Anansi – A Multilevel Summation Method Solver: A Performance Portable Exascale Capable Electrostatic Solver

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We are developing a long-range electrostatic solver that is performance portable and targets HPC centers with hybrid CPU-GPU architectures. The solver uses the Multilevel Summation Method (MSM) which is a local (nearest-neighbor communication) hierarchal grid based algorithm. The current MSM developmental activities can be grouped in two broad categories.

The first category is disentangling the MSM algorithm from the underlying HPC architecture hardware. This is primarily accomplished by software abstraction layers between the MSM algorithm and the CPU and GPU compute devices. This design feature helps performance portability by minimizing the amount of code modifications needed for various HPC CPU/GPU architectures and the ongoing improvements in the GPU hardware and CUDA API.

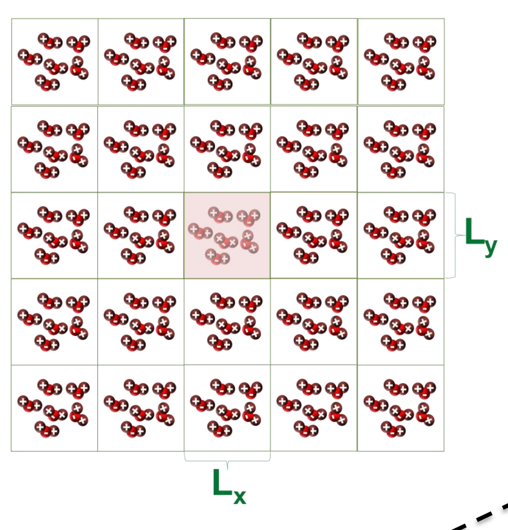
The second activity is the implementation of a CUDA direct kernel for the direct stencil calculation on the grid hierarchies. This direct kernel uses large stencils with minimum dimensions of 13x13x13 and will explore the use of unified memory. Importantly, the direct kernel is not a simple function but a C++ class that is designed by composition and derivation from an abstract base class. This design structure helps attain performance portability and permits rapid implementation of other types of large stencil calculations.

Background

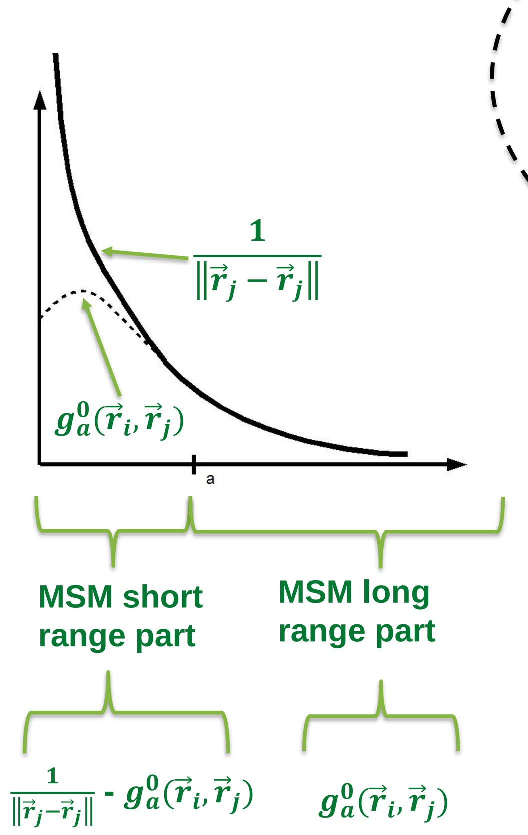
Calculation of long-ranged electrostatics is a major bottleneck in classical MD simulations

$$U_{electrostatic} = \frac{1}{4\pi\varepsilon_o}\sum_{i=1}^{N}\sum_{j<i}^{N}\sum_{n\in\mathbb{Z}^3}\frac{q_i q_j}{\|\vec{r}_j - \vec{r}_j + L^n\|}$$

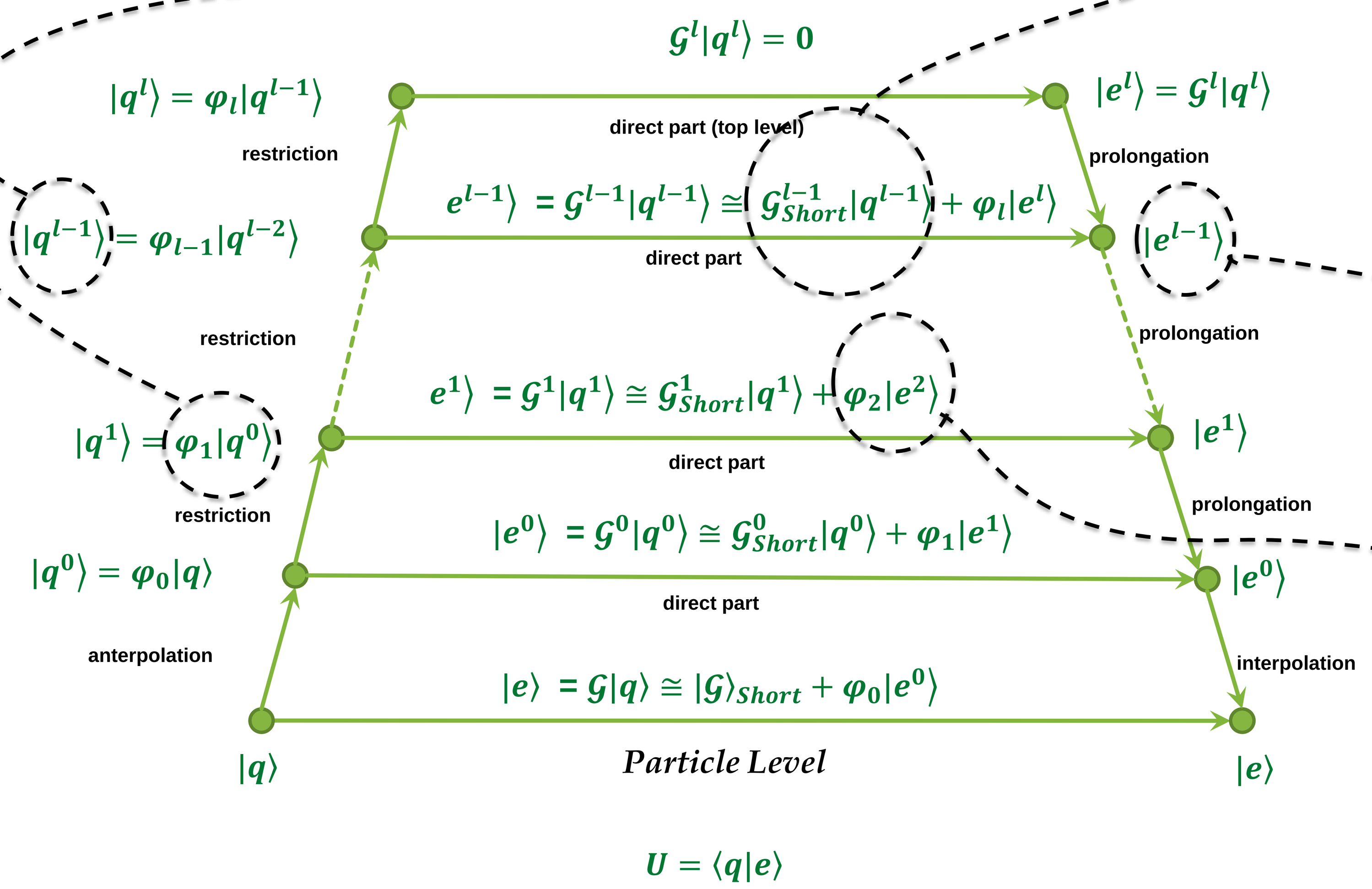
PME is the dominant algorithm for calculating the long-ranged electrostatics, however it has severe communication issues at large system sizes



1. Separation of the electrostatic interaction potential into a MSM short range part plus a MSM long range, slowly varying part
2. Approximate the slowly varying MSM long range part to a grid.
3. Recursive application of the first two ideas on a hierarchy of coarser grids [1].



Graphical representation of MSM



Overview of implementation

Anansi is implemented as a library

C2 Restriction Class
$|q^N\rangle = \varphi_N|q^{N-1}\rangle$

Abstract Base Restriction
- CPU Hardware Architecture Interface
- GPU Hardware Architecture Interface

Direct Restriction Class
$\mathcal{G}^l_{Short}|q^l\rangle$

Abstract Base Direct
- CPU Hardware Architecture Interface
- GPU Hardware Architecture Interface

Prolongation Class
$\varphi_l|e^l\rangle$

Abstract Base Prolongation
- CPU Hardware Architecture Interface
- GPU Hardware Architecture Interface

Charge grid, $|q^N\rangle$

Abstract Base Grid
- Global Arrays Communicator

Potential grid, $|e^N\rangle$

Abstract Base Grid
- Global Arrays Communicator

Global Arrays Communicator

Base Communicator

References/Acknowledgements

[1] **Hardy, David.** "Multilevel Summation For the Fast Evaluation of Forces for the Simulation of Biomolecules" Ph.D. diss., University of Illinois at Urbana-Champaign, 2006.

[2] **Hardy, David., Stone, John., and Schulten, K.** 2009. Multilevel Summation of Electrostatic Potentials Using Graphics Processing Units. Parallel Computing vol 35: pg. 164-177.

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