NAMD Developers Workshop
University of Chicago, May 26-27, 2016
GCIS room W301/303

Day1: Thursday May 26, 2016

08:30	Opening of the workshop		
08:30-09:00	Breakfast		
09:00-09:15	Benoît Roux, Chris Chipot		Welcome, introductory words
09:15-10:00	Keynote 1	Jim Phillips	NAMD software architecture
10:00-10:30	Talk 1	Antti-Pekka Hynninen	Advances in NAMD GPU performance
10:30-11:00	Coffee break		
11:00-11:30	Talk 2	Giacomo Fiorin	Performance improvements in the Colvars module: Towards supramolecular systems
11:30-12:00	Talk 3	Sunhwan Jo	A generic implementation of replica-exchange with solute tempering (REST) algorithm
12:00-01:30	Lunch break		
01:30-02:15	Keynote 2	Sanjay Kalé	General presentation of charm++
02:15-02:45	Talk 4	Brian Radak	Towards a neMD/MC constant pH method in NAMD
02:45-03:15	Talk 5	David Hardy	Multilevel summation method in NAMD
03:15-03:45	Coffee break		
03:45-04:15	Talk 6	Alexandra Heyneman	Introducing SEEKR (simulation-enabled estimation of kinetic rates): A conglomerate of molecular and Brownian dynamics
04:15-04:45	Talk 7	Christopher Mayne	A Tcl-Based implementation of the adaptive multilevel splitting method for computing the kinetics of rare events In NAMD
04:45-06:00	Round table, closing discussion		

Day 2: Friday May 27, 2016

08:45-09:15	Breakfast		
09:15-10:00	Keynote 3	Jim Phillips	Adding features to NAMD
10:00-10:30	Talk 8	Donghyuk Suh	Developing enhanced sampling method with Hybrid non-equilibrium MD/MC scheme
10:30-11:00	Coffee break		
11:00-11:30	Talk 9	Jérôme Henin	Extending the collective variables Module
11:30-12:00	Talk 10	Jeffrey Comer	Implementing unusual force fields in NAMD
12:00-01:30	Lunch break		
01:30-02:00	Talk 11	Charles Matthews	Constant-temperature simulations with holonomic constraints
02:00-02:30	Talk 12	Chris Maffeo	Grid-defined rigid bodies and tabulated bonded potentials for a more versatile NAMD
02:30-03:00	Talk 13	Chris Chipot	An on-the-fly implementation of the extended adaptive biasing force algorithm
03:00-03:30	Coffee break		
03:30-04:00	Round table, closing discussion		
04:00	Closing of the workshop		

Note: Talks are 25-minute long followed by 5 minutes of questions; Keynotes are 40-minute long followed by 5 minutes of questions.