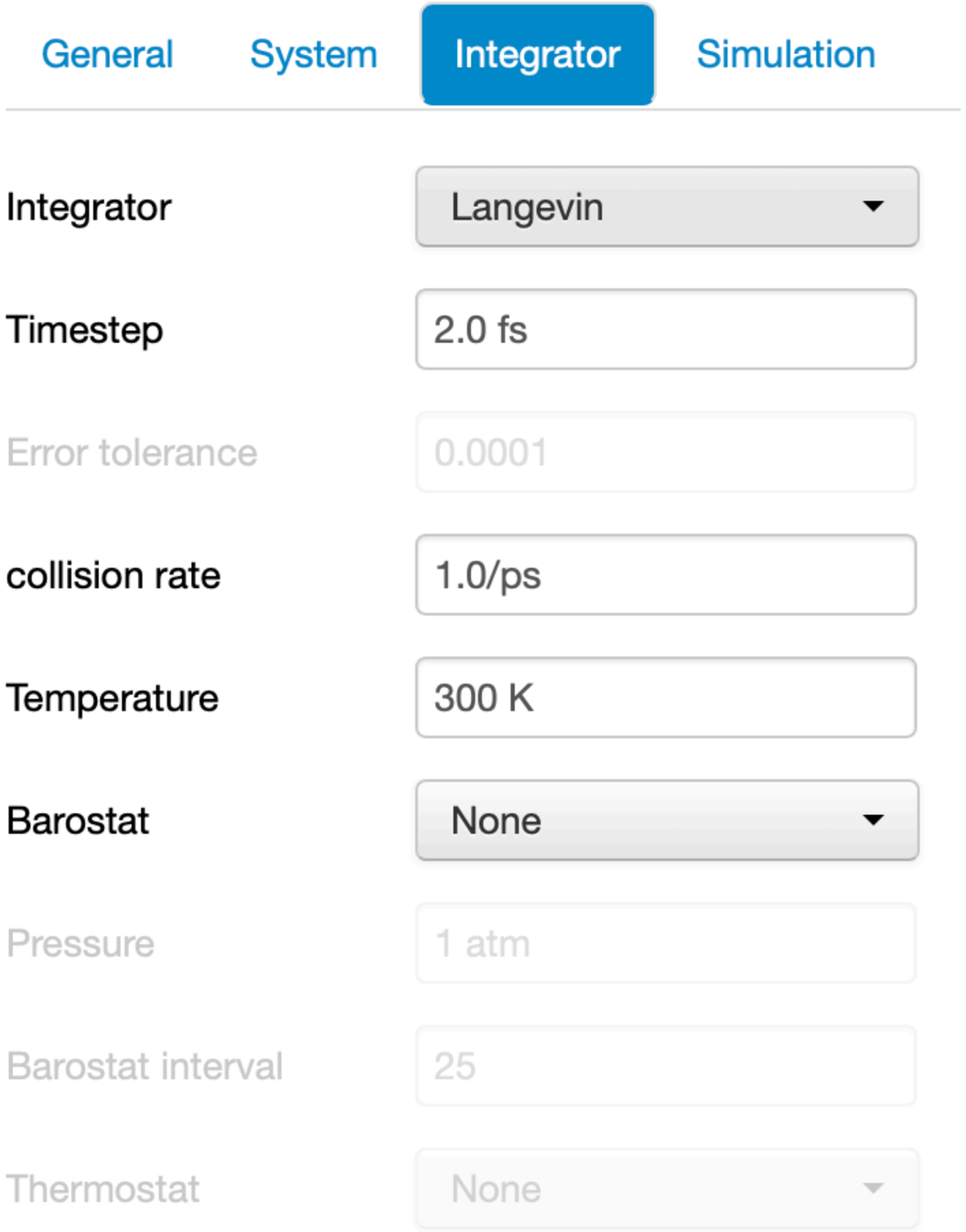
- “Integrator” is the algorithm that goes from one configuration to the next
  - Verlet is completely deterministic
  - Langevin adds some random noise to the motion
  - Brownian is so random that there is no momentum
  - Variable methods use different time steps and depend on an error tolerance
  - 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



- “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