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Adaptive anisotropic network model: generating transition pathways of supramolecular system ZHENG YANG, Univeristy of Pittsburgh, IVET BAHAR, Department of Computaional Biology, Univeristy of Pittsburgh — Generating of functional transition pathways of biomolecular systems is often complicated. This task becomes even more challenging in exploring systems of the order of megadaltons. Coarse-grained models that lend themselves to analytical solutions appear to be the only possible means of approaching such cases. We introduce a new method, *adaptive anisotropic network model* (aANM) for exploring functional transitions, based on the elastic network models, which have been widely used to describe the collective dynamics of biomolecular systems. Application to bacterial chaperonin GroEL highlights the utility of the methodology. Comparisons with experimental data and results from action minimization algorithm support the utility of aANM as a computationally efficient, yet physically plausible, tool for unraveling potential transition pathways sampled by large complexes/assemblies and assessing the critical inter-residue interactions formed/broken near the transition state(s), most of which involve conserved residues.

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