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The gap-tooth method in particle simulations

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Abstract

We explore the gap-tooth method for multiscale modeling of systems represented by microscopic physics-based simulators, when coarse-grained evolution equations are not available in closed form. A biased random walk particle simulation, motivated by the viscous Burgers equation, serves as an example. We construct macro-to-micro (lifting) and micro-to-macro (restriction) operators, and drive the coarse time-evolution by particle simulations in appropriately coupled microdomains ("teeth") separated by large spatial gaps. A macroscopically interpolative mechanism for communication between the teeth at the particle level is introduced. The results demonstrate the feasibility of a "closure-on-demand" approach to solving some hydrodynamics problems.

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Traditional approaches to solving physical problems that manifest separation of scales involve first (a) deriving a set of reduced equations to describe the system, and subsequently (b) solving the equations and analyzing their solutions. Recently an "equation-free" approach has been proposed [1] that sidesteps the necessity of first deriving explicit reduced equations. The approach relies instead on microscopic simulations, enabling them through a computational superstructure to perform numerical tasks *as if the reduced equations were available in closed form*. Both macroscopically coarse-grained equations and atomistic/stochastic simulations can be regarded as "black boxes" from the point of view of appropriately formulated numerical algorithms. They constitute alternative realizations of the same macroscopic input-output mapping. For example, a crystal's elastic response can either be *approximated* by elastic constants, or *evaluated* using a high-accuracy electronic structure program based on density functional theory [2], which, for a given strain, computes the stress on-the-fly. The advantage of a simulator-based approach is that it can be used generally, beyond the region of validity of any given closure—e.g., providing the correct nonlinear elastic responses in the above example. Equation-free methods hold the promise of combining direct physics-

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based simulation with the strength and scope of traditional numerical analysis on *coarse* variables (bifurcation, parametric study, optimization) for certain problems—problems for which coarse equations conceptually exist, but are not available in closed form. An example is the so-called interatomic potential finite-element method (IPFEM) [3], a subset of the more general quasi-continuum method [4], used to identify elastic instabilities leading to defect nucleation in nanoindentation, for which no accurate closed-form constitutive relation is currently available due to the complex triaxial stress state at the critical site of instability.

Microscopic simulations cannot be used directly to attack problems with large spatial and temporal scales ("macrodomains" in space and time); the amount of computation is prohibitive. If, however, the actual behavior can be meaningfully coarse-grained to a representation that is smooth over the macrodomain, the microscopic systems need only to be directly simulated in *small patches* of the macrodomain. This is done by interpolating hydrodynamic variables between the patches in space—the gap-tooth method (see [5])—and extrapolating from one or more patches in time—projective integration [6,7]. In this Letter, we use this "closure-on-demand" approach to solve for the coarse-grained behavior of a particular microscopic system. The illustrative example is the biased random walk of an ensemble of particles, motivated by the viscous Burgers equation,

$$u_t + uu_x = \nu u_{xx}, \tag{1}$$

a 1D version of the hydrodynamics equations used under various conditions to model boundary layer behavior, shock formation, turbulence, and transport. Here, $\nu > 0$ is the viscosity; periodic boundary conditions are used for simplicity, and only non-negative solutions $u(x,t) > 0$ are considered. A particular microscopic dynamics is constructed, motivated by the Eq. (1). For a discussion of particle solvers for given PDEs the reader is referred to [8–11]; our goal here is not to construct such solvers, but rather to solve the (unavailable) equations pertaining to a given particle-based microscopic scheme. In our particle simulation we interpret u as the *density field* of the random walkers; $\int u\,dx = 1$ corresponds to Z walkers, where Z is a large normalization constant.

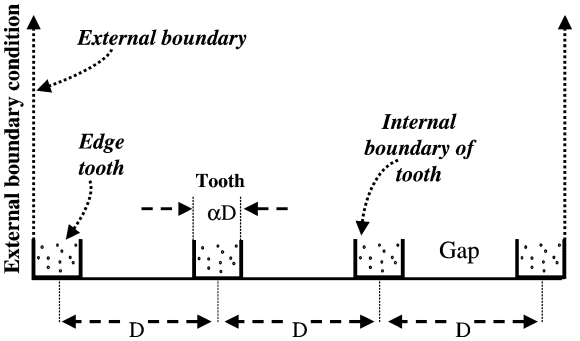


Fig. 1. Teeth and gaps covering space.

In the micro-simulation, random walkers move on $[-\pi,\pi)$ at discrete timesteps $t_n = nh$. At each step, an approximation to the local density, ρ_i, is computed (as discussed later). Then every walker is moved by $\Delta x_i \in N(h\rho_i/2, 2\nu h)$, a biased Gaussian distribution. x_i's are then wrapped around to $[-\pi,\pi)$, and the process repeats. Since ρ_i is a local estimate of u, this process achieves a coarse-grained flux analogous to $j \equiv u^2/2 - \nu u_x$ in Eq. (1) by assigning each walker a drift velocity of $\rho_i/2$.

The gap-tooth scheme, first discussed in [5], covers space with teeth and intervening gaps as shown in Fig. 1 for one dimension. The microscopic evolution is simulated in the interior of each tooth. Clearly appropriate boundary conditions have to be provided at the edges of each tooth. Tooth boundaries coincident with external boundaries have the boundary conditions specified externally, while internal boundary conditions must be generated by the gap-tooth scheme itself. Because this example uses periodic boundary conditions, there are no external boundaries: the teeth can be viewed as equally spaced on a circle.

The microscopic simulation operates on the position of each particle. We are interested in a meaningful *coarse* description, possibly averaged over several realizations of the computational experiment [1]. The *lifting* operator that maps a given $u(x,t)$ to consistent particle positions is straightforward in this case. From the density function over a tooth we can compute its integral, so we know the number of particles that should be present in that tooth. The indefinite integral of the density function over the tooth provides the cumulative distribution function for that tooth which permits the particles to be placed as a discrete representation of that function [12]. If the density approxima-

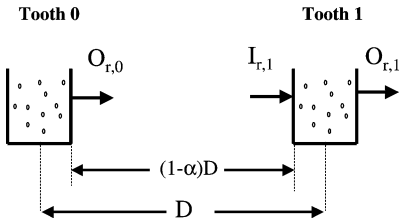


Fig. 2. Right-going input and output fluxes.

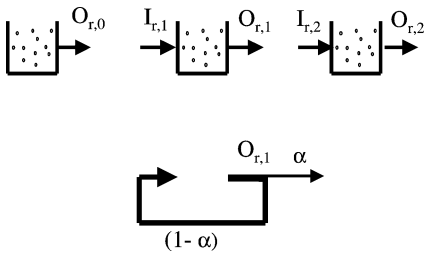


Fig. 3. Flux redistribution for right-going fluxes.

tion is constant in each tooth (as has been found to be adequate in the examples here) this simply means that the particles are uniformly distributed in each tooth according to the density in that tooth.

The mapping of a phase point or points to coarse fields is called a *restriction* operator. In addition to the density field (0th-moment), smooth 1st-moment, momentum (alternatively, velocity) and 2nd-moment, energy (alternatively, temperature) fields can be extracted from molecular microscopic simulations based on maximum likelihood inference (see [13] for the molecular dynamics case). If the interior of a tooth were to be simulated by solving a PDE, we would need to prescribe appropriate boundary conditions at each tooth at each timestep. The same is still true when the tooth is realized using particle simulations. Creating an appropriate match between the coarse fields at the boundaries and the particles in the teeth is an area of extensive research [14,15]. Sometimes one knows so little about the nature of the coarse equation that even the correct *order* for imposing well-posed boundary conditions at the teeth edges is unknown. This issue is addressed in [16].

Here we use an alternative approach suggested in [17], based on "effective smoothness" of the coarse solution. In a 1D particle based random walk simulation we distinguish two "fluxes"—left-going and right-going. The particle simulation in the interior of each tooth generates *outgoing* fluxes, that is, the left(right)-going fluxes at the left(right) boundaries, directly. Boundary conditions are needed to provide matching *incoming* (right(left)-going) fluxes at the same boundaries. In D-dimensions, there will be 2^D boundaries to deal with and the corresponding incoming fluxes to provide.

Consider the estimation of the right-going, incoming flux $I_{r,1}$, as shown in Fig. 2. Assuming macroscopic flux smoothness suggests that we can interpolate its values from neighboring *outgoing* fluxes, in this case $O_{r,0}$ and $O_{r,1}$. If we use linear interpolation, we can write

$$I_{r,i} = \alpha O_{r,i-1} + (1-\alpha) O_{r,i}. \tag{2}$$

The interpolation coefficients depend (in this case through α) only on the gap-tooth geometry.

However, the "fluxes" under discussion here are not continuous quantities, but discrete events as particles cross a boundary, so Eq. (2) needs a different interpretation. Consider instead the role played by each *outgoing* flux in the interpolation for *incoming* fluxes. An interpretation of Eq. (2) for $i = 1$ and $i = 2$ would be that the portion $(1-\alpha)$ of $O_{r,1}$ contributes to the flux $I_{r,1}$ while α of it contributes to $I_{r,2}$. A similar procedure applies to the left-going fluxes. Thus, rather than thinking in terms of flux interpolation we can think in terms of *flux redistribution*. Interpreting the linear interpolation stochastically (on regularly spaced gap-teeth) we direct α of the outgoing particles as input to the neighboring tooth, and redirect $(1-\alpha)$ of them back to the left boundary of the same tooth as shown in Fig. 3.

Flux redistribution has to recognize the position of a particle after it leaves a tooth. If it had moved to a distance δ beyond the boundary of the tooth, it must be inserted a distance δ inside the receiving tooth. If δ were larger than the tooth width, it would have exited a tooth boundary again, and a further redistribution would be required following the same rule. (In multiple dimensions, the boundaries in each dimension are treated independently so that a particle will be redistributed for each boundary that it crosses until it lies inside a tooth.)

The above method implements effective linear interpolation. As discussed in [17], linear interpolation is not adequate for second-order problems: at least quadratic interpolation must be used. A possible

quadratic interpolation formula is

$$I_{r,i} = \frac{\alpha(1+\alpha)}{2} O_{r,i-1} + \left(1-\alpha^2\right) O_{r,i} - \frac{\alpha(1-\alpha)}{2} O_{r,i+1}. \quad (3)$$

As before we consider the impact of each outgoing flux on incoming fluxes. The fractions of output $O_{r,1}$ should be sent to the inputs as follows: $(1-\alpha^2)$ to $I_{r,1}$; $\alpha(1+\alpha)/2$ to $I_{r,2}$; and $-\alpha(1-\alpha)/2$ to $I_{r,0}$. Note that the last value is negative. Any linear higher-order interpolation formula contains negative coefficients. Our solution is to send *anti-particles* to the appropriate teeth. There they must annihilate with regular particles—we simply annihilate with the nearest regular particle. With this approach, the $O_{r,1}$ particles are redistributed as follows: a fraction $(1-\alpha(1+\alpha)/2)$ is sent to $I_{r,1}$; α^2 to $I_{r,2}$; and $\alpha(1-\alpha)/2$ are cloned to get two regular particles sent to $I_{r,1}$ and $I_{r,2}$ and one anti-particle sent to $I_{r,0}$. It is noteworthy that this scheme conserves the total number of particles in the teeth.

There are three sources of numerical error in the computation just described—by "error" we mean the difference between the computed solution and the solution of the closed (continuum) equation. These are (a) the stochastic errors due to the finite number of particles, (b) the errors in interpolation for the teeth boundary conditions, and (c) the error in estimating the local density. The stochastic errors will be proportional to $N^{-1/2}$ where N is the number of particles. Of course, if the actual system contains few particles, errors of type (a) should more appropriately be called "noise". The boundary interpolation errors are going to be of the order of the errors in a finite difference method of the same order based on point values of the density at the center of each tooth. (For this reason, we will show the finite-difference solution for comparison in the tests reported below.) A physically realistic local density estimate should use a suitable particle density influence function, $\sigma(z)$, that specifies the contribution of each particle P_j to the local density at particle P_i, where z is the distance between P_j and P_i. When there are few particles we also get stochastic errors similar to type (a) errors. If differentiability of the density is needed, σ should be smooth, as in Refs. [10,11], which use a Gaussian spreading function for each particle; this, however, requires additional computations. The least expensive technique is to assume that the density is piece-wise constant across each tooth. Its value can be found by simply counting particles in each tooth. It is easy to see that this also leads to errors of the same order as the simplest finite difference method. We will use piece-wise constant density in the tests reported below. Other tests using linear and quadratic approximations to the density in each tooth have given no significant improvement in accuracy. We believe this is because the errors from the other sources are of comparable significance.

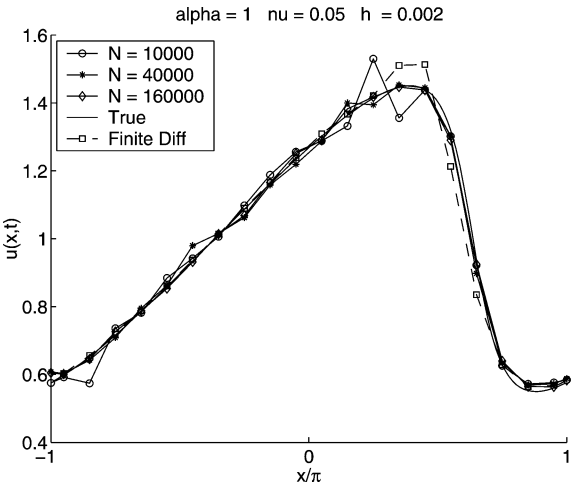
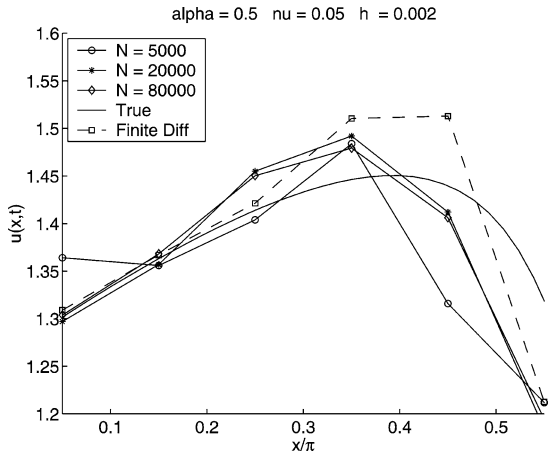


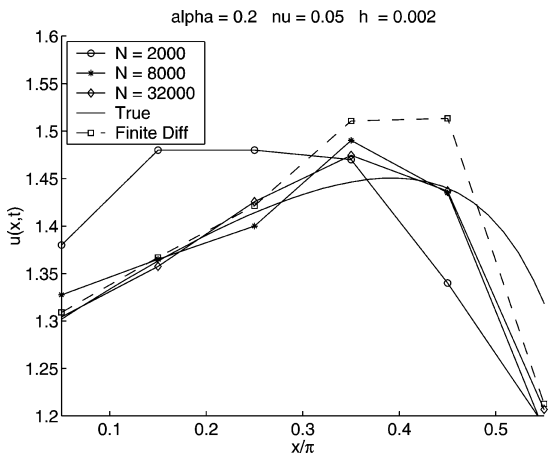
Fig. 4. Simulation results at $t = 2$. N is number of particles, 20 teeth, no gaps ($\alpha = 1$). Piece-wise constant local density estimate in each tooth.

Fig. 4 shows the results for $\alpha = 1$ (no gaps). The microscopic evolution rules were simulated at conditions corresponding to $\nu = 0.05$ and timestep $h = 0.002$ in Eq. (1) over $t \in [0, 2]$ (1000 time steps) using the gap-tooth scheme with 20 equally spaced teeth in the interval $[-\pi, \pi)$. Results are given for three different values of N: 10^4, $2^2 \times 10^4$, and $4^2 \times 10^4$. The analytical solution [18,19] of Eq. (1) is also plotted, as is the finite-difference solution using the same h and $\delta x = \pi/10$.

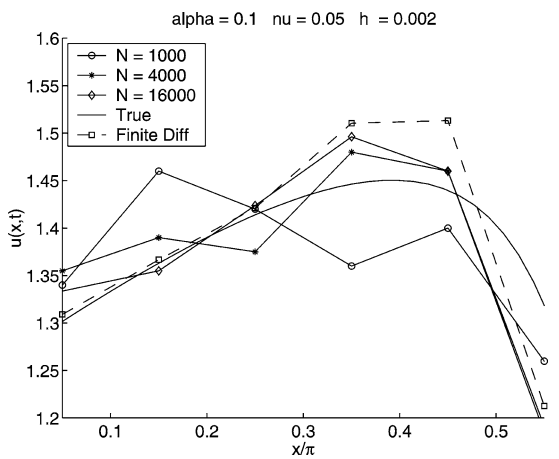
Fig. 5(a)–(c) show the results for the same problem with $\alpha = 0.5$, 0.2, and 0.1 with the three example values of N scaled by α so that the average number of particles per unit distance is unchanged as α changes. Because the largest errors occur near the peak, we have plotted just the vicinity of that region. As can be seen, the results for $\alpha = 0.5$ and 0.2 are comparable to



(a)



(b)



(c)

Fig. 5. Simulation results at $t = 2$ for $\alpha = 0.5$, 0.2, and 0.1.

those for the case of no gaps. Since the computational time is mainly proportional to N, this indicates that the gap-tooth method is achieving some speed-up. The number of particles that cross tooth boundaries increases as α decreases, leading to some increase in cost. A careful study of relative costs will require careful programming of the method rather than the present Matlab coding. The purpose of this Letter is to demonstrate the feasibility of the method.

For $\alpha = 0.1$ the errors appear to be larger. We believe this is because at $\alpha = 0.1$, as a significant number of particles cross multiple teeth in one step, each additional crossing leads to an additional "interpolation" error.

We have demonstrated that the gap-tooth scheme can be successful in solving some problems using microscopic models based on the stochastic simulation of particle motion; we also introduced a novel approach for dealing with the inter-tooth boundary conditions.

In earlier work we have proposed combining this with projective integration [6] and some preliminary numerical experiments have been performed in this direction. However, projective integration requires smoothness of the time derivative estimates. The stochastic nature of the microscopic model leads to significant noise. In this simulation we tried using a least-squares linear estimate from a large number of time steps to get a reasonably accurate time derivative estimate. However, by then, the total time step at the microscopic level was large relative to the size of a projective step in time (which is limited by the smoothness of the solution). If the stochastic noise is reduced by using a much larger number of particles, or a large number of "copies" of the simulation, the time derivative estimates would allow the application of projective integration. In some sense there is a trade-off between saving computation in the spatial domain with fewer teeth and fewer particles, and saving computation in the time domain by getting more accurate estimates of the time derivatives. We believe that for problems in which there is a significant gap between the timescales of the microscopic dynamics and those of the hydrodynamic variables, projective integration would be a useful additional acceleration step. We will report on such "patch dynamics" numerical experiments in a future paper.

Acknowledgements

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