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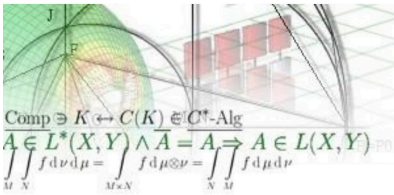

GESELLSCHAFT für
ANGEWANDTE MATHEMATIK und MECHANIK
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Parallel space-time methods for linear hyperbolic systems

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(joint work with W. Dörfler, J. Ernesti, S. Findeisen, and D. Ziegler)

We consider variational space-time discretizations of linear first-order hyperbolic systems. Based on the theory for symmetric Friedrichs systems we establish an analytic framework and we prove inf-sup stability of the continuous variational setting.

Discrete inf-sup stability is obtained for a space-time method with discontinuous Galerkin elements with upwind flux in space and continuous Galerkin elements in time. The discretization is adaptive with independent choice of polynomial degrees p in space and q in time for every space-time cell. The discretization is fully implicit, and the overall linear problem is solved with a parallel Krylov method using a multigrid preconditioner based on a subspace hierarchy. The adaptivity is controlled by a dual weighted residual error estimator with respect to a given linear error functional. The method is evaluated numerically for linear transport and for electro-magnetic, elastic, and visco-elastic waves.

In a second approach we consider a space-time DPG method with degrees of freedom on the space-time skeleton. We introduce a nonconforming variant with discontinuous traces, and the stability is establish by constructing a Fortin operator numerically. Both methods are compared by numerical examples for acoustic waves.

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Space-Time Formulations for the Wave Equation

Silke Glas
Ulm University

We consider a very weak variational formulation of the wave equation in a space-time formulation, i.e., time is treated as an additional variable within the variational formulation of the problem. This results in a setting, where test and trial spaces differ. For a conforming Petrov-Galerkin discretization, we thus need a stable combination of discrete spaces. Instead of adjusting the test space according to the trial space (which is usually done by appropriate stabilization approaches), we start with a suitable test space and derive the trial space subsequently by applying an appropriate differential operator. With these spaces at hand, we can show that the inf-sup constant is equal to one. We provide a numerical realization showing the feasibility of this approach.

Parallel-in-time methods for eddy current problems

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Bergische Universität Wuppertal

The so-called magnetoquasistatic approximation or eddy current problem is a standard approach to simulate the behavior of electrical machines. Thereby Maxwell's equations are simplified by neglecting the displacement current density in Ampère's circuit law. The resulting time-dependent eddy current problem is typically solved by a time-stepping approach, which sequentially solves one time step after the other. For long time periods, as for example at the startup of an electrical machine, the time-stepping approach leads to high computational costs. In contrast, parallel-in-time methods enable parallelism by computing multiple time steps simultaneously and, therefore, are promising techniques for reducing the simulation time of this long range time-dependent problems.

We apply two parallel-in-time algorithms (Parareal and Multigrid Reduction in Time (MGRIT)) to the eddy current problem of a two-dimensional coaxial cable model problem and compare the runtime results of the time-parallel solutions to the runtime of the time-stepping approach.

pySDC: a Parallel Framework for Spectral Deferred Corrections

Robert Speck
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The parallel-in-time method PFASST, the "parallel full approximation scheme in space and time", allows integrating multiple time-steps simultaneously. Based on iterative spectral deferred corrections (SDC) methods, PFASST uses a space-time hierarchy with various coarsening strategies to maximize parallel efficiency. In numerous studies, this approach has been used on up to 448K cores and coupled to space-parallel solvers which use finite differences, spectral methods or even particles for discretization in space. However, since the integration of SDC or PFASST into an existing application code is not straightforward and the potential gain is at least uncertain, we developed the Python prototyping framework pySDC. It allows to rapidly test new ideas and to implement first toy problems more easily. It also provides interfaces to the finite element library FEniCS and the PETSc toolkit. In this talk, we describe the structure of the code and show different examples to highlight various aspects of the implementation, the capabilities and its usage. Moreover, this code sparked the development of a C++-based PFASST implementation, making use of the DUNE framework. The dune-PFASST module specifically targets finite element simulations and is used for reaction-diffusion examples. We will thus also sketch the transition from pySDC to dune-PFASST and show first numerical results.

Automatic Construction of AMG Smoothers

Lisa Claus
Bergische Universität Wuppertal

Algebraic Multigrid (AMG) is used to speed up linear system solves in a wide variety of applications. This talk is concentrated on expanding AMGs applicability to important new classes of problems through algorithms that automatically construct advanced smoothing techniques when needed. AMG algorithms are usually designed by first assuming that the smoother is a simple pointwise smoother, then great effort is put into constructing an interpolation and corresponding coarse-grid correction that complements the smoother and leads to fast O(N) convergence. The so-called weak approximation property and basic two-grid theory are used to guide algorithm development. However, for some classes of problems, pointwise smoothers are not sufficient for achieving the desired O(N) computational complexity. In this talk, we use two-grid theory to motivate the development of new algorithms for automatically constructing more complex (non-pointwise) smoothers. As a relevant application, we consider a curl-curl problem (commonly referred to as the definite Maxwell equations) that often arises in time-domain electromagnetic simulations. We use a Nédélec H(curl)-conforming finite element approach to discretize the problem and demonstrate how our new AMG smoother algorithms recover the well known Arnold-Falk-Winther and Hiptmair smoothers. We also discuss future directions and the potential of these AMG smoothers in more general application settings.

A Heartbeat at a Glance - Space-Time Solution Methods for Cardiac Electrophysiology

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HPC challenges towards realistic simulations of the neuromuscular system

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Realistic simulations of detailed, biophysics-based, multi-scale models require very high resolution and, thus, large-scale compute facilities. Existing simulation environments, especially for biomedical applications, are designed to allow for a high flexibility and generality in model development. Flexibility and model development, however, are often a limiting factor for large-scale simulations. Therefore, new models are typically tested and run on small-scale compute facilities. By using a detailed biophysics-based, chemo-electromechanical skeletal muscle model and the international open-source software library OpenCMISS as an example, we present an approach to upgrade an existing muscle simulation framework from a moderately parallel version towards a massively parallel one that scales both in terms of problem size and in terms of the number of parallel processes. For this purpose, we investigate different algorithmic aspects as well as implementational ones like vectorization. We present improvements addressing both numerical and parallel scalability. In addition, our approach includes a novel visualization environment, which is based on the MegaMol environment capable of handling large amounts of simulated data. It offers a platform for fast visualization prototyping, distributed rendering, and advanced visualization techniques. We present results of a variety of scaling studies at the Tier-1 supercomputer HazelHen at the High Performance Computing Center Stuttgart (HLRS). We improve the node level performance by a factor of up to 2.6 and achieved good scalability on up to 32,768 cores, where the previous implementation used only 4 cores.

Simulation and Sensitivity Optimization for Inverse Problems in Piezoelectricity

Benjamin Jurgelucks, Veronika Schulze, Nadine Feldmann and Leander Claes
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For the optimization of sensitivity for inverse problems in piezoelectricity simulation tools are obligatory. Oftentimes it is especially helpful to also have fast and exact derivatives of the solution computed e.g. via Algorithmic Differentiation. However, for the simulation of piezoelectric ceramics there are, with a few exceptions, mainly closed-source commercial FEM solvers available. In this talk we will present work regarding the instrumentation of the free and open-source FEM package FEniCS for the means of simulation and derivative computation. The resulting tool can then be used to compare and verify results of currently available FEM tools. This leads to new possibilities for further optimization of sensitivity for Inverse Problems in Piezoelectricity.

The Numerical Simulation of Phase Segregation in Electrode Particles of Lithium Ion Batteries

Fabian Castelli and Willy Dörfler
Karlsruhe Institute of Technology (KIT)

Lithium ion batteries are key technologies for mobile power devices, as for example in smartphones, laptops or electric vehicles. For the better understanding of the electrode materials (e. g. LiFePO4) we investigate the temporal evolution of the concentration profile of lithium ions in a single particle of the electrode material during the (dis-)charge process. Due to changes in the host material a separation into lithium rich and lithium poor phases is possible. This behavior can be modeled with the Cahn–Hilliard equation, see [1,2].

Our focus is on the numerical treatment of this forth-order PDE, in particular we are interested in efficient solvers for this problem. The main challenges are on the one hand the non-linearities due to the non-constant mobility as well as the logarithmic free energy density and on the other hand, depending on the electrode material, the almost sharp interface between the lithium rich and the lithium poor phase.

To solve the arising system numerically we employ a higher order standard finite element method ($p \geq 4$) together with an appropriate time integrator. However, for a full resolution of the three-dimensional spatial domain, respecting the very thin interface zone, a huge amount of degrees of freedom is necessary. We therefore use the matrix-free framework within the open-source finite element library deal.II [3], which can be run in parallel with MPI.

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Solving the partitioned heat equation using FEniCS and preCICE

Benjamin Rüth, Peter Meisrimel, Philipp Birken and Benjamin Uekermann
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FEniCS is a general finite element library with high flexibility and very broad functionality. It can be used to solve a wide range of problems from science and engineering using the finite element method; corresponding examples can be found, for example, in the FEniCS documentation. We want to investigate how FEniCS-based solvers can be used to solve coupled problems in a partitioned approach.

This talk explains how to solve the partitioned heat equation – a simple model problem for coupled problems. In our setup, two instances of FEniCS are used to solve the heat equation on two different domains that are non-overlapping. The two domains are only interacting with each other through a common coupling interface, where heat is exchanged. On the algorithmic level, the two domains are coupled at the interface via Dirichlet-Neumann coupling. The coupling and the communication between the two FEniCS-based solvers are realized with the coupling library preCICE. While the FEniCS-based heat equation solver and preCICE were already available, additional glue code (ad- apter) had to be developed to allow interfacing between FEniCS and preCICE. Note that all the software that is necessary for implementing the proposed setup is freely available as open-source. Beyond this study of a proof-of-concept kind, we plan to reuse components of this setup to perform more complex simulations - for example in the area of conjugate heat transfer. Here, the already existing FEniCS-based heat equation solver can be coupled with an appropriate flow solver using preCICE. Additionally, as FEniCS is a general finite element framework, other physical phenomena may be simulated to solve different coupled problems.

Adaptive equation simplification in fluid simulations

Harald Klimach and Sabine Roller
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In flow simulations we are often interested in a larger area of influence, with only smaller perturbations in a large fraction of the considered domain. In those parts it is reasonable to simplify the equations to solve and thereby reduce the computational costs.

In this contribution we are looking at a high-order discontinuous Galerkin scheme and a strategy to locally simplify the equations to solve in adaptation to the solution. With this approach it is possible to consider large domains, while resolving relevant physical effects where required.

The considered scheme is based on the orthogonal Legendre polynomial basis, which is especially effective for linear problems due to its diagonal mass matrix and efficiently computable stiffness matrix. However, for nonlinear terms the computational effort is drastically increased, due to the need for transformations to a nodal basis. Utilizing linearized equations results in accordingly large reductions of computational effort in this scheme. The discontinuous approach further allows for a local decision within elements. This is in turn desirable in parallel computations, as no further communication of synchronization is introduced by the adaptation of the equations to solve.

Efficient Solvers for Density Driven Flow Problems

Arne Nägel
Goethe University Frankfurt
(joint work with Peter Deuflhard and Gabriel Wittum)

When fresh water and brine mix, density effects give rise to many interesting physical effects such as fingering. On the socio-ecnomic level, groundwater salination in coastal areas is an important issue. Problems of this type are described by the problem class of density driven flow, and can be modelled by a transient system of non-linearly coupled PDEs. Developing efficient solvers for these systems is a delicate task, since it includes considering suitable schemes for (i) time integration, (ii) linearization, and (iii) multigrid solvers. In the work at hand, we present results for a linearly implicit method of extrapolation type (LIMEX). After a short theoretical analysis of the problem class, we introduce a suitable norm of estimating the error and discuss various approximations of the Jacobian. Their properties are explored and evaluated in various numerical experiments.

Gradient-based shape optimization of the TU Berlin stator with assembly constraints

Mladen Banovic
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In industrial workflows, geometric design process is driven by Computer Aided Design (CAD) systems. To involve them in a gradient-based shape optimization loop, one requires the calculation of shape sensitivities w.r.t. design parameters of the model to be optimized. So far, these sensitivities are not provided within commercial CAD systems, but calculated using inaccurate finite differences. Here, algorithmic differentiation (AD) is applied to the open-source CAD kernel Open CASCADE Technology (OCCT) to get the exact shape sensitivities. The OCCT kernel is differentiated by integrating the AD software tool ADOL-C (Automatic Differentiation by Overloading in C++) into its sources. Furthermore, it is coupled with a discrete adjoint CFD solver, thus providing a complete differentiated design chain at hand. This differentiated design chain is used to perform gradient-based optimization of the TU Berlin TurboLab stator test-case to minimize the total pressure loss. The stator blade's geometry is re-parametrized with differentiated OCCT, therefore allowing to handle assembly constraints during the optimization loop. One of such constraints specifies that the blade has to accommodate four cylinders used to mount the blade to its casing. The cylinder positioning is accomplished using the gradient information from the differentiated OCCT.

Weak C^n coupling for multi-patch Isogeometric Analysis

Stefan Schuß, Maik Dittmann, Barbara Wohlmuth, Sven Klinkel and Christian Hesch
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Isogeometric Analysis (IGA) has become a widely used methodology. The framework employs the same functions (NURBS) for the geometric design as well as for the analysis. It allows for the construction of finite element basis functions with adjustable continuity across the element boundaries, in contrast to classical Lagrangian basis functions, which are C^0 continuous. This enables the numerical treatment of higher-order problems, e.g. for Kirchhoff-Love shells and Cahn-Hilliard like formulations which require C^1 continuity or the phase-field crystal equation (Elder et. al. 2002) requiring C^2 continuity.

For complex geometries, multi-patch descriptions are necessary, since a single NURBS patch cannot depict arbitrary shapes. Moreover, flexible discretization schemes are employed on various patches to resolve local areas of interest, e.g. near corner singularities, locally large deformations or complex geometries with delicate structures. Along the common interfaces of the patches, domain decomposition techniques are in general used to couple the non-conforming discretizations. The framework of mortar methods, providing weak C^0 continuity at the interfaces, has been applied in recent years to IGA for domain decomposition problems and for contact mechanics. Further works rest on Nitsche's method providing weak C^1 continuity along patch interfaces.

The objective of this contribution is to present a novel methodology to enforce interface conditions preserving higher-order continuity across the interface. We show a natural extension of the mortar method to enforce weak C^n continuity. A particular challenge in realization of a mortar method is the evaluation of the interface integrals. Here it is common to use a quadrature rule based on a merged mesh, i.e. a mesh which respects the reduced smoothness of the master and slave functions at their respective lines. It has been shown, that the construction of the common mesh for higher order elements, especially in case of curved interfaces, results in a noteworthy error contribution. Alternatively one can use a purely slave-element based approach which can be considered as a weighted least square optimization. Moreover, we discuss the implementation of the respective coupling conditions by means of Lagrange multipliers and a basis modification approach. Concluding computational studies of solid systems, Kirchhoff-Love shells, an extended Cahn-Hilliard model and a phase-field crystal equation will finally demonstrate the versatile applicability of the presented method.

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Phase-field Methods on deforming surfaces

Christopher Zimmermann, Deepesh Toshniwal, Chad M. Landis, Thomas J.R. Hughes,
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Phase-field models for phase transitions and brittle fracture on deforming surface structures are presented. For the modeling of phase transitions, the partial differential equation (PDE) is the Cahn-Hilliard equation for curved surfaces, which can be derived from surface mass balance in the framework of irreversible thermodynamics [3]. For the modeling of fracture, the formulation is based on Griffith's theory. For the surface deformation, the PDE is the (vector-valued) Kirchhoff- Love thin shell equation. The mathematical problems are governed by two coupled fourth-order nonlinear PDEs that live on an evolving two-dimensional manifold.

The PDEs can be efficiently discretized using C1-continuous interpolations without derivative degrees-of-freedom. Structured NURBS, locally refinable (LR) NURBS [2] and unstructured spline spaces [1] with pointwise C1-continuity are utilized for these interpolations. The resulting finite element formulations are discretized in time by the generalized-alpha scheme with adaptive time-stepping, and they are fully linearized within a monolithic Newton-Raphson approach.

A curvilinear surface parameterization is used throughout the formulations to admit general surface shapes and deformations. The behavior of the coupled systems are illustrated by several numerical examples exhibiting phase transitions and dynamic brittle fracture on deforming surfaces.

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