

## **Selection of coarse variables, diffusion maps, and effective free energy surfaces**

Yannis G. Kevrekidis

Chemical Engineering and PACM, Princeton University

In performing coarse-grained computations for complex/multiscale systems knowledge of good coarse variables is vital; and when these are not known or suspected from experience, data mining algorithms have an important role to play.

I will present some illustrative examples of equation-free computation and their interplay with a diffusion-map based approach to detecting good "coarse observables" from simulation data.

I will also discuss the exploration of effective free energy surfaces for cases where the appropriate coarse-grained models appear to be low dimensional SDEs.