The Second Chilean Symposium on BOUNDARY ELEMENT METHODS

Friday, December 14, 2018
Universidad Técnica Federico Santa María
Valparaíso, Chile

http://bem2018.usm.cl/

9:25 – 9:30	Welcome	
9:30 – 10:30	Jaydeep Bardhan	*Improving predictions of biomolecule behavior using multiscale boundary conditions and BEM*
10:30 – 11:00	Natalia Clementi	*PyGBe-LSPR: Python and GPU Boundary-integral solver for electrostatics. Simulating nanoplasmonics for biosensing applications.*
11:00 – 11:30	Coffee break	
11:30 – 12:30	Lehel Banjai	*Time Domain Boundary Integral Equations: nonlinear-boundary conditions and BEM/FEM coupling*
12:30 – 13:00	Thomas Führer	*Stable multilevel splittings in* $H^{-1/2}$
13:00 – 14:30	Lunch break	
14:30 – 15:30	Lorena Barba	*Practices for reproducible research in BEM*
15:30 – 16:30	Xavier Claeys	*Two-level preconditioning for BEM based on Generalised Eigenvalues in the Overlaps (GenEO)*
16:30 – 17:00	Coffee break	
17:00 – 17:30	Carlos Pérez Arancibia	*Density interpolation methods for high-order evaluation of nearly-singular, weakly-singular, singular, and hypersingular boundary integral operators and layer potentials*
17:30 – 18:00	Elwin van't Wout	*The Computational Analysis of the Resonances of Bubble Clouds and Fish Schools with Boundary Element Methods*
19:00	Dinner	

Lehel Banjai
Maxwell Institute for Mathematical Sciences
School of Mathematical & Computer Sciences, Heriot-Watt University, United Kingdom

Time Domain Boundary Integral Equations: nonlinear-boundary conditions and BEM/FEM coupling

In this talk I will give a brief overview of time domain boundary integral equation (TDBIE) methods for solving acoustic scattering problems. Numerical methods we will use are the Galerkin boundary element method (BEM) for the spatial discretization and convolution quadrature (CQ) for the time discretization. We will describe CQ based on implicit multistep methods and concentrate on properties important for the application to TDBIE. This will allow us to solve some standard scattering problems.
To broaden the application areas we need to be able to couple the integral equation methods with discretizations of a PDE by, e.g., the finite element method (FEM). The difficulty arises that the hyperbolic PDE would in general be discretized by an explicit scheme such as leapfrog. We describe how energy considerations lead to stable FEM/BEM couplings of the different time discretizations. Working directly in the time-domain also allows us to consider some non-linear problems. We will motivate these and describe how their discretizations can be analysed using analysis methods similar to the ones used for FEM/BEM coupling. Finally, if time allows we will touch upon some new results on high-order methods based on Runge-Kutta CQ.

This talk is based on joint work with Christian Lubich (Tübingen), Alexander Rieder (Vienna), and Francisco Javier Sayas (Delaware).

Lorena A. Barba
Department of Mechanical & Aerospace Engineering
The George Washington University, USA

Practices for reproducible research in BEM

In the field of boundary element methods (BEM), researchers are rigorous with the mathematics, keen to develop improved algorithms, and methodical in using model problems to investigate convergence and computational complexity. But what about the software? When papers present numerical experiments: are they reproducible? Typically, you might report âĂIJCPU timeâĂİ (possibly forgetting to mention what hardware you ran on), you may assert that your algorithm is X times faster than a predecessor, or uses less storage, and you might show results of time complexity of the computation. But if the code is not available, these results are irreproducible. Reproducible research is research published with all the necessary data, source code, and configurations to run the analysis again, re-creating the results and data products [1]. For all these digital artifacts, making available means; using a public license (an OS-approved license for software and a Creative Commons license for data), and depositing in an archival-quality service. Several of the attendees in this symposium use or have contributed to the BEM++ project. This is an open-source project under the MIT license. Great! Computational results using this (or other open source) software, say, in acoustic scattering problems, report physical parameters (like medium density and speed of sound), discuss geometry and incoming acoustic field, and describe the discretization in terms of number of surface triangles and type of basis function. Results may be reported in terms of computation time, number of solver iterations, and perhaps comparison of the physics with another software. In these scenarios, even if the code is open source (and the authors reported the version used), the results are still irreproducible, unless the authors deposit the actual mesh in a data repository, and compile configuration and input files for each run into âĂIJreproducibility packages.âĂİ This talk will propose practices of reproducible research for the BEM field, covering the core set of standards, technologies and preferred tools-of-the-trade that, combined, form the basic reproducibility curriculum.

Jaydeep P. Bardhan
GlaxoSmithKline
USA

Improving predictions of biomolecule behavior using multiscale boundary conditions and BEM

Biological molecules such as proteins and DNA interact strongly with the water and ions that surround them. As a result, understanding biomolecule behavior requires a model for predicting biomolecule-water interactions. Over a century ago, the most basic physics of these interactions were understood and modeled using macroscopic continuum electrostatic models, based on the Poisson equation. Today, thanks to modern computers and algorithms, simulating a protein using such models can be performed in mere seconds. Using macroscopic continuum theory at atomic length scales necessarily means neglecting some important details, however, and these omissions greatly limit the ability of these simulations to reproduce critical experimental results, including the thermodynamics of protein-water interactions. In contrast to macroscopic models are atomically detailed models, which simulate every atom in the protein, as well as many thousands of surrounding water molecules and ions; such models do a much more satisfactory job reproducing those critical experiments, but the tradeoff is that calculations require thousands or even millions of hours of computation. In this talk, I will present our development of a multiscale BEM model that reproduces the important experiments and yet retains the speed advantage of traditional macroscopic models. The core of the approach is a modified boundary condition– modifying the macroscopic dielectric theory to account for the small but vital detail that water's hydrogen atoms are much smaller than water oxygen atoms.

Xavier Claeys
Laboratoire Jacques-Louis Lions
Université Pierre et Marie Curie, France

Two-level preconditioning for BEM based on Generalised Eigenvalues in the Overlaps (GenEO)

Overlapping Domain Decomposition Methods (DDM), such as Additive Schwarz, can be used to precondition linear systems arising from boundary integral equations and, with this approach, two level preconditionners based on coarse spaces have also been proposed and analysed. However, the question of scalability has not yet received much attention in a BEM context. Devising scalable DDM preconditionning strategies is indeed a challenge and, in this respect, important progress has been achieved in recent years for the FEM context.
For the construction of coarse spaces leading to scalable domain decomposition, the method of Generalized Eigenproblems in the Overlaps (GenEO) has emerged as a promising approach. Instead of prescribing the coarse space a priori, GenEO constructs it automatically through the solution of local generalised eigenproblems. As one of its interesting features, this strategy is discretization agnostic, left apart a few reasonable assumptions. In this talk, we will present recent theoretical and numerical results in 2D and 3D aiming at adapting GenEO to the context of boundary integral equations.

This talk is based on joint work with Pierre Marchand and Frédéric Nataf (Paris).

Natalia C. Clementi
Department of Mechanical & Aerospace Engineering
The George Washington University, USA

PyGBe-LSPR: Python and GPU Boundary-integral solver for electrostatics. Simulating nanoplasmonics for biosensing applications

Abstract: PyGBe is a Python library that applies the boundary integral method for biomolecular electrostatics and nanoparticle plasmonics. Its latest release extends the software to nanoplasmonics by treating localized surface plasmon resonance (LSPR) quasi-statically. LSPR is essentially a miniaturization of SPR: the resonance of the electron cloud on a metallic surface (usually a nanoparticle), excited by incident light. This is an optical effect, but electrostatics is a good approximation in the long-wavelength limit. Mathematically, this leads to a coupled system of Poisson equations on complex dielectric regions, which we solve with an integral formulation. The code is accelerated algorithmically with a treecode, and exploits GPU accelerators. PyGBe's LSPR simulations compute the extinction cross-section of the incoming wave due to a scatterer (nanoparticle), which peaks at the resonance frequency. To our knowledge, PyGBe is the only open-source software that uses a fast algorithm - O(N logN), for N unknowns - and hardware acceleration on GPUs to compute the extinction cross-sections of arbitrary geometries. We use our software to study how the presence of a biomolecule affects the resonance frequency, aiming towards assisting the design of LSPR-based biosensors. In particular, we will present results for shifts in resonance frequency due to proteins (Bovine Serum Albumin) near a silver nanoparticle.

Thomas Führer
Facultad de Matemáticas
Pontificia Universidad Católica de Chile

Stable multilevel splittings in $H^{-1/2}$

We define and analyse space decompositions of piecewise constant functions in $H^{-1/2}$. Our analysis is based on extension operators from the space of piecewise constants on the boundary to the lowest-order Nédélec space. These splittings naturally induce preconditioners of additive Schwarz type. We show that the resulting condition number is independent of the mesh-size and number of elements. In particular, our results hold true for locally refined meshes. Numerical studies are presented that confirm the obtained results.

This talk is based on joint work with Alexander Haberl, Dirk Praetorius, Stefan Schimanko (Vienna).

Carlos Peréz Arancibia
Institute for Mathematical and Computational Engineering,
Pontificia Universidad Católica de Chile

Density interpolation methods for high-order evaluation of nearly-singular, weakly-singular, singular, and hypersingular boundary integral operators and layer potentials

I will present an effective and simple-to-implement method for the numerical evaluation of Laplace and Helmholtz boundary integral operators and layer potentials in two and three spatial dimensions. The method relies on the use of Green's third identity and local Taylor-like interpolations of density functions in terms of homogeneous solutions of the underlaying PDE. The proposed technique effectively regularizes the singularities present in boundary integral operators and layer potentials, and recasts the former in terms of integrands that are bounded or even more regular, depending on the order of the density interpolation. The resulting boundary integrals can then be easily, accurately, and inexpensively evaluated by means of standard quadrature rules. A variety of numerical examples demonstrate the effectiveness of the technique in the context of NystrÃűm and boundary element methods.

This talk is based on joint work with Catalin Turc (NJIT) and Luiz Faria (MIT).

Elwin van't Wout
Institute for Mathematical and Computational Engineering,
Pontificia Universidad Católica de Chile

The Computational Analysis of the Resonances of Bubble Clouds and Fish Schools with Boundary Element Methods

At specific frequencies, schools of fish can exhibit a high reflectivity of acoustic signals, resulting in deviations in the sonar signal used for underwater surveillance. This phenomenon happens for fish that have swim bladders filled with air and also for clouds of bubbles. This low-frequency resonance, also known as the Minnaert resonance, can be calculated analytically with spherical harmonics for a single bubble. In the case of multiple bubbles, the observed frequency shifts can be analysed effectively with transmission matrices. However, when the distances between bubbles are small, high-accuracy methods need to be used, such as the boundary element method. This presentation will discuss the use of modern boundary element methods to efficiently compute resonance frequencies and compare the performance with the transmission matrix method. The computational results show a clear impact of different bubble cloud configurations on the resonance frequency.