

1035-37-1148

Yannis Kevrekidis* (yannis@princeton.edu), Department of Chemical Engineering & PACM, Princeton University, Princeton, NJ 08544. *Equation-free and Variable-free computation for complex/multiscale systems.*

I will discuss the equation-free framework for modeling and computation in complex, multiscale systems. The main idea is to circumvent the explicit derivation of coarse-grained, lower-dimensional, effective models. Even without deriving such models, we can perform scientific computing tasks with them through the design, performance, and processing of the results of short bursts of scientific computation with the original, fine-scale code.

This "input-output", design of experiments approach is based on the knowledge of good coarse-grained variables (observables) in terms of which the coarse-grained model would be written. When such variables are not known a priori, data-mining techniques -such as diffusion maps- may be used to detect such good coarse variables on the fly. The work involves several collaborations (C. W. Gear, R. Coifman and others, which will be mentioned in the presentation.) (Received September 18, 2007)