

- “Integrator” is the algorithm that goes from one configuration to the next
  - Verlet is completely deterministic
  - Langevin adds some random noise to the motion
  - 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

General	System	Integrator	Simulation
Integrator		Langevin ▼	
Timestep		2.0 fs	
Error tolerance		0.0001	
collision rate		1.0/ps	
Temperature		300 K	
Barostat		None ▼	
Pressure		1 atm	
Barostat interval		25	
Thermostat		None ▼	

- “Reporters” store data about the simulation
- “StateData” gives various options listed in the check boxes
- “DCD” is a binary file format for molecular dynamics trajectories
- “Report Interval” is how often the data are stored
- “Equilibration” is the number of steps before data is stored
- “Production” is the number of steps the simulation is run
- “Minimize” will minimize the energy before running the simulation.
- Let’s set the options as shown on the right

General
System
Integrator
Simulation

Reporters
StateData, DCD

Report Interval
100

Equilibration steps
0

Production steps
1000

Minimize?
True

Max minimize steps

StateData options
☒ Step index
☒ Time
☒ Speed
☒ Progress
☒ Potential energy
☐ Kinetic energy
☐ Total energy
☒ Temperature
☐ Volume
☐ Density