Explore Refactoring and Accelerating a Molecular Dynamics Application on GPUs

Yuba Bhandari has developed state of art algorithm that matches experimental molecular dynamics results with simulated code.

Eric Stahlberg has explored the optimization of this code in terms of runtime and input interface on intel multicore processors using OpenMP.

Given the availability of GPU accelerator on Biowulf and the national labs supercomputer, it is worth exploring if further speedup can be achieved using GPUs.

Objectives:

1- Implement an GPU version of the time consuming hotspots of the code.

2- Explore the implementation of a web interface to allow users outside the NCI to use the application.

3- Explore further refactoring of the code to enhance the optimization process.

CLICK HERE for the full report.