NAMD developers meeting 2025, Chicago | October 9–10, 2025. University of Chicago
Searle Chemical Laboratory, 5735 S. Ellis, room 240A

Day 1

Time slot	Speaker		
08:30–08:55	Breakfast		
08:55–09:00	Chipot/Roux	Opening. Welcome word	inP
Session I: NAMD development (Chris Chipot moderator)			
09:00–09:20	David Hardy	NAMD recent developments and upcoming challenges	inP
09:20–09:40	Wei Jiang	GPU-accelerated hybrid single-dual topology alchemical free energy approach in NAMD	inP
09:40–10:00	Eric Bohm	Why does `ComputePmeMgr::ungridCalc` devour your Vista allocation?	inP
10:00–10:20	Mahmoud Moradi	Free energy and rate estimation using along-the-path unbiased MD simulations	inP
10:20–10:50	Coffee break		
10:50–11:10	Haochuan Chen	Implementations of GPU-resident Drude force field and Colvars in NAMD	InP
11:10–11:30	David Clark	Prototyping multi-node device migration and distributed PME for GPU-resident NAMD	inP
11:30–11:50	Ke Yue	NAMD3: SYCL and AVX512 implementation status	InP
11:50–12:10	Co Quach	MARTINI3 in NAMD: Implementation challenges and advances	InP
12:10–14:00	Lunch break		

Session II: NAMD development (James Gumbart moderator)			
14:00–14:20	Sarah Moe	neMD/MC simulations of biomolecules with variable ionization states	inP
14:20–14:40	Jay Scott	Implementing relative entropy grid force with GPU-accelerated volumetric density grids in NAMD	rem
14:40–15:00	Hanning Chen	Performance analysis of NAMD3 on supercomputers at the Texas Advanced Computing Center	rem
15:00–15:20	Francis Alipranti	Application of neMD/MC for lipid swapping and protein design	inP
15:20–15:50	Coffee break		
15:50–16:10	Jean-Philippe Piquemal	A foundation model for accurate atomistic simulations in drug design	inP
16:10–16:30	Giacomo Fiorin	Integration and testing in the Colvars library development	rem
16:30–16:50	Benoît Roux	Accelerating SCF for Drude simulations with BFGS and a local, approximate Hessian	inP
16:50–17:10	Jeffrey Comer	Leveraging NAMD's GPU-accelerated alchemical transformation features for enhanced sampling and peptide design	inP
17:10–18:00	Round-table discussion (Benoît Roux moderator)		
19:00–21:00	Dinner at Nella		

Day 2

Time slot	Speaker		
08:30–08:55	Breakfast		
Session III: At the frontier between VMD and NAMD (Benoît Roux moderator)			
09:00–09:20	Haohao Fu	Prioritized quality-of-life (QoL) feedback for routine NAMD simulations: A user perspective	rem
09:20–09:40	Sara Bonella	A constrained MD approach for electrostatic interactions	rem
09:40–10:00	Jérôme Hénin	VMD developers workshop	rem
10:00–10:20	Chenyu Tang	PCCANN and beyond: Revealing transition pathways and mechanisms in rare events via the committor function	rem
10:20–10:50	Coffee break		
10:50–11:10	Marcelo Melo	Tracking information transfer across protein interfaces	rem
11:10–11:30	Diego Barreto Gomes	Toward a unified plugin framework in VMD 2: Setting community priorities and standards	inP
11:30–11:50	Rafael Bernardi	Calcium-stabilized protein mechanics with polarizable (Drude) force fields in GPU-resident NAMD	inP
11:50–12:10	Jodi Hadden	Advancing NAMD/VMD support for carbohydrates, condensates, and protein cages	InP
12:10–14:00	Lunch break		

Time slot	Speaker		
Session IV: Applications (Rafael Bernardi moderator)			
14:00–14:20	Juan Perilla	Extension of shape-based coarse graining to nucleic acids	inP
14:20–14:40	Abhishek Singharoy	Determining protein functions from sequence with the NODES consortium	inP
14:40–15:00	James Gumbart	Exploring the folding pathways of pertactin using enhanced sampling techniques	inP
15:00–15:20	Van Ngo	Large scale simulations of highly flexible and dynamical proteins in cellular signaling	rem
15:20–15:50	Coffee break		
15:50–16:10	Stephen Gee	Applying geometrical restraints with NAMD Colvars to characterize peripheral protein–membrane binding interactions	inP
16:10–16:30	Harper Smith	Martini3 simulations to study lipid scrambling: a NAMD user perspective	inP
16:30–16:50	Josh Vermaas	Pressure profiling in NAMD in 2025 and large scale analysis in VMD	inP
16:50–17:20	Round-table discussion (Chris Chipot moderator)		
17:20–17:30	Chipot/Roux	Closing remarks	inP

inP in person attendance | rem remote attendance

Zoom link: Please, try in advance to connect using your Zoom account to make sure you can get in.
https://illinois.zoom.us/j/81040405864?pwd=D8GZfPsuZgBL8JMMxs2bOdBUr6sAzX.1&from=addon