1056-65-1945 **Patrice Koehl*** (koehl@cs.ucdavis.edu), Genome Center, Room 4319, GBSF Building, University of California, Davis, Davis, CA 95616, and **Joel Franklin**, **Sebastian Doniach** and **Marc Delarue**. *Fast Protein Dynamics Simulations: Dominant Pathways for Protein Conformational Transitions.* Preliminary report.

Both structural and dynamical properties of macromolecules are essential to understand and account for their biological functions. There are numerous examples of biologically important structural rearrangements, including allosteric dynamics of receptors that undergo a transition from an open to a closed state upon ligand binding. While experimental methods can give an atomic description of the two end states, they cannot describe the transition itself. Most studies of structural transitions rely on simulation techniques such as molecular dynamics, but the time scale accessible to such methods is several orders of magnitude smaller than the time scale during which these phenomena occur. Our solution to the problem of finding a path between two states of a molecule is to reformulate the Langevin equation that describes the dynamics as an action minimization problem. We show that this formulation leads to large systems of differential equations that can be efficiently solved using Krylov subspace methods for approximation the product of a function of a matrix times a vector. We perform an illustrative application of these ideas on the dynamics of ion channels in cell membranes. (Received September 22, 2009)