Notes on Normal Modes 2.

I have looked at Paula's notes on the Langevin equation in Normal Nodes and her results coincide fairly well with with our early work. My only real comments are that if we define our N body system as having positions $\mathbf{x} = [x_1, x_2, \cdots, x_{3N}]^{\mathbf{T}}$, velocities $\mathbf{v} = [v_1, v_2, \cdots, v_{3N}]^{\mathbf{T}}$, System forces $\mathbf{F}(\mathbf{x}) = [F_1(\mathbf{x}), \cdots, F_{3N}(\mathbf{x})]^{\mathbf{T}}$, random forces $\mathbf{R} = [R_1, \cdots, R_{3N}]^{\mathbf{T}}$ and the 'mass' and 'coefficient' matrices for the original system as

$$\mathcal{M} = \begin{bmatrix} m_1 & 0 & \cdots & & & & & \\ 0 & m_1 & 0 & \cdots & & & & \\ 0 & 0 & m_1 & 0 & \cdots & & & \\ 0 & 0 & 0 & m_2 & \cdots & & & \\ \vdots & & & & & & & \\ \cdots & & & & m_{N-1} & 0 & 0 & 0 \\ \cdots & & & & 0 & m_N & 0 & 0 \\ \cdots & & & & 0 & 0 & m_N & 0 \\ \cdots & & & & 0 & 0 & 0 & m_N \end{bmatrix},$$

$$\mathbf{\Gamma} = \begin{bmatrix} \gamma_1 & 0 & \cdots & & & & & \\ 0 & \gamma_2 & 0 & \cdots & & & & \\ 0 & 0 & \gamma_3 & 0 & \cdots & & & \\ \vdots & & & & & & & \\ \cdots & & & & 0 & 0 & 0 & \gamma_{3N} \end{bmatrix},$$

then we could write the original system as

$$\mathcal{M}\ddot{\mathbf{x}} = \mathbf{F} - \mathcal{M}\mathbf{\Gamma}\mathbf{v} - \mathbf{R}. \tag{1}$$

Given that we have normal mode 'positions' $\mathbf{c} = [c_1, c_2, \cdots, c_m]^{\mathbf{T}}$, corresponding $3N \times m$ matrix of column eigenvectors $\mathbf{Q}$, initial positions $\mathbf{x}_0$ and

$$\mathbf{x} = \mathbf{x}_0 + \mathbf{Q}\mathbf{c},$$

we can rewrite (1) as

$$\mathcal{M}\mathbf{Q}\ddot{\mathbf{c}} = \mathbf{F} - \mathcal{M}\mathbf{\Gamma}\mathbf{Q}\dot{\mathbf{c}} - \mathbf{R}. \tag{2}$$

If we multiply through by $\mathbf{Q}^{\mathbf{T}}$ we get

$$\mathbf{Q}^{\mathbf{T}}\mathcal{M}\mathbf{Q}\ddot{\mathbf{c}} = \mathbf{Q}^{\mathbf{T}}\mathbf{F} - \mathbf{Q}^{\mathbf{T}}\mathcal{M}\mathbf{\Gamma}\mathbf{Q}\dot{\mathbf{c}} - \mathbf{Q}^{\mathbf{T}}\mathbf{R},$$

as Paula did. However, as Paula pointed out, the term $\mathbf{Q}^{\mathbf{T}}\mathcal{M}\mathbf{Q}$ is not diagonal and so 'mixes' the components of $\mathbf{c}$. As an alternative we can rewrite (2) as

$$\ddot{\mathbf{c}} = \mathbf{Q}^{\mathbf{T}}\mathcal{M}^{-1}\mathbf{F} - \mathbf{Q}^{\mathbf{T}}\mathbf{\Gamma}\mathbf{Q}\dot{\mathbf{c}} - \mathbf{Q}^{\mathbf{T}}\mathcal{M}^{-1}\mathbf{R}, \tag{3}$$

since $\mathbf{Q}$ is orthonormal and $\mathcal{M}$ is invertible.

For the purposes of developing the normal mode integrator code in Protomol, I ignored the two Langevin terms so that we have

$$\ddot{\mathbf{c}} = \mathbf{Q}^{\mathbf{T}}\mathcal{M}^{-1}\mathbf{F}, \tag{4}$$

for the real system forces and

$$\ddot{\mathbf{c}} = \Omega\mathbf{c}, \tag{5}$$

for the normal mode evolution. Here Ω is the diagonal $m \times m$ matrix of eigenvalues of the system corresponding to the eigenvectors in $\mathbf{Q}$, which represent the squares of the frequencies of $\mathbf{c}$.

As a test system I used a single water molecule which has 3 modes, two high frequency and one lower frequency. The results compare the original molecular dynamics with the solutions to (4) and (5), with both all modes and the two fast modes constrained, can be seen at http://www.nd.edu/ csweet1/normalmodes.html.