



EXCELLENCE IN COMPUTER SIMULATION

By Leo P. Kadanoff

EXCELLENT COMPUTER SIMULATIONS ARE DONE FOR A PURPOSE. THE MOST VALID PURPOSES ARE TO EXPLORE UNCHARTED TERRITORY, TO RESOLVE A WELL-POSED SCIENTIFIC OR TECHNICAL QUESTION, OR TO MAKE A GOOD DESIGN CHOICE.

Stand-alone modeling can serve the first purpose; the other two goals need a full integration of the modeling effort into a scientific or engineering program.

Some excellent work, much of it related to the US Department of Energy's laboratories, is reviewed. Some less happy stories are recounted.

In the past, some of the most impressive work has involved complexity and chaos. Prediction in a complex world therefore requires a first principles understanding based on the intersection of theory, experiment, and simulation.

I work within a Department of Energy-supported research program at the University of Chicago called the ASCI/Alliances Center for Astrophysical Thermonuclear Flashes. The main goal of ASCI, the alliance for scientific computing, is to gain knowledge and experience relevant for the construction of large-scale computer simulations, thus supporting computer research on complex systems and thereby helping the DOE maintain a stockpile of nuclear weapons. My interest here is to provide an overview of the art and science of scientific computer simulation.

The Best: Great Examples of Scientific Computing in the Heroic Period

To begin: I am happy to tell you that the Department of Energy's scientific laboratories have supported some of the very best scientific computing ever done. Indeed, in some sense they invented scientific computing. In this section, I describe some of the best examples of scientific computing, and you will see a preponderance of Department of Energy-supported work.

In the Monte Carlo method, a random-number generator is used to perform deterministic calculations.¹ The Rosenbluths, the Tellers, Ulam, and Metropolis played major roles in putting the method together and applying it to the "Metropolis algorithm" for calculating the properties of systems in thermodynamic equilibrium. This paper was cited in *Computing in Science & Engineering* (January/February 2000) as being among the top 10 algorithms having the "greatest influence on the development and practice of science and engineering in the 20th century."

When this calculation was first performed, the idea that a numerical method could be built on the fake, constructed, randomness of a typical computer's random-number generator

seemed almost magical. Indeed, in a famous incident, Alston Householder said he would stop the computational work at Oak Ridge National Laboratory while he waited to be convinced that random-number generators could work.²

Today, we have a fairly clear explanation of why the Monte Carlo method works—namely, that for expectation values, the rapid increase in the number of configurations with energy is compensated for by the rapid decrease of the Boltzmann factor, leaving a narrow window of states that actually have to be explored. Computers' random-number generators are now fully accepted and reasonably well understood. The most powerful and surprising feature that remains from this early calculation is the insight that using an inherently probabilistic algorithm can lead to an enormous compression in the number of computational steps required.

Monte Carlo calculations use a random-number generator to simulate something else, often a system in thermodynamic equilibrium. By contrast, the molecular dynamics approach uses the computer to solve Newton's equations of motion and follow the trajectories of all the particles in the system. Fermi, Pasta, and Ulam performed one of the first calculations of this kind. They studied a linear chain of atoms coupled with anharmonic forces and driven by an initial large tweaking in one mode.³ They then used a simulation to follow the system as the 128 atoms jiggled about and transferred energy from one mode to another. After a time, the energy became satisfactorily mixed (as

expected), but they kept the computer going. At one magic moment, the system returned very nearly to its original starting point, once again having almost all its energy in one mode. These scientists had discovered an almost integrable system—experimentally! By doing exploratory calculations in heretofore unexplored territory, they stumbled across some wonderful new science.

Berni Alder and his collaborator Tom Wainright, working at Livermore National Laboratory, displayed an amazing mastery of the molecular dynamics method. They were involved in not one but two great discoveries. They started by looking at the motion of hard spheres bouncing off one another. To everyone's amazement, in spite of the purely repulsive interactions, they saw a phase transition from a fluid state into a solid one.⁴ Surprise number two was that the motion of these hard spheres—indeed, of any colliding fluid particles—engenders persisting correlations.⁵ These “long time tails” remained a perplexing mystery for a long time, but now they are pretty well understood to be a consequence of the hydrodynamic motion of the fluid as it flows past its own molecules.

Chaotic behavior, now characterized as sensitive dependence on initial conditions (or the “butterfly effect”) was discovered “accidentally” by Edward Lorenz⁶ while working with an early and very primitive program for solving linked sets of ordinary differential equations. It is said that one day the computer prematurely aborted a half-completed and recorded run. Lorenz went back and punched in the numbers corresponding (at least in their first few digits) to the results the computer used on the previous day. To his amazement and our subsequent edification, the resulting run was entirely different. The high-order digits mattered—a lot—and chaos was discovered.

My last “great” example comes from Los Alamos National Laboratory.⁷ Mitchell Feigenbaum was using a not-very-fancy desk calculator to study the properties of models previously investigated by Ulam. The calculator took a number, squared it, formed a linear combination from the square and some fixed coefficients, and generated a new number. Feigenbaum and his trusty computer carried on that simple process through many steps, and patterns emerged—wonderful, unexpected patterns—that showed how systems even simpler than Lorenz's could become “just a little bit” chaotic. An exciting little world unexpectedly opened up.

In all these examples, the scientists involved discovered and explored entirely new pieces of science. In the Monte Carlo case, the novelty was in using a new kind of computer algorithm with new conceptualizations of possible computations. In the other cases, a highly simplified model combined with a new kind of hardware or calculational technique permitted the first scientific investigation of new domains of physics. These researchers discovered new scales of length or time: long-term recurrence or long-range order. They found new scientific ideas that were general and applicable to a broad range of systems. Subsequent experiment, theory, and simulation has delved into each of these ideas in great detail and taken them much further.

Good Recent Examples

We may suspect that the heroic age has passed. The nature of discoveries is somewhat different now. Recent examples illustrate some of the best things computational people are now doing.

One of the best pieces of science done in recent years is the discovery of neutrino mass and neutrino oscillations. The first hint of this major discovery came from a discrepancy between the

flux of neutrinos from the Sun (measured by Ray Davis and others) and the flux of solar reactions and activity predicted by computer models.⁸ For the discrepancy to be taken seriously, one had to believe in the accuracy and reliability of the solar models. It was persuasive that extremely competent people had conducted the experiments, and believed in their results. Another persuasive factor was an observational program seeking additional tests for the models. These models were verified by comparing them with seismographic data recording wave activity within the sun. The seismographic predictions of the models fit the observations. With this increased credibility of the models, the original discrepancy in neutrino fluxes was seen to be a serious problem. Something had to give. Eventually, the part of the picture concerned with elementary particle physics had to be modified. The then-accepted theory assumed that neutrinos have zero mass, but this idea was abandoned to fit the solar data. Later observations have supported this change.

This big discovery was made by the experimentalists who observed and counted neutrinos. Major credit also went to the theorists who held the scientific program together, particularly John Bahcall. The computer-model builders were a third, and quite essential, part of the enterprise. All together, these investigations produced a major unexpected advance in our understanding of the fundamentals of the universe.

Another interesting recent example involves a problem called *single-bubble sonoluminescence*. This phrase describes a situation in which a resonant acoustic field forms a bubble and excites it strongly enough so that the bubble emits light and becomes visible.⁹ Here, once again, experimentalists made the major discoveries and started a pro-

New Feature Section: Perspectives in Computational Science

Computational science is beginning to play an important role in scientific research and development. Modern scientific research—originally grounded in experiment and its theoretical interpretation—is increasingly moving toward becoming a triad of experiment, theory, and computer simulation. This is because the analysis of simulations of complicated systems can be a portal to discovery of important but hitherto unnoticed simplifications and regularities. Computational tools play an important role in the design and testing of new engineering products, and simulation results form part of the basis for many policy decisions. Yet, computational science is not nearly as mature as experimental, theoretical, or engineering science.

The editors of *Computing in Science & Engineering* have established a new feature section we call Perspectives in Computational Science to encourage consideration and discussion of the issues that our field must address on the road to maturity. We will feature invited papers by senior scientists and engineers to share their perspectives on our field. The very positive response to the May/June 2002 article by Robert Laughlin, “The Physical Basis of Computability,” helped us realize the potential utility of this new feature section.

—Douglass Post, Associate Editor in Chief

gram of work in the area. By 1997, they set out the values of some of the most important parameters describing the system. As this understanding of the subject developed, simulations were performed and closely tied to theoretical and experimental work. Thanks to these simulations, very many of the proposed steps and advances were looked at, checked, and more deeply understood.

In this example, simulations played a major integrating role but never led the advances in the field. I would judge that this is the common role for simulation in “tabletop” science. I expect this example will serve as a paradigm for future investigations: a scientific or technical problem involving many branches of science will be largely understood through the interlinked efforts of many investigators who often use simulations to check their arguments.

My third example is drawn from computer simulations cosmology of the early universe.¹⁰ Our colleagues working in this area have a hard task. Experiments are impossible. They can only observe—never manipulate—their system. They are much further away from their system, in both space and time, than are the solar physicists, so even their observational data are quite limited in scope. For this reason, they must be more dependent on simulations than researchers in most other branches of science. Cosmologists construct entire universes—intended to be reasonably realistic—within their computers. They

start from dark matter and baryons and then observe the model bringing together clusters. Step by step, the computers make objects on many scales, down to the size of galaxies. But can these constructed universes give real insight into the processes involved?

One might worry that the model-making gives too much freedom, that simulators will always be able to fit the known facts with a wide variety of schemes. The simulators disagree. Bertschinger states that the “main use [of the calculations] has been and continues to be the testing of the viability of cosmological models of structure formation.”¹⁰ The work takes the theoretical conceptions of the field, casts them into the form of specific models, and then runs them. Many models simply blow up, yielding nothing sensible. The remaining ones give well-defined results that can be analyzed to see whether they agree with observations. Many models fail at this stage.

In the long run, the simulators hope to strain out all but the one correct physical model for the development process. This filtering is a brave goal that the participants believe they can achieve. I cannot tell whether they’re being too optimistic. At the moment, several different models apparently work quite well: “Recent high-resolutions simulations compare remarkably well with many aspects of the observed galaxy distribution.”¹⁰

In all three of these recent examples, simulation’s role was to work with theory, observation, and experiment—essentially, to serve as a cross-check on the

other models and thereby increase the investigators’ confidence that they understood phenomena that were not otherwise open to observation. In the solar neutrino example, simulations made the investigators confident that they understood solar behavior and thus could locate an error in previous assumptions about neutrinos. In the sonoluminescence case, simulations were a necessary part of putting together an intricate puzzle. The early universe investigators hope and expect to weed out incorrect mechanisms and theories by carefully testing their consequences and comparing them with current observations about the universe. In each case, simulation works by being part of a carefully constructed program of activity.

Not So Good: Optimization of Enthusiasm and Misjudgment

Recently, a provocative and controversial experiment conducted at Oak Ridge suggested that fusion was occurring in deuterated acetone via a process involving resonance excitation of bubbles. The reporting paper involved both experimental work and computer simulations.¹¹ “[A] roughly ten-fold increase in the external driving pressure was used in the calculations” beyond the pressure directly produced by the experimental situation “to approximately account for the effect of pressure intensification within the imploding bubble clusters.” As a result, their “[h]ydrodynamic shock code simulation supported the observed

data.” It is remarkable that the referee process for such a high-visibility paper allowed an apparently uncontrolled approximation in a key step in the computer calculation. Subsequent work¹² seemed to disprove Oak Ridge’s experimental result, but that is not the point. Because of the “roughly ten-fold increase,” the simulation was sufficiently uncontrolled so that it neither supported nor could refute the experiment. Neither the authors nor the editors should have permitted it to be published.

This example makes one ask what kind of quality control is appropriate for a computer calculation used to check a controversial experimental result. This problem is broader than just one paper. The whole early history of single-bubble sonoluminescence required step-by-step work to eliminate provocative but incorrect mechanisms. For example, a set of early experiments by Barber and his colleagues¹³ reported very short widths for the emitted pulse of light. This short width opened the door to novel mechanisms for explaining the emitted light’s total intensity. Later developments suggested that the short pulse width was a misstep by the experimentalists. In contrast to the excellent work in sonoluminescence in the post-1997 period, this misstep led simulators and theorists quite astray. A host of incorrect speculations and mechanisms ran through the field, intended to explain the “observed” behavior.

Despite one essentially correct simulation,¹⁴ the pre-1997 simulations¹⁵ did almost nothing to weed out these incorrect discussions, undercutting the hope that simulations might provide a good tool for such a purpose. (Note that this weeding was one of the main goals of the astrophysical modeling.) Instead, the speculations continued unhindered until an experiment by Gompf and his colleagues¹⁶ showed that the pulse width

was much longer than previously believed, which implied a lower temperature for the emitting drop. After this, attention turned away from the incorrect mechanisms so that theory, experiment, and simulation could produce a consensus about what was actually happening.

(There were technical reasons for the failures of the simulations. For example, the earliest simulations¹⁷ used a zero-viscosity code in which heat conduction was also neglected. These codes underestimated the damping mechanisms and hence produced a very strong shock, which would, in the approximations used by the investigators, produce an infinitely high temperature.¹⁸ Later simulations by Vuong and Szeri¹⁴ cast doubt on the relevance of shocks to the observed behavior of sonoluminescence. However, the field did not turn around until new experimental results caught people’s attention.)

The examples of the Oak Ridge paper and some of the earlier sonoluminescence simulations suggest that the models might have been directed toward the wrong goals. Rather than being used in the process of checking, critiquing, and eliminating incorrect possibilities, they were apparently used to support and exemplify the presumptions of the scientists involved. A program of modeling should either elucidate new processes or identify wrong directions. Otherwise, there is no point in performing it.

Another example, which might be entirely mythical, involves a transportation investment model reportedly put together in Britain with the goal of getting the best transportation system while minimizing public spending. The model involved a broad mix of roads, rail, and public improvements; the aim was an overall maximization of benefits, taking into account public spending and the value of time saved. All costs and benefits were converted

into pounds, and an overall optimization was sought and achieved.

The next step was to bring in an outside group of experts to study the model’s recommendations and build a plan for implementing them. This group noticed several apparent anomalies. The strangest, according to the story, was the elimination of all spending for improving pedestrian crossings. This result was considered peculiar, especially since the value of pedestrian time saved was included in the model. A careful look explained how the conclusion was reached: the decreased spending had the effect of increasing accidents at the crossings. According to experience, and also the model, the major result would be increased deaths among older pedestrians, thus spending on pensions would be reduced. The model counted this outcome as a benefit.

The government that paid for the modeling was not amused. (An apparently less mythical recent example concerned an American cigarette company and the Czech government. The government was advised to support cigarette advertising since the early deaths thereby caused would have a beneficial effect on pension spending. Apparently no computer model was needed to reach this conclusion.)

This outcome brings us to a moral: The transportation study failed because the modeling was done too mechanically, without enough thinking about either the actual processes going on or the actual goals of the sponsors. The modelers did not realize that the design goals were actually multidimensional. Modeling efforts should include theory and common sense. The two examples relating to bubbles have a different moral: In those cases, the simulations, both the several wrong ones and even the essentially correct simulation of Vuong and Szeri,¹⁴ did not effectively

refute the incorrect experiments. Instead, the simulations were effectively trumped by experiments, which the community judged to be decisive.

Present Challenges

In this section, I shall describe some work involving simulations in which I have played some role.

Convective Turbulence

In Rayleigh-Bénard flow, a fluid is placed in a box, heated from below and cooled from above. A parameter, called the Rayleigh number gives a dimensionless measure of the heating's strength: the higher the Rayleigh number, the more turbulent the system. To compare with other turbulent systems, one might say that the Rayleigh number is roughly the square of the Reynolds number or the fourth power of the Taylor-Reynolds number.

A little heating of the system from below causes no motion of fluid. However, with increased heating and increased Rayleigh numbers, we see first motion and then chaos. At Rayleigh numbers above roughly 10^8 , turbulent flows and structures form (see Figure 1). As the cartoon in Figure 2 shows, the heated box contains many structures, including plumes, waves, and jets.¹⁹ How far are we from examining this experimental behavior in computer simulations?

Good simulations exist, in both two and three dimensions, but the three-dimensional simulations do not resolve the structures seen in experiments, which reliably reach Rayleigh numbers as high as 10^{14} . Simulations hardly go beyond 10^{12} because of limitations in resolution and computer time. Theory suggests phase transitions—qualitative changes in behavior—at roughly 10^8 , 10^{11} , and 10^{19} . Theorists are unsure of what will happen, and consider a large range of possibilities. Simulations can-

not hope to reach directly into the domains touched by theory and experiment. Nonetheless, we are beginning to learn how to use theoretical ideas to extrapolate simulation results from lower Rayleigh numbers to higher ones. The simulations provide detailed information to help us see what is really happening in much more detail than experiments can currently provide. The high Rayleigh number experiments' data generation is limited by the design, manufacture, and placement of delicate and tiny temperature-measuring devices and by the difficulty of assuring uniform heat transfer into the cell.

One recent example is a simulation by Marcus Brüggén and Christian Kalser describing a hot bubble toward the center of a galaxy (see Figure 3).²⁰ Because we cannot see into the galactic center, this bubble can only be "observed" via computer simulation. Nevertheless, the authors appear confident that they have caught some of the essential features of heat transfer in this region.

Table 1 compares what we might gain from experiment and what we might gain from simulation. Clearly, both are necessary. In the first four rows, experiment does better because it runs longer and with more extreme flows, more repetitions, and hence more flexibility. Experimentalists can measure few things, relatively imprecisely, in hard-to-control situations, but they cannot change the initial data just a little and run again.

Theory is also required to extrapolate a simulation's result into a physically interesting situation. More broadly, theory is required for simulators to

- assess algorithm reliability,
- make better algorithms, and
- help define what is worth "measuring."

Theorists also help bring it all together—recall the work of Oppen-



Figure 1. A shadowgraph showing the spatial distribution of thermal plumes in a Rayleigh-Bénard cell. The fluid is dipropylene glycol, which has a rather high viscosity (Prandtl number = 596), so the pattern of plumes appears in a simplified form. The Rayleigh number is 6.8×10^8 . (The picture was taken by S. Lam in Keqing Xia's laboratory and is part of a joint project with Penger Tong.)

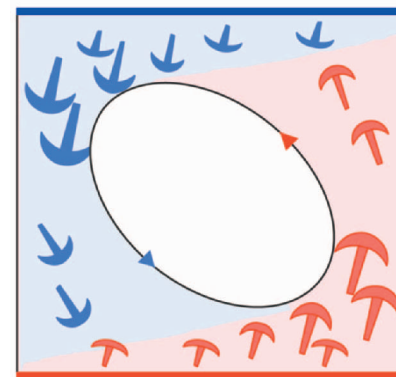


Figure 2. Cartoon view of the central region of a box, a mixing zone containing plumes, and very thin boundary layers at top and bottom. The plumes are believed to arise from the spray thrown up by waves traveling across the boundary layer.¹⁹

heimer, Teller, and Bahcall. Ideally, scientists would do it all, much like Leonardo da Vinci or Enrico Fermi. But usually, different people have different specialized skills. To solve hard problems, all the various kinds of scientific skills must work together and, in the end, pull in the same direction.

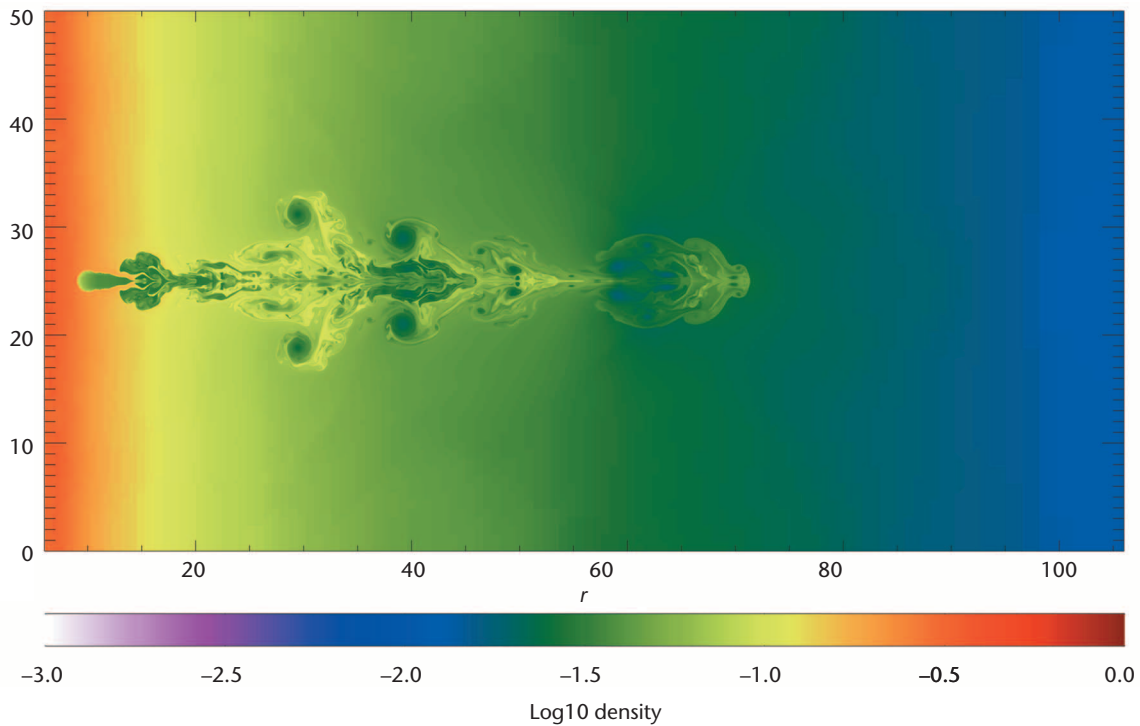


Figure 3. A simulation describing a hot bubble rising from the center of a galaxy. In these pictures, gravity points toward the left. The simulations describe two-dimensional flow with zero viscosity and zero thermal conductivity. The color-coding describes density.

Table 1. How experiment and simulation complement one another.

Quantity	Simulation	Experiment
Turnovers	Five or 10	Thousands
Ra	Up to 10^{11}	Up to 10^{14}
Runs	Few and costly	Many
Flexibility	Low	High
Measure	Anything	Very few things
Precision	Often very high	Variable
Equations	Well known	Often unknown
Small variation in initial data	Easy	Impossible

Jets and Sprays

We shall look at dielectric and conducting fluids moved by an electric field, based on an experiment.

Lene Oddershede and Sidney Nagel’s experimental work starts with oil floating on water (see Figure 4).²¹ They apply a strong electric field, with the regions of strongest field strength near the curved electrode sitting in the oil. The lower fluid, the one with the higher dielectric constant, is pulled upward toward the stronger electric field. Thus, in Figure 4’s first few panels, we see that the water forms itself into a bump.

Here is a nice, simple problem that

we could use as an exercise in a simulation partial differential equations course. The flow looks simple and easy to understand, but in the real world, surprises are possible, even likely (see the last few panels in Figure 4). After a time, the water bump forms itself into a sharp point. Then, starting from the point, something starts moving through the oil. In the next to last frame, that motion resolves itself into a jet of charged fluid. In the final frame, the fluid breaks up into many tiny droplets.

Complex systems sometimes show qualitative changes in their behavior—for instance, if our bump has turned into

lightning and rain. Now our simple problem has developed new phenomena and new scales. Experiment is very good at finding unexpected behavior and describing its overall characteristics; theory often can explain what’s going on. After an appropriate pause for algorithm development, simulations then can test the ideas and fill in the details.

Recently, my student Moses Hohman established the basic mechanism for rain production by doing a simulation investigating the linear stability (in this case, instability) analysis of a charged jet. Working with Michael Brenner, M. Shin, and G.C. Rutledge, he looked for and saw a whipping instability in the motion. This instability produces a turning motion, much like that of a corkscrew; the drops are presumed to be thrown off by the spinning.

In a parallel effort, my student Cheng Yang has looked at the process of singularity formation in the interface between two unlike dielectric fluids in motion in an electric field. He was looking for the structure formed very near the singularity, but he found a surprise—a result

contrary to our initial presupposition. From the previous literature, especially the work of G.I. Taylor, I expected to see the formation of a static cone-like structure that could have a persistent existence in the electric field. Yang actually found a transient dynamical conical structure, which formed for an instant and then broke up (see Figure 5).²² As his thesis adviser, I'm more than slightly proud that his simulation found something unexpected, and that he stuck to his guns long enough to convince his thesis committee that this result was both surprising and correct. So often, simulations only yield what was desired from the beginning.

The Rayleigh-Taylor Instability

The Rayleigh-Taylor instability has been an important focus of recent work, especially within the ASCI program. The instability can arise whenever a heavier fluid sits on top of a lighter one. If the interface between the two remains horizontal, nothing happens, but a wrinkling of the surface can produce a cascade of changes in which jets and plumes of the heavier fluid penetrate into the lighter one and vice versa.

Some experimental studies of this situation have been performed. For administrative reasons, a decision was made early in the ASCI programs to concentrate on simulations—with only minor input from experiment. Recently, this unbalanced approach's weakness was recognized, resulting in plans for an increased emphasis on experiment. Unfortunately, the earlier, unbalanced style has affected some of the Rayleigh-Taylor work.

Many important simulations of the Rayleigh-Taylor system have been performed. To see the fully developed instability, some major simplifications of the physical model are required. Because ASCI is interested in large

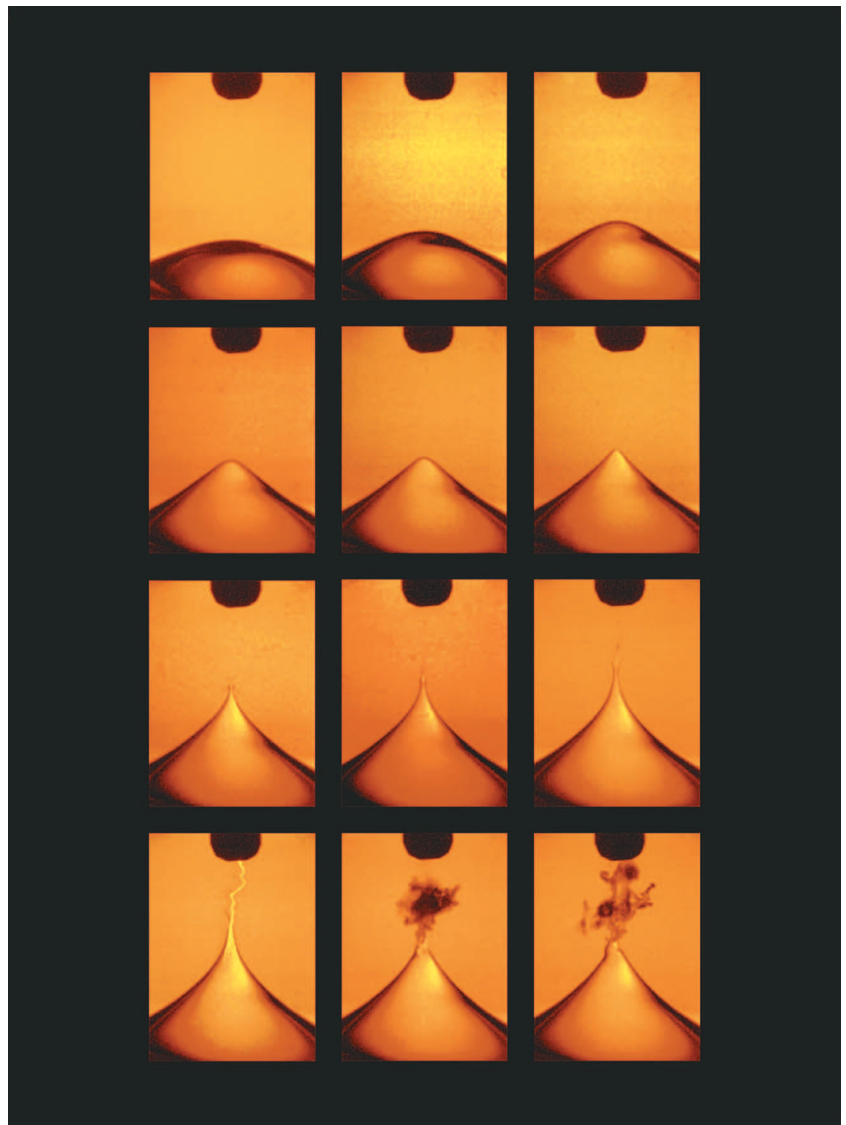


Figure 4. The experimental²¹ production of a singularity at the onset of an electrohydrodynamic spout. Two fluids, oil (above) and water (below), are separated by an interface. A strong electric field points into the electrode shown at the top of each frame. This field carries the water, with its higher dielectric constant, upward into the region of a strong electric field. Eventually, the interface comes to a point and breaks down. A discharge is produced and generates many small droplets of water in the oil.

Reynolds numbers, viscosity is usually neglected in the simulations. Furthermore, to maximize the effect of the instability, you have to neglect the surface tension in the interface between the fluids. These choices have been made to speed up the simulation, and they do so. However, the problem that remains is technically “ill posed:” we cannot prove that it is mathematically meaningful.

The practical meaning is that we cannot promise different approximation approaches will converge to the same answer, and that any one of those will correspond to the experimental system.

The outcome has been, to say the least, quite interesting. A group of studies has been put together—all aiming to measure the degree of penetration of one fluid into another.²³ The

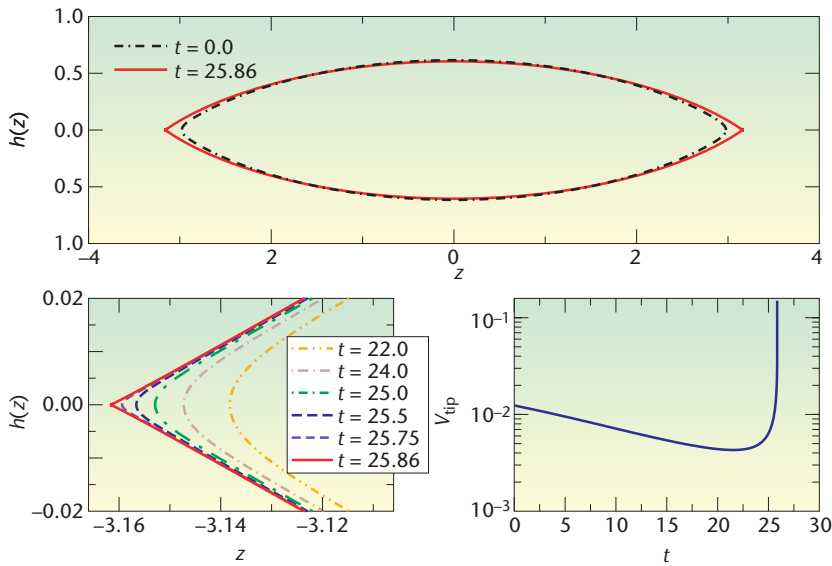


Figure 5. Computer simulation²² of a singularity in a situation in which two fluids with different dielectric constants are separated by an interface. The electric field generates polarization, producing forces on the drop’s surface. Surface tension provides additional forces. The first frame shows the drop’s initial and final shapes. Originally, it had an ellipsoidal shape; after a time, the drop develops cone-like points on the ends. The second frame shows how the cone gradually sharpens. The final frame shows that there is indeed a singularity—the tip’s velocity diverges at a critical time.

penetration is determined in terms of a coefficient called α , which measures the extent of the mixing zone relative to a purely ballistic motion of the fluids. An experiment measuring this quantity has been compared to half a dozen different groups’ simulations, all starting from identical initial conditions. The results fall into two groups. The experiment,²⁴ the theory,²⁵ and one of the simulations²⁶ show an α -value of roughly 0.06; the other simulations give α of the order of 0.03 or less (see Figure 6). Another study²³ takes a different tack by looking at a single penetrating region and using periodic boundary conditions (see Figure 7). Note that the flow is extremely complex and quite sensitively dependent on the computational resolution. If we take the generated pictures at their face value, we would conclude that the shape of the interface given by the simulation would never converge. On the other hand, there is some indication of convergence of the value of α . We still don’t know if the approxima-

tion of zero surface tension and viscosity make any sense, or if the value of α obtained in this way is meaningful.

To drive this point home, let’s look at one more example. Figure 8 shows four calculations of the mixing of the spray produced by a breaking wave.²⁷ All four describe the same, ill-posed problem: wave motion without surface tension or viscosity. All four start from the same initial data, and all four have the same value of the “wind” driving the wave. The only differences are in calculational resolution—and in the answers. The patterns of spray look quite different. The graph on the lower right shows not only that the measured amount of mixing depends on resolution but also that it’s a non-monotonic function of the resolution. In short, much more work will be required before we can, with full reliability, estimate the mixing from this calculational method.

The problems with these calculations illustrate the well-known fact that finding a valid answer from a computer

simulation can be a matter of some subtlety. For example, the calculation in Figure 3 has a range of validity that must be regarded as unknown because the numerical method must still be regarded as unproven. The calculation describes events at the center of a galaxy. We are interested in having an accurate picture of what goes on there, but we can afford to wait for the further scientific developments that should tell us more about the accuracy of the calculational method. In other cases, however, we may need accurate answers to questions involving highly turbulent flows. Unfortunately, we have no proven way of getting them.

To maintain a national capacity for understanding the development of complexity and multiscale phenomena, we should support first principles studies of a variety of different complex systems. Each such study requires a balanced and interdisciplinary program of research in which theory, simulation, and experiment work together to ask and answer incisively posed questions.


The goal of my group’s research at Chicago is to ask important questions about the world. We solve simple model problems, like those I’ve discussed here, and then ask questions like

- How does complexity arise? Why is chaos often observed?
- What dramatic events occur in the fluid? Are they commonplace?
- Why do fluids naturally form structures?

A parallel goal is to teach students to ask incisive questions. These are good problems for students because they are small enough to be solved quickly. They are also down-to-earth enough

so that each student can appreciate what they're about.

In the world outside of schools, we simulators have an important role to play as part of the teams within scientific and engineering groups devoted to understanding design and development. In the past, we have sometimes appeared in a supporting role, filling in the details in understandings constructed by others. We may wish to be more incisive, pointing out where the design won't work, how the theory won't hold water, or why the experiment is wrongly interpreted. We also may wish to be more creative, using our simulations to point the way to overall understanding or good design. Only if we are both more creative and more critical can we expect our work to be evaluated and tested by the hands-on and the pencil-and-paper people who also form a part of our scientific and engineering world. Such a give-and-take approach forms the basis of good design and understanding.

Conversely, if our work only justifies and explains the work done by designers and experimentalists, if we simulators never say that the other guys are dead wrong, then we deserve a situation in which simulation is relegated to the position of a third and lesser branch of science, considerably behind experiment and theory. 

Acknowledgments

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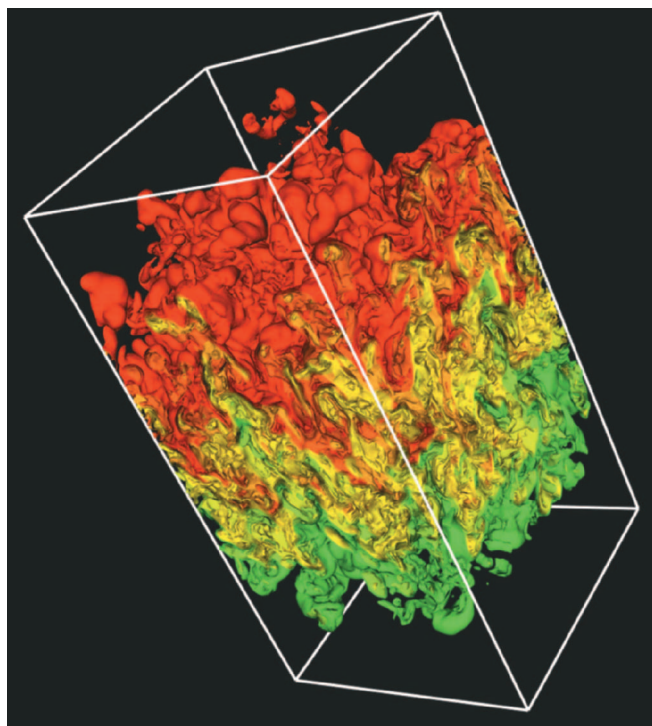


Figure 6. The Rayleigh-Taylor instability. The initial state was a gently wavy interface separating a high-density fluid from a low-density one. Gravity (pointing up!) then destabilizes the interface, producing the mixed regions shown. Unmixed regions are transparent. Red, yellow, and green show successively higher densities. This simulation assumes that both viscosity and surface tension are negligibly small.²³

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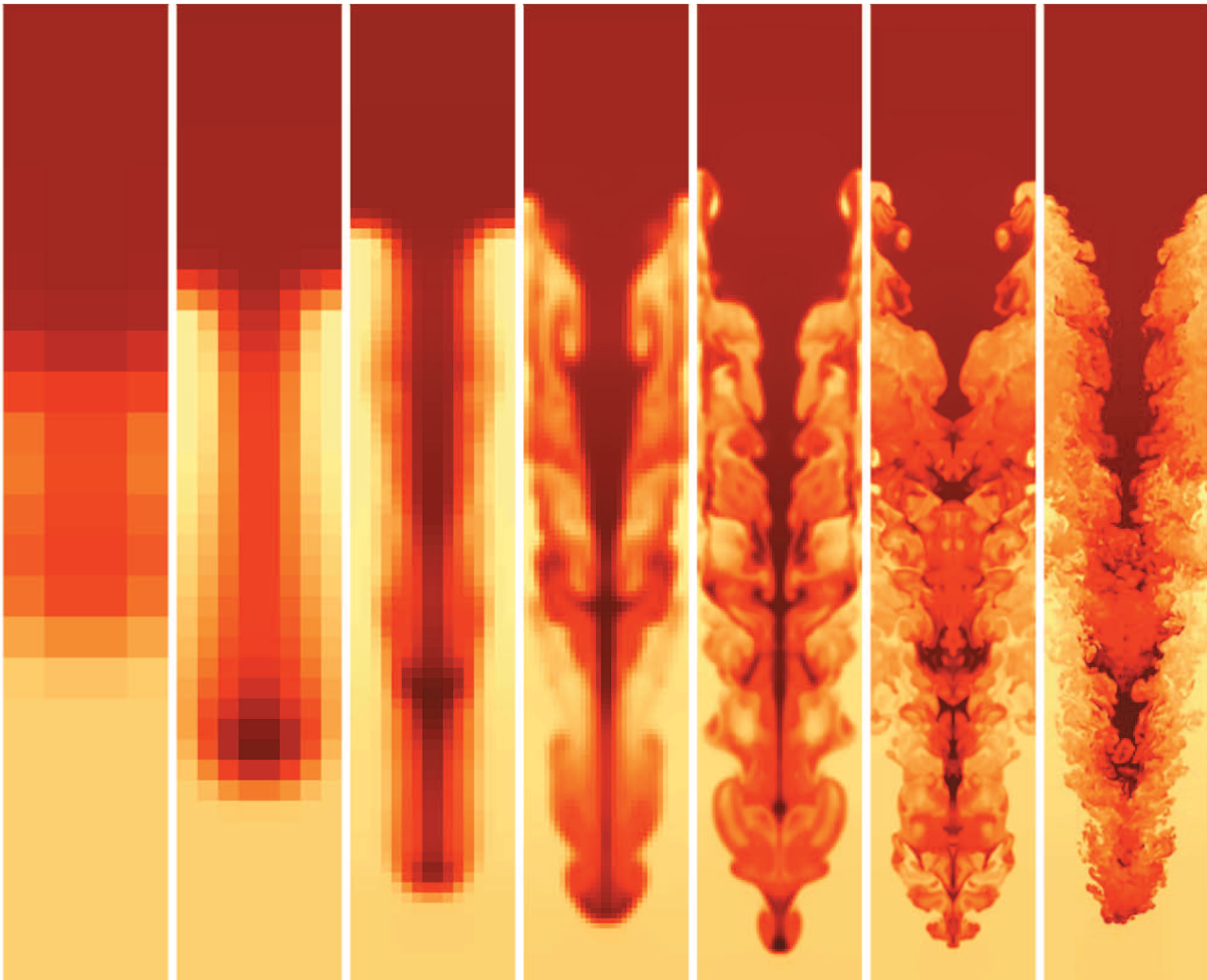


Figure 7. The Rayleigh-Taylor instability, once more. This calculation is done with a simple “one bump” initial state. The effect of resolution is studied by using resolutions differing by a factor of two in successive panels. Note how the results change considerably with resolution. The highest resolution picture is qualitatively different from the others in that the left-right symmetry is broken. (Figure courtesy of Alan Calder, and rather similar to ones appearing in reference 23.)

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Leo P. Kadanoff is the John D. and Catherine T. MacArthur Distinguished Service Professor of Physics and Mathematics, Emeritus, at the University of Chicago. He is also a member of the Committee on the History and Philosophy of Science at this same institution. He has made fundamental contributions to the fields of chaos, statistical, solid-state, and nonlinear theoretical and computational physics. His research has emphasized scaling and the universality particularly in dynamical problems and phase transitions. Contact him at LeoP@uchicago.edu.

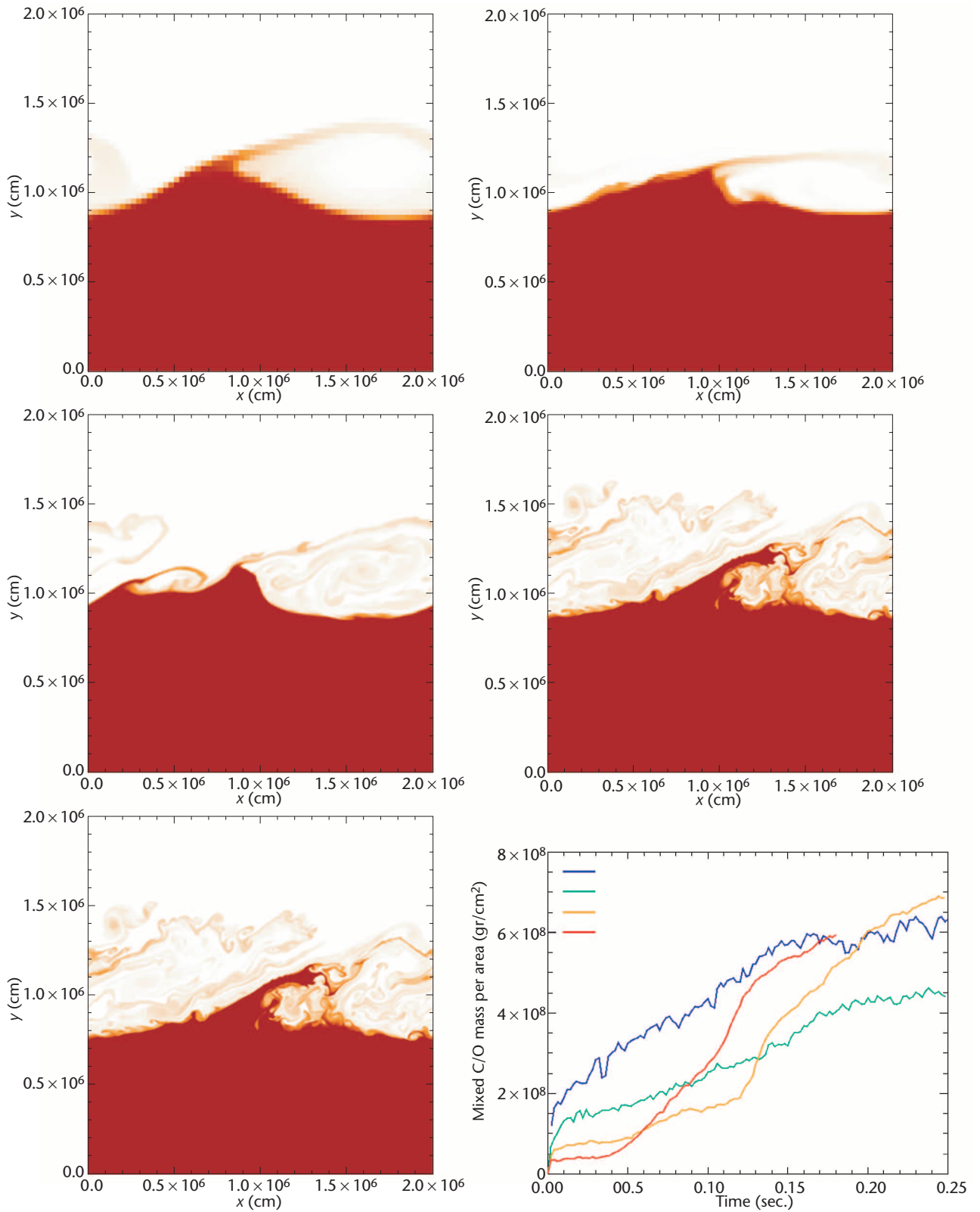


Figure 8. Wave breaking at a white dwarf surface. This figure shows the result of wind-driven instability on the surface of a star. Surface tension and viscosity are assumed to be negligibly small. The different panels show the same initial condition at the same time but the resolutions differ by a factor of two in neighboring panels. On the right, we see plots of mixing versus time for these different resolutions. The take-home message is that resolution matters both in the profile and also in the mixing. (Figure courtesy of Alan Calder; simulations by Alexandros Alexakis.)