

STAVROS NIARCHOS FOUNDATION – FORTH SEMINAR SERIES

Tuesday 2 April 2019

16:00 – 17:00

A. Payatakes Seminar Room

" Path-space variational inference in coarse-graining molecular systems"

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Abstract

A standard methodology to overcome problems of long relaxation times of complex systems is to abandon the chemical detail and describe the molecular system by fewer degrees of freedom. Such particle-based, systematic coarse-grained models of molecular systems are developed by averaging out the details at the molecular level, and by representing groups of atoms by a single coarse particle. The challenge though is to find coarse models that represent the structural and dynamic properties of the all-atom system adequately.

In this talk, we will firstly give a short overview of best-fit procedures to predict parameterized families of CG models at equilibrium. Then, we will present in more detail the use of information-theoretic tools, the minimization of the relative entropy for systems out of equilibrium, and the reduction to the path-space force-matching method. Finally, we will introduce the parametrized stochastic dynamics for a system of liquid methane (at equilibrium and transient time regimes), infer the model parameters with the path-space force-matching minimization approach.