NSF Research Proposal

Bill March

Computer simulations are widely used in chemistry, biology and physics. (Discuss more about exciting applications).

All of these simulations require the scientist conducting them to make basic choices about the level of approximation in the calculations and the scale of the system studied. Most of the effort in developing simulation techniques is spent on determining the right balance between these factors. For example, force field parameters in molecular biology, basis sets in computational chemistry. In order for these methods to progress substantially, there must be new computational methods that allow better accuracy without sacrificing large systems and reasonable computing times.

One of the fundamental simplifying assumptions in these systems is that all interactions are pairwise (rephrase). This approximation is accurate in some systems, but fails on others. Liquid argon, water, etc. These examples are well known, but 3-body terms in other systems are rarely considered. Historically, researchers have had little impetus to study three-body terms, since they are too slow for interesting systems. We believe that if 3-body calculations are made tractable, they will attract more attention.

We propose a general framework for making three-body potentials computationally feasible for large systems. (This paragraph needs to say more, but I'm not sure what). In particular, we will investigate a fast version of the Axilrod-Teller potential [1]. This potential is commonly applied to simulations involving noble gases. In general, we expect our work to be easily applicable to other many-body potentials. Additionally, we intend to investigate similar methods for other computations involving several interactions, such as the repulsion and exchange integrals in Hartree-Fock [4].

Even the simplest simulations are intractable for large systems. For short-range interactions, it is generally acceptable to cut off computations beyond a small radius, thus making these calculations manageable. For long range interactions, especially electrostatics, cutoffs are too imprecise.

The Fast Multipole Method [3] makes large-scale electrostatic computations feasible. The FMM groups charged particles in a space-partitioning tree. The FMM groups charges together. The interaction between two groups of charges can be approximated efficiently.

The space-partitioning and approximation ideas employed in the FMM can be applied to many other problems [2]. Elaborate more on the methods here. Examples are DTFGT etc.

These techniques (meaning series expansions and trees) can be extended to treat multibody potentials.

References

[1] B. M. Axilrod and E. Teller. Interaction of the van der waals type between three atoms. *J. Chem. Phys.*, 11(299), 1943.

[2] A. Gray and A. W. Moore. N-body problems in statistical learning. In T. K. Leen, T. G. Dietterich, and V. Tresp, editors, *Advances in Neural Information Processing Systems 13 (December 2000)*. MIT Press, 2001.

[3] L. Greengard and V. Rokhlin. A Fast Algorithm for Particle Simulations. *Journal of Computational Physics*, 73:325–248, 1987.

[4] A. R. Leach. *Molecular modelling : principles and applications*. Prentice Hall, Harlow, England, 2nd ed edition, 2001.