Scalable Solvers for Inhomogeneous Fluids

Michael A Heroux, Sandia National Laboratories
Laura J D Frink, Sandia National Laboratories

Summary

Density functional theories for inhomogeneous fluids enable the modeling of a wide range of important science problems including porous materials and biological mechanisms at the cell level. Our project is focused on reformulation and solution of the implicit equations in these models with the goals of improving robustness, scalability and efficiency. Our recent efforts include the introduction of Coulomb and diffusion effects to our Schur complement solvers, the first Open Source public release of Tramonto and scalability studies and preparation for petascale class computations.

Introduction

Density functional theories (DFTs) have been tremendously successful in treating a variety of systems at many length scales. In all cases, the fundamental problem is to predict the structure of an inhomogeneous fluid as captured by a density distribution. At the smallest length scale the most well known application of DFT is to predict the structure of quantum mechanical systems. Using a similar mathematical construct but with non-exact density functionals, the structure of atomic, molecular, and polymer fluids can be computed. Fluid inhomogeneities can result from surfaces (e.g. planar interfaces, porous materials, or large geometrically complex macromolecules) or from competing intramolecular and intermolecular interactions that can lead to self-assembly. Mesoscale-DFTs have also been developed for colloidal fluids and biological macromolecules.

Our Approach

Our focus as been on real-space methods for DFTs applied to fluids (Fluid-DFTs). These equations require the simultaneous solution of challenging nonlinear problems on a 2 or 3 dimensional domain, with tens to hundreds of unknowns per grid point. Previous work solved these problems as general sparse system of equations, with some success. Our project looks at Fluid-DFTs from a multi-scale perspective, leading to insights about how to efficiently solve the discrete system of equations using segregated Schur complement preconditioners. Our new algorithms have many attractive properties and have enabled scalable parallel solutions for several important classes of problems, namely hard-sphere models and polymer chains.

Enhanced Model Capabilities

Our previous work established a mathematical framework for efficient scalable solvers for hard-sphere and polymer problems. More recently we have developed scalable algorithms to address Coulomb and diffusion effects. These effects introduce a significant spatial interaction into the equations. However, we are able to address this interaction by leveraging proven scalable preconditioners and direct methods within our global solution algorithms, thereby retaining

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scalability of the global problem. Because of software design we can in fact use existing highly-optimized multi-level preconditioner packages to aid our solution.

Open Source Software Release

All of our algorithms work has been implemented in a scalable application code called Tramonto. Tramonto version 2.1 was release in March 2007 as an Open Source package under the GNU Lesser General Public License (LGPL), and is available for download from the website http://software.sandia.gov/tramonto.

Impact

Using our algorithms within Tramonto has led to fundamentally new calculations for important biology problems. Quotes from Physical Review Letters referees on computations using these solvers include the following:

- "This is (to my knowledge) the first time [Fluid] DFT has been used to analyze the important problem of pore structure in biological membranes."
- "This appears to me to be a highly significant advance in theoretical biophyics, even by the high standards of Physical Review Letters. I suspect that this Sandia group is the only one in the world to have developed classical DFT methods sufficiently sophisticated to deal with such a remarkably complex problem in colloidal physics…"
- "…I would then recommend at least a footnote that gives some introductory hint as to how they have managed to cope numerically with such complex structures; presumably a 3d finite element method with all manner of tricks?

The "tricks" are the solvers. Our initial algorithms work will appear in the paper entitled *Parallel Segregated Schur Complement Methods for Fluid Density Functional Theories*, M. Heroux, L. Frink, A. Salinger to appear in SIAM SISC.

Future Plans: Toward Petascale Capabilities

Although we have solved many challenging problems in the last year and can effectively utilize a thousand or more processors, we have been preparing to run Tramonto on petascale class systems. Several load-balancing challenges exist, but we are otherwise poised to utilize next-generation petascale systems.

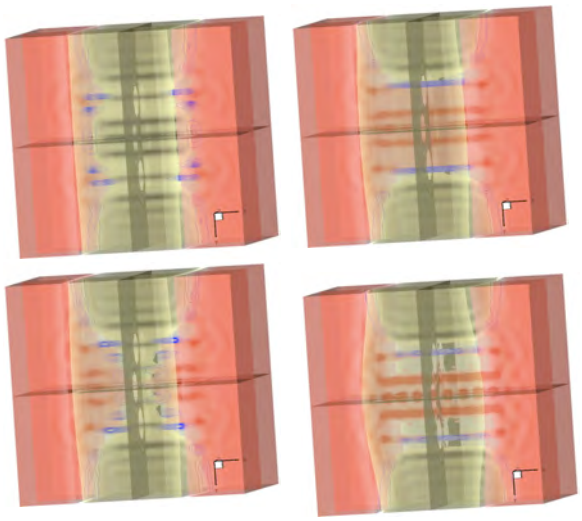

Figure 1: *3D Studies of Antimicrobial Peptide Assemblies in lipid bilayers with Chandler-McCoy-Singer (CMS) DFT formulation. The CMS DFT formulation models freely-jointed linear polymers using second-order functional expansion.*

For further information on this subject contact:
Dr. Anil Deane, Program Manager
Applied Mathematics Research Program
Office of Advanced Scientific Computing Research
Phone: 301-903-1465
deane@mics.doe.gov