Self Consistent Linearly Forced Elastic Network Model

The LFENM model is defined by:

$$V_{\mathtt{mut}}(\mathbf{r}) = V_{\mathtt{mut}}(\mathbf{r}^0_{\mathtt{mut}}) + \frac{1}{2}(\mathbf{r} - \mathbf{r}^0_{\mathtt{mut}})^T \mathbf{K}_{\mathtt{wt}}(\mathbf{r} - \mathbf{r}^0_{\mathtt{mut}})$$

where

$$V_{\mathtt{mut}}(\mathbf{r}^0_{\mathtt{mut}}) = \frac{1}{2}\sum k_{ij}\delta l_{ij}^2 - \frac{1}{2}(\mathbf{r}^0_{\mathtt{mut}} - \mathbf{r}^0_{\mathtt{wt}})^T \mathbf{K}_{\mathtt{wt}}(\mathbf{r}^0_{\mathtt{mut}} - \mathbf{r}^0_{\mathtt{wt}}).$$

The second term of Eq. is 0 at the minimum, because any possible frustration has been included in the minimum-energy first term.

A major weakness of the LFENM model is that:

$$\mathbf{K}_{\mathtt{wt}} \neq \mathbf{K}(\mathbf{r}^0_{\mathtt{mut}})$$

Since ENMs are defined in such a way that $\mathbf{K}$ is derived from the minimum-energy conformation $\mathbf{r}^0$, this is inconsistent with the basic assumption of ENM models.

The previous issue is overcome in the SC-LFENM model that first calculates the mutant's structure using:

$$\mathbf{r}^0_{\mathtt{mut}} = \mathbf{r}^0_{\mathtt{wt}} - \mathbf{K}^{-1}_{\mathtt{wt}}\mathbf{f}$$

Then, we recalculate $\mathbf{K}$:

$$\mathbf{K}_{\mathtt{mut}} = \mathbf{K}(\mathbf{r}^0_{\mathtt{mut}})$$

Thus the full SC-LFENM model is specified by:

$$V_{\mathtt{mut}}(\mathbf{r}) = V_{\mathtt{mut}}(\mathbf{r}^0_{\mathtt{mut}}) + \frac{1}{2}(\mathbf{r} - \mathbf{r}^0_{\mathtt{mut}})^T \mathbf{K}_{\mathtt{mut}}(\mathbf{r} - \mathbf{r}^0_{\mathtt{mut}})$$

whith,

$$V_{\mathtt{mut}}(\mathbf{r}^0_{\mathtt{mut}}) = \frac{1}{2}\sum k_{ij}\delta l_{ij}^2 - \frac{1}{2}(\mathbf{r}^0_{\mathtt{mut}} - \mathbf{r}^0_{\mathtt{wt}})^T \mathbf{K}_{\mathtt{mut}}(\mathbf{r}^0_{\mathtt{mut}} - \mathbf{r}^0_{\mathtt{wt}}).$$

Here, I assume that everything is done in the potential energy surface of the mutant: i.e. firs term sums "stress" energies only over the eges of the mutant's network (new edges have $\delta l_{ij} = 0$, thus they don't contribute, delted edges don't contribute befause their $k_{ij}^{\mathtt{mut}} = 0$); the second term is relaxation of the mutant's from $\mathbf{r}^0_{\mathtt{wt}}$ to $\mathbf{r}^0_{\mathtt{mut}}$. The second term of Eq. is the energy of deformation around the minimum $\mathbf{r}^0_{\mathtt{mut}}$.

We can turn the wild-type into the mutant by a vertical transition at $\mathbf{r}^0_{\mathtt{wt}}$ in which we replace $k_{ij}^{\mathtt{wt}}$ by $k_{ij}^{\mathtt{mut}}$ followed by the relaxation of the mutant from $\mathbf{r}^0_{\mathtt{wt}}$ to $\mathbf{r}^0_{\mathtt{mut}}$.

Problem: the model is not reversible

If I start with the mutant and do the reverse mutation, I don't get the wild-type's potential...

#todo