LA-UR- 01-6964

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Title: ALGORITHM REFINEMENT FOR STOCHASTIC PARTIAL DIFFERENTIAL EQUATIONS

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Submitted to: Whistler Conference Centre
Whistler, British Columbia
July 20-25 2002

Algorithm Refinement for Stochastic Partial Differential Equations

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Abstract. A hybrid particle/continuum algorithm is formulated for Fickian diffusion in the fluctuating hydrodynamic limit. The particles are taken as independent random walkers; the fluctuating diffusion equation is solved by finite differences with deterministic and white-noise fluxes. At the interface between the particle and continuum computations the coupling is by flux matching, giving exact mass conservation. This methodology is an extension of Adaptive Mesh and Algorithm Refinement [*J. Comp. Phys.* **154** 134 (1999)] to stochastic partial differential equations. A variety of numerical experiments were performed for both steady and time-dependent scenarios. In all cases the mean and variance of density are captured correctly by the stochastic hybrid algorithm. For a non-stochastic version (i.e., using only deterministic continuum fluxes) the mean density is correct, but the variance is reduced except within the particle region, far from the interface. Extensions of the methodology to fluid mechanics applications are discussed.

A promising computational strategy for multi-scale and multi-physics problems is to apply a detailed microscopic model only where it is necessary, coupling this computation to a simpler, less expensive method in the rest of the domain. Such "hybrid" methods, also known as Algorithm Refinement, typically couple two structurally (physically and algorithmically) different computational schemes, which are used in different regions of the problem (e.g., interior and exterior of a shock wave). An important class of hybrids involves matching particle methods, such as Direct Simulation Monte Carlo (DSMC), to continuum partial differential equation (PDE) solvers (see [2] and references therein).

An important question is whether the coupling of two algorithms affects the accuracy of either method. Until recently, the testing of hybrid schemes only checked 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 issue is especially important when modeling phenomena where the fluctuations themselves drive (or initiate) a large scale process, such as the onset of instabilities, the nucleation of phase transitions, and the ignition of combustion. Nonequilibrium fluctuations are correctly reproduced by conventional DSMC simulations [6] but coupling with a continuum algorithm could possibly affect these fluctuations.

The present work addresses the issue of fluctuations in hybrid schemes that combine a particle algorithm with a partial differential equation solver. Since our interest is in fluctuations, we consider both deterministic partial differential equations (DPDEs) and stochastic partial differential equations (SPDEs). Spontaneous fluctuations may be introduced into the hydrodynamic equations by including stochastic components to the fluxes, as first proposed by Landau [5]. Our investigation focused on the problem of simple diffusion since much is known about solving the linear diffusion equation (LDE) in both its deterministic and stochastic forms. Moreover, there is a microscopic particle process, namely independent random walkers, that rigorously converges to the LDE in the hydrodynamic scaling limit. [4]

Our numerical experiments simulated a one-dimensional system divided into two parts with a particle region between x =3D 0 to I; elsewhere the continuum density is specified at discrete grid points (see Figure 1). The particle and continuum computations are coupled by flux matching with exact conservation, as described in [2]. At the beginning of each time step, the "handshaking" region is randomly filled with particles according to the density of the underlying grid point. All particles, in the handshaking region and elsewhere, are then displaced as random walkers, i.e., by a distance $\sqrt{2D\Delta t}\,\Re^U$, where D is the diffusion coefficient, Δt is the time step and $\Re^U$ is a uniformly distributed random number in $[0,1)$. The number of particles crossing the interface gives the number flux at the interface, this flux is recorded and used in the continuum portion of the computation. Any particles that end their move outside the particle region are removed from the simulation.

Once the particle update is complete, the number density, ρ, on the continuum grid is updated as

$$\rho_i(t + \Delta t) =3D \rho_i(t) - \left(\frac{F_i^+ - F_i^-}{\Delta x}\right)\Delta t,$$

where the total and stochastic fluxes, respectively, are

$$F_i^{\pm} =3D \mp D\left(\frac{\rho_{i\pm1}(t) - \rho_i(t)}{\Delta x}\right) + f_i^{\pm}, \qquad f_i^+ =3D f_{i+1}^- =3D \sqrt{\frac{D(\rho_i(t) + \rho_{i+1}(t))}{\Delta x \Delta t}}\,\Re_i^G,$$

where Δx is the grid spacing and $\Re_i^G$ are independent, Gaussian distributed, random variables with zero mean and unit variance. The right and left number fluxes, $F^{\pm}$, for each continuum grid point are computed by the above expressions *except* for the grid points adjacent to the particle region. For those points, the number flux recorded during the particles' motion is used. If we set $f_i^{\pm} =3D 0$ then we recover the forward-time centered-space (FTCS) scheme [1] for the deterministic diffusion equation. Note that the coupling by fluxes ensures exact mass conservation for both the DPDE and SPDE versions of the hybrid. The continuum SPDE portion of this hybrid is essentially the same as that presented in [3] but for mass diffusion instead of the Fourier (heat) equation, which has a slightly different form for the stochastic flux.

Our numerical experiments show that this hybrid, constructed to solve the stochastic diffusion PDE and the random walk particle model, produces the correct equal-time density fluctuations in a variety of scenarios, including equilibrium, nonequilibrium steady-state, and time-dependent problems. We also find that the mean density is given correctly by the particle/PDE hybrid using either stochastic or deterministic PDE solvers. However, when the continuum solver does not contain stochastic fluxes (i.e. FTCS scheme) the variance is near zero in the continuum region and suppressed within the particle region near the coupling interface. This reduction of the density fluctuations in the particle region when coupled with a deterministic PDE necessitates placing the interface further away from regions where accurate fluctuations are required.

The talk will present these results in more detail and discuss the extension of this methodology to hybrids coupling DSMC and the fluctuating Navier-Stokes equations.

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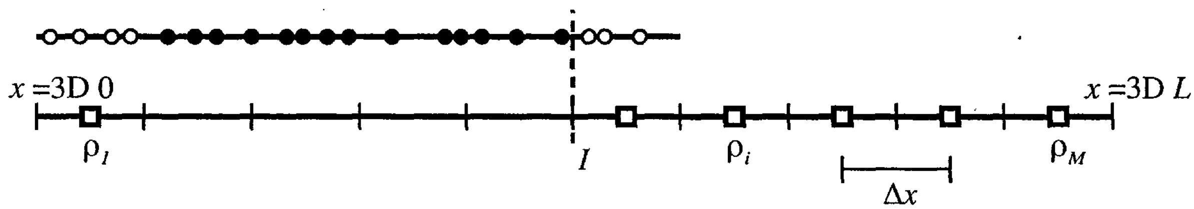

Figure 1 Algorithm Refinement for simple diffusion. A random walk simulation is performed in the region on the left and a PDE solver is used on the right. The methods are coupled at the interface I; new particles (open circles) are generated in the "handshaking" region (right) and at the Dirichlet boundary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