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Supplementary material to accompany: “The pseudo-compartment method for coupling PDE and compartment-based models of diffusion”

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1 Particles diffusing into an empty region from the compartment-based side

Here we present the comparison between the analytical solution of the mean-field model and the density profile given by our algorithms for the initial-boundary-value problem from the main text:

$$\frac{\partial \rho}{\partial t} = D \frac{\partial^2 \rho}{\partial x^2}, \text{ for } x \in [-1, 1], \quad (1)$$

with zero-flux boundary conditions

$$\left. \frac{\partial \rho}{\partial x} \right|_{x=0,1} = 0, \quad (2)$$

and initial condition

$$\rho(x, 0) = H(x) \text{ for } x \in [-1, 1]. \quad (3)$$

This initial condition specifies that all the particles are initially in the compartment-based regime and none in the PDE-based regime. As such this simulation provides a good test of whether the algorithm is converting particles on the compartment-based side to mass on the PDE side appropriately. Clearly, because of the similarity between the mean-field solution and the density profiles given by our algorithms (see Figure 1) we can be confident that both of our algorithms are working correctly. In supplementary Movies M9 and M10 a comparison of the densities through time for algorithm 1 and 2, respectively, can be seen.

In Figure 2 we compare the mass in each regime between our hybrid algorithm 2 and the analytical solution (given by equation (23) of the main text with the minus in front of the sum substituted for a plus) for the initial condition in which all particles are initialised in the compartment-based regime, Ω_C . The expected mass predicted by the hybrid algorithm matches closely the expected mass given by the analytical solution in both Ω_P and Ω_C . The insets demonstrate that the relative error between the masses generated by the analytical solution and the hybrid model are low and have no systematic bias, but instead fluctuate about their expected values in a similar manner to Figure 8 of the main text.

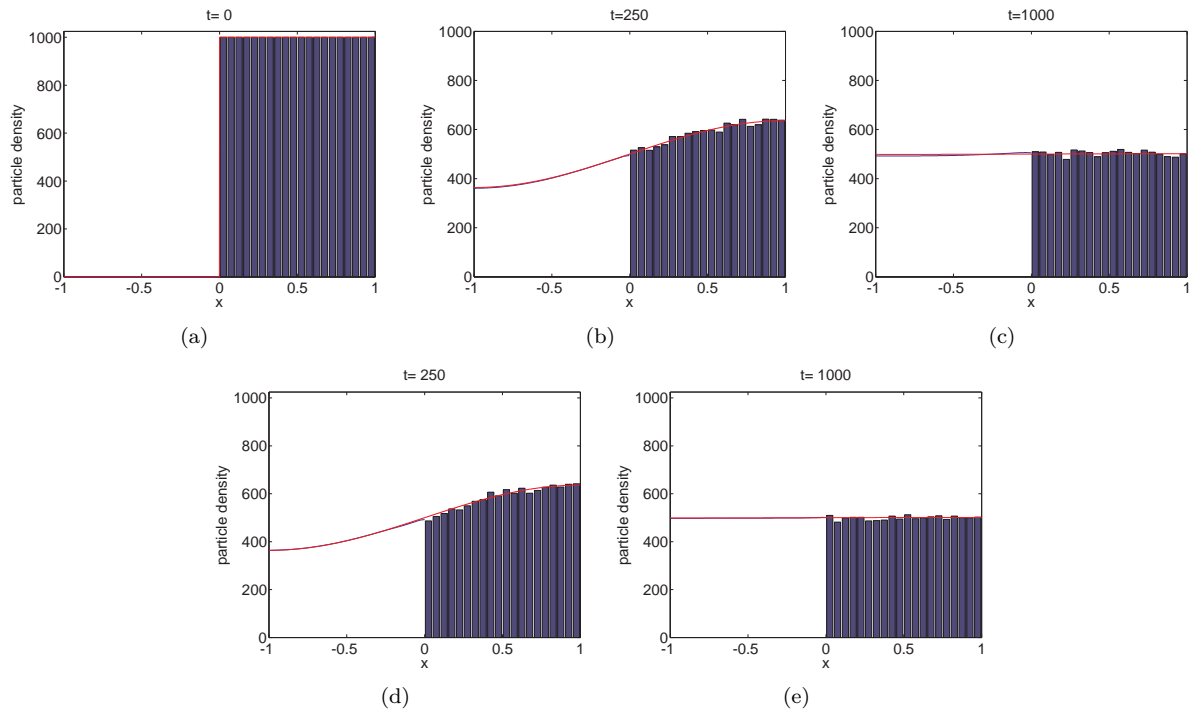


Figure 1. Particles initially in the right-hand half of the domain spread diffusively (with diffusion coefficient $D = 1/400$) throughout the domain eventually reaching steady state. Panel (a) gives the initial condition. By $t = 1000$ the system is assumed to have reached an approximately steady state. Panels (b) and (c) show the particle density profile according to algorithm 1 at times 250 and 1000 respectively. Panels (d) and (e) show the same comparison for algorithm 2. Figure descriptions and particle numbers are as in Fig 4. The simulation results are averaged over 100 repeats.

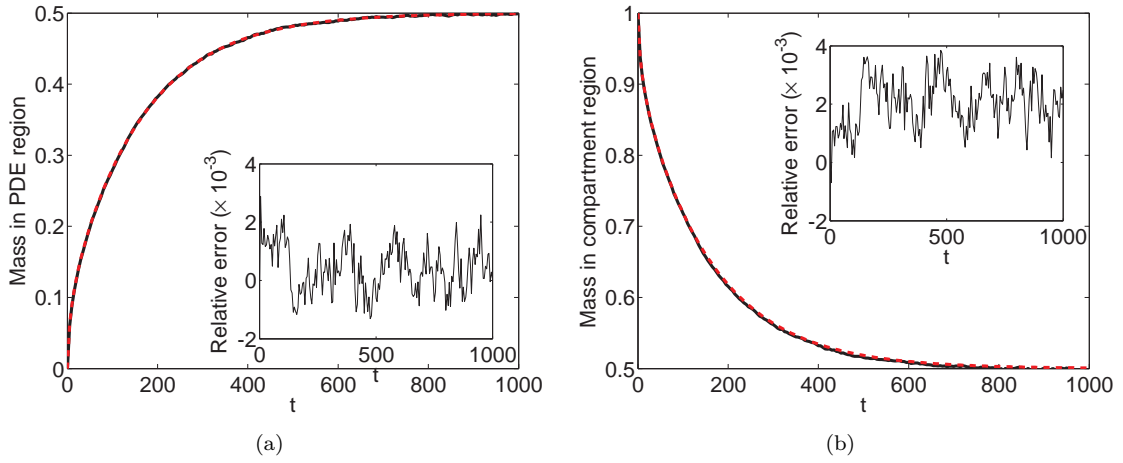


Figure 2. Error plots for test problem 2, in which all particles are initially in Ω_C . In (a) we display the normalised expected value of the total mass in Ω_P given by the analytical solution (red, dashed line) and the normalised average mass in Ω_P (black line) according to our second hybrid algorithm. In 2(b) we display the same comparison but for the compartment-based regime. In each panel, the inset displays the evolution of the relative error (i.e. $(N_{HP} - N_{DP})/N_{DP}$ or $(N_{HC} - N_{DC})/N_{DC}$, respectively) throughout the simulation. Again, the masses generated by our hybrid algorithm are averaged over 100 repeats.