The Good the Bad and the Awful-- Computer Simulation and Prediction

by

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Excellent computer simulations are done for a purpose. The most valid purposes are to explore uncharted territory, resolve a well-posed scientific or technical question, or to make a design choice. Often, one gets useful results from incompletely resolved situations or from computer programs of unknown accuracy. Programs such as these might suggest novel physical mechanisms and behaviors, and thus serve as starting points for larger technical investigations. Of course this kind of works needs a full integration of the modeling effort into a scientific or engineering effort.

Some excellent work, much of it done at Department of Energy Labs, is reviewed. Some less happy stories are recounted. An example of a supernovae calculation is traced in detail.

published version:
Leo P. Kadanoff: Excellence in Computer Simulation, Computers in Science and Engineering. March, April 2004.

Who am I ?

A theoretical physicist and mathematician working in part for ASCI-FLASH.

FLASH is a DOE weapons lab supported program intended to build interaction between the computer efforts at the labs and at the University. At Chicago, we work on building an understanding of novae and supernovae events, using in part large-scale computations

This is a talk about the role of computer simulations in science. The majority of the people at this meeting spend a major portion of their lives constructing and carrying out simulations aimed at advancing scientific knowledge. I do that using small computers, and in fact am proud to have worked with several of the speakers at this conference.

However for the large-scale computations in FLASH my role, is mostly to explain and criticize our efforts. Here it goes..... About Scientific Computing ... what it is good for and where it falls down

The Best: Great Discoveries of the Heroic period

- Alan Turing: Turing Machine, Code breaking, developmental biology
- Monte Carlo: Rosenbluth^2, Teller^2, Metropolis
- Molecular Dynamics: Alder & Wainright
- Fermi, Pasta, Ulam: Integrable Systems
- Ed Lorenz: Chaos in Simple Systems
- Ken Wilson: Renormalization, (Kondo Problem)
- Feigenbaum: Onset of Chaos
- Witten & Sander: Diffusion Limited Aggregation, an Algorithm for Fractals
- Martinus J.G. Veltman: Computer Algebra

Individual work often carried out without benefit of experiment.

Alan Turing: basic theoretical model of a computer. code breaker. morphogenesis.

a. Turing Machine-purely theoretical, conceptualization of computer

b. Enigma, put a "computer" to work in breaking German WWII codes.

c. Morphogenesis. Though out process by which instability could give birth to structure in embryonic development. Invented reaction-diffusion system. He conceptualized morphogenesis as a computer which produces structures and patterns.

Alder and Wainright: Long range Order in Hard Sphere gas; Long Time Tails

Berni Alder and his collaborator Tom Wainright displayed an amazing mastery of the molecular dynamics method. They were involved in not one but two great discoveries. They looked at the motion of hard spheres bouncing off one another. To everyone's amazement, despite the purely repulsive interactions, they nonetheless saw a phase transition from a fluid state into a solid one. Surprise number two is that these hard spheres, and indeed any colliding fluid particles, engender through their motion correlations which persist for a very long time. These "long time tails" remained a perplexing mystery for a long time, but now they are now pretty well understood as a consequence of the hydrodynamic motion of the fluid as it flows past the molecules within the fluid.

New territory yields new insights.

Tom Witten and Len Sander invented an algorithm "DLA" which produced fractal objects. (pictures of algorithm and result)

One of the first examples of a physical system being put forward as an algorithm. Question answered "How can you construct a fractal by a natural process?"

fractals akin to natural ones. picture picture

All these cases: New worlds explored. Highly simplified model permits first exploration. New ideas discovered and explored. Often individual work, not closely tied to group efforts.

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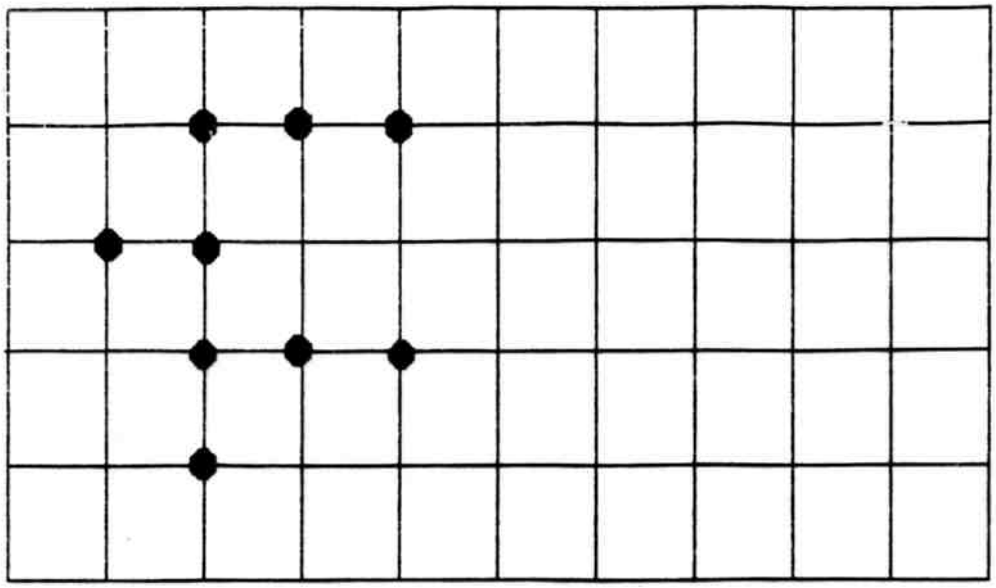
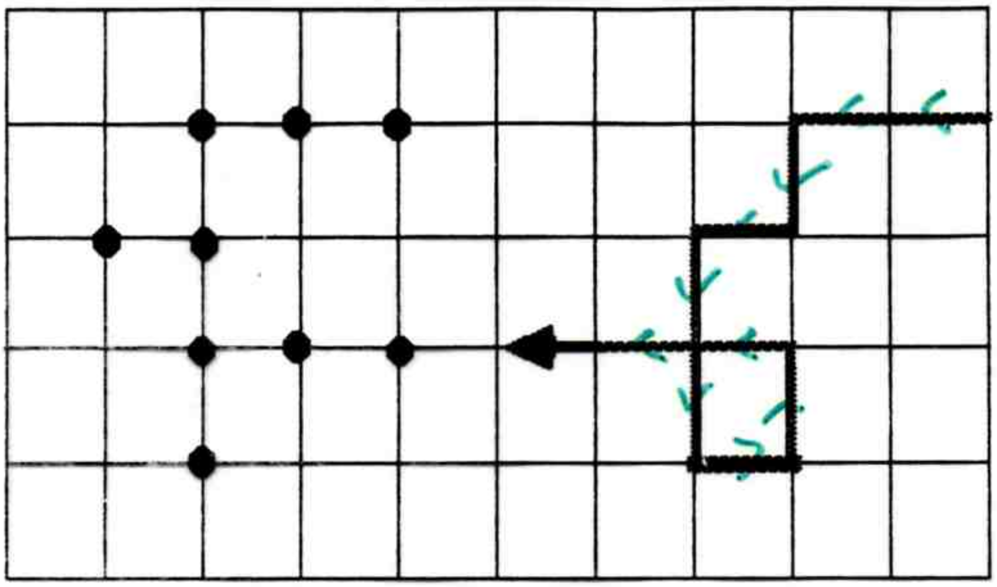
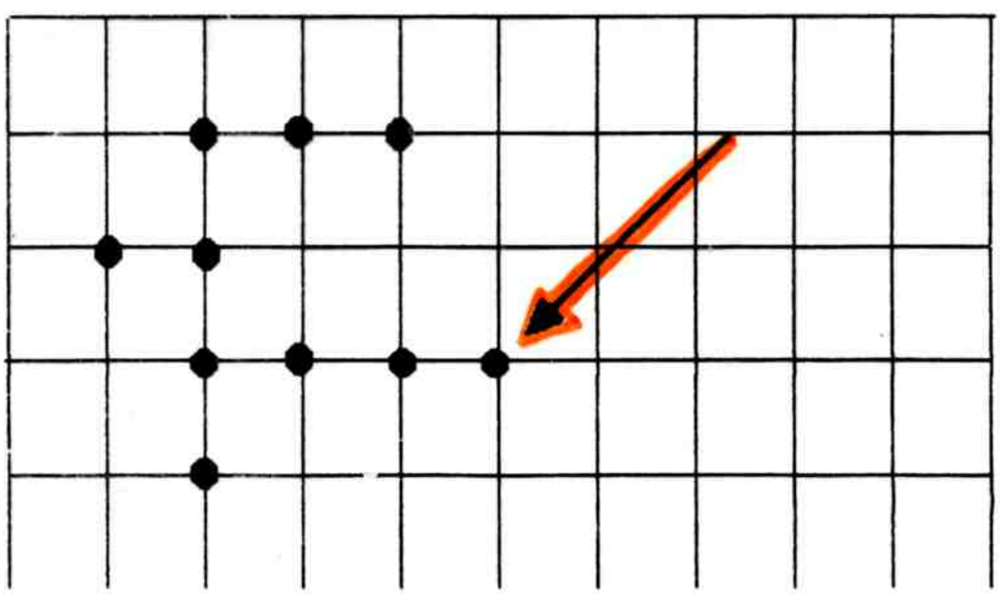


start with
aggregate
on grid.

introduce
random
walker



random walke
walks.
and hits
aggregate



aggregate gro
by one unit.

process start
again.

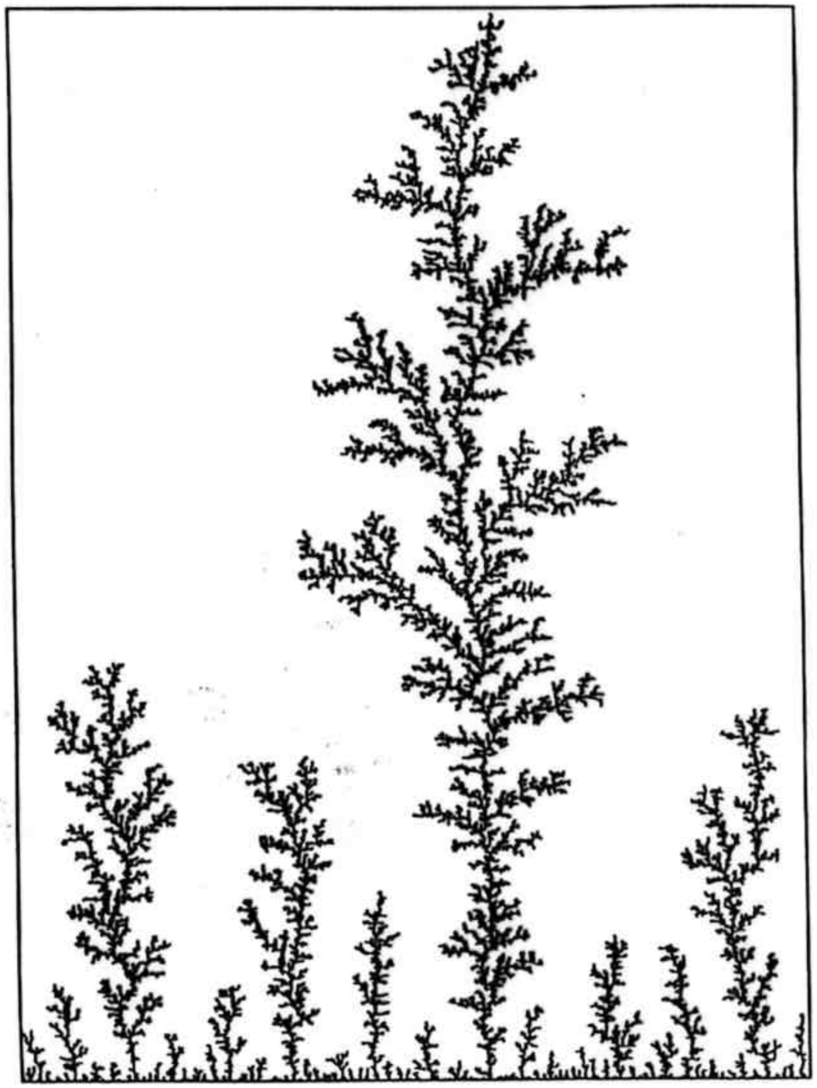


FIGURE 4.12: DLA growth from a line. The particles start on random walk trajectories from the top line and they are reflected from the side walls. The particles attach on contact to the bottom line and to trees connected to the bottom line. The baseline is 801 cells long, and the height of the longest finger is 1099. The number of particles is 47,348 (Hinrichsen et al., 1987).

FIGURE 4.13: Viscous (black) in a two-dimens beads 1 mm in diamete between transparent pla jected along a line show glycerol leaves the mod (Måløy et al., 1987c).

1. Models of Solar Processes

Ray Davis, John Bachall, and others. Experiments catch neutrinos from sun. Solar models predicts neutrino production. But, simulation gives result disagreeing with observation. Is it right? After some time, model is seen to give correct prediction of solar seismic data. Hence model is validated. Therefore people in field come to believe that there is a real disagreement between theory and observation. Eventually, new theory of neutrino is developed. Experiments confirm neutrinos predictions from theory and simulation.

Note integration of computer modeling into scientific program. John Bachall orchestrated melding of theoretical, simulational, and observational efforts. This integration is an essential part of the story.

Mechanism:

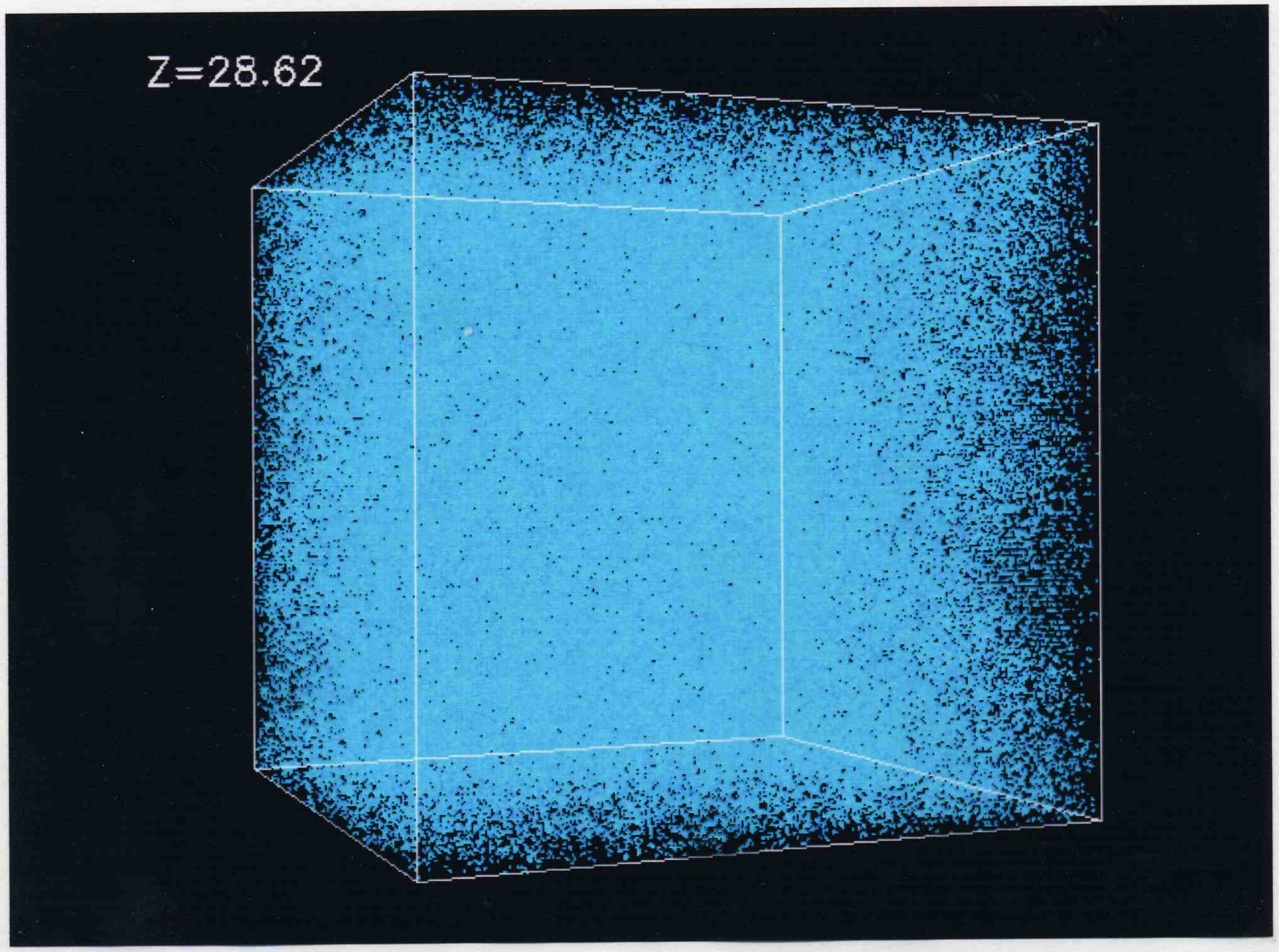
High temperatures, nuclear reactions in sun make neutrinos, which then travel to earth. Solar model describes stratification of different isotopes in sun and their reactions. Predicts neutrino flux here on earth, assuming neutrinos maintain their identity in their passage.

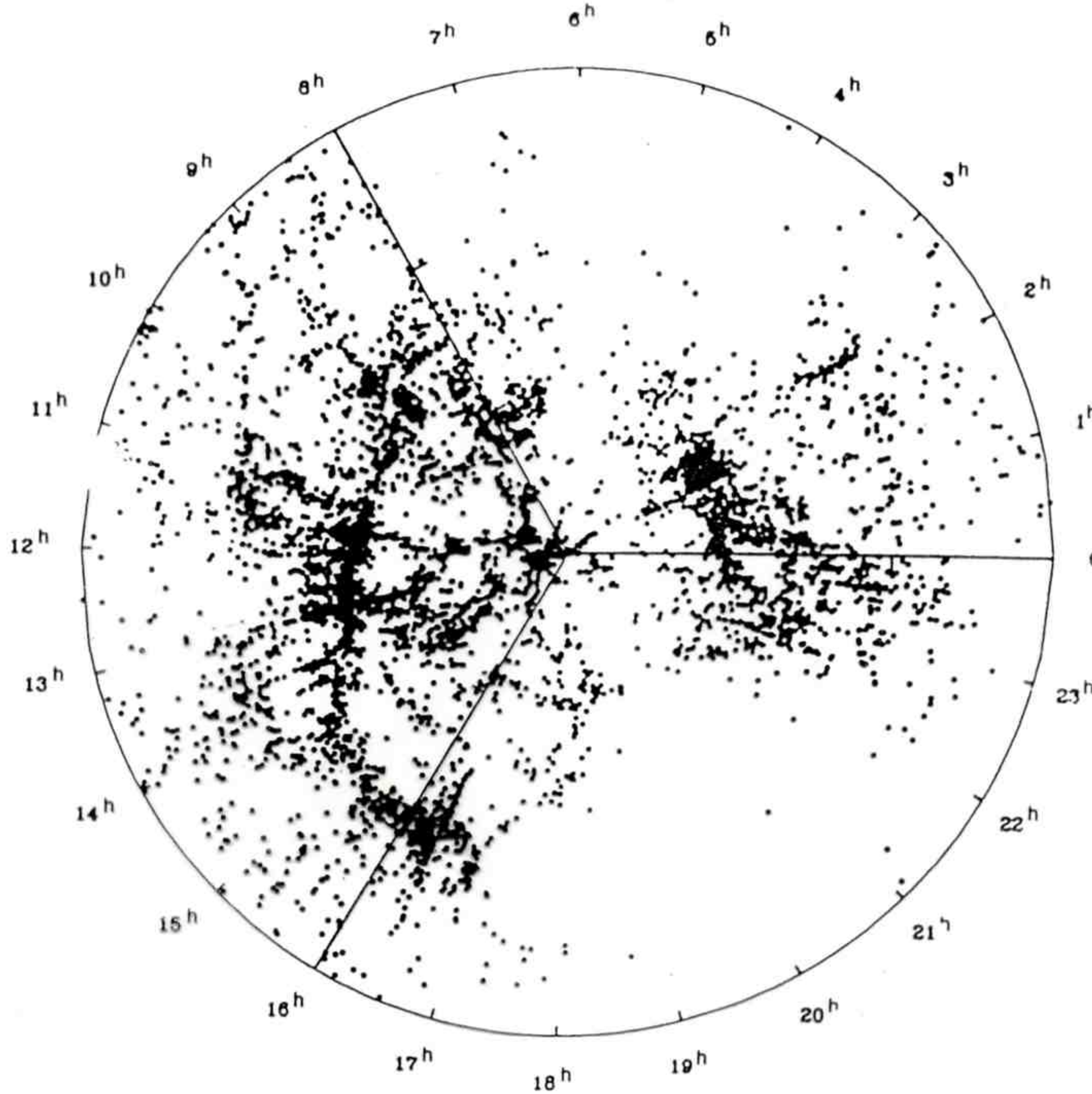
Formation of Structures in the Universe

Simulators have explored the early history of the Universe. Gravity produces instabilities which form fractal?! structures. Simulators follow these events (e.g. Andrey Kravtsov at Chicago.) Theory experiment and-simulations explore phenomena. Progress slowed by complexity of process, huge space of possibilities being explored. Considerable progress made. Some uniminity among investigators.

The hope is that an extensive process of simulation of a wide variety of models may eliminate all but but a few because the others give an answer which is absurd or inconsistent with observations. However in our postheroic period there are practically no examples of computer exploration of new territory, carfried out without the aid of observations and theory, giving information which is both new and correct. So, we can ask of the cosmolgical results

Are they right? And answer: We don't know.


Z=28.62



Maps of the galaxy distribution in the nearby universe reveal large coherent structures ...

– M. J. Geller and J .P. Huchra, Science **246**, 897 (1989)

The Worst

Britain's Transportation Investment Model.

Goal: To get the best transportation system and while minimizing public spending. Broad mix of roads, rail, public improvements. Overall maximization, all expressed in pounds sterling.

Conclusion: Detailed predictions and directions for public spending. Several peculiar features. For example, computer result recommends zero spending on pedestrian road crossings. That's strange because flow of pedestrian traffic is valued in model.

Explanation: Costs of social programs included in minimization. Pensions are a debit. Most people killed at road crossings are old, and the model gives them a negative value. Hence, maximization gives pedestrian safety a negative value.

Moral: Design Goals are usually multidimensional. All sensible modelers ask not only what comes out but also why did we get this outcome? Modeling efforts should include theory and common sense.

This case may be a myth, but ......An apparently less mythical recent example concerned an American cigarette company and the Czech government. The government was advised to support cigarette advertizing since the early deaths they would cause would have a beneficial effect on pension spending.

2. single bubble sonoluminescence

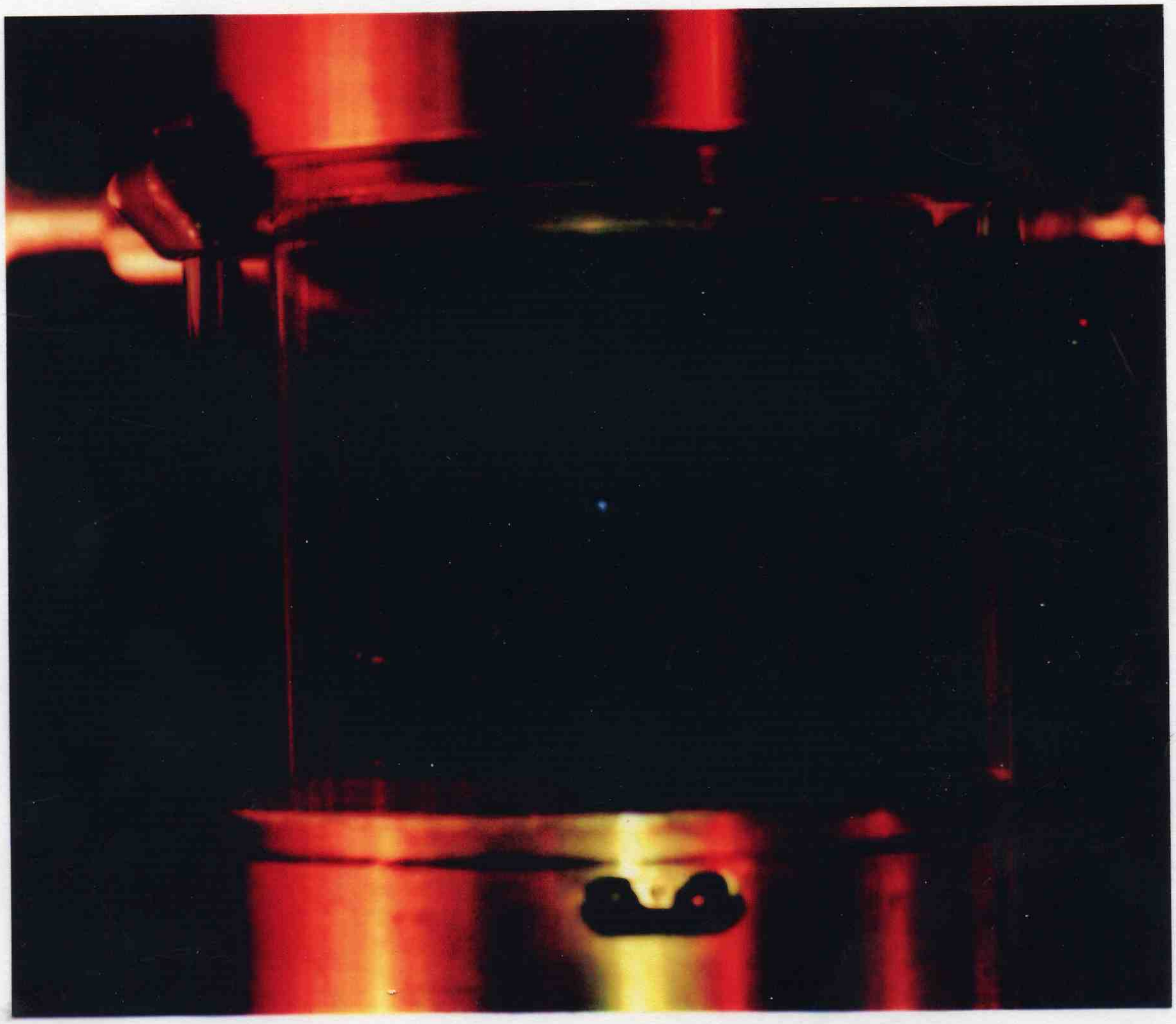
Experiments discover sonoluminescence in single bubble. Theory experiment and simulations explore phenomena. Progress slowed by complexity of process, huge space of possibilities being explored. Experiments measure length of light pulse. Good initial work.

Mechanism:

Sound waves produce pressure oscillations in fluid, shape of container focuses sound

Low pressure makes a bubble.

High pressure produces bubble collapse, concentration of energy, higher temperatures 10,000 or 100,000 degrees and light comes off.



Trouble Arises

However, early workers seem to have been misled, perhaps by their enthusiasm for novel energy sources. Early experiments suggested very short pulse width. Given the measured energy fluxes, these widths suggested very high temperatures and suggested the possibility of novel methods of generating energy, maybe even "fusion power". Early simulations left out viscosity and got shocks and very short pulse width. In fact, without viscosity the width of the shocks would only be limited by the resolution of the computation. A "better", i.e. more expensive, computation would give sharper shocks, shorter pulse width, and higher temperatures, hence suggest the possibility of novel power sources. So early simulations, even the best, led people in the wrong direction.

After Gomph (1997) measured pulse width correctly, simulators get better results (For summary see Lohse, Brenner, Hilgenfeldt in RMP 2002.)

But also see David Flannigan and Kenneth Suslick Nature 434, 52-55 (3 March 2005) which indicates two temperatures and a more complex story than the one I just told.

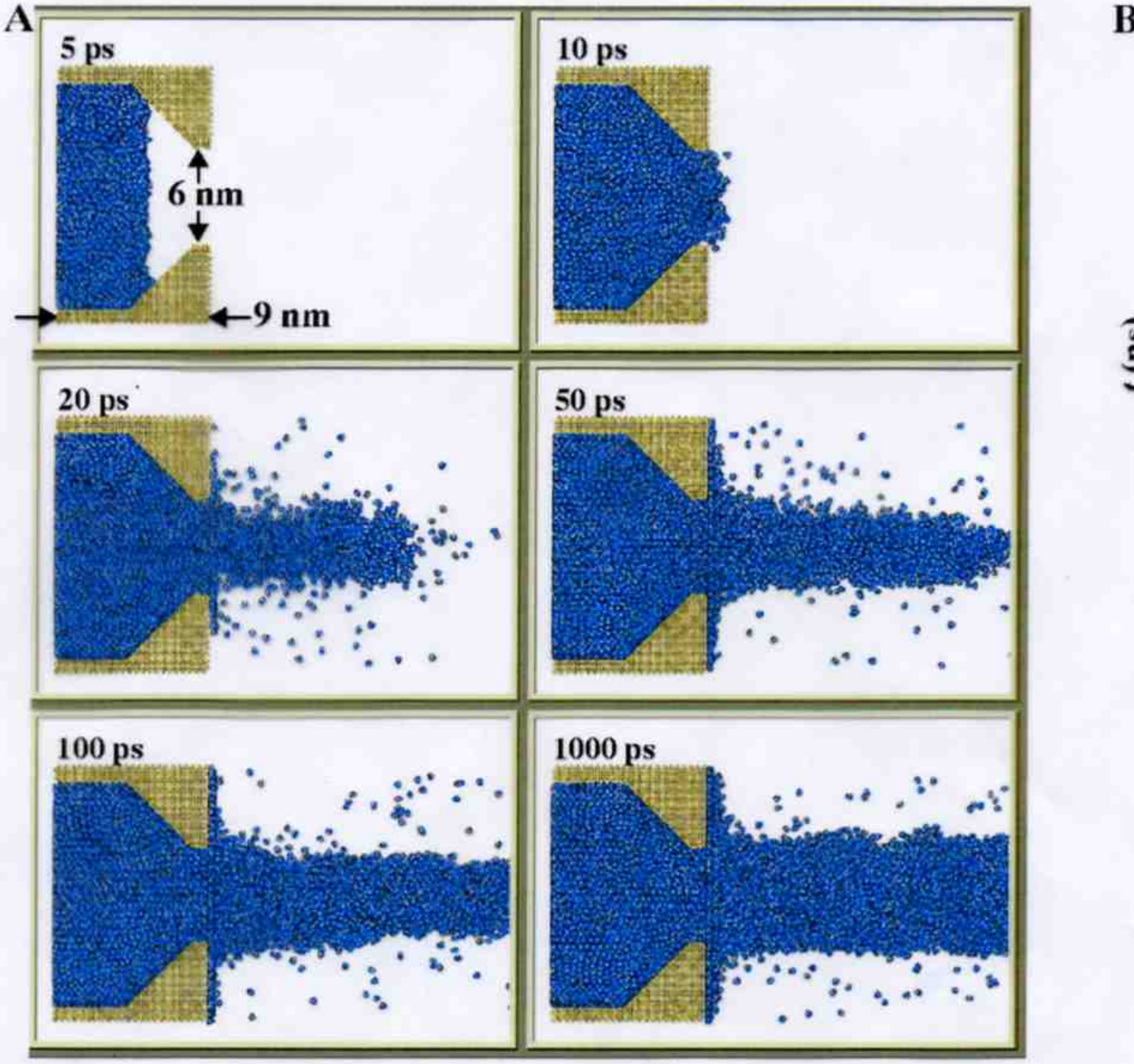
Cool Fusion

An experiment conducted at the U.S. Department of Energy Oak Ridge suggested that fusion was occurring in a system involving resonant absorption of sound in deuterated acetone. The paper, published in Science, involved both experimental work and computer simulations. "[A] roughly tenfold 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". The refereeing process allowed an apparently uncontrolled approximation in a key step in the computer calculation. One might ask what kind of quality control is appropriate for a computer calculation used to check a provocative experimental result. Apparently computer simulations require very little quality control, especially when the paper seems exciting and provocative to the editor, here D. Kennedy. A desire for exciting results led people to publish a computer calculation containing an uncontrolled calculation.

A program of modeling should either elucidate new processes or identify wrong directions. Otherwise there is no point is carrying it out. In many examples concerned with novel mechanisms for the concentration of energy, the simulations were quite pointless and played a somewhat negative role in the advance of the field.

It appeared that the simulations were performed to support a desired result, rather than ask "what is true?".

Question 1: Can one make a nano-jet?
Uzi Landman, Michael Moseler Science **289** 1165 (2000)



Answer: from these simulations the nano-jet described here can work, almost.

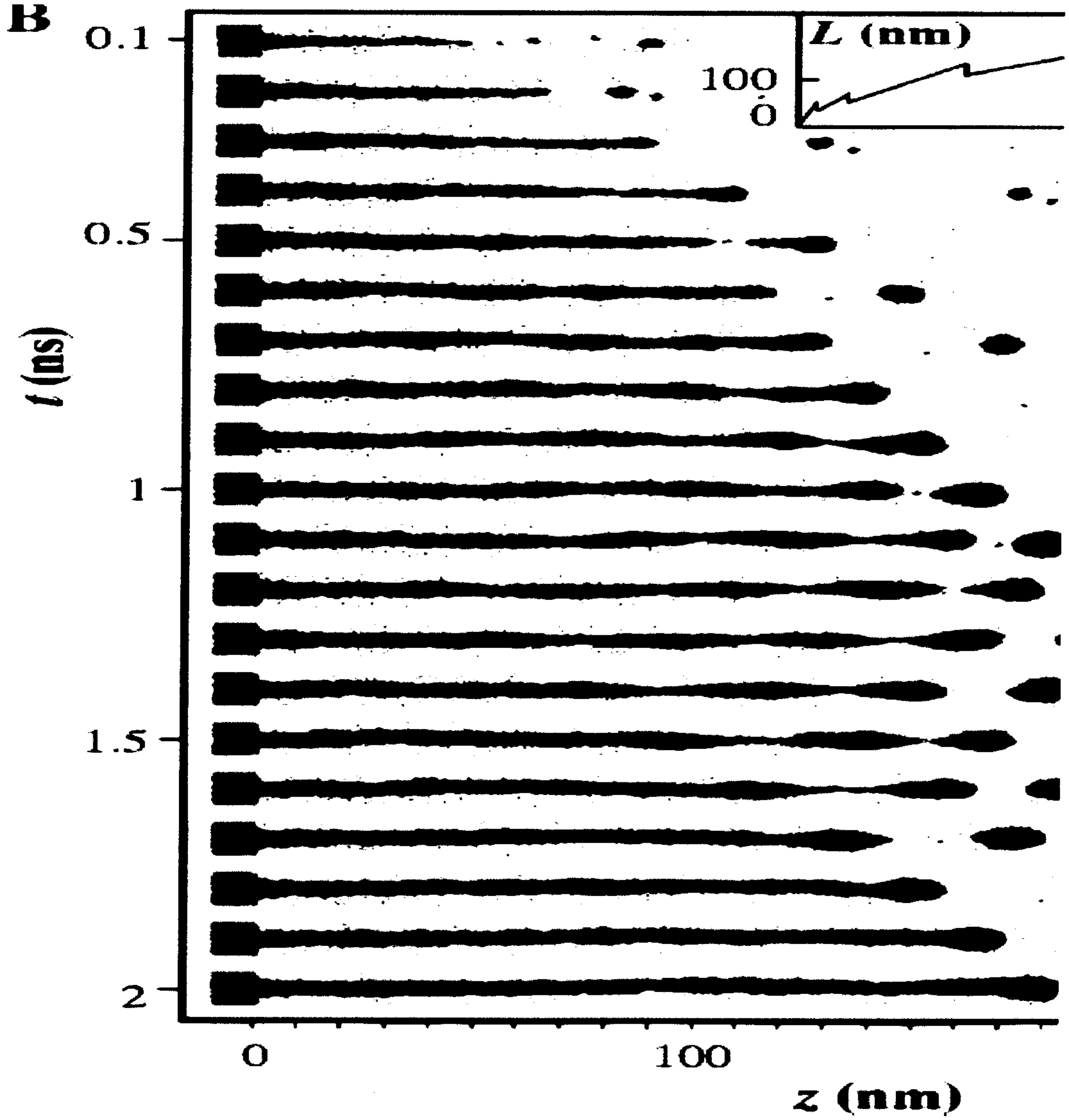
If it works, It can be used, for example to write on chips on the nanoscale.

For now, the available driving pressure is not quite high enough. Another order of magnitude, or a little less, will do the job.

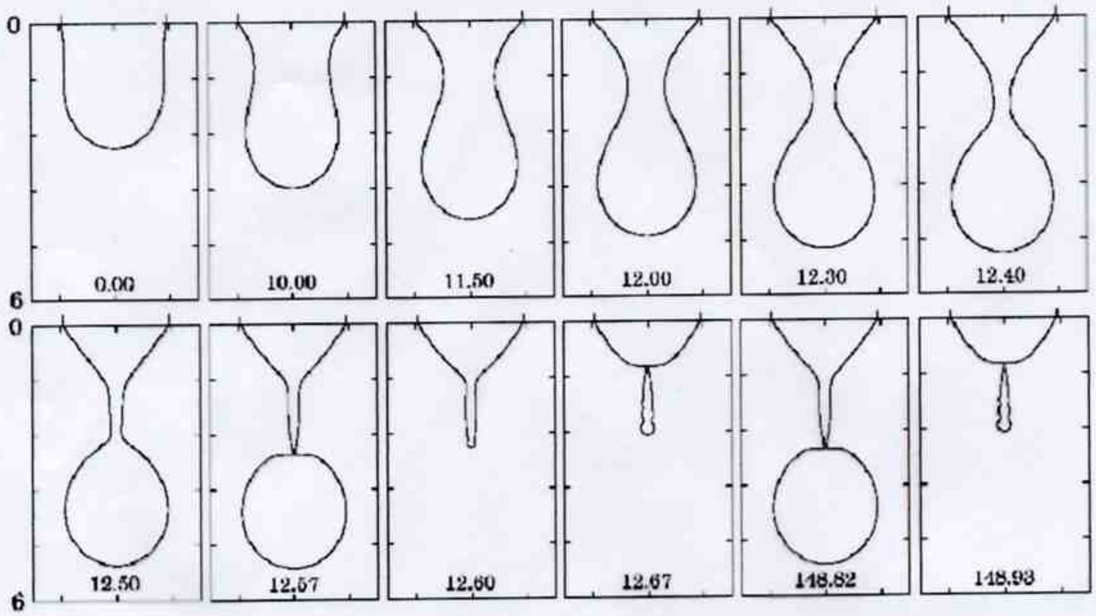
Here is an excellent example of an integrative simulation, used to approach an important engineering question.

This gives us question 2, a focused question: Is shape of jet different because of fluctuations?

look at thin necks



Nagel: shows shape and it looks different:



Not this either;

Jens Eggers PRL **89**, 084502 (2002) argues that shapes are different because fluctuations are important in the nano-study.

Another Example: The Raleigh Taylor Instability.

A high density fluid sits on top of a lower density one. Small deviations from perfect surface flatness triggers an instability. The two fluids penetrate very substantially.

The conventional wisdom says that at low viscosity and surface tensions, the penetration is given by an approximate formula

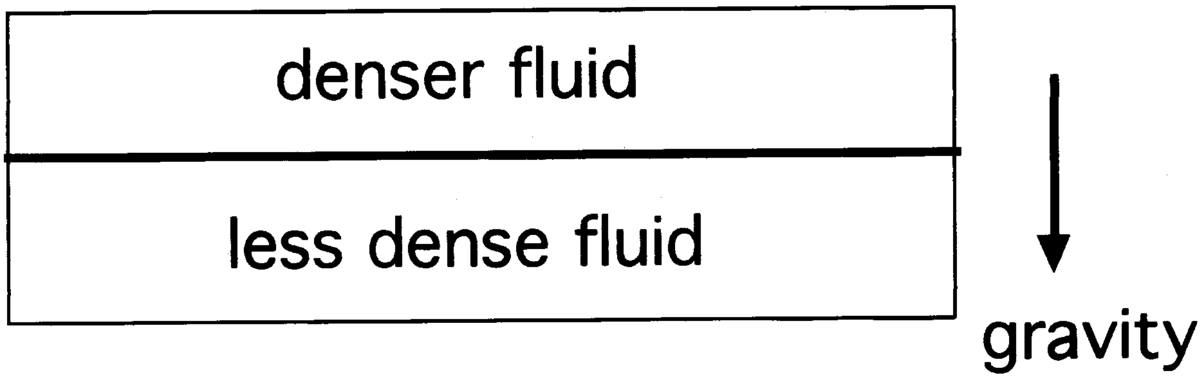
$$h = \alpha A g t^2$$

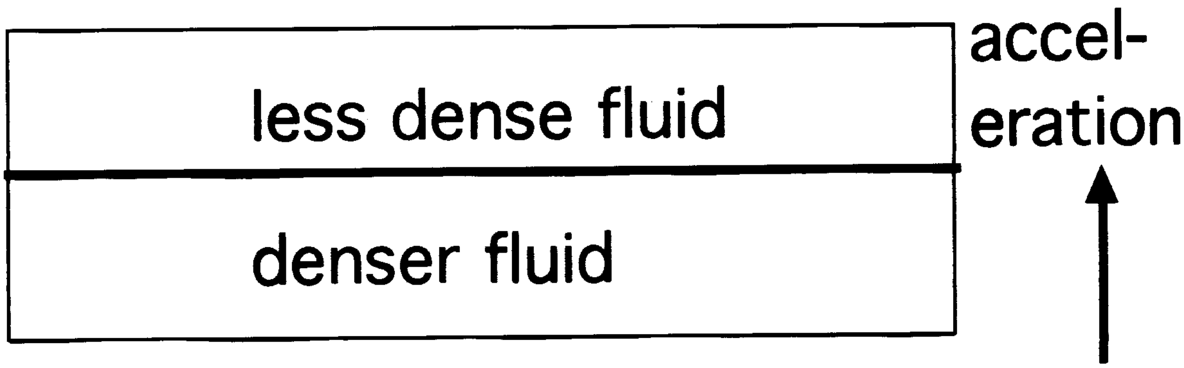
with A being the Atwoods number (density contrast) and α being dimensionless. Almost 10 groups have measured or calculated α, with two values coming out, one bunch getting α =0.06, (e.g, a MD calculation) giving another roughly 0.03 (e.g. a hydrodynamics calculation).

This instability is important for us (a DOE supported astrophysics group) because the instability occurs on the surface of an exploding star. It is also important to the DOE nuclear weapons program who sponsored the ten calculations .

The Simplest Situation

involves a flat interface separating two fluids



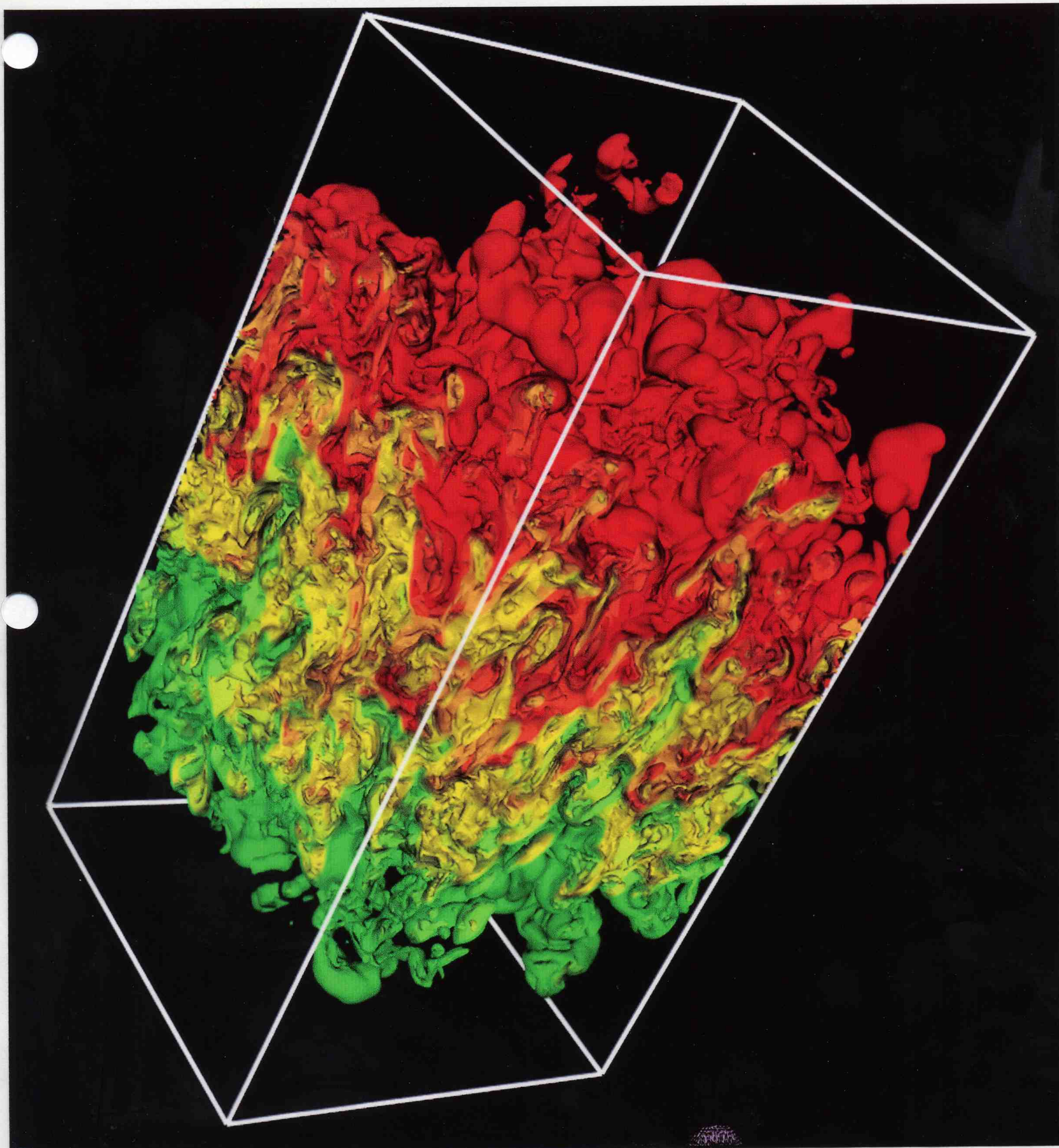


trans

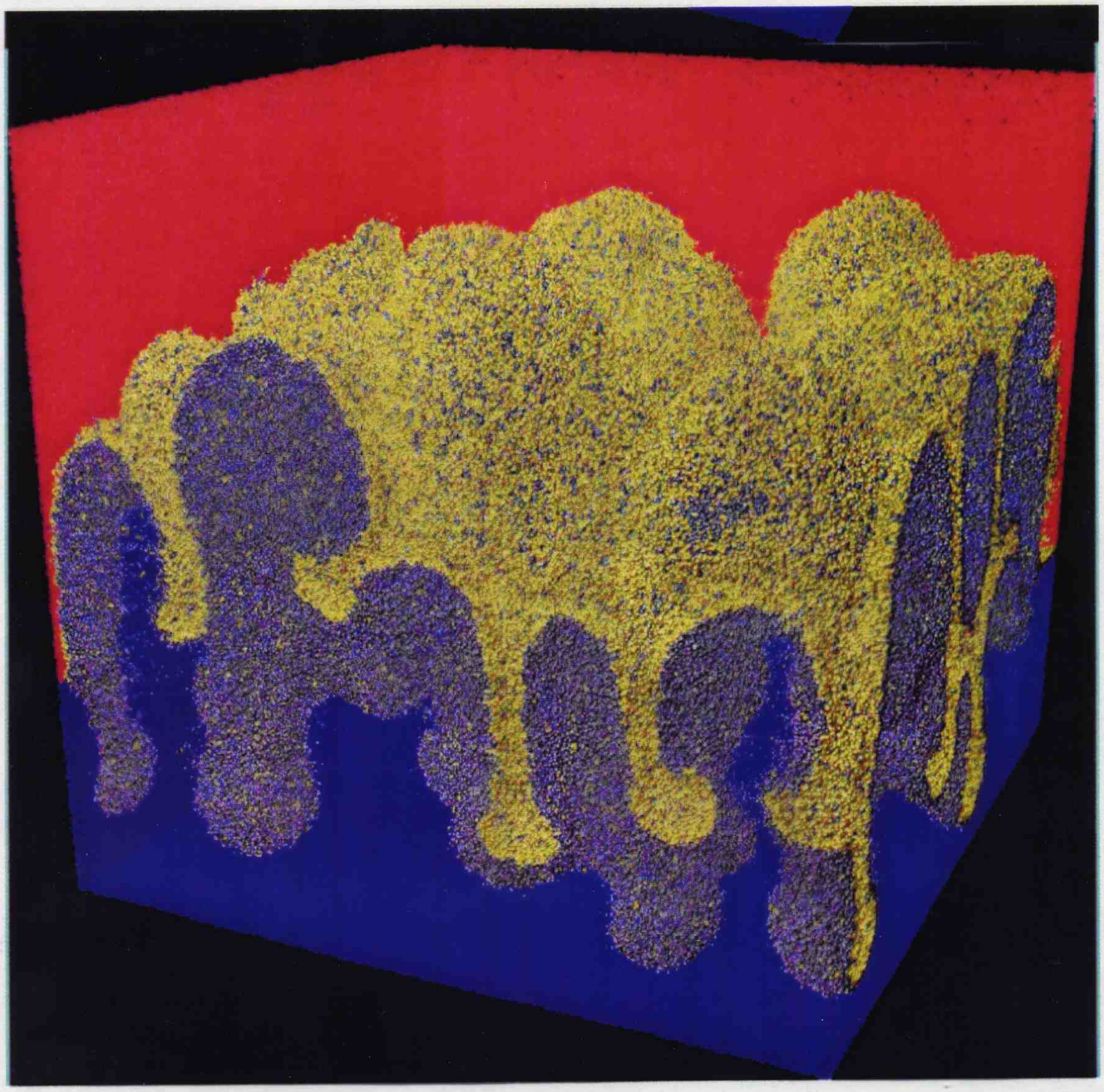
when the fluids have zero viscosity and surface tension dimensional analysis and RG suggest

penetration distance = $g\ A\ \alpha\ t^2$

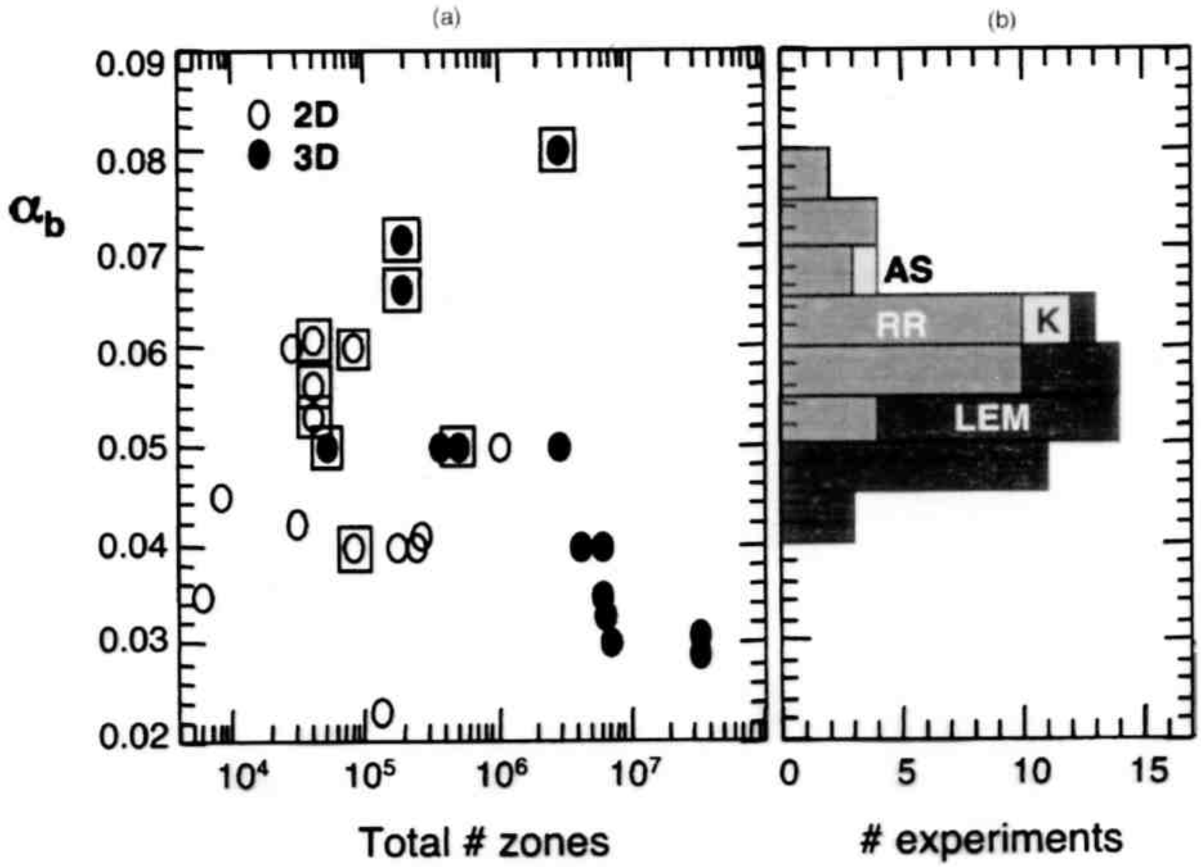
with α being a "universal" constant. Simulations can determine α trans and thus predicting mixing



Another Example:
Do fluctuations matter?



Kai Kadau...Berni Alder,
"Nanohydrodynamics simulation of R-T Instability", '04. $1.3 \bullet 10^8$ particles



A comparative study of the turbulent Rayleigh-Taylor instability using high-resolution three-dimensional numerical simulations: The Alpha-Group collaboration

Guy Dimonte, D. L. Youngs, A. Dimits, S. Weber, M. Marinak, S. Wunsch, C. Garasi, A. Robinson, M. J. Andrews, P. Ramaprabhu, A. C. Calder, B. Fryxell, J. Biello, L. Dursi, P. MacNeice, K. Olson, P. Ricker, R. Rosner, F. Timmes, H. Tufo, Y.-N. Young, and M. Zingale

Physics of Fluids Vol 16(5) pp. 1668-1693. May 2004

The ‘b’ refers to the bubble, which is the mode of penetation of the light fluid

Possibilities

a. The constant α is universal and has the lower measured value. Supported by five numerical calculations with different hydrodynamics codes.

b. The constant α is universal and has the higher measured value. This result is supported by an experiment, a numerical hydrodynamics calculation, another molecular dynamics calculation, and a renormalization group theory.

Either of these results would be good for the existing calculational methods used by the department of energy which (I infer) reach remarkable levels of detail and complexity by using zero viscosity and zero surface tension codes.

Logically, there is a third possibility,

c. The results for low viscosity and surface tension are quite unstable and the computer output depends upon details put in by the code designer rather than nature. (figure)

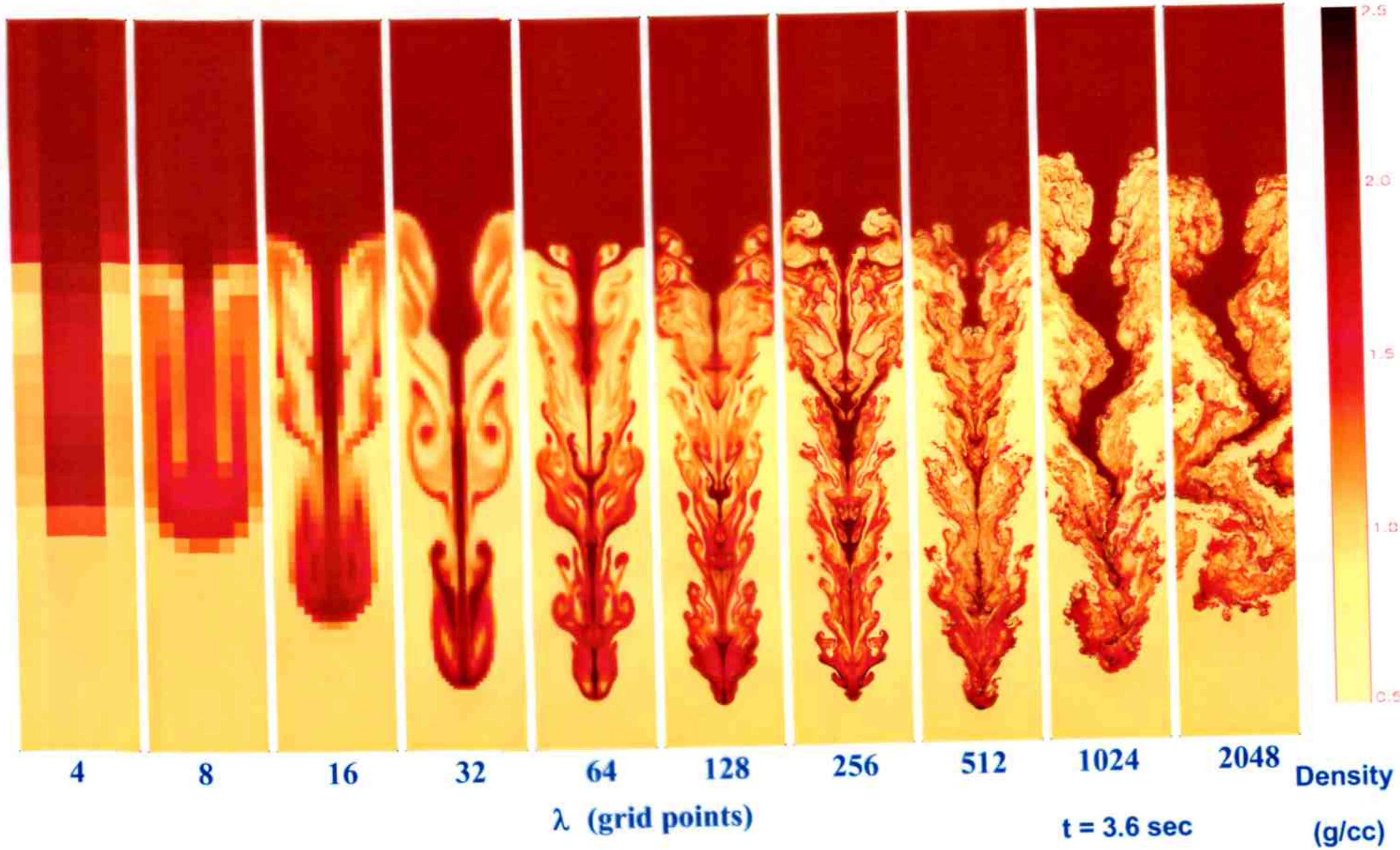
Measurements Support the Third Possibility

c. The results for low viscosity and surface tension are quite unstable and the computer output depends upon details put in by the code designer rather than nature. (figure) .

The result: Neither science nor engineering can depend upon active turbulent mixing simulations. In any new or unexplored situation, the amount of mixing is uncertain to a factor of two.

This result is one important outcome of the FLASH simulation studies.

Single-mode 2-D Rayleigh-Taylor



The ASCI/Alliances Center for Astrophysical Thermonuclear Flashes
The University of Chicago

Why is Resolution So Important?

Problems with an interface and no surface tension are said to be ill-posed. That is a mathematical concept which means that the problem does not make any sense. In such problems, it is often true that tiny changes in initial conditions, or boundary conditions, or calculational method can give very substantial variations in the answer. As, for example, resolution is made finer- the calculational results may not converge, or might converge to the wrong answer, or might even converge smoothly to the correct answer.

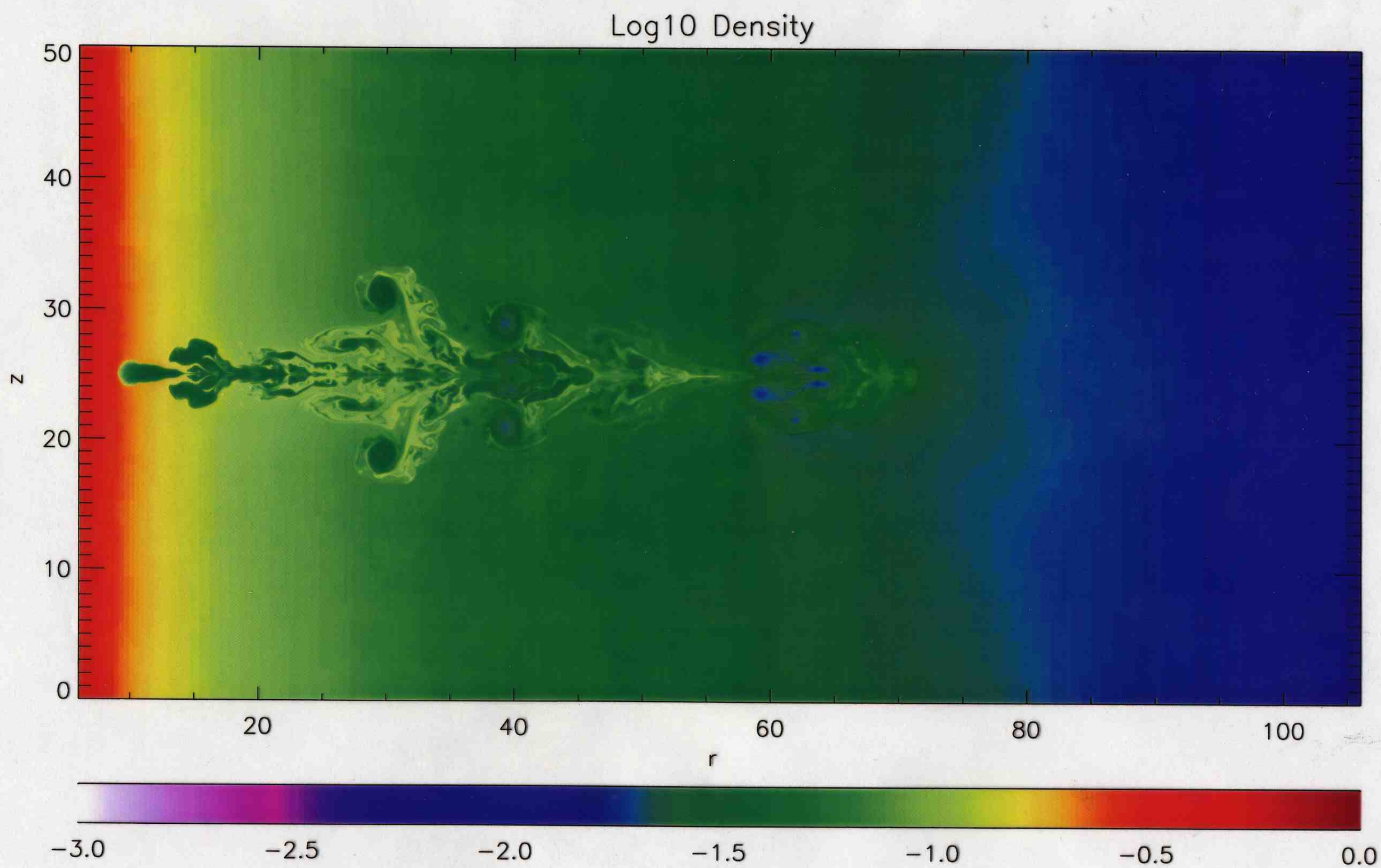
You can generally tell when you have a problem which is ill-posed because adding a parameter. makes a qualitative difference in the solution: Here adding surface tension takes one from infinitely crinkly interface to smooth ones.

Problems which become ill-posed as a small parameter is brought to zero are said to have a singular perturbation. Singular perturbations are also spotted by noticing that setting them to zero produces a qualitative change. In the Raleigh Taylor problem viscosity is also a singular perturbation.

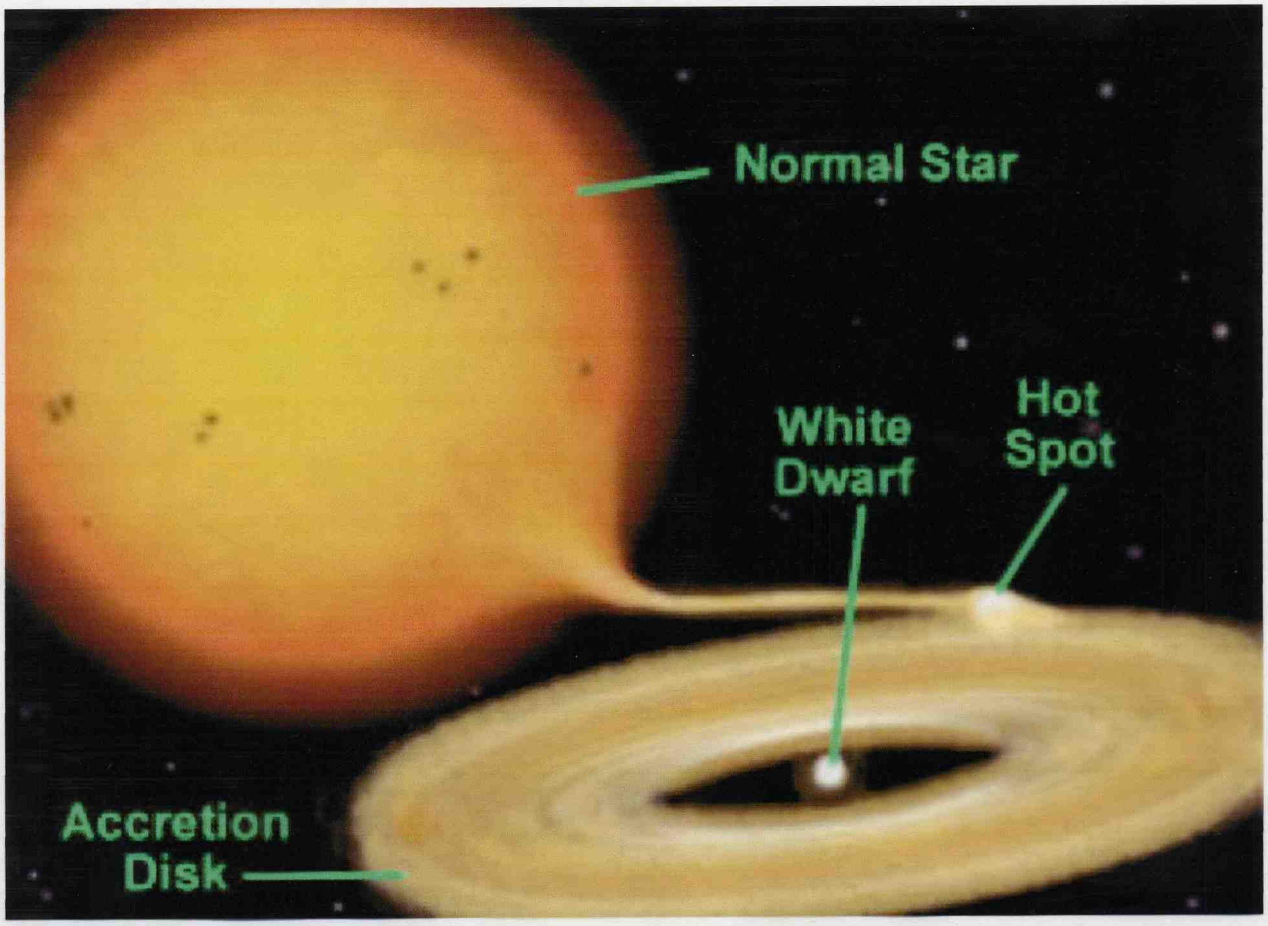
Thus, we do have real caution signs for this problem.

The Center of a Galaxy

A simulation done by Marcus Brüggen and Christian Kalser (Nature **418** 301 (2002)) describing a hot bubble rising from the center of a galaxy. The simulations describe two-dimensional flow with zero viscosity and zero thermal conductivity The color coding describes density. All the details and many of the gross featres in the picture are meaningless. They are artifacts of the resolution employed in the simulation.

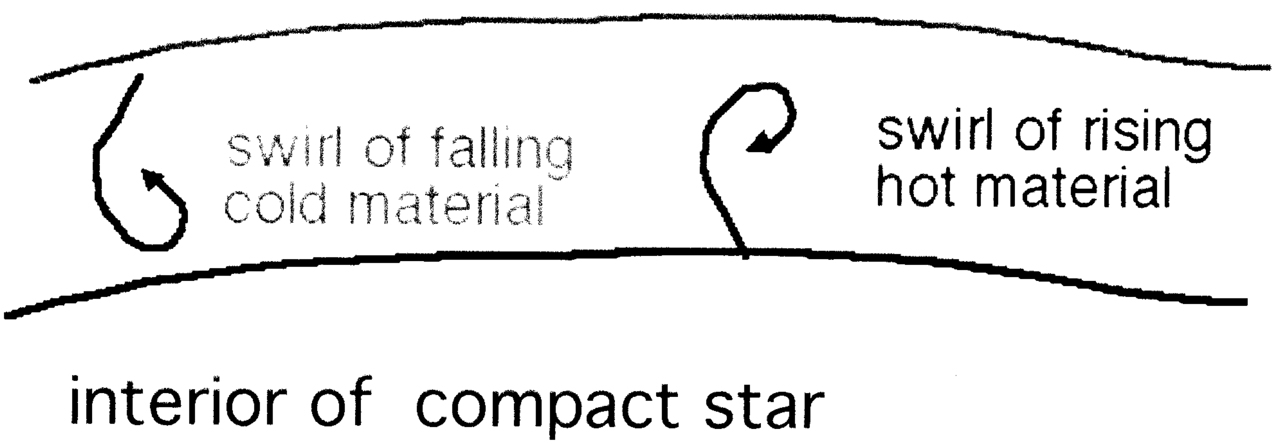


Log10 Density
z
50
40
30
20
10
0
20
40
60
80
100
r
−3.0
−2.5
−2.0
−1.5
−1.0
−0.5
0.0


Normal Star
White Dwarf
Hot Spot
Accretion Disk

RB does not explain mixing in nova: an accomplishment of the astro community

A nova goes boom because material drips off from a companion star. transstars This material forms an overlayer on the compact star. The overlayer can blow up in a nova. One observational fact is that material from the compact star is mixed with and blown off from the nova explosion.



Question: could the swirls dredge up enough materials from below the overlayer to fit the observed composition after the nova explodes?

Rayleigh-Benard instability

cooler,
less dense,
fluid

hotter, more
dense,
fluid

Instability causes fluids to interpenetrate.

RB Does not explain nova results...

In a series of studies, people tried to get their computer simulation to agree with the observed facts on mixing. They hoped that the rising of hot fluid via the RB instability could do the job by dredging up material below the overlayer. Instead, their series of calculations showed that none of their models of the RB instability would dredge up enough material from below to fit the facts.

Several calculations showed that this explanation could not work. See "On the C/O Enrichment of Novae Ejecta" Rosner, R., Alexakis, A., Young, Y.-N., Truran, J.W., & Hillebrandt, W. 2001, ApJ Letters 562, L177-9)

A better mechanism

After the RB-mixing nova studies show a very robust "failure", a Chicago group[4] suggests an entirely new mechanism: a resonant interaction between the wind from the accretion and the surface wave. As oceanographers previously suggested, that resonance can produce huge waves and tons of mixing. The study of "failed" computer simulations drew people attention to the need for a new mechanism. Simulations give an apparently successful test of the resonant mechanism, within the limitations of active mixing work and the factor of 100 uncertainty in wind speed.

The resonant wave theory, developed independently of any simulation, suggests a new mechanism. Then the computer simulation is an after-the-fact argument that all the facts have been taken into account. (Maybe nobody would listen to the qualitative argument if there were no simulations to back it up.) The center has a new proposal for nova behavior, but it is an idea, a suggestion, a proposal ... and not yet known to be correct.

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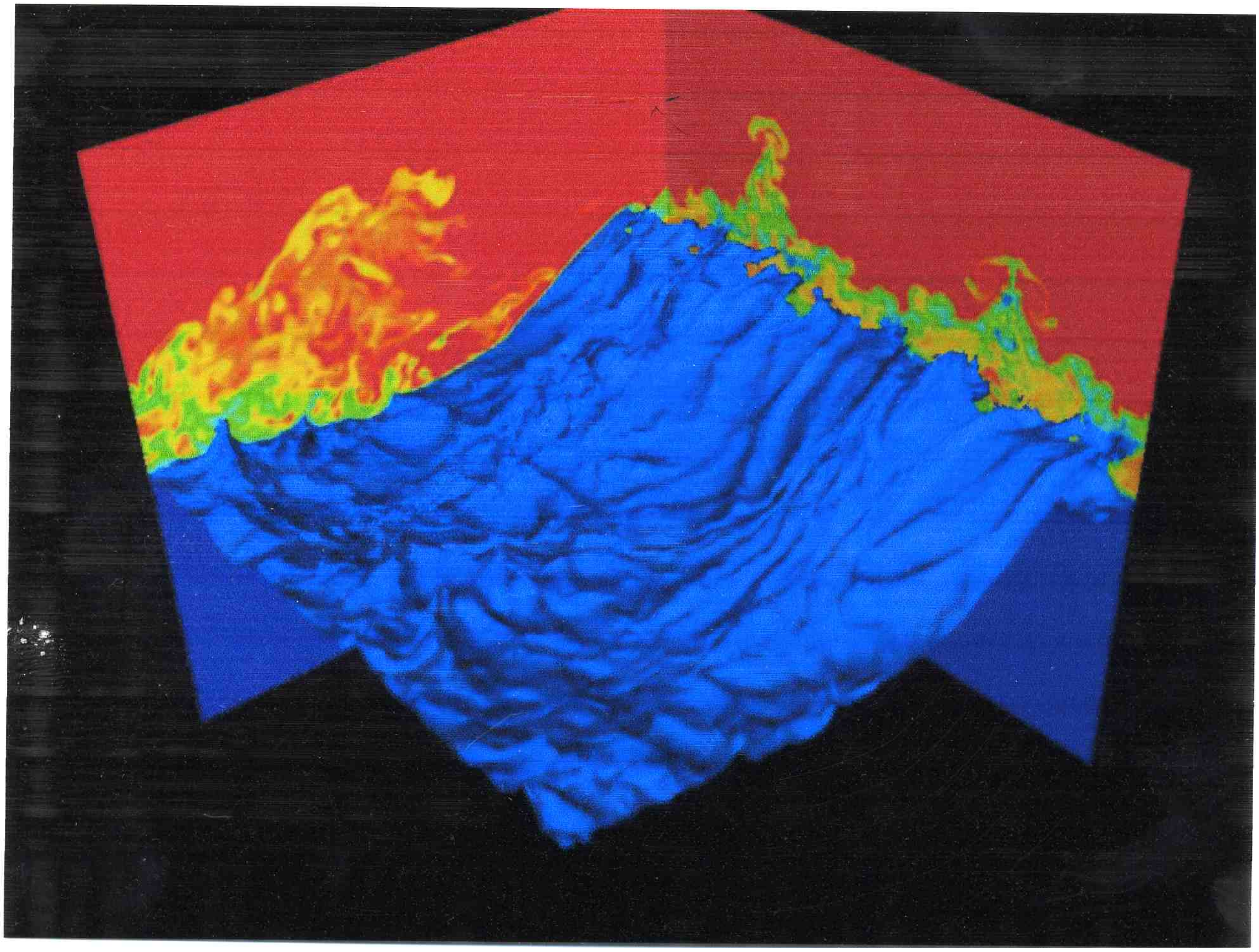
[4] On the nonlinear evolution of wind-driven gravity waves
A. Alexakis, A. C. Calder, L. J. Dursi, R. Rosner, J. W. Truran, B. Fryxell, M. Zingale, F. X. Timmes, K. Olson, and P. Ricker
Physics of Fluids Vol 16(9) pp. 3256-3268. September 2004

image: Daniella Rosner, Adler Museum

resonant interaction produces a very large wave when wind and wave move at the same speed



On to type Ia's: a really hard problem

How does a type 1a supernova go boom? A supernova is a white dwarf with nuclear material all mixed up and ready. But like other high explosives, it needs a really good push to get the nuclear detonation started. It's hard to see where that push comes from. Furthermore, if we just assume that it was somehow detonated in its natural state, maybe by lots of little explosions, still the result is poor because the outcome is mostly lighter elements and does not include the heavier elements actually observed in the explosion.

My colleagues' step I: A new kind of trigger.[4] They know that a local fluctuation produces a hot bubble which rises through the material. Because the RT studies showed the importance of 3D effects, they were ready to believe that instabilities might produce a very unsymmetric bubble. Imagine the pleasure when Alan Calder and coworkers saw small spherical hot region turn into an unsymmetrical bubble rising to the surface, and then unexpectedly making a shock wave. A new kind of rising bubble might produce a new detonation mechanism.

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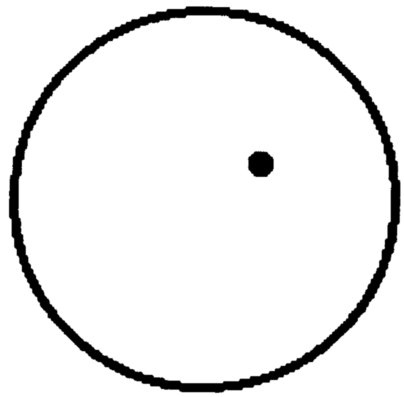
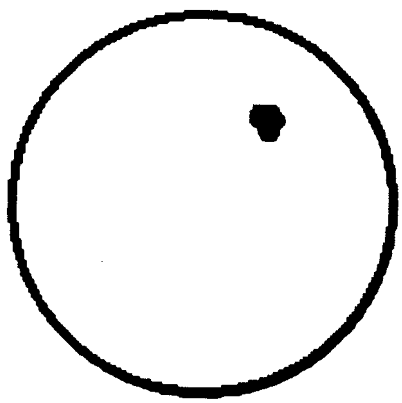
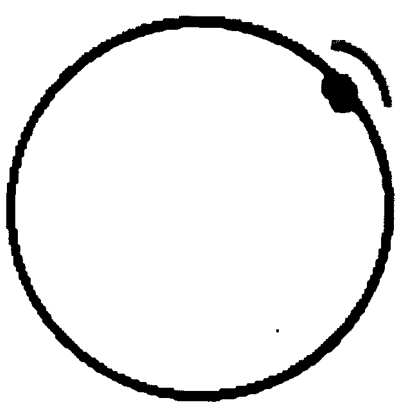
[4] Calder et. al. astro-ph/0405162.



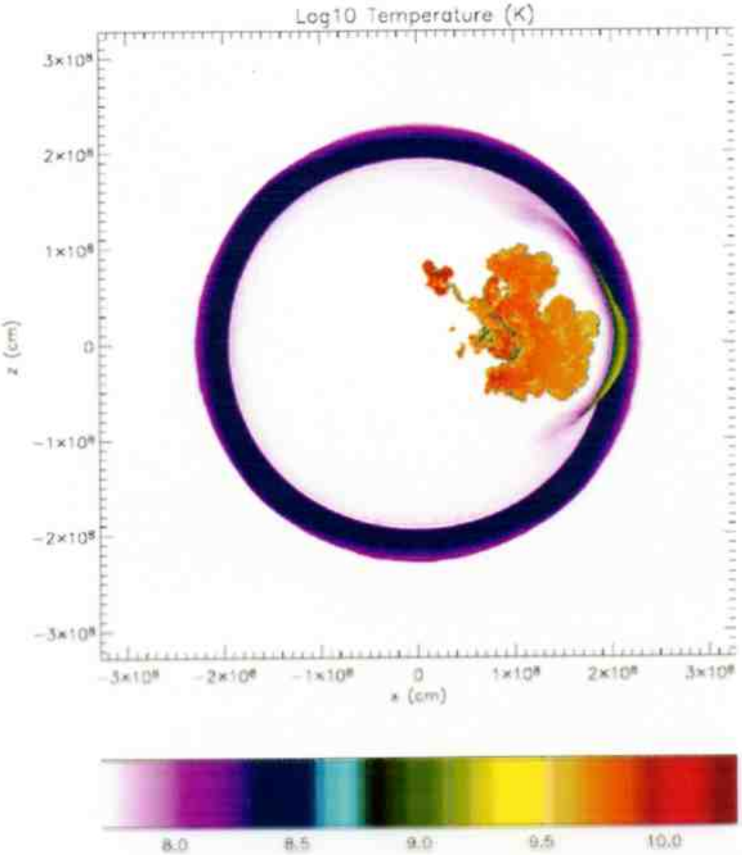
a bubble of hot material nucleates off center

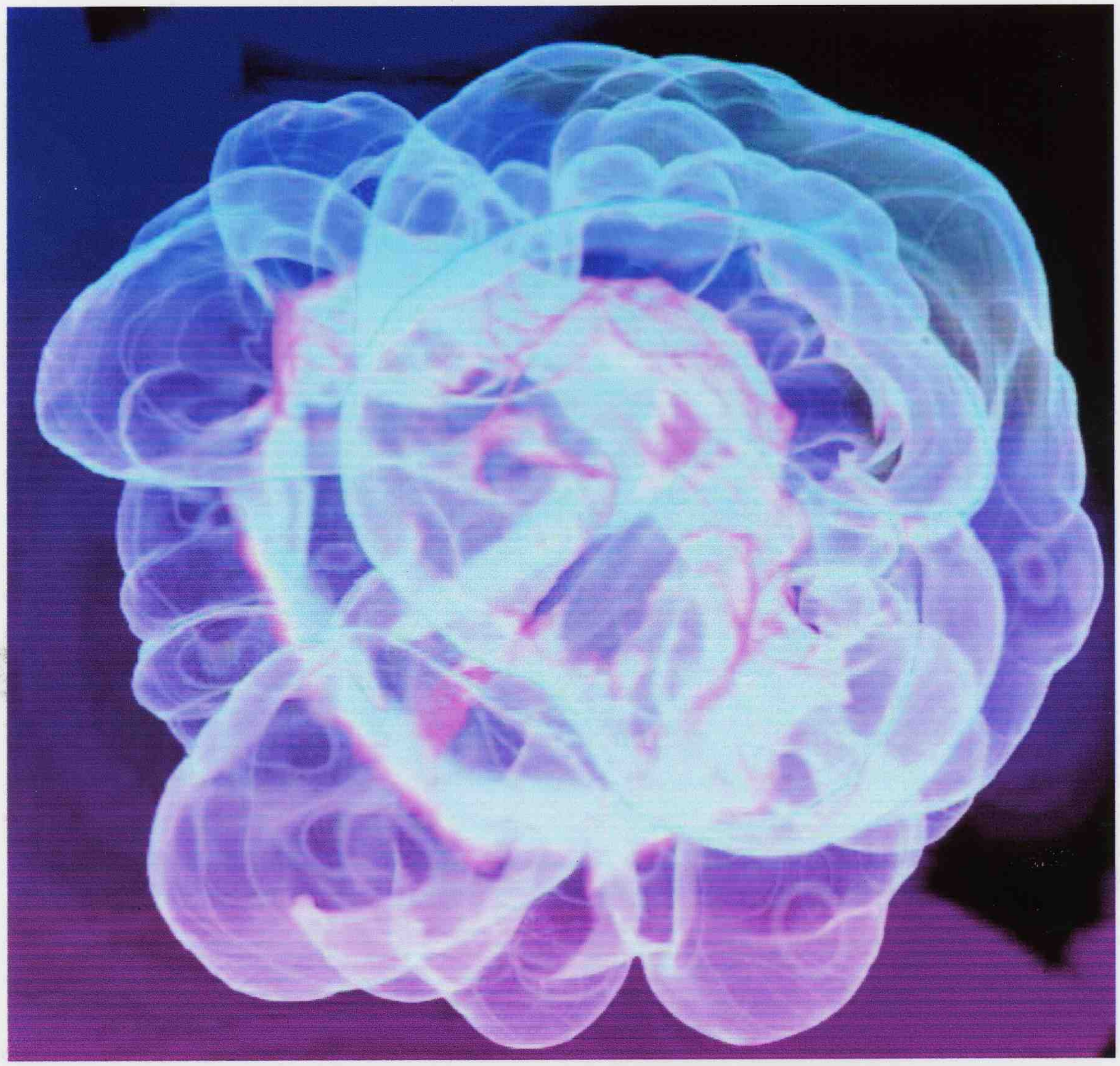


It rises and becomes asymmetrical



It surfaces and produces a shock


Log10 Temperature (K)
3×10^8
2×10^8
1×10^8
0
−1×10^8
−2×10^8
−3×10^8
z (cm)
−3×10^8
−2×10^8
−1×10^8
0
1×10^8
2×10^8
3×10^8
x (cm)
8.0
8.5
9.0
9.5
10.0



The Next Steps

But after a time it was noted that the direct effect of this surfacing was not a detonation. Another idea was needed. This was mostly the product of Tomaz Plewa.[5] Through insight and simulation he showed that hot material would shoot up from the bubble, fly across the star and refocus on the other side. That could detonate the whole show. Meantime, back in the main body of the star, an expansion would occur*, which would increase the radius of the star just enough to change the products of the explosion.

An innovative and unexpected three step mechanism: rising bubble, fluid flying across surface, focus to detonate seems to fit the observed facts. Is it right? How can one tell? There are lots of inaccuracies and unknowns. It's a proposal, an argument, a suggestion, a scenario. Certainly not a proof. A higher degree of certainty might come with more time, more tests, more criticism from the community.

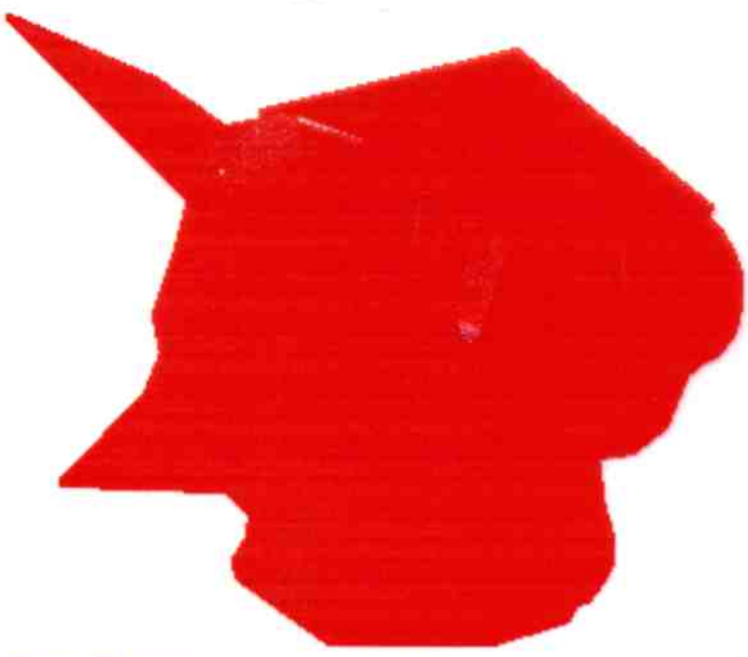
* You see the value of a big integrated simulation where you can watch lots of different process and regions at once.

[5] T. Plewa, A.C. Calder, and D.G. Lamb. ApJ 612, September, 2004.

pressure
and gravity
shoot
material
over
surface

Motion
dredges up
material

Material
comes to a
focus on
opposite side
of star



Star
detonates

Given that the amount of mixing cannot be accurately predicted:

What can one hope to gain from simulations like these

a. Kill off wrong physical arguments

b. Establish ranges of variation for crucial parameters

c. Suggest novel physical mechanisms

d. Discover unexpected behaviors, and thus eliminate surprises.

e. Start off programs for carefully checking suggested mechanisms.

Get effective understanding and eventual control of the range of behaviors in hard problems.

This work represents a scenario, an argument, a discussion !

There is an important technical reason for the increasing use of computers in exploring physical systems. Past analysis of point particles use ordinary differential equations to plot their position and momentum. More recent work has focused upon fluids, plasmas, and even solids that are studied as continuum systems, usually with the aid of partial differential equations. These systems and these sorts of equations can develop structures with very short scales or very long ones. These new processes and structures are often completely unexpected. We need methods to protect ourselves from being overtaken by unexpected occurrences. Computer simulations of simple non-linear systems can be one of our best tools for explorations that uncover unexpected possibilities.

There is More to Say

How do the power of argumentation provided by exploratory simulations compare to that of rhetorical or order-of-magnitude discussions? Since the simulations must include everything to make a star go boom, they provide an internal check of consistency and completeness not available through words. On the other hand, some intermediate steps in the argument may have their weaknesses hidden in unexamined computer processes. Words may be better than computer output for showing up weak arguments. Computer arguments often force us to rely upon the integrity and care of the investigators. So computers provide a useful, but dangerous, tool for the exploration of complex systems.

But, there are also major dangers in simulations. Often simulations are directly aimed at confirming our expectations, thereby throwing away the possibility of finding anything new. In addition, we simulators must be most careful to distinguish between simulations as argument versus simulations as proof. There is a considerable risk of confounding the two approaches. It is tempting to say that "supercomputer simulations show..." when what is meant is more like "recent investigations have raised the possibility that...". In our writing, we all are tempted to replace "it would please us if..." by "we know that ..". And if we scientists and engineers join up with all those around us--in places high and low-- who confound possibility with proof, and desire with truth, who then will believe us in anything we say?