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Title: An introduction to mathematical and computational challenges in hybrid stochastic/deterministic systems

Hybrid systems arise as couplings of stochastic models representing active small scales to deterministic macroscopic equations, and are commonplace in a wide array of applications ranging from catalysis and polymeric flows to stochastic models for tropical and open ocean convection. A major challenge in all these problems arises in the direct numerical simulation of realistic size systems involving both scale and model disparities; furthermore, due to nonlinear interactions across a wide range of scales, the stochasticity inherited from the microscopic model can play a subtle but important role in the dynamic behavior of the overall system.

In this talk we attempt to mathematically formulate these issues in the context of prototype mathematical hybrid models that capture essential features of their complex counterparts. In particular they allow us to derive computationally inexpensive mesoscopic deterministic models for the average behavior of the hybrid systems in various asymptotic limits, and to develop and test deterministic closures and stochastic coarse-graining strategies. A key feature of the the simplified prototype models studied here is that they permit computationally feasible detailed comparisons of the derived deterministic and stochastic coarse-grained models against direct numerical simulations of the full hybrid system.

One of the primary tools we have developed partly for the purpose of coupling systems with disparate scale resolutions, is a hierarchical approach to the stochastic coarse-graining of microscopic dynamics such as lattice Monte Carlo. Computational comparisons of coarse-grained and microscopic simulations along with accompanying rigorous estimates on the loss of information between the time-dependent coarse-grained and microscopic probability distribution functions highlight the validity regimes of the method.

The presented results are joint work with A. J. Majda (Courant), P. Plechac (Warwick), A. Sopasakis (UMass), J. Trashorras (Paris IX) and D.G. Vlachos (Chem. Eng. Delaware).