Langevin Dynamics

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March 2, 2010

1 General solution

The equations of motion are given by the Langevin equation

$$m_i \frac{d\vec{v}_i(t)}{dt} = \vec{F}_i(t) + \vec{\Gamma}_i(t) - \gamma m_i \vec{v}_i(t), \tag{1}$$

where $\vec{v}_i = \frac{d\vec{r}_i}{dt}$ and $\vec{\Gamma}$ is a random force with $\langle \Gamma(t)\Gamma(t')\rangle = 2\gamma m_i T \delta(t-t')$. The general solution for each degree of freedom is

$$v_i(t+\Delta t) = e^{-\gamma \Delta t} v_i(t) + \frac{1}{m_i}\int_t^{t+\Delta t} e^{-\gamma(t+\gamma\Delta t - t')}\left(F_i(t') + \Gamma_i(t')\right)dt'. \tag{2}$$

1.1 Configurational force to first order in Δt

Expanding $F_i(t')$ to first order around $t' = t$, $F_i(t') = F_i(t) + (t'-t)F_i'(t) + O[(t'-t)^2]$, gives

$$\begin{aligned} v_i(t+\Delta t) &= e^{-\gamma \Delta t} v_i(t) + \frac{1}{m_i}\int_t^{t+\Delta t} e^{-\gamma(t+\Delta t - t')}\Gamma_i(t')dt' + \\ &\quad \frac{1}{m_i\gamma}\left(1 - e^{-\gamma\Delta t}\right)F_i(t) + \frac{1}{m_i\gamma^2}\left(\gamma\Delta t - \left(1 - e^{-\gamma\Delta t}\right)\right)F_i'(t) \end{aligned} \tag{3}$$

Since $F_i'(t) = (F_i(t+\Delta t) - F_i(t))/\Delta t + O[\Delta t]$, we have

$$\begin{aligned} v_i(t+\Delta t) &= e^{-\gamma \Delta t} v_i(t) + \frac{1}{m_i}\int_t^{t+\Delta t} e^{-\gamma(t+\Delta t - t')}\Gamma_i(t')dt' + \\ &\quad \frac{1}{m_i\gamma^2}\left(\frac{1 - e^{-\gamma\Delta t}}{\Delta t} - \gamma e^{-\gamma\Delta t}\right)F_i(t) + \\ &\quad \frac{1}{m_i\gamma^2}\left(\gamma - \frac{1 - e^{-\gamma\Delta t}}{\Delta t}\right)F_i(t+\Delta t) \end{aligned} \tag{4}$$

Expanding up to second order in $\gamma\Delta t$, we have

$$\begin{aligned}
e^{-\gamma\Delta t} &= 1-\gamma\Delta t+\frac{(\gamma\Delta t)^2}{2} \\
\frac{1}{\gamma^2}\left(\frac{1-e^{-\gamma\Delta t}}{\Delta t}-\gamma e^{-\gamma\Delta t}\right) &= \Delta t\left(\frac{1}{2}-\frac{\gamma\Delta t}{6}\right) \\
\frac{1}{\gamma^2}\left(\gamma-\frac{1-e^{-\gamma\Delta t}}{\Delta t}\right) &= \Delta t\left(\frac{1}{2}-\frac{\gamma\Delta t}{3}\right)
\end{aligned}$$

and

$$\begin{aligned}
v_i(t+\Delta t) &= \left(1-\gamma\Delta t+\frac{(\gamma\Delta t)^2}{2}\right)v_i(t)+\frac{1}{m_i}\int_t^{t+\Delta t}e^{-\gamma(t+\Delta t-t')}\Gamma_i(t')dt'+ \\
&\quad \Delta t\left(\left(\frac{1}{2}-\frac{\gamma\Delta t}{6}\right)\frac{F_i(t)}{m_i}+\left(\frac{1}{2}-\frac{\gamma\Delta t}{3}\right)\frac{F_i(t+\Delta t)}{m_i}\right). \qquad (5)
\end{aligned}$$

We can then find $r_i(t)$ by integrating $v_i(t')$

$$\begin{aligned}
r_i(t+\Delta t) &= r_i(t)+\int_t^{t+\Delta t}v_i(t')dt' \\
&= r_i(t)+\Delta t\left(1-\frac{\gamma\Delta t}{2}\right)v_i(t)+\frac{\Delta t^2}{2}\left(\frac{F_i(t)}{2m_i}+\frac{F_i(t+\Delta t)}{2m_i}\right)+ \\
&\quad \frac{1}{m_i\gamma}\int_t^{t+\Delta t}\left(1-e^{-\gamma(t+\Delta t-t')}\right)\Gamma_i(t')dt'. \qquad (6)
\end{aligned}$$

1.2 Random force to first order in Δt

We now need to deal with the integrals

$$X_v(\Delta t) = \int_t^{t+\Delta t}e^{-\gamma(t+\Delta t-t')}\Gamma_i(t')dt' \qquad (7)$$

$$X_r(\Delta t) = \frac{1}{\gamma}\int_t^{t+\Delta t}\left(1-e^{-\gamma(t+\Delta t-t')}\right)\Gamma_i(t')dt'. \qquad (8)$$