

- “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

General	System	Integrator	Simulation
Nonbonded method	CutoffNonPeriodic ▼		
Ewald error tolerance	0.0005		
Constraints	HBonds ▼		
Constraint error tol.	0.00001		
Rigid water?	True ▼		
Nonbonded cutoff	1.0 nm		
Random init vels.	True ▼		
Generation temp.	300 K		

- “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	