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Heterogeneous multi-scale methods for oscillatory dynamical systems

Bjorn Engquist

Department of Mathematics, University of Texas at Austin
C1200, Austin, TX 78712-0257, USA
engquist@math.utexas.edu

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ABSTRACT

Highly oscillatory solutions to dynamical systems pose severe challenges for numerical simulations. Details of the oscillations must typically be resolved by the numerical grid over long time intervals resulting in prohibitingly high computational cost. One generic example is molecular dynamics with vibrations on atomistic time scales that may require much longer time integration to model system size reactions.

The framework of the heterogeneous multiscale method for efficient modelling of multiscale phenomena was presented in [1] and recently surveyed in [2]. The basic idea in the approach is to focus on the macroscale variables and the structure of a mecroscale model. Typically the macroscale model is not fully known or may not be valid in all of the computational domain. A higher fidelity microscale model is then used to supply the missing data. The computational efficiency is gained from only using the microscale model in small samples of the computational domain.

When applied to dynamical systems this means that the detailed system is only used for a limited number of micro steps in a short time interval. A local average of the force is then calculated from this data and used for much larger time steps in a numerical macroscale method. This technique was briefly mentioned in [1] and further studied, for example, in [3]. In both these presentations the macroscale and microscale variables were the same as in the original dynamical system. That works well for dissipative cases, linear problems and for certain nonlinear equations with very simple resonance behaviour, [3].

There are other numerical techniques for efficient integration of multiscale problems. The projective integration method in [4] introduced the idea of mixing large and smaller time steps but does not handle oscillatory modes. The book by Heirer et. al. [5] contains many powerful algorithms but those that do not require the computational complexity to grow at least linearly with the inverse of the fastest scale typically require the leading part of the system, to be linear.

In [6] we realised the need to explicitly determine slow variables even in the heterogeneous multiscale method in order to control resonances in general and more realistic nonlinear dynamical systems.

In this presentation we shall describe the recent progress in developing techniques that have the sound theoretical foundation of the original heterogeneous multiscale method but also the does not require knowledge of all slow macroscale variables a priory. We are considering two slightly different approaches. In one, a few slow observables are controlled and they are used to constrain the local microscale simulations. Typically energy is constrained to be constant and relevant averages are predicted from extra differential equations. Here it is natural to compare with thermostats in molecular dynamics that only constrain a few components. Analysis and numerical examples will be given.

In the other technique all slow variables are determined on the fly [7]. This is possible for a fairly general class of systems and works very well for weakly coupled nonlinear oscillators. The analysis of this method also reveals interesting properties of a wide class of dynamical system with oscillatory solutions.

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