

**Stony Brook University  
The Graduate School**

Doctoral Defense Announcement

**Abstract**

Parallel Spherical cutoff 3D FFT and its implementation in SPME algorithm for biophysical simulation studies: Application to the 6D torus QCDOC supercomputer

By

**Bin Fang**

In order to model complex heterogeneous biophysical systems with non-trivial charge distributions such as globular proteins in water, it is important to evaluate the long range forces present in these systems accurately and efficiently. The Smooth Particle Mesh Ewald summation technique (SPME) is commonly employed to determine the long range part of electrostatic energy in large scale molecular simulations. While the SPME technique does not give rise to a performance bottleneck in a single processor or scalar computation, current implementations of SPME on massively parallel, supercomputers become problematic at large processor numbers, limiting the time and length scales that can be reached. Here, two accomplishments have been made in this dissertation to give rise to both improved accuracy and efficiency on both massively parallel and scalar computing platforms. First of all, a new modification of the SPME technique is exploited, which was inspired by the non-linear growth of the approximation error of Euler Exponential Spline interpolation function. Secondly, a well designed parallel framework of 3D complex-to-complex FFT and 3D real-to-complex FFT for the novel QCDOC supercomputer with its 6D-torus architecture is given. The efficiency of this framework was tested on up to 4096 processors. This fine grained parallel implementation of SPME has been embedded into MDoC package. Numerical tests of package performance on up to 1024-processor QCDOC supercomputer residing at Brookhaven National Lab are presented for two systems of interest,  $\beta$ -hairpin solvated in explicit water, a system which consists of 1142 water molecules and a 20 residue protein for a total of 3579 atoms, and HIV-1 protease solvated in explicit water, a system which consists of 9331 water molecules and a 198 residue protein for a total of 29508 atoms.

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