The First Chilean Symposium on
BOUNDARY ELEMENT METHODS

Efficient computational algorithms for simulating wave propagation

A forum for researchers working at the intersection of applied mathematics, engineering, and physics.

Wednesday, December 14, 2016
Pontificia Universidad Católica de Chile
Santiago, Chile

Organized by:
Ingeniería Matemática y Computacional
Pontificia Universidad Católica de Chile

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1. Introduction

Purpose of the symposium
The scientific challenges we face today can only be effectively addressed through interdisciplinary collaborations. The purpose of the symposium is to connect researchers from different scientific fields related to computational science and engineering. Numerical algorithms such as the boundary element method are very powerful as predictive tools for wave propagation and many other physical and engineering problems. The full potential of computational techniques can only be achieved in a collaborative environment of mathematicians, software developers and application scientists.

Overview
The 'First Chilean Symposium on Boundary Element Methods – Efficient computational algorithms for simulating wave propagation,' was held on Wednesday 14 December at campus San Joaquín of Pontificia Universidad Católica de Chile. The symposium attracted 34 attendants consisting of students and academics from Chile and abroad. The participants have been able to enjoy high-quality presentations of the international keynote speakers, invited professors and young researchers. The interdisciplinary character of the symposium was very well appreciated and brought together researchers from applied mathematics, physics and engineering.

Organization committee
Elwin van 't Wout and Clémentine Béchet (*Mathematical and Computational Engineering, UC*).

Sponsors
Vicerrectoría de Investigación, Pontificia Universidad Católica de Chile
Ingeniería Matemática y Computacional, Pontificia Universidad Católica de Chile
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Facultad de Matemáticas, Pontificia Universidad Católica de Chile
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2. Speakers

The keynote presentations were given by two distinguished foreign professors.

Timo Betcke (University College London, United Kingdom)
Biography: Dr. Timo Betcke is a Reader (corresponds to Associate Professor) in the Department of Mathematics at University College London. He finished his DPhil in Numerical Analysis in Oxford in 2006, followed by postdoc positions in Braunschweig (Germany), Manchester and Reading. In 2009 he was awarded a prestigious five year EPSRC Career Acceleration Fellowship and in 2011 moved to University College London, first as Lecturer and since 2013 as Reader in Mathematics. His main interests are in Numerical Analysis and Scientific Computing, in particular the analysis and efficient implementation of boundary element methods. He is the leader of the open-source BEM++ project (www.bempp.org) that develops a widely used boundary element software.

Mahadevan Ganesh (Colorado School of Mines, United States of America)
Biography: Mahadevan Ganesh joined the Department of Mathematical and Computer Sciences at the Colorado School of Mines (CSM) in 2003 as a tenured full Professor, following his seven year tenured position at the University of New South Wales (UNSW), Sydney, Australia. Currently, he is a Professor at the CSM College of Engineering and Computational Sciences (CECS) and he is a Visiting Professorial Fellow at UNSW. At the CSM-CECS he is associated with two departments: Applied Mathematics and Statistics and Electrical Engineering and Computer Sciences. Ganesh is a computational mathematician with research focus on developing, implementing and analyzing fast, high-order, and high-performance computational algorithms for efficient simulation of various physical processes, including wave propagation in random media.

The contributed talks were given by invited academics from Chilean universities:

1. Clémentine Béchet (Mathematical and Computational Engineering, UC);
2. Christopher Cooper (Mechanical Engineering, UTFSM);
3. Christopher Feuillade (Physics, UC);
4. Thomas Führer (Mathematics, UC);
5. Carlos Jerez-Hanckes (Mathematical and Computational Engineering, UC);
6. Michael Karkulik (Mathematics, UTFSM).

Three postgraduate students presented their research as well:

1. María Ignacia Fierro (Mathematical and Computational Engineering, UC);
2. José Pinto (Mentor Graphics *and* Mathematical and Computational Engineering, UC);
3. Gerardo Silva (University of Notre Dame, USA *and* Mathematical and Computational Engineering, UC).

3. Schedule

Time	Speaker	Title
9:00 – 9:25	Registration	
9:25 – 9:30	E. van 't Wout	Opening remarks
9:30 – 10:00	C. Jerez-Hanckes	Electromagnetic wave scattering by random surfaces: uncertainty quantification via sparse tensor boundary elements
10:00 – 10:30	C. Feuillade	Acoustical scattering from single and multiple air bubbles in water
10:30 – 11:00	M. Karkulik	Discontinuous Petrov-Galerkin boundary elements
11:00 – 11:30	C. Béchet	Modeling the beam of a cosmology radiotelescope
11:30 – 12:00	Break	
12:00 – 12:20	I. Fierro	Electromagnetic scattering at a telescope mirror
12:20 – 12:40	G. Silva	Uncertainty Quantification for Electromagnetic Scattering by 1D PEC Gratings
12:40 – 13:40	T. Betcke	Software frameworks for computational boundary element methods
13:40 – 14:50	Break	
14:50 – 15:10	J. Pinto	Efficient and Robust Dyadic Green's Function Evaluation Algorithm for the Analysis of IC Packages and Printed Circuit Boards in the Context of the Method of Moments
15:10 – 15:40	C. Cooper	Simulating protein electrostatics with Python and GPUs: implementation and applications
15:40 – 16:10	T. Führer	On the coupling of DPG and BEM
16:10 – 17:10	M. Ganesh	A hybrid framework with analysis for wave propagation simulation and uncertainty quantification
17:10 – 18:00	Reception	

4. Abstracts

Software frameworks for computational boundary element methods

Timo Betcke (University College London, UK)

Abstract: In recent years Galerkin boundary element methods have become an important tool for large-scale simulations in bounded and unbounded homogeneous media. While the underlying mathematical theory is becoming more mature the development and implementation of fast and robust boundary element methods is still an active field of research. In this talk we present the BEM++ software framework for the solution of a range of boundary element problems from electrostatics, acoustics and computational electromagnetics. The guiding principle of BEM++ is to hide the implementational complexity by providing an interface that is as close to the mathematical description as possible.
We will present the underlying ideas and theory and present a range of interesting applications, in particular in acoustics and computational electromagnetics to demonstrate the design philosophy and capabilities of BEM++.

A hybrid framework with analysis for wave propagation simulation and uncertainty quantification

Mahadevan Ganesh (Colorado School of Mines, USA)

Abstract: We consider a class of exterior wave propagation models with aleatoric and epistemic uncertainties. Using mathematical analysis-based, shape-independent, a priori parameter estimates, we develop offline/online strategies to compute statistical moments of a key quantity of interest in such models. We present a type of cloud computing reduced order model (ROM) and high performance computing (HPC) framework with analysis, for quantifying aleatoric and epistemic uncertainties in the propagation of waves through a stochastic media comprising a large number of three dimensional particles.
Simulation even for a single deterministic three dimensional configuration, using efficient boundary element methods (BEM), is inherently difficult because of the large number of particles. The aleatoric uncertainty in the model leads to a larger dimensional system involving three spatial variables and additional stochastic variables. Accounting for epistemic uncertainty in key parameters of the input probability distributions leads to prohibitive computational complexity. Our hybrid ROM and HPC framework can be used in conjunction with any software to simulate a single particle deterministic wave propagation model.

Modeling the beam of a cosmology radiotelescope

Clémentine Béchet (Mathematical and Computational Engineering, UC)

Abstract: The analysis of the Cosmological Microwave Background and the early age of the Universe requires the development of very specific instruments such

as the Atacama Cosmological Telescope: A six-meter radiotelescope placed at an altitude of 5200m in the Atacama Desert in Chile. In particular the goal of the project ACTPOL is to detect anisotropies of radiation at large angular scales, including some polarized signal of the CMB that constrain the universe models. Such detection requires to have a correct model of the beam of the telescope even at degrees scales, which means in the far sidelobes. We will present the electromagnetic problem of modeling such telescope with its beam, and focus on the difficulties encountered when using commercial and usual software for radio-antennas. I will next present the reasons why we are now studying the problem using Boundary Element Methods, with the benefits we expect from this.

Simulating protein electrostatics with Python and GPUs: implementation and applications

Christopher Cooper (Mechanical Engineering, UTFSM)

Abstract: As opposed to molecular dynamics, implicit-solvent models consider the solvent around a biomolecule as a dielectric region, leading to a coupled system of the Poisson and Poisson-Boltzmann equations. Boundary element methods offer a very efficient way to compute the electrostatic potential in such systems, where the integral equations run over the protein-solvent interface. We implemented a treecode accelerated boundary element Poisson-Boltzmann solver based on Python and CUDA, in a code called PyGBe. In this talk, I will give details on PyGBe and its implementation on GPUs, and show some practical applications on protein solvation, binding, and adsorption.
Towards the end of this talk I will discuss some current developments, related to the improvement of implicit-solvent models, and how we are addressing them from a boundary-element framework.

Acoustical scattering from single and multiple air bubbles in water

Christopher Feuillade (Physics, UC)

Abstract: Acoustical scattering from air bubbles in water is dominated by the monopole resonance response. At the resonance frequency, the scattering cross-section can be significantly greater than the geometrical size of the scatterer. For dense clouds of air bubbles, in the resonance frequency region, radiative interactions between bubbles can cause the ensemble scattering to become highly complex. Additionally, since the wavelength at resonance is generally many times the bubble spacing, the scattered fields interfere strongly. Both features must be incorporated to realistically describe scattering from bubble clouds.
An effective methodology for solving this problem is available through the application of self-consistent multiple scattering techniques, coupled with the solution of sets of coupled differential equations, and incorporating the scattering "kernel" for an individual bubble. All orders of multiple scattering interactions between the bubbles are included, and the aggregate scattering field is calculated by coherent summation.

Results will be presented showing the effects of multiple scattering interactions between bubbles on their ensemble resonance action, and the application of the theory to schools of swim bladder fish.

On the coupling of DPG and BEM

Thomas Führer (Mathematics, UC), joint work with Norbert Heuer and Michael Karkulik

Abstract: We develop and analyze strategies to couple the discontinuous Petrov-Galerkin method with optimal test functions to (i) least-squares boundary elements and (ii) various variants of standard Galerkin boundary elements. Essential feature of our methods is that, despite the use of boundary integral equations, optimal test functions have to be computed only locally. We apply our findings to a standard transmission problem in full space and present numerical experiments to validate our theory. Moreover, the framework extends to more challenging transmission problems with singular perturbations.

Electromagnetic wave scattering by random surfaces: uncertainty quantification via sparse tensor boundary elements

Carlos Jerez-Hanckes (Mathematical and Computational Engineering, UC)

Abstract: For time-harmonic scattering of electromagnetic waves from obstacles with uncertain geometry, we perform a domain perturbation analysis. Assuming as known both the scatterers' nominal geometry and its small-amplitude random perturbations statistics, we derive a tensorized boundary integral equation (BIE) which describes, to leading order, the second-order statistics, i.e., the two-point correlation of the randomly scattered electromagnetic fields. Perfectly conducting as well as homogeneous dielectric scatterers with random boundary and interface, respectively, are considered. Tensor equations for second order statistics of both, Cauchy data on the nominal domain of the scatterer as well as of the far-field pattern are derived, generalizing the work by Harbrecht et al. (2008, Sparse second-moment analysis for elliptic problems in stochastic domains. Numer. Math., 109, 385–414) to electromagnetic problems, and being an instance of the general program outlined by Chernov and Schwab (2013, First order k-th moment finite element analysis of nonlinear operator equations with stochastic data. Math. Comp., 82, 1859–1888). The tensorized BIEs are formulated on the surface of the known nominal scatterer. Sparse tensor Galerkin discretization of these BIEs are proposed and analyzed based on the stability results by Hiptmair et al. (2013, Sparse tensor edge elements. BIT, 53, 925–939); we show that they allow, to leading order, consistent Galerkin approximations of the complete second-order statistics of the random scattered electric field, with computational work equivalent to that for the Galerkin solution of the nominal problem up to logarithmic terms.

Discontinuous Petrov-Galerkin boundary elements

Michael Karkulik (Mathematics, UTFSM), joint work with Norbert Heuer

Abstract: We present an ultra-weak formulation of a hypersingular integral equation on polyhedral surfaces and prove its well-posedness and equivalence with the standard variational formulation. Based on this ultra-weak formulation we present a discontinuous Petrov-Galerkin method with optimal test functions and prove its optimal convergence.
The two-dimensional case on (closed) polygons has been studied in [N. Heuer and F. Pinochet, SIAM-JNA 52, 2703-2721]. In that situation, appearing derivatives are with respect to the arc length, and Sobolev spaces are only of the L^2 and H^1-type. In this talk we study, in particular, open surfaces, where surface differential operators appear and where singularities in the exact solution prohibit to use simple L^2 and H^1 spaces for the ultra-weak formulation, though spaces of orders ±½ are avoided throughout.

Electromagnetic scattering at a telescope mirror

María Ignacia Fierro (Mathematical and Computational Engineering, UC)

Abstract: This presentation is part of a ModEM project, which has as a main objective finding out out how defects on a telescope mirror could cause noise its observations. The hipothesis is that gaps on a telescope surface produce changes on the polarizarion of the field scattered by the mirror. This problem is usually attacked by high frequency methods, as Physical Optics (PO) or Physical Theory of Diffraction (PTD), but in order to validate the results obtained by those methods, we propose to use the Boundary Elements Method on a common problem with the PO/PTD methods. For this reason, in this presentation we show some of the preliminary results that will allow us to decide about the effect of the defects on the telescope mirror and, in the future, to validate or refutate the results obtained by PO/PTD.

Efficient and Robust Dyadic Green's Function Evaluation Algorithm for the Analysis of IC Packages and Printed Circuit Boards in the Context of the Method of Moments

José Pinto (Mentor Graphics and *Mathematical and Computational Engineering, UC), joint work with Giacomo Bianconi and Swagato Chakraborty*

Abstract: We present an algorithm to evaluate each component of the layered media Green's function in fully 3D electromagnetic scenarios such as of IC packages and printed circuit boards. Due to the extremely high cost of each evaluation we present an algorithm to do fast approximations based on local interpolation. The approximations are show to be efficient, accurate and robust, finally we describe how the algorithm is parallelizable.

Uncertainty Quantification for Electromagnetic Scattering by 1D PEC Gratings

Gerardo Silva (University of Notre Dame, USA and *Mathematical and Computational Engineering, UC)*

Abstract: A deterministic numerical method able to calculate the first two statistical moments of the scattered field by a periodic perfect electric conductor surface with stochastic perturbations on its surface was developed and implemented. The electric field integral equation (EFIE) was solved using boundary elements method (BEM), and constant hierarchical bases, called Haar's wavelets. To validate the BEM implementation the method was compared to COMSOL Multiphysics. On the other hand, to validate the stochastic calculations, the algorithm was compared to the Monte-Carlo simulation, obtaining good agreement in both cases. The proposed deterministic approach converges faster than Monte-Carlo simulation, with less computational effort.