A FAST ILU PRECONDITIONING-BASED SOLVER FOR THE CHARGE EQUILIBRATION PROBLEM

Hasan Metin Aktulga, Grad Student,
Department of Computer Science, Purdue University

Friday, February 19, 2010
3:00 PM, Birck 1001

Abstract: Charge equilibration (QEq) is the problem of assigning partial electrostatic charges to individual atoms in a molecular dynamics (MD) simulation. It utilizes the neighborhood information of atoms to determine partial charges which minimize the electrostatic energy in the system subject to the constraint of fixed total charge. The formulation of the QEq problem gives us a large sparse linear system of the form Ax = b which can be solved using well-known Krylov subspace methods such as CG or GMRES. However, application of these solvers to the QEq problem only with simple optimizations such as a diagonal preconditioner and a good initial guess does not yield satisfactory results.

In this talk, I will present an ILU preconditioning-based algorithm which can solve the QEq problem much faster while still using the same CG and GMRES solvers. I will demonstrate the performance of the ILU preconditioner on some sample systems. Due to the difficulties of implementing a parallel ILU factorization algorithm, I will restrict my attention to single-processor calculations and small (< 104 atoms) systems. I will briefly point out some potential problems on a large-scale parallel simulation (> 106 atoms) and some solution approaches that can be used to deal with these large systems.

Bio: Hasan Metin Aktulga is a graduate student in the department of computer science at Purdue University. He joined Purdue in August 2004 after completing his B.S. at Bilkent University in Turkey. His research interests include high performance computing, algorithms and applications (especially on molecular dynamics methods).
Uncertainty Quantification of an Analytical MEMS Beam Model

Michael Snow, Grad Student,
Mechanical Engineering, Purdue University

Friday, February 19, 2010
3:00 PM, Birck 1001

Abstract: As the understanding of mechanical structures at small scales advances, it is critical to understand the effects of the poor tolerances endemic to micro-scale manufacturing. Uncertainty quantification typically entails evaluating a model many times to elicit the sensitivity of parameters and find expected performance distributions. This motivates the creation of analytical models that maintain some of the fidelity of an FEM code but are computationally inexpensive. This talk covers the development of a reduced-order model for an electrostatic MEMS beam and the uncertainty quantification performed on this model. An effort was made to create a model more comprehensive than those available in literature, currently the model accounts for beam stretching, variable electrode geometry, fringing electric field, squeeze film damping and contact. Performance characteristics such as pull-in voltage, closing time, and opening time are found for a few hundred Latin-hypercube samples of the parameter space. A response surface (regression) is fit to this data using MARS (Multiple Adaptive Regression Splines). The response surface for each performance metric can then be sampled hundreds of thousands times to find performance PDFs based on input variation. The response surface can also be analyzed to determine which input parameters are most critical to the beams performance.

Bio: Michael Snow received his B.S. Degree in mechanical engineering from Purdue University in 2008. He is currently a mechanical engineering graduate student working with the PRISM program. His research interests include robotics as well as RF MEMS design, modeling and optimization under uncertainty with a focus on novel RF switches.