NAMD Developer Workshop

University of Chicago, May 22-23, 2017

Gordon Center for Integrative Science (GCIS) room W105

Day1: Monday May 22, 2017

9:15	Opening of the workshop		
09:15-09:30	Welcome, introductory words		
NAMD introductory material			
09:30-10:00	Talk 1	Jim Phillips	NAMD software architecture
10:00-10:30	Talk 2	Ronak Buch	New and upcoming features in Charm++
10:30-11:00	Coffee break		
Collective variables			
11:00-11:30	Talk 3	Giacomo Fiorin	Whole-system collective variables for free-energy calculations
11:30-12:00	Talk 4	Jerome Hénin	Optimization of collective variable calculations through dynamic dependencies
12:00-12:30	Talk 5	Chris Chipot	New variables for standard binding free-energy calculations
12:30-02:00	Lunch break		
Recent developments in NAMD			
02:00-02:30	Talk 6	Brian Radak	Expanded ensemble simulations with NAMD: Free energies, enhanced sampling, and constant-pH
02:30-03:00	Talk 7	David Hardy	Multilevel summation method in NAMD
03:00-03:30	Coffee break		
Developments for modeling cell processes			
03:30-04:00	Talk 8	Noah Trebesch	Atomistic modeling and simulation of cell-scale membrane structures with xMAS builder.
04:00-04:30	Talk 9	Christopher Mayne	Membrane (Re)Shaper: Towards a method and toolset for modeling membrane processes
NAMD roadmap			
04:30-05:30	Round table		
05:30-06:00	Closing discussion		
6:30	Social dinner		

NAMD Developer Workshop

University of Chicago, May 22-23, 2017

Knapp Center for Biomedical Discovery (KCBD) room 3200

Day 2: Tuesday May 23, 2017

9:00	Opening of the second day of the workshop		
New features in NAMD			
09:00-09:30	Talk 10	Jim Phillips	Adding features to NAMD
09:30-10:00	Talk 11	João Ribeiro	Reproducibility in QwikMD and NAMD
10:00-10:30	Talk 12	Risi Kondor	MD meets machine learning
10:30-11:00	Coffee break		
Enhanced sampling methods			
11:00-11:30	Talk 12	Donghyuk Suh	Enhanced sampling in configurational space with hybrid non-equilibrium molecular dynamics/Monte Carlo
11:30-12:00	Talk 13	James Gumbart	Using REST2 in NAMD: Is it worth it?
12:30-01:30	Lunch break		
QM/MM in NAMD			
01:30-02:00	Talk 14	Rafael Bernardi	NAMD goes quantum
02:00-02:30	Talk 15	Marcelo Melo	NAMD goes quantum
02:30-03:00	Coffee break		
03:00-03:30	Talk 16	Chris Maffeo	ARBD: A new GPU-accelerated coarse-grained simulation package
03:30-04:00	Talk 17	Benjamin Jagger	A hybrid MD, BD, and milestoning approach for the calculation of protein-ligand binding and unbinding kinetics in NAMD
Free-energy methods in NAMD — roadmap			
04:30-05:00	Round table		
05:00-05:30	Closing discussion		
5:30	Closing of the workshop		