# Scalable Solvers for Inhomogeneous Fluids

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## 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. To this end we have completed the development of new algorithms for a variety of difficult problems and demonstrated scalable performance leading to one or more orders of magnitude improvement of capabilities.***

## 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.

## Solution properties

Exploiting some of the special structure of Fluid-DFTs equations, we are able to formally reduce the problem size by an order of magnitude or more. Furthermore our numerical results have proven the following desirable properties:

- **Scalability in iterations:** Unlike many preconditioned iterative methods, our algorithm results are invariant to processor count.

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- **Scalability in processor count:** For 3D problems our new solvers have shown linear scalability in arithmetic cost and superlinear speedup in real time (due to cache effects) for fixed size problems (strong scaling).
- **Memory Use:** Memory use is reduced by a factor of 5-20 over previous methods.
- **Tuning parameter:** We require no user-supplied tuning parameters for the preconditioner.
- **Scalability in mesh density:** Our new solvers are not invariant under mesh density changes, but nearly so. In fact, except for the coarsest mesh, the number of solver iterations remains nearly constant as the mesh density increases.
- **Scalability in chain length:** For polymer problems, our new solver has constant iteration count as the chain size increases. Furthermore, the cost of the solver grows approximately linearly with the length of the chain.

## Impact

By providing a scalable, reliable solution capability to the Fluid-DFT application Tramonto, we have enabled the solution of many new problems, as well as detailed studies of families of related problems. As an example, computing interactions of nanoscale surfaces and colloidal particles with lipid bilayers are needed to provide a molecular theory based analysis of surface forces experiments (e.g. surface forces apparatus, atomic force microscope, optical tweezers, etc) for these systems. This type of calculation is also needed for studying the interactions of lipid bilayers with proteins. Figure 1 shows results for one such problem, previously unsolvable because of robustness and scalability issues.

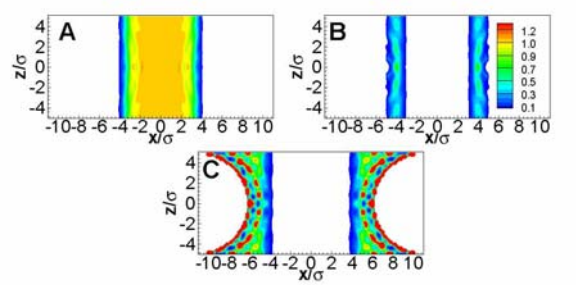


*Figure 1: One slice (at y = 0) through a 3-dimensional computational volume. The color contours show density distributions for lipid tail beads (A), lipid head beads (B), and solvent (C) for a lipid bilayer assembly sandwiched between planar arrays of large spheres. The computational domain is 1/4 of the domain shown in the figure and utilized reflective boundary conditions on all edges. The legend shows the contour scale for all three figures.*

## Future Plans

Although we are able to model a variety of problems already, our present and future work is focused on incorporating Coulomb effects into the model. This feature introduces a spatial Poisson operator that we hope to solve using a multi-level preconditioner as part of our segregated Schur complement framework. Further efforts include mesh coarsening and polymer symmetry efficiencies to reduce model complexity. Finally, we are exploring the use of new parallel partitioning algorithms (hypergraph reorderings) in order to improve load imbalance as we target 1000+ processor systems.

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