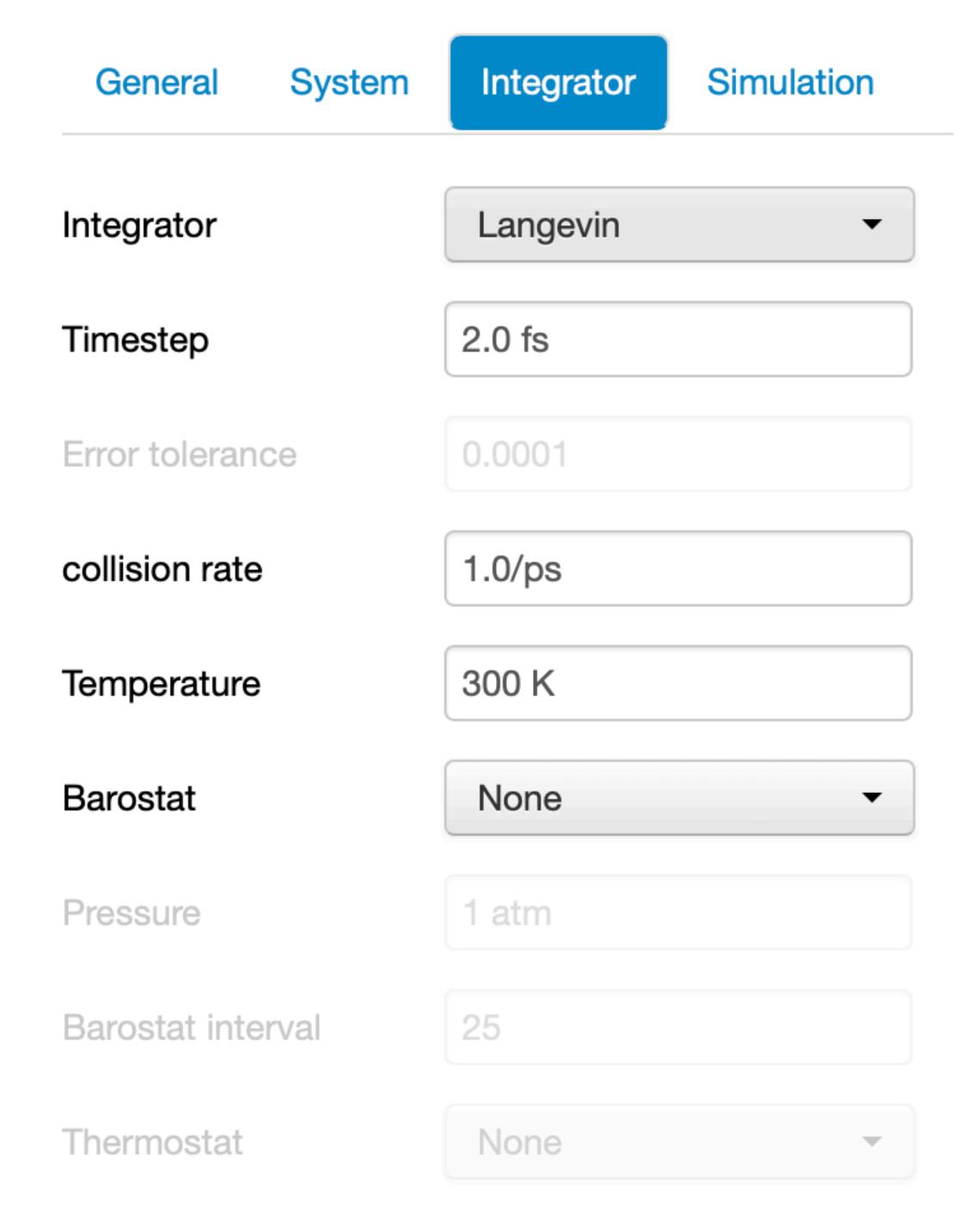
- "Integrator" is the algorithm that goes from one configuration to the next
 - Verlet is completely deterministic
 - Langevin adds some random noise to the motion. The level of noise maintains the system at a certain temperature.
 - Brownian is so random that there is no momentum
 - Variable methods 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



- "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

