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Predictive Simulations for Problems with Solution Non-Uniqueness

James Glimm[1]

[1] Stony Brook University, Stony Brook NY 11794 USA glimm@ams.sunysb.edu
http:www.ams.sunysb.edu/~glimm

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Nonuniqueness for Large Eddy Simulations (LES) of turbulence mixing has been observed in benchmark comparison studies, associated individual variations in the details of numerical algorithms and of the subgrid models, which together emulate the influence of unresolved subgrid phenomena. We resolve this issue with a front tracking/LES algorithm which duplicates experimental values, for predictions of the overall extent of the mixing zone. The experimental validation set is limited to Re = 35,000, and extrapolation methods are presented for verification of turbulent mixing simulations at higher Reynolds numbers.

Issues of reactive chemistry depend on accuracy of solutions at the molecular level, that is convergence of the probability density functions (pdfs) or their integrals, the cumulative distribution functions (cdfs). Cdf convergence.raises accuracy issues far more demanding than the size of the mixing zone. A new notion of convergence, based on coarse-graining of solution values and binning (not averaging) the resulting multiple solution values in a supercell allows convergence of solution cdfs or pdfs for stochastic phenomena. The convergence is in the L_1 norm of the associated cdfs.

Convergence of grid level cdfs to an accurate description of molecular level cdfs depends on scaling laws for turbulence phenomena, the most fundamental of which is the Kolmogorov 1941 law. We have begun V&V/UQ analyses of cdfs, with convergence studies, sensitivity in dependence on parameters and error bounds, both in experimental regimes and with extrapolation beyond these limits.

Slow convergence rates for the cdfs leads to requirements for extreme levels of simulation. Various mathematical theories, such as Young measures, w* convergence, scaling laws, the renormalization group, mathematical existence theories and analysis of subgrid terms have been used and will continue to play a role here. In view of the solution sensitivity to algorithms and to the choice of subgrid terms, validation (comparison to experiment) will be important to control solution nonuniqueness, and will provide a limit on the valid range of extrapolation outside of experimental data. Stochastic (pdf) convergence extends to nonlinear functionals of the solution, thereby reducing the role of models in the convergence process. Models are a major contribution to simulation uncertainties, so that a reduction in their role will improve the simulation reliability. Diagnostic chemical and radiological traces also fall into this category, and their reaction signals, part of the feature extraction outlined above, depend on the fluctuations and pdfs, and are enhanced by convergence issues addressed here.