

- “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

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	<input checked="" type="checkbox"/> Step index <input type="checkbox"/> Time <input checked="" type="checkbox"/> Speed <input checked="" type="checkbox"/> Progress <input checked="" type="checkbox"/> Potential energy <input type="checkbox"/> Kinetic energy <input type="checkbox"/> Total energy <input checked="" type="checkbox"/> Temperature <input type="checkbox"/> Volume <input type="checkbox"/> Density		