Elastic Network Models

- Coarse-Grained at the residue level
- Residues are connected via elastic springs within a cutoff distance
- Interactions are governed by harmonic potentials

**Two main models:**

- **GNM** (Gaussian Network Model)
- **ANM** (Anisotropic Network Model)
Elastic Network Models

Given a protein structure
Elastic Network Models

Coarse grain at residue level

$C_\alpha$ (or $C_\beta$) atoms are selected as representative points
Elastic Network Models

Connect residues that are closer than a selected cutoff ($r_c$)
Elastic Network Models

Connect residues that are closer than a selected cutoff ($r_c$)
Anisotropic Network Model

Assuming harmonic potentials for each spring:

\[ V_{i,j} = \frac{y}{2} \left( S_{i,j} - S_{i,j}^0 \right)^2 \]

Force constant matrix (Hessian) is the second derivative of the potential:

\[
H_{i,j} = \begin{bmatrix}
\frac{\partial^2 V}{\partial x_i \partial x_j} & \frac{\partial^2 V}{\partial x_i \partial y_j} & \frac{\partial^2 V}{\partial x_i \partial z_j} \\
\frac{\partial^2 V}{\partial y_i \partial x_j} & \frac{\partial^2 V}{\partial y_i \partial y_j} & \frac{\partial^2 V}{\partial y_i \partial z_j} \\
\frac{\partial^2 V}{\partial z_i \partial x_j} & \frac{\partial^2 V}{\partial z_i \partial y_j} & \frac{\partial^2 V}{\partial z_i \partial z_j}
\end{bmatrix}_{3x3}
\]

Which also can be written as:

\[
H_{3Nx3N} = B_{3NxM} K_{MxM} B^T_{Mx3N}
\]

\( B \) : Direction Cosine Matrix

\( K \) : Coefficient Matrix
3x3 super element of the inverse Hessian will give the fluctuation correlations:

$$H_{i,j}^{-1} = \Delta R_i \Delta R_j^T$$

The diagonal super element will correspond to the self-correlations.

Normal modes are given by eigenvalue decomposition:

$$H = U \Lambda U^T$$

Diagonals matrix $\Lambda$ will give the frequencies
Columns of $U$ will be the normal modes

In the presence of an external force, following equation holds:

\[ H_{3Nx3N} \Delta R_{3Nx1} = \Delta F_{3Nx1} \]

\( \Delta R \) : Displacement vector
\( \Delta F \) : External force vector

Therefore, one can find the individual displacements for a given force

\[ \Delta R = H^{-1} \Delta F \]
Visualizations by Jmol: an open-source Java viewer for chemical structures in 3D. http://www.jmol.org/
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