UCLA Department of Chemistry & Biochemistry

Physical Chemistry Seminar

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Transforming Molecular Biology Research through Extreme Acceleration of AMBER Molecular Dynamics Simulations: Sampling for the 99%

This talk will cover recent developments in the acceleration of Molecular Dynamics Simulations using NVIDIA Graphics Processing units with the AMBER software package. In particular it will focus on recent algorithmic improvements aimed at accelerating the rate at which phase space is sampled. A recent success has been the reproduction and extension of key results from the DE Shaw 1 millisecond Anton MD simulation of BPTI (Science, Vol. 330 no. 6002 pp. 341-346) with just 2.5 days of dihedral boosted AMD sampling on a single GPU workstation, (Pierce L, Walker R.C. et al. JCTC, 2012 in review). These results show that with careful algorithm design it is possible to obtain sampling of rare biologically relevant events that occur on the millisecond timescale using just a single $500 Graphics Card and a desktop workstation. Additional developments highlighted will include the acceleration of AMBER MD simulations using graphics processing units including Amazon EC2 based automated ensemble calculations, a new precision model optimized for the Kepler architecture, approaches for running large scale multi-dimensional GPU accelerated replica exchange calculations on the Keeneland and BlueWaters supercomputers, recent performance breakthroughs and ways to build your own desktop GPU accelerated MD supercomputer for less than $2000.

Monday, April 15, 2013
4:00 P.M.
2033 Young Hall

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