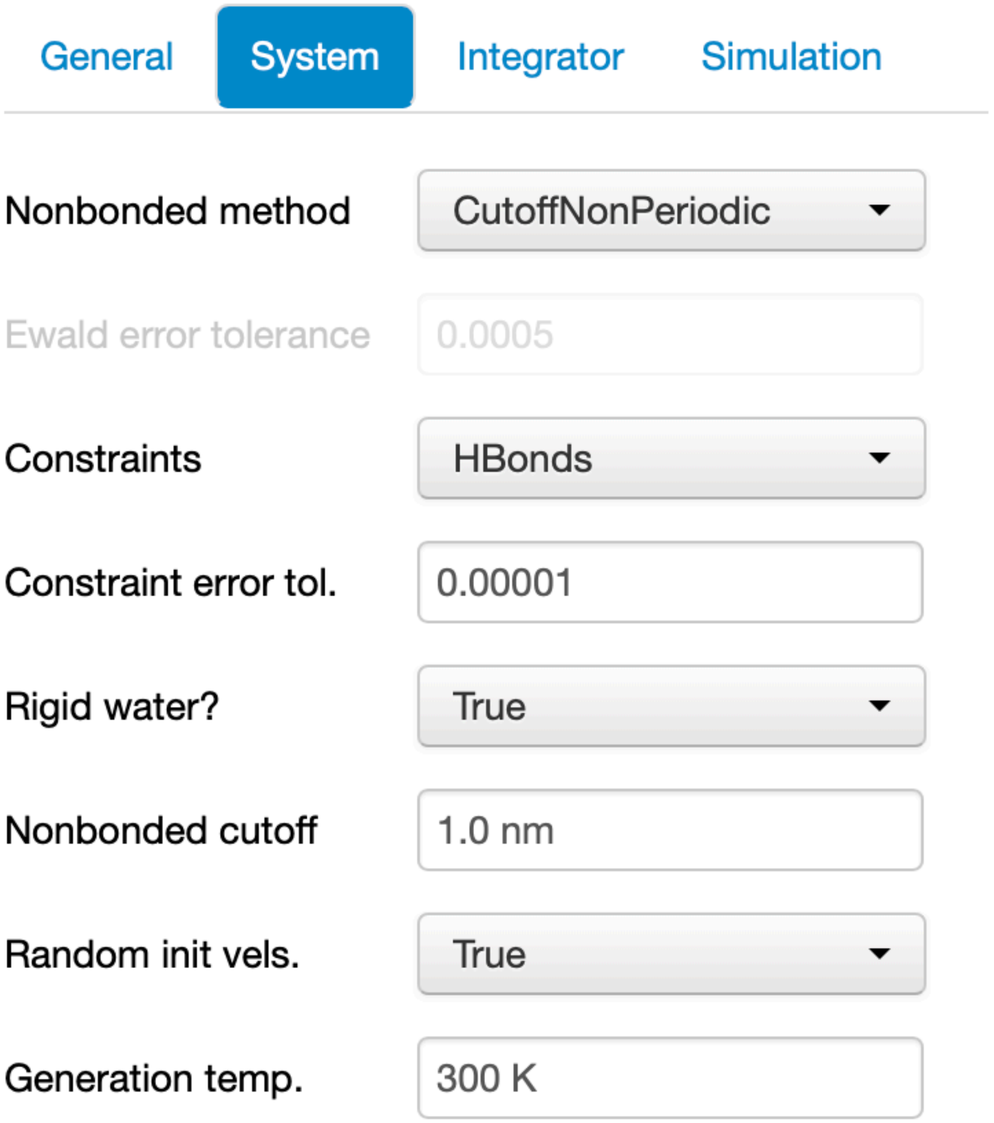
- “Nonbonded method” describes how long-range interactions are treated. The more interactions that need to be computed, the slower an MD simulation will be.
  - Cutoffs don’t perform calculations if two particles are beyond a certain distance apart.
  - Ewald methods calculate long-range interaction energies between a system and its periodic images. It assumes the system repeats indefinitely.
  - Since we are using implicit solvent, we don’t need periodicity.
  - Let’s use “CutoffNonPeriodic”.
- “Constraints”
  - force a degree of freedom to be a certain value
  - allow a larger time step, giving you more bang (simulation time) for the buck (compute time)
- Let’s keep the other “System” parameters as is



- “Integrator” is the algorithm that goes from one configuration to the next
  - Verlet is completely deterministic
  - Langevin adds some random noise to the motion. The level of noise maintains the system at a certain temperature.
  - Brownian is so random that there is no momentum
  - Variable methods use different time steps and depend on an error tolerance
  - Let’s use Langevin and keep default values of other parameters
- “Barostat”
  - allows the volume of the system to change
  - keeps the system at a certain pressure
  - Since we are using implicit water, let’s not use a barostat