Subgrid Modeling and Stochasticity in Multiscale Transport Simulations

C. David Levermore
Department of Mathematics *and*
Institute for Physical Science and Technology
University of Maryland, College Park
lvrmr@math.umd.edu

presented 16 September 2004 at the IPAM/LLNL
Computational Methods in Transport Workshop
11–16 September 2004, Granlibakken, Lake Tahoe

Introduction

One recurring theme that has emerged at this conference is the need for better subgrid modeling in multiscale transport simulations. We saw this in modeling radiation transport through clouds, forest canopies, oceans, and astrophysical media, in modeling neutron transport through pebble-bed reactors, and in modeling neutrino transport in proto neutron stars.

This fundamental problem will challenge the creativity of all our communities for the foreseeable future. Addressing it will require new models and algorithms. It therefore provides an ideal focus for future interdisciplinary workshops involving the larger transport simulation community. This will allow each of our disciplinary communities to quickly benefit from advances in other communities.

Subgrid/Multiscale Modeling

- We can use precomputed and tabulated parametric constitutive relations. (Think of LTE EOS, averaged nuclear cross sections, atomic mix, etc.)

- We can compute constitutive relations "on the fly" from subgrid simulations. (Think of non-LTE, fractal clouds models, canopy models, stochastic mix simulations, gap-tooth simulations, etc.)

- We can use analytic models for unresolved scales. (Think of homogenization, renormalization, stochastic averaging, etc.)

- We can use combinations of the above.

Gap-Tooth Simulations

- Subgrid simulations are carried out "on the fly" at each node *and* time level of a "macroscopic" simulation. These are coupled only through the macroscopic simulation.

- The subgrid simulations are run with stochastically generated data based on parameters from the macroscopic simulation. (Think of a fractal clouds models or a canopy model)

- The subgrid simulation is run past its initial layer. The results are averaged and used to provide constitutive relations used to advance the macroscopic simulation.

Transport through Stochastic Mixtures

- Mix models need to be as simple as possible (but no simpler), depending on a limited number of parameters that can be measured with confidence. (Think of volume fraction, correlation length, mean particle size, etc — not particle size distribution, chord distribution, etc.)

- Transport is usually described by a coupled system of transport equations that must be analytically and numerically tractable. (Think of n coupled equations for an n component mixture.) This is the stochastic analog of homogenization.

- Identify asymptotic regimes that reduce the size of this system, hopefully to a single effective equation. (This can be useful in identifying preconditioners.)

Example: n Component Absorbing Mixtures

- The mix model is an n state plane Poisson process characterized by n volume fractions (summing to one) plus a correlation length. Other models were developed for slab (layered) mixtures.

- Stochastically averaging over this model, stationary transport is described by a coupled system of n transport equations:

$$\omega \cdot \nabla_x F_i + \kappa_i F_i = S_i + \sum_{j=1}^{n} T_{ij} F_j \,,$$

  where F_i is the expected kinetic density in component i.

- There is a single effective transport equation when mix components with relatively thick regimes are rare.

$\boxed{\textbf{Example: } n \textbf{ Component Mixtures with Scattering}}$

- The mix model is an n state plane Poisson process characterized by n volume fractions (summing to one) plus a correlation length.

- Dynamic transport is *approximated* (sometimes badly) by a coupled system of n transport equations:

$$\partial_t F_i + \omega \cdot \nabla_x F_i + \kappa_i F_i = \mathcal{K}_i^S F_i + S_i + \sum_{j=1}^{n} T_{ij} F_j \,.$$

- There is a single effective transport equation when mix components with relatively thick regimes are rare. There is a single effective diffusion equation when there is enough of one thick component to make the F_i's isotropic.

Improvements Needed in Foregoing Example

- A larger zoo of practical mix models needs to be developed. For example, one could allow small fluctuations about a mean for each component.

- Even for the Poisson model, we need to develop a system that correctly describes stationary or dynamic transport through a scattering mixture. To treat scattering one needs the n-point correlations.

- Better (parallel!) numerical schemes need to be developed.

- Such models can also be used for an “on the fly” subgrid simulation.

New Focus: Quantifying Uncertainty

- We need to estimate variances as well as means. As mentioned above, this can be done naturally with some stochastic models. It needs to be developed when subgrid simulations are used.

- We need to estimate sensitivity to the subgrid model. Adjoint methods can be used to compute sensitivities to parameters in the computed model *and to parameters in any model that contains the computed model*.

- Runs with an ensemble of models are far better at quantifying uncertainty than runs of one model with an ensemble of data. We need to identify ensembles of models suited to this task.