Scientific Discovery through Advanced Visualization

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Abstract.
The SciDAC program of the Department of Energy has brought together tremendous scientific expertises and computing resources to realize the promise of terascale computing for attempting to answer some of the most important basic science questions. Scientific visualization is an indispensable path to gleaning insight from the massive data produced by terascale simulations. Unless the visualization challenges presented by the terascale simulations be adequately addressed, the value of conducting these immense and costly simulations is not being fully realized. In this paper, we introduce several key visualization technologies that address the critical need of many SciDAC scientists in the application areas from accelerator simulations, earthquake modeling, plasma physics, supernova modeling, to turbulent combustion simulations.

1. Introduction

J. S. Langer, who was the workshop chair of the 1998 National Workshop on Advanced Scientific Computing, said "The computer literally is providing a new window through which we can observe the natural world in exquisite detail." Visualization has become an indispensable part of that window to facilitate Scientific Discovery through Advanced Computing (SciDAC) because of the ambitious goals of SciDAC scientists to solve challenging scientific problems at a level of accuracy and detail never before achieved. To glean insights in the enormous amounts of data generated by their simulations, innovations in visualization technology must be created.

At the University of California at Davis, we have been developing several new, enabling visualization technologies through close collaboration with SciDAC scientists in five application areas: accelerator simulations, earthquake modeling, plasma physics, supernova modeling, and turbulent combustion simulations. One technique, based on a hybrid rendering approach, makes possible interactive exploration of large-scale particle data from particle beam dynamics modeling [1]. The other technique, based on a compact texture-enhanced representation, exploits the advanced features of commodity graphics cards to achieve perceptually effective visualization of the very dense and complex electromagnetic fields produced from the modeling of reflection and transmission properties of open structures in an accelerator design [2]. In this paper, we give an overview of the visualization techniques that we are presently developing to address the urgent need of SciDAC scientists. First, we show high precision, hardware accelerated rendering can reveal unseen details of the supernova simulations. Second, we describe how to visualize multiple variables simultaneously for understanding the complex chemical process in combustion, and how such a ability helps validate the simulations. Next, we present a hardware accelerated visualization method designed specially for the unique irregular mesh structure employed by gyrokinetic simulations. Lastly, we show a remote interface design for the visualization of modes in the International Linear Collider cavities, and describe a time-accurate technique for visualizing electromagnetic field.

2. High Precision, Quality, and Performance Volume Visualization of Supernova Simulations

In scientific visualization, hardware accelerated rendering is often associated with the creation of real time animation, and interactive exploration of the rendering parameter space. Exploration of the transfer function is crucial for the creation of meaningful visualization since it allows the scientist to add emphasis to those select features that are important to the science being communicated. As such, we have made an effort to fully support this type of data exploration. Furthermore, once these parameters have been set, it is often desirable to create a final high quality animation that illustrates the phenomena in a data set to others. Since these animations only need to be rendered once, and might be played back repeatedly, for visualization of this nature, interactivity is of secondary importance to image quality.

In our work we focus on the task of creating extremely high quality visualizations making use of graphics hardware, and examine every stage of the volume rendering pipeline. For every stage, whenever there is a potential trade-off between performance versus image quality, we focus on preserving the fidelity of the final image without compromise. The resulting visualization can take seconds to render, rather than the several frames per second typically reported with hardware accelerated methods, but the resulting image quality in many ways exceeds that produced using software based techniques that often take minutes per frame. Our work can be broken into three parts for three different stages of the rendering pipeline: classification, lighting, and compositing. For classification we deal with issues related to the precision of the data, and corresponding classification function. For lighting, we have developed a method that avoids lighting aliasing effects from the discrete sampling of boundary surfaces in a volume. Finally, we have carefully addressed the issues related to high precision compositing.

The objective of the Terascale Supernova Initiative (TSI) project is to understand the explosion mechanism for core collapse supernovae, which are the single most important source of elements in the Universe. A complete understanding of core collapse supernovae requires 3D simulations of the turbulence, rotation, radiation, magnetic fields, and strong gravitational fields in massive starts at the ends of their lives, as well as their nolinear coupling. Such simulations are currently generating tens of TeraBytes of data per simulation. Management, analysis, and visualization of terabytes of data present a significant challenge. By exploiting the advanced features of the commodity graphics hardware, we have developed a low-cost, high-quality visualization solution for TSI researchers.

2.1. High Precision Classification

The data sets produces from the Supernovae simulations often have a high dynamic range, with the features of interest occupying only a small portion of the data range. Thus, the 8-bit precision 3D textures traditional used in hardware accelerated methods are not suitable for storing this data. Fortunately support for higher precision textures found on the latest generation of graphics card alleviate part of this problem by allowing data sets to be stored in 16-bit fixed or floating point textures. Modification, however, must also be made to the accompanying transfer function to take advantage of this increased dynamic range. The transfer function refers to the lookup

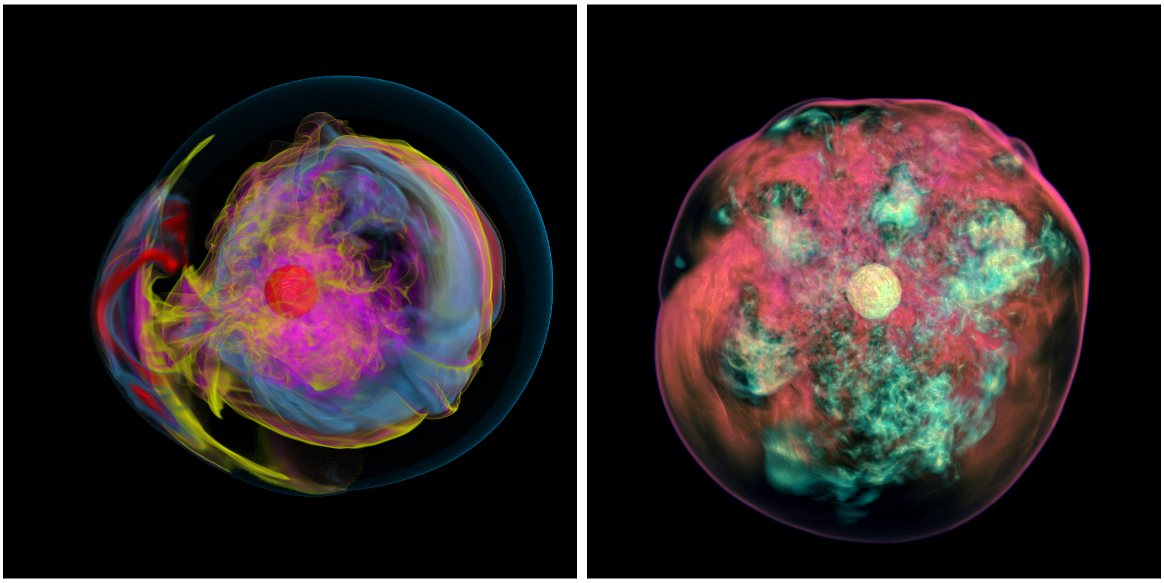

Figure 1. Visual exploration of data generated from a supernova simulation. Left: Entropy. Right: Velocity.

table used to map data scalar values to a color and opacity used for rendering. The size of the lookup table used for the transfer function must also be larger in order to accommodate the wider range of values in data set itself. The latest generation of graphics hardware allows us to store the transfer function as a 32-bit per channel floating point texture so precision of the transfer function is no longer a problem.

2.2. Fast Pre-Integration Volume Rendering

Pre-integration solves many aliasing issues related to the discrete sampling of the transfer function during volume rendering integration. The method pre-computes the integrated color and opacity between any two scalar pairs on the transfer function and stores the values in a 2D lookup table. A naive implementation of the calculation of the large pre-integration tables requires either the use of approximations, which can cause visible artifacts, or $\mathrm{O}(N^3)$ time, which can take tens of minutes for each change to the transfer function when tables are of size, for example, 2048×2048. We have derived an $\mathrm{O}(N^2)$ subrange pre-integration method that does not make approximations [3]. The technique iteratively builds up pre-integration tables along its diagonals, and can compute the 2048×2048 tables used in our work in under a few seconds.

Another source of aliasing occurs from the discrete sampling of surface in a volume. Often a transfer function is specified that creates opacity discontinuities in the volume, which physically take the form of surfaces. Lighting at these surface can show aliasing artifacts for the discrete sampling of the normals used for lighting at positions that do not lie exactly on the intersection between a view ray and the surface. We have developed a pre-integrated lighting method [3], which allows lighting to vary continuously between samples and does not introduce lighting discontinuity artifacts, even if multiple surfaces occur between any two pairs of samples. The method can be though of as Gouroud shaded interpolation between pre-integrated samples in the view direction, and is suited for producing alias free illumination for transfer functions of arbitrary shape.

2.3. High Precision Compositing

The final step in creating high-quality renderings is the use of high-precision compositing. This refers to the accumulated of color and opacity values to the frame buffer during rendering. This is a particularly important problem when one deals with high resolution data sets that require the compositing of a large number of samples that are closely spaced together in world space. This problems stems for the opacity sample spacing relationship. When a high resolution volume is used, and the corresponding world space sample spacing is reduced to accommodate the increased resolution, the opacity values used during composing are reduced. This results in two types of precision issues. First, there can be insufficient precision in the transfer function texture to properly store the reduced small alpha values. Second, the accumulation of these small values in the frame buffer might occur at an insufficient precision. The first problem is solved by making use of a high-precision transfer function texture to store the adjusted values, or applying the α spacing in graphics hardware in the fragment program in floating point precision, allowing the values stored in the texture to be larger. The second problem of frame buffer accumulation errors is made more difficult by the fact that the generation of graphics cards at the time of this writing do not support high precision accumulation. We therefore perform the compositing in the fragment program, reading and writing to the same pixel of the screen as each textured polygon is rendered to the screen. Future generations of graphics cards are expected to support high precision blending.

By combining the techniques we have described it is possible to create volume renderings with visual quality that exceeds those produced using traditional software ray-casting method. In our work we paid special attention to maintaining high precision for all steps of the volume rendering pipeline and paid special attention to reducing aliasing artifacts from the discrete integration of the volume rendering integral. We address the two sources of aliasing that exist despite a volume scalar value Nyquist rate; those being aliasing of the transfer function, and aliasing of illumination.

2.4. Visualization Results

Figure 1 displays volume visualizations of the gas entropy, density, and velocity generated from a 3D supernova simulation. From these images, the shock dynamics in the modeled core-collapse supernova can be clearly observed. Even more powerful is the ability to interactively change the view angle and transfer functions to freely explore the data. If the data size is larger than 512×512, a bricking and data packing technique that we have developed may be used to make visualization possible at near interactive rates [4].

3. Simultaneous Visualization of Turbulent Combustion Simulations

In scientific computing, to gain a better understanding of the intrinsic properties of certain physical or chemical process, scientists often try to simulate and study different aspects of the process. The capability to visualize different variables simultaneously describing the same spatial domain and to determine their correlations is thus desirable. For example, in a multi-disciplinary computing environment, several engineering analysis programs, such as structural and flow solvers, run concurrently and cooperatively to perform a multi-disciplinary design. The goal may be to identify the relevant design variables that can explain the causes of a particular phenomenon, like vortices in a flow field.

Scientists at the Sandia National Laboratory has developed direct numerical simulations of turbulent flames with detailed descriptions of chemistry. These first-principles simulations provide data to validate mixing and combustion models in engineering-level simulations of combustion devices, in addition to fundamental insight into complex turbulence/chemistry interactions in flames. A single run of the simulation can produce multiple terabytes of raw data that is vast in the spatial (0.2 billion grid points), temporal (100,000 time steps) and

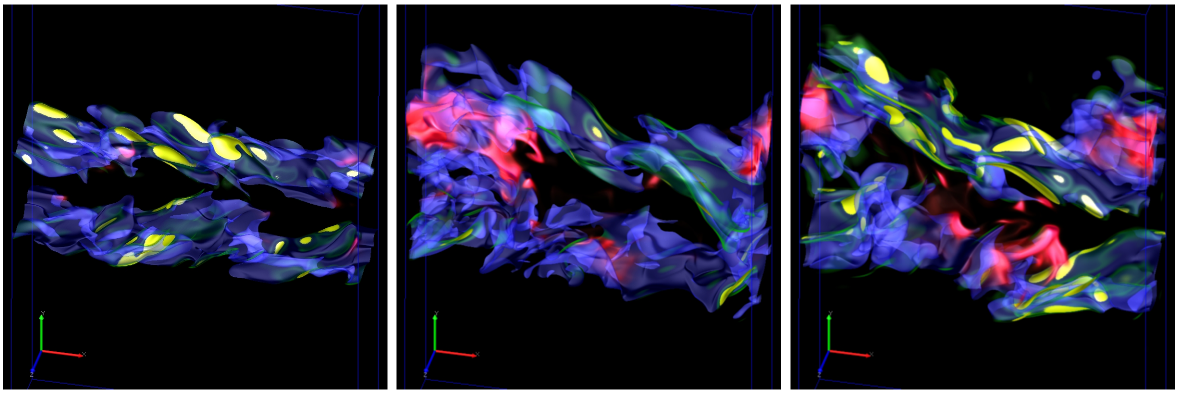

Figure 2. Simultaneous visualization of three variables from simulated combustion data at selected time steps.

variable (tens of variables) domains, creating a formidable challenge for subsequent analysis and interpretation. We and others have addressed such a large data problem using parallel visualization techniques [5, 6, 7] and data reduction methods [8, 9, 10].

In addition to the size of the data-set, the difficulty of knowledge extraction is compounded by the sheer complexity of the turbulent flow-fields, of the phenomena being studied, and by the existence of different types of data (particle and field data). To understand the dynamic mechanisms of extinction and re-ignition in turbulent flames, scientists are thus in need of intuitive and convenient ways of making simultaneous visualization of multiple scalars.

3.1. Simultaneous Volume Visualization

We have studied how to enhance the perception of the relations between two or more scalar variables using advanced volume visualization methods. We aim to develop techniques that can generate effective visualizations which reveal interaction and causal-effect between different scalar properties of the same flow domain. Our approach to the simultaneous visualization problem is to use highly interactive volume rendering, user-controlled data fusion, and mixed rendering styles. Interactive rendering allows the user to freely change rendering and visualization parameters, as well as data fusion schemes. Rendering different volumes with different styles, if done appropriately, may enhance perception of shape, structure, and spatial relationship. The data fusion problem here is to determine how to display multiple data values defined at the same spatial location. Here, we are only concerned with data from the same run of the simulation, unlike in medical imaging or a comparative study of data from different calculations registration and resampling must be done before making a simultaneous visualization.

When rendering multivariate volume data, we must decide how to treat the multiple values defined at the same spatial position. There are basically three approaches to this data fusion problem:

(i) using one value for each color channel,

(ii) using one of the values based on some criterion, or

(iii) computing a weighted sum of all the values.

The first approach is probably the simplest for one to implement and to verify its results. While it is limited to visualization of three or fewer volumes, in practice we hardly need to see more than three volume simultaneously. The problem really limiting this approach is the difficulty for the viewer to interpret the resulting color. An example for the second approach is the alternating sampling used in [11] for rendering two volumes, which seems to work well for medical imaging but not for fluid flow visualization. The third approach gives us more freedom. For example, we could use the opacity transfer function for one volume to enhance or de-enhance some aspects of the other volume. This is similar to the common practice of volume visualization in which gradient magnitude is used to enhance boundary surface. In [12], visualization of multimodality volume data was made by computing values weighted by a function of some or all of other values. Furthermore, the weighted sum might be used with scalings that reflect a desired property, such as distance from the viewer [13].

We use the following linear function to blend colors from multiple variables based on user-specified weights.

$$C = \sum_{i=1}^{k} w_i \alpha_i C_i$$

where k is the number of variables, w_i is the blending weight, and C_i and α_i are the color and opacity correspond to variable i, which are looked up from a 1D transfer function. The key is that the scientists can freely and interactively adjust the weights, and obtain immediate visual feedback. Note that color and opacity must be pre-multiplied before the blending so that color contribution is correctly weighed by its opacity.

Since we use hardware texture volume rendering, this fusing step corresponds to the determination of a fragment color when multiple scalar values, and the associated weight and 1D transfer function for each variable are given. This blending operation is performed for each fragment in the fragment shader which is one of the programmable features in the commodity graphics hardware. The final image is obtained by blending the polygon slices in back-to-front order using the hardware accelerated blending function.

Figure 2 shows simultaneous visualization of three variables using data fusion. In the sequence of selected time steps, mixture fraction isosurface in blue, representing the surface where burning flames are possible was visualized together with other variables, such as OH in red, representing the existence of a burning flame, and χ in yellow and green, representing a local mixing rate. While in isolation these quantities are largely meaningless, together it is possible to understand how the mixing is interacting with the reaction. This data fusion technique may be supplemented with multivariate cut-away to remove occlusion when visualizing highly convoluted flame surfaces resulted from, for example, the cascade of kinetic energy and vortex stretching.

4. Hardware Accelerated Visualization of Gyrokinetic Simulations

Fusion energy research gives promise to environmental attractive, commercially viable, sustainable energy source for the next century. A large part of the worldwide fusion research effort goes into the development of numerical codes to simulate real experiments. By effectively utilizing the full power of modern supercomputers, fusion codes can simulate the movement of billions of particles over thousands of time steps in complex geometry, resulting in enormous amounts of data. Advanced visualization is necessary for extracting the key physics from the large amounts of data generated by these simulations.

In the past, scientists at PPPL mainly relied on commercial software such as AVS/Express to make cross-section and iso-surfaces visualization of the potential data in the simulation results. The software, however, does not take advantage of the advanced features of current graphics hardware, nor it supports volume rendering of irregular-grid data generated by the gyrokinetic simulations. We have developed a hardware-accelerated volume renderer that allows the scientists to interactively explore the potential data.

Visualizing the irregular-grid data generated from the gyrokinetic simulation presents some unique challenge. Simulation results are stored on grid points of a torus-shape, twisted mesh.

The mesh maintains a constant arc distance, $r\Delta\theta$, so the number of mesh points increases as we move out in the radial direction. The mesh twists around the torus, and the twist is different for each radial tube as you go around the torus.

Several parameters, such as density and temperature, are computed at each mesh point for each time step. The largest run of the simulations with 125 million mesh points and one billion particles that has been performed thus far produced 4 terabytes of data. If all of the particle data were stored, the requirements would increase to over 115 terabytes.

4.1. A Hardware-Accelerated Volume Visualization Technique

The 3D texture hardware support of commodity graphics hardware makes possible real time volume rendering. Rendering is performed by drawing a set of view-aligned polygon slices that sample a 3D texture containing the volume data. These slices are composited using hardware alpha blending to derive the final image. However, the graphics hardware is designed around linear interpolation of planar data. The gyrokinetic simulation data is not stored in such a manner so it cannot be rendered directly. To maintain interactive visualization, we have developed a rendering technique that makes use of mixed-coordinate system textures and vertex and fragment shaders [14].

To take the advantage of the 3D texture support on modern graphics hardware, the volume data must be stored in a rectilinear manner. Hence, we must convert the data into the format which is acceptable by the graphics hardware. There are several approaches to achieve this goal. One approach is to resample the whole data set in 3D world coordinates but this approach requires lots of storage and about half of the storage is wasted by the empty region outside the torus-shape mesh. This approach also would generate superfluous samples along the major angular direction, ζ. We have introduced a resample-and-warp strategy [14]. By re-sampling the data along the minor radial direction, r, and the minor angular direction, θ, we can obtain more accurate results because the potential values tend to change less along the mesh line. Furthermore, interpolation therefore should be done along mesh line directions to obtain best accuracy. Using hardware tri-linear interpolation directly would result in artifacts in the image. We have implemented this correct interpolation scheme in the fragment program and obtained accurate and high-quality images as shown in Figure 3. Our design provides scientists an efficient and accurate visualization tool to explore their simulation results.

5. Visualization of Modes in ILC Cavities

The International Linear Collider (ILC) is a proposed future international particle accelerator. The ILC would provide a tool for scientists to address many of the most compelling questions about dark matter, dark energy, extra dimensions and the fundamental nature of matter, energy, space, and time. The ILC components must have their designs modeled, simulated, and optimized before they are built.

One particular problem of the interest of scientists at the Stanford Linear Accelerator Center (SLAC) involves reducing the effects of wake fields. A small bunch of electrons travels at relativistic speeds through the cavity of the accelerating structure. This results in electromagnetic wake fields, analogous to the wake waves arising from a boat speeding along a river. Wakes reflect off of the shores and can set up waves which would be noticed by a second boat following the first. Electromagnetically speaking, these wakes excite higher order modes in the accelerating structure, and the modes can deflect subsequent bunches off of the axis, harming the test results further downstream. Special high order mode couplers are designed to absorb these modes. The optimal placement of the couplers is not obvious, and the way in which the many modes couple to them is an important area of study.

The simulation of the accelerator structure proceeds as follows. A CAD model is meshed using a higher order tetrahedral elements. The parallel code Omega3p solves for the frequency

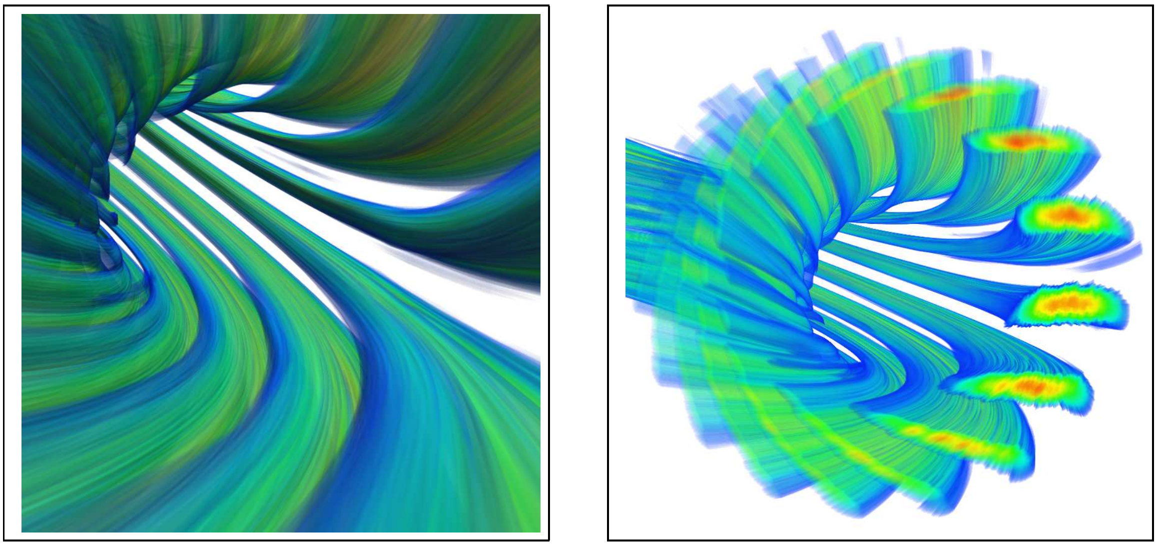

Figure 3. Left: A close-up view of the positive potential values. Right: A cut-away view.

domain description of the E and B fields in this mesh. Each obtained eigenvalue is the frequency of a resonant mode, and the corresponding eigenvector can be used to produce complex E and B field values in the mesh.

These complex 3D field vectors describe periodic behavior of each mode, but not in a visually intuitive way. Therefore, the complex frequency domain vector representation of these fields is converted into a sequence of discrete real-valued fields in the time domain. Time samples are uniformly spaced over one period, and visualization of this sequence is much more intuitive and natural than static images of components of the complex vector fields. Our first approach to the mode visualization is to use scaled cones to show the direction and magnitude of the field. Such glyph visualization, however, is only useful for depicting the properties at a small isolated, local region, and usually does not scale well with the complexity and resolution of the data. We also use a tube-like representation for visualizing the E and B field lines directly. As we can interactively adjust the size, density, transparency, and color of the tubes, it is a more flexibile representation than glyph.

SLAC scientists share these mode visualizations with their collaborators oversea. A collaborative data analysis mechanism is thus needed. We have developed a web-based visualization interface for viewing, manipulating, and annotating the data including images and animations, as shown in Figure 4. The interface displays the Q_e-frequency graph and allows the user to interactively select a particular mode to study. The user can browse through a sequence of images and animations, and select a different mode. Because the graph may potentially contain a very large number of data points, a focus+context display is used. Presently, only precomputed images and animations are shown. In the future, this interface will be integrated with a high-performance visualization server to generate visualizations of interest on the fly.

Electromagnetic visualization differs with fluid flow visualization. For time-varying electromagnetic fields, the motion of the electric or magnetic field is independent with the field itself and generally not along the field lines (i.e. the instantaneous field streamlines). The evolution of the field lines is driven by a motion vector field where the value of this field at a specific point in space and time is the instantaneous velocity of the streamline at the corresponding point of the electromagnetic field. This motion vector field is obtained by computing the crossproduct of the electric field and the magnetic field [15].

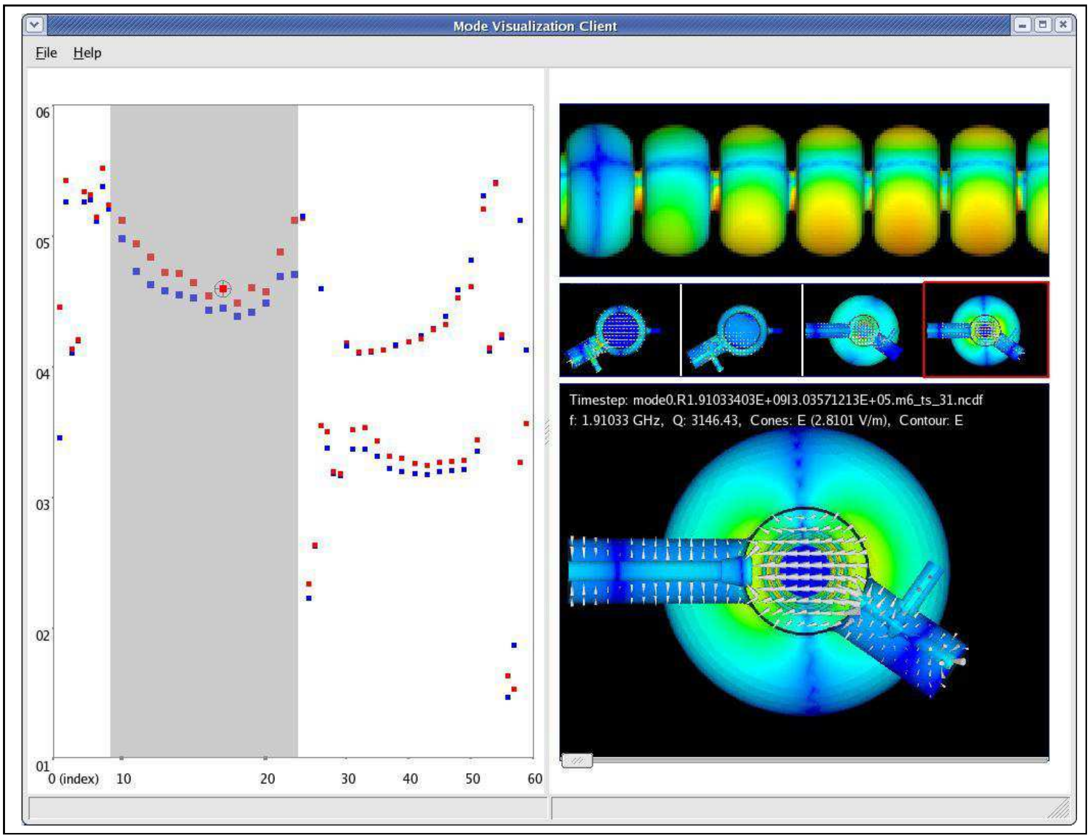

Figure 4. The remote visualization interface for studying modes.

To visualize 3D time-varying electromagnetic fields, the main challenge comes from the visual occlusion. Directly applying LIC generates a 3D texture which presents a visual occlusion problem to the viewer. Thus we present a cut-plane of the LIC volume along with a sparse presentation of the 3D field by explicitly constructing and tracking each field line. The initial seeds for field lines are placed according to the field strength distribution. After that, the lines are drifted by the motion field d with the similar iterative process used in [16]. When the field lines are converging or diverging, we dynamically merge or add field lines to maintain the line density and distribution. The resulting animation effectively exhibits the 3D field evolution.

6. Conclusion

Visualization is an extremely vital component of the SciDAC effort at SLAC in facilitating the design of the next-generation accelerators, and in advancing the understanding of the complex processes that arise in their operation in new parameter regimes. Advanced visualization is also essential for our collaborators at the Lawrence Berkeley National Laboratory to gain insight and understanding of phenomena that are simulated in large, complex computer models involving beams and plasmas. Furthermore, we have shown that how appropriate visualization solutions can drastically lift the ability of scientists to understand the enormous amounts of data generated from their combustion simulations and supernova modeling. The ability to simultaneously visualize multiple variables are essential since combustion is inherently a multi-scalar problem with intricate coupling between reactive scalars and with the flowfield. The realtime, high-fidelity volume visualization capability provides TSI scientists with never-before seen views of the underlying phenomena and are destined to lead to new understanding. These new visualization technologies are also applicable to other areas of SciDAC study.

Next, we will experiment with interactive exploration techniques taking into account particularly the cognitive aspects of visualization. Some of the promising directions include making expressive visualization by mimicking technical illustrators' techniques, employing motion to perceive the complex temporal and spatial relations/structures, and alleviating the occlusion problem with multidimensional cut-away. The other promising approach is to employ machine learning in the complex process of data visualization. We have demonstrated an intelligent system approach to the 4D feature extraction tracking problem [17]. We will begin to apply this approach to SciDAC applications.

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