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Review of the Doctoral Thesis

Parallel Boundary Element Methods in Space and Time

by Ing. Michal Merta

Boundary integral equations and boundary element methods are well established for the approximate solution of partial differential equations, with many applications in science and engineering. While the mathematical and numerical analysis of boundary integral equations in particular for elliptic problems is known for some time, an efficient, accurate, and reliable implementation in particular on state of the art parallel computer facilities is more challenging.

This thesis aims to contribute to the development of parallel fast Galerkin boundary element methods and their implementaion on available supercomputing systems.

The thesis essentially consists of three published research papers, three introductory chapters, and a bibliography with 34 references.

Chapter 1 gives a short introduction into the formulation and analysis of boundary integral equations for the Laplace equation, and for the wave equation. Although this content is rather standard, in particular for the Laplace equation, the presentation is superficial in some aspects: The representation of the normal derivative of the single layer potential, see page 7, line 4, has to be interpreted in the sense of $H^{-1/2}(\Gamma)$, and not pointwise. Moreover, we have $\frac{1}{2}I + K' : H^{-1/2}(\Gamma) \to H^{-1/2}(\Gamma)$, i.e. the mapping properties of K' and D are different, see page 7, the paragraph following equation (1.10). Note that also the presentation of the extended variational problem (1.20) is not correct. In addition to the Laplace equation the author also considers boundary integral equations for the wave equation. Here I miss the rather new monography by F.–J. Sayas in the bibliography, which was availaible as lecture notes for some time. Again, there are some in the notation, see page 13, equation (1.27), and $L^2(\mathbb{R}, X)$ two lines ahead. Finally, I think that the last equality as given on page 17 results from integration by parts.

An introduction into boundary element methods is given in Chapter 2. The discretization os done with respect to an admissible triangulation, nothing is said with respect to shape regularity and globally/locally quasi–uniformity which is of special interest when dealing with adaptive meshes. Topics such as preconditioning and acceleration by using fast methods are mentioned, but without giving any details or references. In the case of the wave equation the discretization is done by separating the spatial and temporal discretizations. In general, no detailed stability and error analysis is given.

Chapter 3 gives an overview on the boundary element software package BEM4I. It is worth to mention that, in particular when comparing to finite elements, only a few boundary element software packages are available. This is mainly due to the complexity of the method, i.e. the use of different formulations and discretizations, and the requirement to handle singular surface integrals and to use fast methods for acceleration. So it can be a break through to have such a library available to be used as simulation tool in future research.

In what follows I will comment on some aspects of the three published journal papers as part of this thesis.

1. **Acceleration of boundary element method by explicit vectorization**
   This paper exploits SIMD instruction sets to speed up the assemby of boundary element matrices, including ACA approximations. I wonder why the exterior Dirichlet problem for the Helmholtz equation was chosen as motivating example. I would expect that the results for the much simpler Laplace equation are similar. Although the exterior Dirichlet problem for the Helmholtz equation is uniquely solvable for all wave numbers, this is due to the radiation condition, this is not true for related boundary integral equations. In fact, spurious modes appear when the wave number coincides with an eigenvalue of the interior Dirichlet eigenvalue problem for the Laplacian. Although the boundary integral equation of the direct approach is solvable all wave numbers, the solution is not unique in the case of a Dirichlet eigenvalue. Note that this does not transfer to the discrete case. Instead, combined or modified boundary integral formulations have to be used to end up with a formulation which is stable for all wave numbers.

2. **A parallel fast boundary element method using cyclic graph decomposition**
   While the parallel assembly of a dense matrix can be rather easy, the situation is quite different when using low rank approximations within a hierarchical matrix approach. In the latter case, small diagonal blocks with cost intensive computatations of singular surface integrals and large low rank blocks have to be distributed to gain optimal load balance. Here the authors propose an optimal parallel distribution of the submeshes and corresponding submatrices by cyclic decompositions of undirected complete graphs.

3. **Efficient solution of time–domain boundary integral equations arising in sound–hard scattering**
   In this paper the authors consider an indirect double layrer potential ansatz for the solution of the Neumann boundary value problem for the wave equation with homogeneous initial data. This paper combines an efficient and parallel assembly of the boundary element matrix with an efficient iterative solution of the resulting linear system. These results are really impressive, and they show the potential of the proposed methods.

This thesis covers new and challenging aspects of a parallel and efficient implementation of boundary element methods. Of particular interest is the space–time discretization of the wave equation which is a hot topic of research world–wide.

From the point of scientific computing I find the thesis excellent since M. Merta showed his ability to formulate and implement state of the art mathematical algorithms on state of the art computing facitilies. Unfortunately, from the point of numerical analysis, this picture is not so clear. Besides some mathematical inconsistencies as mentioned in the report I do miss some more detailed information on the stability and error analysis of the used methods, So combining both ratings I rate the thesis with ·**good** to **very good**.

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