Langevin Notes

Daniel Lay

As a reminder, the equations we are solving are

$$\dot{p}_i = -U_{,i} - \frac{1}{2} m^{-1}_{jk,i} p_j p_k - \gamma_{ij} m^{-1}_{jk} p_k + g_{ij}\Gamma_j(t), \tag{1}$$

$$\dot{q}_i = m^{-1}_{ij} p_j, \tag{2}$$

with the relation $g_{ik}g_{jk} = T\gamma_{ij}$ from the fluctuation-dissipation theorem. The temperature T depends on the excitation energy of the particle at a given time step. $\Gamma_j(t)$ is sampled at each time step from a normal distribution. As such, we can benchmark our Langevin code by comparing the average Langevin trajectory to the deterministic system of differential equations where we just neglect Γ_j.

For now, this will just write out the tensor contractions we're doing, following the paper [CITE]. It will be assumed that the potential, U, and the mass tensor, m, only depend on $\vec{q}$, so that derivative notation can be suppressed.

We start with definitions:

$$h_i = -U_{,i} - \frac{1}{2} m^{-1}_{jk,i} p_j p_k - \gamma_{ij} v_j, \tag{3}$$

$$v_i = m^{-1}_{ij} p_j. \tag{4}$$

Note that, in Appendix A.2 of the paper, this expansion is wrong: it replaces $p \to q$ in the second term in h. The second order expansion (from Appendix A.2 in the paper) is

$$\Delta p_i = t h_i + \frac{1}{2}\left[\frac{\partial h_i}{\partial q_j} v_j + \frac{\partial h_i}{\partial p_j} h_j\right] t^2 + g_{ij}\Gamma_{1j} + \frac{\partial h_i}{\partial p_j} g_{jk}\Gamma_{2k} + g_{ij,k} v_k \Gamma_{3j}, \tag{5}$$

$$\Delta q_i = t v_i + \frac{1}{2}\left[\frac{\partial v_i}{\partial q_j} v_j + \frac{\partial v_i}{\partial p_j} h_j\right] t^2 + \frac{\partial v_i}{\partial p_j} g_{jk}\Gamma_{2k}, \tag{6}$$

with Γs given by

$$\Gamma_{1j} = \sqrt{t}\omega_{1j}, \tag{7}$$

$$\Gamma_{2k} = t^{3/2}\left[\frac{1}{2}\omega_{1k} + \frac{1}{2\sqrt{3}}\omega_{2k}\right], \tag{8}$$

$$\Gamma_{3k} = t^{3/2}\left[\frac{1}{2}\omega_{1k} - \frac{1}{2\sqrt{3}}\omega_{2k}\right]. \tag{9}$$

Both ω_{1j} and ω_{2k} are sampled from independent normal distributions, with variance $\sigma = \sqrt{2}$, at each time step.

For use in writing the code, here's the tensors to construct, in the correct order:

$$v_i = m^{-1}_{ij} p_j \tag{10}$$

$$h_i = -U_{,i} - \frac{1}{2} m^{-1}_{jk,i} p_j p_k - \gamma_{ij} v_j \tag{11}$$

$$\frac{\partial v_i}{\partial q_j} = m^{-1}_{ik,j} p_k \tag{12}$$

$$\frac{\partial v_i}{\partial p_j} = m^{-1}_{ij} \tag{13}$$

$$\frac{\partial h_i}{\partial q_j} = -U_{,ij} - \frac{1}{2} m^{-1}_{kl,ij} p_k p_l - \gamma_{ik}\frac{\partial v_k}{\partial q_j} \tag{14}$$

$$\frac{\partial h_i}{\partial p_j} = -m^{-1}_{jk,i} p_k - \gamma_{ik}\frac{\partial v_k}{\partial p_j} \tag{15}$$