NAMD Features and Capabilities

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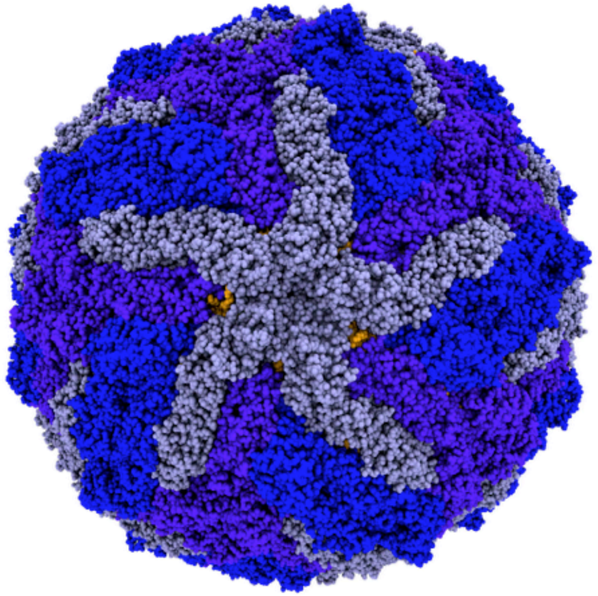
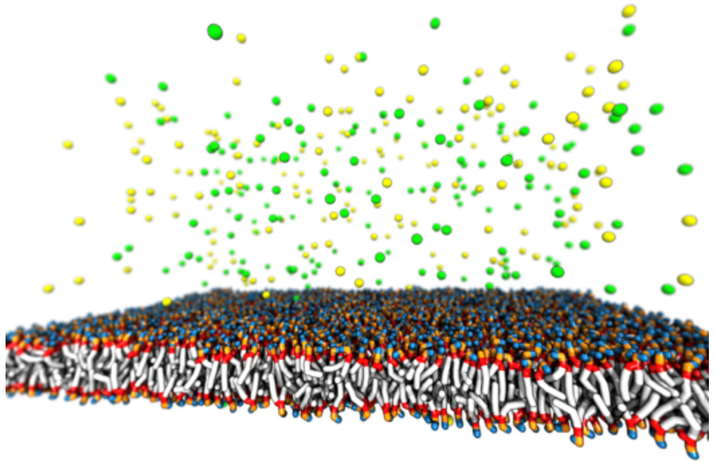
NAMD: Scalable Molecular Dynamics

J. Phillips, D. Hardy, J. Maia, et al. **JCP** 153, 044130 (2020) https://doi.org/10.1063/5.0014475

- Designed for parallel scaling of large biomolecular systems
- Feature development driven by NIH Center driving projects and collaborations
- Developed in object-oriented C++ starting from the mid ‘90s
- Uses Charm++ parallel messaging framework
- Freely available to download and use (but not to redistribute)
- Over 50,000 registered users, over 10,000 citations of the original 2005 reference paper



Zika virus
(equilibrium MD at constant pressure)



Membrane vesicle fusion and formation
(non-equilibrium MD using grid forces)

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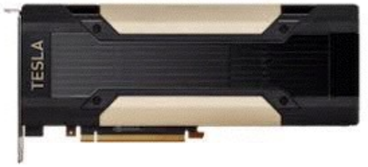
What hardware does NAMD support?

- Designed for Unix/Linux running on x86, POWER, ARM
- Also support Windows and MacOS
- CUDA-accelerated for NVIDIA GPUs since 2007

  ➡ Currently developing support for AMD and Intel GPUs

- Runs on laptops and desktop workstations up through clusters (e.g. AWS and MS Azure) and supercomputers
- Preserves the main command line arguments and can use the same configuration file across all platforms

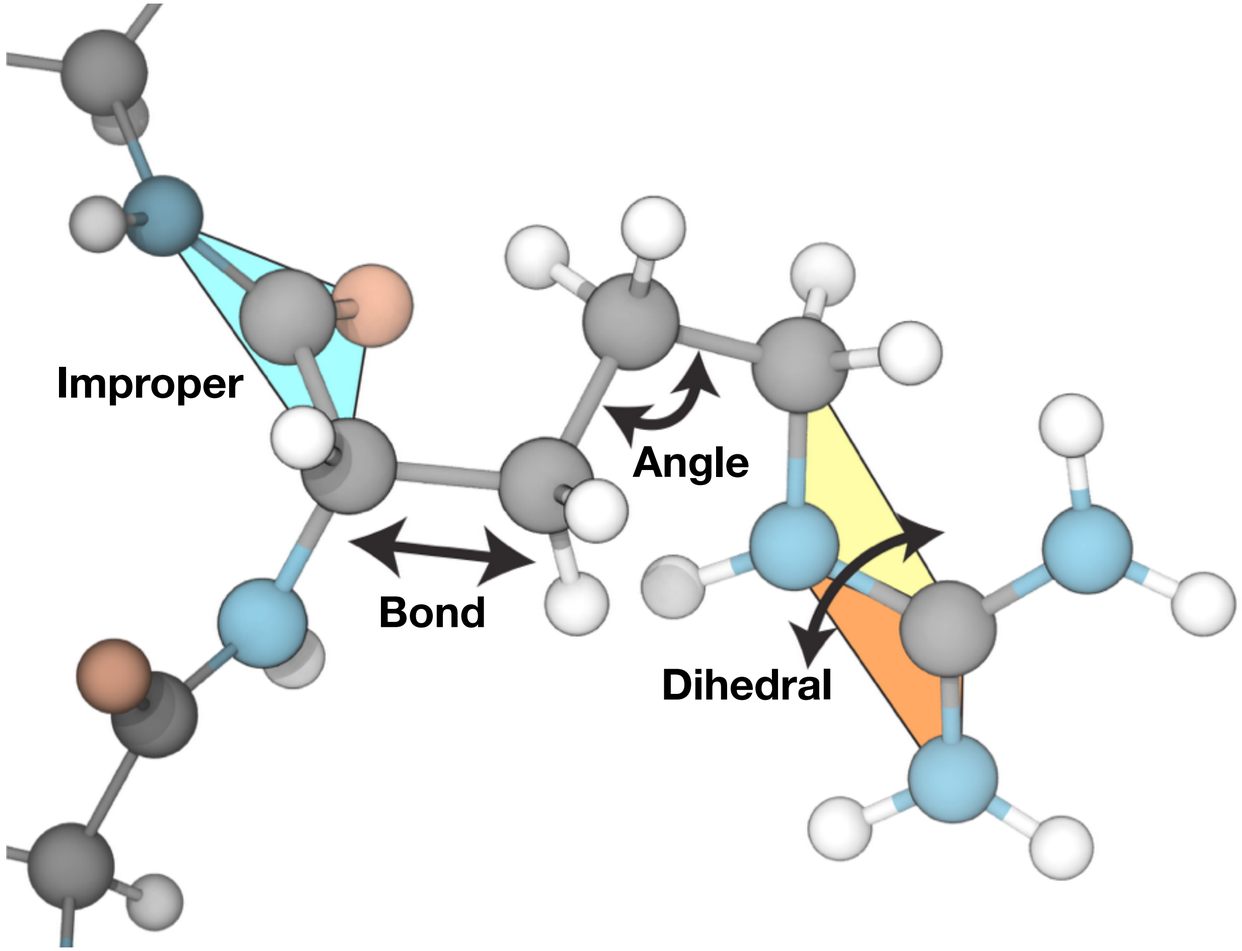


Latest versions of NAMD

- Current stable release is version 2.14 (Aug 2020)
- Current development releases are
  - Version 3.0 alpha 6 (devel branch) - fast single-GPU support
  - Version 2.15 alpha 1 (nightly build from master branch) - explicit AVX-512 support for good scaling on TACC Frontera

NAMD is full-featured MD code

- Optimized for CHARMM force field with TIP3P water
- Support for AMBER input files and force field
- Some support for GROMACS input files
- Lone pairs and TIP4P water
- Drude polarizable force field



NAMD standard features (equilibrium simulation)

Features less common or distinctive among MD codes denoted by 

- Constant energy
- Temperature control
  - Langevin thermostat
  - Stochastic velocity rescaling
- Pressure control
  - Langevin piston
  - Berendsen pressure bath
- Periodic boundary conditions
- Non-periodic with spherical or cylindrical BCs

- Long-range electrostatics
  - Particle-mesh Ewald (for PBCs)
  - Multilevel summation method (for non-periodic or semi-periodic)
- Rigid bond constraints for hydrogen
- Multiple time stepping
- Conserve momentum while still conserving energy (zeroMomentum)
- Energy minimization
  - Conjugate gradient and velocity quenching

NAMD advanced features (non-equilibrium simulation)

- Enhanced sampling methods
  - Apply external forces:
    - Harmonic restraints, fixed atoms, external electric field, steered MD, interactive MD, grid forces
  - Boost or modify interaction potentials to flatten the energy landscape:
    - Accelerated MD, Gaussian-accelerated MD, solute scaling and REST2, replica-exchange MD
- Collective variables (Colvars) module
- Alchemical free energy methods
  - Free energy perturbation (FEP)
  - Thermodynamic integration (TI)
- Constant pH simulation
- Hybrid QM/MM simulation
- Tcl scripting interface accessed through the NAMD configuration file

NAMD: replica-exchange MD

- Loosely-coupled simulations
- Tcl scripting for handling exchanges between systems
  - Provided examples include parallel tempering and umbrella sampling
  - Flexible, e.g., FEP/Hamiltonian-exchange simulations by Benoit Roux's Lab
- Capable of scaling smaller systems extremely effectively
  - Can be used with NAMD 3.0 single-GPU simulation to efficiently use dense GPU architectures

NAMD: Collective variables (Colvars) module

G. Fiorin, M. Klein, and J. Hénin, **Mol. Phys.** 111, 3345 (2013) https://dx.doi.org/10.1080/00268976.2013.813594

- Reduce large number of degrees of freedom to just a few (the “colvars”)
- Statistical distributions of the colvars can be analyzed individually or used to define biasing potentials
- Common use cases:
  - Apply restraints or biasing potentials
  - Calculate potentials of mean force (PMFs) along the set of variables
  - Calculate statistical properties of the variables

Acknowledgments

- NAMD development is funded by NIH P41-GM104601

- NAMD team: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Julio Maia


John Stone


Jim Phillips


Mohammad Soroush Barhaghi


Mariano Spivak


Wei Jiang


Rafael Bernardi


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