Coarse-graining the dynamics of (and on) evolving graphs: Algorithms and Computation.

EQUATION-FREE AND VARIABLE FREE MODELING FOR COMPLEX/MULTISCALE SYSTEMS:
Coarse-grained computation in science and engineering using fine-grained models

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Abstract

We will present and illustrate computer-assisted approaches to coarse-graining the dynamics of evolving graphs, as well as the dynamics taking place *on* graphs, and the combination of the two (the dynamics of adaptive networks). The ideas are those of equation-free multiscale computation: the selection of appropriate macroscopic variables (observables), and the use of traditional numerical methods to design, execute and process the results of brief detailed network evolution simulation. Integrating the design of these computational experiments with *lifting* (the construction of networks with prescribed macroscopic observables), and *restriction* from detailed networks back to coarse observables, we can, in effect, solve the coarse-grained equations without explicitly deriving them.

We will discuss several algorithmic issues. A new development involves the use of mathematical programming to construct networks with prescribed statistics. A collaboration with Balazs Rath illustrates the use of separation of time scales to justify the derivation of explicit coarse-grained equations for validation purposes. It also provides a link of our work with the recent theory of graphons by Lovasz and coworkers. We also discuss an interesting new link between tools for uncertainty quantification and the coarse-graining of networks: when the nodes of a network are heterogeneous (because of their intrinsic properties or because of their connectivity properties in the network or both) we use polynomial chaos coefficients to describe the dependence of their states on the heterogeneity. We also explore the use of data-mining tools (and, in particular, diffusion maps) for the selection of good coarse observables from graph evolution data directly – using graph kernels provides one approach to this task.

We will present an array of illustrative examples, some designed for mathematical validation and theory development, and others arising in social, chemical and neuroscience contexts.