Follow-Up-Workshop to TP

“Multiscale Problems: Algorithms, Numerical Analysis and Computation”

August 19 - 23, 2024

organized by
Susanne C. Brenner (Louisiana State University, Baton Rouge), Björn Engquist (University of Texas, Austin), Max Gunzburger (Florida State University, Tallahassee), Daniel Peterseim (Universität Augsburg), Marc A. Schweitzer (Universität Bonn)

Abstracts

Gabriel Barrenechea (University of Strathclyde)

The Multiscale Hybrid (Mixed) Finite Element Method

Abstract: In this talk I will present a review of the application of the Multiscale Hybrid Mixed (MHM) method to polygonal meshes. In the first part of the talk, based on the work [3], I will present the extension of the MHM method proposed in [1] to the case of polyhedral meshes. The method is based on a hybrid formulation, where static condensation is applied in order to perform upscaling, and solve a system of equations whose only online variables are the Lagrange multipliers in the inter-element boundaries. These Lagrange multipliers are the normal fluxes on the facets of the triangulation. While the continuous hybrid formulation leads to an H(div)-conforming flux, this property is lost at the fully discrete level. So, I will also present recent work on an H(div)-conforming reconstruction of the fluxes. This reconstruction is local, and thus can be done very cheaply. In addition, it presents, at zero cost, a fully computable a posteriori error estimator for the MHM method.
In the second part of the method I will review a recent variant of the MHM method, namely, the Multiscale Hybrid (MH) method, proposed in [2]. The fundamental difference with the MHM method lies on the definition of the Lagrange multipliers. The practical implication of this is that both the local problems to compute the basis functions, as well as the global problem, are elliptic, as opposed to the MHM method (and also other previous methods) where a mixed global problem is solved, and constrained local problems are solved to compute the local basis functions.
The work presented in this talk was done in collaboration with Antonio Tadeu A. Gomes (LNCC, Petropolis, Brazil), Fabrice Jaillet (Universite Lyon 1), Diego Paredes (Universidad de Concepción, Chile), and Frederic Valentin (LNCC, Brazil).

[1] R. Araya, Ch. Harder, D. Paredes, and F. Valentin, Multiscale hybrid mixed method. SIAM Journal on Numerical Analysis, **51** (6), 3505–3531, (2013).

[2] G.R. Barrenechea, A.T. Gomes, and D. Paredes, A multiscale hybrid method. Preprint hal-03907060v2, (2022).

[3] G.R. Barrenechea, F. Jaillet, D. Paredes, and F. Valentin, The multiscale hybrid mixed method in general polygonal meshes. Numerische Mathematik **145**(1), 197–237, (2020).

Carsten Carstensen (Humboldt-Universität zu Berlin)

Adaptive Least-Squares Methods

Abstract: The presentation shall discuss collective and separate marking algorithms for least-squares methods in a model examples. The part on general second order elliptic PDE is joint work with Ma Rui in preparation.

Eric Chung (The Chinese University of Hong Kong)

Multiscale methods for a class of high-contrast heterogeneous sign-changing problems

Abstract: The mathematical formulation of sign-changing problems involves a linear second-order partial differential equation in the divergence form, where the coefficient can assume positive and negative values in different subdomains. These problems find their physical background in negative-index metamaterials, either as inclusions embedded into common materials as the matrix or vice versa. In this paper, we propose a numerical method based on the constraint energy minimizing generalized multiscale finite element method (CEM-GMsFEM) specifically designed for sign-changing problems. The construction of auxiliary spaces in the original CEM-GMsFEM is tailored to accommodate the sign-changing setting. The numerical results demonstrate the effectiveness of the proposed method in handling sophisticated coefficient profiles and the robustness of coefficient contrast ratios. Under several technical assumptions and by applying the T-coercivity theory, we establish the inf-sup stability and provide an a priori error estimate for the proposed method. The research is partially supported by the Hong Kong RGC General Research Fund (Project: 14304021).

Matthias Deiml (University of Augsburg)

Quantum realization of the finite element method

Abstract: This talk presents a quantum algorithm for the solution of prototypical second-order linear elliptic partial differential equations discretized by d-linear finite elements on Cartesian grids of a bounded d-dimensional domain. An essential step in the construction is a BPX preconditioner, which transforms the linear system into a sufficiently well-conditioned one, making it amenable to quantum computation. We provide a constructive proof demonstrating that our quantum algorithm can compute suitable functionals of the solution to a given tolerance $\mathtt{tol}$ with a complexity linear in $\mathtt{tol}^{-1}$ for a fixed dimension d, neglecting logarithmic terms. This complexity is proportional to that of its one-dimensional counterpart and improves previous quantum algorithms by a factor of order $\mathtt{tol}^{-2}$. We also detail the design and implementation of a quantum circuit capable of executing our algorithm, and present simulator results that support the quantum feasibility of the finite element method in the near future, paving the way for quantum computing approaches to a wide range of PDE-related challenges.

Qiang Du (Columbia University)

Asymptotically compatible discretization of parameterized nonlocal models

Abstract: There has been much interest in nonlocal models associated with a horizon parameter δ, which characterizes the effective range of nonlocal interactions. Asymptotically compatible (AC) discretization offers robust numerical approximations for such nonlocal problems by demonstrating insensitivity to variations in the parameter δ. This presentation introduces an abstract framework for the design and mathematical analysis of AC schemes within the context of discretizing a broader class of parameterized problems. Furthermore, we explore their application to specific instances of nonlocal variational problems and nonlocal conservation laws.

Michael Feischl (TU Wien)

Stochastic collocation for dynamic micromagnetism

Abstract: We consider the stochastic Landau-Lifschitz-Gilbert equation, an SPDE model for dynamic micromagnetism. We first convert the problem to a (highly nonlinear) PDE with parametric coefficients using the Doss-Sussmann transform and the Lévy-Ciesielsky parametrization of the Brownian motion. We prove analytic regularity of the parameter- to-solution map and estimate its derivatives. These estimates are used to prove convergence rates for piecewise-polynomial sparse grid methods. Moreover, we propose novel time-stepping methods to solve the underlying deterministic equations.

Dietmar Gallistl (Universität Jena)

Computational multiscale methods for nondivergence-form elliptic partial differential equations

Abstract: This talk proposes novel computational multiscale methods for linear second-order elliptic partial differential equations in nondivergence-form with heterogeneous coefficients satisfying a Cordes condition. The construction follows the methodology of localized orthogonal decomposition (LOD) and provides operator-adapted coarse spaces by solving localized cell problems on a fine scale in the spirit of numerical homogenization. The degrees of freedom of the coarse spaces are related to nonconforming and mixed finite element methods for homogeneous problems. The error analysis of one exemplary approach shows that the favorable properties of the LOD methodology known from divergence-form PDEs, i.e., its applicability and accuracy beyond scale separation and periodicity, remain valid for problems in nondivergence-form.

Patrick Henning (Ruhr-University Bochum)

Multiscale approximations for the stationary Ginzburg-Landau equation

Abstract: In this presentation we discuss recent results on discrete minimizers of the Ginzburg-Landau energy in finite element and multiscale spaces. Special focus is given to the influence of the Ginzburg–Landau parameter κ. This parameter is of physical interest as large values can trigger the appearance of vortex lattices in superconductors. Since the vortices have to be resolved on sufficiently fine computational meshes, it is important to translate the size of κ into a mesh resolution condition, which can be done through error estimates that are explicit with respect to κ and the spatial mesh width h. We present corresponding analytical results for Lagrange finite elements and identify a previously unknown numerical pollution effect. Furthermore, we show how the approximation properties can be enhanced with multiscale techniques.

Frédéric Legoll (ENPC)

Multiscale Finite Element Methods for advection-diffusion and for reaction-diffusion problems

Abstract: The Multiscale Finite Element Method (MsFEM) is a finite element (FE) approach that allows to solve partial differential equations (PDEs) with highly oscillatory coefficients on a coarse mesh, i.e. a mesh with elements of size much larger than the characteristic scale of the heterogeneities. To do so, MsFEMs use pre-computed basis functions, adapted to the differential operator, thereby taking into account the small scales of the problem.
In the first part of the talk, we consider multiscale advection-diffusion problems in the convection-dominated regime. It is well-known that, when the PDE contains dominating advection terms, naive FE approximations lead to spurious oscillations, even in the absence of oscillatory coefficients. Stabilization techniques (such as SUPG) are to be adopted. In the multiscale context considered here, we discuss different ways to define the MsFEM basis functions, and how to combine the approach with stabilization-type methods. In particular, we show that methods using suitable bubble functions and Crouzeix-Raviart type boundary conditions for the local problems turn out to be very effective.
In the second part of the talk, we consider reaction-diffusion equations with oscillating coefficients. The problem is here phrased in terms of an eigenvalue equation. We make partial use of theoretical homogenization results in a periodic framework to guide our intuition in order to define appropriate MsFEM basis functions. Some efficient ways to handle the problem will be presented.
Joint work with Rutger Biezemans, Claude Le Bris, Alberic Lefort and Alexei Lozinski.

Guanglian Li (The University of Hong Kong)

Wavelet-based Edge Multiscale Finite Element Methods for Singularly Perturbed Convection-Diffusion Equations

Abstract: We propose a novel efficient and robust Wavelet-based Edge Multiscale Finite Element Method (WEMsFEM) to solve the singularly perturbed convection-diffusion equations. The main idea is to first establish a local splitting of the solution over a local region by a local bubble part and local Harmonic extension part, and then derive a global splitting by means of Partition of Unity. This facilitates a representation of the solution as a summation of a global bubble part and a global Harmonic extension part, where the first part can be computed locally in parallel. To approximate the second part, we construct an edge multiscale ansatz space locally with hierarchical bases as the local boundary data that has a guaranteed approximation rate without higher regularity requirement on the solution. The key innovation of this proposed WEMsFEM lies in a provable convergence rate with little restriction on the mesh size or the regularity of the solution. Its convergence rate with respect to the computational degree of freedom is rigorously analyzed, which is verified by extensive 2-d and 3-d numerical tests. This is a joint work with Eric Chung (CUHK, Hong Kong) and Shubin Fu (Eastern Institute of Technology, P.R. China).

Robert Lipton (Louisiana State University)

Dynamic brittle fracture as a well posed nonlocal initial value problem

Abstract: A nonlocal model for dynamic brittle damage is introduced consisting of two phases, one elastic and the other inelastic. Evolution from the elastic to the inelastic phase depends on material strength. Existence and uniqueness of the displacement-failure set pair follow from the initial value problem. The displacement-failure pair satisfies energy balance. The length of nonlocality ϵ is taken to

be small relative to the domain. The evolution provides an energy that interpolates between volume energy corresponding to elastic behavior and surface energy corresponding to failure. The deformation energy resulting in material failure over a region is a $d-1$ dimensional integral that is uniformly bounded as $\epsilon \to 0$. For fixed ϵ, the failure energy is nonzero for $d-1$ dimensional regions R associated with flat crack surfaces. This failure energy is the Griffith fracture energy given by the energy release rate multiplied by area of the crack. For flat cracks the nonlocal field theory is shown to recover a solution of Naiver's equation inside intact material adjacent to a propagating flat traction free crack in the limit of vanishing spatial nonlocality. For curved or more generally countably rectifiable cracks the failure energy is Griffith fracture energy but only in the $\epsilon = 0$ limit. The limit deformation is found to be in SBD. A numerical scheme is introduced and shown to be asymptotically compatible to the $\epsilon = 0$ limit.

Roland Maier (Karlsruher Institut für Technologie)

Achieving higher-order convergence rates in numerical homogenization

Abstract: This talk is about the construction of higher-order multiscale methods in the framework of the Localized Orthogonal Decomposition approach. We show how to obtain higher-order estimates in the elliptic setting without restrictive regularity assumptions on the domain, the coefficient, or the exact solution. Further, we discuss extensions to time-dependent problems, where appropriate adaptations are required. Numerical examples are presented to illustrate the theoretical findings.

Axel Målqvist (University of Gothenburg)

Numerical simulation of Timoshenko-beam models of fibre based materials

Abstract: We consider fibre based materials, modelled as spatial networks of connected one dimensional beams. In order to simulate the elastic properties of such materials we use the Timoshenko beam model with rigid joints. The resulting systems of equations are notoriously ill-conditioned. We therefore introduce a subspace decomposition technique and derive an efficient and reliable preconditioner for the arising linear system of equations. The target application is simulation of the mechanical behaviour of paperboard (tensile and bending strength). The work has been done in collaboration with Fraunhofer Chalmers Centre.

Mario Ohlberger (University of Münster)

Localized model order reduction for parameter optimization with multiscale PDE constraints

Abstract: Model order reduction for parameterized partial differential equations is a very active research area that has seen tremendous development in recent years from both theoretical and application perspectives. A particular promising approach is the reduced basis method that relies on the approximation of the solution manifold of a parameterized system by tailored low dimensional approximation spaces that are spanned from suitably selected particular solutions, called snapshots. With speedups that can reach several orders of magnitude, reduced basis methods enable high fidelity real-time simulations for certain problem classes and dramatically reduce the computational costs in many-query applications. While the "online efficiency" of these model reduction methods is very convincing for problems with a rapid decay of the Kolmogorov n-width, there are still major drawbacks and limitations. Most importantly, the construction of the reduced system in a so called "offline phase" is extremely CPU-time and memory consuming for large scale or multiscale systems. For practical

applications, it is thus necessary to derive model reduction techniques that do not rely on a classical offline/online splitting but allow for more flexibility in the usage of computational resources.
In this talk we focus on both, localized training and on-the-fly enrichment strategies [1] for localized model order reduction of multiscale problems in the context of PDE constrained optimization [3, 2]. The approaches are based on the reduced basis - trust region framework, recently developed in [5, 4]. Concepts of rigorous certification and convergence will be presented, as well as numerical experiments that demonstrate the efficiency of the proposed approaches.

[1] Keil T., Ohlberger M., Schindler F., Schleuß J. Local training and enrichment based on a residual localization strategy. arXiv:2404.16537, 2024. doi: 10.48550/arXiv.2404.16537.

[2] Keil T., Ohlberger M.. A relaxed localized trust-region reduced basis approach for optimization of multiscale problems. ESAIM Math. Model. Numer. Anal. 58 (1): 79–105, 2024. doi:10.1051/m2an/2023089.

[3] Keil T., Ohlberger M., Schindler F. Adaptive Localized Reduced Basis Methods for Large Scale PDE-constrained Optimization. In Large-Scale Scientific Computations, edited by Lirkov, I; Margenov, S, 108–116. Cham: Springer Nature, 2024. doi: 10.1007/978-3-031-56208-2_10.

[4] Banholzer S, Keil T, Mechelli L, Ohlberger M, Schindler F, Volkwein S. An adaptive projected Newton non-conforming dual approach for trust-region reduced basis approximation of PDE-constrained parameter optimization. Pure Appl. Funct. Anal. 7(5): 1561–1596, 2022.

[5] T. Keil, L. Mechelli, M. Ohlberger, F. Schindler, S. Volkwein. A non-conforming dual approach for adaptive Trust-Region Reduced Basis approximation of PDE-constrained optimization. ESAIM: Math. Model. and Num. Anal. (M2AN), 55 (3): 1239–1269, 2021. doi: 10.1051/m2an/2021019.

Houman Owhadi (Caltech)

Bridging Scales with Gaussian Processes: Applications to Fluid Dynamics and Nonlinear PDEs

Abstract: This talk presents two examples of applying Gaussian Processes (GP) and Kernel Methods to bridge scales in nonlinear partial differential equations (PDEs). The first example demonstrates how closure can be achieved for the Navier-Stokes/Euler equations by incorporating known physics—such as incompressibility, fluid-structure boundary conditions, the Richardson cascade, and velocity-increment power laws—into the underlying kernel. The second example, a joint work with Yifan Chen and Florian Schäfer, illustrates how near-linear complexity meshless solvers can be obtained for nonlinear PDEs by combining GP/Kernel solvers with sparse Cholesky factorization techniques.

Anna Persson (Uppsala University)

Numerical investigation of vortex formation in Bose-Einstein condensates

Abstract: Bose-Einstein condensates are formed when a gas of Bosons are cooled to ultra-low temperatures. At this point, most of the Bosons occupy the same quantum state and behave like one giant “macro particle”. This is classified as a new state of matter, where some quantum mechanical phenomena can be observed macroscopically. One such phenomenon is superfluidity, which describes

a flow without inner friction. When rotating a superfluid vortex patterns typically occur, which will be the focus in this talk.

We numerically investigate these vortex patterns in ground states of Bose-Einstein condensates using classical finite elements. Similar to a multiscale setting, these are challenging to model because the mesh width needs to be sufficiently small to capture the correct vortex behavior. Increasing the rotational speed typically means more vortices and an even smaller mesh size is needed. However, the precise mesh size needed to achieve reliable approximations has so far been unknown. Our aim is to identify an indicator that can serve as an estimate for this threshold, i.e., the mesh size that is required to achieve accurate approximations.

Robert Scheichl (Heidelberg University)

Multiscale-Spectral Generalized Finite Elements: Efficient Localized Model Order Reduction

Abstract: In this talk, I will present an efficient generalized finite element method with optimal (multiscale spectral) local approximation spaces (MS-GFEM) for PDEs with heterogeneous coefficients. In practice, the local approximation spaces are constructed from local eigenproblems solved on some sufficiently fine finite element mesh with mesh size h. In this work, we will provide rigorous error estimates for the fully discrete method. The error bound of the discrete MS-GFEM approximation is proved to converge as h tends to 0 towards that of the continuous MS-GFEM approximation, which was shown to decay nearly exponentially in previous works. Moreover, even for fixed mesh size h, a nearly exponential rate of convergence of the local approximation errors with respect to the dimension of the local spaces is established. The method can also be used as an effective preconditioner in an iterative solver with a 'tuneable' convergence rate. On the practical side, an efficient and accurate method for solving the discrete eigenvalue problems is proposed by incorporating the discrete-harmonic constraint directly into the eigenproblem via a Lagrange multiplier approach. Numerical experiments that confirm the theoretical results and demonstrate the effectiveness of the method are presented for a second-order elliptic problem, for a large-scale problem of linear elasticity in composite aerospace applications and for a high-frequency heterogeneous Helmholtz problem. Even in this last example, a quasi-optimal and nearly exponential (wavenumber-explicit) global convergence of the method can be theoretically proved, provided the size of the subdomains is O(1/k) (where k is the wavenumber). A two-level restricted additive Schwarz preconditioner with MS-GFEM coarse space can be shown to lead to a tuneable GMRES convergence rate with a very mild dependence of the coarse space size on the wavenumber k.

Li-yeng Sung (Louisiana State University)

DD-LOD

Abstract: DD-LOD is a multiscale finite element method for problems with rough coefficients that is based on a domain decomposition approach to the localized orthogonal decomposition methodology. I will present the construction and analysis of DD-LOD for elliptic boundary value problems with rough coefficients that only require basic knowledge of finite element methods, domain decomposition methods and numerical linear algebra. An application to elliptic optimal control problems will also be discussed.

Barbara Verfürth (Universität Bonn)

Numerical multiscale methods for nonlinear and randomly perturbed problems

Abstract: We consider the construction of problem-adapted multiscale basis functions in the spirit of Localized Orthogonal Decomposition (LOD) methods. These methods are very efficient for linear problems that need to solved many times with the same multiscale coefficient. In this talk, we address two situations that deviate from this setting, namely nonlinear problems and problems with multiscale coefficients with defects, modeled by random perturbations. For nonlinear problems, we discuss and analyze the construction of linearized multiscale basis functions. For random defects, we present and offline-online strategy that allows for a rapid computation of solutions for any realization of the multiscale coefficient.

Lei Zhang (Shanghai Jiao Tong University)

Quantum algorithms for multiscale PDEs

Abstract: Quantum computing has garnered considerable interest in the past few years owing to its potential to offer up to exponential acceleration compared to classical computational methods. In this talk, I will first introduce the Schrödingerisation method by Jin, Liu and Yu [1], followed by its concrete quantum circuit implementation [2]. As examples, I will demonstrate applications to linear multiscale PDEs [3] and multiscale Hamilton-Jacobi equations [4].

[1] Shi Jin, Nana Liu and Yue Yu. Quantum simulation of partial differential equations: Applications and detailed analysis. Phys. Rev. A 108 (2023), no. 3, Paper No. 032603.

[2] Junpeng Hu, Shi Jin, Nana Liu, Lei Zhang. Quantum Circuits for partial differential equations via Schrödingerisation. arxiv:2403.10032.

[3] Junpeng Hu, Shi Jin, Lei Zhang. Quantum algorithms for multiscale partial differential equations. (SIAM) Multiscale Model. Simulation, to appear, arxiv:2304.06902.

[4] Kezhen Wang, Lei Zhang. Quantum Algorithms for Multiscale Hamilton-Jacobi Equation. preprint.
