and Master level. While all departments have strong research groups in computational science, the state of education in the field is lagging behind. This is particularly so with regards to reactions in education on Big Data.

One method to improve the situation would be the introduction of a new interdisciplinary master program with different specalizations, such as Scientific Computing, Computational Chemistry, Computational Earth Sciences and Scientific Assessment. We explain the current ideas behind the program to achieve interdisciplinarity, as well as the improvements that are required in education in programming, statistics and numerical analysis for Bachelor students from different fields to successfully navigate the program. Finally, we take a closer look at the specialization in scientific computing.

SOLELY HYPERBOLIC NUMERICAL APPROXIMATIONS OF ELLIPTIC EQUATIONS

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Problems governed by partial differential equations (PDEs) of elliptic-type necessitate numerical solution techniques that account for their particular behaviour, e.g., non-local exchanges of information. In this talk we describe how to reformulate an elliptic problem into a hyperbolic system of PDEs. Though somewhat strange, the steady state solution of the hyperbolic problem is, in fact, the solution to the original elliptic problem. Converting an elliptic problem into a hyperbolic one allows us to reuse well-developed numerical solvers for conservation laws. As such, we verify that a high-order accurate discontinuous Galerkin (DG) spectral element method approximates such an elliptic PDE solution at steady state.

Then, we apply this hyperbolic formulation for the elliptic problem to simulate self-gravitating flows where the hydrodynamic variables are governed by the compressible Euler equations and the gravity potential by a Poisson equation. To solve this multi-physics problem we use the same DG solver framework for both equation systems where they operate on joint hierarchical Cartesian mesh and are two-way coupled via volumetric source terms. Another benefit to reusing existing DG technologies is that the multi-physics problem can be solved on non-conforming and solution adaptive grids without modification.