Technische Universität Graz

14. Workshop on

Fast Boundary Element Methods in Industrial Applications

Söllerhaus, 13.–16.10.2016

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

Berichte aus dem Institut für Numerische Mathematik

Book of Abstracts 2016/1

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Program

Thursday, October 13, 2016	
15.00	Coffee
18.00–18.30	Opening
18.30–19.30	Dinner
19.30–20.15	J. Zapletal (Ostrava, Czech Republic) A note on the multi– and many–core implementation of the boundary element method
20.15–21.00	S. Christophersen (Kiel, Germany) Fast boundary integral operator setup with Green cross–approximation on the GPGPU
Friday, October 14, 2016	
8.00–9.00	Breakfast
9.00–9.45	E. P. Stephan (Hannover, Germany) Collocation with trigonometric polynomials for integral equations for mixed boundary value problems
9.45–10.30	M. Zank (Graz, Austria) Space-Time Boundary Integral Equations for the Wave Equation
10.30–11.00	Coffee
11.00–11.45	R. Hiptmair (Zürich, Switzerland) Second–kind BIE for multi–domain diffusion problems
11.45-12.30	K. Niino (Graz, Austria; Kyoto, Japan) A preconditioning for the electric field integral equation discretized with the H(div) inner product
12.30	Lunch
14.00–14.45	F. Wolf (Darmstadt, Germany) IGA BEM for Maxwell eigenvalue problems
14.45–15.30	G. Unger (Graz, Austria) Numerical analysis of boundary element methods for time–harmonic Maxwell's eigenvalue problem
15.30–16.00	Coffee
16.00–16.45	G. Of (Graz, Austria) Computational aspects of the fast multipole method in adaptive boundary element methods
16.45–17.30	Z. Adnani (Paris, France) Fast multipole accelerated boundary element method for soil impedance operator computation
17.30–17.45	Break
17.45–18.30	M. Peters (Basel, Switzerland) Bayesian Inversion for Electrical Impedance Tomography
18.30	Dinner

Saturday, October 15, 2016	
8.00–9.00	Breakfast
9.00–9.45	C. Urzua–Torres (Zürich, Switzerland) Optimal operator preconditioning for boundary elements on screens
9.45–10.30	S. Dohr (Graz, Austria) Preconditioned space–time boundary element methods for the heat equation
10.30–11.00	Coffee
11.00–11.45	J. Dölz (Basel, Switzerland) $\mathcal{H}$–matrix techniques for uncertainty quantification of PDE on random domains
11.45–12.30	S. Bonkhoff (Graz, Austria) Boundary integral solution of the time fractional diffusion equation
12.30	Lunch
13.30–18.00	Hiking Tour
18.30	Dinner

Sunday, October 16, 2016	
8.00–9.00	Breakfast
9.00–9.45	H. Harbrecht (Basel, Switzerland) A fast sparse grid based space–time boundary element method for the nonstationary heat equation
9.45–10.30	O. Steinbach (Graz, Austria) Boundary element methods for shape optimization problems
10.30–11.00	Coffee

Fast multipole accelerated boundary element method for soil impedance operator computation

Zouhair Adnani
Paris-Saclay University, France

The evaluation of accurate structural responses under seismic loading is an important issue for the safety assessments of operational power plants. Available experimental data show that site effects can significantly modify the seismic ground motion reaching the structure, thus causing, in some cases, either an amplification or an alteration of the spectrum of the signal. The quantification of these site effects generally involves expensive numerical simulations in terms of memory requirements and CPU time, due to the complexity of the model (topography and geology) and to the large spatial scale of the problems.
This work aims at developing a new numerical approach to solve soil-structure interaction (SSI) problems that accounts for site effects. We use a substructuring technique: the structure is modeled using the Finite Element Method (FEM) while the unbounded soil domain is represented by an impedance operator computed using the Boundary Element Method (BEM). The FEM part of the model may include a portion of the soil in addition to the structure itself. However, the BEM involves fully-populated matrices thus reducing the capabilities of the method to deal with large-scale geometries or broadband seismic signals. To overcome these limitations, the Fast Multipole Method (FMM) is used to accelerate the BEM (FM-BEM). However, since the FM-BEM requires the use of an iterative solver, the soil impedance matrix must be assembled using an indirect approach, which entails solving judiciously chosen problems by means of the FM-BEM and combining these solutions appropirately. Accordingly, the present work proposes a numerical approach to evaluate soil impedance matrices in a reduced modal basis defined over the FEM/FM-BEM interface. The obtained results are validated by comparison to literature values and classical BEM solutions. The validation models include rigid and flexible foundations on homogeneous and stratified basin.

Boundary integral solution of the time fractional diffusion equation

Sarah–Lena Bonkhoff
TU Graz, Austria

In the last years fractional partial dfferential equations are gaining more and more interest since they are a useful approach for the description of recently investigated phenomena in physics. We consider the time fractional diffusion equation in a space-time cylinder with a time derivative of order $\alpha \in (0, 1)$. For this purpose, fractional order derivatives are introduced and replace the first order time derivative of the standard diffusion equation. We can construct a fundamental solution and represent the solution of the time fractional diffusion equation in terms of layer potentials. This approach lead to boundary integral equations and we investigate the behaviour of the layer potentials in appropriate function spaces.

Fast boundary integral operator setup with Green cross-approximation on the GPGPU

Sven Christophersen
Universität Kiel, Germany

The *boundary element method* is advantageous with respect to matrix dimensions compared to the *finite element method*. The fact that these matrices are densely populated and their entries arise from four-dimensional integration with a singular kernel function has always been a drawback of these method.
Therefore fast approximative algorithms have been developed in the past, that not only reduce the storage complexity to $\mathcal{O}(n \log n)$ or even $\mathcal{O}(n)$, but also reduce setup times dramatically. Methods that achieve this goal can be categorized into three groups: purely analytical methods like *tensor interpolation*, purely algebraic methods like *adaptive cross-approximation* and hybrid methods like *hybrid cross-approximation*, that combine both approaches.
Recently we developed a new hybrid method, the *Green cross-approximation method (GCA)*, that constructs a degenerate approximation of the kernel function g utilizing *Green's representation formula* with quadrature. Upon that, a subsequent cross-approximation step further reduces the local ranks and therefore also the memory and time requirements.
We can show that this method has complexity of $\mathcal{O}(n)$ and we can also prove rigorous error bounds. For the construction on the analytical part, it is sufficient to know the Green's function g as well as their normal derivatives. Therefore it is easier to implement for various PDEs than the famous *fast multipole methods*.
In the context of Galerkin discretization with $\mathcal{H}^2$-matrices the entries of both nearfield and coupling matrices still consist of four-dimensional singular integrals in 3D, which introduce a high amount of computational effort to setup these boundary integral operators.
Since quadrature has a high computational intensity, this is a very suitable task for vector computers, e.g. GPGPUs. Therefore we have developed an efficient algorithm, that is capable of computing all these entries entirely on the GPGPU. By this approach we can easily outperform multi-socket servers at relatively low costs for the GPU hardware.

Preconditioned space-time boundary element methods for the heat equation

Stefan Dohr
TU Graz, Austria

Regarding time-dependent initial boundary value problems, there are different numerical approaches to compute an approximate solution. In addition to finite element methods and time-stepping schemes one can use boundary element methods to solve time-dependent problems. As for stationary problems, one can use the fundamental solution of the partial differential equation and the given boundary and intial conditions to derive boundary integral equations and apply some discretization method to compute an approximate solution of those equations.
In this talk, we describe the boundary element method for the discretization of the time-dependent heat equation. In contrast to standard time-stepping schemes we consider an arbitrary decomposition of the space-time cylinder into boundary elements. Besides adaptive refinement strategies, this approach allows us to parallelize the computation of the global solution of the whole space-time system. In addition to the analysis of the boundary integral operators and the derivation of boundary element methods for the Dirichlet initial boundary value problem, we state convergence properties and error estimates of the approximations. Those estimates are based on the approximation properties of boundary element spaces in anisotropic Sobolov-spaces, in particular in $H^{\frac{1}{2},\frac{1}{4}}(\Sigma)$ and $H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)$. The systems of linear equations, which arise from the discretization of the boundary integral equations, are being solved with GMRES. For an efficient computation of the solution we need preconditioners. Based on the mapping properties of the single layer- and hypersingular boundary integral operator we construct and analyse a preconditioner for the discretization of the first boundary integral equation. Finally we present numerical examples for the spatial one-dimensional heat equation to confirm the theoretical results.

$\mathcal{H}$-matrix Techniques for Uncertainty Quantification of PDE on Random Domains

Jürgen Dölz, Helmut Harbrecht
Universität Basel, Switzerland

We are interested in the first and second moment of the solution of PDE with random input data. Previous works have shown that these moments can be computed by the $\mathcal{H}$-matrix arithmetics in almost linear time if the solution depends linearly on the data. However, in the case of random domains the dependence of the solution of the data is nonlinear. Extending previous perturbation approaches we can linearize the problem and can compute the first moment up to third order accuracy and the second moment up to second order accuracy in almost linear time.

A fast sparse grid based space-time boundary element method for the nonstationary heat equation

Helmut Harbrecht

Universität Basel, Switzerland

This talk is dedicated to a fast sparse grid based space-time boundary element method for the solution of the nonstationary heat equation. We make an indirect ansatz based on the thermal single layer potential which yields a first kind integral equation. This integral equation is discretized by Galerkin's method with respect to the sparse tensor product of the spatial and temporal ansatz spaces. By employing the $\mathcal{H}$-matrix and Toeplitz structure of the resulting discretized operators, we arrive at an algorithm which computes the approximate solution in a complexity that essentially corresponds to that of the spatial discretization. Nevertheless, the convergence rate is nearly the same as in case of a traditional discretization in full tensor product spaces.

Second-kind BIE for multi-domain diffusion problems

Xavier Claeys[1], Ralf Hiptmair[2], Elke Spindler[2]

[1]LJLL, UMPC Paris, France, [2]Seminar for Applied Mathematics, ETH Zürich, Switzerland

We consider isotropic scalar diffusion boundary value problems on $\mathbb{R}^d$, whose diffusion coefficients are piecewise constant with respect to a partition of space into Lipschitz subdomains. We allow so-called material junctions where three subdmains may abut. We derive a boundary integral equation (BIE) of the second kind posed on the skeleton of the subdomain partition that involves, as unknown, only one trace function at each point of each interface. We prove the well-posedness of the corresponding boundary integral equations. We also report numerical tests for Galerkin boundary element discretizations, in which the new approach proves to be highly competitive compared to the well-established
rst-kind direct single-trace boundary integral formulation. In particular, for the discrete second-kind BIEs, GMRES enjoys fast convergence independent of the mesh resolution.

A preconditioning for the electric field integral equation discretised with the H(div) inner product

Kazuki Niino

Kyoto University, Japan

A discretisation method with the Hdiv inner product for the electric field integral equation (EFIE) and preconditioning for this discretised integral equation are discussed. It is known that the boundary element method for Maxwell's equations suffer from bad accuracy in low-frequency problems. One of the remedies for this bad accuracy is the discretisation method using the Hdiv inner product. The BEM with this discretisation, however, shows slow convergence of iteration methods and, what is worse, a naive application of the Calderon preconditoining is not effective for this problem.
In this talk, I will propose a different approach of preconditioning, which can efficiently reduce the computational time of the BEM discretised with the H(div) inner product.

Computational Aspects of the Fast Multipole Method in Adaptive Boundary Element Methods

Günther Of

TU Graz, Austria

We will address computational aspects of fast methods in adaptive boundary element methods for 3d computations for the Laplace equation. In the computational examples we will use the (h - h/2)-error estimation strategy [1]. An important aspect is the automatic choice of parameters of the Fast Multipole method with respect to error estimation and in adaptive boundary element methods.

References

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Bayesian Inversion for Electrical Impedance Tomography

Michael Peters
Universität Basel, Switzerland

In this talk, we consider a Bayesian approach towards Electrical Impedance Tomography, where we are interested in computing moments, in particular the expectation, of the contour of an unknown inclusion, given noisy current measurements at the surface. By casting the forward problem into the framework of elliptic diffusion problems on random domains, we solve a suitably parametrized version by means of the domain mapping method. This straightforwardly yields parametric regularity results for the system response, which we exploit to conduct a rigorous analysis of the posterior measure, facilitating the application of sophisticated quadrature methods for the approximation of moments of quantities of interest. As an example of such a quadrature method, we consider an anisotropic sparse grid quadrature. To solve the forward problem numerically, we employ a fast boundary integral solver. Numerical examples are provided to illustrate the presented approach and validate the theoretical findings.

Boundary element methods for shape optimization problems

Niels Köster, Olaf Steinbach
TU Graz, Austria

The shape derivative of cost functionals in shape optimization problems can be represented in the Hadamard–Zolesio form which implies the choice of the new search direction. We will recall the computation of the shape derivative, and we comment and discuss the choice of different cost functionals and search directions. First numerical results are given which illustrate the potential of the proposed approach.

Collocation with trigonometric polynomials for integral equations for mixed boundary value problems

Ernst P. Stephan, M. Teltscher
Leibniz Universität Hannover, Germany

We consider the direct boundary integral equation formulation for the mixed Dirichlet-Neumann bvp for the Laplace equation on a plane domain with a polygonal boundary. The resulting system of integral equations is solved by a collocation method which uses a mesh grading transformation and trigonometric polynomials. The mesh grading transformation method yields fast convergence of the collocation solution by smoothing the singularities of the exact solution. Special care is taken for handling the hypersingular operator as in [1]. With the indirect method in [2] this was avoided. Using Mellin transformation techniques a stability and solvability analysis of the transformed integral equations can be performed, in a setting in which each arc of the polygon has associated with it a periodic Sobolev space [3].

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Numerical analysis of boundary element methods for time–harmonic Maxwell's eigenvalue problems

Gerhard Unger
TU Graz, Austria

We consider Galerkin approximations of boundary integral formulations of different kinds of Maxwell's eigenvalue problems. An analysis of the boundary integral formulations and their numerical approximations is given in the framework of eigenvalue problems for holomorphic Fredholm operator-valued functions. We use recent results from [1] to show that the Galerkin approximation provides a so-called regular approximation of the underlying operator of the eigenvalue problem. This enables us to apply the abstract results of the numerical analysis of [2,3] which guarantee convergence of the eigenvalues as well as of the eigenspaces. In addition quasi-optimal error estimates are given. Numerical examples confirm the theoretical results.

References

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IGA BEM for Maxwell eigenvalue problems

Felix Wolf, Stefan Kurz, Sebastian Schöps
TU Darmstadt, Germany

Superconducting cavities are standard components of particle accelerators. Their design is typically described by parametrized ellipses and determined by mathematical optimization. The simulation model is subject to demanding requirements, such as a relative accuracy of 10^{-9} for the resonance frequency of the accelerating mode. Since the geometry and the electromagnetic fields are smooth, an approach in the gist of isogeometric analysis (IGA) suggests itself. The geometry is modeled by a NURBS mapping, while the electromagnetic fields are discretized by the B-spline de Rahm complex [2]. An IGA finite element method (FEM) for the Maxwell eigenvalue problem was investigated and showed promising results [3]. For the same accuracy, the number of required degrees of freedom was reduced by a factor $3 \ldots 9$ compared to classical FEM. However, CAD systems feature surface descriptions only, so the volumetric spline model had to be created manually.
To live up to the promises of IGA, namely closing the gap bewteen design and analysis, we suggest an IGA boundary element method (BEM). We will review the state-of-the-art of all relevant building blocks. We will address the B-spline de Rham complex on a boundary manifold, the Galerkin discretization of the electric field integral equation, and present a convergence result. We will discuss a recent contour integral method [1] to solve the resulting non-linear eigenvalue problem. Aspects of integrating so-called "fast methods" will also be presented, in particular Adaptive Cross Approximation [5] and Calderón preconditioning [4].

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Optimal operator preconditioning for boundary elements on screens

Ralf Hiptmair[1], Carlos Jerez–Hanckes[2], Carolina Urzua–Torres[1]
[1]Seminar for Applied Mathematics, ETH Zürich, Switzerland,
[2]PUC Santiago de Chile, Chile

In this presentation, we introduce Calderón-type preconditioners for the hypersingular and weakly singular operators arising from the Laplacian on screens. For their construction, we use operator preconditioning [1] and the bilinear forms induced by their recently found inverse boundary integral operators (BIOs) over the disk.
By using this approach, for any screen that can be parametrized over the unit disk by a bi-Lipschitz diffeomorphism, we obtain bounded condition numbers that remain constant when increasing the number of degrees of freedom. Moreover, we are able to apply this preconditioning strategy to non-uniform meshes [3].
Numerical examples illustrate the optimality of our preconditioner for the hypersingular operator when applied to different screens [2]. For the case of the weakly singular operator, the direct implementation of its inverse BIO is impractical due to its hypersingular nature. Instead, we build our preconditioner by using a regularized bilinear form and show promising preliminary numerical results.

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Space-Time Boundary Integral Equations for the Wave Equation

Marco Zank
TU Graz, Austria

For the discretisation of the wave equation by boundary element methods the starting point is the so-called Kirchhoff's formula, which is a representation formula by means of boundary potentials. In this talk different approaches to derive weak formulations of related boundary integral equations are considered. First, weak formulations based on the Laplace transform and second, space-time energetic formulations are introduced. In both cases coercivity is shown in appropriate Sobolev spaces. To derive an adaptive scheme an a posteriori error estimator based on the representation formula is used.
Finally, numerical examples for a one-dimensional spatial domain are presented and discussed.

A note on the multi- and many-core implementation of the boundary element method

Lukas Maly, Michal Merta, Jan Zapletal
TU VSB Ostrava, Czech Republic

Although the clock frequency of modern CPUs has not been growing as rapidly as in the previous decades, the hardware manufacturers still look for ways of increasing the theoretical performance limits. One possibility is the transition from multi-core to many-core architectures. Instead of several high-performance cores the modern many-core chips, including the Intel's Xeon Phi technology, feature many rather simple cores ready to deliver the power of several TFLOPS in total. However, this puts higher demands on the developers of scientific codes, since the peak performance can only be reached if the application scales well up to tens or even hundreds of employed threads. Moreover, the newest Xeon Phi processor series introduces the AVX-512 instruction set able to operate on 8 (16) double (single) precision operands at once. Failing to exploit this feature again results in low performance of the code. In this talk we present an efficient implementation of the regularized boundary element quadrature deployable at both multi- and many-core architectures. The local element contributions are distributed to the individual threads by standard OpenMP pragmas. In addition, the SIMD vectorization is achieved by suitable loop collapsing, data replication and transformation, and subsequently by the OpenMP SIMD pragmas available since its 4.0 version. We present numerical experiments for both full and ACA assembly performed at the multi-core Haswell architecture and two generations of the many-core Intel Xeon Phi chips, namely the Knights Corner and Knights Landing.

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Erschienene Preprints ab Nummer 2014/1

2014/1 K. Bandara, F. Cirak, G. Of, O. Steinbach, J. Zapletal: Boundary element based multiresolution shape optimisation in electrostatics.

2014/2 T. X. Phan, O. Steinbach: Boundary integral equations for optimal control problems with partial Dirichlet control.

2014/3 M. Neumüller, O. Steinbach: An energy space finite element approach for distributed control problems.

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2014/6 T. Apel, O. Steinbach, M. Winkler: Error estimates for Neumann boundary control problems with energy regularization.

2014/7 G. Haase, G. Plank, O. Steinbach (eds.): Modelling and Simulation in Biomechanics. Book of Abstracts.