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Idealization and modeling

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Abstract This paper examines the role of mathematical idealization in describing and explaining various features of the world. It examines two cases: first, briefly, the modeling of shock formation using the idealization of the continuum. Second, and in more detail, the breaking of droplets from the points of view of both analytic fluid mechanics and molecular dynamical simulations at the nano-level. It argues that the continuum idealizations are explanatorily ineliminable and that a full understanding of certain physical phenomena cannot be obtained through completely detailed, non-idealized representations.

Keywords Models · Idealizations · Simulations · Explanation · Fluid dynamics · Scaling · Molecular dynamics

1 Introduction

Physical applied mathematics is in the business of constructing and investigating models of physical phenomena. Typically these mathematical models take the form of an equation or set of equations which are then manipulated in various ways. Fowler (1997) discusses the nature of this art:

> Applied mathematicians have a procedure, almost a philosophy, that they apply when building models. First, there is a phenomenon of interest that one wants to describe or, more importantly, explain. Observations of the phenomenon lead, sometimes after a great deal of effort, to a hypothetical mechanism that can

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> explain the phenomenon. The purpose of a model is then to formulate a description of the mechanism in quantitative terms, and the analysis of the resulting model leads to results that can be tested against the observations. Ideally, the model also leads to predictions which, if verified, lend authenticity to the model. It is important to realize that all models are idealizations and are limited in their applicability. In fact, one usually aims to oversimplify; the idea is that if a model is basically right, then it can subsequently be made more complicated, but the analysis of it is facilitated by having treated a simpler version first. (Fowler 1997, p. 3)

I think that this is an accurate statement of a fairly widespread view about mathematical modeling and, while I agree with the overall sentiment, I also believe that in several ways it potentially misleads. For instance, I agree with Fowler that all models are or involve idealizations; although I disagree that this necessarily means that they are limited in their applicability. I agree that mathematical modelers usually aim to over-simplify; although I will argue that sometimes (often, in fact) if one tries to make the model more complicated, one fails to realize the stated goal of providing an *explanation* of the phenomenon. Finally (though I will not consider this here), I think that in many instances the search for a mechanism—at least if this is understood rather narrowly in causal terms—is not an important feature of the explanation provided by the mathematical model.

In what follows I would like to discuss these features of mathematical modeling. In particular, I will concentrate on the explanatory goals of modeling. In order to do so we must examine more closely the role of idealization and the proper understanding of that role in describing and explaining various features of the world. However, in order to do this we need to grasp what counts as the physical phenomenon to be modeled. I believe that most discussions of modeling simply take it for granted that we have an appropriate understanding of "the physical phenomenon". But, I think a proper investigation of this concept will help us (at least) to make some distinctions between different views about modeling. Thus, in the next section I try to say something about the nature of the phenomena that are often investigated, and how certain important features of those phenomena demand a particular way of thinking about the role of idealizations in the model—a way that is largely at odds with some of the things Fowler mentions. Following that in Sect. 3 I discuss, qualitatively, an example of the modeling of shocks. In Sects. 4 and 5 I consider in much more detail, first, the analytical modeling of the behavior of breaking droplets and, second, molecular dynamical simulations of the formation of droplets at the nano-level. These two problems are intimately related to one another and serve as good exemplars of the different roles played by idealizations in mathematical modeling. I conclude by arguing that some idealizations are explanatorily ineliminable. That is to say, I argue that the full understanding of certain phenomena cannot be obtained through a completely detailed, nonidealized representation.

2 Idealization and the phenomena

There are (at least) two views about the nature and role idealizations play in modeling and representing physical phenomena. There is what one might call a traditional view,

according to which one aims for the most exact and detailed representation of the phenomenon of interest. On this view, the use of idealizations is, in effect, justified pragmatically: We need to introduce idealizations into our equations in order to simplify them so as to make them tractable or solvable. (As the passage above indicates, Fowler appears to endorse something like this traditional view.) A second view finds virtue where the traditional view sees vice; namely, in the particular kinds of simplification that idealizations typically provide. This other view, which for lack of a better term I will call "nontraditional," maintains that in some cases (and actually in many cases) idealized "overly simple" model equations can *better* explain and characterize the *dominant* features of the physical phenomenon of interest. That is to say, these idealized models better explain than more detailed, less idealized models.

Let us consider the traditional view in a bit more detail. As noted this approach to modeling holds that one should try to find the most accurate and detailed mathematical representation of the problem at hand.[1] This fits nicely with Fowler's "philosophy" of modeling. If the model fails to capture adequately those features of the phenomenon one is interested in, then there are a couple of things one can do. For instance, one can try to add more detail to the mathematical representation,[2] or one might try to adjust the parameters already appearing in the model so as to better reflect what is going on. Most crucially, on this view, the aim is to try to effect a kind of convergence between model and reality. Ultimately, the goal is to arrive at a complete (or true) description of the phenomenon of interest. Thus, on this view, a model is better the more details of the real phenomenon it is actually able to represent mathematically. In effect, idealizations are introduced only to be removed later through further work on those details. This, too, fits nicely with Fowler's "philosophy" of modeling.

Before considering the contrasting approach, we need to get clear about the nature of the so-called "phenomenon of interest." As I noted, I think there is virtually no discussion of this in the literature on modeling and idealization. However, a proper understanding of the kinds of phenomena that are most often of interest will enable us to appreciate better the second, nontraditional, role of idealization in mathematical modeling.

It is an incontrovertible fact that nature presents us with patterns and regularities. And, much of scientific theorizing involves trying to understand how these regularities arise. This is not to say that every pattern we observe reflects a genuine lawful feature of the world. Humans are all too ready to see patterns in just about anything.[3] Neither is it to say that we are interested only in investigating "real" regularities and patterns. *Sui generis* phenomena are, of course, also worthy of investigation. As an example of the latter one might think of studying the nature of the transient behavior in a particular electrical circuit before it settles down to a steady state.

[1] I consider the work of Ronald Laymon as representative of this approach to idealization. See for instance, Laymon (1980).

[2] By this I mean, one might include mathematical representations of additional factors that may be relevant for the phenomenon under investigation.

[3] Fine, in his excellent discussion of computational complexity, randomness, and probability, puts the point as follows: "Too keen an eye for pattern will find it anywhere" (Fine 1973, p. 120).

Nevertheless, most often it seems that our attention is captured by regularities—by repeatable phenomena. It is, in part, the repeatability of phenomena that makes it dominant and captures our interest. That is to say, the repeatability itself is a salient feature that leads us to ask about what is responsible for that very repeatability. When we couple this feature—the salience of the phenomenon—with the fact that for all but the simplest empirical generalizations we need to idealize so as to find an adequate mathematical representation, we gain a fuller understanding of the meaning of "dominant feature."

One goal of mathematical modeling is, surely, to capture these salient features of the regularity in a mathematical formula. The repeatability of the phenomenon places a constraint on the nature of the mathematical model: The model must be sufficiently robust or stable under certain kinds of changes to reflect the fact that the phenomenon is repeatable in various situations where many details have changed. The world is constantly changing in myriads of ways; yet despite this, we see the same patterns over and over again in different situations. Idealizing is a means for focusing on exactly those features that are constitutive of the regularity—those features that we see repeated at different times and in different places. Equivalently, the process of idealization, understood in this way, is most broadly seen as a means for removing details that distract from such a focus—those details that can change without affecting the dominant, repeatable behavior of interest. The mathematical operation that represents the removal of such irrelevant details involves the taking of limits.

Let me now return to the discussion of what I have called the "nontraditional view" of the nature and role of mathematical modeling. Recall that the traditional view aims, ultimately, to "de-idealize" by adding more details so as to bring about a convergence to a complete and accurate descriptions. The nontraditional view, to the contrary, holds that a good model does not let these details get in the way. In many cases the full details will not be needed to characterize the phenomenon of interest, and those details may, in fact, actually detract from an understanding of that phenomenon. This nontraditional approach requires that one find a minimal model—a model "which most economically caricatures the essential physics" (Goldenfeld 1992, p. 33). The adding of details with the goal of "improving" the minimal model is self-defeating—such improvements are illusory.[4]

Once one arrives at a representative equation, there is, to some extent, a set of procedures the modeler typically follows in order to gain insight from the model. (These procedures are largely independent of ones view of the nature of modeling; though, as will become evident, I believe they best fit the nontraditional conception.) In effect, these procedures characterize the modeler's methods of simplification. Two features of this recipe stand out. First, one typically nondimensionalizes the equation or system of equations. This enables one to compare parameters appearing in the equation as to their importance or "size" even though they have been expressed in different units. Second, one takes limits thereby reducing the equation. Typically these limits involve letting a "small" nondimensionalized parameter approach the limiting value of zero or a "large" nondimensionalized parameter is taken to infinity. The aim is to simplify by

[4] See Batterman (2002) for a detailed discussion.

idealizing in this fashion. This is not by any means *solely* an exercise in pragmatics: It is not simply a means for finding exactly solvable solutions. In today's world of extraordinary computing capabilities, this analytical practice continues to play a major role in the investigation of physical phenomena. If all we cared about were correct and accurate numerical predictions, then we would not bother with these analytic investigations. (As Fowler puts it, sounding here as if he endorses the nontraditional conception of modeling, "computation can limit insight, because of an inability to pose questions properly" (Fowler 1997, p. 6).)

The hope is that if done correctly, one will end up with a model which exhibits the *dominant* features of the system. It will be a limiting model that displays the essential physics. As a qualitative example, consider the case of shocks. (A more detailed example is discussed in Sect. 4.)

3 Modeling shocks

Let us say we are interested in understanding the behavior of a gas as it moves through a tube. See Fig. 1. If a collection of the molecules are given a push (say by blowing into the tube at one end), then they will begin to catch up to those in front resulting in a more densely populated region separating two regions of relatively less molecular density. Across this region, molecules will exchange momentum with one another as if some kind of permeable membrane were present. The region occupied by this "membrane" is a shock. Of course it is very difficult to track the behavior of the individual molecules as they move through the tube and undergo the collisions in the shock region. (This is not to say that computational simulations cannot approximately track such behavior. I will have more to say about molecular dynamical simulation and this notion of approximation below.) But, often the applied mathematician will approach the problem by taking a continuum limit. This is a model in which the collection of molecules in the tube is treated as a continuous fluid. Such a limit will shrink the shock region onto a two-dimensional boundary. Upon either side of the boundary, the behavior of the fluid will be governed by the relevant (partial) differential equations of fluid mechanics. However, the behavior across the boundary is not governed by

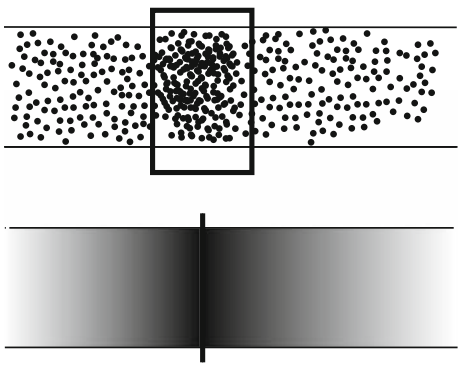


Fig. 1 Modeling shocks

any differential equation at all, but rather by algebraic "jump conditions"—singular behavior across the boundary.

One might think (if you held the more traditional approach to modeling) that the idealization of the collection of molecules to a continuous fluid would be to make the boundary region unimportant to the physics. After all, the boundary shrinks to two dimensions and is not "law governed." (All those ignored molecular details ought to be put back in!) In fact, traditional (covering law) accounts of explanation hold that laws do the essential explanatory work, and initial conditions and boundary conditions are given a sort of secondary status. Further, as the boundary is a place where the laws apparently break down, how can the boundary function in a covering *law* explanation?

Mark Wilson has argued that this view—the view that the boundary becomes unimportant to the physics—is mistaken. In fact, the boundary is the most important feature when it come to understanding the behavior of interest. As Wilson notes "the allegedly 'suppressed details' have become crushed into a singular (hence not law-governed) factor that still dominates the overall behavior through the way in which it constrains the manner in which the 'law governed regions' piece together" Wilson (2003, personal communication).[5] The idea is that such boundaries dominate the physics and that often the mathematical modeler's search focuses on those features to explain what is going on. The limits often yield boundaries that shape or constrain the phenomena. And, it is the elucidation of these shapes that is important for understanding.

Thus, the continuum limit provides a means for ignoring details about molecular interactions in the development of shocks. Most importantly, the taking of limits in this way often imposes mathematical constraints on the equations or formulas that represent the phenomenon of interest. In particular, it requires our models to exhibit the appropriate kind of stability under perturbation of various details—those details that are effectively eliminated by the taking of the limit. Our attempt to represent the dominant features of the phenomenon—genuine features of the world—dictates to some extent the nature of the appropriate mathematical representation. That representation, in turn, leads us to investigate in detail the nature of the imposed constraints. It turns out that in many instances such investigations lead to the discovery of singularities—places where the governing laws "breakdown." The example of shocks is just one such instance. In the next section I consider another example in considerably more detail.

4 Modeling drops and jets

As water drips from a faucet it undergoes a topological change—a single mass of water changes into two or more droplets. This is the most common example of a hydrodynamic discontinuity that arises in a finite period of time. In Victorian times Lord Rayleigh recognized that drops form as a result of a competition between gravitational force and surface tension. He was able to determine the typical size of a droplet and was able to set the time scale upon which a drop would form (Eggers 1997, p. 866).

[5] See Wilson (2006) for much more detailed discussions of these and related issues.

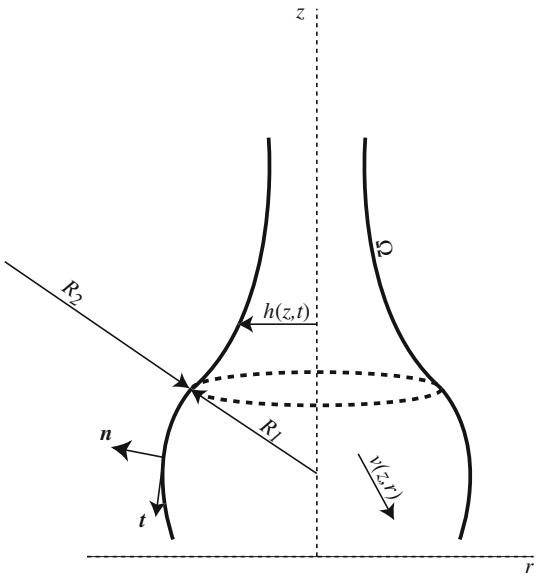


Fig. 2 Geometry of a falling drop

Recent work on the problem has focused on characterizing the shape of the fluid interface at and near the time of breakup. One needs to examine the nonlinear Navier–Stokes equations for free surface flows. These problems are considerably more difficult to solve than those where the fluid is constrained (say by the walls of a pipe).[6] The Navier–Stokes equations must develop a singularity in finite time that is characterized by divergences both in the fluid velocity and in the curvature of the interface at the point of snap-off.

To begin we assume that the typical geometry of a dripping drop is exhibits axial symmetry about the z-axis. Figure 2 provides the relevant details. Assuming axial symmetry, the velocity field inside the fluid is given by a function $v(z, r)$. One can define a time dependent radius function, $h(z, t)$, describing the shape of the drop at any given time. R_1 and R_2 are the principal radii of curvature of the axisymmetric surface Ω. In this geometry, using cylindrical coordinates, the Navier–Stokes equations are given by

$$\frac{\partial v_r}{\partial t} + v_r \frac{\partial v_r}{\partial r} + v_z \frac{\partial v_r}{\partial z} = -\frac{1}{\rho}\frac{\partial p}{\partial r} + \nu\left(\frac{\partial^2 v_r}{\partial r^2} + \frac{\partial^2 v_r}{\partial z^2} + \frac{1}{r}\frac{\partial v_r}{\partial r} - \frac{v_r}{r^2}\right), \tag{1}$$

$$\frac{\partial v_z}{\partial t} + v_r \frac{\partial v_z}{\partial r} + v_z \frac{\partial v_z}{\partial z} = -\frac{1}{\rho}\frac{\partial p}{\partial z} + \nu\left(\frac{\partial^2 v_z}{\partial r^2} + \frac{\partial^2 v_z}{\partial z^2} + \frac{1}{r}\frac{\partial v_z}{\partial r}\right) - g, \tag{2}$$

$$\frac{\partial v_r}{\partial r} + \frac{\partial v_z}{\partial z} + \frac{v_r}{r} = 0. \tag{3}$$

[6] In such cases (at least for laminar flows) one can conquer by dividing the problem into two asymptotically related regimes—one near the wall (the boundary layer where viscous effects will dominate), and the other, far from the wall, where such effects are subdominant.

The acceleration due to gravity (g) is in the negative z-direction; v_z and v_r are, respectively, the velocities in the axial and radial directions; p is the pressure; ρ is the fluid density; and ν is the kinematic viscosity. Equation 3 expresses the continuity of the fluid. Equations 1 and 2 express the force balance. The accelerations on the left-hand-sides are due to a pressure gradient (from surrounding the air), viscous stresses, and to gravity (in the z-direction).

These equations are subject to two boundary conditions. The first comes from a balance of normal forces

$$\mathbf{n}\sigma\mathbf{n} = -\gamma\left(\frac{1}{R_1} + \frac{1}{R_2}\right), \tag{4}$$

and the second from a balance of tangential forces

$$\mathbf{n}\sigma\mathbf{t} = 0. \tag{5}$$

Here σ is the stress tensor and γ is the surface tension and Eq. 4, called the "Young-Laplace equation," says that the stress within the fluid normal to the interface and near the surface must be balanced by a stress that acts normal to the surface due to surface tension. The formula "$(1/R_1 + 1/R_2)$" appearing here is equal to twice the mean curvature of the surface Ω at the point of evaluation. Equation 5 expresses the fact that sheer stresses vanishes at the interface. It is possible to express the mean curvature in terms of the radial "shape" function $h(z, t)$.[7] This allows us to write the equation of motion for $h(z, t)$ as follows:

$$\frac{\partial h}{\partial t} + v_z\frac{\partial h}{\partial z} = v_r\mid_{r=h}. \tag{6}$$

This says that the surface must move with the fluid at the boundary.

These equations define a difficult and complex moving boundary value problem. We are interested in what happens near the point at which the fluid breaks—at the singularity. Prima facie, that should make the problem even more difficult, as nonlinear effects will dominate. Nevertheless, by focusing on the behavior of the fluid near the singularity, it is possible to simplify the problem dramatically and provide exact solutions to these equations. (This is the modeling recipe mentioned above.) There are two aspects of the problem that allow this to happen.

The first (Eggers 1995, p. 942) derives from the fact that, near breakup, the axial extension of the fluid is much greater than its radial extension. This allows us to make the simplifying assumption that the singularity is line-like. In turn this allows us to find a one-dimensional solution to the full Navier–Stokes equations by introducing a characteristic axial length scale l_z that is related to a radial length scale l_r according to the following scheme:

$$l_r = \epsilon l_z, \tag{7}$$

[7] See Eggers (1995).

where ϵ is a small parameter. If, in addition, we introduce a characteristic time scale t_z we can nondimensionalize the quantities appearing in above equations. The characteristic scales l_z, l_r, and t_z are, of course, constants and so have zero time derivatives. Nevertheless, as the singularity forms, these characteristic scales will be different at different stages of the singularity formation (Eggers 1995, p. 942).

The second feature of the moving boundary problem that allows for simplification is the fact that near the singularity, surface tension, viscous forces, and inertial forces all become equally important (Eggers 1995, p. 942). Surface tension is related to the radius of curvature which diverges at the singularity, viscous forces are also important, and inertial forces must also be considered as the fluid velocity is increasing with greater pressure gradients due to the increasing curvature. Given this, the fluid acceleration diverges leaving the constant acceleration of gravity out of the picture near the singularity.

Furthermore, *and this is extremely important*, close to the singularity, all of the length scales become arbitrarily small in comparison with any external length scale such as the nozzle size of the faucet. This is an indication that one should expect the singular solutions of the one-dimensional Navier–Stokes problem to possess *similarity* or *scaling* properties. To a large extent and for a wide range of fluids, this turns out to be the case.

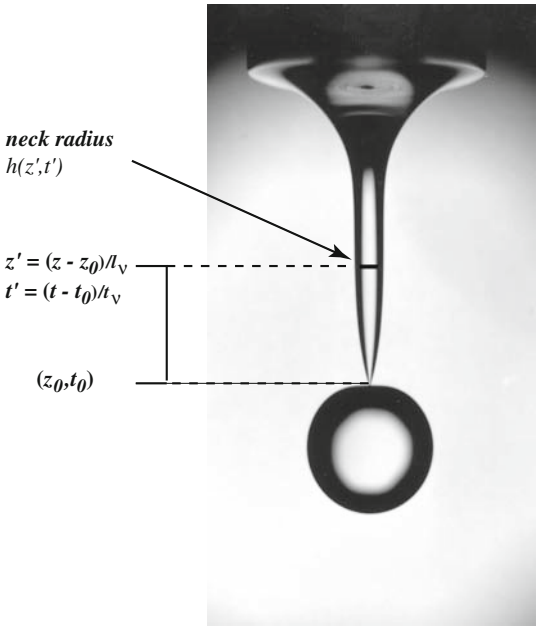
It is worth stressing the importance of discovering a similarity solution to a physical problem. This discovery will mean that one can expect essentially identical behavior in the system when "viewed" at different (appropriately chosen) scales. Such solutions are crucial in standard cases of modeling in which one builds a model, experiments with it, and then argues that the same observed properties will hold at different scales. For instance, consider the investigation of the aerodynamic properties of wings through experimentation on model wings in a wind tunnel.[8] In addition, however, the existence of similarity solutions and their corresponding scaling laws play essential roles in our understanding of why different systems exhibit identical or nearly identical behavior when described in the appropriate (dimensionless) variables. Another way of putting this is to say that the existence of a similarity solution is an indication of a kind of robustness or stability of the phenomenon under perturbation of various details. This, will become clear as the argument below progresses.

Returning to the process of drop formation, recall the following fact. "External" length and time scales that are determined by the initial conditions and the boundary conditions become irrelevant in the description of the singularity. This is critical for our understanding of the nature of the singularity. It means, for example, that it is possible to describe the flow near the breakup using only "internal" length and time scales, defined in terms of the fluid parameters. One introduces the so-called viscous length scale and the viscous time scale as follows:

$$l_v = \frac{\rho \nu^2}{\gamma} \tag{8}$$

[8] An excellent discussion of dimensional analysis, similarity solutions, scaling laws can be found in Barenblatt (2003).

Fig. 3 Water droplet at breakup



$$t_\nu = \frac{\rho^2 \nu^3}{\gamma^3} \tag{9}$$

These scales imply that when the viscosity ν is doubled, the breakup will look the same at length scales four times as large and at time scales eight times as large. This is an instance of scaling.

On the supposition that the breakup occurs at a single point z_0, and at an instant t_0, we can measure spatial and temporal distance from the singularity in terms of the dimensionless variables:

$$z' = \frac{z - z_0}{l_\nu} \tag{10}$$

$$t' = \frac{t - t_0}{t_\nu}. \tag{11}$$

See Fig. 3.[9]

In effect, the scales l_ν and t_ν characterize the width of the critical region around the singularity. For a specific fluid, they are fixed constants and do not change with time as do the characteristic scales mentioned above (l_z, l_r, l_t).

[9] The pictures of water drops in Figs. 3–6 are courtesy of Sidney R. Nagel and appear in Nagel (2001).

It is possible now to demonstrate that a scaling or similarity solution in the variables z', t' exists that describes the drop radius or shape function

$$h(z', t') = |(t')|^{\alpha} \Phi(\xi), \tag{12}$$

where the similarity variable ξ is defined as follows.

$$\xi = \frac{z'}{|t'|^{\beta}}. \tag{13}$$

One can determine the values of the scaling exponents α and β from dimensional analysis. Eggers then shows, both analytically and numerically, that the similarity solution (12) does hold for the problem. One finds the function Φ by inserting the similarity solution into a nondimensionalized version of the fundamental differential Eq. 6.[10] Furthermore, such a solution is in excellent agreement with the full solutions for the (one-dimensional) Navier–Stokes equations at low viscosities.[11]

The existence of such a similarity solution in the variable ξ indicates that the shape of breaking drops is universal. One can see evidence of this by examining the shapes in Figs. 4 and 5.

Notice the cone-to-sphere shape in Fig. 4 and note the *identical* shape at the top of the about-to-break satellite drop in Fig. 5. This demonstrates that how the drop is formed (whether, for instance, it drips solely under the influence of gravity or is sprayed in the air by a crashing wave) is irrelevant for the shape it takes on as it breaks.[12]

In fact, this similarity solution characterizes an entire *class*—a universality class—of fluids at breakup. This class is, in part, determined by the ratio of the viscosity of the fluid to the viscosity of the surrounding medium. For example, the shape of water drops dripping from a faucet surrounded by air (Figs. 4, 5) in which $\nu_{int} \gg \nu_{ext}$ is different than that of a drop forming in a fluid surrounded by another fluid of approximately the same viscosity (Fig. 6) where $\nu_{int} \approx \nu_{ext}$.[13]

That these shapes are to be expected is completely accounted for by the nature of the similarity solution (12) just prior to breakup. Furthermore, Eggers has shown that for scales sufficiently larger than the microscopic, it is actually possible to continue, uniquely, the similarity solution before breakup to one that holds beyond the singularity, after breakup. At breakup some molecular mechanism must come into play, but the uniqueness of this continuation is an indication of the self-consistency of the hydrodynamic description. *The striking conclusion is that the evolution of the fluid both before and after breakup is independent of the molecular microscopic details.*

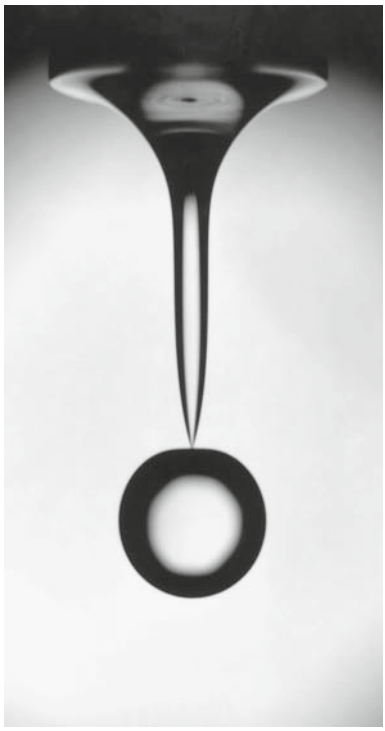
[10] This equation is nondimensionalized using Eqs. 10 and 11.

[11] Shi et al. (1994) argue that Eggers' and Dupont's solution needs to be corrected as there are perturbations (noise) that play an essential role in determining the character of the fluid shape near breakup.

[12] See Nagel (2001).

[13] Interestingly, Doshi et al. (2003) have recently demonstrated a third regime, characterized by $\nu_{int} \ll \nu_{ext}$ that fails to exhibit universal behavior. The breakup profiles in this latter regime are nonuniversal and depend upon initial and boundary conditions in a way that the other two regimes do not.

Fig. 4 Water droplet at breakup



So the existence of the scaling solutions to the one-dimensional Navier–Stokes equations provide evidence for the universality of the phenomenon. And, as a result, it is possible to explain why different fluids, of different viscosities, dripping from different nozzles, etc., will exhibit the same shape upon breakup.

5 Molecular dynamics and simulations

Let me now describe the drop breakup problem from the point of view of state-of-the-art simulations in molecular dynamics. (After all, as just noted, some molecular mechanism must be involved near breakup.) Moseler and Landman (2000) investigate the formation, stability, and breakup of jets at the nanolevel.They model propane as it is injected into a vacuum through a nozzle of diameter 6 nm. The simulation involves following approximately 200,000 propane molecules as they are pushed through a nozzle composed of gold molecules at various pressures. The molecules interact according to the Lennard-Jones 12-6 potential:

$$\phi_{\mathrm{LJ}}(r) = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^{6} \right], \tag{14}$$

where ϵ and σ are, respectively, energy and length scales appropriate to the materials. The term proportional to $(\frac{1}{r^{12}})$ dominates at short distances and represents the repulsion

Fig. 5 Water droplet after breakup

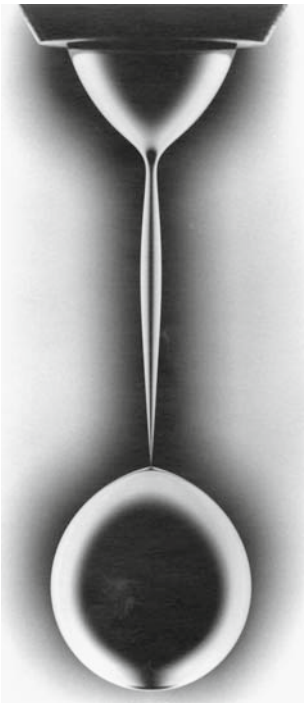
between molecules in very close proximity to one another. The $(\frac{1}{r^6})$ term dominates at large distances and represents the attractive forces between the molecules. Thus the potential has an attractive tail at large r, reaches a minimum near $r = 1.122\sigma$, and is strongly repulsive for $r < \sigma$.[14]

The nanojets in Fig. 7 were simulated by pressurizing the nozzle downstream at 500 MPa and with a controlled temperature at the nozzle of 150 K.[15] This results in a 200 m/s flow velocity for the jet. For $t < 1$ nanosecond following the initial exit of the fluid, the flow exhibits transient behavior. One can see the beginnings of the formation of fast moving droplets and molecular clusters in this initial period, and after that one sees the formation of necking instabilities resulting in breakup and the formation of drops. Moseler and Landman note that for $t \geq 1$ns, a steady state is

[14] The use of the Lennard-Jones potential is justified in investigation of this sort (interactions between closed-shell atoms) for the following reasons. It exhibits long-range van der Waals attraction, extremely strong short-range repulsion and has a potential well. Given these features, along with its relative ease of computational implementation, it is the potential of choice for investigations into generic properties of many molecular dynamical interactions. For a detailed discussion of molecular dynamical simulations see Ercolessi (1997).

[15] Figures 7 and 8 are courtesy of Uzi Landman and appear in Moseler and Landman (2000, p. 1166 and p. 1168, respectively).

Fig. 6 Two fluid breakup: $v_{\text{int}} \approx v_{\text{ext}}$



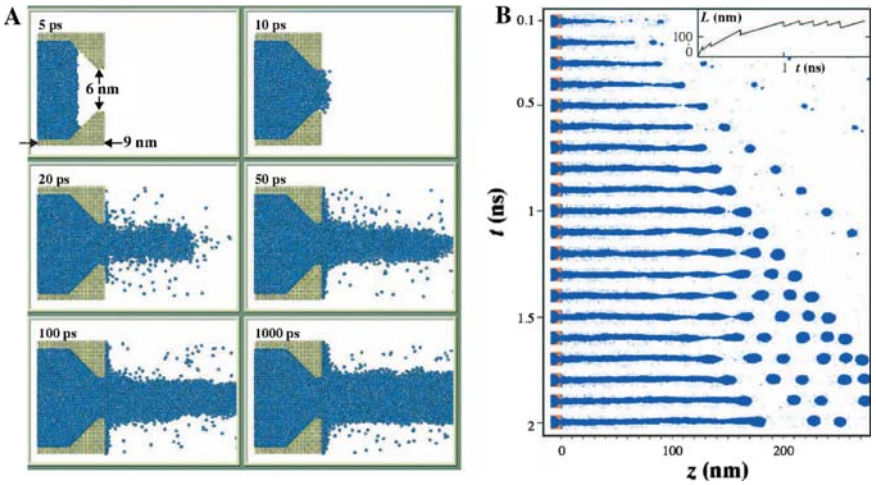


Fig. 7 Formation of nanojets

achieved with an average breakup length of 170 nm. They report that, upon repeated simulations, the typical shape at breakup resembles a double cone as shown in Fig. 8b and the upper image in Fig. 8d. Occasionally, however, they witness the formation of nonaxisymmetric necks as in Fig. 8a and an elongated neck configuration as in Fig. 8c

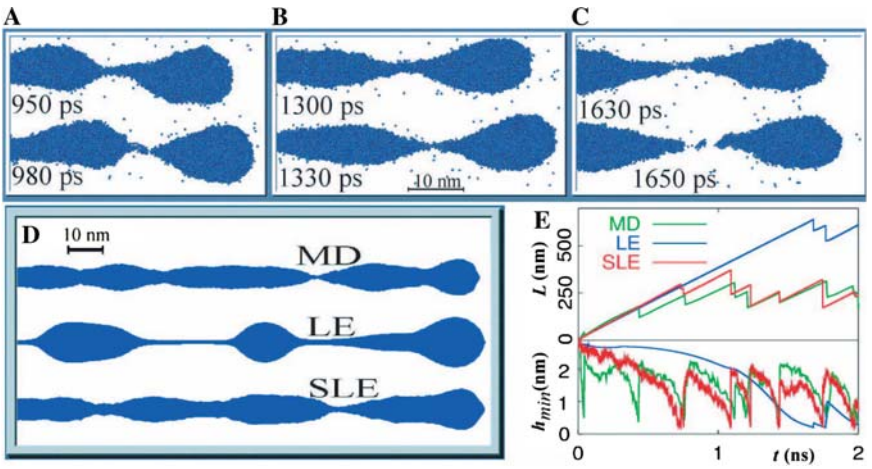


Fig. 8 Molecular dynamical configurations of nanojets

which was accompanied by the formation of small "split-off" molecular clusters or "satellite drops".

If we suppose that the hydrodynamic equations discussed in the last section could apply to the nanoscale drop formation problem, then we would expect the propane (at the nanoscale) to be quite viscous. (Even though, at larger scales, propane is surely not very viscous.)[16] Viscous fluids such as glycerol or honey exhibit long necks prior to breakup. (Just think about the honey that you drip into your cup of tea, or the maple syrup you pour over your pancakes.) In fact, Moseler and Landman apply the hydrodynamic equations (particularly, Eq. 6) and show that as expected for a viscous fluid, the propane jet should develop long necks prior to breakup. This is shown in Fig. 8d and is the simulation labelled "LE" for "lubrication equations."

The discrepancy between the double cone shape of the the molecular dynamical simulation and the hydrodynamic description of the same process is a direct indication that continuum deterministic hydrodynamics fails to apply at the nanoscale. Large hydrodynamic fluctuations become important at the nanolevel signaling a break down of the deterministic continuum description. As Moseler and Landman note,

> …the continuum description of such small systems requires the use of exceedingly small volumes, each containing a very limited number of particles, and consequently, continuum variables associated with such small volume elements, which represent (local) averages over properties of the microscopic constituents are expected to exhibit large fluctuations. (Moseler and Landman 2000, p. 1168)

[16] The reason for this depends upon the scale of observation. For "macroscopic" observation, the scale (l_{obs}) is on the order of one micron (10^{-6} m), and at this level of observation the ratio $l_{\text{obs}}/l_{\nu} \gg 1$. This ratio is what we expect for low viscosity fluids such as water that yield the asymmetric cone-to-cap shape at breakup. However, at the nanolevel—at the level of molecular dynamics—l_{obs} is on the order of a few *nanometers* (10^{-9} m). At this level, $l_{\text{obs}}/l_{\nu} \ll 1$. This ratio holds of viscous fluids such as glycerol and leads to an expectation of thin neck formation prior to breakup (Moseler and Landman 2000, p. 1167).

Moseler and Landman introduce a stochastic term (Gaussian noise) into the hydrodynamic equations and solve the stochastic continuum equations. They demonstrate remarkable agreement with the dominant double cone shape of the molecular dynamical simulations. This agreement is displayed in Fig. 8d. Compare the top molecular dynamical run with the stochastic continuum equations labelled SLE. This agreement "strongly suggests that in [nanojets] the very nature of the dynamical evolution is influenced strongly by hydrodynamic fluctuations, deviating in a substantial way from the behavior predicted through the analysis of the deterministic [continuum equations]" (Moseler and Landman 2000, p. 1168). Further analysis shows that it is possible to see the failure of the deterministic continuum equations as a consequence of a new length scale becoming important at the nanolevel. Moseler and Landman introduce this so-called "thermal capillary length" that for most materials is on the order of interatomic distances.

The fact that a new length scale becomes important at the nanolevel is, according to Moseler and Landman, further indication that the universality described above (provided by the scaling solutions to the Navier–Stokes equations) breaks down. As they say,

> The appearance of an additional length scale in the [stochastic continuum] simulations …is a direct consequence of the extension to include temperature-dependent stress fluctuations, and its magnitude determines the nature of the jet evolution, including the appearance of *solutions other than the universal ones predicted through the deterministic [continuum equations]*. (Moseler and Landman 2000, p. 1168, My emphasis.)

Let me make a few observations and pose a couple of questions concerning the molecular dynamical simulations and their potential for providing explanations for certain aspects of very small-scale drop phenomena. First of all, notice that every molecular dynamical simulation of nanojet formation is different.[17] The images in Fig. 8a–c attest to this. While Moseler and Landman assert that "[t]he most frequently observed breakup process [exhibits] close to pinch-off formation of an axisymmetric double cone shape of the neck …," this amounts to a statistical claim based solely upon generalizations from different simulation runs (Moseler and Landman 2000, p. 1168). And, while it is sometimes appropriate to say that the explanatory buck must stop somewhere, one might, in this situation, ask for an explanation of why *this* is the statistically dominant shape for nanojet breakup.

As we have seen, one important virtue of the scaling solutions to the Navier–Stokes equations discussed in Sect. 4 is that they allow for exactly such an answer to the analogous explanatory why-question on larger scales. We can explain and understand (for large scales) why a given drop shape at breakup occurs and why it is to be expected. The answer depends essentially upon an appeal to the existence of a genuine singularity developing in the equations of motion in a finite time. It is because of this

[17] One might think that this is merely an artifact of simulation and that it counts against treating the molecular dynamical simulations as genuinely providing *theoretical* information about the formation of nanojets. This would be a mistake. The differences in simulations can be attributed to difference in initial conditions, and, as a result, are to be expected.

singularity that there is a decoupling of the breakup behavior (characterized by the scaling solution) from the larger length scales such as those of the faucet diameter. Without a singularity, there is no scaling or similarity solution. *Thus, the virtue of the hydrodynamic singularity is that it allows for the explanation of such universal behavior*. The very break-down of the continuum equations enables us to provide an explanation of universality. This is completely analogous to the renormalization group explanation of the universality of critical phenomena.[18]

No such explanation—one that appeals to a singularity to explain the statistically universal double cone structure, is available from the "fundamental" theory employed in the molecular dynamical simulations. If one looks, for example, at any of the results presented in Fig. 8a, b, or c, one cannot locate the actual breakup location in either time or space. There is no well-defined singularity in the equations. And, of course, one would not expect there to be, since the Newtonian molecular dynamical equations do not develop singularities in finite times.

6 Analytical modeling versus simulation: a reconciliation?

So the question is whether it is possible to provide some kind of theoretical answer to the question of why the double cone structure is to be expected in nanojet breakup. Moseler and Landman show that if one introduces fluctuations into the continuum hydrodynamic equations, and solves those equations, the shape is similar to that typical of many molecular dynamical simulations. But the challenge is to understand the qualitative change in the breakup shape that occurs in the regime in which fluctuations apparently make a leading contribution to the shape function. To put this another way, we would like to have an account of the *statistical universality* of the double cone structure—one that provides the kind of understanding that the scaling solutions provide for the breakup profile at larger scales by demonstrating that most of the details of the evolution are by and large irrelevant.

In a paper entitled "Dynamics of Liquid Nanojets" Eggers (2002) provides the desired explanation. Eggers notes that Moseler's and Landman's stochastic continuum equations suggests that "hydrodynamics, at least when suitably generalized to include fluctuations, is fully capable of describing free surface flows down to the scale of nanometers" (Eggers 2002, p. 084502-1). There is a simple physical argument to understand what goes on at the nanolevel. One can think of the random noise introduced into the continuum equations as representing a kind of effective force that is generated by the fluctuations.

> [A] random fluctuation which increases the thread radius also increases its effective mass, slowing down the motion. Any fluctuation towards a smaller neck radius, on the other hand, accelerates the motion. On average, the fluctuations thus drive the thread towards breakup, in fact more effectively than surface tension …(Eggers 2002, p. 084502-2)

[18] See Batterman (2005) for a discussion.

As Eggers notes, however, conventional perturbative analysis around the deterministic continuum solution cannot describe this mechanism. This is because the fluctuations—the noise—makes the dominant contribution. The idea that one can average about a fixed time

> no longer makes sense for this problem, because there is a finite probability for pinchoff to have occurred, so the original formulation ceases to be valid. Thus a valid description has to be conditioned on the event of breakup to take place at a fixed time t_0. It is then natural to ask for the *most probable* sequence of profiles that brings one from the initial condition to a "typical" breakup event. (Eggers 2002, p. 084502-2)

Eggers develops an ingenious and difficult argument involving path integrals to determine probability of the "optimal" path to breakup. For our purposes here, the interesting feature is that to solve this problem he needs to *assume*, for a fixed breakup time t_0, that the solution is *self-similar*. He finds that the unique solution, on this assumption, is the symmetric profile of a double cone unlike the asymmetric long-neck similarity profile for the deterministic equations. The crucial feature is that the similarity solution is only possible on the assumption that there is a *singularity* at t_0 in the (stochastic) hydrodynamical equations. The result is an explanation for why such a symmetric profile seen in the *molecular dynamical simulations* is to be expected—one that is grounded in the "less fundamental" continuum theory of hydrodynamics.

A further consequence of this explanation is that we can understand why so few satellite drops are formed in nanojets and why there is a very narrow distribution in the size of the droplets that are formed. If one looks back at Fig. 5, one sees that a satellite drop is about to detach itself from the nozzle at the upper end of the picture. This is a consequence of the asymmetric, long-neck nature of the dripping process. That smaller satellite molecular clusters, such as that in Fig. 8c, are unlikely to form is a direct consequence of the universality of the double cone profile for nanojets. They occur only for large fluctuations in the neck region; and such fluctuations are statistically rare.

So, surface tension driven pinching at larger scales essentially determines the breakup time. Nevertheless, at times very close to that, a different process dominated by fluctuations takes over, speeding up the breakup at the nanoscale. The transition between these different scaling regimes can be understood in terms of the emergence, as one approaches the nanolevel, of a new length scale—the thermal capillary length. Most importantly, however, our understanding of this transition and of the universality of the different profiles, depends essentially upon the development of finite time singularities in the continuum hydrodynamical equations. These singularities entail that the breakup behavior at small length and time scales decouples from larger length and time scales. The details of the molecular dynamics drops out of our explanation of the origin of the different universality classes. Thus, the very breakdown of the continuum equations enables us to provide an explanation of the universal shapes.

However, from the point of view of pure molecular dynamical simulation, we can have no explanation of the universal shape of breaking drops and jets. The molecular dynamical equations do not exhibit any singularities—there are no blow-ups allowing for the scaling solutions that is required for this sort of understanding.

7 Conclusion

Fowler's characterization of the nature of idealization in mathematical modeling conforms well with what I have called the traditional conception. Recall that from that point of view, idealizations are pragmatically justified and (paradoxically) receive their ultimate warrant from the "fact" that they are to be (can in principle be) eliminated by further work on the details. In the context of our discussion of the nanojet simulations, one can think of the simulations as attempts to provide all of those details—to fully de-idealized a continuum description by tracking all of the molecular motions. Such simulations do surely provide significant and interesting information about the nature of those dynamical systems.

However, one lesson to be learned from this discussion is that, sometimes at least, such simulations do not tell us the whole story. The understanding of the process that they provide is only partial. They cannot, I have argued, provide an explanation for the universality of the shapes that appear in the jets at breakup. The gaps in the full story *can*, as I have tried to show, be filled in by employing (limiting) idealizations—idealizations that are ubiquitous in the mathematical analysts' approach to modeling. In particular, by appealing to the idealized continuum theory of hydrodynamics. Furthermore, it seems that these idealizations are in many instances explanatorily *ineliminable*. That is to say, they play an essential role in the proper explanation of the phenomenon of interest. They are not, as the traditional view of the use of idealization in modeling suggests, put in only to be subsequently removed by more detailed work.

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