(a) (b) (c)

Figure 3. Continuum dislocation dynamics. Simulation results at t = 1.0 of our CDD Equation 1 at different grid sizes (h), starting from a smooth initial condition. (a) h = 1/128, (b) h = 1/256, and (c) h = 1/512. We use periodic boundaries in both horizontal and vertical directions, and all physical quantities are constant along the perpendicular direction.

look significantly different as the grid spacing decreases. Again, this is analogous to the corresponding simulations of our dislocation dynamics shown in Figure 4, where larger cells continue to distort and shift as the grid spacing decreases.

Simulation Analysis

If the simulations aren't convergent, how can we decide if the theory is physically relevant and can be trusted to interpret experiments? In turbulence, it has long been known that, as vortices develop, self-similar patterns arise in the flow and exhibit power laws in the energy spectrum and in the velocities' correlation functions.[10] A successful simulation of fully developed turbulence isn't judged by whether the flow duplicates an exact solution of Navier-Stokes! Turbulence simulations study these power laws, comparing them to analytical predictions and experimental measurements.

Our primary theoretical focus in our plasticity study[3] has been to analyze power-law correlation functions for the dislocation density, plastic distortion tensor, and local crystalline orientation. As Figure 5 shows, like turbulence simulations, these statistical properties seem to converge nicely in the continuum limit.

It's worth noting that, in both cases, nonconvergence emerges when small-scale features appear on the wall (see Figure 6) or the interface (see Figure 7).

In the case of our simulations of plastic flow (Equation 1), starting from smooth initial density profiles, finite time singularities develop in the form of -shocks. The existence of finite-time singularities was shown in a 1D variant of these equations, which is associated with the Burgers equation.[11] Figure 6 shows how this effect occurs by considering the two-norm differences (the integrand in space of the L_2 norm discussed earlier). At t = 0.04 (see Figure 2a), when the N = 512 curve starts to cross all the other curves, singular features start to appear around a wall (as in Figure 6b). Although the boundaries are nonconvergent when specific locations and times are considered (Figure 2a), the statistical properties and associated self-similarity (Figure 5) are convergent.

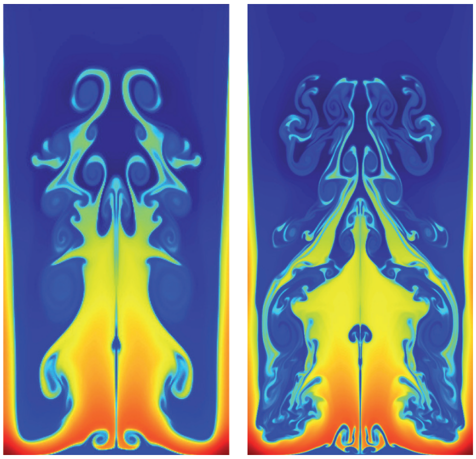
(a) (b) (c)

Figure 4. The Rayleigh-Taylor instability of the Navier-Stokes equation. The Rayleigh-Taylor instability is a fluid-mixing phenomenon that occurs when an interface between two different fluid densities is pulled by gravity. These simulation results here are of the Rayleigh-Taylor instability at t = 4.0, for $\mu \to 0$, at different grid spacings (h) with periodic boundaries in the horizontal direction and fixed boundaries along the vertical. (a) h = 1/128, (b) h = 1/256, and (c) h = 1/512. The initial condition has density interface with a single mode perturbation in the vertical velocity. The system size is (L_x, L_y) = (1.0, 2.0).

In the case of Navier-Stokes simulations (see Figure 7), the existence of finite-time singularities

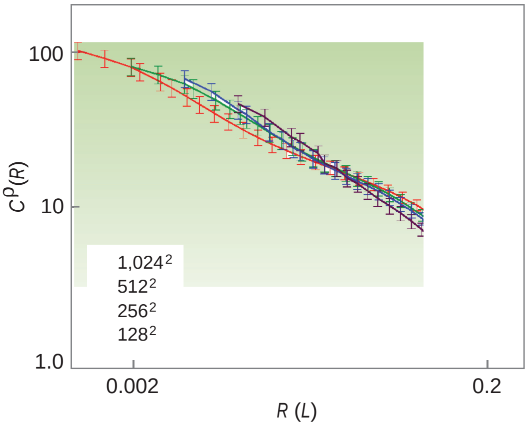

Figure 5. Statistical properties and convergence. Although the continuum dislocation dynamics (CDD) simulations with different grid sizes are nonconvergent (Figure 2a), the statistical properties are the same. The dislocation density correlation function is plotted here for different simulation sizes at the same time, exhibiting consistent power laws.

is a topic of active research: even though local-in-time analytic solutions are easily shown to exist, global-in-time analytic solutions can be proven to exist only for special cases, such as in the 2D incompressible genuine Euler equation.[12] In 3D, the mechanism of vortex stretching is conjectured to lead to finite-time singularities,[13] even though there are still crucial open questions. Despite its complexity, turbulence can be concretely studied in special cases. For our example of the Rayleigh-Taylor instability, the two-fluid interface gets distorted and bubbles form (Figure 3); over time, the bubbles exhibit emergent self-similar characteristics,[9] showing statistical convergence. However, there's no spatiotemporal convergence, because the interface develops complex, turbulent features as the grid becomes finer (see Figures 2b and 7).

Sometimes science seems to be fragmented, with independent fields whose vocabularies, toolkits, and even philosophies almost completely separate. But many valuable insights and advances arise when ideas from one field are linked to another. Computational science is providing a new source of these links, by tying together fields that can fruitfully share numerical methods.

Our use of well-established numerical methods from the fluids community made it both natural and easy to utilize their analytical methods for judging the validity of our simulations and interpreting their results.

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(a) (b) (c) (d)

Figure 6. Nonconvergence and singularity for CDD. (a) h = 1 256, (b) h = 1 512, (c) h = 1 256, and (d) h = 1 512. For (a) and (b), t = 0.04; for (c) and (d), t = 1.00. The two-norm difference between h and h/2 are plotted. At short time, t = 0.04, the differences are small: (a) is empty and (b) nearly so. At later times, t = 1.00, the two-norm difference becomes significant especially where the walls are forming (see Figure 4 for wall locations).