Meet the Scientists

Kwan-Liu Ma[*]
University of California, Davis

John Blondin[†]
NC State University

Jacqueline H. Chen[‡]
Sandia National Laboratories

Mark Rast[§]
University of Colorado, Boulder

Ravi Samtaney[¶]
Princeton Plasma Physics Laboratory

1 INTRODUCTION

Scientific visualization has become an active area of research. Most researchers and students in the field of visualization, however, do not have access to data sets generated by the state-of-the-art simulations. In the case they have access to some of these data sets, they often do not get to directly interact with the scientists who generated the data sets. This interaction is crucial for obtaining the understanding of what scientists really need to get out of their data sets and what visualization functionalities are missing in existing visualization software tools. This panel will provide such interaction. Through the DOE SciDAC Institute for Ultrascale Visualization (Ultravis Institute) [6], scientists in representative areas from astrophysics, combustion, to plasma physics will be sponsored to attend the Visualization 2007 Conference and participate in the panel. Each scientist will describe his/her application, data sets, and the corresponding visualization and data analysis needs and challenges, and then answer questions. By making their data sets openly available through the Ultravis Institute after the Conference, more visualization researchers will be given the chance to work on the problems truly faced by the scientists. The panel will thus provide these researchers the correct understanding of the problems, and subsequently help accelerate the development of the field of scientific visualization. The following sections introduce the four participating scientists and their application areas.

2 SUPERNOVA MODELING

John Blondin is a Professor of Physics at the North Carolina State University. He is carrying out research in the field of Circumstellar Gas-Dynamics using the time-dependent hydrodynamics code VH-1. His work covers a vast array of objects observed by astronomers both from ground-based observatories and from orbiting satellites. The two primary subjects under investigation are interacting binary stars - including normal stars like the Algol binary, and compact object systems like the high mass X-ray binary SMC X-1 - and supernova remnants - from very young, like SNR 1987a, to older remnants like the Cygnus Loop. Other astrophysical processes of current interest include radiatively driven winds from hot stars, the interaction of stellar winds with the interstellar medium, the stability of radiative shockwaves, the propagation of jets from young stellar objects, and the formation of globular clusters.

Professor Blondin participated in the Terascale Supernova Initiative, an effort sponsored by the DOE SciDAC program to understand the mechanism behind core-collapse supernovae. Visualization of time-dependent datasets generated by large, three-dimensional simulations is a key component of this hunt to discover the mechanism behind core-collapse supernovae, the violent death of short-lived massive stars. As examples, visualization played a key role in understanding the origin of a dynamical instability of the supernova shock wave at an age of less than one second. This spherical accretion shock instability, or SASI, shown in Figure 1, is driven by the response of an initially spherical shock wave to global acoustic modes trapped in the interior. This instability, discovered in the early stages of TSI, provides a natural explanation for the asymmetry observed in most core-collapse supernovae. Following these 3D supernova models to later time, visualization of a spiral flow generated by the SASI led to the discovery of a new mechanism for creating the rapid spins of observed radio pulsars [4]. The new model he is developing includes substantially more physics in 3D and will generate hundreds of terabytes to several petabytes of data from one simulation. His approach is to create complex models involving all relevant physical processes and a wide range of time and length scales, using the largest computing platforms available. This process is one of discovery, where he is hunting for new clues generated in a virtual laboratory within a supercomputer. As such, this work demands interactive visualization, where one can quickly visualize different combinations of variables (scalars and vectors) or isolate features by manipulating the transparency of the rendered data. The dynamical nature of this problem also demands the ability to quickly produce animations from a time-series of 3D data. But whatever visualization technique is employed, it is clear that the key to scientific discovery is interactive visualization of the

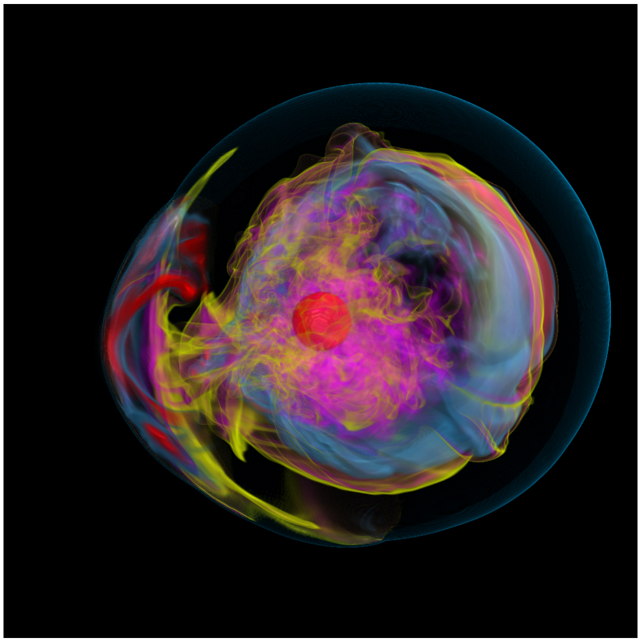

Figure 1: Direct volume visualization of a supernova simulation displaying entropy field.

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[*]e-mail: ma@cs.ucdavis.edu
[†]e-mail:john_blondin@ncsu.edu
[‡]e-mail:jhchen@sandia.gov
[§]e-mail:mark.rast@lasp.colorado.edu
[¶]e-mail:samtaney@pppl.gov

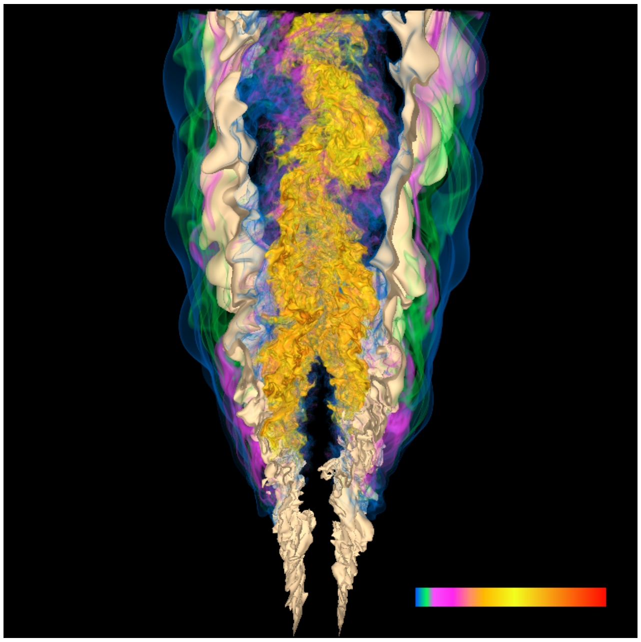

Figure 2: Direct volume visualization of a turbulent combustion simulation displaying mixture fraction isosurface along with HO_2 concentration.

data.

3 TURBULENT COMBUSTION SIMULATIONS

Jacqueline H. Chen is a Distinguished Member of Technical Staff at the Sandia National Laboratories, and a director on the Board of Directors of the Combustion Institute. She has contributed to research in terascale simulations of turbulent combustion focusing on turbulence-chemistry interactions in combustion based on the S3D code. She has worked closely with computer scientists on time-varying visualization of terascale simulated data, topology of combustion features, and parallel feature detection and tracking algorithms for combustion. She received the DOE INCITE Award in 2005 and 2007 and the DOE Office of Science Leadership Computing Facility Award in 2006.

S3D is the Sandia 3D Direct Numerical Solver [10], which presently is capable of generating tens of terabytes of raw data per run in a parametric study of several runs, presenting a significant challenge for subsequent analysis and interpretation. The current approach is to store the raw data at prescribed time intervals, and then either analyze it on a supercomputer or access it via a local analysis and visualization cluster at Sandia. The raw data is archived so that various modeling groups in the combustion community can interrogate it to test model assumptions. To understand the correlation of scalar fields such as temperature, mixing rates, and species concentrations in turbulent flames, scientists must be able to visualize two or more scalars simultaneously. Conventional visualization tools do not directly support such a capability. Scientists often must make side-by-side comparisons of images of different variables by hand, which is tedious and time-consuming. Furthermore, the information that scientists can derive by looking at separate images is quite limited. Thus, they need effective methods for simultaneously visualizing multiple time-varying variables from large data sets in an interactive fashion [1].

The data rates of S3D are expected to increase by tenfold in the next two years, demanding new analysis and visualization capabilities to extract physical insights from such large time-varying, multi-scale complex data. Due to the enormous data volume, scientists need parallel feature detection, extraction, and tracking tools to automate reduction of the data for analysis of intermittent combustion phenomena. An extensible set of feature identification and tracking algorithms needs to be developed into a parallel feature analysis pipeline that is efficient and scalable to petascale computers and beyond so that the automated data analysis can be performed online or offline. The algorithms need to be efficient so as not to impose a significant runtime penalty. Furthermore, a library of parallel turbulent combustion analysis tools needs to be developed for structured grids to understand turbulence interaction with flames and ignition kernels. The tools need to be accessible as part of the feature borne analysis and also in a postprocessing mode. The library of tools must support flame surface analysis, chemistry analysis, conditional statistics, turbulence and scalar spectra, multi-scale representation of combustion data, Lagrangian particle tracking, and scalar topology.

4 TURBULENT PLUME SIMULATIONS

Mark Rast is an associate professor in the Department of Astrophysical and Planetary Sciences at the University of Colorado, Boulder. His primary research interests are astrophysical fluid dynamics with an emphasis on stellar convective dynamics and scale selection, turbulence, the excitation of the solar p-modes, and the origin of solar/stellar irradiance variations. His interest in large scale numerical simulations includes the development of visualization and analysis techniques essential to their scientific understanding. In addition to these theoretical and computational efforts, Professor Rast serves as the principal scientist of the Precision Solar Photometric Telescope (PSPT) at Mauna Loa Solar Observatory, which obtains full disk images of the Sun at five wavelengths with 0.1% photometric precision.

Sun-like stars are convectively unstable in their outer layers. Turbulent motions are driven by heat production in the interior and radiative loss from the photosphere. The radiative losses are nonuniform over the solar surface, and vigorous new downflow plumes form at those sites where advective heat supply from below fails to support the radiative energy losses from above. These plumes play a crucial role in the dynamics of the flow [8], interacting to form larger convective scales in the surface layers, and possibly descending through the entire highly stratified convective layer to play a key role in the transport of heat, momentum, and magnetic field into the overshoot region below. The dynamics, stability, and transport properties of these flows are just beginning to be understood. That understanding is being achieved through very high resolution hydrodynamic and magnetohydrodynamic simulations.

While resources exist for such simulations of sizes 2048^3 and larger, the essential scientific analysis and visualization of the results proves daunting. Post-simulation analysis is essential because these studies typically focus on physical process within the domain rather than statistical properties of the solution. The locations of interest, the nature of the analysis to be undertaken, and the relevant secondary quantities to be derived, are often not known or even knowable before the simulation is computed. Visualization to locate sites of interest and illuminate spatial relations between variables and analysis to quantitatively test scientific hypotheses on interactive time scales are both essential in order to interrogate the data and learn from the solution. Typically, many hundreds or thousands, and soon tens of thousands, of central processing units are available for batch mode simulations, but only a few to post-processing scientific analysis. This mismatch means that the scientific return realized from the computational investment is limited by the availability, or lack there-of, of appropriate post-processing resources, both software and hardware.

The volume visualization in Figure 3 shows the enstrophy of a fully-developed compressible downflow plume. The plume was initiated and maintained by a fixed temperature perturbation imposed

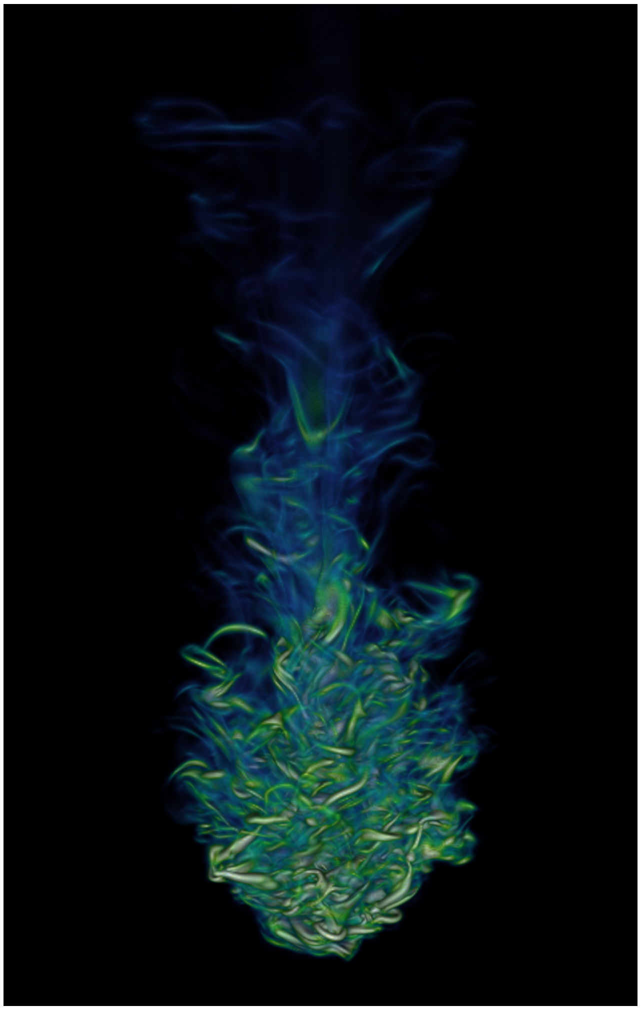

Figure 3: Volume visualization of the enstrophy of a fully developed compressible downflow plume

on the upper boundary (threedimensional version of Case E in [7]). It is subject to vigorous secondary instability that leads to the successive penetration and disruption of the leading vortex torus by the stem flow from behind. This process generates the tangled mass of vortex filaments at the plume head. The computational grid employed was horizontally periodic and highly nonuniform. Only the central one-third and bottom one-third of the domain is shown after uniform resampling. The image was produced using an open source analysis/visualization package developed at NCAR named VAPoR [5].

5 SIMULATION OF PELLET INJECTION IN TOKAMAKS

Ravi Samtaney is a research physicist in the Computational Plasma Physics Group at the Princeton Plasma Physics Laboratory (PPPL), Princeton University. His research interests include magnetohydrodynamics, numerical methods, and high performance computing. He is developing adaptive mesh refinement (AMR) numerical methods for magnetohydrodynamics (MHD). The AMR MHD code is a fully three dimensional nonlinear MHD code in toroidal geometry. It is a unique simulation tool, primarily used for simulating pellet injection into tokamaks, a problem of substantial interest to ITER. Furthermore, he is investigating fully implicit Jacobian-Free Newton-Krylov methods to overcome the temporal stiffness in MHD simulations.

ITER ("The Way" in Latin), a joint international research and development project that aims to demonstrate the scientific and technical feasibility of fusion power, is now under construction at Cadarache, France. Refueling of ITER is a practical necessity due to the burning plasma nature of the experiment, and longer pulse durations. An experimentally proven method of refueling tokamaks is by pellet injection. Pellet injection is currently seen as the most likely refueling technique for ITER. Thus it is imperative that pellet injection phenomena be understood via simulations before very expensive experiments are undertaken in ITER. The emphasis of the present work is to understand the large-scale macroscopic processes involved in the redistribution of mass into a tokamak during pellet injection. Arguably, such large scale processes are best understood using magnetohydrodynamics (MHD) as the mathematical model.

The physical processes of pellet injection in tokamaks span several decades of spatio-temporal scales which has prevented effective simulations of these processes. There is a large disparity between the pellet size and device size ($O(10^3)$). Naive estimates indicate that the number of space-time points required to resolve the region around the pellet for simulation of ITER-size parameters can exceed 10^{19}. The large range of spatial scales and the need to resolve the region around the pellet is somewhat mitigated by the use of Adaptive mesh refinement (AMR). Our approach is to employ block structured hierarchical meshes as championed by the seminal work of Berger and Oliger [2], and Berger and Colella [3]. We employ the Chombo library for AMR developed by the APDEC SciDAC Center at LBNL for AMR. We have developed an upwind conservative flux-surface coordinate MHD code. A critical component is the modeling of the highly anisotropic energy transfer from the background hot plasma to the pellet ablation cloud via long mean-free-path electrons along magnetic field lines. Further details on the approach can be found in [9].

Figure 4 shows the mesh structure in computational coordinates wherein the pellet is buried within the finest mesh which occupies less than 0.015% of the volume of the coarsest mesh – a visual illustration of the resolving power afforded by the AMR technology. The speed up of these AMR simulations over similar single mesh simulations is estimated to be greater than two orders of magnitude Results from pellet injection from the low-field-side (LFS) and high-field-side (HFS) are presented in Figure 5 in which the top panel shows a time sequence of the density in LFS injection while the bottom panel shows density evolution in HFS injection. The dominant motion of the ablated pellet mass is along field lines accompanied by transport of material across flux surfaces towards the low field side. The interchange instability is the mostly likely cause of the pellet material to move towards the low field side. This observation is also qualitatively consistent with experimental observations leading to the conclusion that HFS pellet injection is a more efficient refueling technique than LFS injection.

It ought to be recognized by the visualization community that several physical applications are beginning to employ adaptive meshes; and developments in data analysis and visualizations of such data would accelerate the speed of discovery. As evident from our graphical presentation of the data, there are still very limited ways of visualizing field quantities on hierarchical adaptive meshes, particularly when the data on each grid is in generalized curvilinear coordinates. Furthermore, our data representation is unique in the sense that the mapping is from cylindrical (as opposed to Cartesian) coordinates to a curvilinear one in which the toroidal angle is preserved. Several visualization packages surveyed do not provide even rudimentary support for hierarchical mapped meshes. Standard visualization techniques such as iso-surfaces, and projections of the field data on 2D planes and 1D curves would be extremely valuable to the scientist in interpreting the simulation data. Going beyond the mundane visualizations one would like to investigate the vector field topology (for magnetic fields in MHD), which ought to

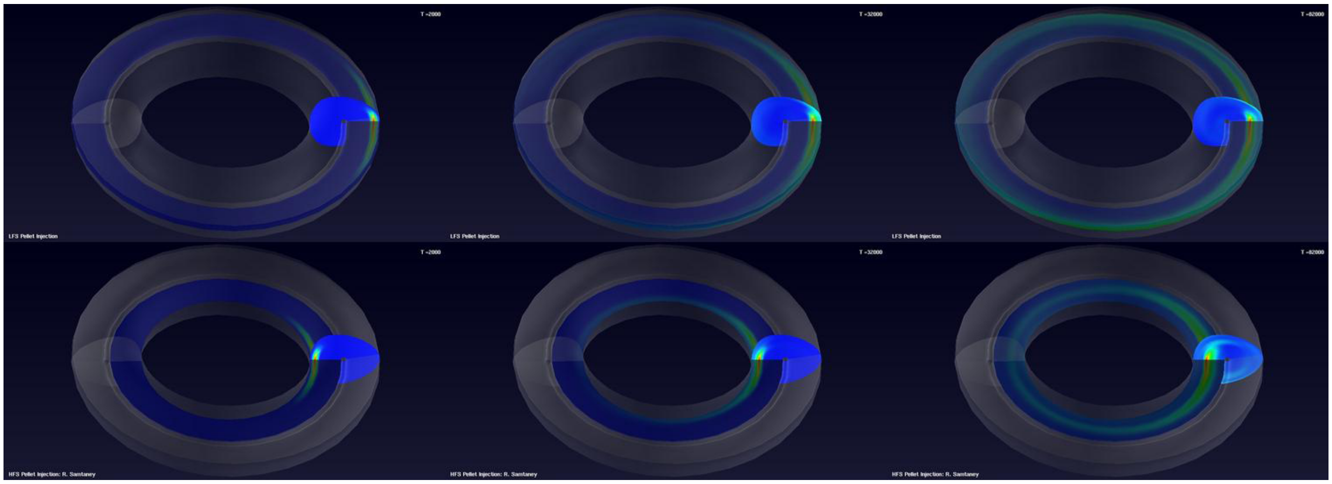

Figure 5: Top: Time sequence of the density in LFS injection. Bottom: Density evolution in HFS injection.

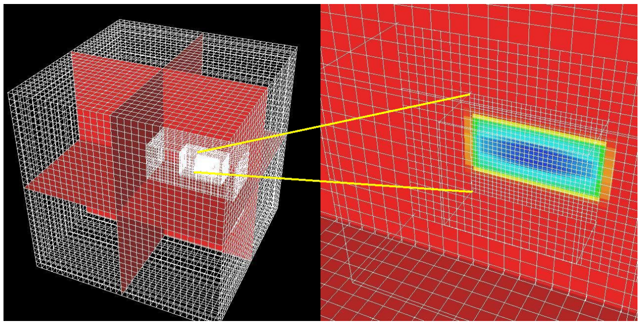

Figure 4: Mesh structure in computational coordinates. The finest mesh area occupying less than 0.015% of the volume contains the pellet. The equivalent single-mesh resolution of this simulation is 1024^3.

be driven by intuitive and interactive ways of picking seed points to generate stream lines, path lines, and streaklines, and extracting information such as local curvature of such streamlines. Other data analysis techniques which are conspicuously missing include volume rendering on hierarchical adaptive mapped meshes, techniques to choose appropriate stencils and specify boundary conditions to obtain derived quantities (such as divergence, curl of vector fields), and interactive ways to identify and quantify correlations among various derived quantities (e.g. 2D histograms, structure functions, convolutions).

6 CONCLUSION

While these studies present some representative visualization challenges, each of them also has some unique requirements, from the desire to see the interaction between multiple variables in both spatial and temporal domains, the need to address the widely varying time and length scales, to the ability to render adaptive mesh refinement data at high quality and interactivity. More information about these studies, respective data sets, and their visualization requirements can be found at: `http://vis.cs.ucdavis.edu/VisFiles`. Through this panel presentation and discussion, we hope to better direct the visualization research community's effort to collectively solve some of the most challenging problems facing us.

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