Masha Sosonkina

Iterative solution techniques for flexible approximation schemes in multiparticle simulations

Ames Laboratory DOE
Ames IA 50011
masha@scl.ameslab.gov
Igor Tsukerman, Elena Ivanova, Sergey Voskoboynikov

The paper examines various parallel iterative solvers for the new Flexible Local Approximation MEthod (FLAME) [5, 6] applied to colloidal systems. The electrostatic potential in such systems can be described, at least for monovalent salts in the solvent, by the Poisson-Boltzmann equation (see e.g. [2]). Classical Finite-Difference (FD) schemes would require unreasonably fine meshes to represent the boundaries of multiple spherical particles at arbitrary locations with sufficient accuracy. In the Finite Element Method, mesh generation for a large number of particles becomes impractical. The Fast Multipole Method works well only if the particle sizes are neglected and the Poisson-Boltzmann equation is linearized [1].

Classical FD schemes rely on Taylor expansions that break down near material interfaces (such as particle boundaries) due to the lack of smoothness of the field. In FLAME, Taylor expansions in the vicinity of the particles are replaced with much more accurate approximations. Namely, the local FLAME bases are constructed by matching (via the boundary conditions) the spherical harmonics for the electrostatic potential inside and outside the particle; see [5, 6] for details.

The system matrices of FLAME and classical FD have the same sparsity structure for the same grid stencil on a regular Cartesian grid; for example, the standard seven-point stencil leads to a seven-diagonal matrix. However, the FLAME matrix is generally nonsymmetric. Several parallel iterative solution techniques have been tested with an emphasis on suitable parallel preconditioning for the nonsymmetric system matrix. In particular, flexible GMRES [3] preconditioned with the distributed Schur Complement [4] has been considered and compared with Additive Schwarz and global incomplete ILU(0) preconditionings. It has been observed that Schur Complement preconditioning with a small amount of fill and a few inner iterations scales well and exhibits good solution times while attaining almost linear speedup. The number of iterations and the computational time depends only mildly on the Debye parameter of the electrolyte.

Bibliography

[1] L. F. Greengard and J. Huang. A new version of the Fast Multipole Method for screened Coulomb interactions in three dimensions. *J. Comput. Phys.*, 180(23):642–658, 2002.

[2] A. Yu. Grosberg, T. T. Nguyen, and B. I. Shklovskii. Colloquium: The physics of charge inversion in chemical and biological systems. *Reviews of Modern Physics*, 74(2):329–345, 2002.

[3] Y. Saad. *Iterative Methods for Sparse Linear Systems, 2nd edition*. SIAM, Philadelpha, PA, 2003.

[4] Y. Saad and M. Sosonkina. Distributed Schur Complement techniques for general sparse linear systems. *SIAM J. Scientific Computing*, 21(4):1337–1356, 1999.

[5] I. Tsukerman. Electromagnetic applications of a new finite-difference calculus. *IEEE Trans. Magn.*, 41(7):2206–2225, 2005.

[6] I. Tsukerman. A class of difference schemes with flexible local approximation. *J. Comput. Phys.*, 211(2):659–699, 2006.