Algorithm Refinement for Stochastic Partial Differential Equations

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Abstract. We construct a hybrid particle/continuum algorithm for linear diffusion in the fluctuating hydrodynamic limit. The particles act as independent random walkers and the fluctuating diffusion equation is solved by a finite difference scheme. At the interface between the particle and continuum computations the coupling is by flux matching, and yields exact mass conservation. This approach is an extension of Adaptive Mesh and Algorithm Refinement [*J. Comp. Phys.* **154** 134 (1999)] to stochastic partial differential equations. We present results from a variety of numerical tests, and in all cases the mean and variance of density are obtained correctly by the stochastic hybrid algorithm. A non-stochastic hybrid (i.e., using only deterministic continuum fluxes) results in the correct mean density, but the variance is diminished except in particle regions away from the interface. Extensions of the approach to other applications are discussed.

INTRODUCTION

An increasingly important and growing class of computational problems involves systems where the detail required for an accurate and effective description differs (possibly significantly) from one spatial region to another. One efficient approach to solving these spatio-temporal, multi-scale problems is to perform detailed calculations, using an expensive algorithm, only where absolutely required and coupling this computation to a simpler, less expensive method, which is used in the rest of the domain. Such "hybrid" methods typically couple (at least) two structurally (physically and algorithmically) different computational schemes, which are used in different regions of the problem (e.g., near and far from a shock or combustion front). One class of hybrids involves matching a continuum partial differential equation (PDE) solver to a particle method, such as Direct Simulation Monte Carlo ([1]-[7]) or Molecular Dynamics ([8]-[12]). Such a multi-algorithm approach, also known as Algorithm Refinement, is advantageous when the computational expense of a hybrid calculation is much less than that of performing the entire calculation using the more expensive of the two algorithms.

To make Algorithm Refinement a reliable numerical tool, one must address a variety of issues. From a numerical analysis perspective, one issue is how the marriage of two very different algorithms affects the accuracy of both the individual and combined methods. Another issue is that of noise. Until now, the testing of Algorithm Refinement schemes has focused on mean values such as average density, temperature, etc. Yet for simulations of microscopic systems, one is also interested in the variations of these quantities due to spontaneous fluctuations. This is likely to be important for modelling phenomena where the fluctuations themselves drive (or initiate) a large scale process, such as the onset of instabilities and the nucleation of phase transitions.

Here we address the issue of fluctuations in hybrids, focusing specifically those schemes that combine a particle algorithm with a partial differential equation solver. We consider both deterministic and stochastic partial differential equations. Our investigation deals with Fickian diffusion since much is known about solving the linear diffusion equation (LDE) in both its deterministic and stochastic forms. In addition, the microscopic particle process of independent random walkers rigorously converges to the LDE in the hydrodynamic scaling limit.

The outline of the paper is as follows: First we comment on the random walk model and the linear diffusion equation (LDE) including its stochastic form. Then numerical schemes for simulating this model and for computing this stochastic PDE are described. Following that we discuss ways to couple the two representations and present the

results of our numerical investigations, closing with a discussion of our results and a list of further directions.

SIMPLE DIFFUSION: PARTICLE AND CONTINUUM THEORIES

Consider the well-known random walk model. Specifically, take a system of N independent (i.e., non-interacting) particles that evolve according to the following stochastic dynamics

$$dX_k(t) = DdW_k, \tag{1}$$

where X_k is the location of particle k, D is the diffusion constant and W is a standard Wiener process [13].

Define the density of particles in a region

$$\rho(x,t) = \sum_{k=1}^{N} \delta(x - X_k(t)). \tag{2}$$

The Fokker-Planck equation for the random walker dynamics, in the hydrodynamic limit, yields the one-dimensional, fluctuating diffusion equation, [13]

$$\frac{\partial \rho}{\partial t} = -\frac{\partial F}{\partial x} = D\frac{\partial^2}{\partial x^2}\rho - \frac{\partial f}{\partial x}, \tag{3}$$

where F is the total particle flux, whose deterministic component is given by Fick's law, $-D\partial\rho/\partial x$. Its fluctuating component, f, is a Gaussian white noise with zero mean and correlation

$$\langle f(x,t) f(x',t') \rangle = A(x,t)\delta(x-x')\delta(t-t'), \tag{4}$$

where the angle brackets indicate an ensemble average. The noise amplitude, $A(x,t)$, is related to the equal-time correlation of density fluctuations, which is taken to be,

$$G(x,x') = \langle \delta\rho(x,t)\delta\rho(x',t) \rangle = \bar{\rho}(x,t)\delta(x-x') + C, \tag{5}$$

where $\delta\rho = \rho - \bar{\rho}$ and the deterministic density is given by the solution of

$$\frac{\partial \bar{\rho}}{\partial t} = D\frac{\partial^2 \bar{\rho}}{\partial x^2}, \tag{6}$$

with the same initial and boundary conditions as (3). For an open system (a system in contact with a particle or density reservoir) the constant $C = 0$; for a closed system of length L,

$$C = -\frac{N}{L^2} \qquad ; \qquad N = \int_0^L \rho(x,t)\,dx = \int_0^L \bar{\rho}(x,t)\,dx, \tag{7}$$

due to mass conservation. Given (5), the noise amplitude is [13]

$$A = 2D\bar{\rho}(x,t). \tag{8}$$

Note that for open systems the variance in the number of particles within an interval equals the mean number in that interval, as with the Poisson distribution; for closed systems the variance is reduced due to mass conservation.

SIMPLE DIFFUSION: PARTICLE AND CONTINUUM ALGORITHMS

The numerical simulation of the random walk model is straightforward: integrating both sides of (1) over a time increment Δt yields

$$X_k(t+\Delta t) - X_k(t) = \sqrt{2D\Delta t}\,\Re_k, \tag{9}$$

where $\Re_k$ are independent, Gaussian distributed random values with zero mean and unit variance. At each time step every walker is given a random displacement, as in Equation (9).

If we discretize space and time in the continuum formulation, we may write the stochastic diffusion equation, (3), as

$$\frac{\rho_{i;n+1}-\rho_{i;n}}{\Delta t} = -\left(\frac{F^+_{i;n}-F^-_{i;n}}{\Delta x}\right), \tag{10}$$

where $\rho_{i;n} = \rho(x_i,t_n)$ with $x_i = (i-\frac{1}{2})\Delta x$, $i = 1,\ldots,M$, and $t_n = n\Delta t$, $n = 0,1,\ldots$. The discretized fluxes (right and left) are

$$F^{\pm}_{i;n} = \mp D\left(\frac{\rho_{i\pm1;n}-\rho_{i;n}}{\Delta x}\right) + f^{\pm}_{i;n}. \tag{11}$$

The discretized correlation of the fluctuating particle flux may be written as [14]

$$\langle f^+_{i;n} f^+_{j;m}\rangle = \frac{(A_{i;n}+A_{i+1;n})\delta_{i,j}\delta_{n,m}}{2\Delta x\Delta t} \quad ; \quad \langle f^-_{i;n} f^-_{j;m}\rangle = \frac{(A_{i;n}+A_{i-1;n})\delta_{i,j}\delta_{n,m}}{2\Delta x\Delta t}, \tag{12}$$

and $F^+_{i;n} = F^-_{i+1;n}$, so

$$f^+_{i;n} = f^-_{i+1;n} = \sqrt{\frac{(A_{i;n}+A_{i+1;n})}{2\Delta x\Delta t}}\,\Re_{i;n}, \tag{13}$$

where $\Re_{i;n}$ are independent, Gaussian distributed, random variables with zero mean and unit variance.

Collecting the above yields a Langevin-type numerical scheme for the density,

$$\begin{aligned}\rho_{i;n+1} &= \rho_{i;n} + \frac{D\Delta t}{\Delta x^2}\left(\rho_{i+1;n}+\rho_{i-1;n}-2\rho_{i;n}\right) \\ &- \sqrt{\frac{D\Delta t}{\Delta x^3}}\left(\sqrt{\bar\rho_{i;n}+\bar\rho_{i+1;n}}\,\Re_{i;n} - \sqrt{\bar\rho_{i;n}+\bar\rho_{i-1;n}}\,\Re_{i-1;n}\right),\end{aligned} \tag{14}$$

since $A_{i;n} = 2D\bar\rho_{i;n}$.

This scheme is essentially the same as that presented in reference [14] for the Fourier (heat) equation except for the form of the noise amplitude. For mass diffusion the amplitude is linear in the density while for temperature diffusion it is quadratic in the temperature, which leads to long-ranged spatial correlations of equal-time fluctuations [14, 15, 16].

Using (14), the equal-time correlation function $G_{i,j} \equiv \langle \delta\rho_{i;n}\delta\rho_{j;n}\rangle$, is

$$\begin{aligned}4\left(1-\frac{D\Delta t}{\Delta x^2}\right)G_{i,j} &- \left(1-\frac{2D\Delta t}{\Delta x^2}\right)\left(G_{i,j+1}+G_{i,j-1}+G_{i+1,j}+G_{i-1,j}\right) \\ &- \frac{D\Delta t}{\Delta x^2}\left(G_{i+1,j+1}+G_{i+1,j-1}+G_{i-1,j+1}+G_{i-1,j-1}\right) \\ &= \frac{1}{\Delta x}\left(B_iB_j\delta_{i,j} - B_iB_{j-1}\delta_{i,j-1} - B_{i-1}B_j\delta_{i-1,j} + B_{i-1}B_{j-1}\delta_{i-1,j-1}\right),\end{aligned} \tag{15}$$

where $B_i = \sqrt{\bar\rho_{i;n}+\bar\rho_{i+1;n}}$. Note if the deterministic density is linear (i.e., $\bar\rho_{i+1;n}-\bar\rho_{i;n}$ is independent of i) then

$$\begin{aligned}&B_iB_j\delta_{i,j} - B_iB_{j-1}\delta_{i,j-1} - B_{i-1}B_j\delta_{i-1,j} + B_{i-1}B_{j-1}\delta_{i-1,j-1} \\ &\quad = 4\bar\rho_{i;n}\delta_{i,j} - \left(\bar\rho_{i;n}\delta_{i,j+1} + \bar\rho_{i;n}\delta_{i,j-1} + \bar\rho_{i+1;n}\delta_{i+1,j} + \bar\rho_{i-1;n}\delta_{i-1,j}\right).\end{aligned} \tag{16}$$

In the limit $\Delta t \to 0$, the static correlation is $G_{i,j} = \bar\rho_{i;n}\Delta x^{-1}\delta_{i,j} + C$, in agreement with the continuum result, equation (5).

The above formulation is somewhat cumbersome in that the deterministic PDE (6) must be evaluated separately to obtain the space and time dependent $\bar\rho$, since the noise amplitude is $A = 2D\bar\rho$. For the linear, stochastic diffusion equation we may extend the additive noise to be multiplicative, that is, $A = 2D\rho(x,t)$, in the limit where the fluctuations about the mean are small [17]. In the discrete numerical scheme, (14), we may replace $\bar\rho_{i;n}$ with $\rho_{i;n}$ in the noise terms; this generalization is tested and validated by the numerical simulations in SIMULATION RESULTS section.

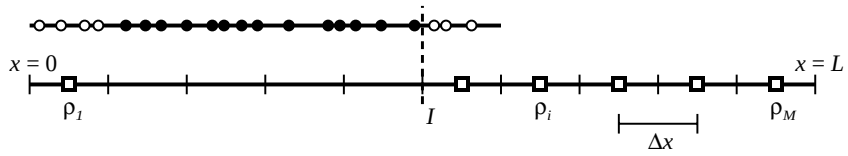

FIGURE 1. Algorithm Refinement for simple diffusion. A random walk simulation is performed in the region on the left and a PDE solver is used on the right. The methods are coupled at the interface I; new particles (open circles) are generated in the "handshaking" region (right) and at the Dirichlet boundary (left).

PARTICLE/CONTINUUM HYBRID ALGORITHM

Having presented the stochastic PDE corresponding to independent, random-walk particle dynamics and outlined the numerical schemes for each representation (particle and continuum), we now describe how to couple the two numerical methods. Figure 1 illustrates a typical hybrid calculation with a particle region within the interval from $x = 0$ to I; elsewhere the continuum density is specified at discrete grid points. For the purpose of statistical measurements and plotting *only*, the density in the particle regions is evaluated on the same grid as the discretized continuum calculation. Specifically,

$$\rho_{i;n} = \frac{1}{\Delta x} \sum_{k1}^{N} \delta[x_i - \tfrac{1}{2}\Delta x < X_{k;n} < x_i + \tfrac{1}{2}\Delta x], \tag{17}$$

where $X_{k;n}$ is the position of particle k at time $t = n\Delta t$; the boolean delta function is defined as $\delta[A] = 1$ if A is true, and 0 otherwise. Initially, a density is assigned to all M grid points and particles are generated within the particle region.

At the beginning of a time step, the particle region is extended by one grid point into the continuum region. This added "handshaking" region is uniformly filled with $N_{i;n}$ particles according to the density of the underlying grid point, taking $N_{i;n} = \rho_{i;n}\Delta x$, rounded to an integer. Other ways of filling the region were tested (nonuniform distribution of particle positions using $\nabla\rho$, Poisson distribution for $N_{i;n}$ with mean $\rho_{i;n}\Delta x$, etc.) but were found to give equal or poorer results. All particles, in the handshaking region and elsewhere, are then displaced as $X_{k;n+1} = X_{k;n} + \delta X_{k;n}$ where the distance $\delta X_{k;n} = \sqrt{2D\Delta t}\,\Re_{k;n}$ (see equation (9)). The number of particles crossing the interface gives the number flux at I, this flux is recorded and used in the continuum portion of the computation (see below) . Any particles that end their move outside the particle region are removed from the simulation.

Once the particle update is complete, (11) is used to compute the left and right number fluxes for each continuum grid point *except* for the grid point adjacent to the particle region. For that point, the number flux recorded during the particles' motion is used instead of F^-. The number density on the continuum grid is computed using (10), which is equivalent to using (14) for non-interface grid points. This completes one time step for the hybrid.

Notice that because the particle region and discretized continuum regions use the same time step and because the former is updated before the latter, no separate synchronization (i.e., "refluxing") is required at the end of a time step. The algorithm can also be formulated using different time steps; the region using the larger time step (typically the continuum calculation) is evaluated first and refluxing (i.e., correcting the density according to the actual flux across the interface) is performed when the two parts are synchronized [7].

Both stochastic and non-stochastic (i.e., deterministic) PDE solvers are tested. In the former, the noise amplitude is computed using the *instantaneous* value of the local density; in the latter, $A_{i;n} = 0$. The deterministic method is similar to that used earlier in particle/continuum hybrids for fluid mechanics (e.g. the DSMC/Euler hybrid in [7]).

Dirichlet boundary conditions are used in our simulations, that is, $\rho_{1;n}$ and $\rho_{M;n}$ have fixed (mean) values. If either of these cells is within the particle region, then the cell is re-initialized with a number of particles selected randomly from a Poisson distribution with means $\rho_{1;n}$ and $\rho_{M;n}$, respectively. The particles are then distributed in the same fashion as the handshaking region. If the density is fixed at a boundary grid point in the stochastic PDE region, then the density at each time step is drawn from a Poisson distribution with the appropriate mean value.

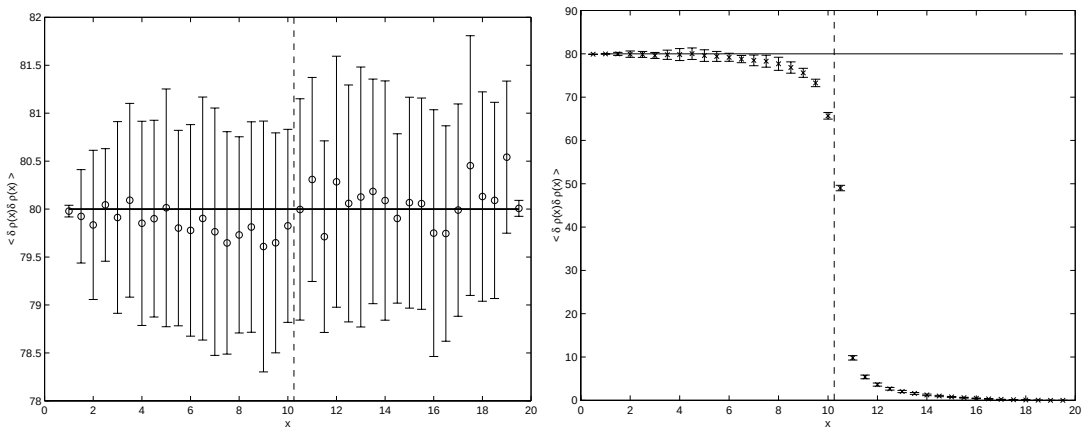

FIGURE 2. Variance of density in a cell, $G_{i,i} = \langle \delta\rho_{i;n}^2 \rangle$, for the open, equilibrium system. The data from the particle/stochastic-PDE hybrid (left) and from the particle/deterministic-PDE hybrid (right) are shown; solid line is $\langle \delta\rho_{i;n}^2 \rangle = \rho_0/\Delta x$; dashed line indicates particle/PDE interface.

SIMULATION RESULTS

Open, equilibrium system

The first test case is an open system in equilibrium. Specifically, we have Dirichlet boundary conditions with (mean) density ρ_0 at the endpoints. The deterministic steady state is taken as the initial condition so $\rho_{i;1} = \bar{\rho}_{i;n} = \rho_0$. For both the particle/stochastic-PDE and particle/deterministic-PDE hybrids we take $\Delta x = 0.5$, $M = 40$, $\Delta t = 0.001$, $\rho_0 = 40$, and the diffusion constant $D = 1.0$. From $x = 0$ to $x = L/2$ there are independent random walkers and from $x = L/2$ to $x = L$ the diffusion equation is computed on a grid of 20 cells. Our statistics are long-time averages over 10 independent samples. In both cases, the mean value of the density agrees with the expected value $\langle \rho_{i;n} \rangle = \rho_0$.

The stochastic and deterministic hybrids give different results for the spatial dependence of the variance, as seen in Fig. 2 . The stochastic hybrid is within statistical errors of the expected value of the variance, $\langle \delta\rho_{i;n}^2 \rangle = \rho_0/\Delta x$ (i.e., Poisson distribution). In the deterministic hybrid, the variance is close to zero in the continuum region while in the particle region it is significantly reduced in the cells near the interface. Note that for both the deterministic and stochastic-PDE hybrids the fluctuations in the cells near the Dirichlet boundary (where $\rho_{1;n}$ is fixed) are *not* reduced.

Open, steady-state, non-equilibrium system

The second test case is a system in which a (constant) density gradient is maintained. We take Dirichlet boundary conditions, but with different (reservoir) densities at the endpoints; $\rho_{1,n} = \rho_0$, and $\rho_{M,n} = \rho_L$. The system is initialized with the linear density profile, $\rho_{i,1} = \rho_0 + (\rho_L - \rho_0)(i-1)/(M-1)$, which is the steady state, $\bar{\rho}_i$. (This initialization leads to faster convergence of statistics; any other would lead to the correct steady-state.) Both particle/stochastic-PDE and particle/deterministic-PDE hybrids were tested. Again, for both cases $\Delta x = 0.5$, $\Delta t = 0.001$ and the diffusion constant, $D = 1.0$; densities at the endpoints were $\rho_0 = 40$, $M = 40$, $\rho_L = 80$. From $x = 0$ to $x = L/2$ there are independent random walkers and from $x = L/2$ to $x = L$ the diffusion equation is computed on a grid of 20 cells. As before, in the stochastic case, for the noise amplitude we use the *instantaneous* value of the local density.

Figure 3 shows the mean density as a function of position for the hybrids using the stochastic and deterministic PDE solvers, respectively. Our statistics are long-time averages over 10 independent samples. In both cases, the mean value of the density agrees with the expected value of $\langle \rho_{i;n} \rangle = \bar{\rho}_i$, which is linear in x. For the stochastic hybrid the variance is within statistical errors of its exact value, $\langle \delta\rho_{i;n}^2 \rangle = \bar{\rho}_i/\Delta x$ (see Fig. 4). The variance in the particle region of the non-stochastic hybrid is significantly reduced near the interface and goes quickly to zero within the continuum region.

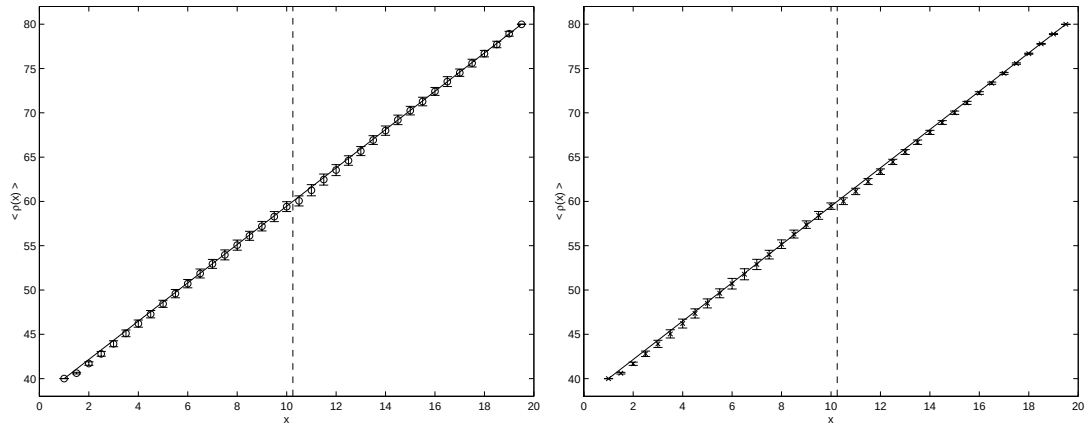

FIGURE 3. Mean density, $\langle \rho_{i;n} \rangle$, for the open, non-equilibrium system. The data from the particle/stochastic-PDE hybrid (left) and from the particle/deterministic-PDE hybrid (right) are shown; solid line is $\langle \rho_{i;n} \rangle = \bar{\rho}_i$; dashed line indicates particle/PDE interface.

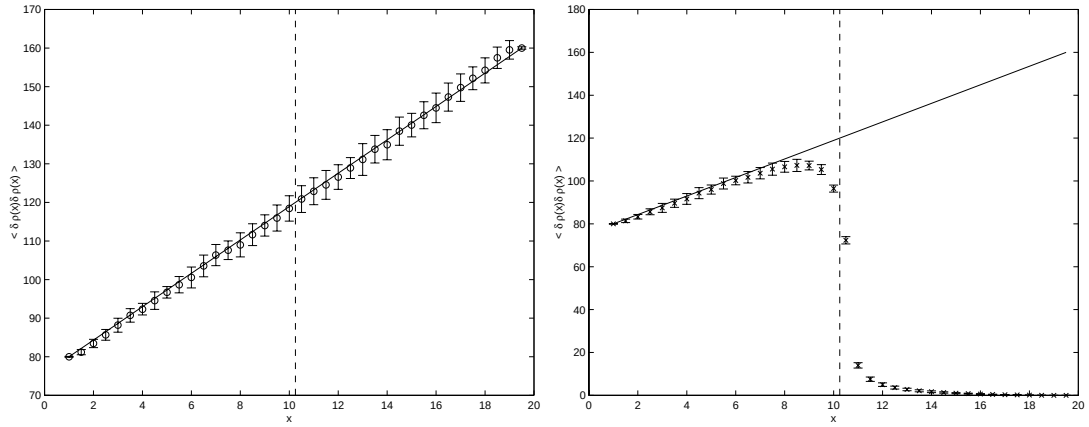

FIGURE 4. Variance of density in a cell, $G_{i,i} = \langle \delta\rho_{i;n}^2 \rangle$, for the open, non-equilibrium system. The data from the particle/stochastic-PDE hybrid (left) and from the particle/deterministic-PDE hybrid (right) are shown; solid line is $\langle \delta\rho_{i;n}^2 \rangle = \bar{\rho}_i/\Delta x$; dashed line indicates particle/PDE interface.

CONCLUDING REMARKS

Our aim in this study was to determine how accurately particle/continuum hybrids, such as those used in Algorithm Refinement, could model hydrodynamic fluctuations. Our results show that such hybrids, constructed to solve the linear diffusion PDE and the random walk particle model, are capable of capturing *some* fluctuations correctly for both equilibrium and nonequilibrium problems. We find that the mean density is given correctly by particle/PDE hybrids using either stochastic or deterministic PDE solvers; a longer exposition, with more results, will appear elsewhere [19]. The variance can be recovered everywhere with a particle/stochastic-PDE hybrid but is only correct within the particle region far from the coupling interface when the continuum solver does not contain stochastic fluxes. This reduction of the density variance in the particle region when coupled with a deterministic PDE necessitates placing the interface further away from regions where accurate fluctuations are required. If such measures are not taken, we believe this can have a deleterious effect when using a deterministic PDE solver in hybrids that simulate strongly interacting systems (e.g., nonequilibrium solids and dense liquids).

It is important to note that the linear diffusion equation is a particularly simple PDE, and while the results presented here are encouraging, one should not assume that particle/continuum hybrids will do equally well for other physical systems. For simple fluids, the extension of the present formulation to the stochastic PDEs of linearized fluctuating

hydrodynamics is straightforward [14, 20]. Furthermore, different hybrid coupling schemes will have different effects on the fluctuations, even for the linear diffusion equation. [21]

In our study of fluctuations in simple diffusion we focused our attention on the variance of density but for other physical systems equal-time correlations are also of interest. A common feature found in the stochastic PDEs arising from fluctuating hydrodynamics is the existence of long-range correlations of equal-time fluctuations at non-equilibrium steady-states [22]. The linear diffusion equation for density does *not* have such long-range correlations but one does find them in other simple cases, such as the linear Fourier equation [14] and the Train Model for viscous diffusion [23]. Preliminary studies of the Train Model indicate that the correlation of equal-time fluctuations in a stochastic PDE hybrid are identical to those obtained in a pure particle simulation while a deterministic PDE hybrid preserves the long-range nature of the correlations but with diminished amplitude. [24]

Though we find that a hybrid scheme constructed with a simple, explicit stochastic-PDE solver can reproduce the correct fluctuations, it is not our intent to promote the present scheme as being optimal. A topic for future study is the analysis of a variety of stochastic-PDE schemes to establish the most accurate and efficient methods for particle/continuum hybrids. In particular, the details of how the coupling is implemented may affect the convergence properties of a hybrid.

In this paper we consider explicit schemes because these are the most commonly used methods for the continuum calculations in hybrids. Elliptic PDEs, such as the diffusion equation, are often solved by implicit methods (e.g., Crank-Nicolson). Because such schemes introduce a non-local coupling, the modification to the fluctuations may be significant especially in hybrids using deterministic-PDEs. While semi-implicit PDE solvers have been used in particle/continuum hybrids [7], the study of implicit, stochastic hybrids is a topic best treated in a separate paper.

Finally, we have not addressed the question of how one selects the regions in a calculation that should be computed by a microscopic, particle scheme versus a macroscopic, continuum method. For example, when a hybrid is fully "adaptive" the particle regions can grow, shrink, shift, merge, and fission throughout the calculational domain. In adaptive mesh refinement, gradient detection is a commonly used refinement criteria (e.g., using a fine grid near a shock front). Spontaneous fluctuations in a stochastic or particle-based algorithm can trigger such criteria, even in regions that are at thermodynamic equilibrium, causing unnecessary refinement. Preliminary studies using an adaptive DSMC/Euler hybrid indicate that this problem may be overcome by a judicious choice of multiple refinement criteria [25] but this important computational issue merits further study.

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