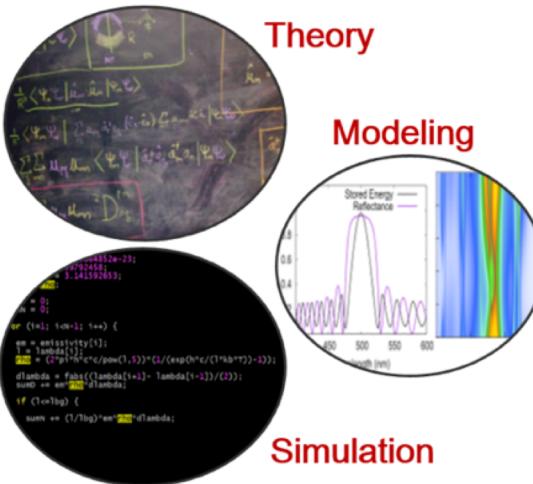


@Foley_Lab

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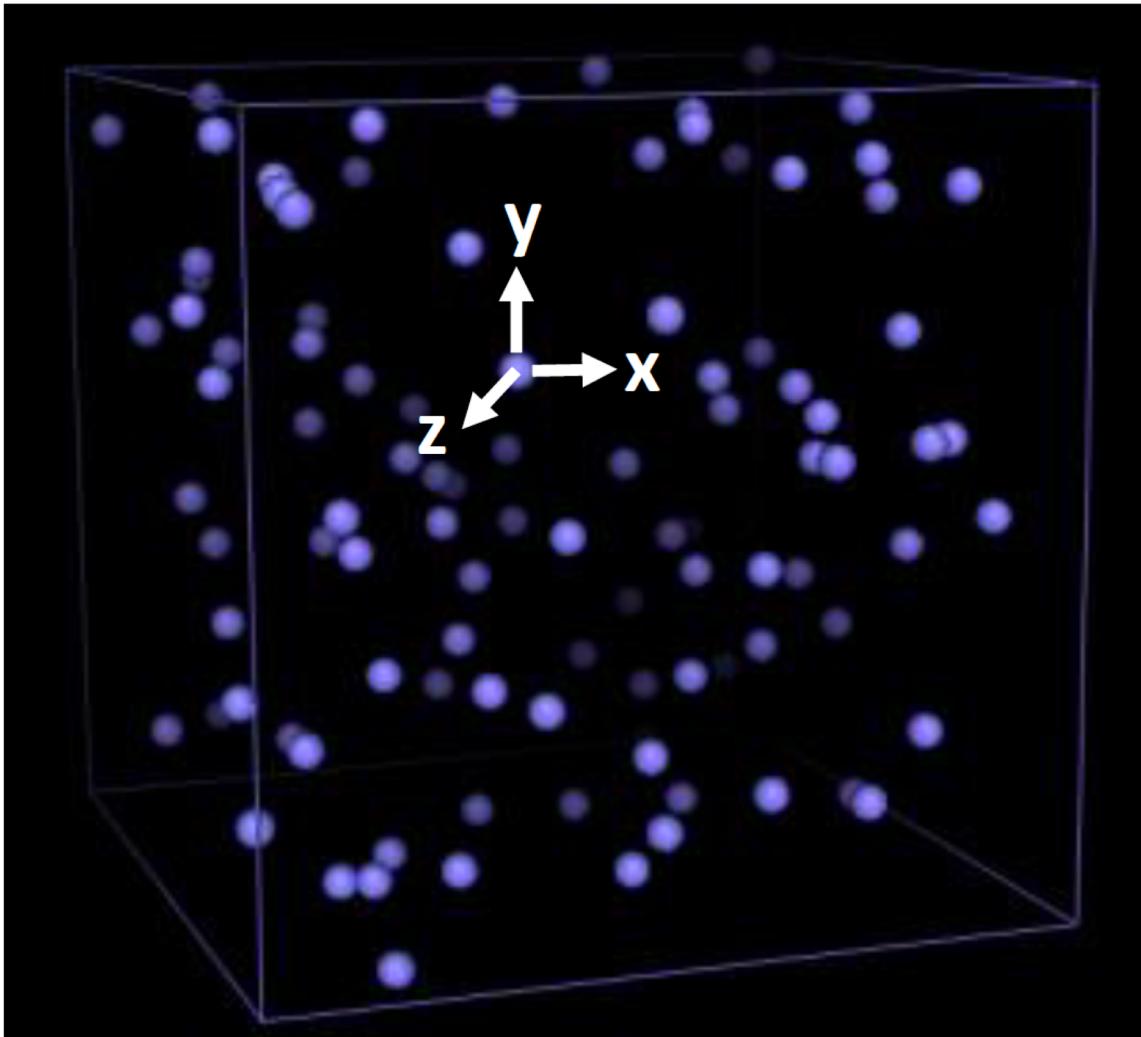
wptherml

<https://foleylab.github.io/wptherml/>

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Brief overview of molecular dynamics simulations



Newton's equations are numerically integrated for a system of N particles

$$\frac{\mathbf{F}_i(t)}{m_i} = \mathbf{a}_i(t) = \frac{-\partial V_i(\mathbf{r}(t))}{\partial \mathbf{r}_i(t)}$$

$$\mathbf{v}_i(t + dt) = \mathbf{v}_i(t) + \frac{1}{2} (\mathbf{a}_i(t + dt) + \mathbf{a}_i(t)) dt$$

$$\mathbf{r}_i(t + dt) = \mathbf{r}_i(t) + \mathbf{v}_i(t) dt + \frac{1}{2} \mathbf{a}_i(t) dt^2$$

molecular dynamics simulation in a flow chart

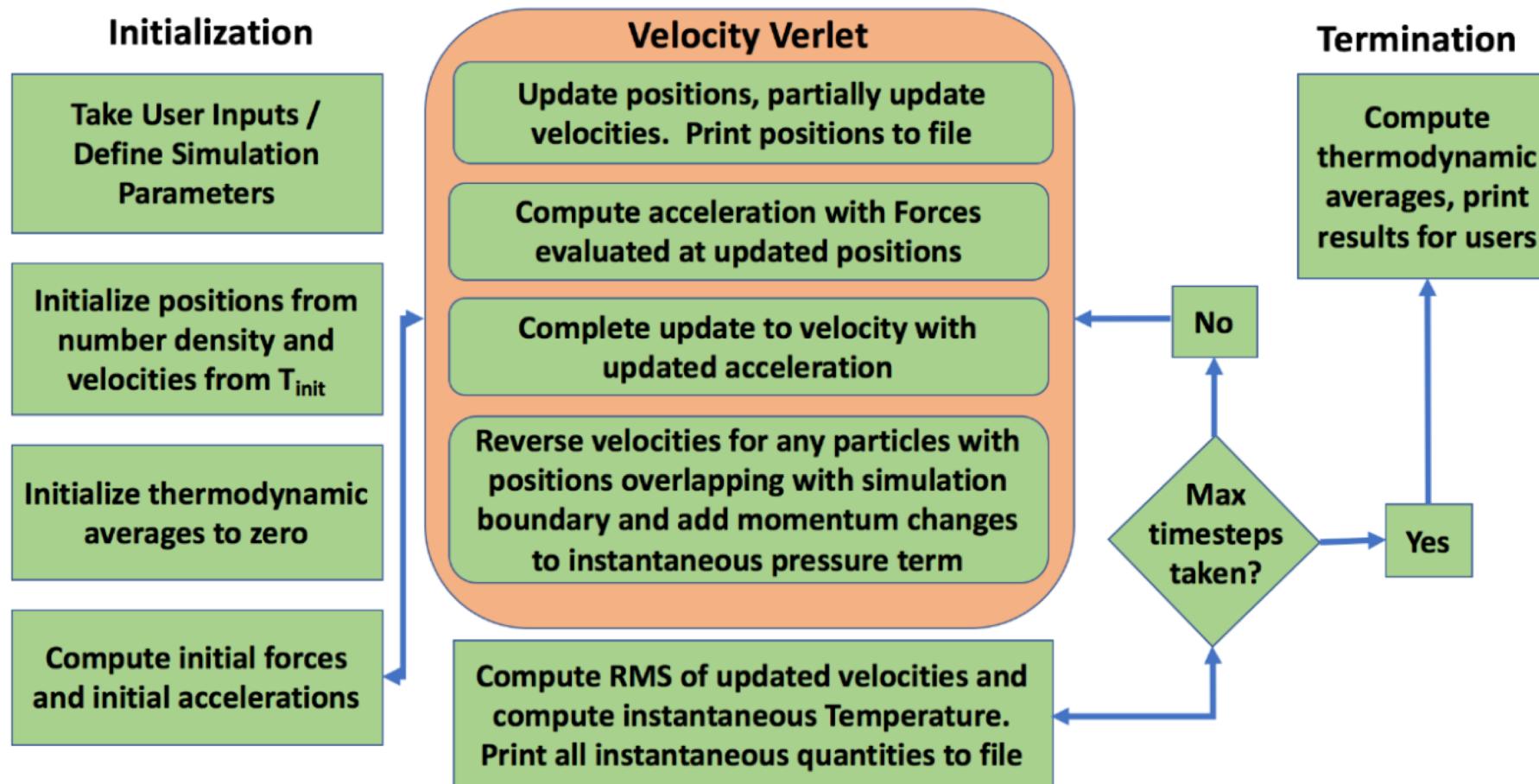
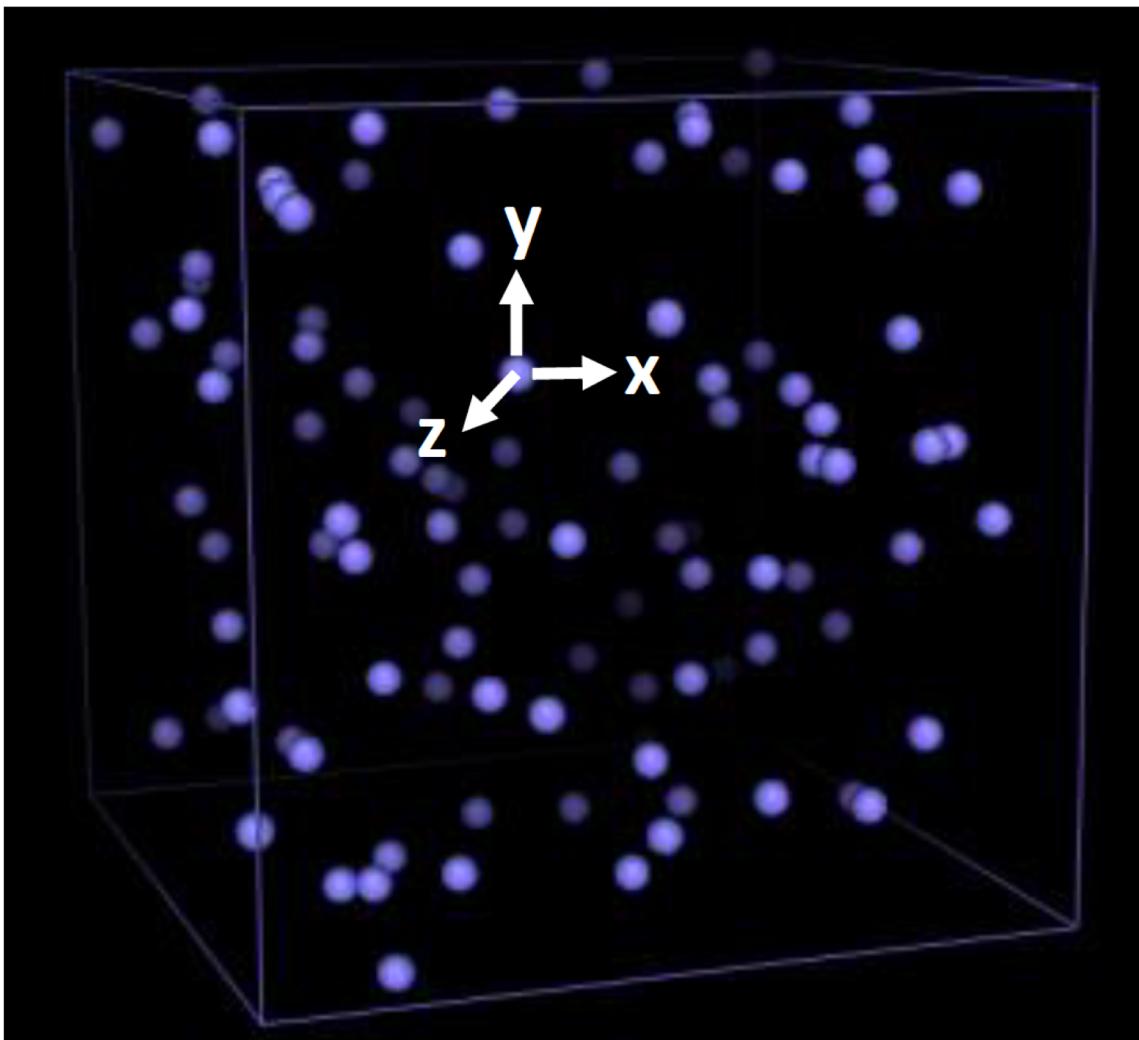


Figure S1 Block diagram illustrating flow of a Molecular Dynamics Simulation

This is how we know things are classical!



Instantaneous position and velocity/momentum of all particles are the quantities that are directly simulated

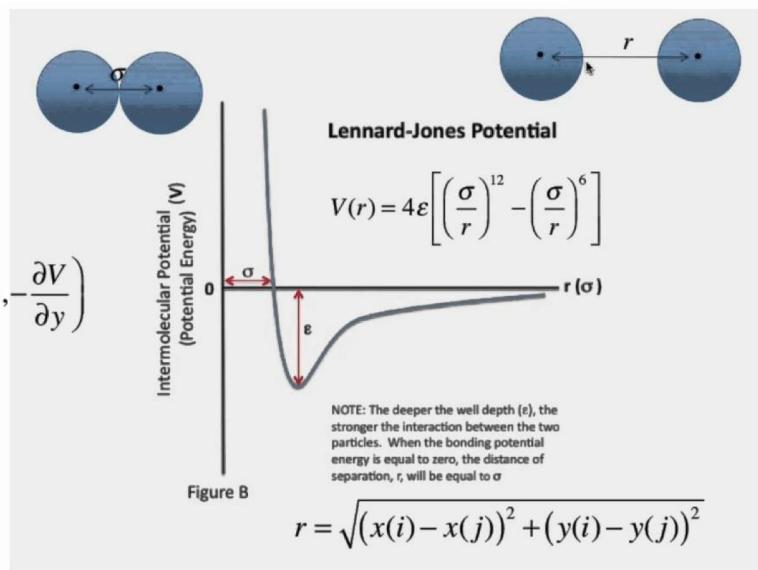
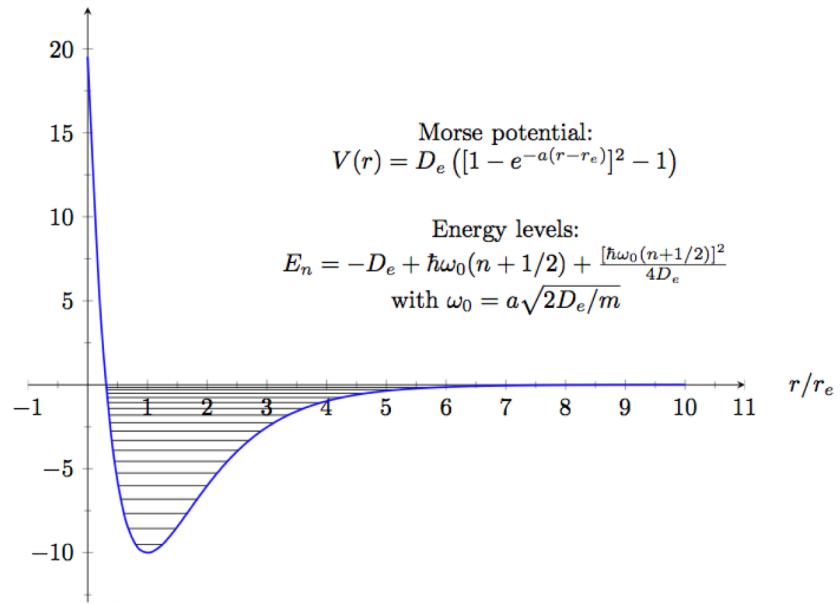
$$\frac{\mathbf{F}_i(t)}{m_i} = \mathbf{a}_i(t) = \frac{-\partial V_i(\mathbf{r}(t))}{\partial \mathbf{r}_i(t)}$$

$$\mathbf{v}_i(t + dt) = \mathbf{v}_i(t) + \frac{1}{2}(\mathbf{a}_i(t + dt) + \mathbf{a}_i(t))dt$$

$$\mathbf{r}_i(t + dt) = \mathbf{r}_i(t) + \mathbf{v}_i(t)dt + \frac{1}{2}\mathbf{a}_i(t)dt^2$$

The potential governs the forces, and by extension, the dynamics

$E/\hbar\omega_0$

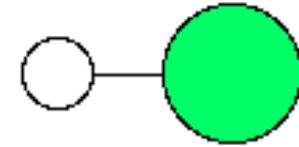


$$\frac{\mathbf{F}_i(t)}{m_i} = \mathbf{a}_i(t) = \frac{-\partial V_i(\mathbf{r}(t))}{\partial \mathbf{r}_i(t)}$$

Potential/Force Field can be derived in a number of ways:

- (a) Model functions (e.g. Lennard-Jones, Morse) with parameters extracted from experimental observables, *ab initio* calculations, or both
- (b) Forces computed by *ab initio* calculations at each configuration as simulation is run

Overview of what we will do!



- Compute potential at a range of separations for HF using *ab initio* methods with psi4numpy
- Fit potential to a spline using scipy – permits us to compute potential at arbitrary separations
- Differentiate spline using scipy – permits us to compute the force at arbitrary separations
- Implement and validate Velocity Verlet integrator
- Simulate HF's vibrational motion with a model and *ab initio* potential