Singularities and Blowups

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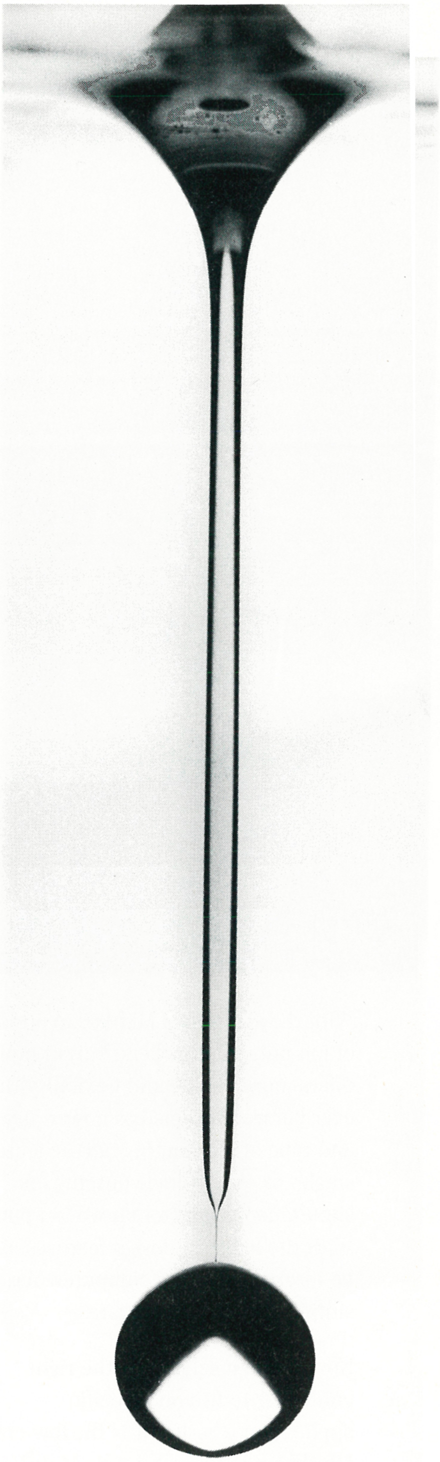
We have gotten spoiled in physics. Our mathematics works so very well. Most of our problems involve differential equations, and most of our fundamental differential equations continue to make sense in a quite global fashion. Maxwell's equations or the Schrödinger equation have the property that, if you start out with a physically reasonable situation, the equation's time development gives you another physically reasonable solution and so on to eternity, or at least to the eternity defined by the equation.

But these equations are quite special. They are linear, and wonderfully robust. In recent years, physicists, mathematicians and others have turned their attention to equations that develop mathematical singularities from nothing. You start from a very smooth initial situation and just wait. After a time, an infinity shows up in the solution or in one of its derivatives. Sometimes you can continue the solution past the singularity. Sometimes you need new physics (perhaps an additional boundary condition) to see what happens next. Sometimes you can say nothing at all beyond the singularity time.

The simplest example of singularity formation is drawn from the elementary study of ordinary differential equations. Look at the equation $\mathrm{d}x / \mathrm{d}t = ax$, with a being positive and constant, and an x that is positive at time zero. This could be the growth equation for something—perhaps the concentration of some compound in the atmosphere. Note that the solution grows exponentially in time, but x remains positive and well-behaved for all finite times. Perhaps this outcome is bad, but the worst takes an infinitely long time to arise. In contrast, imagine that the growth rate, a, is itself linear in the concentration of the contaminant: $a = cx$, with c being constant. A quick calculation shows that the concentration obeys: $x(t) = 1 / c(t^* - t)$, with ct^* being an abbreviation for the positive quantity $1 / x(0)$. Notice that the concentration blows up at t^* and subsequently has the senseless property of being negative.

This example, drawn from the theory of ordinary differential equations, is too trivial for research-style investigation. However, examples of singularity formation based upon partial differential equations are hot research topics. One example is provided by black hole formation in general relativity. Black holes are singularities. In an elegant numerical study, Matt Choptuik[1] showed that in contrast to the generally held view, holes of mass smaller than the Chandrasekhar limit could be formed and that, in the process of formation, the solutions would oscillate periodically in $\ln(t^* - t)$. Many others published papers that agreed with and extended this conclusion.

Choptuik's study is one of a series of recent works that study how partial differential equations develop singularities that are universal and scale-invariant. These properties go together. For example, a group of us (Michael Brenner, Peter Constantin, Leonid Levitov, Alain Schenkel, Shankar C. Venkataramani and I) are studying a problem in which bacteria are attracted by something that they produce. This attractant undergoes a rapid diffusion process.[2] As the bacteria produce a more concentrated region of attractant, they are bound together into a tight little clump in which their



A DROP IS PRODUCED by the flow through a faucet of a glycerol/water mixture with a viscosity of 1 poise. The singularities occur at the precise space/time points at which the thread breaks. (Photo from S. D. Shi, M. P. Brenner, S. R. Nagel, Science **265**, 219 (1994).)

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density, ρ, goes to infinity near a singular point as

$$\rho(\mathbf{r}, t) = (t* - t)^{-1} F\left(\frac{|\mathbf{r}-\mathbf{r}_0|}{(t* - t)^{1/2}}\right) + \text{(smaller terms)}$$

Note that the singular term always has the same basic shape, but its size and extension vary in time. Hence we call it scale-invariant. We use the word "universal" to suggest that the result will remain the same if the initial situation is varied slightly, or even perhaps if the differential equation is changed a little bit. The equation describes the simplest way in which a solution to a partial differential equation can "go bad."

This same sort of mathematical structure appears time and time again. For example, scientists have long studied situations in which a mass of fluid forms a thin neck and that neck breaks so that the fluid separates into two pieces. (See the figure on page 11.) A group of theorists here at the University of Chicago looked for similarity solutions in these situations. Using simulations, we[3] found a whole zoo of such solutions, one of which was, in parallel, achieved experimentally.[4] In this solution, the derivative of the pressure blew up at the breaking point. This situation of broken necks is part of a broader problem, discussed by Pierre-Gilles de Gennes[5] and others, in which one must understand fluid flow on a surface that is partially wet and partially dry. The first time a dry spot appears on an initially wet surface, there is a mathematical singularity. After that time, one must somehow deal with the new boundary conditions required to describe the motion of the interface. The number and type of those boundary conditions can, in principle, be determined by studying another kind of similarity solution, the one that describes the wet–dry edge.

There is a classical, and unsolved, problem related to these singularity issues. The most fundamental equations for fluid flow are the Navier–Stokes and Euler equations. These equations[5] have a large number of near-singular behaviors that interfere strongly with the construction of economical, accurate and reliable simulations. These difficulties, in turn, limit advances in such fields as weather prediction and the design of explosive devices.

Accurate simulation of singular or near-singular behavior is both difficult to achieve and hard to assess. In the bacterial example, we ran into a particularly favorable situation in which we had theorems and stability analysis that told us what to expect. In one region of behavior, the theorems ruled out any singularity, yet each single simulation that we did showed some apparent singularity. Only the most careful comparisons of solutions obtained by different methods sufficed to show that the computed singularities were artifacts of the computational technique.

Choptuik concluded that the best approach to computational understanding of singularity formation was to have a maximum opportunity for "on line" human intervention in the simulation process. He designed techniques for achieving interactivity in the context of the Cray supercomputer at the University of Texas at Austin. We had a simpler computational problem so we could get where we wanted with workstations. For us too, interaction with the computer and extensive tests of computational technique were necessary before we could feel any confidence in our results.

Perhaps this experience gives some practical lessons. The Department of Energy is now in the process of learning how to use another generation of supercomputers, bigger and faster than the previous ones but, for the moment, more weakly supplied with software. These computers will be used in part to replace understanding that might have been obtained from testing of nuclear weapons. If the experience of the singularity work is any guide, in this new design and testing process, human understanding will remain essential. It is not sufficient to set up the code and let the computer zip along. It zips alright, but to where? It will remain crucially important to monitor the computational process in detail, to see and understand the steps involved in each stage of the computation. The weapons designers should require many internal tests of the consistency of the numerical technique. To enhance reliability, they should test their computer results against previous experiment and observation as much as possible. Even then, one cannot have absolute confidence that the computer will produce truth. Computer simulation is, at the edge, an art as much as a science. ■

References

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