EUROPHYSICS LETTERS 15 March 2005

Europhys. Lett., **69** (6), pp. 959–965 (2005)
DOI: 10.1209/epl/i2004-10431-y

Fluctuations and continuity in particle-continuum hybrid simulations of unsteady flows based on flux-exchange

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received 21 September 2004; accepted in final form 14 January 2005
published online 4 February 2005

PACS. 47.11.+j – Computational methods in fluid dynamics.
PACS. 02.70.Ns – Molecular dynamics and particle methods.
PACS. 47.85.Np – Fluidics.

Abstract. – This letter describes the treatment of unsteady liquid flow by a hybrid particle-continuum scheme. The scheme couples a particle region described by molecular dynamics with a coarse-grained domain solved by continuum fluid dynamics. The particle and continuum domains overlap in the coupling region, where two-way transfer of momentum flux is established. We demonstrate that this flux-coupling scheme is able to describe high-frequency oscillatory flows and to ensure the continuity of velocity across the particle-continuum interface. The effect of fluctuations within the particle system is also analysed and establishes the range in frequency and flow wave number for which hydrodynamic fluctuations need to be taken into account within the continuum description.

Many systems are governed by a dynamic interplay between rapid molecular processes occurring within a small localised region and slower long-ranged hydrodynamic processes mediated by hydrodynamic interactions with the bulk fluid. This sort of scenario is broadly encountered in complex flows near interfaces, wetting, drop formation, melting, crystal growth from a fluid phase or moving interfaces of immiscible fluids or membranes. Such problems are usually too computationally expensive for any standard molecular dynamics (MD) simulation, while they cannot be solved by continuum fluid dynamics (CFD). An alternative is to retain the atomistic description only where it is needed and solve the bulk flow by much faster CFD methods. This multiscale approach is the essential idea of the present hybrid particle-continuum model.

A quite general procedure used in hybrid particle-continuum models, based on domain decomposition, is to connect the particle (P) and the continuum (C) domains at an overlapping or handshaking region consisting in two buffers, C $\rightarrow$ P and P $\rightarrow$ C, where the two-way exchange of information is performed. At C $\rightarrow$ P, the particle dynamics are modified to adhere to the local prescriptions of the C-flow, while within the P $\rightarrow$ C domain the microscopic

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variables are coarse-grained to supply boundary conditions for C [1,2]. The kind of information which needs to be transferred across the handshaking region has been the subject of some discussion. The first hybrid schemes to appear in the literature (see [2] for a cursory review) considered steady shear flow and were based on *variable coupling*, that is, on imposing the values of the continuum and the averaged particle velocities within the overlapping region [3]. The second coupling strategy, based on the exchange on fluxes, was first developed for hybrid simulations of gases by Garcia *et al.* [4]. The first flux-based hybrid formulation for liquids was then introduced by Flekkøy *et al.* who considered steady flows involving momentum [1] and also energy exchange [5]. Delgado-Buscalioni and Coveney [2] introduced modifications into the flux scheme at C $\to$ P and demonstrated that it admits generalised open boundary conditions which provide correct propagation and relaxation of shear, sound and heat waves [2].

The most important advantage of the flux scheme is that it guarantees the conservation laws. For a particle-continuum hybrid model the implications of this fact are widespread. Fluxes are directly evaluated from the particle dynamics and flux conservation does not require *a priori* knowledge of the constitutive relation for the P-region (actually not known in many of the applications meant for the hybrid approach, *e.g.*, complex fluids near surfaces). Also, flux boundary conditions are required if one needs to treat the P domain as an open system which exchanges mass, momentum and energy with C. For instance, any heat or density wave originating within P can only be consistently propagated to the C-region if flux boundary conditions are used. This was illustrated in ref. [2], where it was shown that if a Dirichlet boundary condition is used at the overlapping region (*i.e.*, variable coupling), heat is not properly removed from P [2]. Finally, according to the Landau description for fluctuating hydrodynamics [6], variable fluctuations arise only as a consequence of momentum flux and heat flux fluctuations. Hence the coupling of a particle system and a fluctuating hydrodynamics model should be based on fluxes. However, if the main goal of the hybrid scheme resides in solving the mean flow, one disadvantage is that fluxes across the coupling interface involve larger statistical noise than variables averaged within the overlapping volume [7].

Nevertheless, we note that an excessive noise reduction is not desirable when it comes from fluctuations playing an important part in the phenomena under study. The most important limitation of the flux scheme comes from the fact that a flux does not prescribe the variable value, and therefore variable continuity at the interface is not guaranteed. Indeed, discontinuities can be induced by particle fluctuations if the mean flow amplitude is small enough. This letter provides a way to correct the flux scheme to ensure continuity and also optimise the signal-to-noise ratio. The coupling scheme introduces an extra relaxation term which acts *only* on the C boundary condition and does not affect the flux conservation. This relaxation term ensures variable continuity with no further alteration of the particle dynamics at the interfacing region. This is relevant because the bias introduced by strong alteration of the particle dynamics (such as an external imposition of the particle velocities) can affect the statistical quantities at the P $\to$ C region. We show that the present scheme preserves the correct momentum flux variance at the P $\to$ C interface and therefore opens the possibility of MD/fluctuating-CFD hybrid models for liquids. A more favourable signal-to-noise ratio is obtained by averaging the particle flux over the interfacing volume ΔV_{PC} (instead of measuring the particle flux across the interface surface [4]). We derive the conditions under which fluctuations should be included in the C model and in the last section we demonstrate our scheme by solving the problem of unsteady forced flow. To the best of our knowledge, this is the first work dealing with hybrid descriptions of oscillatory liquid flow, which has direct applications to rheology of complex fluids.

A typical spatial domain decomposition structure for our hybrid scheme is depicted in fig. 1. Here the system ranges from $x = 0$ to $x = L_x$ and from $[-L_\alpha/2, L_\alpha/2]$ in the other two periodic directions ($\alpha = \{y, z\}$). The particle region (P) spans from $x = 0$ to $x = l_P$, the continuum

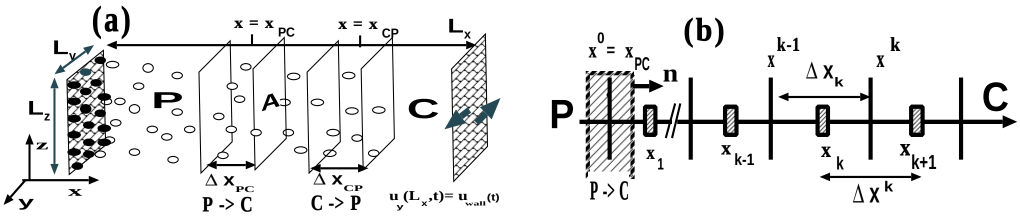

Fig. 1 – (a) The domain decomposition of the hybrid scheme in the present set-up. The coupling region consists in the C → P and P → C buffers whose volumes are $\Delta V_{CP} = A\Delta x_{CP}$ and $\Delta V_{PC} = A\Delta x_{PC}$, with $A = L_y L_z$ the interface area. The P domain, $x \leq l_P = x_{CP} + \Delta x_{CP}/2$, includes the wall around $x \sim 0$ formed by two layers of LJ particles (black circles) tethered by hard springs to a hexagonal lattice and interacting with the fluid with an increased cutoff and potential well $r_w = 1.311\sigma$ and $\epsilon_w = 1.303$, ensuring vanishingly small slip velocities. The C domain, $l_C = x_{PC} \leq x \leq L_x$, is divided into M cells centred at $x_k = (x^k + x^{k-1})/2$, where x^k denote the cell faces. (b) shows three consecutive cells of the finite-volume discretisation and the P → C buffer around $x^0 = x_{PC}$.

region (C) from $x = l_C$ to $x = L_x$ and both subdomains overlap within $l_C \leq x \leq l_P$. The particle region (P) contains $N(t)$ particles at time t, interacting through a truncated Lennard-Jones (LJ) potential $\psi(r) = \psi_{\rm LJ}(r) - \psi_{\rm LJ}(r_0)$, where $\psi_{\rm LJ}(r) = 4\epsilon^{-1}\left[(\sigma/r)^{12} - (\sigma/r)^6\right]$ and $r_0 = 2^{1/6}\sigma$. Each particle has a mass m, velocity $\boldsymbol{v}_i$ and experiences a force $\boldsymbol{f}_i^T = \boldsymbol{f}_i^{\rm ext} + \boldsymbol{f}_i$, where $\boldsymbol{f}_i$ is due to inter-particle interactions and $\boldsymbol{f}_i^{\rm ext}$ is the external force released by the continuum (see below). The equations of motion for the particles, $\dot{\boldsymbol{r}}_i = \boldsymbol{v}_i$ and $\dot{\boldsymbol{v}}_i = \boldsymbol{f}_i^T$, were solved via standard molecular dynamics (MD) using the velocity-Verlet algorithm with a time step $\Delta t_P \simeq 10^{-3}\tau$, where $\tau = (m\sigma^2/\epsilon)^{1/2}$ is the characteristic time of the LJ potential. In what follows all quantities will be expressed in reduced LJ units.

Within the C-region the relevant variables are the macroscopic local densities associated with the conserved quantities, Φ. The conservation law is expressed as $\partial\Phi/\partial t = -\nabla \cdot \boldsymbol{J}$. Momentum conservation, in particular, corresponds to $\Phi = \rho\boldsymbol{u}(\boldsymbol{r}, \boldsymbol{t})$, where ρ is the density and $\boldsymbol{u}$ the continuum velocity. In this work we shall consider fluids at fixed temperature T and focus on the flux of momentum across the P-C interface, $\boldsymbol{J} \cdot \boldsymbol{n} = (\rho\boldsymbol{u}\boldsymbol{u} + P\boldsymbol{I} + \mathbf{T}) \cdot \boldsymbol{n}$, where the interface vector $\boldsymbol{n}$ points towards C (see fig. 1). The pressure tensor $P\boldsymbol{I} + \mathbf{T}$ includes the hydrostatic pressure P and the stress tensor $\mathbf{T}$ for the Newtonian LJ fluid with shear viscosity η (see [2] for references). The coupling scheme is a twofold communication between C and P, as can be understood from fig. 1. In a previous work [2], we explained how the mass, momentum and energy fluxes evaluated from C are imposed on the particle dynamics. For consistency, we now briefly describe this part of the hybrid protocol and refer to ref. [2] for further details. This part of the coupling scheme takes place within the C → P domain which comprises the volume ΔV_{CP} around the interface position $x = x_{CP}$ (see fig. 1a). The flux of momentum across $x = x_{CP}$ is given by $(P_{CP} + \mathbf{T}_{CP}) \cdot \boldsymbol{n}_{CP}$, where the surface vector is $\boldsymbol{n}_{CP} = -\boldsymbol{n}$. This flux is introduced within the particle dynamics by adding an external force $\boldsymbol{f}_i^{\rm ext} = A(P_{CP} + \mathbf{T}_{CP}) \cdot \boldsymbol{n}_{CP}/N_{CP}$ to the $N_{CP}(t)$ particles within ΔV_{CP} (if $\boldsymbol{r}_i \notin \Delta V_{CP}$, then $\boldsymbol{f}_i^{\rm ext} = 0$). In order to maintain a desired density ρ_c within the particle system, the hydrostatic pressure needs to be given by the correct equation of state $P_{CP} = P(\rho_c, T)$.

The P → C *scheme ensuring variable continuity.* – At the P → C interface (see fig. 1b), the flux measured in the particle system must be imposed onto the continuum system as a flux boundary condition. To coherently communicate both descriptions, the particle flux transferred to the continuum domain has to be averaged over the local time and length scales of the continuum level. The mean value of any particle quantity ϕ_i within a volume ΔV of a cell centred at position $\boldsymbol{R}$ is $\phi_R(t) = \sum_i^{N_R} \phi_i(t)/N_R$, where the sum is made over the N_R particles within ΔV. The coarse-grained quantity is defined by time-averaging over Δt_{av}, *i.e.*, $\bar{\phi}_R(t) \equiv \int_0^{\Delta t_{\mathrm{av}}} \phi_R(t-\xi)\,\mathrm{d}\xi/\Delta t_{\mathrm{av}}$. In particular, the momentum flux across the P $\to$ C interface is obtained by averaging $\boldsymbol{\phi}_i = \Delta V_{PC}^{-1}[m\boldsymbol{v}_i\boldsymbol{v}_i - (1/2)\Sigma_j^N \boldsymbol{r}_{ij}\boldsymbol{f}_{ij}]\cdot\boldsymbol{n}_{PC}$ over the volume ΔV_{PC} and over Δt_{av}. This flux, denoted $\bar{\boldsymbol{j}}_{PC}\cdot\boldsymbol{n}$ is decomposed as $\bar{\boldsymbol{j}}_{PC}\cdot\boldsymbol{n} = (\bar{\boldsymbol{s}}_{PC} + \bar{\boldsymbol{\tau}}_{PC})\cdot\boldsymbol{n}$, where $\bar{\boldsymbol{s}}_{PC} \equiv \bar{\rho}\,\bar{\boldsymbol{v}}_{PC}\bar{\boldsymbol{v}}_{PC} + \bar{p}_{PC}\boldsymbol{I}$ contains the mean momentum advection ($\bar{\rho}\,\bar{\boldsymbol{v}}_{PC}$) and the particle pressure $\bar{p}_{PC}$, while $\bar{\boldsymbol{\tau}}_{PC} = \bar{\boldsymbol{j}}_{PC} - \bar{\boldsymbol{s}}_{PC}$ is the local viscous stress tensor.

We use the finite-volume method to solve the flow within the continuum region because it is based on flux conservation [8]. The coupling procedure is explained in the one-dimensional example of fig. 1b. We divide the C domain into $k = \{1,\ldots,M\}$ cells centred at x_k and separated by M + 1 faces located at x^k. The variable's value at x_k is Φ_k while Φ^k stands for its value at the cell face x^k. The time evolution of Φ_k is obtained by integrating the conservation equation $\partial\Phi/\partial t = -\nabla\cdot\boldsymbol{J}$ between each consecutive cell face $x^{k-1} \le x \le x^k$ (see fig. 1b). This yields $\dot{\Phi}_k = [J^{k-1} - J^k]/\Delta x_k$, where $\Delta x_k \equiv x^k - x^{k-1}$. To close this set of equations one requires a spatial discretisation of the flux J^k. As customary [8], we split the flux into $J^k = \mathsf{T}^k + S^k$. The term S^k includes contributions from pressure, advection or any other directly evaluable flux source, while the diffusive flux T^k is obtained from the constitutive relation $\mathsf{T}^k = -D(\Phi_{k+1} - \Phi_k)/\Delta x^k$, where $\Delta x^k \equiv x_{k+1} - x_k$ and D is the corresponding transport coefficient. We use a first-order discretisation for the time derivative $\dot{\Phi}_k \simeq [\Phi_k(t+\Delta t_C) - \Phi_k(t)]/\Delta t_C$, where the C time step Δt_C satisfies $\Delta t_P \ll \Delta t_C \le \Delta t_{\mathrm{av}}$. Introducing $r_e \equiv D\Delta t_C/(\Delta x^k \Delta x_k)$ and $r_w \equiv D\Delta t_C/(\Delta x^{k-1}\Delta x_k)$, the resulting explicit scheme for the $k = \{1,\ldots,M\}$ cells is

$$\Phi_k(t+\Delta t_C) = (1 - r_e - r_w)\,\Phi_k(t) + r_w\Phi_{k-1}(t) + r_e\Phi_{k+1}(t) + \left(S^{k-1} - S^k\right)\frac{\Delta t_C}{\Delta x_k}\,. \qquad (1)$$

Note that for the explicit scheme (1) to be stable one requires the standard Courant condition, $r_k \le 1/2$ [8]. In order to close eq. (1) for $k = 1$ and $k = M$, one needs to assign the value to the flow variables at the cells outside the C domain: Φ_0 and Φ_{M+1}. To that end, one uses the boundary conditions at x^0 and x^M. Here we focus on the evaluation of Φ_0 which must be obtained from $J^0 = \bar{j}_{PC}$, *i.e.*, from the flux conservation across the P-C interface $x^0 = x_{PC}$ (see fig. 1b). The particle flux due to pressure and advection is simply set by $S^0 = \bar{s}_{PC}$ (see eq. (2) below). In what follows, we discuss the imposition of the diffusion flux T^0, which shall provide Φ_0. In order to set the standard flux boundary condition, one imposes flux conservation $T^0 = \bar{\tau}_{PC}$ into a discretized expression for T^0 involving Φ_0; such as $T^0 = -D(\Phi_1 - \Phi_0)/\Delta x^0$. This provides $\Phi_0 = \Phi_1 + \Delta x^0\bar{\tau}_{PC}/D$, which is then inserted in eq. (1) to close the time marching scheme for the boundary cell Φ_1. In our case, however, at x_1 the system is represented both by particles and continuum variables. This leaves us with a freedom of choice for the expression of T^0, as it can involve either Φ_1 or the coarse-grained P-variable $\bar{\phi}_1$. To fully analyse the implications of such choice, we propose the linear interpolation $\hat{\Phi}_1 \equiv (1-\alpha)\Phi_1 + \alpha\,\bar{\phi}_1$. A stable scheme is obtained by expressing T^0 with a "hybrid" gradient $T^0 = -D(\hat{\Phi}_1 - \Phi_0)/\Delta x^0$ [9] which contains information on the particle variable $\bar{\phi}_1$ if $\alpha > 0$ is chosen. The outer cell value is then $\Phi_0 = \hat{\Phi}_1 + \Delta x^0\bar{\tau}_{PC}/D$ and inserting this in eq. (1) for $k = 1$ provides

$$\Phi_1(t+\Delta t_C) = (1-r_e)\,\Phi_1(t) + r_e\,\Phi_2(t) + \frac{\bar{\tau}_{PC}\Delta t_C}{\Delta x^0} + \left(\bar{s}_{PC} - S^1\right)\frac{\Delta t_C}{\Delta x_1} + \alpha r_w\left(\bar{\phi}_1(t) - \Phi_1(t)\right). \quad (2)$$

For $\alpha > 0$, the last term on the right-hand side of eq. (2) acts as a relaxation term that drives the continuum variable at the boundary cell $x = x_1$ towards the particle average $\bar{\phi}_1$. This term becomes negligible once continuity is established, $\Phi_1 \simeq \bar{\phi}_1$. The scheme of eq. (2) was first tested under steady Couette flows using densities $0.4 \le \rho \le 0.85$, temperature $1.0 \le T \le 4.0$ and shear rates $10^{-3} \le \gamma \le 0.5$ (where $\gamma \equiv u_y^{\rm wall}/L_x$). In all simulations and for any α used, the flux balance is respected within less than around 3%. Concerning variable continuity, the standard flux-coupling scheme ($\alpha = 0$) gives rise to a velocity discontinuity at the overlapping region which grows to a size comparable to that of particle velocity fluctuations. Instead, using $\alpha = 1$ in eq. (2), continuity was ensured within $\Delta t_{\rm av} \sim 1$ and seamless linear velocity profiles are obtained at arbitrary shear rates. Similar seamless velocity profiles are obtained for any $\alpha > 0$ used indicating that the scheme is not sensitive to this relaxation parameter. This result is expected because, as deduced from eq. (2), the relaxation time required for variable continuity to hold is of order $\Delta t_C/(r_w \alpha)$ (where $r_w \le 1/2$). Continuity is ensured if this relaxation time is much smaller than the mean flow time scale, *i.e.*, $\alpha \gg \omega \Delta t_C$, where ω is the flow characteristic frequency. This condition is always fulfilled for steady flow $\omega = 0$, and it imposes no restriction (see below) for unsteady flows (unless at very high frequencies $\omega \sim {\rm O}(1)$ for which, in any case, the continuum picture would be no longer valid).

Shear stress fluctuations and accuracy limits. – The flux balance across the P $\to$ C interface establishes $\overline{\boldsymbol{\tau}}_{PC} = \mathsf{T}_{PC} + \mathsf{T}'_{PC}$, where we have decomposed the viscous stress into a deterministic part T_{PC} and a random contribution T'_{PC}. Clearly, one can only neglect fluctuations in the C description of the hybrid scheme if the signal-to-noise ratio of the exchanged flux $\overline{\tau}_{PC}$ is sufficiently large. We denote this ratio as $E \equiv \langle \overline{\tau}_{PC} \rangle / \langle (\overline{\tau}'_{PC})^2 \rangle^{1/2}$, where $\langle [\overline{\tau}'_{PC}]^2 \rangle$ is the variance of $\overline{\tau}_{PC}$. We now identify the implications for the sizes of ΔV_{PC} and $\Delta t_{\rm av}$ with respect to the value of E. To illustrate the discussion we shall focus on the xy component of the viscous tensor $\mathsf{T} \equiv \boldsymbol{x}\mathsf{T}\boldsymbol{y}$ (*i.e.*, on shear flows). In order to evaluate E, we need the variance of $\overline{\tau}_{PC} = \int_0^{\Delta t_{\rm av}} \tau_{PC}(t-\xi){\rm d}t/\Delta t_{\rm av}$, which is calculated by averaging a certain number of samples of the instantaneous stress τ_{PC} over a time window $\Delta t_{\rm av}$. If the time interval between samples is made larger than the proper particle decorrelation time t_λ [10], these samples are uncorrelated and the central-limit theorem tells us that $\langle [\overline{\tau}'_{PC}]^2 \rangle \propto 1/\Delta t_{\rm av}$. The prefactor can be obtained by carrying out the Landau-Lifshitz analysis for fluctuating fluids [6], which results in $\langle [\overline{\tau}'_{PC}]^2 \rangle = 2\eta T/(\Delta V_{PC} \Delta t_{\rm av})$ (see ref. [7] for a kinetic derivation for gases). We measured the variance $\langle [\overline{\tau}'_{PC}]^2 \rangle$, from the simulations of Couette flows mentioned above, obtaining good agreement (within 10%) with the Landau expression. This result is important because it indicates that the present scheme does not significantly bias the particle dynamics within the P $\to$ C cell, and consistency with fluctuating hydrodynamics is preserved.

The flux signal in a simple shear flow is $\langle \overline{\tau}_{PC} \rangle = \eta \gamma_{PC}$, where γ_{PC} is the local shear rate; so $E^2 = \gamma_{PC}^2 \eta \Delta V_{PC} \Delta t_{\rm av}/(2T)$ and the signal is larger than its noise ($E > 1$) if

$$\Delta V_{PC} \Delta t_{\rm av} > \frac{2T}{\gamma_{PC}^2 \eta} \,. \qquad (3)$$

Equation (3) can be used to control the signal-to-noise ratio of the coarse-grained momentum flux. Clearly, when solving a steady flow the inequality (3) can always be fulfilled by extending the averaging time $\Delta t_{\rm av}$. However, when solving an unsteady flow, $\Delta t_{\rm av}$ cannot be larger than the characteristic flow period ω^{-1}. Similarly, Δx_{PC} has to be smaller than the characteristic length of variation of the shear stress, $k_{PC}^{-1} \equiv |({\rm d}\mathsf{T}/{\rm d}x)_{PC}/\mathsf{T}_{PC}|$. For temporal and spatial resolution one requires that, at least, $\Delta t_{\rm av}\omega \le {\rm O}(0.1)$ and $\Delta x_{PC} k_{PC} \le {\rm O}(0.1)$ and if so, eq. (3) indicate that fluctuations can be neglected if $k_{PC}\omega < \gamma_{PC}^2 \eta \Delta V_{PC}/(T \Delta x_{PC})$.

If required, flux fluctuations can be easily coupled in the present scheme using the Landau formalism in the C fluid model. Stress fluctuations at each cell volume of the C domain ΔV_k are inserted into the discretized continuum equations by adding a random stress T'_k with zero mean and correlation $\langle \mathsf{T}'_k(t) \mathsf{T}'_{k'}(t') \rangle = [2T\eta/(\Delta V_k \Delta t_C)]\delta_{kk'}\delta_{tt'}$ [6, 11]. Hence, the variance of the stress fluctuations $\langle(\mathsf{T}'_{PC})^2\rangle = 2T\eta/(\Delta V_{PC}\Delta t_C)$ will coincide with that of the coarse-grained P-flux by simply setting $\Delta t_{\rm av} = \Delta t_C$. This means that the present flux scheme is naturally suited to interface an MD domain with any mesoscopic model based on the Landau formalism for fluctuating hydrodynamics [11–13]. Such hybrid models have not yet been developed for liquids; however Alexander and coworkers implemented a similar model to study Fickian diffusion [14] in gases. They showed that if the proper stochastic representation is used for C, both the mean and variance of the density are correctly matched.

Application to oscillatory shear flow. – To demonstrate the proposed scheme in the case of unsteady scenarios, we consider isothermal fluid flow in a slot driven by the oscillatory motion of one of the walls in its own plane: the so-called Stokes problem. The flow is uniquely driven by the wall at $x = L_x$ which introduces a velocity $u_y^{\rm wall}(t) = u_{\max}\sin(2\pi\omega t)$ as a Dirichlet boundary condition for C at $x^M = L_x$ (*i.e.*, $u_y^M = u_y^{\rm wall}$). The mean density is ρ_c and the fluid is taken to be incompressible. Within the P domain the temperature T_c is kept constant by thermostatting the x and z translational degrees of freedom. There are no transfers of mean energy or mass along the x-direction and in the particle system this condition is ensured by using the scheme described by Barsky *et al.* [15]. Under these circumstances the mean pressure is constant throughout the domain and the equation for the transversal velocity is $\partial u_y/\partial t = \nu\partial^2 u_y/\partial x^2$ with $\nu = \eta/\rho_c$. The finite-volume discretisation of this equation is obtained by letting $\Phi = \rho_c u_y$, $S^k = 0$ and $D = \nu$ in eq. (1). As usual [8], the Dirichlet boundary condition is imposed by setting $u_{y,M+1} = 2u_y^{\rm wall} - u_{y,M}$ in eq. (1). We used a regular grid, $\Delta x_k \sim 0.5$ and $\Delta t_C < \Delta x^2/(2\nu)$ to ensure the stability of the explicit scheme of eq. (1) [8]. The flow profiles in fig. 2 show the good agreement between the hybrid simulations and the analytical solution. The frequencies considered ranged from $\omega = 0$ (Couette flow) to $\omega = 0.01$. We note that oscillatory shear flow is widely used in rheology of complex fluids and, in particular, the range of frequencies and flow amplitudes considered here are relevant

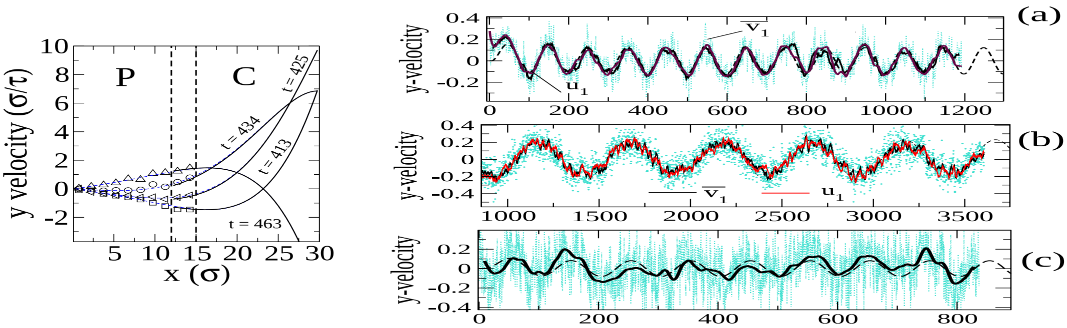

Fig. 2 – Left: snapshots of the y velocity profile of a LJ fluid at $\rho = 0.8$ and $T = 1.0$. The wall velocity is $u_y^{\rm wall}(t) = u_{\max}\sin(2\pi\omega t)$, with $u_{\max} = 10$ and $\omega = 0.01$ and $L_y = L_z = 9$. The overlapping region is indicated with vertical dashed lines. Symbols within the P region indicate the mean velocities within slices of width $1.6(= \Delta x_{PC})$ and averaged over $\Delta t_{\rm av} = 1$. Solid lines are the C-flow profile and dashed lines are the analytical profile [16]. Right: the velocity within the overlapping region for $u_{\max} = 0.5$, $\Delta t_{\rm av} = 10$ and (a) $T = 1$ and $\omega = 0.01$, (b) $T = 1$ and $\omega = 0.002$ and (c) $T = 4$ and $\omega = 0.01$. Case (b) is solved using $\alpha = 0.1$ and the rest with $\alpha = 1$. The value of $5\,(T/\rho\Delta V_{PC})^{1/2}$ is 0.49 in cases (a) and (b) and $0.98 (> u_{\max})$ in case (c). Solid lines correspond to the coarse-grained particle velocity $\overline{v}_1$; in (a) and (b) we compare it with the continuum velocity at the same cell u_1. The strongly fluctuating line corresponds to the instantaneous mean velocity $v_1(t)$ and dashed lines to the analytical solution. All quantities are given in reduced LJ units.

to the rheology of polymer brushes [16]. In recent work we used this hybrid scheme to study the dynamics of tethered polymers under steady uniform shear flow [15]; the oscillatory case will be discussed in future publications.

We used a deterministic model for C, so the accuracy of the scheme can be compared with the prediction of eq. (3). In the Stokes flow, the momentum introduced by the moving wall penetrates up to a viscous fluid layer of width $\delta \sim \sqrt{\pi\nu/\omega}$ and tends to zero diffusively as the other wall is approached. Within the viscous layer the shear rate is $\gamma \sim u_{\max}/\delta$. We used $\Delta t_{\mathrm{av}}\omega \leq 0.1$ and inserting these two relations into eq. (3) one gets that the signal-to-noise ratio $E > 1$ if $u_{\max} > 5(T/\rho\Delta V_{PC})^{1/2}$. As illustrated in fig. 2, we choose $u_{\max}$ in cases (a) and (b) to consider a flow slightly above the $E \sim 1$ threshold. In fig. 2a we compare the P-velocity $\overline{v}_1$ and C-velocity u_1 at the same cell to illustrate that continuity is perfectly satisfied. Also, we solved case (a) using $\alpha = 1$ and case (b) with $\alpha = 0.1$ to show that the flow solution does not depends on the value of α used, as long as $\alpha \gg \omega\Delta t_C$. In case (c) we increased the temperature from $T = 1$ to $T = 4$ and, according to eq. (3), this is enough for the noise to overpower the signal. Indeed, as seen in fig. 2c, $\overline{v}_1$ is a strongly fluctuating signal meaning that fluctuations should be taken into account in the C-flow.

In conclusion, the present hybrid particle-continuum scheme based on flux-exchange can describe oscillatory shear flows over a broad range of frequencies. We showed that using hybrid gradients across the particle-continuum interface is a simple and robust way to ensure variable continuity. The resulting "variable-coupling" term acts *only* on the C boundary condition and does not directly bias the particle dynamics. The scheme thus preserves the variance of the averaged P-flux across the coupling region consistent with the Landau expression [6] and is naturally suited to interface an MD region with a fluctuating hydrodynamics domain, *à la* Landau [11–13].

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This research was supported by the European Commission through a Marie Curie Fellowship to RD-B (HPMF-CT-2001-01210) (2000-02) and by the EPSRC RealityGrid project GR/R67699. RD-B also acknowledges support from project BFM2001-0290.

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[9] Instead one could fix $T^0 = \overline{\tau}_{PC}$ and evaluate T^1 using the "hybrid" gradient $T^1 = -D(\Phi_2 - \hat{\Phi}_1)/\Delta x^1$. However, the resulting scheme $\dot{\Phi}_1 = r_e(\Phi_2 - \Phi_1) + \overline{j}_{PC}/\Delta x_1 - \alpha r_e(\overline{\phi}_1 - \Phi_1)$ is unstable.
[10] Given by $t_\lambda = \int_0^\infty \langle \tau'_{PC}(t)\tau'_{PC}(0)\mathrm{d}t\rangle / \langle [\tau'_{PC}]^2 \rangle$. From MD simulations we obtained $t_\lambda \simeq 0.06$.
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