NAMD Developer Workshop

Room 3269 - Beckman Institute, University of Illinois, Urbana Illinois.
August 19-20, 2019

Day 1: Monday, August 19, 2019

8:30	Participants Reception - Outside Room 3269, 3rd Floor		
09:00-09:15	Emad Tajkhorshid - Welcome/Introductory Remarks Overview of NAMD Vision and Major Areas of Development		
Morning Session			
09:15-10:00	Talk 1	David Hardy	NAMD Development Progress and Plans, Potential migration to GitHub
10:00-10:45	Talk 2	Julio Maia	NAMD on GPUs: Ongoing efforts and future challenges
10:45-11:00	Coffee break - TCB Courtyard I, 3rd Floor		
11:00-11:45	Talk 3	Jim Phillips	Experiences with NAMD and Charm++ on the Summit POWER9/Volta Supercomputer
11:45-12:15	Talk 4	Ronak Buch	Recent Developments in Charm++
12:15-01:15	Lunch break - TCB Courtyard I, 3rd Floor		
Afternoon Session			
01:15-01:45	Talk 5	Peng Wang	NAMD CUDA development update
01:45-02:15	Talk 6	Joao Ribeiro	Accessible molecular modelling environment with VMD and NAMD
02:15-02:45	Talk 7	Mariano Spivak	Multiple QM levels in hybrid QM/MM simulations
02:45-03:00	Coffee break - TCB Courtyard I, 3rd Floor		
03:00-03:30	Talk 8	Rafael Bernardi	QM/MM MD: Using NAMD's enhanced sampling tools in hybrid simulations
03:30-04:00	Talk 9	Marcelo Melo	Dimensionality reduction on-the-fly: concurrent generalized correlations analysis within MD calculations
04:00-04:30	Talk 10	Juan Perilla	Analysis of petascale molecular dynamics simulations
NAMD Roadmap			
04:30-06:30	Round Table + Roadmap Elaboration		
6:30	Social dinner		

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Day 2: Tuesday, August 20, 2019

8:30	Participants Reception - Outside Room 3269, 3rd Floor		
9:00	Opening of the second day - Room 3269, 3rd Floor		
Morning Session			
09:00-09:30	Talk 11	Chris Chipot	Roadmap for Free Energy Methods in NAMD
09:30-10:00	Talk 12	Benoit Roux	Revisiting the fundamental issues of molecular dynamics alchemical free energy calculations
10:00-10:30	Talk 13	Ron Elber	Milestoning and MDAS
10:30-10:45	Coffee break - TCB Courtyard I, 3rd Floor		
10:45-11:15	Talk 14	Jeffrey Comer	Hybrids of adaptive biasing force and replica exchange in NAMD
11:15-11:45	Talk 15	Wei Jang	Input setup tool for relative free energy computations
11:45-12:15	Talk 16	Kosar Khajeh	Implementation of magnetic field force in molecular dynamics algorithm: NAMD source code
12:15-01:15	Lunch break - TCB Courtyard I, 3rd Floor		
Afternoon Session			
01:15-01:45	Talk 17	John Vant	MDFF: An Investigation of Systematic Error in GridForces Potential and It's Edification
01:45-02:15	Talk 18	Chris Rowley	ANI Machine Learned Potential to Represent Ligand Intramolecular Terms
02:15-02:45	Talk 19	Sepehr Dehghani-Ghahnaviyeh	Coarse-Grained Molecular Dynamics in NAMD
02:45-03:15	Talk 20	Daipayan Sarkar	String-like simulations outside the friction dominated regime
03:15-03:30	Coffee break - TCB Courtyard I, 3rd Floor		
NAMD Roadmap			
03:30-05:30	Round Table + Roadmap Elaboration		
5:30	Closing of the workshop		