

An Analysis of Local Quasi-Continuum-Like Model Reduction Techniques in Material Science Applications

Mihai Anitescu

**Argonne National Laboratory, Mathematics and Computer Science
Division, Argonne, IL**

<mailto:anitescu@mcs.anl.gov>

<http://www-unix.mcs.anl.gov/~anitescu/>

We present a local quasicontinuum-like approach for model reduction of minimum energy problems in materials science, and we give sufficient conditions for the wellposedness of the reduced problem. The approach includes a recent multiscale model reduction approach for orbital-free density functional theory electronic structure calculations that was proposed by the authors as well as the local quasicontinuum approach for potential-based calculations. Numerical results validate our findings.

Algorithms and Designs for Mesh-Free Methods in High Dimensions: Where some of the Challenges Lie

Greg Fasshauer

**Department of Applied Mathematics, Illinois Institute of
Technology, Chicago, Illinois, USA**

<mailto:fasshauer@iit.edu>

<http://math.iit.edu/~fass>

Mesh-free methods are based on a choice of symmetric positive-definite kernel, which is the reproducing kernel of a Hilbert space (also called the native space). Often these kernels are defined as positive definite functions of the Euclidean norm of $x - y$, hence the notion of a radial basis function. Computing radial basis function approximations naively requires solving a dense system of N linear equations, and thus $\mathcal{O}(N^3)$ operations. Alternatives, such as Krylov subspace, fast multipole, fast transform, and moving least squares methods can reduce the operation count, while sometimes increasing the truncation error. Error analysis for function approximation depends on the smoothness of the

kernel and the quality of the design. Unfortunately, traditional radial basis function methods suffer from the curse of dimensionality. Algorithms based on non-Euclidean distances and designs spreading points evenly with respect to these distances are required to make radial basis functions practical in high dimensions. This talk discusses some of the progress made and the important problems not yet solved. This is joint work with Fred Hickernell.

Estimation of L^p -Errors of Itô-Riemann Quadratures for Stochastic Integrals Along Wiener Paths

Henri Schurz

Department of Mathematics, Southern Illinois University,
Carbondale, IL

<mailto:hschurz@math.siu.edu>

<http://www.math.siu.edu/schurz/personal.html>

The L^p -error and its rate of convergence of numerical quadratures of non-anticipative Itô integrals (see Itô, 1944) based on Itô-Riemann sums along non-random partitions of Wiener paths are studied. Simple examples with non-Lipschitzian integrands are given. The main results can be extended to stochastic integrals along diffusion processes (see upcoming papers of the author).

This talk is related to the papers

[1] Henri Schurz: On Estimation of L^p -Errors of Itô-Riemann-Type Numerical Quadratures for Stochastic Integrals Along Wiener Paths, Preprint m-06-001, SIU, 2006 (Proceedings NPSC 3, Dynamic Publishers, Atlanta, p. 221-225).

[2] Henri Schurz: Stochastic α -calculus, a fundamental theorem and Burkholder-Davis-Gundy-type estimates, *Dynam. Syst. Applic.* 15 (2), p. 241-268, 2006.

Simulating Circuits with Diodes and Transistors

David Stewart

Department of Mathematics, University of Iowa, Iowa City, IA

<mailto:dstewart@math.uiowa.edu>

<http://www.math.uiowa.edu/~dstewart/>

Diodes and bipolar junction transistors can be modeled using complementarity conditions. Solving the resulting differential equations with inequality constraints can be done using implicit time-stepping methods where a complementarity problem is solved at each step. This can be done efficiently using

nonsmooth Newton methods.

Boundary Conditions for the Incompressible Stokes and Navier-Stokes Problems – The Struggle Continues...

Dietmar Rempfer

MMAE Department, Illinois Institute of Technology, Chicago, IL

<mailto:Rempfer@iit.edu>

<http://mmae.iit.edu/dietmar/BioPage/>

In a number of recent publications, some authors claim to present well-posed Stokes and Navier-Stokes problems based on "modified" pressure Poisson equations that do not need pressure boundary conditions. We show that, and why, such claims are wrong. A straightforward proof of the ill-posedness of some of these alternative formulations is given.

A Dynamic Viscoelastic Contact Problem with Adhesion

Jeongho Ahn

**Department of Math & Physics, Alfred State SUNY College of
Technology, Alfred, NY**

<mailto:ahnj@alfredstate.edu>

<http://web.alfredstate.edu/ahnj/>

We consider dynamic adhesive contact between a thin viscoelastic body and a stationary rigid obstacle, based on the Signorini's contact conditions. The adhesion process with the bonding field is included in the contact conditions. We prove the existence of solutions for the problem and investigate an energy balance. Employing time-discretization and the finite element method, we compute numerical solutions. The complementarity problem which is formulated in the numerical method is solved, using non-smooth Newton's method.