Comments on the Papers

Weinan E

- Section 2: The paper by Car and Parrinello presents the most compelling example for using microscale models (here the density functional theory for electronic structure analysis) to help bypassing empirical macroscale models (here molecular dynamics of the atoms with empirical inter-atomic potential).

  I chose the Knap-Ortiz version of the quasicontinuum method since it is more closely related to the renormalization multi-grid, HMM and "equation-free" – the small clusters in the Knap-Ortiz version play the role of the "small windows".

  I should also post a representative paper on the kinetic scheme for gas dynamics. I am still not sure which one to pick.

- Section 3: Brandt's paper proposed a general framework for capturing the macroscopic behavior of a system using microscopic models, bypassing empirical macroscale models, using an "interpolation-equilibration-restriction" strategy. Brandt also recognized the possibility of simulating microscopic models on "small windows" and for a "few sweeps". This is a long paper. The reader might consult directly section 14.

  I am using an old terminology and calling this "renormalization multi-grid". Achi now calls this "systematic upscaling".

- Section 4: The first paper lays down the framework of HMM. The second paper describes the background. The third paper is a nice example of an algorithm formulated in HMM framework. It should be pointed out that Eric had his initial ideas before HMM came into market. The 4th paper is a review of HMM.

- Section 5: The first paper is what I usually use as the paper that inaugurates the general framework of "equation-free".

  I should point out that from the viewpoint of multiscale modeling, what is done in the third paper (Erban et al.) and the second half of the second paper (Hummer et al.) is "equation-based" precomputing (i.e. sequential multiscale modeling, a simple form of which is called "parameter passing". What is done here is "coefficient passing"). Among the many such papers that Yannis is involved with, I chose these two for their interesting examples. Here the authors assume that the probability density satisfies a specific form of the Fokker-Planck equation, precompute the coefficients using microscopic models and then solve the

Fokker-Planck equation. I think these are very nice applications of ("equation-based") sequential coupling. However, calling it "equation-free" has caused confusion. It seems that, if anything, it should be called "equation-unfree". In numerical linear algebra, if we precompute the matrix, we would not call it "matrix-free" computation.

- Section 6: Here is an interesting case: Many years ago, Eric Vanden-Eijnden proposed multiscale algorithms for stochastic ODEs using the HMM framework (he had his initial ideas before HMM came to the market). Later Givon et al. studied more or less the same algorithm, but called it "projective integrators". I like the analysis results in the paper by Givon et al. and I have suggested my former student Di Liu to look for sharp estimates. But as before, I feel it is inappropriate to call the algorithm they analyzed "projective integrators".

  If precomputing and HMM are all called "equation-free", what is not "equation-free" among all multiscale algorithms?

- Section 7: The last paper represents an attempt to understand "equation-free". We looked at the difficulties with the "equation-free" approach using very simple examples. While it might be possible to do, fixing these problems seems require substantial deviation from the original philosophy of "equation-free", as was laid out in the first paper in section 5. One attempt to fix the difficulties with patch dynamics is presented in the last paper in section 5. One can see that this is an attempt to put the macro-solver information in the "lift-run-restrict-extrapolate" strategy of patch dynamics via the lifting step. This makes patch dynamics strictly less useful than HMM: It now has all the limitations of HMM (requiring a macro-solver to begin with), but it is definitely harder to implement than HMM since everything has to be done through the already difficult lifting step. In addition to the requirement that the lifted micro-state has to be consistent with the macro-state (the same requirement for the interpolation step of the multi-grid method or the reconstruction step of HMM), it also has to have the correct macroscopic behavior such as upwinding. This is hard to do when we don't know the direction of the wind.

  Note that the convention in multiscale modeling is to put macro models on top and micro models on the bottom. For examples, the "lifting schemes" in wavelet analysis is a way of getting coarse-scale wavelet coefficients from fine-scale ones. So calling an operator that maps macro states to micro states "lifting operator" may generate some confusion since it is opposite to that convention.