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BEMPP-CL: FAST GPU AND CPU ASSEMBLY OF INTEGRAL OPERATORS WITH OPENCL

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The Bempp boundary element library is a UCL lead project that has been developed since 2011. It consists of a fast C++ core and a user friendly Python interface. It supports the Galerkin discretisation of Laplace, Helmholtz and Maxwell boundary integral operators, either as dense matrices or via ACA based H-Matrix compression.

However, over the last 10 years a revolution has taken place in advanced computing architectures. Massively multicore Xeon CPUs with up to 56 cores are expected to be released in 2019. Each of these cores supports AVX-512 registers that allow the parallel execution of eight double precision or sixteen single precision instructions. At the same time GPU architectures have become mainstream with the fastest Nvidia Volta V100 GPUs having over 5000 compute cores with a peak performance of almost 16 TFlops per second in single precision.

While Bempp performs well on classical multi-core architectures with a few parallel cores, performance issues arise in massive multicore environments. Moreover, it is not able to take advantage of modern vectorized instructions or GPU computing environments.

These considerations have lead to the decision to completely redevelop the library with modern compute architectures in mind. The new library should support advanced vector instruction sets on CPUs and vendor-independent GPU computing. Moreover, the new library should consist only of Python code that would not require any pre-compilation of C or C++ modules. The outcome of these efforts is the Bempp-cl library, which is expected to be released in May 2019. So far it supports the dense Galerkin assembly of Laplace, Helmholtz and Maxwell operators. The performance profiles are significantly improved compared to Bempp, making it possible to assemble dense matrices in the dimension of tens of thousands within seconds on a modern CPU or GPU node. This is especially useful for highly oscillatory problems, which are challenging for standard H-Matrix compression algorithms. Indeed, we will demonstrate high-frequency examples, where the dense assembly in Bempp-cl is significantly more performant than the H-Matrix assembly in previous Bempp versions.

In this talk we present an overview of Bempp-cl, discuss the optimised implementation of assembly routines on modern vector CPU and GPU devices, and present a number of application benchmarks.

MAXWELL-LLG COUPLING VIA CONVOLUTION QUADRATURE

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We consider the Landau-Lifshitz-Gilbert-equation (LLG) on a bounded domain Ω with Lipschitz-boundary Γ coupled with the linear Maxwell equations on the whole space. As the material parameters outside of Ω are assumed to be constant, we are able to reformulate the problem to a MLLG system in Ω coupled to a boundary equation on Γ. We define a suitable weak solution (which still has a reasonable trace for the boundary equation) and propose a time-stepping algorithm which decouples the Maxwell part and the LLG part of the system and which only needs linear solvers even for the nonlinear LLG part. The approximation of the boundary integrals is done with convolution quadrature. Under weak assumptions on the initial data and the input parameters we show convergence of the algorithm towards weak solutions, which especially guarantees the existence of solutions to the MLLG system.

Keywords: convolution quadrature · maxwell · maxwell-LLG · linear scheme · ferromagnetism · boundary elements · transparent boundary conditions · convergence

Mathematics Subject Classifications (2010): 35Q61, 65M12, 65M38, 65M60

ANISOTROPIC HIGH-ORDER ADAPTIVE BOUNDARY ELEMENT METHODS FOR 3D WAVE PROPAGATION

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The main advantage of the Boundary Element Methods (BEMs) is that only the domain boundaries are discretized. They are also well suited to problems in large-scale or infinite domains since they exactly account for radiation conditions at infinity. This dimensional advantage is offset by the fully-populated system matrix, with solution times rapidly increasing with the problem size.

Mesh adaptation is a technique to reduce the computational cost of a numerical method by optimizing the positioning of a given number of degrees of freedom on the geometry of the obstacle. For wave scattering problems, adaptation is particularly important for obstacles that contain geometric or solution singularities. The best strategy to achieve these goals is via so-called "anisotropic" mesh adaptation for which an extensive literature exists for volume-based methods. However, there is relatively little research attention being paid to mesh adaptation in a boundary element context. With the development of fast BEMs, the capabilities of BEMs are greatly improved such that efficient adaptive mesh strategies are needed to optimize further the computational cost. So far BEM adaptivity methods have been confined to isotropic techniques (by using Dörfler marking) and formulated specifically for a system of equations.

The first originality of our work is the extension of metric-based anisotropic mesh adaptation (AMA) [3] to the BEM [2]. The metric-based AMA generates a sequence of non-nested meshes with a specified complexity. The different meshes are defined according to a metric field derived from the evaluation of the linear interpolation error of the (unknown) exact solution on the current mesh. The advantages of this approach are that it is ideally suited to solutions with anisotropic features, it is independent of the underlying PDE and discretization technique, and it is inexpensive. The second originality is the combination of two acceleration techniques, namely metric-based AMA and Fast Multipole accelerated BEM [1]. If no fast BEM is used, the capabilities of anisotropic mesh techniques cannot be fully demonstrated for realistic large scale scattering scenarios.

In this talk, we will show the performance of the strategy to recover optimal convergence rates for simple and complex real-world scattering problems. We will also show the importance of the proposition of an efficient preconditioner if highly anisotropic meshes are used.

References

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A TIME DOMAIN COMBINED FIELD INTEGRAL EQUATION FREE FROM CONSTANT-IN-TIME AND RESONANT INSTABILITIES

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Time domain boundary integral equations are used for the modelling of transient scattering by reflecting or penetrable bodies [F. Sayas, Retarded Potentials and Time Domain Boundary Integral Equations: A Road Map, Springer, 2016]. Their advantages include that solutions to these integral equations automatically fulfil radiation conditions, and that only the boundary of the scatter needs to be modelled.

Time domain as opposed to frequency domain solvers have the additional advantages that solutions include information over a broad range of frequencies and that the equations can be coupled to non-linear lumped element circuits or boundary conditions.

Unfortunately, straightforward implementations of the single and double layer based time domain integral equations for the Maxwell equations suffer from a number of problems: (i) the condition number of the system to be solved grows as the mesh parameter tends to zero, (ii) the condition number also grows as the time step tends to infinity, (iii) the system support constant and/or linear in time regime solutions stemming from the scatter's topology, and (iv) the system supports regime solutions related to internal resonances supported by the interior of the scatterer [Y. Beghein at al., A DC-Stable, Well-Balanced, Calderon Preconditioned Time Domain Electric Field Integral Equation, IEEE Trans. AP, vol. 63, no. 12, 2015].

In this contribution, an integral equation is introduced alongside a discrretisation scheme that eliminates these problems. The solver methodology relies on both Calderon or operator preconditioning techniques to control the condition number and a combined field approach to eliminate spurious resonances. To render the system immune from constant and linear in time regime solutions, a non-tensorial space-time discretisation is required subject to a well-chosen Helmholtz decomposition for the discrete currents. The details of the operator preconditioning for the single layer and double layer terms of this combined field equation differ in a technical but critical manner to achieve this.

The discretisation is carefully introduced and its properties are discussed. It will be demonstrated both by investigating late-time solutions and by considering polynomial eigenvalue distributions that the method is free from constant-in-time regime solutions and that, as a result, the method is more robust in the presence of quadrature error and when applied to scattering off multiply connected obstacles.

A FAST DIRECT SOLVER FOR SCATTERING PROBLEMS IN QUASI-PERIODIC LAYERED MEDIUM

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Being able to accurately and efficiently solve quasi-periodic scattering problems involving multi-layered medium is important for the design of composite materials. This talk presents a fast direct solver for the linear system that results from discetizing a robust integral equation. The direct solver scales linearly with respect to the number of discretization points and the precomputation is able to be reused for all right hand sides.

FINITE-ELEMENT AND BOUNDARY-ELEMENT SIMULATIONS FOR HIGH-INTENSITY FOCUSED ULTRASOUND MODELLING

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High-intensity focused ultrasound (HIFU) is a promising non-invasive, non-radioactive technology for the ablation of tumours. By focusing energy on a small target region the tissue temperature in the target region can be elevated such that with sufficient treatment time the tissue is destroyed. Challenges in planning HIFU treatments in the abdomen include the presence of a large number of scatterers, nonlinear effects and the presence of transport mechanisms for heat.

In this talk, I will compare a range of different finite-element and boundary-element formulations for the non-linear wave equation in practically relevant HIFU scattering scenarios. These include classical implicit and explicit time-stepping schemes, high-order methods, and convolution quadrature. We aim to isolate the main challenges in such high-frequency, non-linear wave simulations and identify the most fruitful directions towards the development of accurate methods that are fast enough to be clinically relevant, and which will hopefully support patient treatment planning in the future.

The presented methods are implemented in the open source FEniCS (`https://fenicsproject.org`) and Bempp (`https://bempp.com/`) libraries.

BOUNDARY ELEMENT METHODS FOR ACOUSTIC SCATTERING BY FRACTAL SCREENS

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We consider time-harmonic acoustic scattering by a planar screen, i.e. a subset of a two-dimensional hyperplane embedded in a three-dimensional propagation domain. In contrast to previous studies we allow the relative boundary of the screen to be arbitrarily rough - in particular, the screen could have fractal boundary (Koch snowflake), or itself be a fractal (Sierpinski triangle). Such problems are of interest in the study of fractal antennas in electrical engineering, light scattering by snowflakes/ice crystals in atmospheric physics, and in laser optics.

The fractal nature of the screen presents challenging questions concerning how boundary conditions should be enforced, and the appropriate function space setting. But progress is possible and there is interesting behaviour to be discovered: for example, a sound-soft screen with zero area (planar measure zero) can scatter waves provided the fractal dimension of the set is large enough [1,2]. Accurate computations are obviously challenging because of the need to capture the fine structure of the fractal. A natural approach to numerical simulation is via boundary element method approximations on sequences of smoother "prefractal" approximations. As well as presenting numerical results for such an approach, I will outline some of our recent theoretical results, and some outstanding open questions, regarding convergence analysis [3].

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FAST CALDERÓN PRECONDITIONING FOR HELMHOLTZ BOUNDARY INTEGRAL EQUATIONS

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Calderón multiplicative preconditioners are an effective way to improve the condition number of first kind boundary integral equations yielding provable mesh independent bounds. However, when discretizing by local low-order basis functions as in standard Galerkin boundary element methods, their computational performance worsens as meshes are refined. This stems from the barycentric mesh refinement used to construct dual basis functions that guarantee the discrete stability of L^2-pairings. Based on coarser quadrature rules over dual cells and H-matrix compression, we propose a family of fast preconditioners that significantly reduce assembly and computation times when compared to standard versions of Calderón preconditioning for the three-dimensional Helmholtz weakly and hyper-singular boundary integral operators. Several numerical experiments validate our claims and point towards further enhancements.

A PARALLEL SPACE-TIME BOUNDARY ELEMENT METHOD FOR THE HEAT EQUATION

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We present a parallel boundary element solver for space-time boundary integral equations of the heat equation. The related system matrix is huge, but it allows for additional parallelization with respect to time. The related space-time boundary mesh is decomposed into submeshes and the system matrix is decomposed into related blocks. These blocks are distributed among computational nodes by an algorithm based on a cyclic decomposition of complete graphs to achieve load balance. In addition, we employ vectorization and threading in shared memory to ensure intra-node efficiency. We present scalability experiments to evaluate the performance of the proposed parallelization techniques and observe almost optimal speedup.

ADAPTIVE BEM WITH INEXACT PCG SOLVER YIELDS ALMOST OPTIMAL COMPUTATIONAL COSTS

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In our talk, we will sketch our recent work [Führer et al., Numer. Math. 141, 2019]. We consider the preconditioned conjugate gradient method (PCG) with optimal preconditioner in the frame of the boundary element method (BEM) with adaptive mesh-refinement. As model problem serves the weakly-singular integral equation $V\phi = f$ associated with the Laplace operator. Given an initial mesh $\mathcal{T}_0$, adaptivity parameters $0 < \theta \leq 1$ and $\lambda > 0$, counter $j = 0$ (for the mesh-sequence $\mathcal{T}_j$) and $k = 0$ (for the PCG steps per mesh $\mathcal{T}_j$), as well as a discrete initial guess $\phi_{00} \approx \phi$ on $\mathcal{T}_0$ (e.g., $\phi_{00} = 0$), our adaptive strategy reads as follows:

(i) Update counter $(j, k) \mapsto (j, k + 1)$.

(ii) Do one PCG step to obtain ϕ_{jk} from $\phi_{j(k-1)}$.

(iii) Compute refinement indicators $\eta_j(T, \phi_{jk})$ for all elements $T \in \mathcal{T}_j$.

(iv) If $\lambda^{-1} \|\phi_{jk} - \phi_{j(k-1)}\|^2 > \eta_j(\phi_{jk})^2 = \sum_{T\in\mathcal{T}_j} \eta_j(T, \phi_{jk})^2$, continue with (i).

(v) Otherwise determine marked elements $\mathcal{M}_j \subseteq \mathcal{T}_j$ such that $\theta\, \eta_j(\phi_{jk})^2 \leq \sum_{T\in\mathcal{M}_j} \eta_j(T, \phi_{jk})^2$.

(vi) Refine all $T \in \mathcal{M}_j$ to obtain the new mesh $\mathcal{T}_{j+1}$.

(vii) Update counter $(j, k) \mapsto (j + 1, 0)$ and continue with (i).

For *a posteriori* error estimation, we employ the weighted-residual error estimator. If the final ϕ_{jk} on each mesh $\mathcal{T}_j$ is the exact Galerkin solution, then linear convergence of adaptive BEM, even with optimal algebraic rates, has been proved independently in [Feischl et al., SIAM J. Numer. Anal. 51, 2013] and [Gantumur, Numer. Math. 124, 2013]. As a novel contribution, we now extend this result to adaptive BEM with inexact PCG solver.

We prove that the proposed adaptive algorithm does not only lead to linear convergence of the error estimator (for arbitrary $0 < \theta \leq 1$ and $\lambda > 0$) with optimal algebraic rates (for $0 < \theta, \lambda \ll 1$ sufficiently small), but also to almost optimal computational complexity, if $\mathcal{H}^2$-matrices (resp. the fast multipole method) are employed for the effective treatment of the discrete integral operators. In particular, we provide an additive Schwarz preconditioner which can be computed in linear complexity and which is optimal in the sense that the condition numbers of the preconditioned systems are uniformly bounded (see [Feischl et al., Calcolo 54, 2017] in the context of the hypersingular integral equation).

FAST BOUNDARY ELEMENT METHODS FOR COMPOSITE MATERIALS

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In this talk, we discuss numerical solutions to the problems in the field of solid mechanics by combining the Boundary Element Method (BEM) with interpolation by means of radial basis functions, [1]. The main task is to find an approximation to a particular solution of the corresponding elliptic system of partial differential equations. To construct the approximation, the differential operator is applied to a vector of radial basis functions. The resulting vectors are linearly combined to interpolate the function on the right-hand side. The solubility of the interpolation problem is established. Additionally, stability and accuracy estimates for the method are given. A fast numerical method for the solution of the interpolation problem is proposed. These theoretical results are then illustrated on several numerical examples related to the Lamé system.

References

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WEAKLY IMPOSING BOUNDARY CONDITIONS ON THE BOUNDARY ELEMENT METHOD USING A PENALTY METHOD

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In recent years, Nitche's method has become increasingly popular within the finite element community as a method for weakly imposing boundary conditions. Inspired by this, we propose a penalty-based method for weakly imposing boundary conditions within boundary element methods.

We consider boundary element methods where the Calderón projector is used for the system matrix and boundary conditions are weakly imposed using a particular variational boundary operator. Regardless of the boundary conditions, both the primal trace variable and the flux are approximated.

Due to using the full Calderón projector, the number of unknowns—and hence the computational cost—is higher for problems such as those with pure Dirichelt conditions. As such, we focus on more complex boundary conditions: mixed Dirichlet–Neumann, Robin, and Signorini contact conditions. The focus of this talk is on Laplace's equation, although the imposition method is also applicable to other problems.

The theory is illustrated by a series of numerical examples using the software library Bempp.

SPACE-TIME BEM FOR THE HEAT EQUATION

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In this talk we present a new framework for the numerical analysis of space-time boundary element methods for the heat equation. As for elliptic problems we first consider domain variational formulations in anisotropic Sobolev spaces of Galerkin-Petrov type, or equivalently of Galerkin-Bubnov type when using a Hilbert type transformation. From this we derive all mapping properties of boundary integral operators and we discuss unique solvability of related boundary integral equations.

For the space-time discretization we consider boundary element spaces which are defined with respect to either tensor product or rather general boundary element meshes of the space-time boundary. For the approximate solution we provide related a priori error estimates, and we discuss the iterative solution when using preconditioning by operators of opposite order.

This presentation is based on joint work with Stefan Dohr and Marco Zank.

PARALLEL ADAPTIVE CROSS APPROXIMATION FOR DISTRIBUTED MEMORY SYSTEMS

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We present a parallel version of the boundary element method accelerated by the adaptive cross approximation (ACA). The boundary of the computational domain is decomposed into patches defining a block structure of boundary element matrices. The blocks are then distributed across computational nodes by a graph algorithm providing a load balancing strategy. Each block is compressed individually by a slightly modified ACA algorithm able to recognize zero blocks generated e.g. by double-layer kernels. The intra-node implementation further utilizes threading in shared memory and in-core SIMD vectorization to make use of all features of modern processors. The suggested approach is validated on a series of numerical experiments presented in the paper.

Furthermore, we present preliminary results of the application of the algorithm for scattering problems with composite scatterers. The problem is modeled by the local version of the multi-trace formulation which allows for operator preconditioning even for skeletons with junction points. Individual Caldern projectors are treated independently, i.e. the boundary of every homogeneous subdomain is decomposed into clusters of elements. The algorithm then proceeds as in the case of single domain problems.