Enabling Tools for Extreme Scale Computation of Nanoscale Fluids

Linear Algebra for Extreme Scale Computing of Nanoscale Fluids

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Abstract

Fluid density functional theories applied to inhomogeneous fluids (fluid-DFTs) enable modeling and simulation of a wide range of applications, including fluids at interfaces, colloidal fluids, wetting, porous media, and biological mechanisms at the cellular level. The ability to solve the fluid-DFT governing equations in 3D and at large scales is crucial to continued scientific progress. To realize the promised performance of modern high-end multicore systems, we must develop new algorithmic capabilities to efficiently use multicore nodes by reducing our node-level memory bandwidth and size usage. The core of our solution strategy utilizes and builds upon Segregated Multi-level Schur Complement Methods (SMSC methods), which efficiently leverage a rich block structure inherent in the fluid-DFT governing equations.

One enabling tool we discuss is the development of block Krylov recycling methods, which improves solver performance in two ways. First, recycling methods solve a family of linear systems by reusing subspace information from previous solutions, reducing the number of required iterations. Second, block methods have superior convergence properties and computation to bandwidth requirements, improving processor utilization.

A second enabling tool we discuss is mixed-precision algorithms. Solver kernels utilizing 32-bit precision are more amenable for multicore systems, but must be deployed in such a way as to not compromise robustness or the accuracy of the final computed solution. To provide for mixed-precision algorithms, we require multiple ingredients. The first ingredient is the ability to utilize our fluid-DFT solvers with single precision, which we achieve by leveraging the Tpetra and Kokkos packages within the Trilinos project. The second ingredient is utilization of least-squares methods that, when coupled with mixed precision computations, can be used to solve linear problem formulations that are numerically singular due to the use of lower precision.

We discuss progress on development and deployment of these and other techniques in the Sandia National Laboratories fluid-DFT code, *Tramonto*.