# VISIOMETRICS, JUXTAPOSITION AND MODELING

High-performance computers that allow users to visualize and diagnose numerical simulations and interact with them rapidly are boosting scientific productivity in the study of complex and turbulent systems.

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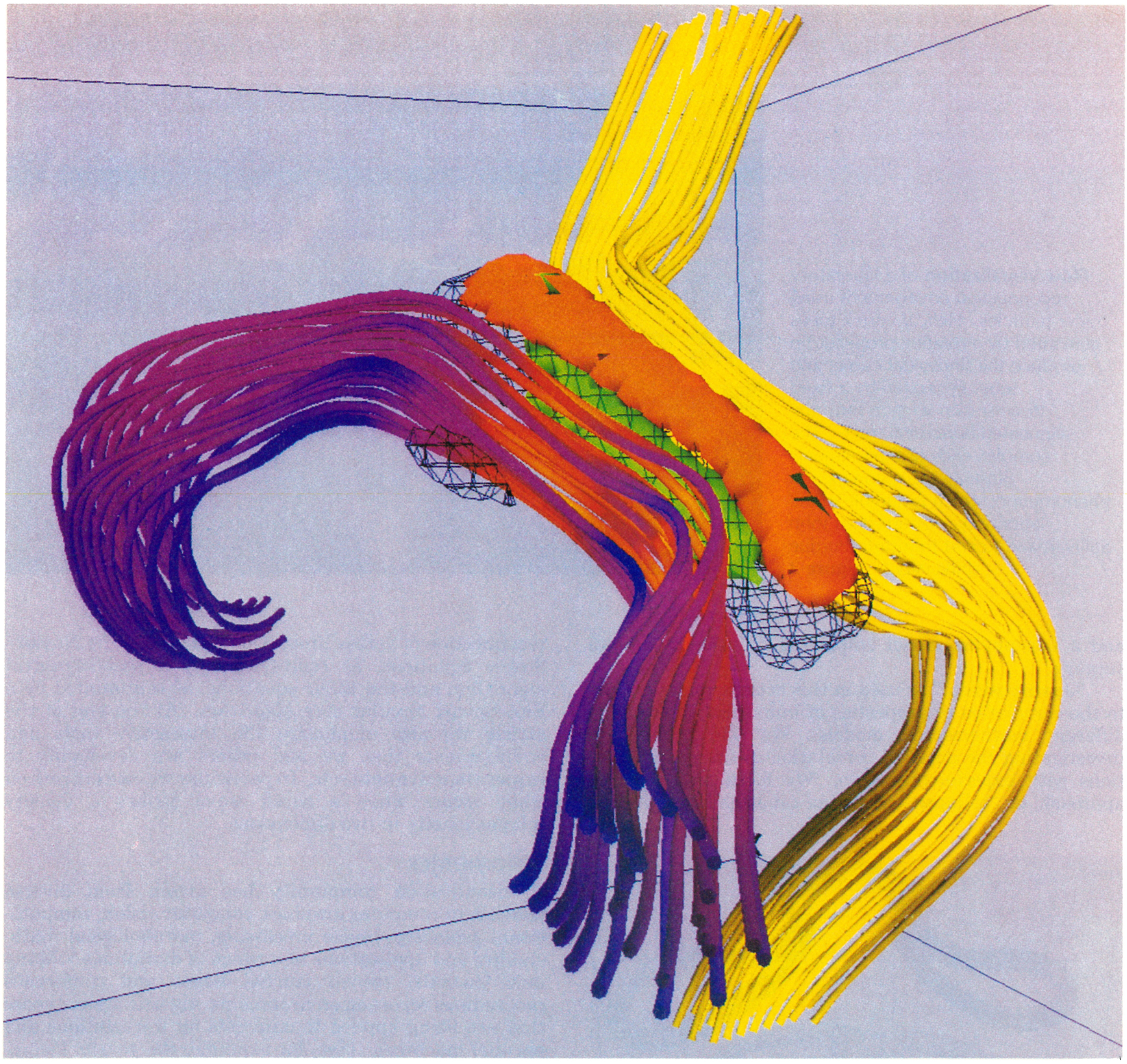
With the advent of massively parallel computers, the evolution of nonlinear dynamical systems such as fluids and plasmas is being investigated in three dimensions at increasingly high resolutions. Today a typical physical volume is represented by $100^3$ grid points, and we may expect the resolution to increase to $1000^3$ by the end of the decade.

The nonlinear processes under investigation are typically unstable and turbulent. Often they are unpredictable and evolve into complex topologies with near-singular space–time events. (An example, which we discuss below, is the "collapse" of nearly antiparallel vortex tubes in a fluid, as shown in figure 1.) To acquire a deeper understanding of these phenomena, we will often find it useful to formulate models with reduced parameters, or low degrees of freedom, based on insights gained by juxtaposing solutions from computer simulations having many degrees of freedom with the results of laboratory and field experiments.

By "juxtaposition" we mean the detailed and quantitative comparison of experimental images with adjacent or superimposed computer simulation images of similar or different functions at the same or different times.

Juxtaposition is a step in the visiometric process—the process of visualizing and quantifying evolving features within space–time data sets to obtain information for validating candidate mathematical models.[1,2] The goal is to juxtapose visualized and quantified data sets from various simulations and experiments interactively and automatically. This will allow one to make cogent and timely decisions on selecting new directions, such as model parameters, for future study.

We use the term "modeling" to refer to several processes. First, in the usual physical modeling of real processes, one introduces many parameters to define a space–time domain with many interacting physical processes and scale sizes. Examples are a weather prediction model for the entire planet or the design of a magnetic fusion reactor (tokamak). Second, in reduced modeling, there occur a smaller number of phenomena that are

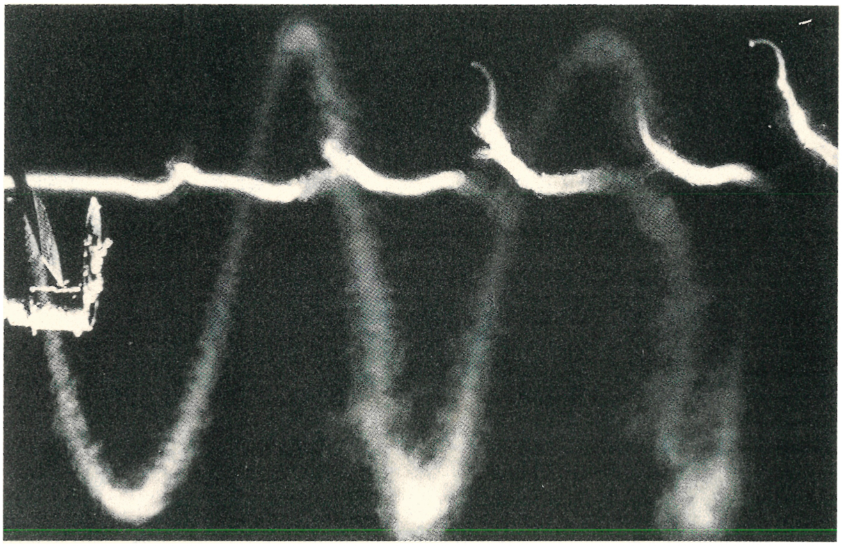


**Vorticity field lines** in a computer simulation of fluid flow with high Mach number (0.9). The strongly compressible zone between the two vortex tubes prevents collapse and large increases in vorticity. The "wire frame" shows the isosurface for Mach number 1. The antiparallel configuration induces a velocity "jet" that shoots up between the tubes. The lower isosurface (green) indicates where expansion of the flow is strong, a region of positive divergence. A shocklet forms at the isosurface where the jet velocity becomes subsonic again (orange), a region of negative divergence. (Simulation by Thomas Scheidegger, Rutgers University.) **Figure 1**

controlled by fewer system parameters—that is, a low-degree-of-freedom representation.

The discovery of the soliton by Zabusky and Martin Kruskal in 1965 is a paradigm for the latter modeling process. They tried to understand unexpected observations in simulations performed by Enrico Fermi, John Pasta and Stanislaw Ulam in the early 1950s. They obtained waveforms of displacement and energy spectra as numerical solutions of the ordinary differential equations of a one-dimensional nonlinear spring-mass lattice with fixed boundary conditions. Of particular interest in their solutions was the near-recurrence of initial waveforms of displacement. Kruskal suggested that modeling the lattice by the third-order nonlinear Korteweg–de Vries (KdV) partial differential equation with periodic boundary conditions would yield a reduction in complexity. (See the article by Zabusky in PHYSICS TODAY, July 1984, page 36.) Gary Deem, Zabusky and Kruskal obtained numerical solutions, which represented a combination of time derivatives and spatial differences of the lattice waveform and showed clearly the presence of coherent pulses colliding and reappearing. This inspired a group at Princeton to find an exact mathematical solution to the KdV problem in 1967. It also led a host of people to new mathematical connections and insights and to many analytical solutions to related nonlinear systems such as deep water waves and nonlinear optics. Recently the soliton idea has been applied to the analysis of ocean wave data through a technique called "nonlinear Fourier analysis"[3] and to the development of commercially useful fiber-optic transmission systems.[4]

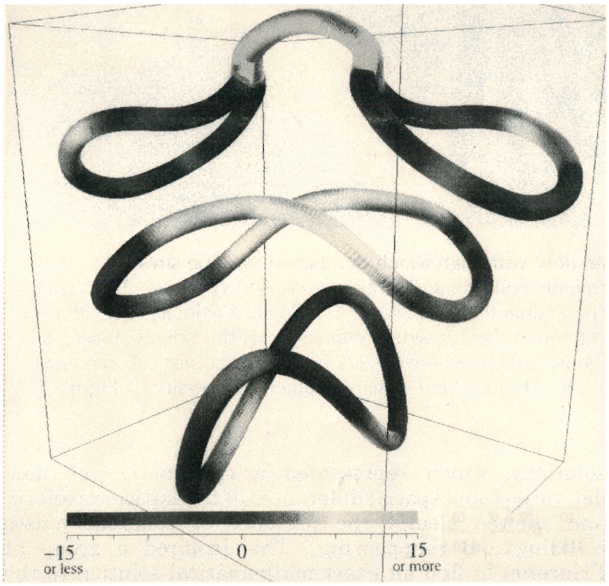
The companion article by David Dritschel and Bernard Legras (page 44) gives an excellent example of model juxtaposition in two dimensions. They are studying two-dimensional incompressible vortex dynamics and turbulence with an Eulerian continuum pseudospectral model



**Flow visualization** of a laboratory reconnection environment using tracer particles. Helical vortex tubes generated by a rotating propeller tip produce the sinusoidal curve, and tubes generated by a fixed downstream wingtip form the segmented horizontal trace. The complex ends of the segments illustrate the reconnection phenomenon, which is audible in the laboratory. (Courtesy of John Sullivan and Robert Johnston, Purdue University.) **Figure 2**

and a Lagrangian model employing "contour dynamics surgery."

"Juxtaposition," as used in this article, refers mainly to the correlation of properties of numerical solutions of different mathematical models. We and others are investigating the detailed correlation of numerical solutions with experimental data. We focus on the rapid approach, or "collapse," of vortex tubes and the ensuing reconnection of vortex lines. Our models are the Navier–Stokes equations, as represented by a pseudospectral algorithm, and the Euler equations, as represented by a Biot–Savart circular core algorithm. At the end of the article we also emphasize the interactive tools and environments that we and others are developing to explore massive data sets. In particular we concentrate on what occurs when a shock wave strikes a density inhomogeneity in two dimensions.




**Evolution** of an upwardly translating Lissajous elliptical vortex ring. The ring is shown at three times during the Biot–Savart simulation: the initial condition (bottom), a near-collapsed state (middle) and a collapsed state (top). The arch-shaped region in the collapsed state symbolizes overlap but is not physical. Dark shading indicates low scalar strain, or intensification of the vorticity on the vortex tubes; light shading indicates high strain. (Simulation by Victor Fernandez, Rutgers University.) **Figure 3**

## Visiometrics

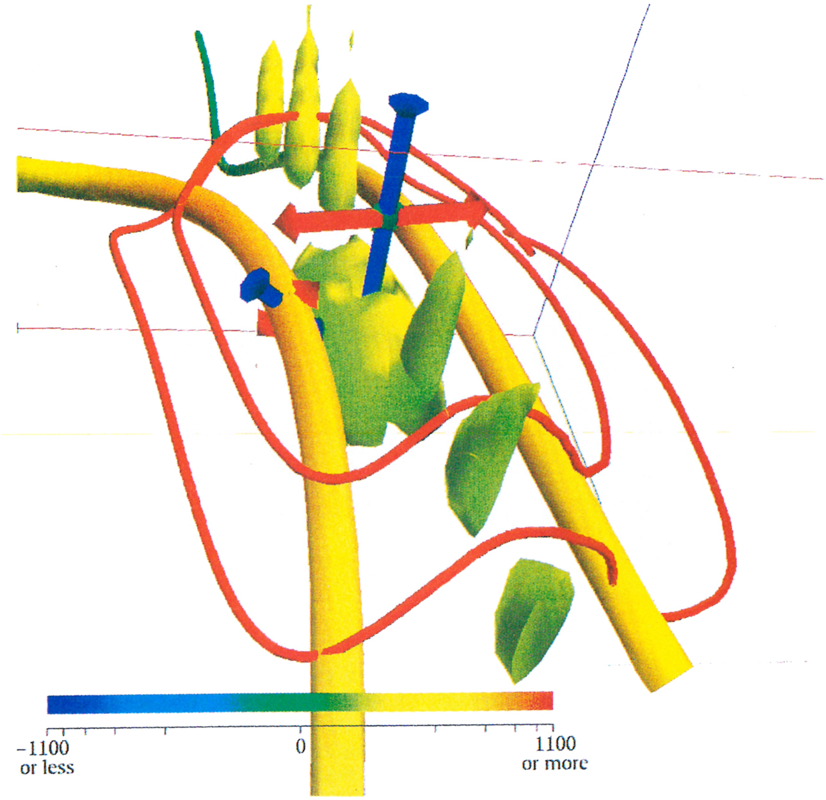
A visualization community has arisen from diverse workers in computer graphics, computer vision, computational geometry, image processing, morphological mathematics and applications in a range of disciplines.[5] Many new journals, special journal issues and conference proceedings report on environments, algorithms and codes that are being applied to data sets on workstations and parallel machines. (See, for example, the yearly *Visualization Conference Proceedings.*) Several visualization packages and environments are available for mainframes and workstations, including AVS (Advanced Visual Systems), Data Explorer and others. Several government-affiliated laboratories also provide visualization software, including the National Center for Atmospheric Research and the NASA Ames Research Center.

Visualization alone is not enough. Insight toward new models requires the quantification of evolving morphologies of features such as wave packets, solitons, dislocations, shock waves, eddies, vortex rings and vortex tubes. Quantification of a feature or region involves its isolation, extraction, classification and correlation. Next one tracks features to determine how they interact with other regions, how they change their form, where they have moved and—the focus of this article—how they compare with features from other experiments and simulations. Interacting features include scattering of waves, roll-up of shear layers, formation and collapse of bubbles, collisions of galaxies, and the merging and winding of vortices in turbulent fluids.

The individual steps of quantification and juxtaposition, to be discussed in detail below, are as follows:

▷ Visualization: rendering a "picture" of the data set using standard visualization and computer graphics techniques.

▷ Identification: isolating and extracting persistent and




**Ellipsoids** of vorticity (yellow) and of normalized stretching (green) traversed by five-element vector bundles. Also evident are a zoomed vortex tube (orange and yellow), rate-of-strain isosurfaces (light green domains) and the corresponding vector field (red), whose toroidal shape is a signature of collapse. (Simulation by Fernandez.) **Figure 4**

localized—that is, coherent—regions.

▷ Quantification: measurement of a coherent region—volume, area, circulation, charge, current, moments and so on.

▷ Classification: identifying this region as either a known or possibly new phenomenon.

▷ Tracking: following the region in time.

▷ Juxtaposition: comparing and correlating features from simulations and observations.

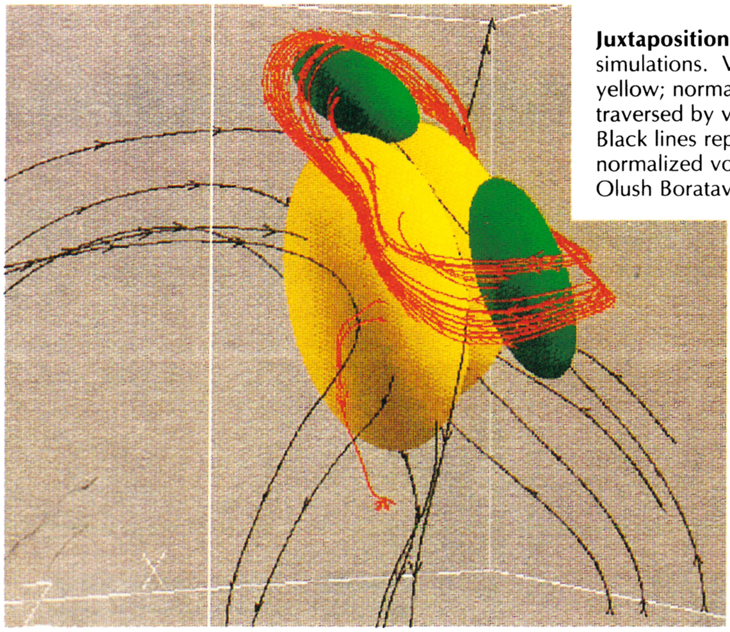
The ultimate goal is to understand the original problem well enough to formulate models that describe the interaction of observed localized phenomena and the way processes scale.

**Visualization** converts data into a variety of pictures. First, we preprocess the data (to reduce noise or size) and categorize it by choosing appropriate color maps, opacity parameters, contour levels and so on. It can then be transformed to an appropriate geometric model for display. Standard visualization techniques include continuous-tone contour maps in two dimensions; volume rendering (integrating along rays in three dimensions);[6] displaying isosurfaces, or "contours," from connected polygons that bound regions of functions above some threshold;[7] and, for vector fields, drawing icons or "hedgehogs" (arrows) and tracers (streamlines, vector field lines and so on) and then tracking critical points.[8]

New advances in both hardware and software have opened exciting possibilities. One can now interactively visualize and quantify larger and more complex data sets as the computation is executed, a capability made possible by multiprocessor supercomputers with massive internal and external storage systems; by multiprocessor workstations for interactive three-dimensional manipulation; and by high-bandwidth networks such as the gigabit-per-second network test-beds sponsored by the Corporation for National Research Initiatives. Advanced visiometric environments and virtual reality techniques such as three-dimensional eyephones, stereo sound, force feedback and holography are also being used to help present all the data to the user in a meaningful and more intuitive format.[9]

**Identification.** The simplest type of structure to visualize is an isovalued cluster in a scalar field, which can be detected using volume rendering or isosurface contouring. Object regions consist of a set of neighboring interior points above a certain threshold value and their boundaries. The entire data set can be segmented, using a particular threshold value, into coherent regions and a surrounding sea. These regions—a set of node points—can be stored in a hierarchical data structure, such as an octree structure,[10] for efficient computation and retrieval. Different threshold values will generate different sets of regions. A "seed" algorithm is used to grow the regions from local maxima. This is similar to methods used in other domains.[2,11] Histograms, or number distribution functions, for various threshold values are revealing.[12] Isolating regions in this way provides a handle on the objects of interest for quantification and tracking.

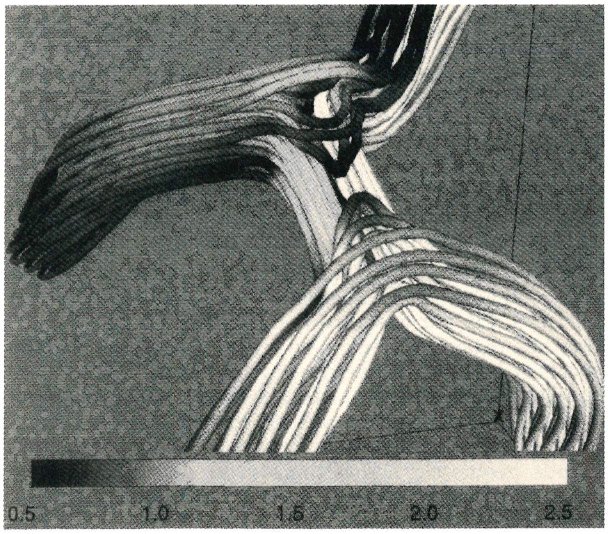
**Quantification and classification.** Quantification involves computing general and domain-specific parameters to describe the extracted regions. These parameters include geometric descriptions such as volume, area, genus, curvature, torsion, medial axis and simplified shape abstractions as well as domain-specific quantities such as moments, circulation and field lines. These region parameters are also required for classifying regions into a set of known objects or a set of generic shapes. These shapes, which appear across disciplines, include line-like structures found in images of two-dimensional projections of jet streams, storm fronts and galaxy formations; three-



**Juxtaposition** from pseudospectral simulations. Vorticity ellipsoids are shown in yellow; normalized stretching ellipsoids traversed by vector-field bundles, in green. Black lines represent vorticity; red lines, normalized vortex stretching. (Simulation by Olush Boratav, Rutgers University.) **Figure 5**

dimensional tube-like structures such as tornadoes, typhoons and contrails of flying aircraft; sheet-like pancake domains found in vortex collapse (described below); and ellipsoid-like structures such as bubbles or regions near extrema of any function. For filamentary and tube-like objects, skeletal representations are efficient quantifiers.[13] These abstractions can also help in simplifying procedures for tracking objects such as vortex tubes.

**Tracking** involves searching the output in time for the previously isolated and identified coherent structures. However, correlating objects automatically is difficult, because they are constantly evolving and interacting—merging or splitting, for example. Therefore feature tracking also involves classifying interactions—identifying what is happening to the feature so as to maintain tracking through close interactions. (Reference 2 describes a sample of interactions.) Some of our interactions are between nearest neighbors. Therefore to properly track features one must maintain a list of neighbors and potential interactions. Furthermore one must parameterize all the interactions possible for a given domain—that is, list under what conditions they occur and some of the signatures that precede these occurrences. Limiting region movement and tracking extrema can be used to follow objects under certain conditions.[2]



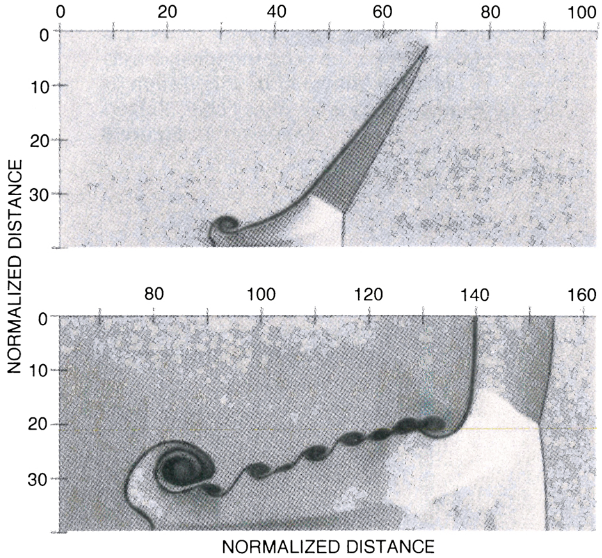

**Reconnection** of vorticity field lines at low Mach number (0.3). The X point is clearly visible, with a vorticity zero-crossing at the center. (Simulation by Scheidegger.) **Figure 6**

## Collapse, intensification and reconnection

The quintessential nonlinear space–time domain of basic and practical interest is the dynamics of fluids—liquids, gases and plasmas. Vortex tubes are one of the fundamental structures in fluid mechanics. They are produced at the tips of wings and propellers and as evanescent "hairpin" structures in boundary layers, or they can result from unstable nonuniform parallel flows. The stretching and intensification of vortex tubes in a turbulent flow is believed to be the main way in which energy is distributed, or "cascades," to different scale sizes. Research has suggested that the interaction of vortex tubes leads to singularities of vorticity in a finite time in inviscid flows and to bursts in viscous flows. The literature is rich and growing.[14,15]

The collapse of vortex tubes to antiparallel configurations was first found in regularized Biot–Savart simulations of an elliptical vortex ring and was confirmed experimentally by M. R. Dhanak and D. De Bernadinis at Imperial College in London. Such a process is also manifested in the late-time evolution of the Crow instability for vortex tubes that are initially weakly perturbed and antiparallel. The latter phenomenon is often visible to those who stare at the vapor-seeded contrails of high-flying jets.

Here we examine the juxtaposition of vortex collapse and reconnection phenomena in three-dimensional space and time using the Navier–Stokes equations for incompressible and compressible fluids and the Biot–Savart form of the Euler equations for incompressible fluids. The generic nature of this process is under investigation, and




**Density images** show development of the interaction of a Mach-number-2 shock with an air–freon interface inclined at 60° to the vertical from time $t = 28$ (top) to $t = 83$ (bottom). (Simulation by Ravi Samtaney, Rutgers University.) **Figure 7**

we discuss results and new approaches to understanding the process.

**Laboratory realizations.** In 1987 Paul Schatzele and Donald Coles at Caltech beautifully and carefully investigated the collision of low-Reynolds-number vortex rings approaching at an angle. Coparallel vortex ring collisions have also been carefully investigated by others for both same-axis and offset-axis configurations.

Recently John P. Sullivan and Robert Johnston of the Purdue University Aerospace Science Laboratories developed a new laboratory environment for investigating large-scale vortex tube interactions.[16] Figure 2 shows a flow visualization done by them of tracer particles that define helical and horizontal vortex tubes generated by a rotating propeller tip (sinusoidal trace) and a fixed downstream wingtip (segmented near-horizontal trace), respectively. The complex ends of the segments illustrate the reconnection phenomena discussed below. In the future we hope to juxtapose the real events with model simulations.

**Model juxtaposition.** As initial conditions for our simulation studies, we take either a Lissajous ellipse, $(x,y,z) = (\cos\theta, b\sin\theta, c\sin 2\theta)$, for the Biot–Savart simulations, or two compact, orthogonally offset (that is, perpendicular and with displaced axes) vortex tubes, for the pseudospectral periodic domain simulations.

The Biot–Savart equations use the simplifying model of a circular core for incompressible filaments, or tube-like topologies. The assumption of a circular core breaks down during collapse and filament overlap, and the model does not characterize Euler or Navier–Stokes solutions for all times. Eric Siggia of Cornell University and Alain Pumir of the Ecole Normale Supérieure in Paris used it to describe aspects of collapse.[17] Figure 3 shows three stages in the evolution of an upwardly translating ring: the initial condition, the near-collapsed state and a collapsed state in which the arch-shaped segment symbolizes overlap but is not physically correct.

In figure 4 we juxtapose a portion of the collapsing elliptical ring with strain quantifications (diagnostic quantities) in a box that surrounds the high-strain region of the Biot–Savart simulations. A zoomed vortex tube (orange and yellow), rate-of-strain isosurfaces (light-green domains) and the corresponding vector field $\omega\cdot\nabla\mathbf{u}/|\omega|$ (shown in red) are evident. The red toroidal region is a signature of collapse. Also shown are two sets of eigenvectors of the rate-of-strain tensor (red and green are positive, and blue is negative). Note that the mid-eigenvalue (parallel to the vortex field during collapse) is relatively small and is virtually hidden.

Figure 5 shows a corresponding juxtaposition from the pseudospectral simulations.[14] One sees vorticity $|\omega|$ ellipsoids (yellow) and "strain" $|\omega\cdot\nabla\mathbf{u}|/|\omega|$ ellipsoids (green). The ellipsoids are fit to thresholded spatial domains of scalars. Again, a bundle of vectors emanates from the ellipsoids. The yellow ellipsoids are pancake-like, with aspect ratio 7.61:6.94:1.08.

As expected, one sees the oppositely directed black vorticity field lines through the yellow ellipsoids. As in the Biot–Savart simulations, the red toroidal field bundle appears. The yellow pancake-like regions, however, are not modeled in the circular-core Biot–Savart simulations. Furthermore, the green regions of stretching, which are nearly symmetric in the Biot–Savart simulations, are offset toward the head of the dipolar (yellow) pair in the pseudospectral simulations.

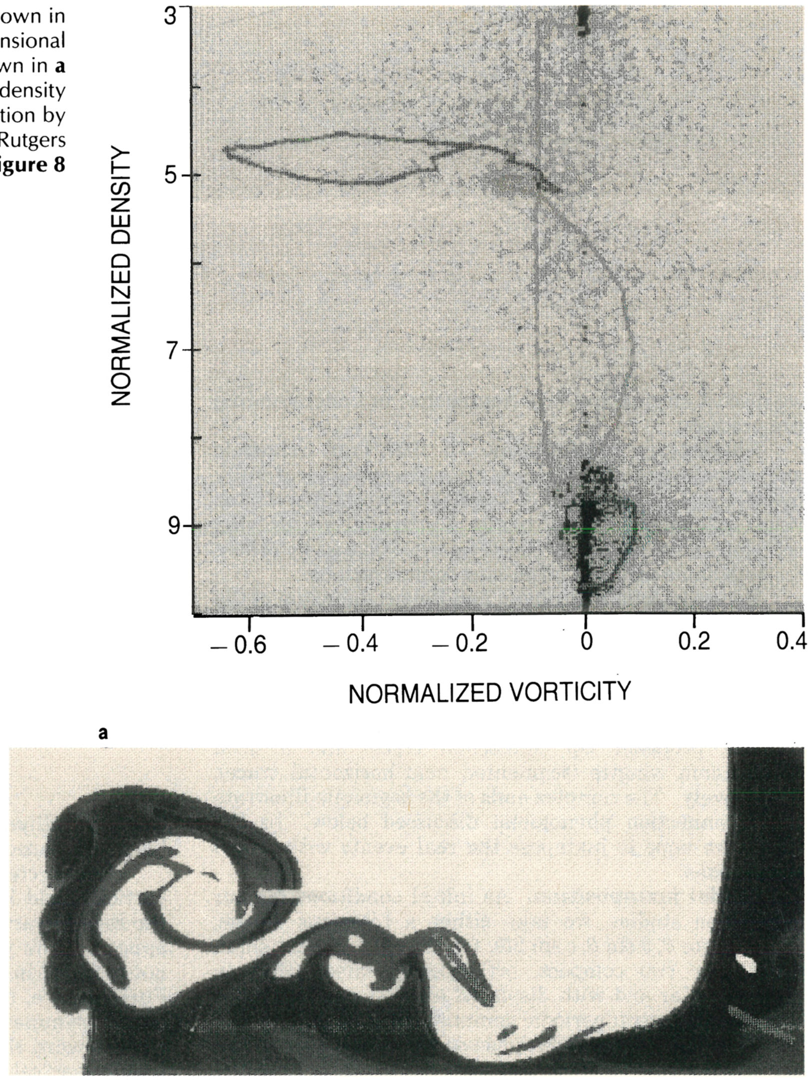
At present we have no detailed mathematical explanation, such as a prediction of collapse time as a function of the initial geometric parameters. We have observed and noted generic properties of both viscous and inviscid simulations for future modeling.

We expand the physical modeling domain by allowing compressibility, which we find inhibits vortex reconnection. The initial condition consists of the same orthogonally offset, divergence-free tubes. We quantify the time scale for reconnection by tracking vortex lines. Lines are launched at a certain magnitude of vorticity at each grid point on the boundary face where one or both tubes enter the computational domain. This is done for consecutive times, and the beginning or end of the reconnection process is taken when, respectively, the first or last vortex line switches from one tube to the other.

As shown in figure 6, at low Mach numbers the vortex lines that undergo reconnection first form an X point with a large increase in vorticity. Subsequently these lines move out of the interaction zone, and the topology resembles a double Y point. Viscous dissipation limits the growth of vorticity and causes reconnection of low-amplitude vorticity. Eventually all lines originating in one tube are connected with one branch of the other tube.

As shown in figure 1, if the Mach number is increased, a highly divergent expansion–compression (orange–green) flow region develops where formerly both vortex tubes

**Shock–interface interaction** shown in figure 7 develops the two-dimensional distribution of density and vorticity shown in **a** at time $t = 194$. The corresponding density image is shown in **b**. (Simulation by Samtaney; interface by Akos Feher, Rutgers University.) **Figure 8**




would normally pinch. This compressible region inhibits the collapse process. Thus for sufficiently high Mach numbers, the vorticity intensification is reduced substantially, and the entire flow field decays due to dissipation before the tubes are fully reconnected.

From such juxtapositions we hope to continue to identify the causal effects involved in the reconnection process. Furthermore, for an incompressible medium, we may be able to simulate processes for longer times with an augmented Biot–Savart model where the invariant circular core is replaced by a "complex" filament composed of one or more concentric sheets or many intersecting sheets. Certainly the use of a multiplicity of such complex filaments would be required to model reconnection and turbulence, provided some "surgery" algorithm were introduced to allow for changes in topology.

## Shock–interface interactions

The interaction between shock waves and density inhomogeneities is of fundamental importance in compressible hydrodynamics and turbulence. The study of this interaction illuminates the nonlinear aspects of the instability in a shock-perturbed interface, known as the Richtmyer–Meshkov instability.[18] Furthermore, the elemental processes that occur are of great interest in the study of astrophysical interiors and of great practical interest in work on supersonic combustion and inertial confinement fusion. Here we discuss some ongoing work and illustrate some new tools for exploring large data sets. Compared with our mathematical and physical understanding of solitons, the study of shock–interface interactions is at its beginning.

The Richtmyer–Meshkov instability describes the growth of perturbations on a density interface separating a gas of density $\rho_1$ from a gas of density $\rho_2$ after the interface is struck by a shock wave. Usually the plane of a shock wave is parallel to the plane of the interface, and the perturbations break the one-dimensional symmetry. To validate the numerical simulations—a first step in model building—we have found it useful to examine the interaction between a shock and an inclined planar interface where $\rho_2 > \rho_1$.

During the rapid interaction between shock and interface, a velocity discontinuity, or vortex sheet, develops on the interface due to the misalignment of the density and pressure gradients—the so-called "baroclinic" source term. For certain parameter configurations, a rigorous time-independent analysis provides results for vorticity deposition on the interface. Our numerical simulations of the compressible Euler equations are in excellent agreement with these analytical results. The simulations also illustrate the errors that could result from inadequately resolving the fluid structures.

Figure 7 shows the density at two times. In the upper frame, the shock is about to leave the interface, and in the lower frame, the vortex layer deposited by the shock has begun to roll up—a nonlinear manifestation of the velocity-shear, or Kelvin–Helmholtz, instability. These vortices merge with one another until finally we have a few coherent vortices surrounded by filamentary structures.

Let us illustrate how we are using our DAVID quantification environment to explore the simulation's data sets.[1] We simultaneously juxtapose two variables—density and vorticity. Figure 8a shows the two-dimensional distribution of density and vorticity for the density image at a later time. The "round" coherent vortices in that image (figure 8b) are dominantly in the low-density fluid, while the filamentary structures are distributed uniformly across the interface. This is made apparent if one draws a line across the coherent structures and observes that the map of this line in the distribution lies in the low-density region. A horizontal line drawn across a filament appears across the interface (the vertical part of the large curve in the distribution). Such a migration of dominant vorticity into lower-density regions may decrease the turbulent mixing at the interface.

## Future prospects for visiometrics

Nearly five decades ago John von Neumann envisioned the "penetration" that computation would make in enhancing our understanding of "all types of nonlinear partial differential equations . . . particularly . . . in the field of fluid dynamics."[19] Each decade since, the march of technology has enhanced the physics, dimensions and scale sizes that we have been able to study. It is more difficult to fathom and comment on how this technology, when harnessed by visiometrics, will enhance our visual literacy—that is, our ability to recognize and understand ideas conveyed through images. The development of physical insight arises from an amalgam of processes: sight, touch and focused immersion. They enhance our ability to recall, juxtapose and review various kinds of information in a way that, for some, synergizes the creation of mathematical abstractions. The ability to work in an environment (at a terminal) that will be sensitive to inputs from a keyboard, body movement, voice and touch and that will steer the computer through the parameter space of a model will lead to enhanced productivity for the visiometrically trained scientist. Integrating many of the visualization and quantification algorithms with the simulation code is a necessary step for rapid results. Such integration should involve parallelizing the visualization, quantification and data compression algorithms.

Environments in computational science must provide interactive and automatic data management so that new results appear with sufficient accuracy and minimal delay. These data must be presented to the scientist in a form suitable for cogent assimilation. Juxtaposition, feature extraction, tracking and quantification are crucial parts of this process. The robust management of these abundant data for recall, communication and training is the grand challenge for computational science designers of the future.

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*Computations were done on the Cray Y-MP and the Thinking Machines CM-2 at the Pittsburgh Supercomputer Center.*

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