THE MULTILEVEL SUMMATION METHOD: A PYTHON IMPLEMENTATION

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1. Problem Statement. -Multilevel summation method[2]: Efficient method for evaluation of long-range interactions in n-body type problems. Traditionally used to calculate forces in molecular dynamics simulations.

-MSM important because permits linear time algorithm for evaluation. Traditionally FFT used, efficient but requires periodic domain; results in unwanted interactions from copies of domain in surrounding periodic repeats.

-Algorithm has similar structure/idea to multigrid v-cycle approaches: smoothing, restriction of smooth part to coarser grid, evaluation of new short range interactions (repeat until coarsest level), then interpolation of smooth parts back down cycle until finest level[1].

2. Approach. -Implement main parts of algorithm in Python: smooth part separation, restriction, short-range interaction, interpolation.

-For simplicity a serial implementation will be used.

-After implementation will test various random charge distributions with increasing number of charges to evaluate scaling performance for number of bodies.

3. Numerical Results. Smoothing (separation of short/long-distance parts of interaction) is first part of numerics being worked on currently.

-Example plot of smoothing implementation:

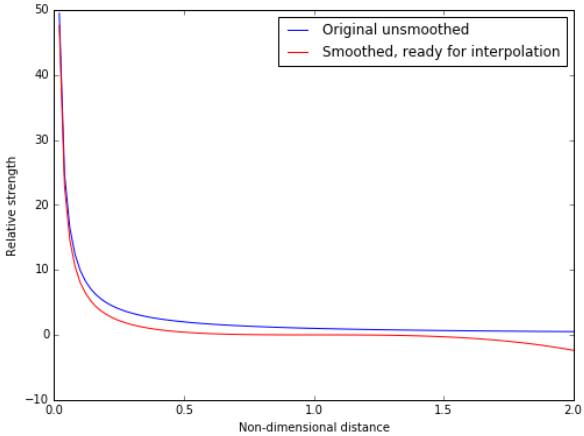

FIG. 1. *Comparison of original and smoothed interaction for a single particle.*

-Uses same smoothing approach as described in 2015 Hardy paper [1].

4. Conclusions.

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REFERENCES

[1] David J. Hardy, Zhe Wu, James C. Phillips, John E. Stone, Robert D. Skeel, and Klaus Schulten. Multilevel Summation Method for Electrostatic Force Evaluation. Journal of Chemical Theory and Computation 2015 11 (2), 766-779 DOI: 10.1021/ct5009075

[2] Hardy, D. J. Multilevel summation for the fast evaluation of forces for the simulation of biomolecules. Ph.D. thesis, University of Illinois at UrbanaChampaign, Champaign, IL, 2006; Also Department of Computer Science Report No. UIUCDCS-R-2006-2546, May 2006.