GPU-Accelerated Molecular Dynamics Simulation of Rigid Water

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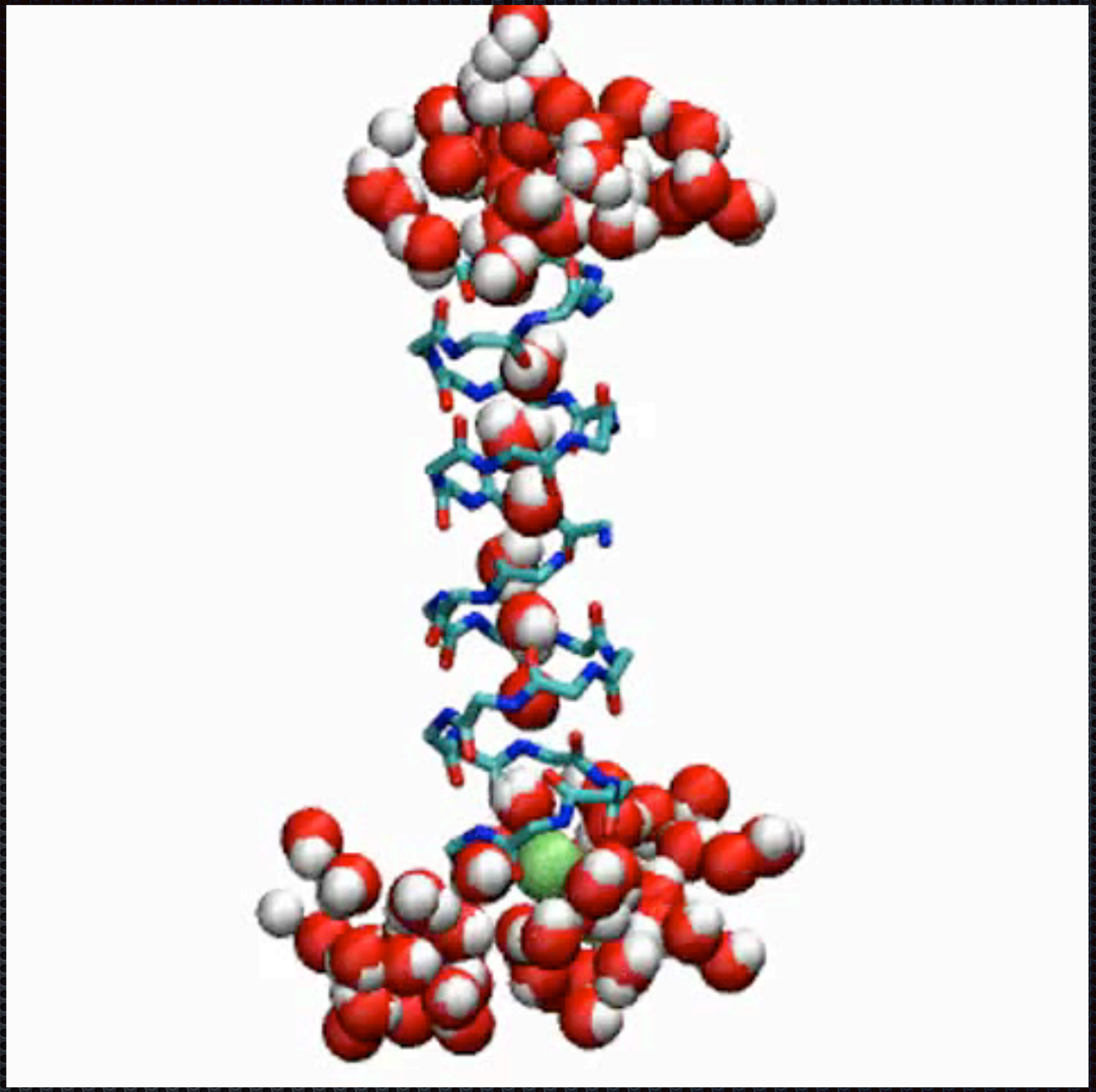
Molecular dynamics (MD)

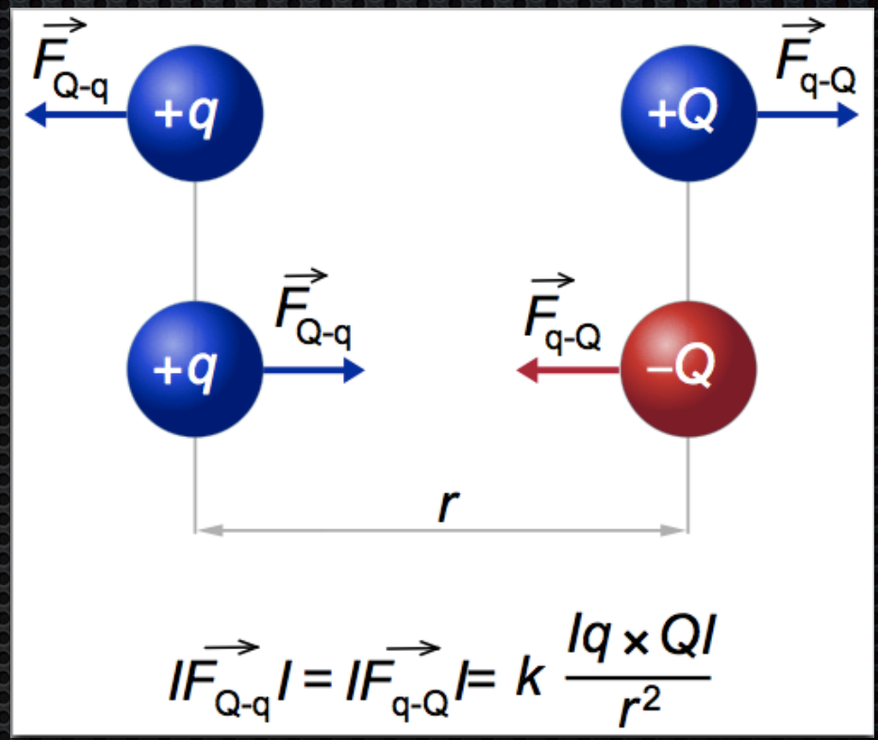
- Processes occurring over 10^{-9} second
- Simulation of atoms/molecules
- Newtonian mechanics, quantum mechanics
- Biochemistry, drug design, materials science



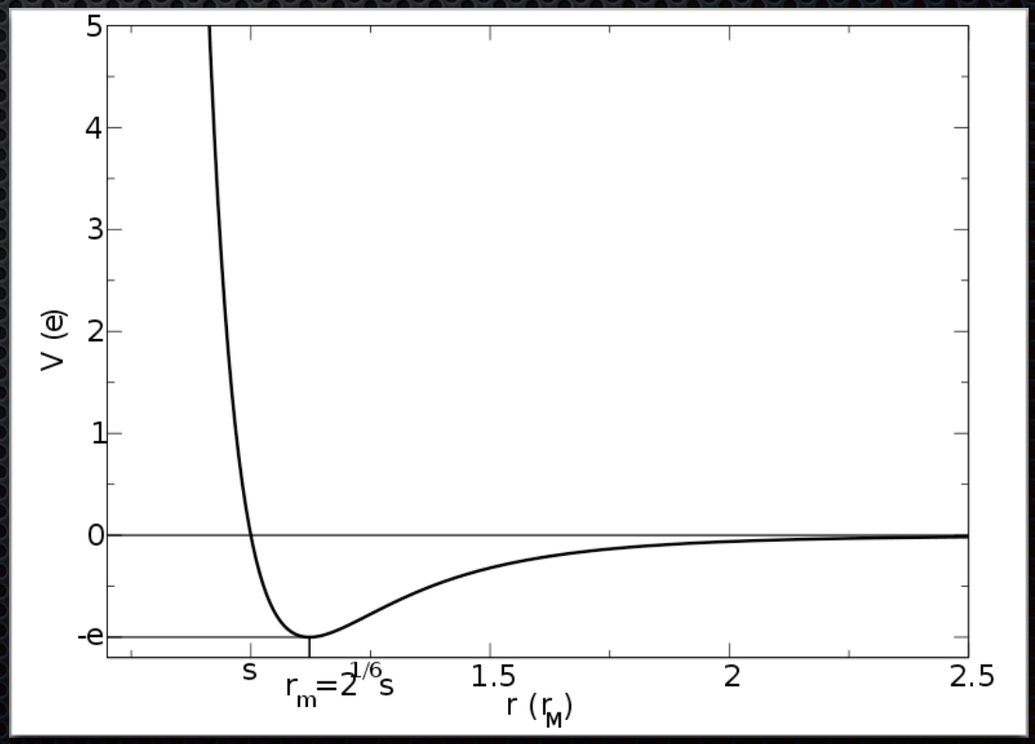
http://vimeo.com/3173968

MD Interactions

- Coulomb
  - Charged atoms
- Lennard-Jones
  - Neutral atoms



Wikipedia: Coulomb's law



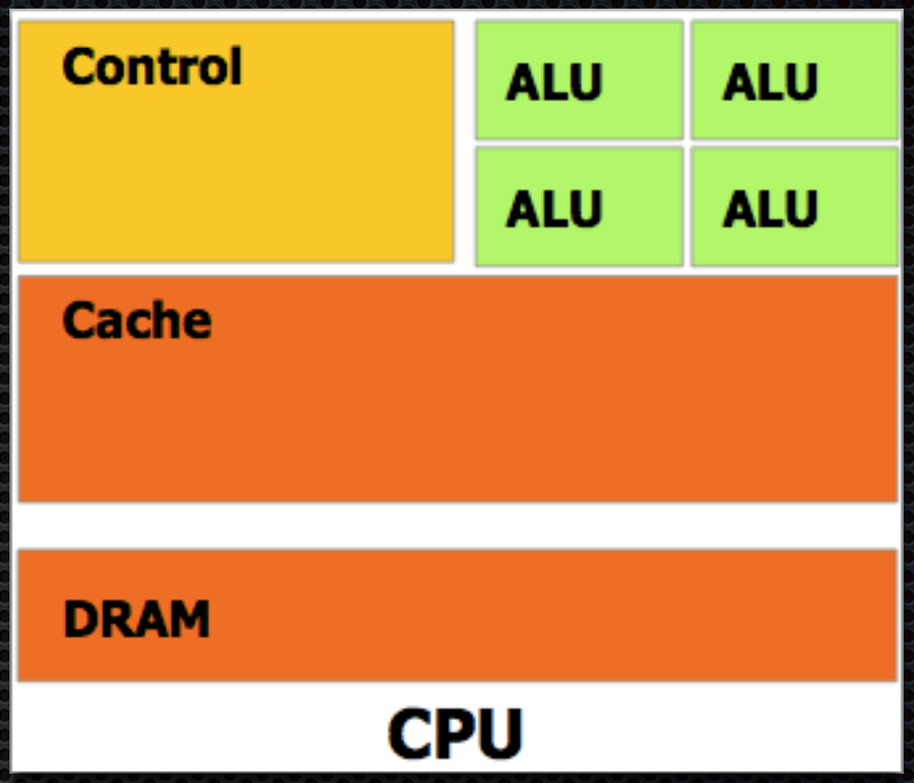
Wikipedia: Lennard-Jones Potential

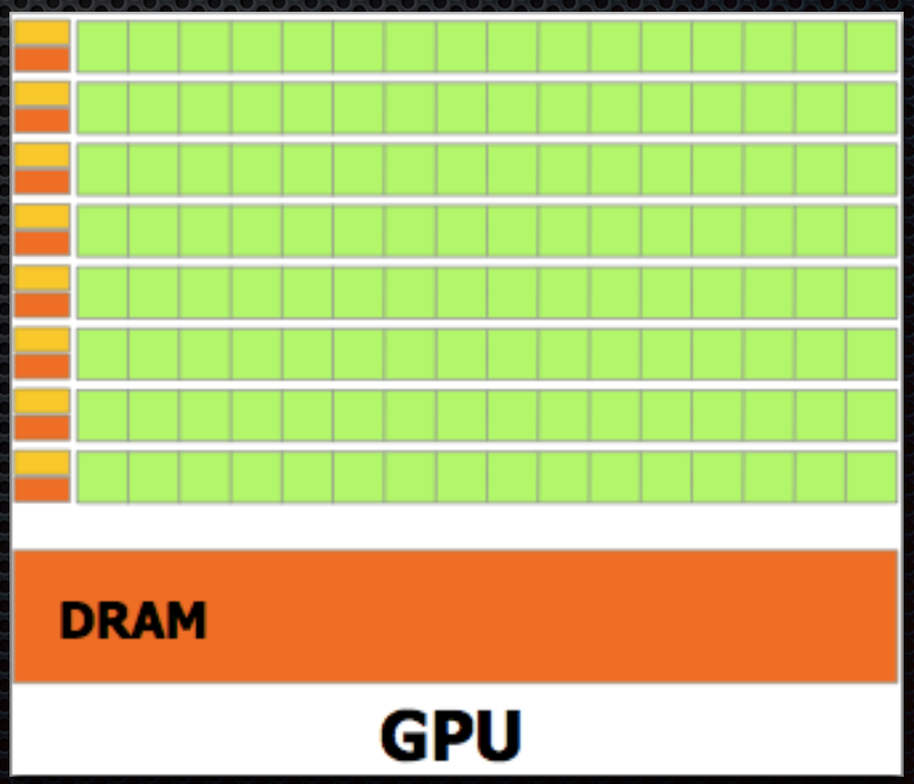
MD Approximations

- Interaction “cutoff” distances
- Water approximations
  - Thin shells
  - Cutoffs
- Charged systems
  - Non-negligible effects from polar water

GPU Computing

- More power
- Parallelization
- Evolution of GPU
- Cheap, fast, easy

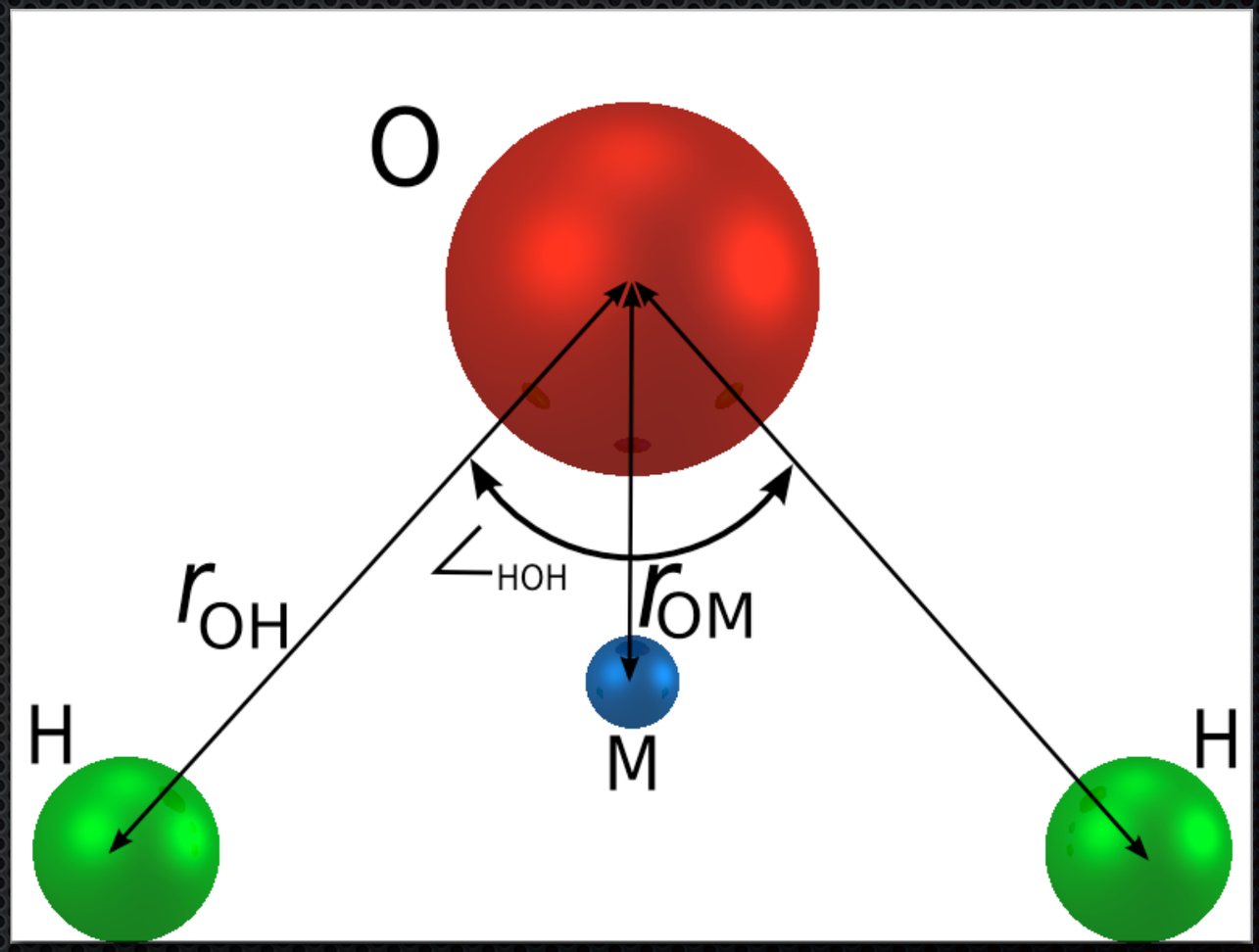




CUDA C Programming Guide

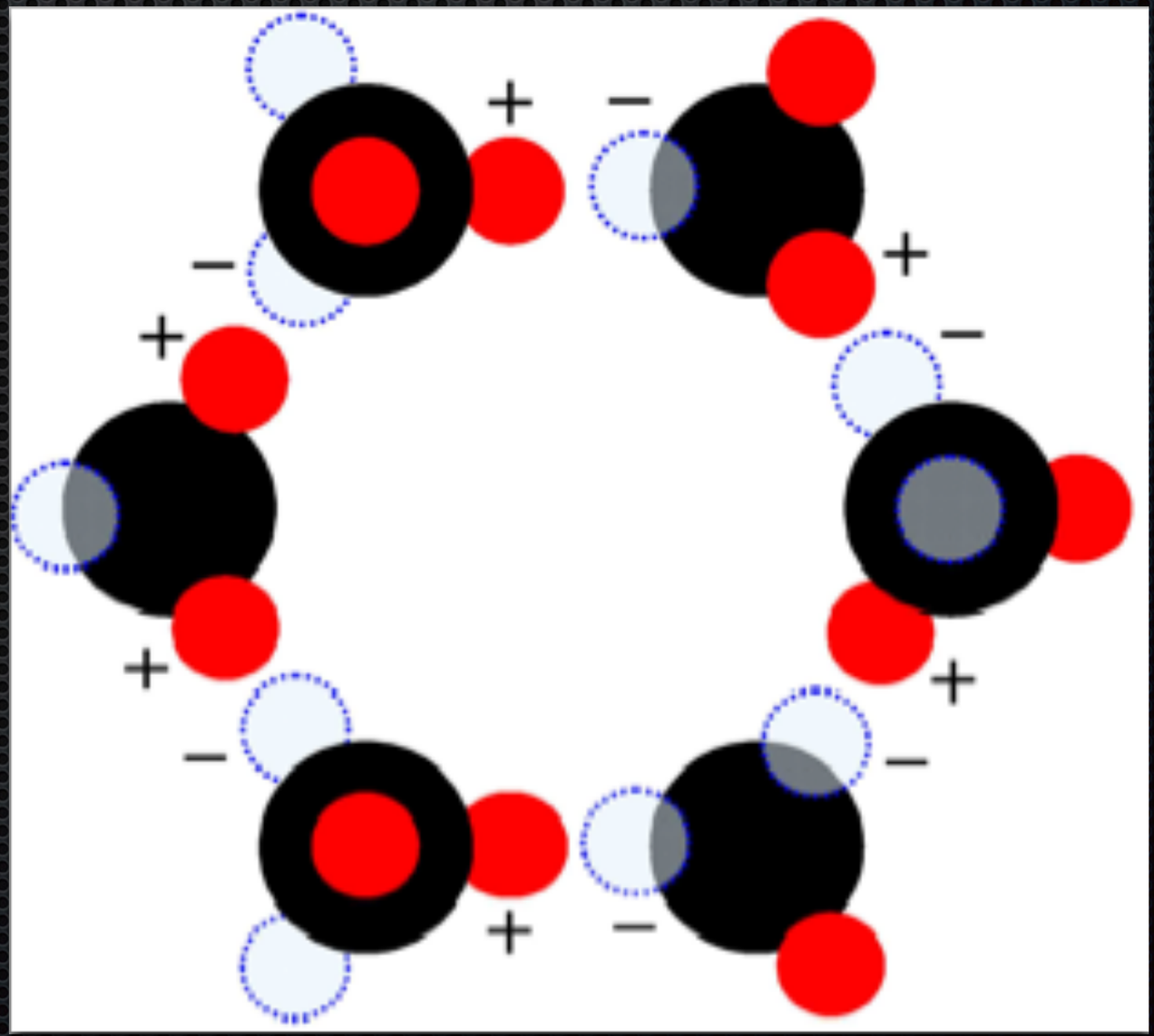
Water model

- Rigid or flexible
- Number of “sites”
- TIP4P/2005



Initialization

- Ice lattice
  - Random orientations
  - Replicate unit cell
- No rotation, no speed

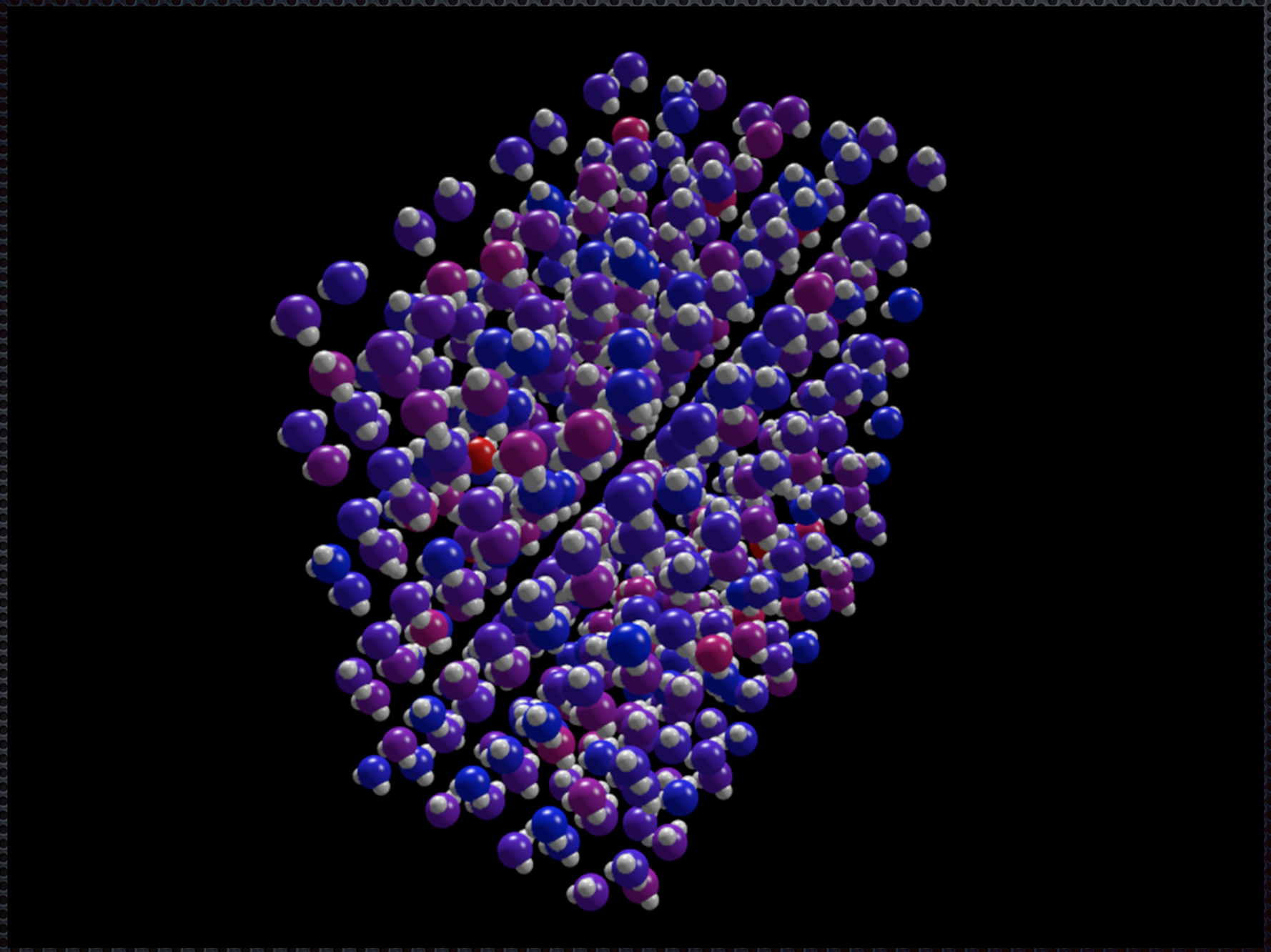


storyofsnow.com

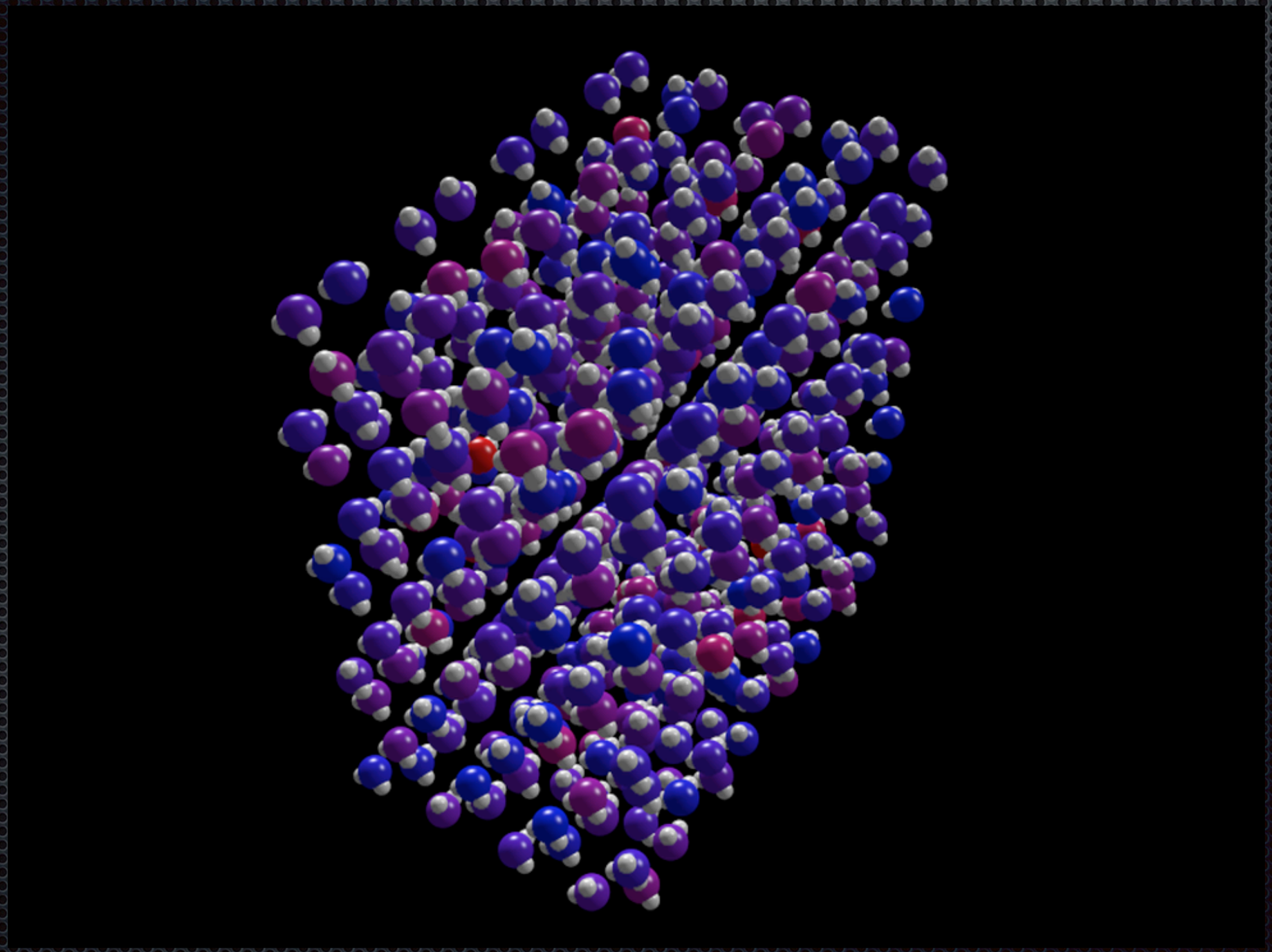
Thermostat

- Two types of motion
  - Rotational
  - Translational
- Temperature ~ $E_{kinetic,\ average}$
- Rescale motion to low temperature
  - Take energy out of system

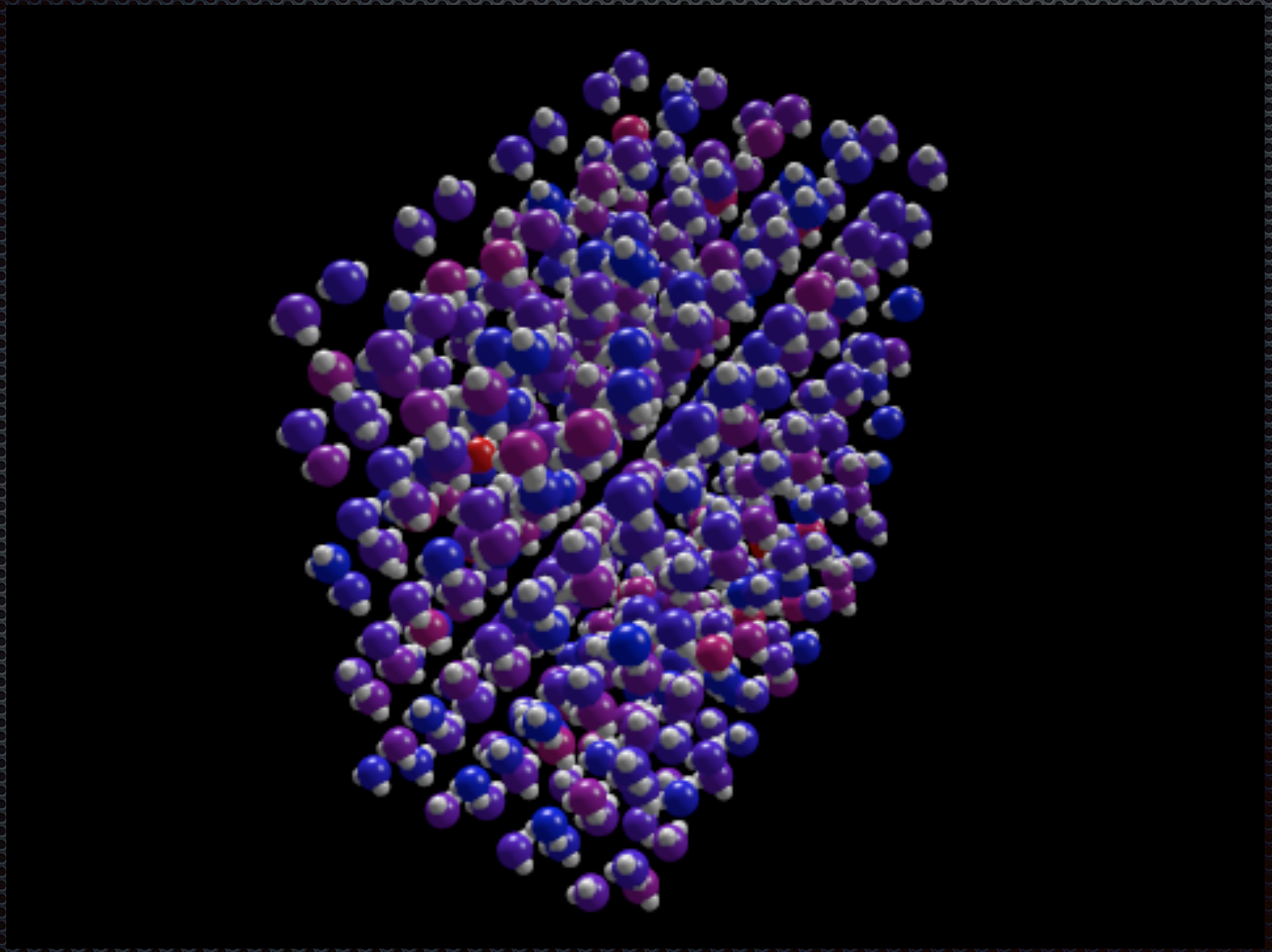
Ice (is cold)

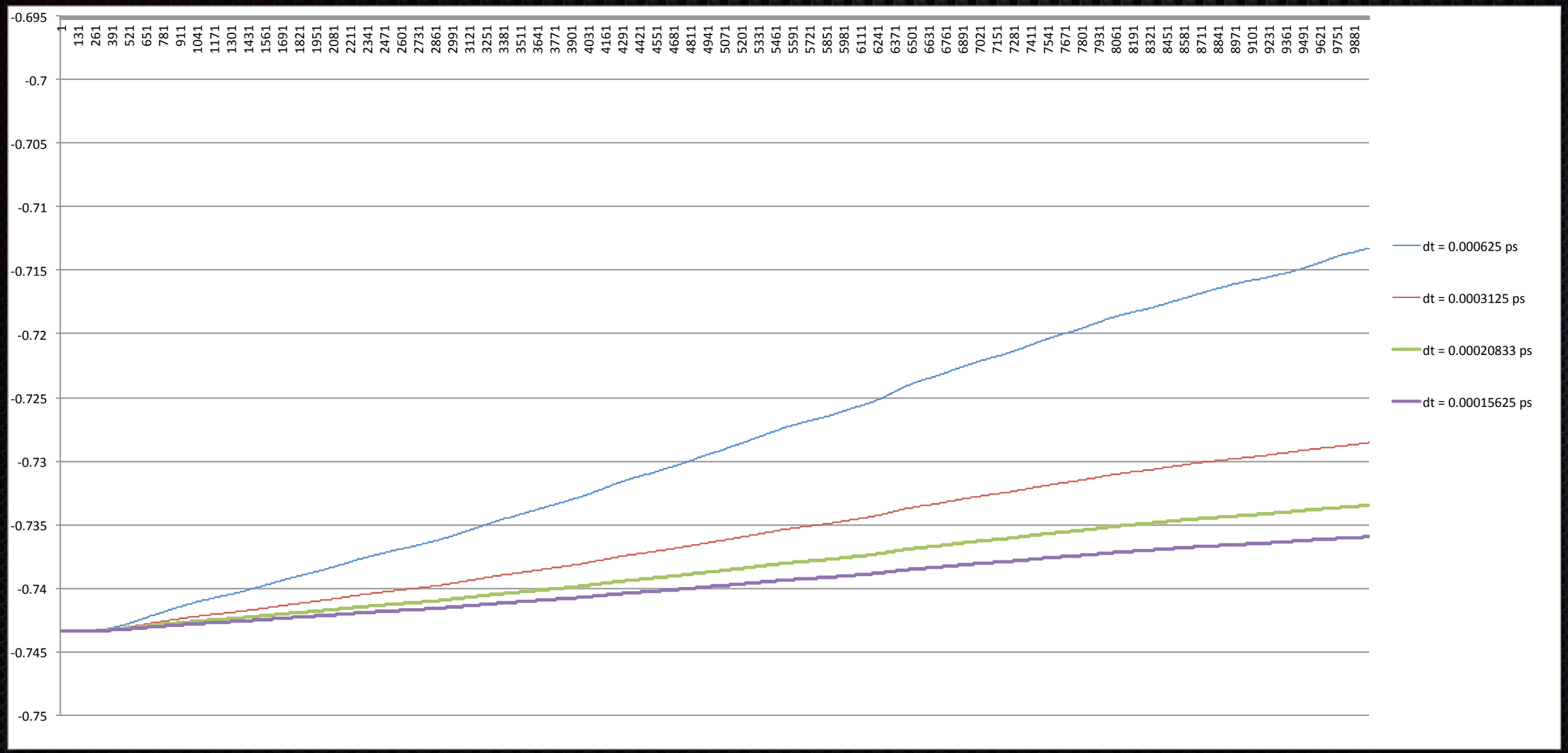


Liquid water (is warm)



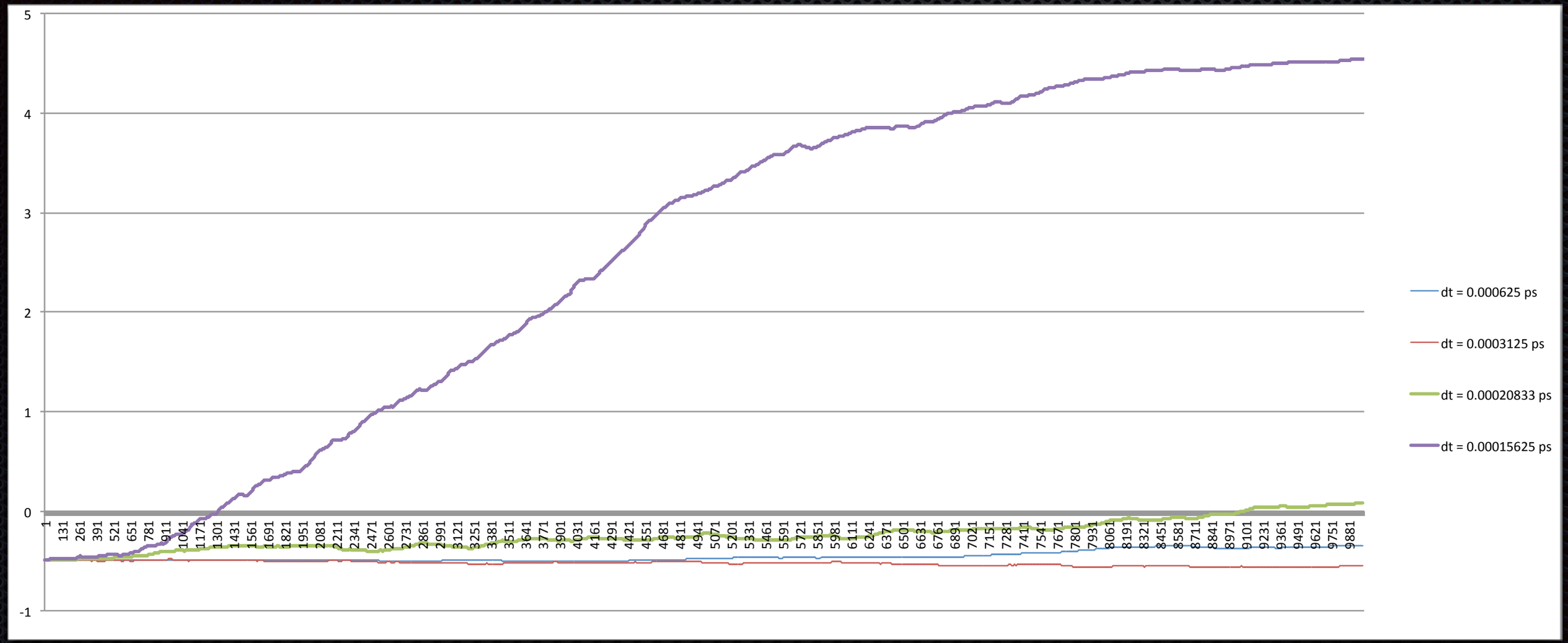
Gas (is hot)





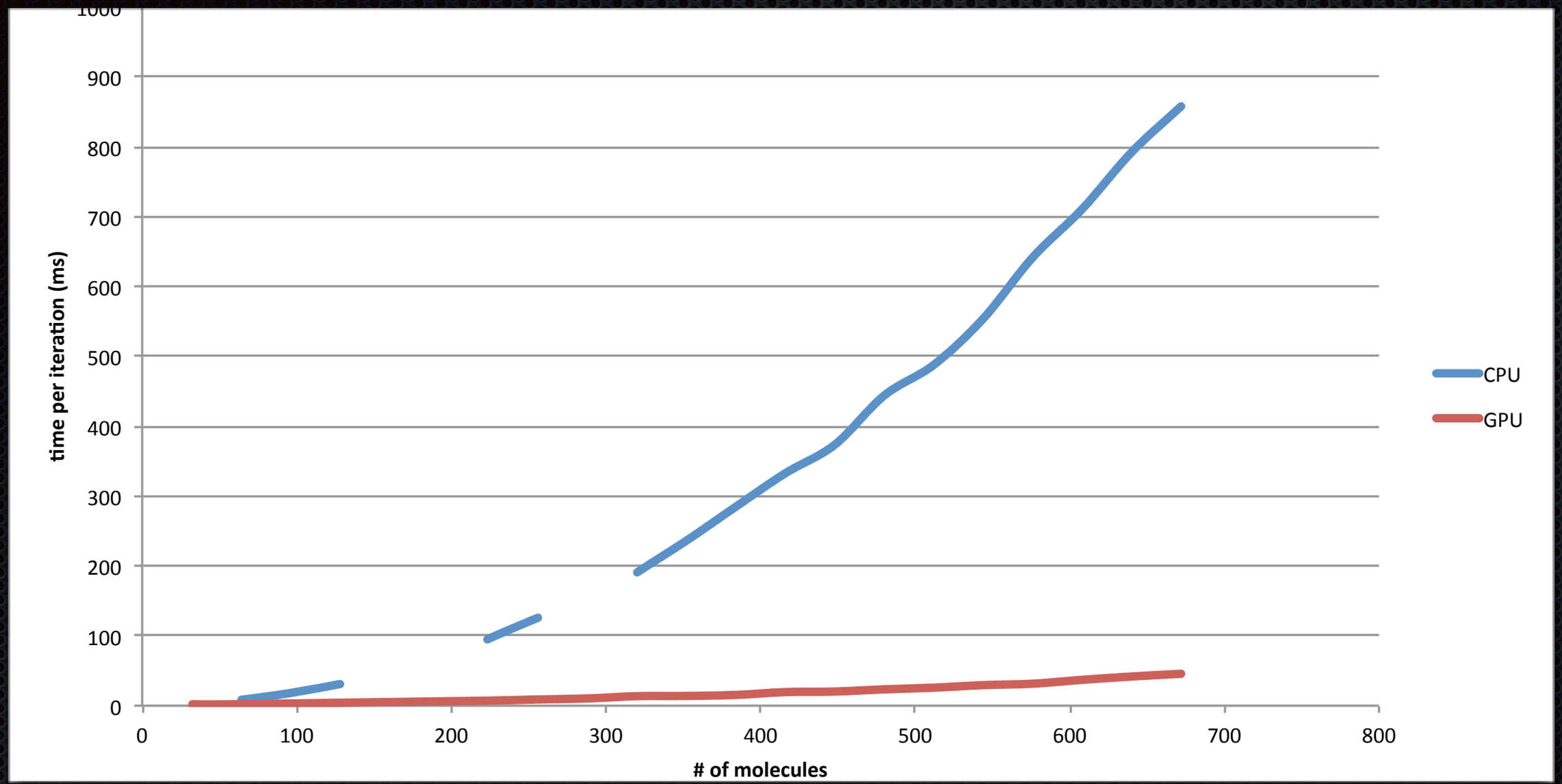
Energy conservation

Double precision



Energy conservation

Floating-point errors



CPU vs. GPU Benchmark

Conclusions/Future Work

- Periodic boundaries
- Control pressure/volume
- Reconstruct/validate previous TIP4P/2005 data
- Insert ions into system of water

Acknowledgments

- Dr. John Deisz
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