Physikalisches Institut
Albert-Ludwigs-Universität Freiburg

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Free energy landscape analysis of complex dynamics:
from protein folding to chess and biomarkers

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Dimensionality reduction is ubiquitous in analysis of complex dynamics. The conventional dimensionality reduction techniques, such as principal component analysis, however, focus on reproducing properties of the underlying configuration space, rather than the dynamics itself. The constructed low-dimensional space does not provide complete and accurate description of the dynamics. I will describe how to perform dimensionality reduction while preserving the essential properties of the dynamics. Three recent applications will be presented: the analysis of the atomistic simulation of protein folding dynamics by Shaw et. al. Science 330, 341 (2010), the analysis of the dynamics of the chess game and the construction of a biomarker from longitudinal cohort studies.

Molecular Dynamics Seminars 2012
Seminar Room of Gustav Mie Haus, Ground Floor, 16:15

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