CREATION OF THE WHORLED

COMPUTATIONS PROBE THE SUBTLE PRINCIPLES GOVERNING TURBULENCE

In the world of physics, the difficulty of understanding turbulence in fluids is legendary. A humorous legend has Albert Einstein (or Werner Heisenberg, or Horace Lamb) saying on his deathbed, "I'm going to ask God two questions: Why relativity (or quantum electrodynamics), and Why turbulence? I'm rather optimistic about getting an answer to the first question."

A famous quotation is also variously attributed to Einstein, Heisenberg, Richard Feynman, or Arnold Sommerfeld: "Turbulence is the last great unsolved problem of classical physics." Whether any of those luminaries actually uttered those words is beside the point — everyone agrees with the statement.

Fluids (including air) are everywhere, and their motions are usually turbulent. You can create an exception by turning on a water tap just a little bit: the water flow will be smooth and constant, or in the jargon of physics, "laminar." Turn on the water full blast, and the flow becomes disorderly and turbulent. The same change happens to smoke rising from a cigarette into still air: the smoke immediately above the cigarette is laminar, but a little higher up it becomes rippled, chaotic, and diffusive — turbulent.

Fluid motion becomes turbulent when the speed of the fluid exceeds a specific threshold, below which frictional ("viscous") forces prevent the chaotic behavior. The mathematical expression of that threshold is the Reynolds number, sometimes described in simplified terms as the ratio of inertial to viscous forces (although viscous effects remain significant even at very high Reynolds numbers). The Reynolds number is variable because it is proportional to both the size of the object and the flow velocity. The Reynolds number for air flowing over a cruising aircraft might be in the range of 100 million, while for blood flowing through an artery, it might be around 1,000. But for any given problem, the higher the Reynolds number, the more turbulent the flow — and the more mathematically complicated.

The motion of fluids is described mathematically by the Navier-Stokes equations, which express basic principles of conservation of mass and momentum. Solving the Navier-Stokes equations for high Reynolds number turbulent flows requires massive calculations; so to make the problem manageable, most full-scale engineering calculations use approximations or models of some variables.

But a method called "direct numerical simulation" (DNS) is available that solves the exact conservation equations for mass, momentum, and chemical species concentration and mixing without any approximations. DNS is a powerful research tool that can supply data at a level of detail well beyond what is possible in experiments. Researchers use DNS results to improve their understanding of turbulent phenomena and to develop and test more accurate statistical models of turbulence. Those models in turn can be used to analyze experimental results; to simulate data that cannot be readily obtained by experiment, such as correlations between variables; or to solve engineering problems.

"The complexities of turbulence limit our ability to predict natural phenomena, such as weather, and to design improved engineering devices, ranging from

FIGURE 1 NASA photo of a cloud vortex with smaller vortices over the Madeira Islands.

engines to airplane wings to artificial heart valves," says P. K. Yeung, Professor of Aerospace Engineering at the Georgia Institute of Technology, and principal investigator of the INCITE project "Fluid Turbulence and Mixing at High Reynolds Number." This project used close to 2 million processor hours at NERSC in 2004 in the quest to find the underlying order in apparently disorderly motion and to help develop statistical models of turbulent mixing and dispersion.

"DNS is very CPU intensive, so it provides a grand challenge for high performance computing," Yeung says. "Our INCITE award has allowed us to perform the largest simulation of fluid flow turbulence ever done in the U.S., at a level of detail and within a time frame not possible otherwise. We have used as many as 8 billion grid points to probe deeply into a problem arising in multiple fields of science and engineering. Our simulation has achieved a Reynolds number comparable to or higher than that observed in many laboratory experiments."

An important feature of turbulent flows is that they are composed of fluctuating eddies or vortices of many sizes, which are constantly forming and breaking down (Figure 1). When the smallest eddies succumb to viscosity, their energy dissipates into heat. The first person to apply mathematics to weather forecasting, British meteorologist Lewis Richardson, described this process in verse:

Big whorls have little whorls,
That feed on their velocity;
And little whorls have lesser whorls,
And so on to viscosity.

The flow of energy between the large, intermediate, and small scales was first expressed mathematically by Kolmogorov in 1941. His theory predicts a universal constant and a –5/3 exponent for the energy spectrum at intermediate scales for all flows if the Reynolds number is high enough. While the Kolmogorov constant is still considered a good approximation, over the years researchers have found that some features of the theory are not confirmed by experiment.

"High Reynolds number simulations can help answer unresolved questions like this," Yeung says. "Although our focus in this project is on small scales, the high grid resolution allows a wide enough range of scales to test the Kolmogorov constant and other theories and models used to describe flow behavior in applications."

Yeung's DNS simulations examine the most basic, simple form of turbulence, which is isotropic, that is, uniform in all directions. With high resolution and long runs, these simulations produce more detailed and realistic data than can be obtained from shorter, low-resolution simulations. DNS data from multiple computer runs can be analyzed to derive important statistical characteristics of turbulent flows, as well as information that can be used to model complex real-world turbulence. The INCITE project has made significant contributions to a database that now encompasses Taylor-scale Reynolds numbers from 38 to 700 and grid resolutions from 64^3 to 2048^3.

As if turbulence were not difficult enough, the mixing or diffusion of substances or heat in turbulent flows adds further mathematical complications. Diffusion is important for anyone studying the spread of pollutants released into water or the atmosphere, and it is especially important in the study of combustion, where chemical reactions depend on the proximity of the reactants. For example, when a homogeneous mist of fuel is injected into a combustion chamber, the turbulence of the gases already present breaks up the uniformity of the fuel mist at first, making it uneven and disorderly. But a high level of turbulence eventually tends to mix the fuel with the gases more or less evenly. Better control of diffusion in a combustion chamber results in less unburned fuel and fewer undesirable byproducts.

The mathematical representation of the mixed substance in a turbulent flow is called a "passive scalar." Obukhov and Corrsin independently extended Kolmogorov's theory to the study of passive scalar fluctuations. Of course, turbulent mixing of several different substances requires multiple scalars, resulting in even more complex calculations, so the reliability of the Obukhov-Corrsin constant is critical. One of the earliest results of this INCITE project was the best demonstration to date of Obukhov-Corrsin scaling in the spectrum of fluctuations in turbulent mixing, supporting the validity of this theory.

One of the ways in which scalar dissipation differs from energy dissipation in turbulence is that scalar dissipation is less uniform in both space and time. A phenomenon called intermittency — intense, localized fluctuations of any quantity in a turbulent flow — can result in localized extinction and reignition of a combustion process, so calculating intermittency accurately is important in combustion modeling and engineering applications, as well as many others.

To help Yeung and his collaborators understand the patterns of intermittency in their simulations, the Berkeley Lab/NERSC Visualization Group created images showing energy and scalar dissipation for various "slices" of the data, with data magnitude mapped to both color and height for easy visual recognition of differences. Figure 2 shows that at high Reynolds number, scalar dissipation has much higher "peaks" than energy dissipation. Figure 3 compares scalar dissipation at low and high Reynolds numbers, and shows more intense and localized peaks at the higher Reynolds number.

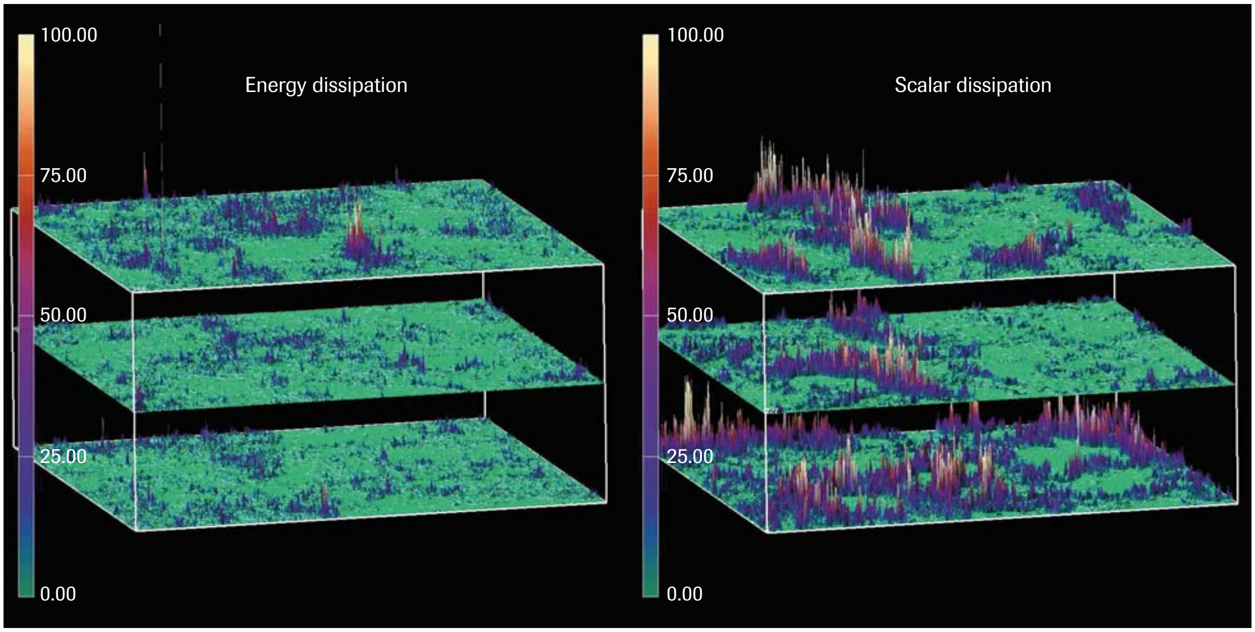

FIGURE 2 Energy and scalar dissipation at Taylor-scale Reynolds number (R_λ) ~700 (2048^3 grid points). Scalar dissipation shows higher peaks.

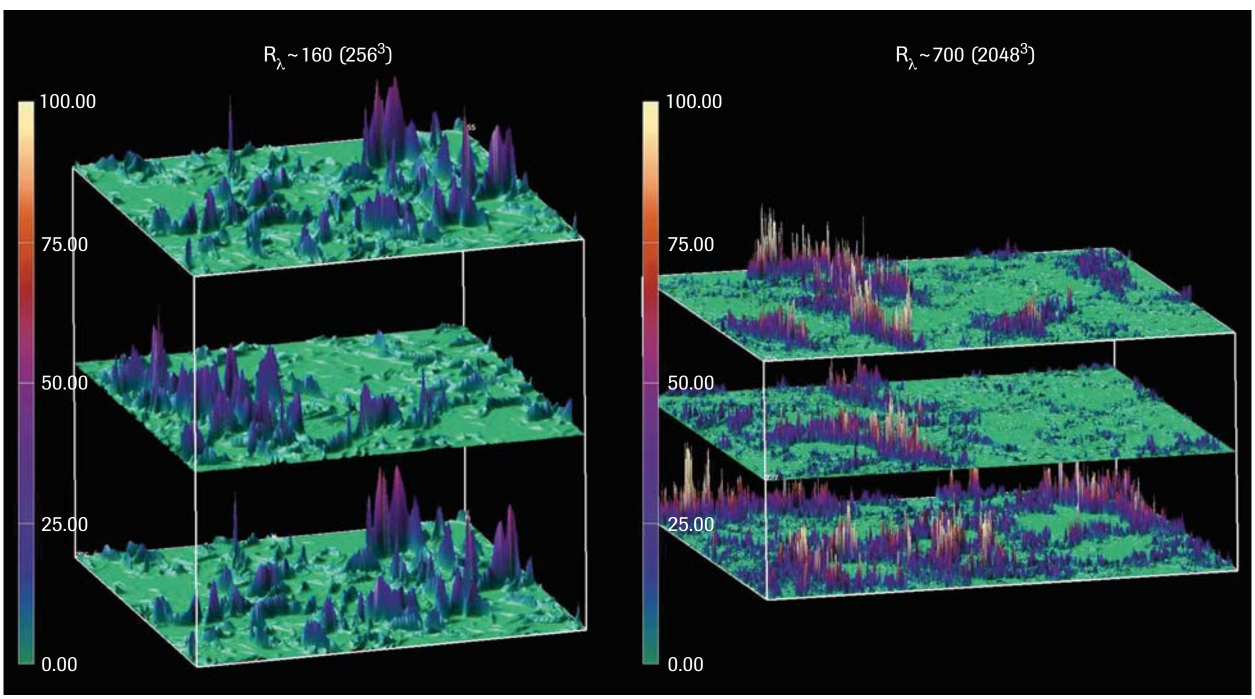

FIGURE 3 Scalar dissipation for low (left) and high (right) Reynolds numbers. The peaks are more intense and localized at the higher Reynolds number.

Figure 4 presents a three-dimensional depiction of scalar dissipation data.

"Our successes with the INCITE program have drawn attention in both the science and supercomputing communities, and created a very broad range of opportunities for the future," Yeung says. "More than twenty leading scientists in the field have indicated a strong desire to access our database to answer questions that they have long sought to resolve. We are extending the simulations to turbulent reacting flows where phenomena such as extinction and reignition are strongly dependent on small-scale mixing and intermittency."

Besides Yeung and his Ph.D. student Diego Donzis of the Georgia Institute of Technology, this project also involves close collaborations with K. R. Sreenivasan, who is both Distinguished University Professor at the University of Maryland and Director of the International Centre for Theoretical Physics in Trieste, Italy, and, more recently, Rodney Fox, who holds both an endowed chair professorship at Iowa State University and an Associate Scientist position at the Ames Laboratory. The first publication of results from this research is P. K. Yeung, D. A. Donzis, and K. R. Sreenivasan, "Turbulence and scalar transport in numerical simulations at 2048^3 resolution," Bull. Am. Phys. Soc. **49,** 22 (2004).

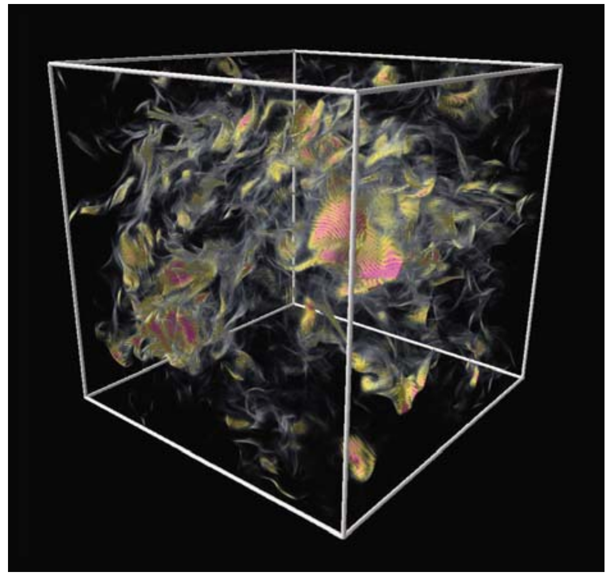

FIGURE 4 Using an imaging method called volume rendering, data values from the 3D scalar dissipation data slice are mapped onto color and opacity, revealing more features of the data. A movie of this image rotating can be viewed at http://www-vis.lbl.gov/Events/SC04/Incite3/scdiss2_vol_2.mpg.

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