

University Center for Mathematical Modeling, Applied Analysis and Computational Mathematics

Semester Seminar, hybrid form (in person and via Zoom),
Room K3, Wednesdays, November and December, 09:00-10:00

SCHEDULE

Time	Speaker	Title
Nov 19		
9:00–9:20	Santolo Leveque	An Augmented Lagrangian preconditioner for the control of the Navier–Stokes equations
9:20–9:40	Ritesh Khan	Accelerating Dense Matrix Computations Using Hierarchical Matrices
9:40–10:00	Yuxin Ma	On a shrink-and-expand technique for symmetric block eigen-solvers
Dec 3		
9:00–9:20	Petr Šácha	Are atmospheric gravity waves accelerating or decelerating the jet stream?
9:20–9:40	Alexei Gazca	A Nitsche method for fluid flow with dynamic and set-valued boundary conditions
9:40–10:00	Petr Pelech	Constitutive model for NiTi-based SMA including plasticity
Dec 10		
9:00–9:20	Vojtěch Patočka	Polar motion on Venus: outlooks and perspectives
9:20–9:40	Laëtitia Lebec	Cracking Europa: Salts distribution and the tectonic secrets of dilation bands
9:40–10:00	Ondřej Chrenko	Towards 3D simulations of radiative circumplanetary disks
Dec 17		
9:00–9:20	Michal Outrata	Multiprecision computations with Schwarz methods
9:20–9:40	Marc Fehling	Numerical optimization in nonlinear elasticity
9:40–10:00	Jan Blechta	On traction computation in viscous flow

ABSTRACTS

Jan Blechta: On traction computation in viscous flow (20 mins). Forces exerted by fluid flow on a solid structure are of great importance in engineering. For the total force exerted on the structure by the fluid it is well known that the variational method, known as the Babuška–Miller trick, provides superior results in comparison to the direct evaluation of traction from the Cauchy stress and surface integration. Similarly, for boundary traction distribution, there is some evidence that the variational method provides an advantage but the overall picture is rather blurry. Theoretical results are available only for elliptic problems. The matter is further complicated by other issues, such as geometry approximation errors or a certain over-consistency paradox exhibited by some divergence-free methods under no-slip boundary conditions.

I will give an overview of the aforementioned issues and present some numerical evidence based on the recently submitted study with J. Cach, K. Tůma, and S. Schwarzacher.

Ondřej Chrenko: Towards 3D simulations of radiative circumplanetary disks (20 mins). Simulating interactions of newborn planets with their natal circumstellar disk is a challenging multi-scale problem. While planet-driven spiral arms and planet-induced gas gaps can stretch over tens of astronomical units, the gas flow in the closest neighborhood of the planets can develop a small circumplanetary sub-disk, orbiting around the planet itself. Such a circumplanetary disk is of high importance for protoplanet detection and plays a pivotal role in mediating

accretion of massive gaseous envelopes and formation of satellites (such as the Galilean moons of Jupiter). The only way to study both the circumplanetary and circumstellar disk in a single numerical simulation is to introduce some form of mesh refinement. Here, I will present new upgrades of my radiative model based on Fargo3D, using non-uniform mesh density functions and aiming at resolving the circumplanetary environment in sufficient detail. I will present my first test simulations that resolve the thermal structure around a Jupiter-mass protoplanet.

Marc Fehling: Numerical optimization in nonlinear elasticity (20 mins). Large deformations in elastic solids require nonlinear theory. Associated constitutive relations are often highly complex, posing significant challenges for numerical simulation.

We propose an approach that formulates the large deformation problem as a numerical optimization over continuous piecewise polynomials. Given boundary displacements and an energy functional derived from the constitutive law, we compute the displacement field that minimizes the total energy of the body.

Our prototype implementation leverages both open-source libraries ROL for numerical optimization and deal.II for finite element discretization. We present preliminary results for a buckling problem to demonstrate the method's potential.

Alexei Gazca: A Nitsche method for fluid flow with dynamic and set-valued boundary conditions (20 mins). The classical no-slip (or homogeneous Dirichlet) boundary condition for fluid flow is not appropriate in many situations, as many fluids will often slip at solid walls. In this work we propose a theoretical framework that is able to capture a wide variety of slip models, including linear (Navier) slip, non-linear (and possibly non-smooth) slip described by monotone graphs, non-monotone slip, and dynamic (time-dependent) slip. A finite element scheme is proposed, in which the non-penetrability condition at the wall is enforced with a Nitsche formulation. One of the key tools in the convergence proof is an inhomogeneous Korn inequality that includes a normal trace term. Numerical experiments implemented in firedrake will also be presented. This is joint work with F. Gmeineder, E. Maringová-Kokavcová and T. Tschepel.

Ritesh Khan: Accelerating Dense Matrix Computations Using Hierarchical Matrices (20 mins). Dense matrices arise frequently across many areas, such as PDEs, inverse problems, integral equations, machine learning, kernel methods, etc. In many practical applications, these dense matrices can be very large, making matrix operations involving them quite challenging. For example, the direct evaluation of the dense matrix-vector product in the potential theory requires $O(N^2)$ operations and solving a dense linear system using naive direct methods (such as LU) requires $O(N^3)$ operations. Both operations become computationally prohibitive for large N . To address this, large dense matrices are usually approximated using block low-rank representations, commonly known as hierarchical matrices. In this talk, I will discuss different types of hierarchical matrices and how they can be used to design fast and scalable solvers. I'll also show a few interesting applications that highlight the power of hierarchical matrices.

Laëtitia Lebec: Cracking Europa: Salts distribution and the tectonic secrets of dilation bands (20 mins). Icy moons have become a major focus of interest in planetary science due to their internal structure and dynamics. Among them, Europa is one of the most promising candidates in the search for life in the Solar System. This interest is largely driven by the potential existence of a subsurface liquid water ocean in direct contact with a rocky core, which enables strong water-rock interactions as well as efficient heat and mass exchanges. Meanwhile, Europa's very young surface indicates intense tectonic activity. In particular, the oscillating thickness of the ice shell, between 3 km and 70 km, leads to global contraction and dilatation of the surface. The extension process may cause rifting, facilitating mass exchanges between the ocean and the surface. Taken together, these elements could provide a consistent explanation for the significant fraction of salts found along the large dilatation bands crisscrossing Europa. In our study, we investigate the conditions leading to the formation of these bands and how, in this context, tectonic extension and convection may together drive the transport of salts from the ocean to the surface.

Santolo Leveque: An Augmented Lagrangian preconditioner for the control of the Navier–Stokes equations (20 mins). Optimal control problems with PDEs as constraints arise very often in scientific and industrial applications. Due to the difficulties arising in their numerical solution, researchers have put a great effort into devising robust solvers for this class of problems. An example of a highly challenging problem attracting significant attention is the distributed control of incompressible viscous fluid flow problems. In this case, the physics is described by the incompressible Navier–Stokes equations. Since the PDEs given in the constraints are non-linear, in order to obtain a solution of Navier–Stokes control problems one has to iteratively solve linearizations of the problems until a prescribed tolerance on the non-linear residual is achieved.

In this talk, we present efficient and robust preconditioned iterative methods for the solution of the stationary incompressible Navier–Stokes control problem, when employing an inexact Newton linearization of the first-order optimality conditions. The iterative solver is based on an augmented Lagrangian preconditioner. By employing saddle-point theory, we derive suitable approximations of the (1,1)-block and the Schur complement. Numerical experiments show the effectiveness and robustness of our approach, for a range of problem parameters.

Michal Outrata: Multiprecision computations with Schwarz methods (20 mins). We explore and analyze the use of multiprecision arithmetic for several classes of Schwarz methods and preconditioners, where the approximate solution of the local problems is performed at a lower precision, i.e., with fewer digits of accuracy than in the underlying (double precision) computation. Conditions for the appropriate round-off criteria for the lower precision are presented. Several numerical experiments illustrate the obtained results.

Yuxin Ma: On a shrink-and-expand technique for symmetric block eigensolvers (20 mins). In symmetric block eigenvalue algorithms, such as the subspace iteration algorithm and the locally optimal block preconditioned conjugate gradient (LOBPCG) algorithm, a large block size is often employed to achieve robustness and rapid convergence. However, using a large block size also increases the computational cost. Traditionally, the block size is typically reduced after convergence of some eigenpairs, known as deflation. In this work, we propose a non-deflation-based, more aggressive technique, where the block size is adjusted dynamically during the algorithm. This technique can be applied to a wide range of block eigensolvers, reducing computational cost without compromising convergence speed. We present three adaptive strategies for adjusting the block size, and apply them to four well-known eigensolvers as examples. Detailed theoretical analysis and numerical experiments are provided to illustrate the efficiency of the proposed technique. In practice, an overall acceleration of 20% to 30% is observed.

Vojtěch Patočka: Polar motion on Venus: outlooks and perspectives (20 mins). Internal and external planetary processes such as mantle convection, deglaciation, or large meteorite impacts cause bodies to move as a whole relative to their rotation axis. The rotation poles of planets and moons thus wander on their surfaces, as shown by paleomagnetic, astrometric, and geological observations (true polar wander). In a recent study, polar motion dynamics of the slow rotating Venus was shown similar to that of fast rotating planets such as Earth or Mars. One of the implications is that it is difficult to explain the offset between the rotation and figure axis of Venus by internal processes, in particular by mantle convection. Here I outline other possible explanations of the offset, and address the role of atmospheric drag in the angular momentum conservation of the solid Venus.

Petr Pelech: Constitutive model for NiTi-based SMA including plasticity (20 mins). Among metallic materials, shape memory alloys (SMA) are distinguished by their capacity to respond to mechanical loading through deformation, which can be subsequently recovered by either releasing the load (superelasticity) or by varying temperature (shape memory effects). Attempts to capture the influence of the transformation processes in SMA on their mechanical response via models date back to 1980s. Macroscale constitutive models, stemming from the combination of continuum thermodynamics and internal variables theory, are the first choice tool for design and engineering analysis purposes. They relate the mechanical response to the evolution of microstructural descriptors (internal variables).

The functional fatigue (“shakedown”) related to cyclic loading/training has been tackled in many works. In these models, additional accumulated martensite-dependent descriptors – representing retained, irrecoverable martensite, residual stress, residual strain, etc. – and/or cumulated martensite-dependent material parameters are used. Usually, this is referred as transformation induced plasticity (TRIP). Models that also consider the other scenario – in which plastic yielding represents a distinct/separate deformation process not directly linked to the phase transformation – are much less frequent in the literature. Generally, the martensitic transformation and plastic yielding of martensite can occur simultaneously and influence each other.

Petr Šácha: Are atmospheric gravity waves accelerating or decelerating the jet stream? (20 mins). In this talk I will present the latest research of my group concerning the dynamical effect of internal gravity waves in the terrestrial atmosphere.

The first (boring) part of the study was already published and confirmed the textbook knowledge and expectations regarding the gravity wave role in atmospheric dynamics (gravity waves as a mechanism for wind deceleration aloft).

However, the second part, which is currently under preparation, underwent a transition from being internally labelled as an obvious methodological error to an exciting novel mechanism, how gravity waves can locally accelerate and sharpen the jet.

The research is based on atmospheric reanalysis data, which are a joint product of numerical modelling and atmospheric observations through involved data assimilation techniques and the talk will devote substantial time for explaining them.