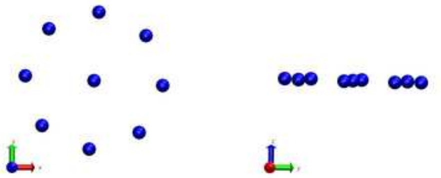
Testing fix rigid langevin

A planar rigid body consisting of 9 atoms was created, and a fix rigid langevin applied.



A unit vector $\mathbf{u}$ is defined as the direction connecting the position of the central atom and one of the other atoms. Outputting $\mathbf{u}(t)$ at regular time intervals allows the correlation function

$$\langle \mathbf{u}(t) \cdot \mathbf{u}(t') \rangle = \langle \cos\phi \rangle \approx e^{-(t-t')k_B T \tau_r / I} \tag{1}$$

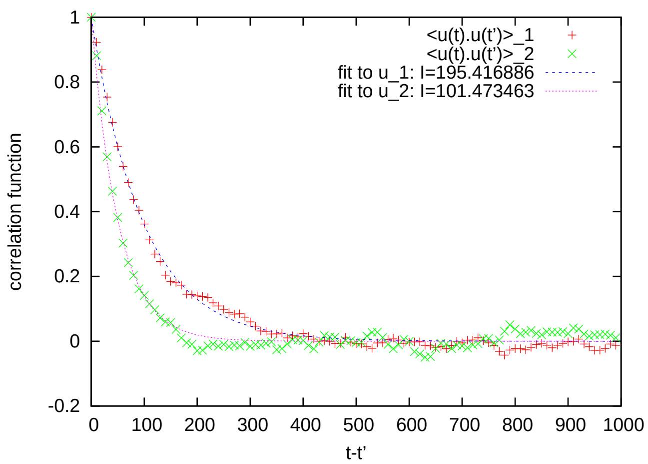
to be calculated. Here τ_r is the rotational velocity damping time, I the moment of inertia, and ϕ is the angle between the vectors $\mathbf{u}(t)$ and $\mathbf{u}(t')$.

Two planar indenters (using fix indent) were used to constrain the rigid body's motion to the $z = 0$ plane; $\mathbf{u}(t)$ was then recorded for 5×10^7 steps. This means that rotations are constrained to be about the axis perpendicular to the plane of the rigid body. Assume that any extra drag due to the indenters is the same in each case below.

Then the indenters were removed and two new ones applied so as to re-orientate the rigid body and constrain it so that moves only along the $y = 0$ plane. The rotations are still constrained to be about the axis perpendicular to the plane of the rigid body — but are in a different axis relative to the system. $\mathbf{u}(t)$ was again recorded for 5×10^7 steps.

For each case the correlation function $\langle u(t) \cdot u(t') \rangle$ can be calculated, and the above equation fit to the data to find I about the axis of rotation. Since the axis of rotation relative to the rigid body is the same in each case, I should be the same.

Results:



The same was done again, after modifying `fix_rigid.cpp`, so as to take into account that the arrays `inertia` and `omega` are in different frames of reference: