



## Circus 2015

Numerical Mathematics and Computational Science

Umeå University, August 26-27, 2015



# Abstracts of presentations

### Producing a Menu of Stationary Solutions to the Axially-Symmetric Einstein-Vlasov System

*Ellery Ames, Chalmers*

We present a code for numerically solving the time-independent Einstein-Vlasov system in axial symmetry. Solutions to these equations model a large collection of collisionless bodies interacting gravitationally through the Einstein equations. In the Vlasov model, position and momenta of the bodies are obtained via a distribution function on phase space. Under the stationary ansatz the equations become a nonlinear integro-differential system of PDEs, which we solve using an iteration scheme and finite element methods. Our solver has been implemented in FEniCS. In this talk I will present the equations, finite element discretization and solution algorithms, as well as numerical results in the form of numerical solutions, convergence results and adaptive meshes.

### High order FEM computation of resonances in nanostructures (POSTER)

*Juan Carlos Araujo-Cabarcas, Umeå University*

In the study of wave propagation in open domains with dielectric scatterers, the localization of energy peaks is closely related to the scattering resonances. Computing resonances of the transverse electromagnetic scattering problem in open domains requires setting up an outgoing condition. In particular we compare two well-known methods to do so: Dirichlet to Neumann maps (DtN) and the perfectly matched layer (PML). The use of the DtN results in a fully nonlinear eigenvalue problem where the spectral parameter is argument of transcendental functions in dimensions 2 and 3. While the PML method gives the advantage that the resulting rational eigenvalue problem can be straightforwardly linearized. However, the PML method introduces spectral pollution. We discretize in space by using high order finite element methods and observe that in both cases spurious eigenvalues appear due to the discretization. We notice that the spurious eigenvalues and the polynomial order in use are closely related to the number of spurious eigenvalues and we present a way of reducing/eliminating them.

### Lagrangian-Eulerian based immersed boundary method for large scale simulations

*Rahul Bale, RIKEN, Japan*

A Lagrangian-Eulerian approach is used in an immersed boundary framework for modelling fluid structure interaction. The structure and the fluid are represented on a Lagrangian and an Eulerian mesh, respectively. The Eulerian flow field is solved on a hierarchical Cartesian mesh called Building Cube Method (BCM). BCM allows for an efficient parallelization with low communication costs that can scale to hundreds of thousands of cores. The structure is represented on a BCM based Lagrangian data structure. The Lagrangian allows us to accurately capture complex geometries. The Lagrangian IBM is developed such that it does not necessitate special consideration for reparation of dirty CAD data or mesh generation, thereby reducing preprocessing time from weeks to minutes. BCM based Lagrangian data structure is designed for efficient parallelization and scalability.



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## **Coupled Sylvester-Type Matrix Equations and Block Diagonalization**

*Andrii Dmytryshyn*, Umeå University

We prove Roth's type theorems for systems of matrix equations including an arbitrary mix of Sylvester and \*-Sylvester equations, in which also the transpose or conjugate transpose of the unknown matrices appear. In full generality, we derive consistency conditions by proving that such a system has a solution if and only if the associated set of  $2 \times 2$  block matrix representations of the equations are block diagonalizable by (linked) equivalence transformations. Various applications leading to several particular cases have already been investigated in the literature, some recently and some long ago. Solvability of these cases follows immediately from our general consistency theory. We also show how to apply our main result to systems of Stein-type matrix equations.

## **Schur complement matrix and its (elementwise) approximation: A spectral analysis based on GLT sequences**

*Ali Dorostkar*, Uppsala University

Using the notion of the so-called spectral symbol in the Generalized Locally Toeplitz (GLT) setting, we derive the GLT symbol of the sequence of matrices  $\{A_n\}$  approximating the elasticity equations. Further, as the GLT class defines an algebra of matrix sequences and Schur complements are obtained via elementary algebraic operations on the blocks of  $A_n$ , we derive the symbol  $f$  of the associated sequences of Schur complements  $\{S_n\}$  and that of its element-wise approximation.

## **A multilevel subset simulation for estimation of rare events**

*Daniel Elfversson*, Uppsala University

We want to estimate the probability that a functional is below or above some critical threshold. Standard Monte Carlo is infeasible due to the huge amount of samples that are needed to produce even a single rare event. Remedies for this are using variance reduction techniques, e.g., subset simulation. In this work we consider a multilevel subset simulation approach with a varying number of samples on the different levels. The key idea in our new method is to use a posteriori error estimators to guarantee the critical subset property that may be violated when changing the model resolution from one failure set to the next.

## **A Vertex-centered Discontinuous Galerkin Method (POSTER)**

*Sven-Erik Ekström*, Uppsala University

The most common type of solver in industry for CFD is the vertex-centered finite volume methods. The emerging high-order discontinuous Galerkin methods are in their standard form cell-centered, and thus not compatible with existing codes. The presented method is a vertex-centered discontinuous Galerkin method, which is backwards compatible with existing codes and can be seen as a high-order generalization of the classical vertex-centered finite volume method.

## **Spectral Graph Partitioning and a Generalization to Tensors**

*Lars Eldén*, BIT Editor in Chief, Linköping University

Spectral graph partitioning is a method for clustering data organized as undirected graphs. The method is based on the computation of eigenvectors of the graph Laplacian. We give a brief account of spectral graph partitioning and a couple of applications in information sciences. In many areas one wants to cluster data from a sequence of graphs. Such data can be organized as a large sparse tensor. We present a spectral method for tensor partitioning based on the computation of the best multilinear rank approximation of the tensor. A few applications are briefly discussed.



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## **NUMA-Aware Blocked Hessenberg Reduction Using Parallel Cache Assignment (POSTER)**

*Mahmoud Eljammaly, Umeå University*

Eigenvalues and eigenvectors play an important role in many aspects of science and engineering. The needs are increasing every day to compute accurate eigenvalues and eigenvectors in a fast way. A key step in computing all eigenvalues for dense matrices is reducing the matrix to Hessenberg form. The Hessenberg reduction can be classified as a memory-bound computation problem, which makes it slow. Overcoming this problem requires a high degree of data locality. Local data access on the memory level can be achieved using NUMA-aware algorithms, while for small matrices local data access on the cache level will be required. Both of these requirements can be achieved using a recently published technique by Castaldo and Whaley called parallel cache assignment (PCA). Using PCA we present a fine-grain parallelization of the Hessenberg reduction that is also NUMA-aware. The new technique gives a noticeable improvement compared to multi-threaded LAPACK. In addition, we discuss a study made on the algorithm parameters to determine which parameters have a big impact on performance and what is the possible gain of tuning them. An automatic-tuning mechanism based on this research is intended as a future work to achieve the highest performance.

## **Coupling Requirements for Well Posed and Stable Multi-physics Problems**

*Fatemeh Ghasemi Zinatabadi, Linköping University*

A well posed initial boundary value problem requires that a unique solution that can be estimated in terms of the data, exist. The so called energy-method is the most common method for showing well-posedness. In this method one multiply the governing partial differential equations (PDEs) with the solution, integrate by parts and impose boundary conditions. But this may not be wide-spread when it comes to the mathematical coupling of multi-physics problems. Finding accuracy relations such that combinations of variables for one set of PDEs at the interface is equal to combinations of variables and fit both equations is commonly the most difficult part of these problems. We will derive the coupling conditions by only demanding a well posed problem for a general multi-physics problem.

## **Convergence analyses of the Peaceman-Rachford and Douglas-Rachford Schemes for Semilinear Evolution Equations**

*Erik Henningson, Lund University*

We present new results concerning the convergence analysis of the Peaceman-Rachford and Douglas-Rachford time discretization schemes for semilinear evolution equations. The vector field of the equation is assumed to be the sum of two unbounded dissipative operators. A setting in which the Peaceman-Rachford and Douglas--Rachford splitting methods exhibit excellent stability properties. Applications include semilinear reaction-diffusion systems. For the two aforementioned splitting schemes optimal convergence orders are given when the vector field is the sum of a linear and a nonlinear operator. Further, in the setting of linear evolution equations, we combine the splitting methods with convergent spatial discretizations and prove optimal, simultaneous, space-time convergence orders.

## **Megapixel Topology Optimization using Quasi-Arithmetic Mean Based Filters**

*Linus Hägg, Umeå University*

One of the most popular strategies to achieve mesh-independent designs is to use the material distribution approach to topology optimization in combination with a filtering procedure. We have recently proposed an algorithm that applies quasi-arithmetic mean based filters over polytope shaped neighborhoods on regular grids, with a computational cost that scales linearly with the number of design variables. We show results from megapixel topology optimization using a multigrid-CG finite element solver, together with various combinations of filters. The presented results illustrate that these filter combinations can produce almost binary designs, and provide independent size control on structural members and void regions.



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## Towards large-scale multiphysics simulations on the K computer

*Niclas Jansson, RIKEN, Japan*

We present our work on developing a unified simulation method that enables efficient computation of time resolved approximations for complex multiphysics industrial applications. All discretized equations are mapped onto the same grid and solved as a unified continuum. To address the challenges of modern and emerging supercomputers, efficient data structures and communication patterns are needed. Here, we use a hierarchical Cartesian grid together with an immersed boundary method to accurately capture complex geometries. A multithreaded halo-exchange algorithm allows for an efficient parallelization that can scale to hundreds of thousands of cores (one third of the K computer).

## Full system Co-simulation for analysis and design of vehicular mechatronic systems (POSTER)

*Mats Johansson and Claude Lacoursière, Umeå University*

Complex mechatronics systems are used in the automotive industry to improve fuel efficiency, manoeuvrability, safety, and ease of use. They are prone to systemic errors due to interactions. Reliable system simulations are needed to detect these during the early design process. Today's simulation software packages are reliable for any given component but not for full system simulations. The project Virtual Truck & Bus promotes integration testing, which will enable the automotive industry to reduce the number of prototypes and redesigns of their products. It will also increase the efficiency of the systems as a large design space can be examined in search for optimal solutions. We intend to systematically rely on FMI to allow software and ECUs to communicate in a uniform way and interchangeably within a client-server architecture. In addition, we will develop a robust numerical time-integration scheme for co-simulation. For the mathematical model, we are opting for a hard kinematic coupling. We believe that stable, fast, linearized methods can be developed based on previous experience and state of the art.

## StratiGraph and the Matrix Canonical Structure Toolbox (POSTER)

*Stefan Johansson, Umeå University*

We present StratiGraph and the Matrix Canonical Structure (MCS) Toolbox for Matlab. StratiGraph is a Java software tool for computing and visualizing closure hierarchy graphs of orbits of matrices, polynomial matrices, and various system pencils. An orbit is a manifold of matrices with the same canonical structure (Jordan, Kronecker, etc.) and the stratification (the closure hierarchy graph) reveals how (small) perturbations in the matrices may change the canonical structure. The MCS Toolbox is a framework with datatype objects for representing canonical structures of matrices, matrix pencils, and system pencils. The toolbox can both be used on its own in Matlab and together with StratiGraph, which enables import and export of canonical structures between Matlab and StratiGraph. Under development are new Matlab routines for computing the staircase form of matrices and matrix pencils. The staircase form reveals the canonical structure of the matrix or matrix pencil.

## Convergency of Leap-frog Discontinuous Galerkin Methods for Solving Time-Domain Maxwell's Equations with Anisotropic Materials

*Maryam Khaksar Ghalati, Coimbra University*

Modelling light propagation in biological tissue has become an important research topic in biomedical optics with applications in diverse fields as for example in ophthalmology. It may be worthwhile to model waveguides with induced anisotropy as they could play a role in biological waveguides. For instance, there is a strong correlation between retinal nerve fiber layer thinning and reduction in tissue birefringence. Simulating the full complexity of the retina, in particular the variation of size and shape of each structure, distance between them and refractive indexes, requires a rigorous approach that can be achieved by solving Maxwell's equations. The finite difference time domain method (FDTD) was the first commonly used technique to find a time-domain



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solution of Maxwell's curl equations on spatial grids. The first application of the FDTD to cellular level biophotonics was reported in 1994.

In the last decades, many papers in electromagnetic simulations have shown interest in discontinuous Galerkin time domain methods (DGTD) to solve Maxwell's equations. The DGTD methods present some well-known major advantages compared with more classical FDTD and finite element time domain methods. In opposition to the traditional FDTD methods, the DGTD method is a high-order accurate method that can easily handle complex geometries. Moreover, the method is suitable for parallel implementation on modern multi-graphics processing units and local refinement strategies can be incorporated due to the ability of the method to deal with irregular meshes with hanging nodes and local spaces of different orders. This also represents an advantage when compared to finite element methods. Despite the relevance of the anisotropic case, most of the formulations of the DGTD methods have been restricted to isotropic and dispersive materials. In this work we consider models with anisotropic permittivity tensors which arise naturally in our application of interest. Here we combine the DGTD method (considering central and upwind fluxes) with a leap-frog type time integration, arriving at a fully-discrete explicit leap-frog DG scheme. We give a rigorous proof of the stability and the high-order convergence of the scheme. We provide the results of some numerical tests to illustrate the theoretical results.

### An exponential integrator for polynomially parameterized linear ODEs

*Antti Koskela, KTH*

Consider the initial value problem  $\dot{u}(t) = (\sum_{\ell=0}^N \epsilon^\ell A_\ell) u(t)$ ,  $u(0) = u_0$ , where  $A_0, A_1, \dots, A_N \in \mathbb{C}^{n \times n}$  and  $u_0 \in \mathbb{C}^n$ . We present results that allow us to evaluate  $u(t)$  efficiently for several values of  $\epsilon$  and  $t$ . We propose a new Krylov subspace method which uses the approximation of the product of the matrix exponential and a vector. The approach is based on the Taylor expansion of the exact solution  $u(t)$  with respect to  $\epsilon$ . We show that the coefficient vectors of this expansion are given by the matrix exponential of a block Toeplitz matrix. This result can be seen as a generalization of a result given by Najfeld and Havel (1995). A priori error bounds are derived for the approximation which show a superlinear convergence for any  $N$ .

### Parameterless stopping criteria for density matrix expansions

*Anastasia Kruchinina, Uppsala University*

We propose parameterless stopping criteria for recursive polynomial expansions for the construction of the density matrix from the effective Hamiltonian matrix in linear scaling electronic structure calculations. Our new type of stopping criteria automatically and accurately detect when the calculation is dominated by numerical errors. Stopping criteria of this type can straightforwardly be derived for recursive expansions based on various choices of polynomials and may be used together with any method for removal of small matrix elements in a linear scaling sparse matrix setting. Our parameterless stopping criteria stand in contrast to the standard approach to stop as soon as some error measure goes below a user-defined parameter or tolerance. In the present work we derive and evaluate new stopping criteria for the regular and accelerated McWeeny and SP2 recursive expansions.



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## A New High Order Mimetic Arakawa-Like Jacobian Differential Operator for the Incompressible Vorticity Equation

*Cristina La Cognata*, Linköping University

Mimetic schemes are widely used in long-time computations of geophysical flows. A high order mimetic expression for the celebrated Arakawa's Jacobian for the two-dimensional incompressible vorticity equation is developed. Mimetic properties such as skew-symmetry, energy and entropy conservation for the semi-discretization are proved using summation-by-parts operators. A new form of well-posed boundary conditions is derived on a general two-dimensional domain. The discrete version of the boundary conditions is weakly imposed. Numerical experiments corroborate the results.

## Uniformly best wavenumber approximations

*Viktor Linders*, Linköping University

We construct difference stencils for problems involving high frequency waves or multi-frequency solutions over long time intervals with a relatively coarse spatial mesh, and with an easily obtained bound on the dispersion error. This is done by demonstrating that the problem of constructing difference stencils that have minimal dispersion error in the infinity norm can be recast into a problem of approximating a continuous function from a finite dimensional subspace with a basis forming a Chebyshev set. In this new formulation, characterising and numerically obtaining optimised schemes can be done using established theory.

## Molecular Structure Reconstruction From Single-Particle Imaging Using GPUs (POSTER)

*Jing Liu*, Uppsala University

Modern techniques allow X-ray laser beams to produce ultrashort high energy pulses, and such pulses could create single-particle images. Through machine learning methods the collected data can be transformed into a three-dimensional volumetric intensity map of the particle itself. The computational complexity associated with this problem is very high, so that clusters of data parallel accelerators are required. We have implemented a distributed and highly efficient algorithm for inversion of large collections of diffraction patterns targeting clusters of hundreds of GPUs. With the expected enormous amount of diffraction data to be produced in the foreseeable future, this is the required scale to approach real time processing of data at the beam site.

## Matrix-Free Finite-Element Computations on Graphics Processors

*Karl Ljungkvist*, Uppsala University

Modern processors such as GPUs require a high amount of arithmetic operations per memory access to be fully utilized. For traditional finite-element methods, this is an issue since the sparse matrix-vector product constituting its major part is dominated by memory bandwidth usage rather than computations, in particular for high dimensionality and element order. By using a matrix-free approach the bandwidth usage can be reduced considerably which leads to a corresponding speedup for the bandwidth-bound case. In addition, the matrix-free method uses significantly less memory allowing for larger problems to be solved. Finally, since the matrix-free method eliminates the matrix, no assembly is needed which further reduces the run time, especially for non-linear problems.



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## **Uncertainty Quantification for High Frequency Waves**

*Gabriela Malenova, KTH*

We consider the scalar wave equation with highly oscillatory initial conditions where the wave speed and/or the initial data are stochastic. A spectral asymptotic method for the uncertainty quantification of high frequency waves subject to stochastic uncertainty is presented. The method consists of Gaussian beam superposition in the deterministic space and collocation on sparse grids in the stochastic space. In the presence of stochastic regularity, the method exhibits a faster rate of convergence compared to the Monte Carlo techniques. We show theoretical and numerical evidence that certain quadratic quantities of interest are indeed smooth in stochastic space, and exhibit fast convergence.

## **Stochastic diffusion simulations under molecular crowding**

*Lina Meinecke, Uppsala University*

Living cells have a high level of spatial organization, such as a confined nucleus in eukaryotes or membrane bound reaction complexes. Hence it is important in systems biology to not only model the biochemical reactions between molecules but also their movements by either active transport or diffusion. Moreover, key proteins such as transcription factors are only present in very low copy numbers, introducing intrinsic noise. To simulate cells stochastically we use the mesoscopic model of reaction-diffusion kinetics, described by a continuous time, discrete space Markov process. In order to represent complicated geometries the jump coefficients of stochastic diffusion are obtained by a discretization of the macroscopic diffusion equation on unstructured grids. The intracellular environment is considered crowded, meaning that while each molecular species is present at only low copy numbers the total fraction of occupied volume is a tenfold higher than in test tube experiments. We use more detailed results from microscopic Brownian dynamics simulations to examine how to incorporate molecular crowding effects on both the mesoscopic stochastic level and the macroscopic deterministic level.

## **The waveguide eigenvalue problem and the tensor infinite Arnoldi method**

*Giampaolo Mele, KTH*

We present a new iterative algorithm for nonlinear eigenvalue problems, the tensor infinite Arnoldi method, which is applicable to a general class of NEPs and we show how to specialize the algorithm to a specific NEP: the waveguide eigenvalue problem, which arises from a finite-element discretization of a partial-differential equation used in the study of waves propagating in a periodic medium. The algorithm is successfully applied to solve (with high precision) benchmark problems as well as complicated waveguides. We study the complexity of the specialized algorithm with respect to the number of iterations  $m$  and the size of the problem  $n$ , both from a theoretical perspective and in practice. Link to the preprint: <http://arxiv.org/abs/1503.02096>

## **A Family of Runge-Kutta Starters for Discontinuous ODEs**

*Fatemeh Mohammadi, Lund University*

In this talk we present a class of Runge–Kutta methods designed to start multistep methods applied to ODEs with frequent discontinuities. Multistep methods use information from previous steps to approximate the next value. A single step of these Runge–Kutta methods provides sufficiently accurate initial values to start a high order multistep method, whereas classical algorithms either apply a Runge–Kutta method several times or start with a variable order implementation. Both classical schemes can lead to inefficiency when the integration has to be interrupted frequently due to discontinuities. We demonstrate the advantage of this approach by an extension of Assimulo together with original LSODE.



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## **Preconditioning techniques for discrete PDE-constrained optimization problems**

*Maya Neytcheva*, Uppsala University

We consider various preconditioning methods for the algebraic systems, arising from discrete PDE-constrained optimization problems and compare their numerical and computational efficiency.

## **Element-free elastoplastic solid for nonsmooth multidomain dynamics**

*John Nordberg*, Umeå University

A mesh free, constraint based model of elastoplastic solids is derived from the strain energy density function.

The model is presented within a mathematical framework for simulation of complex physical systems and nonsmooth dynamics. This is demonstrated simulating a vehicle interacting with deformable terrain.

## **Energy balanced time integration for electrical machines**

*Lauri Perkiö*, Aalto University

Computation of magnetic fields in electric motors involves solving a heat-equation like PDE. FEM-discretization of such problem leads to a index-1 DAE. One part of our work concerns finding a time integration method that is suitable for such a problem, and in addition the method should compute the energy changes such that the sum of stored energy, energy loss and input energy is zero. Our proposed methods are based on collocation methods involving Gauss quadrature points (subfamily of implicit Runge-Kutta). This is related to torque and force computations in electrical machines. One proposed method for torque computation involves computing the torque from the energy balance of the system, and one can naturally ask if the integration method itself loses significant amounts of energy.

## **Singularity of the discrete Laplacian operator**

*Andrea Alessandro Ruggiu*, Linköping University

The one-dimensional Poisson equation with two boundary conditions given at different nodes is studied both in the continuous and discrete setting. The discretization for the continuous problem is given in terms of an algebraic equation,  $\mathbf{Av} = \mathbf{G}$ . We prove that the matrix  $\mathbf{A}$  is singular if the continuous problem is ill-posed. The converse implication holds if, and only if, a condition on a rank of a discretized differential operator is satisfied.

## **Numerical evaluation of the roots of orthogonal polynomials**

*Diego Ruiz Antolín*, Universidad de Cantabria

A well-known method for finding the real zeros of classical orthogonal polynomials is the Golub-Welsch algorithm, which consists in computing the eigenvalues of the Jacobi matrix associated to the recurrence relation satisfied by the orthogonal polynomials. However, the method becomes less efficient as more nodes are required, because the cost of finding the eigenvalues of the tridiagonal Jacobi matrix scale as  $n^2$ , where  $n$  is the desired number of roots to be computed. For high values of  $n$ , a more efficient way to proceed is to compute the roots by standard techniques like the Newton-Raphson method, starting from sufficiently accurate initial estimations. But then the problem is how to be sure that the initial values guarantee convergence. We discuss how the consideration of Sturm comparison theorems for ODEs gives rise to fourth order fixed point methods which converge with certainty to the roots. We discuss how the implementations of these methods lead to efficient methods for computing classical Gaussian quadrature rules.



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## **A multibody dynamics model of bacterial biofilms**

*Martin Servin, Umeå University*

A coarse grain multibody dynamics model for bacterial biofilms is presented. The bio film is modeled by a collection of rigid bacteria interacting through contact forces and by a pili organelles. The interactions are formulated as kinematic constraints, and the numerical integration algorithm is based on a nonsmooth dynamics approach. Preliminary results are presented.

## **Stabilized Nitsche Cut-Elements for Wave propagation**

*Simon Stålka, Uppsala University*

The idea of immersed methods is to use a uniform computational background mesh which is not aligned with the boundary of the problem-domain. One such method, based on finite elements, is cut-elements. We discuss the cut-element method in the context of wave propagation problems. In particular we give a weak formulation for solving the scalar wave equation. Here, boundary conditions are enforced weakly by Nitsche's method and additional penalty terms ensure a non-stiff temporal system. For standard piecewise linear elements we give optimal a priori error estimates. Numerical experiments verify the theory. Since higher order methods are known to perform better for wave propagation problems we discuss the use of higher order Lagrange elements on quadrilaterals.

## **Spectral properties of non-selfadjoint rational operator functions and applications to wave propagation in photonic crystals (POSTER)**

*Axel Törshage, Umeå University*

The poster will present a rational spectral value problem with applications in for example electromagnetic wave propagation in metallic photonic crystals and microwave cavities containing lossy dielectric materials. The spectral value problem will be non-selfadjoint which results in a complex spectrum and complicates the analysis. By rewriting the rational spectral value problem as an equivalent linear problem it is noted that the problem is almost selfadjoint in a Krein space, from which analytic outer bounds of the numerical range is obtained. These bounds are only slightly larger than the computationally expensive numerical range and very cheap to compute regardless of the size of the problem.

## **Robust Boundary Conditions for Stochastic Incompletely Parabolic Systems of Equations**

*Markus Wahlsten, Linköping University*

We study an incompletely parabolic system in one space dimension with stochastic boundary and initial data. The goal is to show how the variance of the solution depends on the boundary conditions imposed. Estimates of the variance of the solution are presented both analytically and numerically.

## **Accelerated granular matter simulation (POSTER)**

*Da Wang, Umeå University*

Modelling and simulation of granular matter has important applications in both natural science and processing and transportation industry. One widely used method is the discrete element method. It can be used for simulating granular matter in the gaseous, liquid as well as solid regime whereas many of the alternative methods are best suited for a single regime. Analysis of large-scale systems is limited by long computational time. A number of solutions for increasing the computational efficiency of conventional DEM are presented. These include treating the material as a non-smooth dynamical system, allowing large time-step integration, and methods for improving the convergence of the solver for the resulting mixed linear complementarity problem. The solutions are validated and applied for design exploration of iron ore pelletizing systems.



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## **Convergence of summation-by-parts finite difference methods for the wave equation (POSTER)**

*Siyang Wang*, Uppsala University

In this poster, we present our results on the convergence analysis of summation-by-parts finite difference methods applied to the second order wave equation. The spatial derivative is approximated by the central finite difference stencil in the interior with an error  $\mathcal{O}(h^{2p})$ , while near the boundary the one sided stencil is used and the error is increased to  $\mathcal{O}(h^p)$  for stability reason. Here  $h$  is the grid spacing and  $2p=2,4,6,8,10$  is the order of accuracy. We show the relation between the convergence rate  $q$  and the accuracy order  $2p$  for the problem with the Dirichlet condition and Neumann condition, and also the problem solved on a grid with a grid interface. The relation is proved by the normal mode analysis, and is verified by numerical experiments.



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