

- For “Input coordinates”, enter 1ubq.pdb
- “Forcefield” is the set of parameters and functions that describes the energy of a system. Let’s keep “AMBER99sb-ildn”
- “Water Model” includes
 - descriptions that vary in the number of point charges
 - a description that doesn’t actually model water at all, but its effect on the electrostatic energy and a penalty for forming surfaces. For computational speed, let’s pick this “Implicit Solvent” version
- “Platform” describes the version of the code and the hardware it will run on
 - “Reference” is meant to be the most readable code
 - “CUDA” and “OpenCL” are meant for GPUs, which make MD simulations much faster. “CUDA” only works with Nvidia GPUs and “OpenCL” on others
 - “CPU” is a faster version of Reference.
 - Since the laboratory machines don’t have GPUs, let’s use “CPU”
- The other options are GPU-specific

General System Integrator Simulation

Input coordinates

Input topology

Forcefield

Water Model

Platform

Precision

Device index

OpenCL platform indx

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General System Integrator Simulation

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Input topology

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Platform
TIP3P
TIP4P-Ew
TIP5P
Implicit Solvent (OBC)

Precision

Device index

OpenCL platform indx

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OpenCL
CPU
CUDA

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OpenCL platform indx

- “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		