NAMD Developer Workshop

Room 3269 - Beckman Institute, University of Illinois, Urbana Illinois.

June 11-12, 2018

Day1: Monday, June 11, 2018

8:30	Participants Reception - TCB Courtyard I, 3rd Floor		
09:00-09:15	Welcome, Introductory Words - Room 3269, 3rd Floor		
NAMD Design Overview & Performance			
09:15-10:00	Talk 1	David Hardy	NAMD Design Overview and Ongoing Challenges
10:00-10:30	Talk 2	James Phillips	Experiences with NAMD on the Summit POWER9/Volta Supercomputer
10:30-11:00	Coffee break		
11:00-11:15	Talk 3	Ronak Buch	Possible GitHub Migration Discussion
Free-Energy and Alchemical Calculations			
11:15-11:45	Talk 4	Chris Chipot	Free Energy in NAMD: Then, Now and Tomorrow
11:45-12:15	Talk 5	Giacomo Fiorin	Collective Variables Module Updates
12:15-01:45	Lunch break		
01:45-02:15	Talk 6	Ronald Tse	Double Wide Free Energy Perturbation
02:15-02:45	Talk 7	Wei Jiang	Development of Single Topology Alchemical Free Energy Calculation and User Interface
02:45-03:15	Coffee break		
03:15-03:45	Talk 8	Brian Radack	Developing a Roadmap for Alchemical Calculations in NAMD
Free-Energy Methods in NAMD Roadmap			
03:45-05:45	Round Table + Roadmap Elaboration		
6:30	Social dinner		

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Day 2: Tuesday, June 12, 2018

9:00	Opening of the second day - Room 3269, 3rd Floor		
NAMD Features and Performance			
09:00-09:45	Talk 9	David Hardy	NAMD Software Architecture
09:45-10:15	Talk 10	James Phillips	NAMD and Charm++ Performance Tuning for Users and Developers
10:15-10:45	Coffee break		
10:45-11:15	Talk 11	Ronak Buch	New and Future Features in Charm++
Enhanced Sampling			
11:15-11:45	Talk 12	Jérôme Hénin	Efficient Implementations of Adaptive Multilevel Splitting and Double-Wide Sampling
11:45-01:15	Lunch break		
01:15-01:45	Talk 13	James Gumbart	Hydrogen-Mass Repartitioning Using NAMD
01:45-02:15	Talk 14	Yinglong Miao	Gaussian Accelerated Molecular Dynamics in NAMD
02:15-02:45	Coffee break		
Experimental Data in MD Simulations			
02:45-03:15	Talk 15	Juan Perilla	CryoEM Structure Refinement by Integrating NMR Chemical Shifts with Molecular Dynamics Simulations
03:15-03:45	Talk 16	Noah Trebesch	Modeling and Simulation of Geometrically Accurate, Multibillion Atom Cellular Membrane Structures with xMAS Builder
QM/MM in NAMD			
03:45-04:15	Talk 17	Rafael Bernardi	NAMD and VMD combined for easy and fast QM/MM simulations
NAMD — roadmap			
04:15-05:30	Round Table + Roadmap Elaboration		
5:30	Closing of the workshop		