

Multiscale Mathematics for Complex Reacting Flow Simulations

Developing the next generation of energy technologies that will satisfy growing US energy needs without increasing our dependence on foreign energy suppliers while meeting the emissions levels mandated by public health issues is a daunting task. Potential concepts that have been proposed to address these issues include developing methodologies for clean burning of coal, lean combustion technologies and hydrogen-based systems. High fidelity numerical simulation will be critical to developing these technologies; however, the requirements for the needed computational tools are extremely demanding. We will need to be able predict the chemical behavior of turbulent reacting flows to within a few parts per million; we will have to predict both the dynamics and chemistry of microscopic particulates; we will need to be able to model catalytic surface reactions that are not currently understood at a fundamental level. These capabilities, which are difficult in their own right, must be incorporated into simulations of large-scale systems where there is a coupling between acoustic waves on the scale of meters, turbulence scales on the order of millimeters and chemical scales on the order of microns.

Current modeling tools in the combustion community will not be able to meet this challenge. The standard Reynolds averaged Navier-Stokes (RANS) methods currently used for full-scale simulations only approximate the mean properties of the system with turbulent motions and fluctuations modeled across all scales. They are inherently unable to predict the behavior of systems with the fidelity required for to develop new energy technologies. Direct numerical simulation approaches that use brute force computing to resolve all of the relevant length scales have the ability to provide accurate predictions but their computational requirements make them unusable for realistic systems. The fundamental issues with these approaches are that they are inherently single scale; to provide the simulation capabilities needed for chemically reacting flow new approaches that reflect the multi-scale character of the problems are required.

Developing the multiscale computational tools required for chemically reacting flows is essentially a three-stage process. In the near term we need to establish a computational framework for simulation that exploits the natural scale separation inherent in chemically reacting flows. In the next phase of the development we need to develop new closure approaches that can capture the communication between continuum scales inherent in the physics. Completion of the first two phases will provide comprehensive multiscale methodologies for continuum simulation of reacting flows. This capability needs to be augmented to include processes that are not well described at the continuum level and require some type of atomistic modeling. Development of tools to support the hybridization of continuum and atomistic modeling is the third-stage of the development.

Exploiting natural scale separation

Chemically reacting flows are characterized by phenomena at a wide range of scales. Typical flows are low Mach number so there is a natural separation between acoustic and convective scales. For small-scale systems this separation has been exploited to develop

low Mach number approaches that allow acoustic scales to be removed from the system. We need to develop a generalization of the low Mach number approach that allows us to exploit the scale separation while incorporating the acoustic effects that play a critical role in instabilities for larger scale systems. Developing such a capability will require new multi-scale asymptotic analysis to derive the appropriate formulation combined with careful algorithm design to develop discretization approaches that exploit the new model.

Another important scale separation is that reactions typically occur on time scale much faster than the large-scale fluid motion. As a result, regions of intense reaction are typically localized in space. This localization can be exploited by various approaches that focus computational effort such as adaptive mesh refinement techniques, front-tracking and Lagrangian discretization approaches. Although there has been significant progress much work is still required. New techniques that integrate adaptivity for rigorous control of discretization errors and an understanding of modeling accuracy on unresolved scales are required.

New approaches to closure

Numerical methodology that effectively exploits the natural scale separation of chemically reacting flows is a necessary starting point but the chemical reaction scales are too small to be fully resolved in large-scale simulations. Existing methodologies for representing reaction kinetics enforce an explicit separation of scales to separate turbulence scales from chemical scales. However, in most situations turbulent transport and reaction scales that are strongly coupled; new approaches are required to represent the reaction process that respect this coupling. One approach to developing new closure approaches is to adopt tools such as renormalization group ideas originally developed in statistical physics to nonlinear partial differential equations. This type of approach provides a framework for elucidating the coupling between fine and coarse scales and for developing mathematically rigorous approximations to this coupling. However, unlike the statistical mechanics setting, we do not have the necessary scaling laws to perform this development analytically. Instead, we will use detailed simulations to derive the necessary coupling to bootstrap across scales. One feature of these approaches is that small-scale deterministic behavior is represented stochastically at the larger scales. Thus, developing numerics for these models will raise new issues in algorithms for stochastic partial differential equations.

Hybrid modeling

Many of the important phenomena in chemically reacting flows such as catalytic surface reactions or the synthesis and oxidation of particulates are not well represented at the continuum level. These types of effects must be modeled at the atomistic level; integrating their treatment into a continuum simulation will require hybrid discretizations that couple atomistic and continuum scales. The critical issue in developing these hybrids is determining statistical distributions from the atomistic scale that are needed to express the coupling between atomistic and continuum scales.

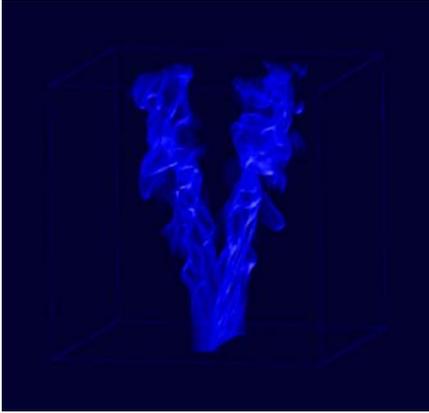


Figure 1. Low Mach number simulation of a laboratory-scale turbulent flame

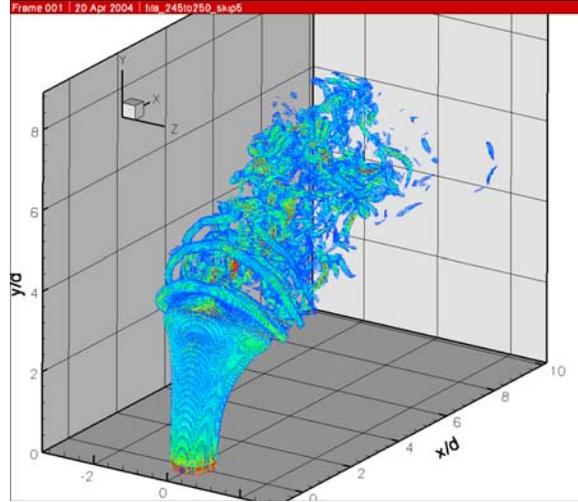


Figure 2. A high resolution simulation of a transverse jet, similar to that used in the combustion experiment to stabilize the flame by hydrogen injection, depicting the vorticity structure in a specific range.

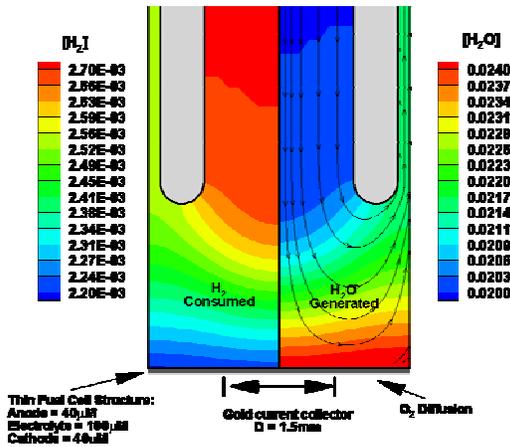


Figure 3. Two-dimensional model of a solid oxide fuel cell using phenomenological models for surface electrochemical reactions, charged particle transport and estimation of overpotentials

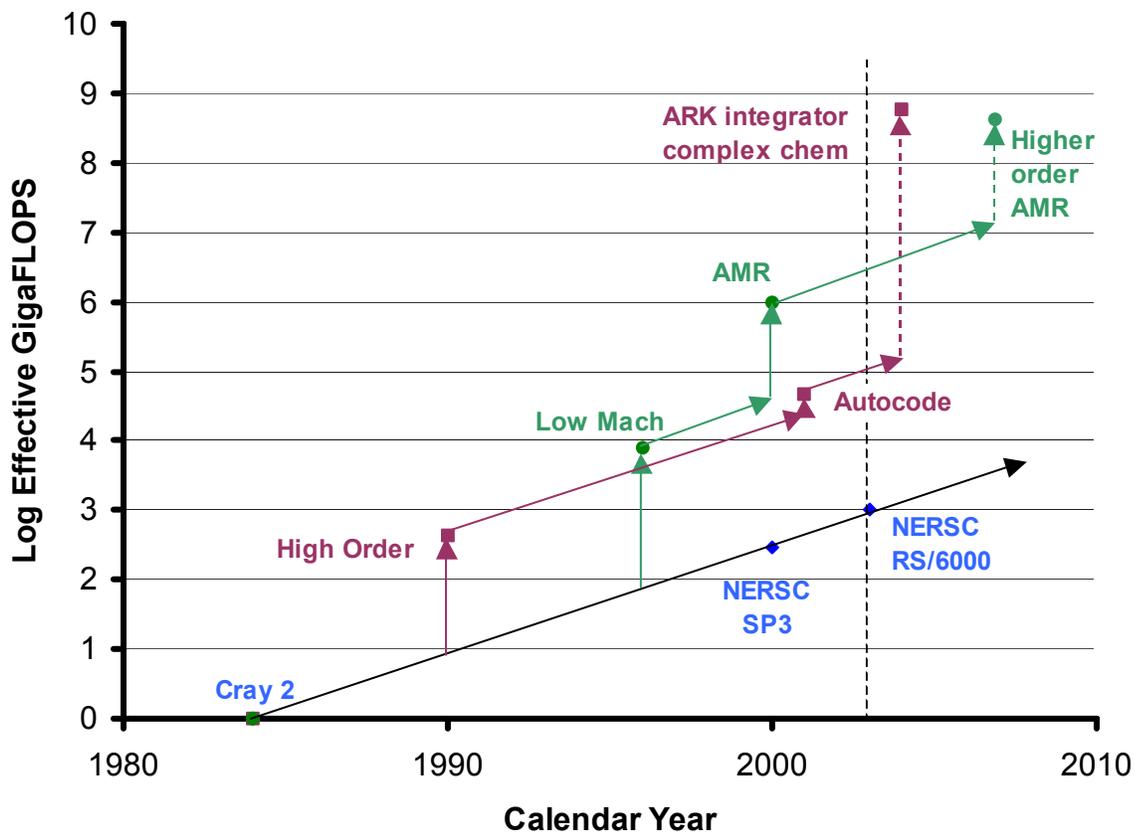


Figure 4. Turbulent gas-phase combustion simulations are modeled using either the compressible reacting flow equations or a low Mach number model. In both formulations, the equations include models for fluid dynamics, chemical kinetics and transport. Algorithmic advances for both types of simulations continue to yield enhancements to our computational capability comparable to, if not exceeding, those obtained through improved hardware capabilities. (From SCALES Report)