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Large-Scale Relaxation Motion of Complex Elastic Networks: as Prototypes of Molecular Machines

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Molecular machines such as enzymes play a fundamental role in biology, and construction of similar devices is a major challenge in nanotechnology. It is recently discovered that elastic network models [1] can reproduce slow conformational motions, essential for the machine functions, in various proteins.

An elastic network model for a protein is constructed in such a way: replace each atom or residue (α-carbon) with a node (identical material particle), and connect two nodes by a link (elastic spring with the same stiffness) if they are within a certain cutoff distance[1]. In this study, instead of choosing networks corresponding to particular proteins, we investigate artificially generated structures.

We show that relaxation behavior of random elastic networks is usually complicated with many modes around the equilibrium states, and thus inconvenient for repeatable machine operations under fluctuations. However, elastic networks with a distinctive slow relaxation mode can be constructed by evolutionary optimization[2]. In contrast to random networks, the optimized networks have long and narrow attractive path(s), along which relaxation proceeds, in the conformational space. These networks may undergo large-scale well-defined motions along the path without strong internal strains, and can be viewed as prototypes of molecular machines.

We demonstrate a constructed elastic network operating as a stochastic cyclic machine powered by binding a ligand. Relevance to biological protein machines such as molecular motors is also discussed.

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[1] M. M. Tirion, *Phys. Rev. Lett.* **77**, 1905–1908 (1996).

[1] The equation of motion for an elastic network in the overdamped limit is

$$\dot{\mathbf{R}}_i = -\sum_{j=1}^{N} A_{ij} \frac{\mathbf{R}_i - \mathbf{R}_j}{|\mathbf{R}_i - \mathbf{R}_j|} \left(|\mathbf{R}_i - \mathbf{R}_j| - \left|\mathbf{R}_i^{(0)} - \mathbf{R}_j^{(0)}\right| \right), \tag{1}$$

where $\mathbf{R}_i^{(0)}$ are initial (equilibrium) positions of the nodes, $\mathbf{R}_i(t)$ their actual coordinates, and A is the adjacency matrix of the network ($A_{ij} = 1$, if $\left|\mathbf{R}_i^{(0)} - \mathbf{R}_j^{(0)}\right|$ is smaller than the cutoff; $A_{ij} = 0$ otherwise).

[2] The equation (1) can be linearized around the equilibrium as

$$\dot{\mathbf{r}}_i = -\sum_{j=1}^{N} \mathbf{\Lambda}_{ij} \mathbf{r}_j = -\sum_{j=1}^{N} A_{ij} \frac{\mathbf{R}_i^{(0)} - \mathbf{R}_j^{(0)}}{\left|\mathbf{R}_i^{(0)} - \mathbf{R}_j^{(0)}\right|^2} \left[\left(\mathbf{R}_i^{(0)} - \mathbf{R}_j^{(0)} \right) \cdot (\mathbf{r}_i - \mathbf{r}_j) \right] \tag{2}$$

for small deviations $\mathbf{r}_i = \mathbf{R}_i - \mathbf{R}_i^{(0)}$. The relaxation is described by a sum of independent exponentially decaying modes; each eigenvalue of $\mathbf{\Lambda}$ corresponds to the decay rate of the mode. Such normal mode analysis (ANM) is often adopted for proteins. Here, we construct networks with a large spectral gap between the lowest and second lowest nonzero eigenvalues, $\log_{10}(\lambda_2/\lambda_1)$, which corresponds to a large difference in the decay rates.