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2000 Europhys. Lett. 52 271

(http://iopscience.iop.org/0295-5075/52/3/271)

EUROPHYSICS LETTERS 1 November 2000

Europhys. Lett., **52** (3), pp. 271–276 (2000)

Hybrid model for combined particle and continuum dynamics

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(received 20 April 2000; accepted in final form 12 September 2000)

PACS. 47.11.+j – Computational methods in fluid dynamics.
PACS. 83.20.Di – Microscopic (molecular) theories.
PACS. 83.20.Lr – Boundary conditions.

Abstract. – Differential equations for continuum fields describe many macroscopic phenomena. Hydrodynamics, for example, is described by the Navier-Stokes equations, and their solutions depend on boundary conditions. However, boundary conditions are set by the interactions at the atomistic or molecular scale. We introduce a "hybrid model" that permits a continuum description in one region to be coupled to an atomistic description in another region. The coupling is symmetric in the sense that the fluxes of the conserved quantities are continuous across the particle-field interface. As an example, we couple a Lennard-Jones liquid and the compressible Navier-Stokes equations and show that the hybrid model is consistent with hydrodynamic predictions.

Conflicting views on matter as either continuous or discrete date back at least to early Greek philosophy: Aristotle has been taken to represent the continuous point of view and Democritus the discrete, atomistic standpoint. Modern physics has reconciled the conflicting views by considering continuum descriptions as local averages of the underlying, fundamentally discrete, atoms. Theoretically one may proceed from the atomistic equations of motion to continuum equations, such as the Navier-Stokes equation [1], via kinetic theory [2] or some other coarse-graining theory.

While discrete particle descriptions, such as molecular dynamics (MD) [3], are useful and necessary on microscopic or mesoscopic scales, they cannot be handled on a macroscopic scale: the computational effort is prohibitive. Indeed, continuum descriptions are absolutely crucial for the description of macroscopic systems.

However, there are processes on macroscopic length scales that, for fundamental reasons, cannot be described by continuum theory; they must be treated on the discrete atomistic scale. Famous examples of such processes include the moving contact line [4], the breakup and merging of fluid droplets [5], strong shear localization, dynamic melting processes [6] and the evolution of a fracture tip [7–9]. In all of these examples dense systems self-organize to produce strong gradients on the atomic scale, thus coupling the macroscopic behavior to microscopic processes in ways that are not easily captured by constitutive relations or other average descriptions.

For the modeling of such processes it is of fundamental interest to combine a local and detailed particle description with a continuous field description of greater numerical economy. Particle models that seek to bridge the gap between the microscopic and the macroscopic scale do exist, most notably the hydrodynamic models known as dissipative particle dynamics [10, 11]. Even though these models have recently evolved to include an adaptive range of particle scales [12], they remain mesoscopic in the sense that their particles are coarse-grained representatives of the underlying micro-dynamics.

Much progress has been made in the description of multi-scale processes in solids. For instance, in recently developed hybrid descriptions of fracture [7,8], the continuum mechanics equations are solved using an adaptive mesh that follows the atomic motion in lock step at the continuum-particle interface. The same approach cannot be applied to hydrodynamic problems in which the particles follow random trajectories and mass flow across the continuum-particle interface may occur.

Recently, several multiscale coupling schemes designed specifically to explore hydrodynamic problems were presented. Hadjiconstantinou and Patera [13–15] used the flow field observed in conventional molecular dynamics simulations to provide the boundary conditions for separate finite-element computations. Thus microscopic and macroscopic length scales were coupled elegantly; at the price of limiting the approach to the study of steady-state solutions. Li *et al.* [16] studied the general problem of obtaining boundary conditions from a particle ensemble. Finally, O'Connel and Thompson [17] studied the Couette flow problem using an overlap region mediating between a particle ensemble and a continuum described by the incompressible Navier-Stokes equation. This approach is limited to scenarios in which there is no mass and energy exchange between the discrete and the continuous phases. Moreover, in their model momentum is conserved only in the special case in which the continuum equations *exactly* describe the particle system. Garcia *et al.* [18] have coupled multigrid continuum equations to a Direct Simulation Monte Carlo particle simulator. This sophisticated approach includes the exchange of mass, momentum and energy but is limited to dilute systems.

Here we focus on the general principles for coupling a particle and a field description in possibly dense systems and develop a model that is applied to some simple hydrodynamic examples. Our approach represents the first coupling scheme that is explicitly based on direct flux exchange. As such, it has the advantage that it directly implies adherence to the relevant conservation laws. Garcia *et al.* introduce a "refluxing" correction step to ensure flux continuity in dilute systems. The other existing coupling schemes [13–15,17], however, rely on the use of the *exact* constitutive relations and equations of state to maintain the conservation laws. This is generally a problematic requirement in contexts where particle methods are needed to replace inadequate continuum descriptions. The problem is thus to communicate between the two representations in a way that conserves mass, momentum and energy, even when the representations have somewhat different macroscopic properties. In order to obtain a generally valid coupling scheme, the different representations must interact by the symmetric exchange of *fluxes* of the conserved *densities*. This is qualitatively illustrated in fig. 1. Existing hydrodynamic coupling schemes for hydrodynamic flows [13,17] are based on the exchange of densities (mass, momentum, and energy), rather than on flux exchange.

The hybrid model presented here is based fully on flux boundary conditions and is conservative in general. This is demonstrated to good accuracy in two-dimensional flow simulations in which the particle system cannot easily be described in terms of a single Newtonian viscosity. Figure 1 illustrates how the discrete and continuous phases couple. While both phases are thought to represent the same underlying physical system, they may simultaneously be considered as two interacting systems. In region P←C the continuum fluxes are imposed on the particles; in region P→C the particle fluxes are measured and imposed on the continuum.

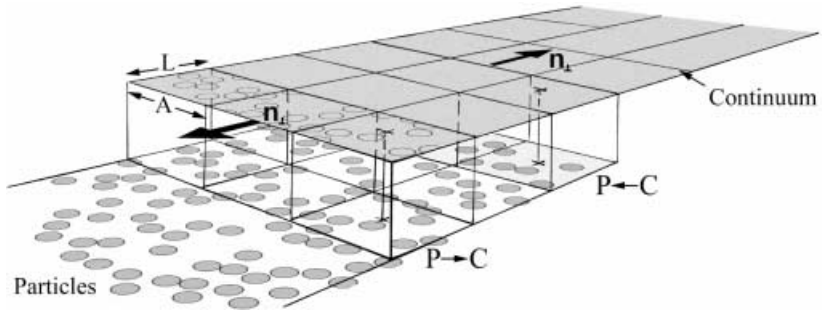

Fig. 1 – A schematic illustration of the interaction between the particles and the continuum in 2*d*. The narrow strips on the edges of the two spaces receive the local flux values of the other phase.

This ensures that whatever flows out of one representation, flows into the other. The two regions cannot coincide since this would impose a hierarchy given by the order of flux exchanges; in each region the interaction is one way.

The continuum equations that describe mass and momentum conservation are given in the general form [1]

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0 \quad \text{and} \quad \frac{\partial \rho \boldsymbol{u}}{\partial t} + \nabla \cdot \boldsymbol{\Pi} = 0\,, \tag{1}$$

where ρ and $\rho\boldsymbol{u}$ are the mass and momentum densities, $\boldsymbol{u}$ the velocity, and $\boldsymbol{\Pi}$ the momentum flux tensor. For a compressible Newtonian liquid in two dimensions we have

$$\boldsymbol{\Pi} = \rho \boldsymbol{u}\boldsymbol{u} + P - \mu \left(\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^{\mathrm{T}} - \nabla \cdot \boldsymbol{u} \right) - \lambda \nabla \cdot \boldsymbol{u}\,, \tag{2}$$

where μ and λ are the dynamic and bulk viscosities, respectively, P is the pressure, and $^{\mathrm{T}}$ denotes the transpose of the $\nabla \boldsymbol{u}$ tensor. For simplicity, we take both the continuum and the particles system to be at a constant temperature T. In order for the above description to hold for the particle system, the value of μ as well as the equation of state $P = P(\rho, T)$ must be measured in separate particle simulations for the relevant range of ρ-values.

Imposing boundary conditions on the continuum is straightforward. In the continuum region the derivatives of the flux densities, $\nabla \cdot \rho \boldsymbol{u}$ and $\nabla \cdot \boldsymbol{\Pi}$, are computed as finite differences across nodes; these differences are used to propagate the continuity equations (1) in time. Flux boundary conditions are imposed by substituting the fluxes at the boundary by the averaged particle fluxes. We measure and coarse-grain the mass and momentum flux density [3] of the particles in region P→C. This results in average flux densities that replace the original continuum flux densities on the nodes in region P→C:

$$\frac{1}{V} \sum_i m \langle \boldsymbol{v}_i \rangle \cdot \boldsymbol{n}_\perp \to \rho \boldsymbol{u} \cdot \boldsymbol{n}_\perp \quad \text{and} \quad \frac{1}{V} \sum_i \left(m \langle \boldsymbol{v}_i \boldsymbol{v}_i \rangle + \frac{1}{2} \sum_{j \neq i} \langle \boldsymbol{F}_{ij} \boldsymbol{r}_{ij} \rangle \right) \cdot \boldsymbol{n}_\perp \to \boldsymbol{\Pi} \cdot \boldsymbol{n}_\perp\,, \tag{3}$$

where i labels individual MD particles of mass m in a subregion of volume V pertaining to one node, $\boldsymbol{v}_i$ is their velocity, $\boldsymbol{F}_{ij}$ is the force acting from particle j on particle i and $\boldsymbol{r}_{ij}$ is their separation vector. The unit vector $\boldsymbol{n}_\perp$ is defined in fig. 1 and the average $\langle .. \rangle$ is taken over the time step Δt with which the continuum equations are integrated in time. In addition, the velocity $\boldsymbol{u}$ on the boundary nodes is replaced by the coarse-grained particle velocity, in order to compute the velocity gradients in $\boldsymbol{\Pi}$ on the nodes next to region P→C in a consistent fashion.

Imposing boundary conditions on the particles implies that the few degrees of freedom described by the continuous fields must be used to set the many degrees of the particles in region P←C. For the mass flux into the particle system to equal the mass flux out of the continuum, we introduce $s(\boldsymbol{x},t)$ particles per unit time in region P←C according to $ms(\boldsymbol{x},t) = A\rho\boldsymbol{u}\cdot\boldsymbol{n}_\perp$, where A is the surface area (or length) corresponding to one node spacing L. Note that s may be negative, corresponding to the removal of particles from region P←C. Likewise, to obtain momentum flux continuity, we impose the averaged condition $ms(x,t)\langle\boldsymbol{v}'\rangle + \sum_i \boldsymbol{F}_i = A\,\boldsymbol{\Pi}\cdot\boldsymbol{n}_\perp$, where $\boldsymbol{v}'$ is the velocity of the introduced particles and $\boldsymbol{F}_i$ an external force acting on particle i in region P←C. The left-hand side is thus the momentum per unit time introduced in the particle system averaged over Δt. Now, inserting the result for $s(\boldsymbol{x},t)$ and comparing with eq. (2) we observe from the last equation that momentum continuity is satisfied if the particles are introduced with the average velocity $\langle\boldsymbol{v}'\rangle = \boldsymbol{u}$ and that the overall force $\sum_i \boldsymbol{F}_i$ on the particles equals the stress force $A\boldsymbol{\sigma}\cdot\boldsymbol{n}_\perp$, where $\boldsymbol{\sigma} = \boldsymbol{\Pi} - \rho\boldsymbol{u}\boldsymbol{u}$.

Since only the *sum* of the forces on the particles from the continuum is determined, it may be shown that the particles may spread arbitrarily far to the right of region P←C if $\boldsymbol{F}_i$ is position-independent. To fix the volume available to the particles, we introduce an arbitrary *weight function* $g(x)$ that obeys $g(x) = g'(x) = 0$ for $x \le 0$ and that diverges as $g(x \to L/2) \sim (L/2 - x)^{-1}$ on the edge of region P←C ([1]) (see fig. 1). The coordinate x runs parallel to $\boldsymbol{n}_\perp$ and $x = 0$ in the middle of the $P \to C$ region. The precise form of the weight function is not important. The stress force acting on the i-th particle is $\boldsymbol{F}_i = (g(\boldsymbol{x}_i)/\sum_i g(\boldsymbol{x}_i))A\sigma\cdot\boldsymbol{n}_\perp$, where the sum includes all N_A particles in a given section A of region P←C. By construction, the fraction $\boldsymbol{F}_i$ of the total stress force imposed by the continuum increases as the i-th particle approaches the edge of region P←C, driving the particle back into the bulk. This solves the potential stacking problem posed by the insertion of particles as these may always be placed sufficiently deep into region P←C, and yet avoid the vicinity of other particles.

In this work we disregard energy flux exchange and limit ourselves to an isothermal continuum at temperature T. Future applications will include energy exchange on the same footing as mass and momentum exchange. Each particle must have then an average kinetic energy of $k_\mathrm{B}T$, where k_B is Boltzmann's constant; new particles are inserted with a velocity vector $\boldsymbol{v}'$ picked randomly from the Maxwellian distribution $P(\boldsymbol{v}') \propto \exp[m(\boldsymbol{v}' - \boldsymbol{u})^2/(2k_\mathrm{B}T)]$.

The imposed continuum stress forces will perform work on the particles and thus change their thermal energy. To compensate the stress work, it is necessary to thermalize the particles in region P←C. This is done by adding the Langevin force $\boldsymbol{F}_{\mathrm{L}i} = -\alpha(\boldsymbol{v}_i - \boldsymbol{u}) + \tilde{\boldsymbol{F}}$ to $\boldsymbol{F}_i$. Here $\boldsymbol{v}$ is the particle velocity, α is a friction coefficient and $\tilde{\boldsymbol{F}}$ is a fluctuating force of zero mean and a Gaussian distribution with the correlation function $\langle\tilde{\boldsymbol{F}}(t)\tilde{\boldsymbol{F}}(t')\rangle = 2k_\mathrm{B}T\alpha\delta(t-t')$. To correct for fluctuations $-(\sum_{i\epsilon(\mathrm{P}\leftarrow\mathrm{C})} \boldsymbol{F}_{\mathrm{L}i}/\sum_{i\epsilon(\mathrm{P}\leftarrow\mathrm{C})} 1)$ is added to all $\boldsymbol{F}_{\mathrm{L}i}$. In this way an independent net momentum input due to the Langevin forces is prevented.

There is an inherent asymmetry in the coupling scheme as only the particle system supplies fluctuations, while the continuum is intrinsically non-fluctuating. As a consequence, the continuum does not fully play the role of a thermodynamic bath. For instance, fluctuations in the total particle number will be smaller than those predicted by statistical mechanics, and they will in general decrease as L is increased.

The present coupling scheme was implemented and tested for elementary flow scenarios. The interaction forces governing the molecular dynamics were derived from the shifted Lennard-Jones potential [3] $V_\mathrm{LJ} = 4\varepsilon\left[(\sigma/r)^{12} - (\sigma/r)^6\right] - V_\mathrm{c} - B(r - r_\mathrm{c})$, where ε is the characteristic interaction energy and σ the characteristic interaction distance, and the constants V_c and B are chosen so as to ensure vanishing forces at the cut-off distance $r_\mathrm{c} = 2.5\sigma$. The

([1])In the simulations reported here, we used $g(x) = 2[(L-2x)^{-1} - L^{-1} - 2xL^{-2}]$ for $0 \le x \le L/2$.

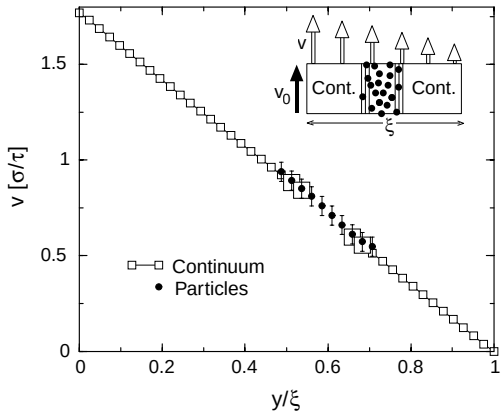

Fig. 2

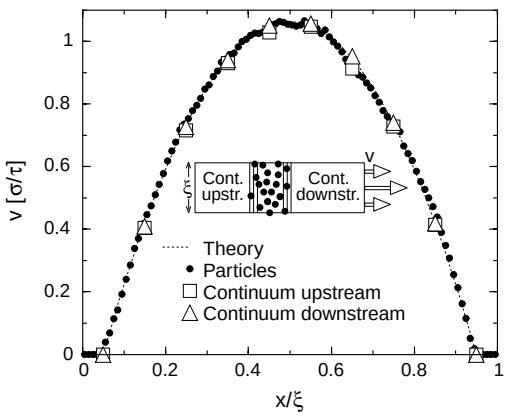

Fig. 3

Fig. 2 – Plot of the steady-state velocity profile $v(y)$ as a function of distance y/ξ, where ξ is the width of the channel in the Couette flow setting. Squares and circles indicate continuum and particle averages, respectively. Error bars and square sizes indicate the standard deviation of the mean.

Fig. 3 – Plot of velocity profile v across the flow channel in the Poiseuille flow setting, measured in the upstream and downstream continuum region and in the particle region. Also shown is the parabolic prediction.

Newtonian equations of particle motion were integrated using the velocity Verlet algorithm [3] with a time step $\Delta t_{\mathrm{MD}} = 0.0017\tau$, where $\tau = (m\sigma^2/\varepsilon)^{1/2}$ is the characteristic time of the potential. At $T = 0.7\epsilon/k_{\mathrm{B}}$ and a density of $\rho = 0.4\sigma^{-2}$, the MD particles formed a fluid with $\mu = 0.58\epsilon\tau\sigma^{-2}$.

The continuum equations were integrated using the MacCormack predictor-corrector algorithm [19] on a grid of spacing $L = 7.6\sigma$, a time step $\Delta t = 100\Delta t_{\mathrm{MD}}$, and the measured shear viscosity. The bulk viscosity was set to $\lambda = \mu/3$. The magnitude of the time steps reflects the stability requirements of the MacCormack scheme and the steepness of the Lennard Jones potential. The size of Δt_{MD} could be increased if a softer, non-divergent potential were used. The length L must be sufficiently large that the fluctuations in the measured particle fluxes do not cause stability problems in the continuum solver (here the MacCormack scheme). A central region in the grid was used only by the particles, and boundary sections $3L$ wide each formed two continuum-particle interfaces according to fig. 1.

Couette shear flow parallel to the continuum-particle interfaces was imposed by fixing the velocities at the impermeable walls of the channel. Periodic boundary conditions were used in flow direction. Initially both walls were at rest; in steady state one moved with velocity $v = 1.77\sigma/\tau$. Figure 2 shows that the fluctuations in the continuum velocities decreased away from the particle region. This effect is due to the viscous damping of continuum velocity fluctuations induced by fluctuations in the particle velocities. A small difference in the slope in the particle and continuum regions is attributed to the discrepancy between the initially measured particle viscosity, which is used in the continuum simulations, and the actual value that results under the present flow conditions. This is the typical rather than the exceptional situation and does not bear on the validity of the scheme. The good equality of the slopes on both sides of the particle region demonstrates that the model works as this reflects the correct transfer of shear forces. Correct treatment of mass and pressure transfer was tested in the Poiseuille flow simulations illustrated in fig. 3. Here the flow direction was perpendicular to

the continuum-particle interfaces. In the continuum, no-slip boundary conditions were used at the channel walls, and periodic boundaries in flow direction. In the particle region, boundaries of fixed particles were used parallel to the flow. Good agreement is found between the velocity profiles obtained by the averaging of particle motion and the up- and downstream continuum solutions. Also the parabolic prediction obtained from the continuum viscosity and forcing agrees well with the measurements.

In conclusion, we have established and tested a general strategy for the consistent coupling of different physical representations of hydrodynamic systems by means of the exchange of *fluxes* of the conserved quantities. This scheme is general in the sense that it allows the construction of a "particle window" of arbitrary boundaries within a continuum simulation—provided potential practical difficulties with the corners of such a window are dealt with. It does not require parallel orientations between the flow direction and the continuum-particle interface. More importantly, it obeys the basic conservation laws even without the exact continuum description of the particles, which may break down or not even be known in the regions of interest. Moreover, the scheme is in principle applicable to the coupling of conservative descriptions in general. It may be used to couple partial differential equations and molecular dynamics in arbitrary dimensions, as in the present case, or it could be applied to couple different particle descriptions, such as dissipative particle dynamics and molecular dynamics.

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We gratefully acknowledge many fruitful discussions with A. Aharony and O. Entin-Wohlmann on the subject. GW was partially supported by Tel Aviv University and by Schweizerischer Nationalfonds. This research was also supported by the research contract 462000-98/0 between Norsk Hydro ASA and Fracton as.

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