Technische Universität Graz

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20. Workshop on

Fast Boundary Element Methods in Industrial Applications

Söllerhaus, 13.–16.10.2022

U. Langer, M. Schanz, O. Steinbach, W. L. Wendland (eds.)

Berichte aus dem
Institut für Angewandte Mathematik

Book of Abstracts 2022/5

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Technische Universität Graz
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Program

Thursday, October 13, 2022	
15.00	Coffee
16.30–16.45	Opening
16.45–17.15	S. Hardesty (Albuquerque) Approximate shape gradients with boundary element methods
17.15–17.45	M. Ferrari (Torino) Development on the stability of the coupled finite element and one-equation boundary element methods
17.45–18.15	I. Labarca (Zürich) Volume integral equations and single-trace formulations for acoustic wave scattering in an inhomogeneous medium
18.30	Dinner
Friday, October 14, 2022	
8.00–9.00	Breakfast
9.00–9.30	B. Stamm (Stuttgart) Fast numerical methods for integral equation-based continuum solvation models
9.30–10.00	M. Hassan (Paris) Numerical analysis of integral equations for N-body polarisable electrostatics
10.00–10.30	H. Harbrecht (Basel) Boundary integral operators for the heat equation in time-dependent domains
10.30–11.00	Break
11.00–11.30	G. Of (Graz) A time-adaptive fast multipole boundary element method for the heat equation
11.30–12.00	D. Lukas (Ostrava) Preconditioned Galerkin BEM for the 3d Laplace equation accelerated on a GPU
12.00	Lunch
15.00	Coffee
15.30–16.00	C. Özdemir (Graz) A 3D finite element-boundary element coupling method in time domain
16.00–16.30	D. Hoonhout (Delft) Stability of space-time boundary element methods for 1D wave problems
16.30–17.00	R. Löscher (Graz) Adaptive FEM for distributed optimal control problems subject to the wave equation with variable energy regularization
17.00–17.30	Break
17.30–18.00	M. Wolfmayr (Jyväskylä) A posteriori error estimates for the optimal control of time-periodic eddy current problems
18.00–18.30	M. Liebsch (Geneve) Boundary element methods for the field reconstruction in accelerator magnets
18.30	Dinner

Saturday, October 15, 2022	
8.00–9.00	Breakfast
9.00–9.30	E. P. Stephan (Hannover) High-order finite element methods for the fractional Laplacian: graded meshes and hp
9.30–10.00	H. Gimperlein (Innsbruck) Time-domain boundary elements for 2d elastodynamics
10.00–10.30	C. Urzua–Torres (Delft) Calderón preconditioners for boundary elements on multi-screens
10.30–11.00	Break
11.00–11.30	J. Rivero (Albuquerque) On the accuracy of the test integral on EFIE
11.30–12.00	E. Schultz (Zürich) Boundary integral exterior calculus
12.00	Lunch
13.00–18.00	Hiking Tour
18.30	Dinner
Sunday, October 16, 2022	
8.00–9.00	Breakfast
9.00–9.30	M. Schanz (Graz) Application of 3D-ACA in time domain boundary element method
9.30–10.00	O. Steinbach (Graz) Space-time finite and boundary element methods for a parabolic-elliptic interface problem with rotating subdomains

21. Söllerhaus Workshop on
Fast Boundary Element Methods in Industrial Applications
28.9.–1.10.2023

Development on the stability of the coupled finite element and one-equation boundary element methods

Matteo Ferrari

Dipartimento di Scienze Matematiche, Politecnico di Torino, Italy

We consider the non-symmetric coupling of finite and boundary elements to solve second order uniform elliptic partial differential equations defined in unbounded domains. We present a novel condition that ensures the ellipticity of the associated bilinear form, keeping track of its dependence on the linear combination of coefficients of the interior domain equation with the boundary integral one. We show that an optimal ellipticity condition, relating the minimal eigenvalue of the diffusion matrix to the contraction constant of the shifted double-layer integral operator, is guaranteed by choosing a particular linear combination. This latter condition is always satisfed when the interface is a circle. These results generalize those obtained in Of and Steinbach [1] and [2], and in Steinbach [3] where the simple sum of the two coupling equations has been considered. Numerical examples confirm the theoretical results on the sharpness of the presented estimates.

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[2] G. Of, O. Steinbach: On the ellipticity of coupled finite element and one-equation boundary element methods for boundary value problems. Numer. Math. 127 (2014) 567–593.

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Time-domain boundary elements for 2d elastodynamics

H. Gimperlein
Universität Innsbruck, Austria

We discuss recent and on-going progress for boundary element methods in linear elastodynamics, with a focus on locally refined meshes and two dimensions. Solutions of the time-dependent Lamé equations exhibit singularities due to geometry (corners), mixed or nonlinear (contact) boundary conditions. We discuss well-posed formulations for such problems as well as their approximation on locally refined meshes by h- and hp-versions. A priori and a posteriori estimates for the approximation error are presented for both the weakly singular and the hypersingular integral equations. The a posteriori estimates lead to an adaptive mesh refinement procedure. Numerical experiments illustrate the theoretical results. (joint with A. Aimi, G. Di Credico, C. Guardasoni and E. P. Stephan)

Boundary integral operators for the heat equation in time-dependent domains

Rahel Brügger, Helmut Harbrecht, Johannes Tausch

This talk provides a functional analytical framework for boundary integral equations of the heat equation in time-dependent domains. More specifically, we consider a non-cylindrical domain in space-time that is the C^2-diffeomorphic image of a cylinder, i.e., the tensor product of a time interval and a fixed domain in space. On the non-cylindrical domain, we introduce Sobolev spaces, trace lemmata and provide the mapping properties of the layer operators. Here it is critical that the Neumann trace requires a correction term for the normal velocity of the moving boundary. Therefore, one has to analyze the situation carefully.

Approximate shape gradients with boundary element methods

Sean Hardesty
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Approximate shape gradients with finite element methods were carefully studied by Hiptmair, Paganini and Sargheini in 2015. They showed that for piecewise-linear elements, the volume method is $\mathcal{O}(h^2)$, whereas the boundary method is $\mathcal{O}(h)$. With boundary element methods, there is no direct analogue to the volume method since everything lives on the boundary. However, there are two distinct approaches: the ëxtractionmethod of Schwab and Wendland, and the tensor ACA method that I developed with Mario Bebendorf. In this talk, I'd like to give these two methods some additional context and ask the question: how do their numerical properties compare?

Numerical analysis of integral equations for N-body polarisable electrostatics

M. Hassan[1], B. Stamm[2]
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[2]University of Stuttgart, Germany

We consider the problem of calculating the electrostatic interaction between N dielectric spherical particles embedded in a polarisable continuum, undergoing mutual polarisation. In order to tackle this problem, a possible approach is to express the sought-after surface electrostatic potential as the solution of a boundary integral equation (BIE) of the second kind, and employ a Galerkin discretisation based on local spherical harmonics expansions on each sphere. Efficient computational scaling can then be achieved by making use of the Fast Multipole Method (FMM).

The current talk will present results on the numerical analysis of such an algorithm with the aim of proving that the method is linear scaling in accuracy with respect to the number of spheres N, i.e., in order to compute physical quantities of interest *up to a given relative error*, the computational cost of the algorithm scales as $\mathcal{O}(N)$. In contrast with fixed-domain problems, for which the behaviour of second-kind BIEs in relation to the discretisation parameter is relatively well understood, our analysis focuses on the properties of second kind BIEs when the size of the domain (expressed by the number of spherical particles N) changes. We show that for such problems, it is possible to derive N-independent continuity and (discrete) inf-sup constants for the second-kind BIE. This allows us to derive relative error estimates for several quantities of interest that do not explicitly depend on N and to demonstrate exponential convergence under suitable regularity assumptions. We also analyse the conditioning of the solution matrix associated with the Galerkin discretisation, and show that the maximum number of Krylov solver iterations required to obtain a solution (up to a given tolerance) is also independent of N. Combining this analysis with an FMM implementation that allows computing matrix vector products in $\mathcal{O}(N)$ yields the required linear scaling in accuracy.

Stability of space-time boundary element methods for 1D wave problems

D. Hoonhout, C. Urzúa–Torres
Delft University of Technology, Delft, Netherlands

We consider stable space-time boundary element methods (BEM) for transient wave problems with prescribed Dirichlet data and zero initial conditions. For this, we use the formulations proposed in [1], for which the related boundary integral equations have continuity and inf-sup conditions in trace spaces of the same regularity. In [2], the stability of space-time BEM in 1D has already been shown with the used of the modified Hilbert transform [3].

In this talk, we study when standard low-order BEM leads to discrete inf-sup conditions for both first kind and indirect second kind boundary integral equations (BIE) in 1D. Moreover, when the discrete inf-sup condition is violated, we present simple regularisations. Although additional numerical error is introduced, the use of these regularisations recovers unique solvability, preserves the expected asymptotic convergence rate, and is computationally considerably cheaper than the modified Hilbert transform. These results give us further understanding related to unstable behaviour sometimes observed in 1D, and pave the way towards computationally cheaper stable space-time BEM for the wave equation in higher dimensional problems.

References

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Volume integral equations and single-trace formulations for acoustic wave scattering in an inhomogeneous medium

Ignacio Labarca
ETH Zürich

We study frequency domain acoustic scattering at a bounded, penetrable, and inhomogeneous obstacle. By defining constant reference coefficients, a representation formula for the pressure field is derived. It contains a volume integral operator, related to the one in the Lippmann–Schwinger equation. Besides, it features integral operators defined on the boundary of the obstacle and closely related to boundary integral equations of single-trace formulation (STF) for transmission problems with piecewise constant coefficients. We show well-posedness of the continuous variational formulation and asymptotic convergence of Galerkin discretizations. Numerical experiments in 2D validate our expected convergence rates.

Boundary element methods for the field reconstruction in accelerator magnets

Melvin Liebsch[1], Stephan Russenschuck[1], Stefan Kurz[2]
[1]CERN, European Organization for Nuclear Research, Geneva, Switzerland
[2]University of Jyväskylä, Jyväskylä, Finland

Magnetic fields generated by normal or superconducting electromagnets are used to guide and focus particle beams in storage rings, synchrotron light sources, mass spectrometers, and beamlines for radiotherapy. The accurate determination of the static magnetic field by measurement is critical for the prediction of the particle beam trajectory and hence the design of the accelerator complex. In this context, state-of-the-art numerical field computation makes use of boundary element methods (BEM) to express the magnetic field. This enables the accurate computation of higher-order derivatives and local expansions of magnetic potentials used in efficient numerical codes for particle tracking [1,2].

In this presentation, some use-cases for BEM in the field of magnetic measurements are presented. Two dimensional formulations are used to express the integrated fields in cases where the magnet bore is not cylindrical. This enables the accurate reconstruction of fields in arbitrarily shaped domains and requires only the determination of the Dirichlet or Neumann data by measurement. Field measurements along the domain boundary are achieved by single stretched wire measurement systems [3].

There are circumstances where it is infeasible to bring the sensor towards the boundary of the domain of interest. This is due to the dimension of the sensor housing and supporting structure, especially for measurements of three dimensional field distributions. In these cases, the boundary data needs to be inferred from measurements within the domain, yielding potentially ill-posed inverse problems.

As a regularization measure we follow a Bayesian approach and we construct a Gaussian prior from a numerical field simulation. Moreover, an iterative learning algorithm is proposed that uses the spatial distribution of uncertainty in the predicted field to explore the spatial domain. The measurement uncertainty can be propagated successively to the boundary data, the magnetic field and also to beam related quantities. We provide results obtained from real measurement data of a curved dipole magnet using a Hall probe mapper system.

References

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Adaptive FEM for distributed optimal control problems subject to the wave equation with variable energy regularization

Richard Löscher, Olaf Steinbach
TU Graz, Austria

We present a space-time finite element approach for a distributed optimal control problem for the wave equation. In particular, we are interested in bounding the L^2-norm between the computed solution and the target function with respect to the relaxation parameter, the regularity of the target and the approximation property of our finite element space. An abstract framework is outlined to rigorously analyze the problem, which will lead to a so-called energy regularization. We give numerical examples, validating the theory and comparing the energy regularization with the, more standard, L^2-regularization. Furthermore, we propose an adaptive refinement strategy. Moreover, we briefly discuss the direct solution of the wave equation. First, by means of a saddle point formulation in space-time, which requires a discrete inf-sup condition. Second, by introducing a stabilization, circumventing the inf-sup and CFL-condition, which can be analyzed with the tools we saw for the optimal control problem.
This talk is based on joint work with U. Langer, O. Steinbach and H. Yang.

References

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Preconditioned Galerkin BEM for the 3d Laplace equation accelerated on a GPU

D. Lukáš
TU VŠB Ostrava, Czech Republic

We present a matrix-free implementation of the Galerkin BEM for the 3d Laplace equation where the intensive numerical quadratures within both the system matrix and an operator preconditioner are implemented on GPUs. We discuss implementation details of Sauter-Erichssen-Schwab quadratures. Further, an extension of the 2-dimensional operator preconditioner of Steinbach and Wendland, published in 1998, to three dimensions is suggested. We study and document numerically its robustness with respect to the discretization step. In terms of the overall computational time the GPU simulations outperform the CPU ones by factors of 10 to 50, while allowing to solve densely populated systems up to 1e5 degrees of freedom on a laptop with a single GPU within an hour.

A time-adaptive fast multipole boundary element method for the heat equation

M. Merta[2], G. Of[1], R. Watschinger[1], J. Zapletal[2]
[1]TU Graz, Austria, [2]TU VŠB Ostrava, Czech Republic

We consider a space-time boundary element method for the solution of initial boundary value problems of the heat equation in three spatial dimensions. In particular we deal with tensor product meshes with adaptive decompostions of the considered time interval. We present a related new time-adaptive version of the fast mutipole method and apply shared and distributed memory parallelization with respect to space and time. This combination enables fast computations of the space-time method. Finally, we present numerical experiments that demonstrate the benefits of the new method.

References

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A 3D finite element-boundary element coupling method in time domain

H. Gimperlein[1], C. Özdemir[2], E. P. Stephan[3]
[1]Universität Innsbruck, Austria
[2]TU Graz, Austria
[3]Leibniz Universität Hannover, Germany

We consider a transmission problem, where the homogeneous wave equation on a bounded Lipschitz domain Ω is coupled with another homogeneous wave equation on the exterior $\Omega^c = \mathbb{R}^3 \backslash \Omega$. We derive a variational formulation based on the Poincare-Steklov operator. We use a tensor product ansatz and derive an efficient time stepping scheme, precisely the Marching-on-in time (MOT) scheme. Finally, we conclude the presentation with different numerical examples.

On the accuracy of the test integral on EFIE

Javier Rivero[1], Francesca Vipiana[2], Donald. R. Wilton[3], William A. Johnson[4]
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[3]University of Houston, Houston, TX USA
[4]Private Consultant, Jemez Springs, NM, USA

An accurate solution of electromagnetics problems using surface integral equation formulations needs the accurate and cost-effective numerical evaluation of double surface reaction integrals. There is a lot of literature written on how to deal with the source integral and it is widely accepted that once this integral is smoothed, the test integral should be easy to integrate numerically. However, that affirmation is not always true. Recently, some papers have considered the possibility of treating the double surface integral as a whole [1-2]. These approaches demonstrate good accuracy, but their implementation is non-trivial and may require extensive modification of an existing code.

Here, we focus on the numerical evaluation of the outer test integral. To handle this integral we will use the definition of the vertex functions proposed in [3]. We propose a radial-angular scheme for each vertex function, allowing us to evaluate the integrals of the vertex functions very efficiently, since, as can be seen in [3], the vertex functions have a linear radial dependence. The approach is compared to standard Gauss-triangle schemes to demonstrate its effectiveness.

References

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Application of 3D-ACA in time domain boundary element method

A. M. Haider, M. Schanz
TU Graz, Austria

The acoustic wave equation is solved in time domain with a boundary element formulation. The time discretisation is performed with the convolution quadrature method and for the spatial approximation standard elements and a collocation schema is applied. In the interest of increasing the efficiency of the boundary element method a low-rank approximation such as the adaptive cross approximation is carried out. We discuss about a generalization of the adaptive cross approximation to approximate a three-dimensional array of data, i.e. usual boundary element matrices at several complex frequencies. This approximation is used within the generalized convolution quadrature method to obtain a time domain method. Results for Dirichlet and Neumann problems are presented.

Boundary integral exterior calculus

Ralf Hiptmair[1], Erick Schulz[1], Stefan Kurz[2]
[1]ETH Zürich, Switzerland
[2]University of Jyväskylä, Finland

We develop first-kind boundary integral equations for Hodge–Dirac and Hodge–Laplace operators associated with de Rham Hilbert complexes on compact Riemannian manifolds and in Euclidean space. We show that from a variational perspective, the first-kind boundary integral operators associated with Hodge–Dirac and Hodge–Laplace boundary value problems posed on submanifolds with Lipschitz boundaries are Hodge–Dirac and Hodge–Laplace operators as well, this time spawned by trace de Rham Hilbert complexes on the boundary whose spaces are equipped with non-local inner products defined through boundary potentials.

Fast numerical methods for integral equation-based continuum solvation models

Benjamin Stamm
Universität Stuttgart, Germany

Since the seminal paper by Mennucci and Cancès in the nineties, numerical methods for so-called continuum solvation models in theoretical chemistry that are based on integral equations are very popular and widely used in this community. We will give an overview of a new family of meshless methods that combine integral equation discretizations with the domain-decomposition method in order to achieve linear scaling with respect to the number of atoms of the solute molecule. En gros, the cavity of a solute molecule is divided into a union of van der Waals balls where in each of them the solution is discretized based on spherical harmonics. Then, the local representations of the unknown are coupled through integral operators. We will also show aspects that are important in theoretical chemistry but which a numerical analyst is not necessarily aware of. A few numerical examples will demonstrate the performance of the methods.

Space-time finite and boundary element methods for a parabolic-elliptic interface problem with rotating domains

Olaf Steinbach
TU Graz, Austria

When considering the eddy current approximation of the Maxwell system in two space dimensions this results in a parabolic-elliptic interface problem. While the elliptic problem is considered in the fixed stator domain, the parabolic problem is formulated in the rotor. Using the Dirichlet to Neumann map which is related to the elliptic problem we end up with a parabolic problem in the rotor. We discuss the well-posedness of the space-time variational formulation, and its discretization using space-time finite element methods. In addition we comment on the use of boundary element methods for the solution of the elliptic problem.
This talk is based on joint work with P. Gangl (Linz) and M. Gobrial (Graz).

High-order finite element methods for the fractional Laplacian: graded meshes and hp

Ernst P. Stephan
Leibniz Universität Hannover, Germany

This talk considers efficient approximations for the Dirichlet boundary problem for the integral fractional Laplacian. The solutions of such problems exhibit singular behavior at the boundary, resulting in slow convergence of Galerkin approximations by an h-method on quasi-uniform meshes. We discuss recent results on the a priori analysis of h, p and hp-versions, based on the analysis of the singularities near boundaries and corners. In particular, exponential convergence of the hp-finite element method is obtained on geometrically graded meshes.
(joint work with H. Gimperlein and J. Stocek).

Calderón preconditioners for boundary elements on multi-screens

Kristof Cools[1], Carolina Urzúa–Torres[2]
[1]Department of Information Technology, Ghent University, Belgium
[2]Delft Institute of Applied Mathematics, Delft University of Technology, Netherlands

We are interested in the numerical solution of time-harmonic scattering by so-called multi-screens, which are geometries composed of panels meeting at junction lines. This is modelled via first kind integral equations using the framework proposed in [2,3]. The key realisation is that solutions of the related boundary integral equations belong to jump spaces, that can be represented as the quotient-space of a multi-trace space and a single trace space.

As shown in [1], the corresponding Galerkin discretization via quotient-space boundary element methods is up to the task. However, it does not address the ill-conditioning of the arising Galerkin matrices and the performance of iterative solvers deteriorates significantly when increasing the mesh refinement.

As a remedy, we introduce a Calderón-type preconditioner and discuss two possible multi-trace discretizations. First, we work with the full multi-trace discrete space, which contains many more degrees of freedom (DoFs) than strictly required. Then, we propose a representation of the quotient-space that reduces significantly the number of degrees of freedom while still allowing for efficient Calderón preconditioning. For this, we exploit the fact that the solution to the scattering problem is determined only up to a function in the single trace space. This implies that if we modify the single trace subspace of the multi-trace discrete space, the solution, as an element of the quotient-space, is unaffected.

References

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A posteriori error estimates for the optimal control of time-periodic eddy current problems

Monika Wolfmayr
Institute of Information Technology, Jyväskylä University of Applied Sciences, Finland

The multiharmonic analysis of a distributed eddy current optimal control problem is presented. The problem is situated in a time-periodic setting. A posteriori estimates of functional type can be derived by taking advantage of inf-sup and sup-sup conditions. They have been used in order to prove existence and uniqueness for the optimality system. Sharp, guaranteed and fully computable bounds of the approximation error for the optimal control problem are presented derived by applying functional type a posteriori estimation techniques.

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