MAR06-2005-000044

Abstract for an Invited Paper
for the MAR06 Meeting of
the American Physical Society

Flexibility in Biomolecules: Beyond Molecular Dynamics.[1]

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Molecular dynamics is unable to explore the conformations large protein complexes, viral capsids etc. Using Lagrange constraints for covalent bonds, hydrogen bonds, hydrophobic tethers, and van der Waals excluded volumes, Monte Carlo dynamics uses ghost templates to efficiently guide rigid clusters via the flexible joints between them. The generation a new protein conformation typically requires about 100 milliseconds CPU time. Specifically, input from a single X-ray crystallographic structure can generate an ensemble of structures remarkably similar to those observed in NMR. Further applications are pathways for ligand docking, misfolding proteins and viral-capsid swelling. The software used for this work is available either interactively or for downloading via flexweb.asu.edu.

[1]Work done in collaboration with Stephen Wells, Dan Farrell, Scott Menor and Brandon Hespenheide - see Constrained Geometric Simulation of Diffusive Motion in Proteins, Physical Biology (October 2005)