CORE PROGRAM
GENOME SCALE BIOLOGY & BIOINFORMATICS

BIOZENTRUM Universität Basel

[BC]^2 Special Seminar

Dr. István Kolossváry

D. E. Shaw Research, New York, NY, USA

"Novel algorithms in Desmond enabling practical microsecond-scale molecular dynamics simulations in the Maestro environment"

Although molecular dynamics (MD) simulations of biomolecular systems often run for days to months, many events of great scientific interest and pharmaceutical relevance occur on long timescales that have remained beyond reach. We recently introduced several algorithms that significantly accelerate classical MD simulations compared with current state-of-the-art codes.
These algorithms include parallel decompositions that reduce interprocessor communication requirements and numerical techniques that maintain high accuracy even with single-precision computation. Using these methods, we have developed an MD code called Desmond which achieves unprecedented speed and parallel scalability for all-atom, explicit-solvent simulations, enabling simulation rates above a microsecond per week on commodity clusters. These simulation rates represent an order-of-magnitude performance improvement over several widely used MD codes, broadening the range of biological problems amenable to study by MD simulation.

Please note:

- *Dr. Kolossvary will discuss implementation and application details of Desmond calculations. This seminar is intended for a molecular dynamics audience and will go into more technical details than his presentation at the [BC]^2 conference, which aims at a broader audience.*
- *The talk will be prepended with a brief introduction to correct protein preparation in Maestro by Dr. Jianxin Duan, Schrödinger, Llc. After the presentations, there will be sufficient time for additional Q&A.*

Date: **Wednesday, March 12th, 2008**

Time: **14:15**

Room: **Hörsaal 2, Pharmazentrum**

Contact: Dr. Michael Podvinec, Biozentrum Research IT (michael.podvinec@unibas.ch)

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