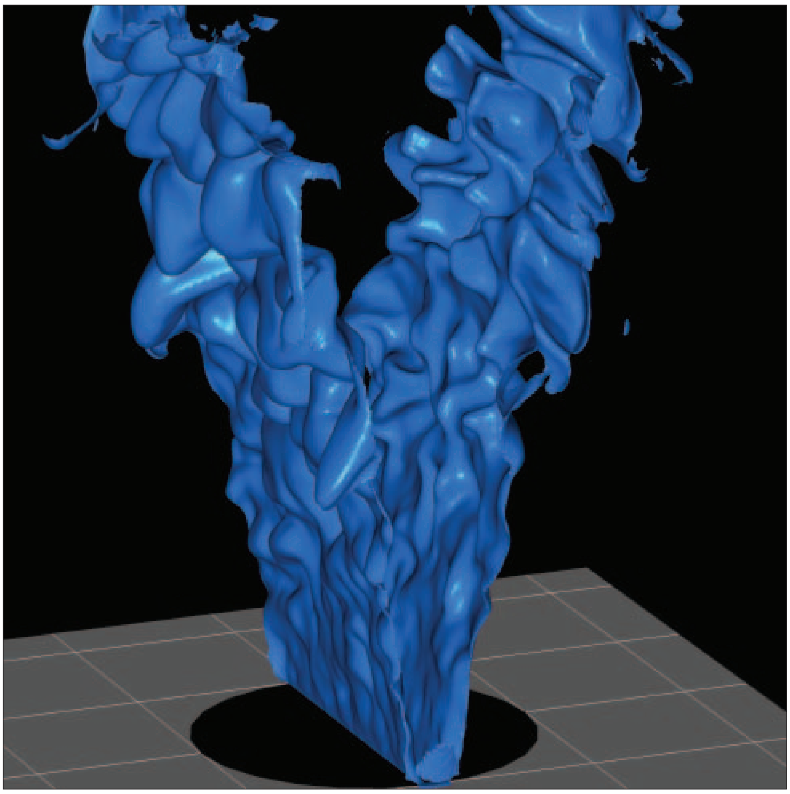
SIMULATING Turbulent Flames

New three-dimensional simulations, developed with the support of SciDAC-funded infrastructure, are advancing scientific knowledge of turbulence-chemistry interactions.



J. B. Bell et al., 2005, LBNL Report LBNL-54198; Proc. Natl. Acad. Sci. U.S.A., 102(29), 10006–10011.

Figure 1. *The three-dimensional flame surface of the V-flame.*

Exploiting fire for heat and light was a vital advancement in human history. The basic chemistry of combustion was established long ago, but details of this important reaction are still being actively pursued so that combustion can be more efficiently utilized in modern applications. One of the most critical problems in combustion science has been the turbulence-chemistry interactions that can cause a flame to burn faster or slower, and to create more or less pollution. Current three-dimensional simulations are beginning to provide detailed information on the structure and dynamics of turbulent flames necessary to design new low-emission, fuel-efficient combustion systems.

Dr. John Bell and his colleagues have achieved the first three-dimensional simulation of a laboratory-scale turbulent flame from first principles. The simulation of "a laboratory-scale turbulent rod-stabilized premixed methane V-flame" (figure 1) was unprecedented in several aspects—the number of chemical species included, the number of chemical reactions modeled, and the overall size of the flame. This impressive accomplishment is the result of a SciDAC-funded collaboration between computational and experimental scientists at Lawrence Berkeley National Laboratory (LBNL).

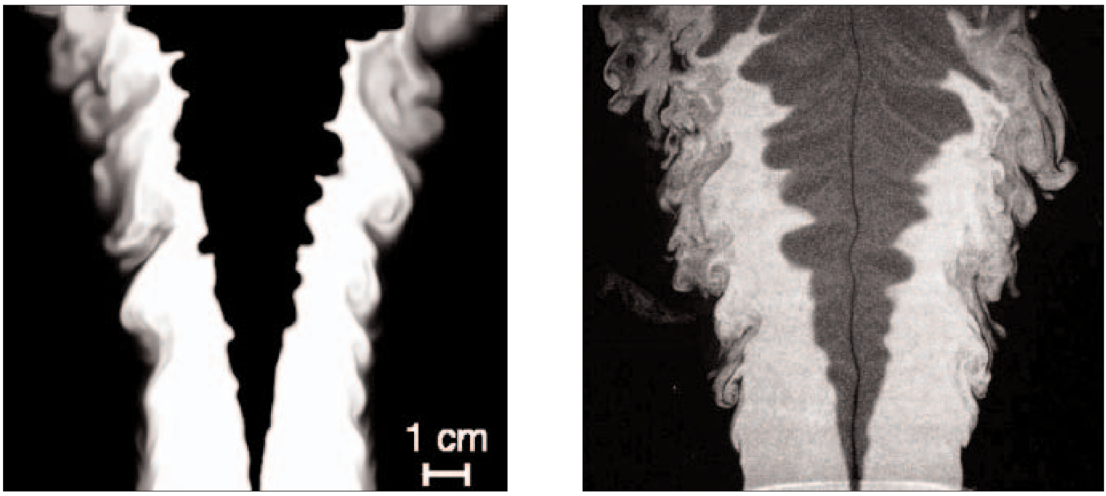
Supported in part by the Algorithmic and Software Framework for Applied PDEs (APDEC)—a SciDAC Integrated Software Infrastructure Center (ISIC)—this simulation employed a different mathematical approach than has typically been used for combustion. Most combustion simulations designed for basic research use compressible flow equations that include sound waves, and are calculated with small time steps on very fine, uniform spatial grids—all of which make them very computationally expensive. Because of limited computer time, such simulations often have been restricted to only two dimensions, to scales less than a centimeter, or to just a few carbon species and reactions.

In contrast, the collaborative effort led by Dr. Bell has developed an algorithmic approach

"A much closer interaction with experimentalists allows us to bring experiment and simulation together."

Dr. John Bell
LBNL

> "For simulation to be an equal partner, you need to be simulating real experiments. Our goal is to be able to simulate laboratory experiments."
>
> **Dr. John Bell**
> LBNL



J. B. Bell et al., 2005, LBNL Report LBNL-54198; Proc. Natl. Acad. Sci. U.S.A., 102(29), 10006–10011.

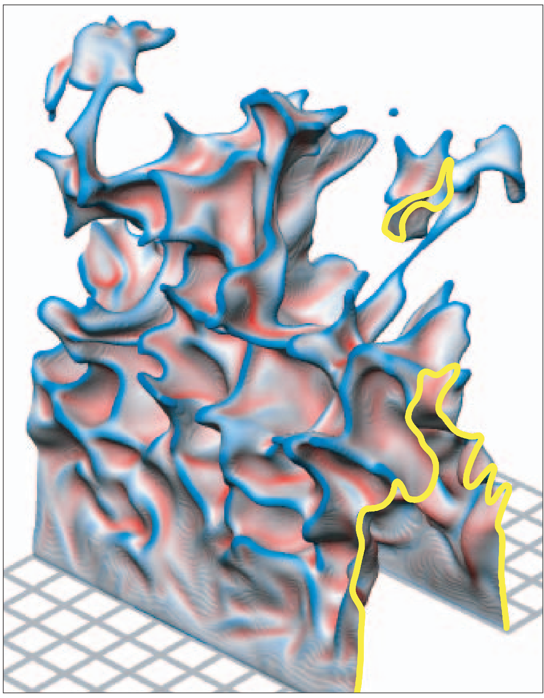
Figure 2. *Left: A typical centerline slice of the methane concentration obtained from the simulation. Right: Experimentally, the instantaneous flame location is determined by using the large differences in Mie scattering intensities from the reactants and products to clearly outline the flame. The wrinkling of the flame in the computation and the experiment is of similar size and structure.*

that combines low Mach-number equations, which remove sound waves from the computation, with Adaptive Mesh Refinement (AMR), which bridges the wide range of spatial scales relevant to a laboratory experiment. This combined methodology strips away relatively unimportant aspects of the simulation and focuses computing resources on the most important processes, thus slashing the computational cost of combustion simulations by a factor of ten thousand.

Using this approach, combustion researchers have modeled turbulence and turbulence-chemistry interactions for a three-dimensional flame approximately twelve centimeters high, including twenty chemical species and eighty-four chemical reactions. The simulation captured with remarkable fidelity some major features of the experimental data, such as flame-generated outward deflection in the unburned gases, inward flow convergence, and a centerline flow acceleration in the burned gases (figure 2). The simulation results were found to match the experimental results within a few percentage points.

In more recent work with the same collaborators, Dr. Bell's team performed three-dimensional simulations of the core region of a low-swirl stabilized turbulent premixed flame. A novel adaptive control algorithm enabled them to efficiently simulate just the core region of the flame where turbulence-chemistry interactions can be studied unperturbed by mechanical stabilization devices.

The long-term goal is to develop high-resolution adaptive methods for partial differential equations and to implement them into production-quality software tools that are applicable to a number of Department of Energy (DOE) Office of Science research programs, including magnetic fusion, accelerator design, and turbulent reacting flows in both chemical combustion and Type Ia supernovae.



J. B. Bell et al., 2005, LBNL Report LBNL-59245; Proc. Natl. Acad. Sci. U.S.A., 102(29), 10006–10011.

Figure 3. *A slot-burner flame from a laboratory-scale simulation.*

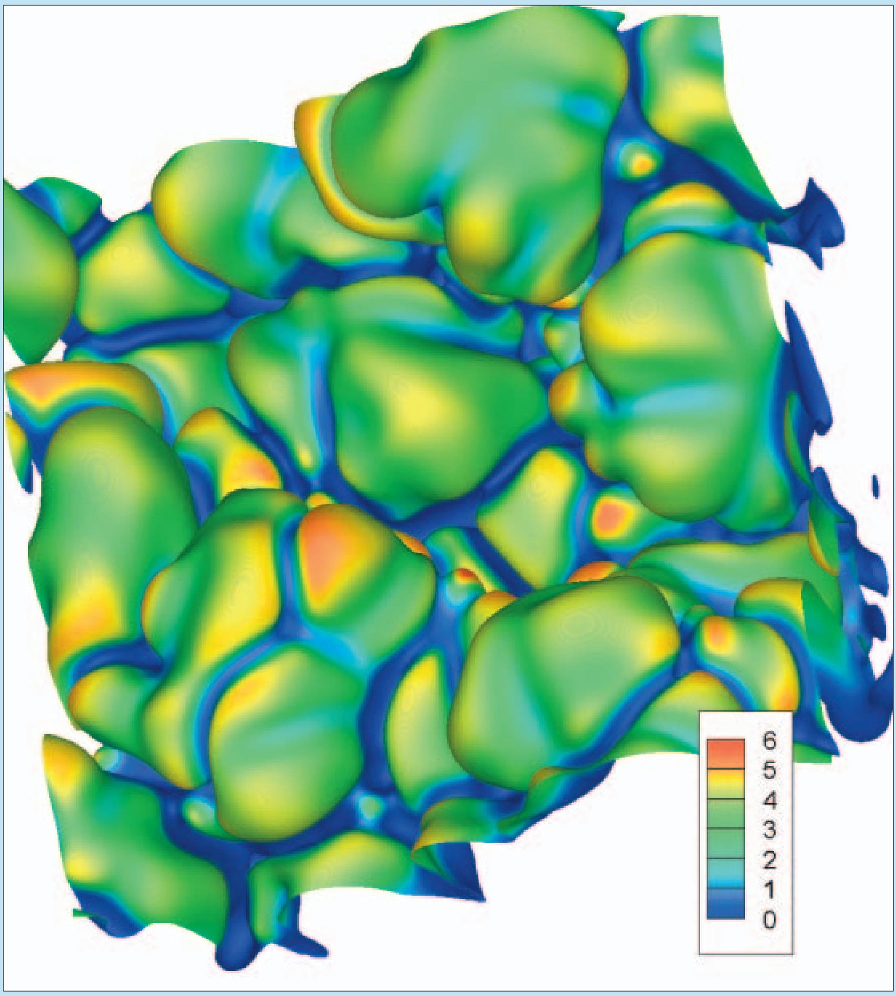
Writer: John Hules, LBNL

Further Reading

J. B. Bell et al. 2005. Numerical simulation of a laboratory-scale turbulent V-flame. *Proc. Natl. Acad. Sci. U.S.A.*, **102**: 10006.

J. B. Bell et al. 2006. Active control for statistically stationary turbulent premixed flame simulations. *Commun. Appl. Math. Comput. Sci.*, **1**: 29.

A Conversation with Dr. John Bell



J. Bell, LBNL

Figure 4. *The flame surface of an ultra-lean hydrogen flame, colored by the local burning rate.*

Dr. John Bell and his collaborators have been striving to connect simulation results to experiments. What researchers wanted to know, Dr. Bell says, is “can we simulate a laboratory-scale flame directly? What are the issues that arise if you want to do that?”

Dr. Bell stresses that comparing simulations and experiments requires careful attention to the conditions of each. In the past, combustion research has involved isolated efforts by specialists in different fields. “One of the things that we hope to accomplish by doing these laboratory-scale experiments is to bring all the things together and see if we can make the whole process work synergistically, instead of having everyone push their own piece of the science. It’s only when you can actually simulate a real turbulent flame that you can actually talk about doing that.”

“If you want to have impact on what experimentalists do, you need to look at turbulence that has the same sort of features,” says Dr. Bell. The characteristic eddies that carry most of the energy are a few millimeters in size, and “you want to represent a bunch of them, so to do a realistic simulation you need to be in a domain that’s many centimeters on a side.”

The burning of hydrogen under lean conditions (figure 4) is a difficult challenge Dr. Bell’s team is currently exploring. With methane, “the turbulence causes the flame to wrinkle up, but for the most part the flame is moving at the same speed all along,” like a smooth, laminar flow. In contrast, with hydrogen “you get gaps in the flame. You don’t have this continuous surface. This is an area where we’re not just trying to match experiment, but we can actually contribute to understanding what they see,” explains Dr. Bell. “At lean conditions, burning hydrogen is very bizarre.”

In the Bunsen simulation and other work, Dr. Bell and his team speed calculations by treating sound waves separately from the fluid motion. “We exploit the fact that there’s a separation between the time scales of acoustics and the scales of fluid motion.” In this low Mach number approximation, the sound waves are not eliminated, but are assumed to achieve equilibrium before the fluid motion changes significantly. “If the acoustic time scale is really fast, I can pretend that instead of that taking a finite amount of time, it happened instantaneously.”

This type of approximation is similar to the Born-Oppenheimer approximation for calculating molecular motions. In that scheme, the electronic structure of a solid or molecule is assumed to adapt instantaneously when the positions of atoms change. The motion of the atoms in response to forces that this electronic structure generates is then calculated.

Instead of tracking the sound waves bouncing around a combustion system, Dr. Bell says, “I can actually set the time scale that I do the simulation on based on how fast the fluid is moving, not how fast the sound waves move.” The time scale can be fifty times longer than what would be required to capture acoustics properly, so the computation can proceed much faster. Achieving this efficiency requires extra effort. “You don’t just blithely write down these new equations and integrate them.” Because the new equations are more complicated, computing their evolution over time is more difficult.

Adaptive Mesh Refinement (AMR) is another technique the researchers use. “For these kinds of flames that we’re doing, you need some level of resolution to resolve the incoming turbulence, but you need a finer resolution to resolve the flame front itself.” The resolution around the flame is typically ten to one hundred microns, but the turbulent eddies can be captured with a resolution of a few hundred microns because the turbulence in these experiments is not overly intense. AMR allows the researchers to concentrate the computational resources where they are needed. “The idea is to change the local resolution to match the local requirements, both in space and time.”

Writer: Don Monroe, Ph.D.