Multiple copy algorithms in NAMD & force field development

Why do we need Mira?
How do we use Mira?

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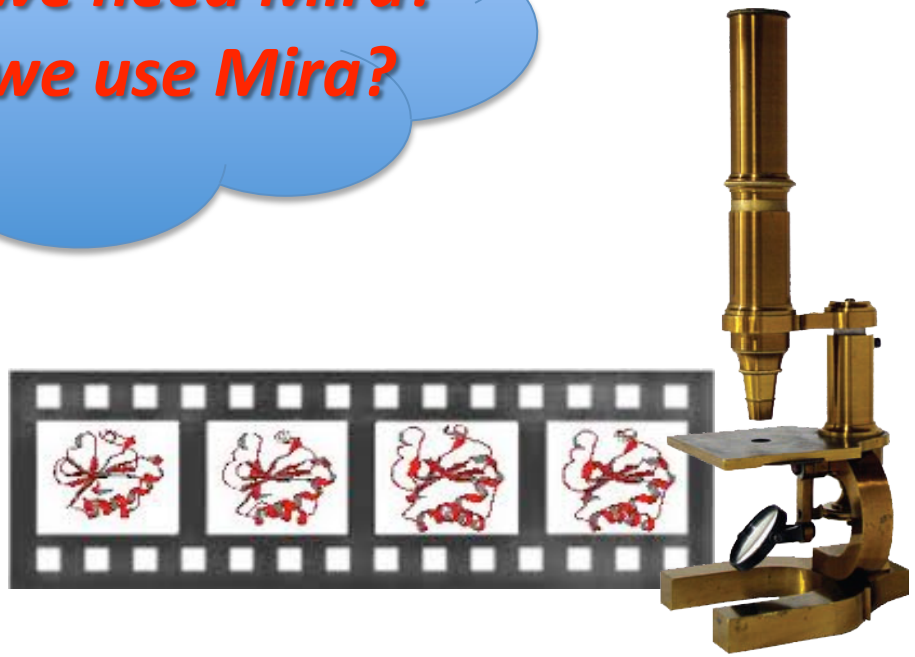


Project Goal

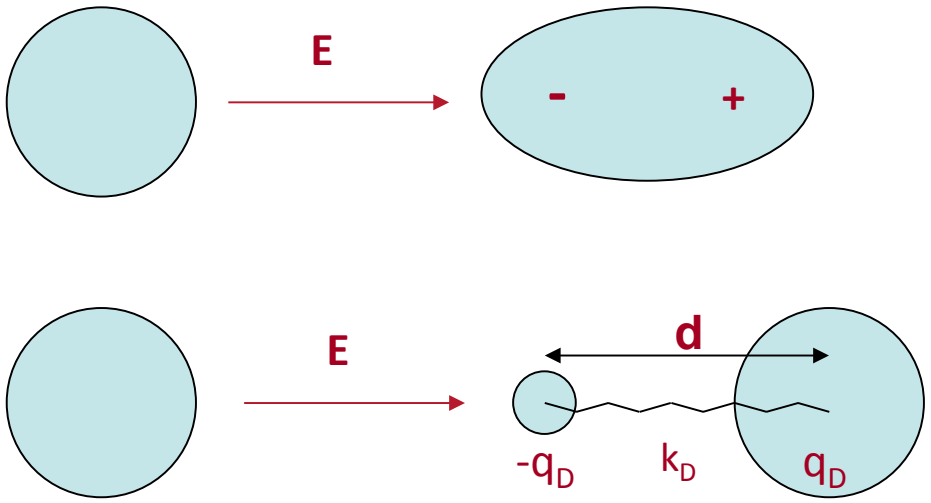
NAMD - The Engine for Large-Scale Classical Molecular Dynamics (MD) Simulations of Biomolecular Systems Based on a Polarizable Force Field

More complex and larger system

More accurate force field

Drude Model

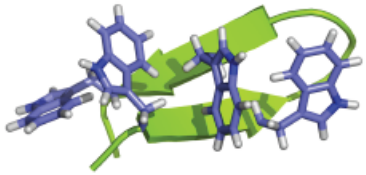
•Classical Drude oscillator model takes into account the electronic polarizability in molecular systems.

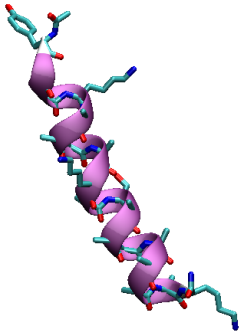


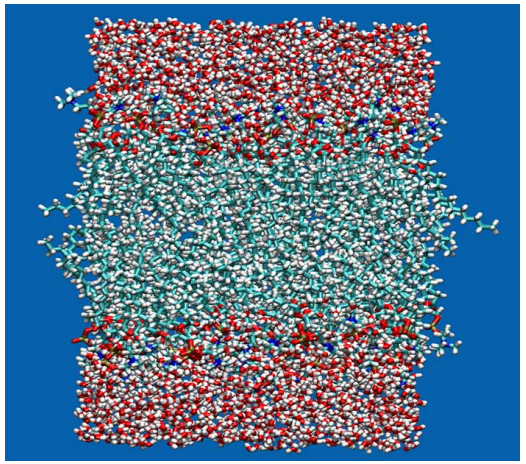
W. Jiang, et. al. J. Phys. Chem. Lett. 2011

Why do we need Mira?

- **Validating new force field requires efficient large scale sampling**







3 sets of new parameters
5 model systems
298k to 398k
200 ns per replica

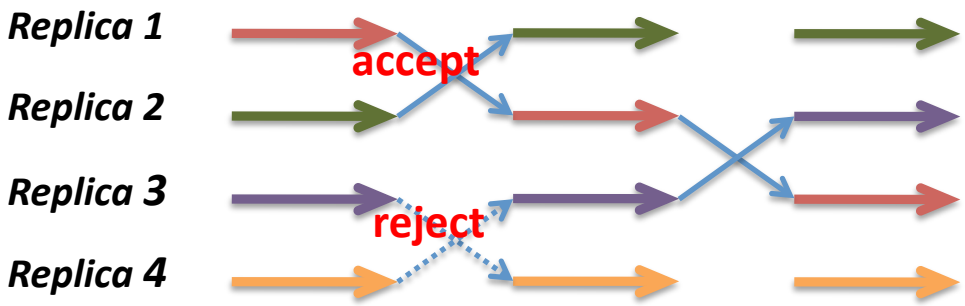
3*5*100*200 ns =300 µs !

How to use Mira?

Allow multiple copies to run in parallel

Allow information to exchange between copies

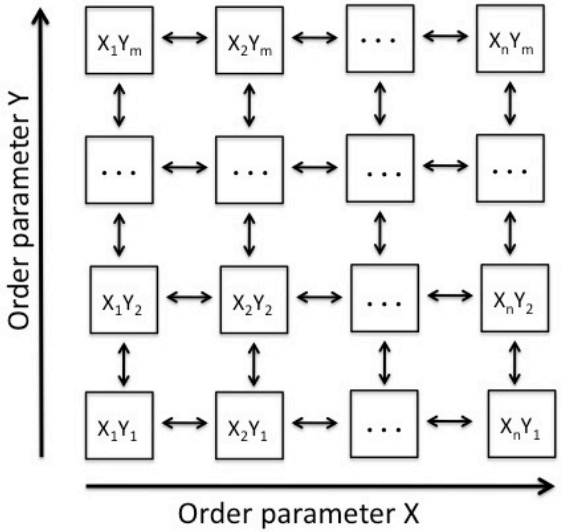
Replica Exchange (REMD)



- **Different Temperature or Hamiltonian (order parameters)**
- **Metropolis criterion to guarantee Boltzmann distribution**
- **Enhance sampling and free energy convergence**

Newly Implemented REMD in NAMD2.9

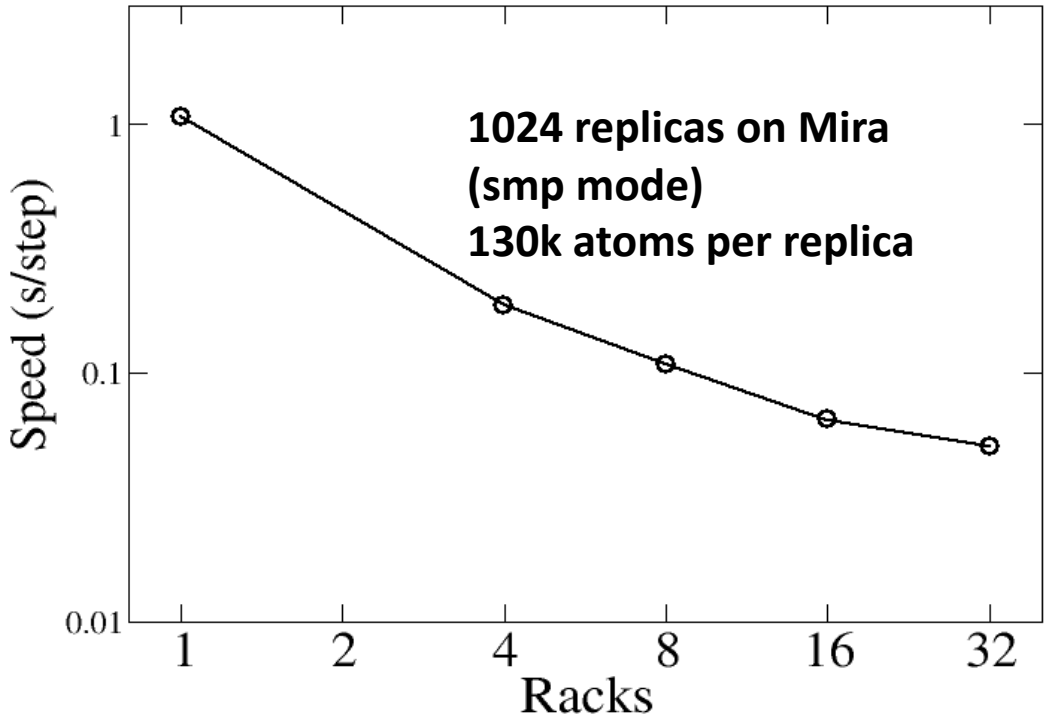
Previous implementation	New implementation
Driven by external job script (small cluster)	MPI based (supercomputer)
Small number of replicas (<100)	Thousands of replicas
Low frequent exchange (<1ps^{-1})	High frequent exchange (>0.1 ps^{-1})
One dimensional exchange	Multi dimensional exchange



Jiang, W., Luo, Y. *et al., J. Chem. Theory Comput.* (2012)

Scalability on Mira

- **Communication overhead is minimized by swapping order parameters instead of coordinates**
- **Pthread is implemented in charm++ for NAMD to run in SMP**



Generality and Flexibility

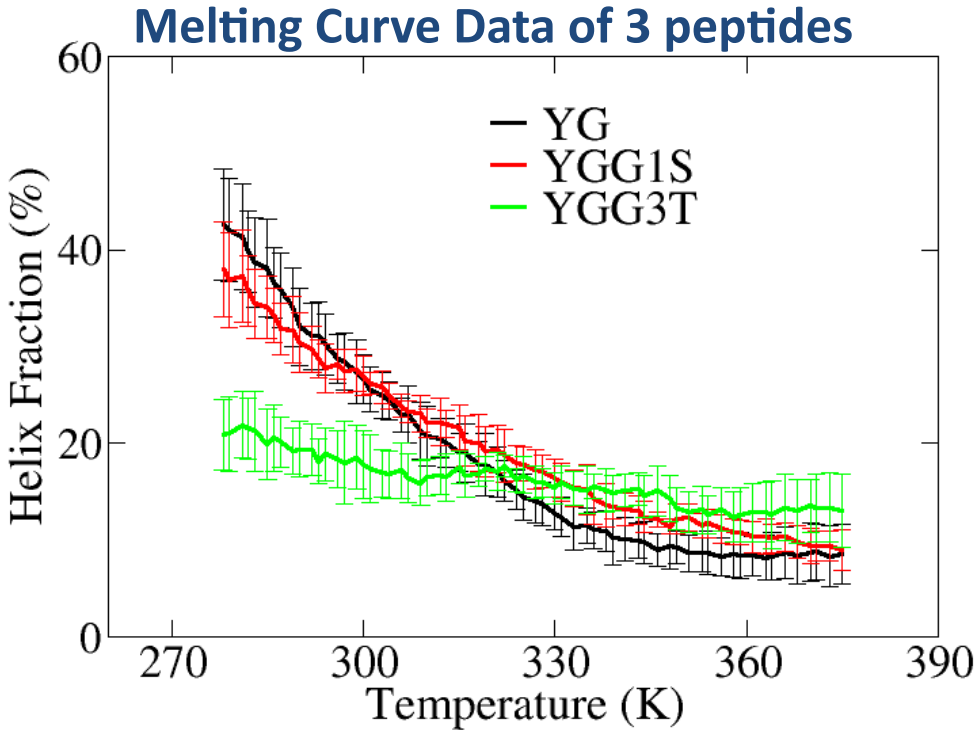
- **Can be used with variant of REMD algorithms without changing the source code**
  - **T-REMD: temperature replica exchange**
  - **FEP/REMD: free energy perturbation replica exchange**
  - **US/REMD : umbrella sampling replica exchange**
  - **REXAMD: accelerated molecular dynamics replica exchange**
  - **Swarms-of-trajectories method**

- **Tcl script allows user to define exchange parameters**
  (temperature, lambda or biasing potential in *ColVars module*)

- **User-defined exchange topology: *replica_neighbors* Tcl**

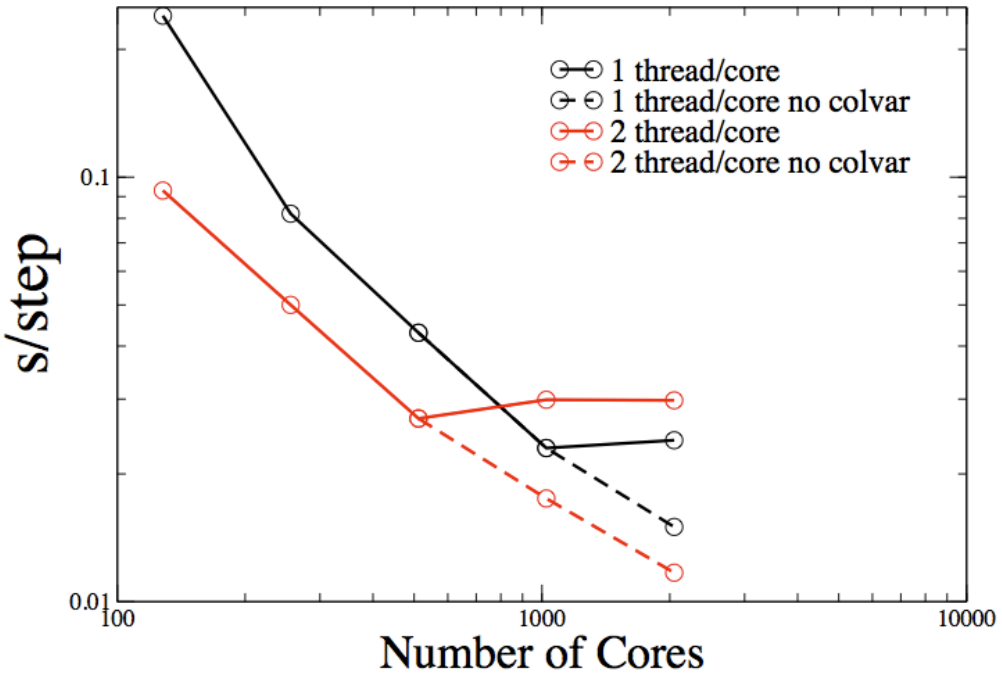
Easy post processing and data analysis

- .history files: save replica ID and energies
- .colvars.traj files: save biasing potential applied
- .sortreplicas: namd2 binary directory, un-shuffle replica trajectories



Future improvement

1. **Charm++ base REMD on BG/Q**
2. **NAMD's *colvar* module has a scaling limit**



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CHARMM FF Parameters

Alex MacKerell,
Pedro Lopes, Jihyun Shim