Skalenkaskaden in komplexen Systemen

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Hierarchical Dynamics of Biomolecular Processes: Molecular Dynamics Simulation and Langevin Modeling

Abstract:

Biomolecules exhibit structural dynamics on a number of timescales, say, from 10^{-12} to 10 seconds. Despite this substantial separation of timescales, fast and slow degrees of freedom appear to be coupled in a nonlinear manner, e.g, there is theoretical and experimental evidence that fast structural fluctuations are required for slow functional motion to happen. Adopting Aib peptide as a simple model system, we perform extensive molecular dynamics simulations to discover a hierarchy of (at least) three tiers of the molecule's free energy landscape [1]. Providing a simple mechanism of hierarchical dynamics, picosecond hydrogen bond dynamics is found to be a prerequisite for the nanosecond local conformational transitions, which in turn are a prerequisite for the microsecond global conformational rearrangement of the peptide. As a consequence of the hierarchical coupling, the various processes exhibit a similar temperature behavior which may be interpreted as a dynamic transition. Using principal component analysis techniques to define a five-dimensional essential space, the hierarchical energy landscape and conformational dynamics of the system is modeled by a data driven Langevin equation [2]. As the multidimensional Langevin fields describing deterministic drift and stochastic driving are estimated locally, the

method can be used in enhanced sampling methods such as the construction of the overall energy landscape of a system from short trajectories.

[1] S. Buchenberg, N. Schaudinnus and G. Stock, "Hierarchical biomolecular dynamics: Picosecond hydrogen bonding regulates microsecond conformational transitions", J. Comp. Theo. Chem. 11, 1330 (2015).

[2] N. Schaudinnus and B. Bastian and R. Hegger and G. Stock", "Multidimensional Langevin modeling of nonoverdamped dynamics", Phys. Rev. Letters 115, 050602 (2015).