Noise in Algorithm Refinement Methods

Hybrid or algorithm refinement (AR) schemes have focused mainly on the mean behavior of system states. However, variances in these behaviors, such as spontaneous fluctuations, are important for modeling certain phenomena. This article discusses the effects of statistical fluctuations on hybrid computational methods that combine a particle algorithm with a partial differential equation solver.

Hybrid or algorithm refinement (AR) methods facilitate the simulation of multiscale phenomena (see the Guest Editors' Introduction on page 14). An important consideration when designing hybrid algorithms is how the coupling of two types of solvers impacts the accuracy of the individual methods. For the most part, the development and testing of these schemes have focused on the mean behavior of system states, such as the average density or temperature in a fluid hybrid. Yet simulations of many systems can require computing the higher moments (for example, variances) of these quantities, which capture spontaneous fluctuations. This is important for modeling phenomena in which the microscopic fluctuations drive a macroscopic phenomenon. Fluctuations, for example, initiate the onset of instabilities and the nucleation of phase transitions out of a metastable state.

This article focuses on fluctuations, in particular how different algorithms treat random variations and how these fluctuations affect the algorithms' coupling. Figure 1 shows a molecular simulation coupled to a continuum hydrodynamic calculation in which fluctuations of density, temperature, and so on occur in the former algorithm because of the particles' random motion. Correctly treating fluctuations is especially important for stochastic, nonlinear systems, such as those undergoing phase transitions, nucleation, noise-driven instabilities, or chemical reactions. In these and similar applications, the nonlinearities can exponentially amplify the fluctuations' strength and affect the phenomenon of interest.

Accurate simulations of these noise-driven phenomena must ensure that the noise is properly generated, propagated, and dissipated. The challenge is that particle and continuum methods treat noise in completely different ways. In the former, spontaneous fluctuations are inherent to the particle dynamics, as the phenomena of Brownian motion and self-diffusion illustrate. Continuum methods typically rely on partial differential equations (PDEs), which we can make stochastic by including the appropriate noise terms.[1] The challenge is ensuring that the numerical coupling of the particle and continuum computations doesn't adversely impact the underlying physics.

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Linear Diffusion

We begin by considering simple linear diffusion for a system modeled by particles (independent ran-

dom walkers) on the interval $x \in [0, I)$ and by the linear diffusion equation for the coarse-grained density $\rho(x)$ on the remaining interval $x \in [I, L]$, as Figure 2 illustrates. The right interval treats two cases of the diffusion equation: the deterministic case and the randomly fluctuating case.

During a time step, the walkers on the left side of the system move by random displacement. A handshake region, just right of the interface I, is filled with particles according to the density of the leftmost continuum cell. This boundary acts as a reservoir of particles coupling the continuum region to the particle region.

Specifying the mass flux across the interface $x = I$ couples the particle method, in turn, to the continuum calculation. Particles that "walk" across the interface during a time step define this flux between the particle and continuum regions. In addition to guaranteeing strict mass conservation, this yields favorable numerical stability.

For the bulk of the continuum region, Fick's law $F = -D\nabla\rho$ gives the mass flux for the deterministic case. For the stochastic case, we add a random component to the Fickian flux; this random flux is white in space and time with variance $2D\rho$.

This simple hybrid uses the same time step in the particle and discretized continuum regions, and, because we update the former before the latter, the algorithm requires no separate synchronization (that is, refluxing) at the time step's end. In more complicated applications, however, hybrid algorithms are likely to use much larger time steps in the region with coarse-grained computations. Then, the researcher should perform refluxing—that is, correct the density according to the actual flux across the interface—when synchronizing the two regions.[2]

To analyze this relatively simple hybrid's robustness and accuracy, we conducted various computational experiments for both steady-state and time-dependent diffusion.[3] Although we've dealt with various boundary conditions, here we focus on deterministic Dirichlet boundary conditions $\rho = \rho_0$ prescribed at $x = 0$ and $x = 1$. Because of the system's linear nature, both deterministic and stochastic hybrids capture the mean behavior correctly.

Figure 3 shows that the deterministic hybrid significantly underestimates the density variance, except in the particle region ($x \in [0, I)$), well away from the interface $x = I$. This result is not entirely unexpected as there is no way to maintain fluctuations in the deterministic PDE region. On the other hand, the stochastic hybrid is within a statistical error of the variance's expected value, $\langle \delta\rho_{i;n}^2 \rangle = \rho_0/\Delta x$ (that is, the Poisson distribution). Note that the density variance doesn't reduce the fluctuations in the cells near the Dirichlet boundary (where $\rho_{1;n}$ is fixed) for either the deterministic or stochastic-PDE hybrids.

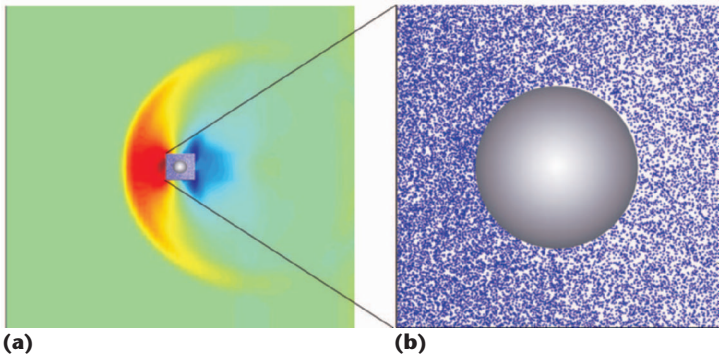

Figure 1. Example of a particle/continuum adaptive mesh algorithm refinement (AMAR) hybrid computation. (a) Pressure distribution for an impulsively started cylinder moving at Mach 2. (b) The simulation uses a hydrodynamic partial differential equation (PDE) solver everywhere except around the cylinder, where it performs a direct simulation Monte Carlo (DSMC) calculation.

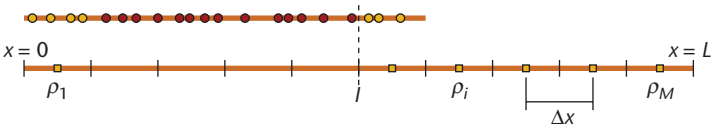

Figure 2. Algorithm refinement for simple diffusion. The region on the left shows a Monte Carlo random walk simulation, and the region on the right illustrates a PDE solver. The methods are coupled at the interface *I*; the algorithm generates new particles (open circles) in the handshaking region (right) and at the Dirichlet boundary (left).

These results clearly illustrate that even for a simple linear phenomenon, such as Fickian diffusion, hybrid methods require that researchers pay special attention to the implementation details. These range from the obvious, such as the dependence of time-dependent density on the specific particle initialization process, to the nontrivial, such as the dependence of a mean solution on the statistical distribution (for example, uniform or Poisson distributions) of particles used to fill the handshake region.

The very different constructions (discrete versus continuum) of the two algorithms complicate the mathematical analysis of AR hybrids. However, if a stochastic continuum solver couples transparently to a particle algorithm, we can use the former in place of the latter. That is, to analyze a hybrid that couples a particle scheme with a deterministic continuum scheme, we replace the particle dynamics

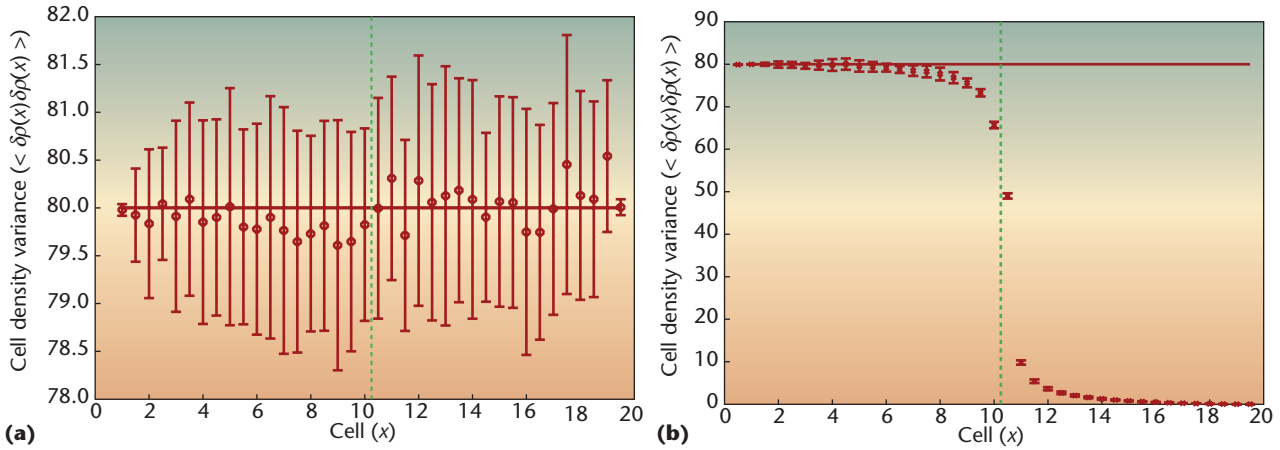

Figure 3. Density variance in the open equilibrium system. (a) Variance for cell $\langle \delta\rho^2_{i,n} \rangle$ using the stochastic hybrid, and (b) variance for cell $G_{i,i} = \langle \delta\rho^2_{i,n} \rangle$ using the deterministic hybrid (the same variance we'd find had the entire simulation been done using particles). The dashed line indicates particle/PDE interface; the solid line is $\langle \delta\rho^2_{i,n} \rangle = \rho_0/\Delta x$.

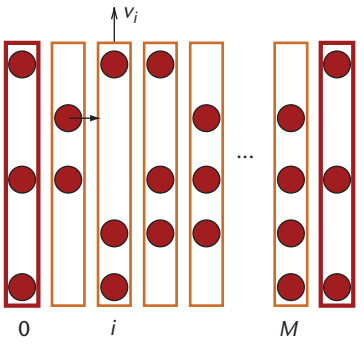

Figure 4. Schematic illustration of the train model, with *M* trains and two platforms. A passenger on train *i* – 1 jumps to train *i*, changing its velocity v_i.

with the corresponding stochastic diffusion equation in the region $x \in [0, I)$ while retaining the deterministic diffusion equation in the region $x \in [I, 1]$. We refer to this method as a *half-stochastic hybrid*.[3] Such a model is ideally suited for testing the effects of noise in hybrids because we're coupling two systems of the same type (both PDE solvers). Our studies indicate that the results from these half-stochastic hybrids are similar to particle/deterministic-continuum AR hybrids and far more amenable to theoretical analysis.

Particle/continuum AR hybrids could accurately model hydrodynamic fluctuations in Fickian diffusion when the appropriate stochastic PDE is used. However, this only gives us confidence in the methodology for linear systems. We therefore examine a more complicated model for which the noise amplitude is nonlinear.

Train Model

We generalize our analysis by considering a nonlinear system that intrinsically has long-range spatial correlations due to the nonlinearity of its stochastic fluxes. Specifically, we analyze a train model of viscous transport in a gas.[4] The train model falls into a general class of random walk models that exhibit these long-range correlations. Other models of this class include lattice gases[5] and the Knudsen chain.[6] These long-range correlations are generic to realistic hydrodynamic systems, as various theoretical approaches predict and numerical simulations and laboratory experiments confirm.[7–9]

One train model formulation[4] considers two railroad cars traveling on parallel tracks with initial velocities v_a and v_b. The train cars initially have N_a and N_b passengers, respectively; the passengers have mass m whereas the mass of the cars is negligible. Passengers jump at random between the trains at a rate $1/\tau$, where τ is the mean free time between a passenger's jumps to an adjacent train. The jumps from train a to train b result in the exchange of momentum mv_a, which preserves the velocity of train a, $v'_a = v_a$, and modifies the velocity of train b, $v'_b = N_b v_b/(N_b + 1) + v_a/(N_b + 1)$. Over a long time period, this random process reaches a steady state in which the mean number of passengers on each train car is $(N_a + N_b)/2$, and the mean velocity is $(N_a v_a + N_b v_b)/(N_a + N_b)$.

A generalized formulation of the train model[10] includes a set of cars on M parallel tracks (see Figure 4). Passengers on the trains jump left or right with equal probability, as in the unbiased random walk. Adjacent to the first and last tracks are plat-

forms moving with constant numbers of passengers N_0 and N_{M+1}, at constant velocities v_0 and v_{M+1}. These platforms act as reservoirs of passengers who jump at half the rate of train passengers because they can only jump in one direction. Starting from an initial state, a random passenger is chosen to jump in a random direction. A passenger jumping onto a train changes that train's velocity. If the passenger jumps from a platform onto a train, a new passenger is added to the system; vice versa, a passenger is removed. After each jump, the time is advanced by $(\tau/N_\Sigma)\Re_e$, where N_Σ is the total number of passengers in the system, and $\Re_e$ is an exponentially distributed random number. Florence Baras and colleagues discuss a numerical implementation of this particle (random walk) algorithm.[10]

A system of PDEs for the mass density $\rho(x, t)$ and the fluid momentum $p(x, t)$ gives a continuum description of the generalized train model

$$\frac{\partial \rho}{\partial t} = -\frac{\partial F(\rho)}{\partial x},$$

$$\frac{\partial p}{\partial t} = -\frac{\partial G(\rho, v)}{\partial x}, \qquad (1)$$

where F is the mass flux, G is the momentum flux, and $v = p/\rho$ is the fluid velocity. We establish the correspondence between these two descriptions by discretizing Equation 1 with, for example, finite differences

$$\frac{\rho_{i;n+1} - \rho_{i;n}}{\Delta t} = -\frac{\left(F_{i;n}^{+\rightarrow} - F_{i;n}^{+\leftarrow}\right) - \left(F_{i;n}^{-\rightarrow} - F_{i;n}^{-\leftarrow}\right)}{\Delta x}, \qquad (2)$$

where $\rho_{i;n} = \rho(x_i, t_n)$ with $x_i = (i - 1/2)\Delta x$ for $i \in [1, M]$, and $t_n = n\Delta t$ for $n = 0, 1, \ldots$. The superscript + (or –) indicates that the flux is through the side between cells i and $i + 1$ (or $i - 1$), and the superscript $\rightarrow$ (or $\leftarrow$) indicates that the term is the flux contribution caused by particles moving left to right (or right to left). If a grid point x_i is associated with a single discrete train i, then $N_i = \rho_i \Delta x/M$. For the mass density, the train model is equivalent to the linear diffusion model because the dynamics of the random walkers are independent of the trains' velocities. The equation for the momentum is similar to Equation 2, with the momentum flux directly linked to the mass flux as $G = vF$.

The boundary conditions fix the density and velocity of the first and last grid points (that is, a platform). In the particle simulations, the system immediately replenishes (or removes) the last grid point with particles as they leave (or enter). In the continuum simulations, we prescribe either a velocity gradient only, or both density and velocity gradients. The case of a density gradient only is equivalent to our earlier study of simple diffusion.

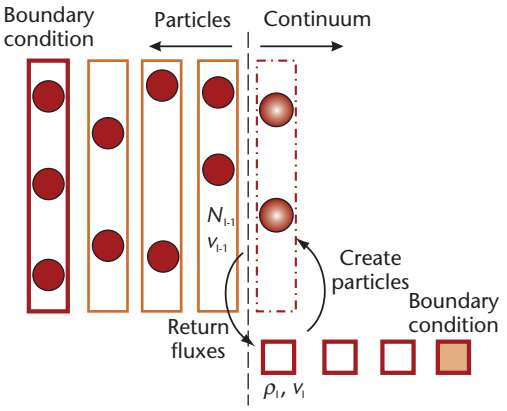

Figure 5. Algorithm refinement hybrid for the train model. We use particle simulation in the region on the left (from 0 to *I* – 1) and a PDE solver on the right (*I* to *M*), coupling the methods at the interface. The particle algorithm generates new particles (open circles) in the handshaking region (cell *k*) and at the Dirichlet boundary (left platform). For the continuum algorithm, we obtain the fluxes $F_{I;n}^{\leftarrow}$, $F_{I;n}^{\rightarrow}$ $G_{I;n}^{\leftarrow}$, and $G_{I;n}^{\rightarrow}$ (between cells *I* – 1 and *k*) from the particle computation.

An AR hybrid consists of a coupling of the particle and continuum descriptions, as Figure 5 shows. The particle and continuum simulations occur to the left and right of the dashed line, respectively. For simplicity, we take the continuum grid spacing Δx equal to the particle grid spacing (width of a train). We executed the simulations in 10^8 steps using a time step of $\Delta t = \Delta t_{\max}/20 = 0.025$, which is enough for solutions to reach steady state.

Similar to the linear diffusion analysis, we consider the deterministic and stochastic hybrids that are constructed by having the continuum solver use deterministic or stochastic currents, respectively. Because of the train model's weakly nonlinear nature, both deterministic and stochastic hybrids correctly capture the mean profiles of density $\langle \rho(x) \rangle$ and velocity $\langle v(x) \rangle$. Differences in the two hybrids' performance manifest in the higher statistical moments of ρ and v—specifically, their variances and correlations.

Figure 6 demonstrates that the stochastic hybrid accurately reproduces the correlation of velocity

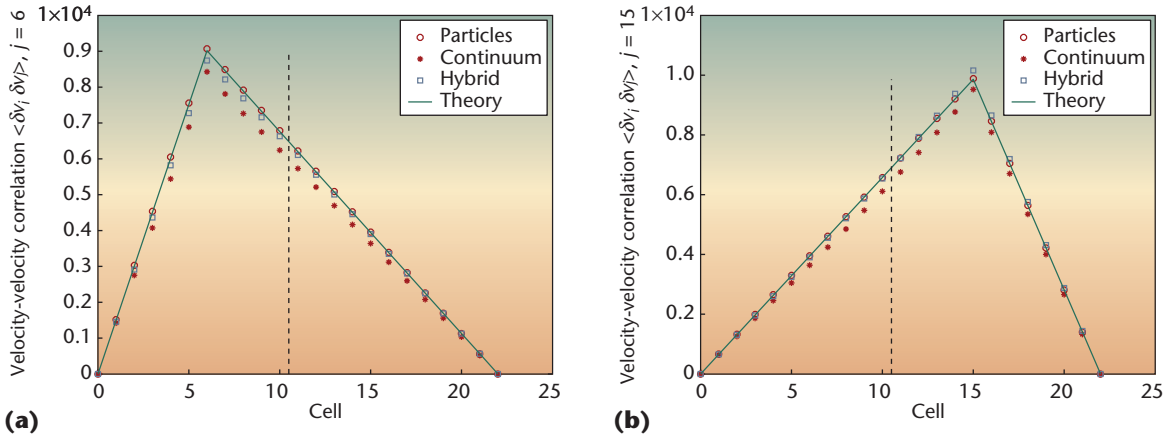

Figure 6. Results for stochastic hybrid. Velocity–velocity correlation $\langle \delta v_i \delta v_j \rangle$ as functions of position i for (a) $j = 6$ and (b) $j = 15$. The solid line is the theoretical result.

fluctuations when both velocity and density gradients exist. These results indicate that the AR hybrid with stochastic fluxes correctly captures the long-range nature of these nonequilibrium fluctuations. This result is significant because these long-range correlations are generic to hydrodynamic systems out of global equilibrium.[7]

Figure 7 shows the same quantities computed with the deterministic hybrids. The absence of noise in half the system (the deterministic PDE side) roughly reduces by half the amplitude of velocity correlations $\langle \delta v_i \delta v_j \rangle$, yet the correlations are still long-ranged, spanning the system's length.

This result contrasts the findings in our linear diffusion study. In that study, we showed that the variance of density fluctuations $\langle (\delta \rho_i)^2 \rangle$ goes quickly to zero in the simulation's deterministic region. No contradiction exists, however, because the long-range nature of hydrodynamic correlations is not due to the presence of noise throughout the system. Rather, the hydrodynamic transport propagates the correlation, and the hybrid correctly computes it. In other words, local fluctuations are produced in the particle region and propagated by the hydrodynamic transport, which is purely viscous in the train model, to produce the correlations.

In brief, the effect of long-range correlations is still present, albeit at a reduced amplitude, even if only one part of the hybrid is stochastic. On one hand, this result is good news because it means that even when using a deterministic PDE solver, which is far more common for AR hybrids, we can preserve some of the qualitative features of long-range correlations. On the other hand, reducing (or for that matter, enhancing) the fluctuations by a factor of two can greatly alter time-dependent behavior. This is a serious concern for modeling noise-driven phenomena where fluctuations and their correlations are often exponentially amplified (first-passage time problems, spontaneous transitions at unstable points, explosive ignition, and so on). Clearly, the nature of the physical process and the relative importance of fluctuations to the correct modeling of that process govern the construction of stochastic and deterministic AR hybrids.

Reducing the density variance in the particle region when coupled with a deterministic PDE necessitates placing the interface further away from regions in which the algorithm requires accurate fluctuations. Not taking such measures can have a deleterious effect when using a deterministic PDE solver in hybrids that simulate strongly interacting systems (for example, nonequilibrium solids and dense liquids). Our study focused on static (that is, equal-time) correlations of velocity fluctuations because they're long-range when the system is out of equilibrium, a generic feature of fluctuating hydrodynamics.[7] Hybrids that capture static correlations correctly should successfully reproduce dynamic correlations because the latter are given by the former plus hydrodynamic transport. That said, it would still be interesting to confirm this expectation by measuring time-dependent correlations in AR hybrids and comparing the results with pure particle systems. For some physical problems, generating time-dependent fluctuations and correlations cor-

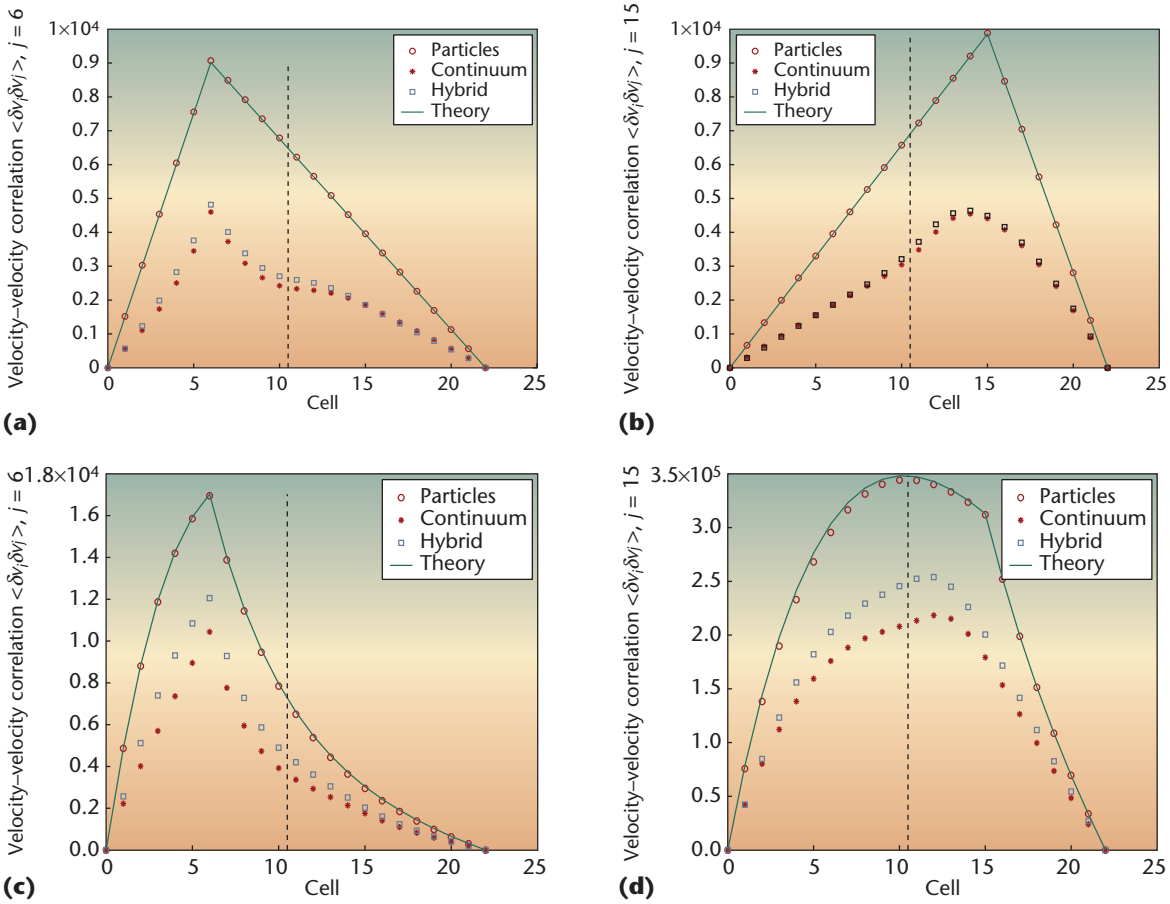

Figure 7. Results for deterministic hybrid. Velocity–velocity correlations as functions of position *i*. (a) Correlations $\langle \delta v_i \delta v_j \rangle$ for $j = 6$ and (b) $j = 15$ in the case of velocity gradient only. (c) Correlations $\langle \delta v_i \delta v_j \rangle$ for $j = 6$ and (d) $j = 15$ in the case of density and velocity gradients. Hybrid uses a deterministic PDE solver for the right-hand side of the system.

rectly will be crucial for accuracy.

Our future work will focus on strongly nonlinear systems. We're currently investigating AR hybrids that combine the fluctuating Burger's equation and the Landau fluctuating Navier-Stokes equations with corresponding particle algorithms (for example, DSMC for the latter).

For highly nonlinear equations or for systems with more general multiplicative noises, deterministic hybrids aren't guaranteed to yield mean values that are correct across the coupling interface, even in equilibrium. These cases require special care in constructing the hybrid; renormalized noises or effective potentials (from which we derive the PDE) might prove useful. This is likely to play an important role in nonlinear time-dependent Ginzburg-Landau models of solids and is currently under investigation.

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