Algorithmic Challenges in solving Density Functional Theories for Fluids at Interfaces

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Density functional theories for fluids at interfaces occupy a unique mathematical niche, and are often characterized as systems of integral equations of finite extent. As a result of the unique mathematical properties, the optimization of algorithms for solving these systems of equations requires new and different approaches than have been developed for solution of systems based on partial-differential equations (PDEs). This seminar will briefly overview the field from a physics and engineering perspective in order to illustrate the importance of this class of problems both for both nanoscale and multiscale modeling of materials and biological systems. In addition, we will discuss the challenges presented by these systems of equations from an algorithms perspective. Specifics will include the properties of the matrices found in these systems, some recent work on solvers designed specifically for these DFTs, and progress on parallel partitioning. The seminar will demonstrate the rich opportunities available for both algorithms and physics research in nanoscale modeling of interfacial fluids.