Diffusion maps for model reduction: exploiting data mining to accelerate simulation

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***Abstract*— In many complex/multiscale systems, the long-term dynamics are reducible: they lie on a low-dimensional manifold parameterized by appropriate coarse variables (observables). Knowing these observables *a priori*, through experience or intuition, can be crucial in accelerating the computational extraction of information from detailed, "fine scale" simulators. Indeed, when such variables parameterizing the slow dynamics are known, the so-called equation-free approach [1] [2], provides a systematic way of designing computational "wrappers" that enable fine scale simulators to perform accelerated simulation as well as a wide range of additional tasks (coarse-grained stability and bifurcation computations, parametric continuation, coarse controller design etc.).**

When such coarse observables are not known, data-mining tools can be used to extract them from simulation databases. Linking data-mining tools (and, in particular, the diffusion map approach of Coifman and coworkers [3]) and the design of equation-free computational experiments provides an integrated framework for coarse-grained computations of complex/multiscale systems. We will illustrate these two components as well as their combination through a number of computational examples. In particular, we will focus on the exchange of information between fine-scale and coarse-scale descriptions. We will explore coarse projective integration alternating between diffusion map and physical settings, and discuss the construction of physical initial conditions consistent with new, "out of sample" diffusion map coordinate values [4].

References

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