GPU Technology Conference 2010 Sessions on Molecular Dynamics (subject to change)

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2269 - Bringing GPUs to Mainstream Molecular Dynamics Packages

Recent work in close collaboration with NVIDIA has produced a GPU accelerated version of the AMBER Molecular Dynamics Code PMEMD that runs between 20 and 130 times the speed of a single 2.8GHz Intel Nehalem Processor, with even higher performance on multiple GPUs, but which does not make sacrifices in the accuracy or validity of such calculations to achieve this. The GPU accelerated version supports both explicit solvent particle mesh ewald (PME) and implicit solvent simulations and is available as part of the new AMBER 11 package. This talk will provide an overview of the AMBER software, background behind this GPU work, benchmarks, the impact that GPU accelerated MD can have on the field, the techniques used to achieve the performance seen without sacrificing accuracy and finally the validation methods used to ensure simulations are directly equivalent to CPU based calculations. Ensuring that a GPU implementation of a MD package provides results that are indistinguishable from the CPU code is extremely tricky and often the desire to take shortcuts to boost performance can affect accuracy with unpredictable results. We have developed a comprehensive validation suite that can be used to perform the detailed testing that is required to ensure the approximations necessary for GPU performance do not impact the scientific results. Additionally we will discuss how we have made careful use of mixed single and double precision arithmetic in the AMBER implementation to achieve equivalence in the results without excessively compromising performance. Finally we provide examples of recent breakthrough simulations conducted using GPU enabled AMBER 11.

Speaker: Ross Walker, San Diego Supercomputer Center

Topic: Molecular Dynamics

Time: Thursday, September, 23rd, 10:00 - 10:50

2007 - Folding@home: Petaflops on the Cheap Today; Exaflops Soon?

Learn how Folding@home has used petascale computing with GPUs to make fundamental breakthroughs in computational biology and how this technology can make an impact in your work.

Speaker: Vijay Pande, Stanford University

Topics: Life Sciences, Cloud Computing, High Performance Computing, Molecular Dynamics

Time: Thursday, September, 23rd, 11:00 - 11:50

2086 - GPGPU DL_POLY

Discover DL_POLY.

1. DL_POLY: an MD code ICHEC has ported to CUDA. The presentation especially focuses on the auto-tuning of the work distribution between CPU and GPU

Speaker: Gilles Civario, ICHEC

Topics: Molecular Dynamics, High Performance Computing

Time: Thursday, September, 23rd, 16:00 - 16:50

2062 - HOOMD-blue: Fast and Flexible Many-Particle Dynamics

See the newest capabilities and performance enhancements in HOOMD-blue, a general-purpose many-particle dynamics application written for GPUs. Speedups of 80-100x are attained for a wide range of simulation types. Topics for this presentation include an overview of HOOMD-blue, design and implementation details of the underlying algorithms, and a discussion on how generality is maintained without sacrificing performance.

Speaker: Joshua Anderson, University of Michigan

Topics: Molecular Dynamics, High Performance Computing, Life Sciences, Physics Simulation

Time: Thursday, September, 23rd, 15:00 - 15:50

2073 - High Performance Molecular Simulation, Visualization, and Analysis on GPUs

This talk will present recent successes in the use of GPUs to accelerate interactive visualization and analysis tasks on desktop computers, and batch-mode simulation and analysis jobs on GPU-

accelerated HPC clusters. We'll present Fermi-specific algorithms and optimizations and compare with those for other devices. We'll also present performance and performance/watt results for NAMD molecular dynamics simulations and VMD analysis calculations on GPU clusters, and conclude with a discussion of ongoing work and future opportunities for GPU acceleration, particularly as applied to the analysis of petascale simulations of large biomolecular complexes and long simulation timescales.

Speaker: John Stone, University of Illinois at Urbana-Champaign

Topics: Molecular Dynamics, Algorithms & Numerical Techniques, High Performance Computing, Life Sciences

Time: Wednesday, September, 22nd, 16:00 - 16:50

2128 - Hybrid Quantum Mechanics/Electrodynamics (QM/ED) Modeling of Solar Cells on a CUDA Cluster

One of the greatest challenges of the twenty-first century is the utilization of renewable energy. In providing a theoretical explanation and guidelines for computer-aided design of dye-sensitized solar cell (DSSC), we recently developed a hybrid multi-scale quantum mechanics/classical electrodynamics (QM/ED) methodology.

Our numerical simulations were tested on a CUDA enabled Linux cluster using CP2K. We extended its CUDA implementation to MPI parallel environment. Our preliminary results demonstrated a superior performance advantage of hybrid MPI/GPGPU programming that could potentially shorten the total simulation wall time by an order of magnitude.

Speaker: Hanning Chen, Northwestern University

Topics: Quantum Chemistry, Energy Exploration, Molecular Dynamics, Physics Simulation

Time: Wednesday, September, 22nd, 17:00 - 17:50

2168 - Interactive Molecular Dynamics for Nanomechanical and Nanochemical Experiments

Hear how the combination of GPU accelerated molecular dynamics simulation software, 3D TV displays, affordable haptic game controllers, and high performance molecular visualization is leading to new ways to study materials and objects on the nanoscale. We will present the concept of an appliance for integrated virtual nanoscale experiments and challenges related to software and hardware.

Speaker: Axel Kohlmeyer, Institute for Computational Molecular Science, Temple University

Topic: Molecular Dynamics

Time: Wednesday, September, 22nd, 10:00 - 10:50

2054 - NAMD, CUDA, and Clusters: Taking GPU Molecular Dynamics Beyond the Desktop

A supercomputer is only as fast as its weakest link. The highly parallel molecular dynamics code NAMD was one of the first codes to run on a GPU cluster when G80 and CUDA were introduced in 2007. Now, after three short years, the Fermi architecture opens the possibility of new algorithms, simpler code, and easier optimization. Come learn the opportunities and pitfalls of taking GPU computing to the petascale.

Speaker: James Phillips, University of Illinois

Topics: Molecular Dynamics, High Performance Computing, Life Sciences, Physics Simulation

Time: Thursday, September, 23rd, 14:00 - 14:50

2218 - Redesigning Molecular Dynamics for GPUs and GPU Clusters

Generalized Born and Particle Mesh Ewald (PME) molecular dynamics are two computationally intensive algorithms for simulating biological molecules. While several adaptations of Generalized Born have attained excellent speedup on GPUs, high performance Particle Mesh Ewald has been more elusive. Here we describe in detail a recent port of PME implemented within AMBER 11 that has achieved performance on par with up to 128 nodes of a top ten supercomputer.

Speaker: Scott Le Grand, NVIDIA

Topics: Molecular Dynamics, Algorithms & Numerical Techniques, High Performance Computing, Life Sciences

Time: Wednesday, September, 22nd, 15:00 - 15:50

2006 - Short-Range Molecular Dynamics on GPU

Learn how to accelerate short-range molecular dynamics using CUDA C. We will cover building the neighbor list and calculating the forces on the GPU. To handle the case where a few particles have significantly more neighbors than most other particles, we propose a hybrid data

structure for the neighbor list that can achieve a good balance between performance and storage efficiency. A CUDA C implementation of the technique for Leonard-Jones forces can be found in the LAMMPS molecular dynamics open source code.

Speaker: Peng Wang, NVIDIA

Topic: Molecular Dynamics

Time: Wednesday, September, 22nd, 17:00 - 17:50

2035 - Simulations of Large Membrane Regions

Learn how to study membrane-bound protein receptors by moving beyond the current state-of-the-art simulations that only consider small patches of physiological membranes. Towards this end, this session presents how to apply large-scale GPU-enabled computations of extended phospholipid bilayer membranes using a GPU code based on the CHARMM force field for MD simulations. Our code enables fast simulations of large membrane regions in NVT and NVE ensembles and includes different methods for the representation of the electrostatic interactions, i.e., reaction force field and Ewald summation (PME) methods. Performance and scientific results for dimyristoylphosphatidylcholine (PC) based lipid bilayers are presented.

Speakers: Michela Taufer, University of Delaware, Narayan Ganesan, University of Delaware, Sandeep Patel, University of Delaware

Topics: Molecular Dynamics, High Performance Computing, Physics Simulation

Time: Wednesday, September, 22nd, 11:30 - 11:50