Dimension Reduction Method for Large ODE Systems

New Dimension Reduction Methods and Scalable Algorithms for Multi-Scale Nonlinear Phenomena

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Abstract

Many natural physical processes allow different mathematical descriptions on different scales. A microscale description is usually based on fundamental conservation laws that form a closed system of ordinary differential equations (ODEs) or partial differential equations (PDEs). The numerical discretization of these equations may produce a system of ODEs with an enormous number of unknowns. Furthermore, time integration of the microscale equations usually requires time steps that are smaller than the observation time by many orders of magnitude. A direct solution of these ODEs can be extremely expensive. On the other hand, an accurate closed-form macro-scale description of the same phenomenon is often unavailable. This necessitates development of new effective dimension reduction methods.

The starting point of many reduction methods is to apply volume averaging to a system of ODEs governing the dynamics of microscale variables. Averaging procedure usually results in non-local mesoscale balance equations for the corresponding spatial averages. That is, the mesoscale equations contain flux terms that are explicit functions of the microscale variables. No rigorous closure methods are available for many non-linear non-ergodic systems with large relaxation times, and most of the existing closure methods rely on empirical models. I will describe a new computational closure for non-local mesoscale equations. The key idea of the closure is to use an iterative deconvolution to approximate microscale variables from their spatial averages and to use these microscale variables to calculate non-local flux terms in the mesoscale balance equations. Then the mesoscale equations are integrated in time, and the closure procedure is repeated. The main advantage of the proposed dimension reduction method is that the computational closure is not empirical and does not require assumptions of ergodicity and/or local equilibrium. Deconvolution approximation of a microscale variable from its average is a classical example of an unstable ill-posed problem. We employ regularized iterative deconvolution method, a method for regularizing ill-posed deconvolution problems, to obtain stable approximates of the microscale variables.

The dimension reduction method was used to solve systems of ODEs describing Newtonian particle dynamics with application to reactive transport in porous media. Our results show that the dimension reduction method can significantly accelerate solution of large ODE systems. The reduction method provides an accurate prediction of the average behavior of the modeled systems and is able to recover important features of a direct solution of the ODE systems, while using a significantly reduced number of degrees of freedom and, in general, a significantly larger time step than that required for the direct solution of the ODEs.