Chaos and Ergodicity of Realistic Hamiltonian Systems
Le chaos et l'ergodicité pour des systèmes Hamiltoniens réalistes
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Physical Structure, Graph Structure and Uncertainty in Complex Systems

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Abstract

Complexity of systems can be roughly represented on 2 axes, one parametrizing complexity of structure, the other complexity of system dynamics. These two are often not independent, and disentangling their interdependence is not trivial. I will begin by addressing complexity of the system in the context of its behaviours under parameter and initial condition uncertainty in the framework of ergodic theory. Then I will discuss how graph-theoretic decompositions on state variables allow for an extension of that analysis to higher dimensional systems. In this approach, it is not the statistics of the graph that plays the dominant role, but its functional submodules. Algorithms for finding such submodules involve a combination of graph theory, control theory and dynamical systems theory.

Biomolecular systems represent a rich source of interesting complex systems behaviour but are not easily decomposed using above mentioned graph theoretic methods on the standard position-velocity description. I will discuss features of dynamics of a specific model on various scales and the underlying spectral theory that allows for reduced representations of a model biomolecular system that concurrently exhibits robustness and flexibility. An interesting phenomenon occurs, where specific structured perturbations effect global change is system conformation, while non-structured ones do not affect its stability. This enables the system to perform its function in an uncertain environment. The phenomenon is driven by a resonant interaction and

captured accurately by a suitable spectral projection on a small number of modes. In this system there is no separation of scales, but a finite-dimensional representation is possible.

Finally I will discuss approaches to computation of uncertainty and present a modulation of Quasi-Monte Carlo method using a construction that samples the space of parameters or initial conditions using uniformly ergodic dynamical systems that preserve the specified prior.