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Editorial

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Computational Methods in Applied Mathematics (CMAM 2022 Conference, Part 1)

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Abstract: This paper introduces the contents of the first of two special issues associated with the 9th International Conference on Computational Methods in Applied Mathematics, which took place from August 29 to September 2, 2022 in Vienna. It comments on the topics and highlights of all twelve papers of the special issue.

1 Introduction

Computational methods are fundamental tools to numerically investigate the behavior of complex systems and thus advance knowledge in a variety of scientific disciplines. The aim for more and more efficient and sophisticated computational tools cannot disregard the need of a rigorous mathematical analysis of any developed numerical method, as this is the only way to fully understand its properties and the limitations of its applicability, and to certify its reliability.

In this context, the biennial international CMAM conferences on Computational Methods in Applied Mathematics, organized under the aegis of this journal, are focused on various aspects of mathematical modeling and numerical analysis and aim at fostering cooperation between researchers working in the area of theoretical numerical analysis and applications to modeling, simulation, and scientific computing. The 9th edition of the conference (CMAM 2022) took place from August 29 to September 2, 2022 at TU Wien (Vienna, Austria), and featured a rich scientific program consisting of overall 149 presentations, 15 plenary talks and 134 contributed talks, organized in 21 thematic minisymposia.

This CMAM special issue, the first one of overall two issues dedicated to the conference, collects twelve selected works from conference participants. The central theme is the numerical analysis of partial differential equations (PDEs), with a particular focus on wave propagation problems [3, 7, 12], preconditioning [8] and implementational [1] aspects, low regularity problems [4], computational fluid dynamics [5], eigenvalue problems [11], nonstandard applications [2], stochastic PDEs [10], as well as on the modeling and numerical analysis of PDEs in quantum physics [6, 9].

2 Wave Propagation

Wave propagation in complex media is a central topic of numerical analysis as it poses several interesting challenges to any numerical solver. Both forward and inverse problems are tackled in this special issue. The work [3] delves into the dynamics of wave propagation in media characterized by high-contrast coefficients, addressing both one-dimensional (1D) and higher-dimensional structures. Initial discussions focus on periodic structures, where established homogenization results for low-contrast scenarios are revisited, and a novel asymptotic

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result for high-contrast situations is introduced. The complexity of extending these results to higher dimensions is thoroughly examined. Moving beyond periodicity, the research explores the approximation of wave propagation problems using the Localized Orthogonal Decomposition (LOD) method, extending its application from low-contrast, stationary settings to high-contrast cases.

An inverse wave propagation problem is considered in the work [7], which investigates vibro-acoustography, focusing on proving the well-posedness of forward model equations and the convergence of a frozen Newton method for solving the inverse problem. The study aims at reconstructing sound speed and nonlinearity parameter from boundary measurement data, a challenge due to the complexities of boundary observations. Utilizing theoretical frameworks from previous works, it establishes the forward problem's well-posedness and tackles the inverse problem by combining an ill-posed linear and a well-posed nonlinear problem. The paper successfully demonstrates the convergence of the Newton method and thus contributes to the modeling and analysis of vibro-acoustography.

When it comes to *a posteriori* error estimation, wave problems are particularly difficult as they usually do not posses a nice inf-sup structure which is the basis for many error estimators. The work [12] introduces a multiharmonic approach to analyze and derive functional-type *a posteriori* estimates for a distributed eddy current optimal control problem and its corresponding state equation within a time-periodic framework. While eddy current problems are a simplification of the full Maxwell equation, they offer more mathematical tools to establish inf-sup and sup-sup conditions and to prove the existence and uniqueness of the solution for both the optimality system and the forward problem through a weak space-time variational formulation. Leveraging these conditions, the paper provides guaranteed, precise, and fully calculable error bounds for both the optimal control problem and the forward problem as part of the functional-type *a posteriori* estimation methodology. This paper also showcases the initial computational findings based on these derived estimates.

3 High-dimensional FEM, Space-time, and Time-stepping

Space-time methods enjoy a surge of mathematical interest in the recent years as they offer attractive analytical and practical advantages such as: increased efficiency through parallel implementation, more flexible discretization, and often a better control of inf-sup properties of the underlying equations.

In the work [8], the authors focus on preconditioning of square block matrices (PRESB) for space-time finite element methods for discretizing parabolic problems, including the heat equation and the approximation of the Maxwell system for eddy currents. The discretization employs a space-time tensor product mesh tailored to the systems discussed and fast diagonalization methods are used to decouple the resulting linear systems such that they can be solved concurrently in time. Numerical results in a four-dimensional space-time domain are presented to back the theoretical analysis.

Space-time methods require the discretization of one more dimension than classical time-stepping methods. Hence, the need for efficient implementations of high-dimensional FEM is higher than ever. The work [1] propose a Matlab implementation of FEM for solving a general linear second-order elliptic partial differential equation (PDE) with mixed Dirichlet–Neumann boundary conditions in subsets of $\mathbb{R}^d$ for any dimension d. The authors use the lowest-order (P1) conforming finite element method on a grid created from simplicial subdivisions of a set of covering cubes. The implementation also includes an adaptive algorithm designed to refine the grid locally via iterated newest vertex bisection steered by *a posteriori* error estimates. The implementation of FEM, error estimators, and grid refinement is detailed for Matlab, with considerations for portability to other vectorized languages like Julia. Particular focus is put on the efficiency and challenges of implementing FEM and mesh refinement in higher dimensions within vectorized programming environments.

When it comes to stochastic partial differential equations (SPDEs), classical time-stepping methods dominate the literature. The work [10] explores the weak convergence of the Rosenbrock semi-implicit method when applied to semilinear SPDEs with additive noise, particularly focusing on equations where the nonlinear component is more significant than the linear one. Such SPDEs often cause standard numerical schemes to lose stability. While exponential Rosenbrock and Rosenbrock-type methods have been shown to be effective for these equations, only their strong convergence has primarily been examined until now. This paper presents an analysis of weak convergence for these methods, revealing that the weak convergence rate is double that of the strong convergence rate. Importantly, the analysis forges a path without relying on Malliavin calculus, instead using the Kolmogorov equation and leveraging the smoothing effects of the resolvent operator inherent in the Rosenbrock semi-implicit method.

Finally, the work [5] proposes and analyzes a numerical scheme for Bingham flows with variable density, which are described by Navier–Stokes-type equations with a particular fluid-stress tensor. There are several challenges: First, one has to deal with a numerically involved transport equation that describes the mass conservation, and second, one has to deal with the fact that the stress-strain relation is nonlinear and nonsmooth. The mass conservation equation is handled by using dG methods, the nonsmoothness of the stress-strain relation is treated with Huber regularization, and the nonlinearity by a semismooth Newton method.

4 Low-regularity, Eigenvalues, and Non-standard Applications of Numerical Analysis

Low data regularity poses an extraordinary challenge for many numerical methods and is therefore often overlooked in numerical analysis. The work [4] examines variations of the mixed finite element method (mixed FEM) and the first-order system least-squares finite element (FOSLS) approach for solving the Poisson problem by incorporating a regularization that accommodates H^{-1}-loads. The main result states that any bounded H^{-1} projector onto piecewise constants can serve as the basis for this regularization, ensuring quasi-optimality for the lowest-order mixed FEM and FOSLS in weaker norms. The paper provides construction methods for such projectors, including one derived from the adjoint of a weighted Clément quasi-interpolator, which is shown to possess second-order approximation capabilities. Additionally, it reveals that the adapted mixed method achieves optimal convergence rates for postprocessed solutions under minimal regularity conditions, a performance not mirrored by the lowest-order mixed FEM without regularization.

The work [11] analyzes the use of the conforming finite element method (FEM) for the eigenvalue problem associated with the Steklov differential operator, aimed at offering reliable lower bounds for the eigenvalues. These lower bounds are derived using *a priori* error estimations for FEM solutions to non-homogeneous Neumann boundary value problems, achieved through the construction of hypercircles for the relevant FEM spaces and boundary conditions.

The mathematical tools of numerical analysis often prove to be useful in nonstandard applications. One example is the work [2], which adapts Binev's optimal tree refinement algorithm and applies it to image compression inspired by JPEG. Instead of using an 8×8 pixel grid, as is standard for JPEG compression, the algorithm generates an optimal subdivision of the source image and applies JPEG compression techniques on all the subimages. The main difficulty is the fact that images in general do not satisfy the assumptions for optimal tree refinement. The authors show, however, that a tiny random perturbation of the image allows the theory developed by Binev to be applied with high probability. Numerical experiments confirm a significant improvement in storage size compared to standard JPEG.

5 PDEs in Quantum Physics

The work [9] introduces the self-consistent Pauli equation as a semi-relativistic model designed to describe charged spin-$\frac{1}{2}$ particles interacting with the electromagnetic field. This equation is derived as an approximation of the fully relativistic Dirac equation, contrasting with the Dirac–Maxwell equation that naturally incorporates spin and magnetic fields. In non-relativistic scenarios, the Schrödinger–Poisson equation, which omits spin and magnetic field effects and focusses solely on electric field interaction, is typically used. The authors propose the Pauli–Poisson equation as an extension that emerges from the mean field limit $N \to \infty$ of the linear N-body

Pauli equation with Coulomb interaction, emphasizing the importance of considering the fermionic nature of particles. Furthermore, the paper discusses the semiclassical limit of the Pauli–Poisson equation to the Vlasov equation with Lorentz force, coupled to the Poisson equation, through the Wigner method.

The work [6] examines a numerical approach for solving the time-dependent linear Pauli equation across three spatial dimensions. The Pauli equation, which extends the Schrödinger equation to semi-relativistic scenarios for 2-spinors, incorporates effects of both magnetic fields and spin – an aspect not covered in earlier numerical analyses of the linear magnetic Schrödinger equation. Employing a quartet of operator splits for temporal analysis, we establish the method's stability and convergence, offering error assessments and meshing guidelines specifically for scenarios with constant electromagnetic potentials. This work thus broadens the scope of existing findings related to the magnetic Schrödinger equation.

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