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MULTISCALE FLOW SIMULATIONS USING PARTICLES

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■ **Abstract** Flow simulations are one of the archetypal multiscale problems. Simulations of turbulent and unsteady separated flows have to resolve a multitude of interacting scales, whereas molecular phenomena determine the structure of shocks and the validity of the no-slip boundary condition. Particle simulations of continuum and molecular phenomena can be formulated by following the motion of interacting particles that carry the physical properties of the flow. In this article we review Lagrangian, multiresolution, particle methods such as vortex methods and smooth particle hydrodynamics for the simulation of continuous flows and molecular dynamics for the simulation of flows at the atomistic scale. We review hybrid molecular-continuum simulations with an emphasis on the computational aspects of the problem. We identify the common computational characteristics of particle methods and discuss their properties that enable the formulation of a systematic framework for multiscale flow simulations.

1. INTRODUCTION

The simulation of the motion of interacting particles is a deceivingly simple, yet powerful and natural, method for exploring physical systems as diverse as planetary dark matter and proteins, unsteady separated flows, and plasmas. Particles can be viewed as objects carrying a physical property of a system, that is being simulated through the solution of Ordinary Differential Equations (ODEs) that determine the trajectories and the evolution of the properties carried by the particles. Particle methods amount to the solution of a system of ODEs:

$$\frac{d\mathbf{x}_p}{dt} = \mathbf{u}_p(\mathbf{x}_p, t) = \sum_{q=1}^{N} \boldsymbol{K}(\mathbf{x}_p, \mathbf{x}_q; \boldsymbol{\omega}_p, \boldsymbol{\omega}_q) \tag{1}$$

$$\frac{d\boldsymbol{\omega}_p}{dt} = \sum_{q=1}^{N} \boldsymbol{F}(\mathbf{x}_p, \mathbf{x}_q; \boldsymbol{\omega}_p, \boldsymbol{\omega}_q), \tag{2}$$

where $\mathbf{x}_p, \mathbf{u}_p$ denote the locations and velocities of the N particles, $\boldsymbol{\omega}_p$ denote particle properties (such as density, temperature, velocity, vorticity), and $\boldsymbol{K}, \boldsymbol{F}$ represent the dynamics of the simulated physical system. In flow simulations particles are implemented with a Lagrangian formulation of the continuum equations, as in the vorticity formulation of the Navier-Stokes equations, or with systems that are discrete by nature, as in molecular flows at the nanoscale. Continuum flows, such as flows in porous media and unsteady separated and turbulent flows, are inherently multiscale due to the range of scales that govern the underlying physical phenomena. The continuum assumption fails in flow regions containing contact lines and shocks, and suitable molecular descriptions become necessary. A consistent and systematic framework is necessary to couple molecular and macroscale descriptions because the macroscale flows determine the external conditions that influence the molecular system, which in turn influences the larger scales by modifying its boundary conditions.

Particle methods such as Vortex Methods (VMs) and Smooth Particle Hydrodynamics (SPH) present an adaptive, efficient, stable, and accurate computational method for simulating continuum flow phenomena and for capturing interfaces such as vortex sheets. On the other hand, particle methods encounter difficulties in the accurate treatment of boundary conditions, while their adaptivity is often associated with severe particle distortion that may introduce spurious scales. Ongoing research efforts attempt to address these issues as outlined in the review.

In molecular and mesoscopic simulations particle methods, such as Molecular Dynamics (MD) and Dissipative Particle Dynamics (DPD), are the methods of choice because the discrete representation of the underlying physics is inherently linked to interacting particles. Particle methods for continuum and discrete systems present a unifying formulation that can enable systematic and robust multiscale simulations, as we outline in this review.

A remarkable feature of particle methods is that their computational structure involves a large number of common abstractions that help in their computational implementation, while at the same time particle methods are distinguished by the fact that they are inherently linked to the physics of the systems that they simulate.

In this review we focus on updating the reader in methodological advances in Lagrangian particle methods since the first related such review by Leonard in 1985 (Leonard 1985), with an emphasis toward describing methodologies that enable multiresolution simulations. In the simulation of discrete systems, starting from the review of Koplik & Banavar (1995), we focus on hybrid continuum-molecular flow simulations. In this article we do not discuss particle methods for the simulation of kinetic equations, for which we refer the reader to Chen & Doolen's (1998) work.

The review is structured as follows: We introduce particle methods for continuous systems by illustrating unifying concepts such as function and derivative particle approximations. We discuss the fundamental problem of particle distortion and remeshing associated with the Lagrangian formulation and introduce multiresolution particle methods. We briefly outline the key characteristics of molecular

simulations and discuss recent advances in hybrid continuum-molecular simulations. We conclude by describing efficient tools for large-scale simulations using particle methods and provide an outlook for future developments in particle methods in this new era of multiscale modeling and simulation.

2. PARTICLE METHODS FOR CONTINUOUS SYSTEMS

Particle methods for continuum flow simulations include VMs and SPH. The key common characteristic of these methods involves the approximation of the Lagrangian form of the Navier-Stokes equations by replacing the derivative operators through equivalent integral operators that are in turn discretized on the particle locations.

2.1. Particle Function Approximations

Point particle approximations were the first to attract attention in solving fluid mechanics problems because their evolution can be formulated in terms of conservation laws. An approximation of a smooth function f in the sense of measures (Raviart 1986) can be formulated as:

$$f^h = \sum_{p=1}^{N} w_p \, \delta(\mathbf{x} - \mathbf{x}_p), \tag{3}$$

where w_p denotes the weights of the particles. Although the point particle approximation has several interesting properties, particularly when considering exact formulations of conservation equations, smooth function approximations are often desirable, allowing recovery of the function between particle locations and a regularized formulation of the particle motion. Smooth function approximations can be constructed by using a mollification kernel $\zeta_\varepsilon(\mathbf{x})$:

$$f_\varepsilon(\mathbf{x}) = f \star \zeta_\varepsilon = \int f(\mathbf{y}) \, \zeta_\varepsilon(\mathbf{x} - \mathbf{y}) \, d\mathbf{y}, \tag{4}$$

where ε denotes a characteristic length of the kernel.

The particle approximation of the regularized function is defined as

$$f_\varepsilon^h(\mathbf{x}) = f^h \star \zeta_\varepsilon = \sum_{p=1}^{N} w_p \, \zeta_\varepsilon(\mathbf{x} - \mathbf{x}_p). \tag{5}$$

The error introduced by the quadrature of the mollified approximation f_ε^h for the function f can be distinguished in two parts as

$$f - f_\varepsilon^h = (f - f \star \zeta_\varepsilon) + (f - f^h) \star \zeta_\varepsilon. \tag{6}$$

The first term in Equation 6 denotes the mollification error that can be controlled by appropriately selecting the kernel properties. The second term denotes the

quadrature error due to the approximation of the integral on the particle locations. Since the early 1980s, mollifier kernels have been developed in VMs with an emphasis on the property of moment conservation to comply with vorticity moments conserved by the Euler equations. The accuracy of these methods is related to the moments that are being conserved, and a method is of order r when:

$$\begin{cases} \int \zeta(\mathbf{x})\, d\mathbf{x} = 1 \\ \int \mathbf{x}^{\mathbf{i}} \zeta(\mathbf{x})\, d\mathbf{x} = 0 \quad \text{if} \quad |\mathbf{i}| \leq r-1 \\ \int |\mathbf{x}|^r |\zeta(\mathbf{x})|\, d\mathbf{x} < \infty \end{cases} \tag{7}$$

The overall accuracy of the method is then:

$$\| f - f_\varepsilon^h \|_{0,p} \sim \mathcal{O}(\varepsilon^r) + \mathcal{O}\left(\frac{h^m}{\varepsilon^m}\right). \tag{8}$$

For equidistant particle locations at spaces h in a d-dimensional space, the weights can be chosen as: $w_p = h^d f(\mathbf{x}_p)$ with $m = \infty$ for certain kernels and for positive kernels such as the Gaussian, $r = 2$. Kernel cutoffs of arbitrary order (Beale 1986) are possible by giving up the positivity of the cutoff. These error estimates reveal an important, albeit often overlooked, fact for smooth particle approximations: to obtain accurate approximations smooth particles must overlap. Note that the moment conditions expressed by the integrals of the mollifier functions are not often well represented for discrete particle sets. These moment conditions can be ensured by appropriate normalizations (Cottet & Koumoutsakos 2000).

2.1.1. PARTICLE DERIVATIVE APPROXIMATIONS Although the representations of functions by particles can be considered a post-processing step, the approximation of derivatives is a key aspect in the development of particle methods for solving the governing flow equations.

Particle approximations of the derivative operators can be constructed through their integral approximations. This can be easily achieved by taking the derivatives of Equation 4 as convolution and derivative operators commute in unbounded or periodic domains. These approximations can be cast in a conservative formulation and are extensively employed in SPH.

An alternative formulation involves the development of integral operators that are equivalent to differential operators such as the Laplacian. Motivated by the need to construct high-order viscous algorithms for VMs, in 1987 Mas-Gallic introduced the method of Particle-Strength Exchange (PSE). The PSE scheme can be derived starting from a straightforward Taylor expansion of f around $\mathbf{x}$:

$$f(\mathbf{y}) = f(\mathbf{x}) + (\mathbf{y}-\mathbf{x}) \cdot \nabla f(\mathbf{x}) + \sum_{i,j} (x_i - y_i)(x_j - y_j) \frac{\partial^2 f}{\partial x_i \partial x_j} + \cdots. \tag{9}$$

Convolving this expansion with an even function η, the first-order terms and the cross-terms involving the second-order derivatives of f drop out in the righthand

side of Equation 9 and, using the normalization conditions,

$$\eta_\varepsilon(\mathbf{x}) = \varepsilon^{-d}\eta\left(\frac{\mathbf{x}}{\varepsilon}\right), \qquad \int x_i^2\eta(\mathbf{x})\,d\mathbf{x} = 2 \qquad i = 1, \cdots, d \tag{10}$$

leads to the approximation (Degond & Mas-Gallic 1989a):

$$\Delta_\varepsilon f(\mathbf{x}) = \varepsilon^{-2}\int (f(\mathbf{y}) - f(\mathbf{x}))\,\eta_\varepsilon(\mathbf{y}-\mathbf{x})\,d\mathbf{y}, \tag{11}$$

where $\Delta_\varepsilon f(\mathbf{x})$ denotes the mollified approximation of the Laplacian operator. High-order approximations can be obtained by choosing suitable functions η. The anisotropic extension of this method is defined as

$$\nabla\cdot\,[B\nabla f](\mathbf{x}) \simeq \varepsilon^{-2}\sum_{i,j=1}^{d}\int \psi_{ij}^{\varepsilon}(\mathbf{x}-\mathbf{y})M_{ij}(\mathbf{x},\mathbf{y})\,[f(\mathbf{y}) - f(\mathbf{x})]\;d\mathbf{y}, \tag{12}$$

where $M_{ij}(\mathbf{x},\mathbf{y})$ are symmetric functions and ψ_{ij}^{ε} are cut-off functions, related to each other and to the matrix B through conditions that are detailed in Degond & Mas-Gallic (1989b). Starting from the PSE formulation Eldredge et al. (2002) presented a general deterministic integral representation for derivatives of arbitrary order. The error analysis of particle derivative approximations strengthens the requirement for particle overlap.

In particle methods the precise connectivity of the computational elements (as, for example, in finite difference methods) is not required to discretize the governing equations, but neighboring elements need to overlap to provide consistent approximations.

2.2. Vortex Methods

Vortex particle methods have been used since the 1930s (Rosenhead 1930) to describe the evolution of vortical structures in incompressible flows.

Navier-Stokes equations describe the evolution of the vorticity field in 3D, incompressible, viscous flows in a velocity-vorticity ($\mathbf{u}$, $\boldsymbol{\omega} = \nabla\times\mathbf{u}$) formulation as

$$\frac{\partial\boldsymbol{\omega}}{\partial t} + (\mathbf{u}\cdot\boldsymbol{\nabla})\,\boldsymbol{\omega} = (\boldsymbol{\omega}\cdot\boldsymbol{\nabla})\,\mathbf{u} + \nu\Delta\boldsymbol{\omega} \tag{13}$$

The velocity field $\mathbf{u}$ is obtained by solving the Poisson equation

$$\nabla^2\mathbf{u} \;=\; -\nabla\times\boldsymbol{\omega} \tag{14}$$

with suitable boundary conditions (Cottet & Koumoutsakos 2000). Velocity calculations, satisfying explicitly far-field boundary conditions, are based on the Biot-Savart law:

$$\mathbf{u} = \int \mathbf{K}(\mathbf{x}-\mathbf{y}) \;\times\; \boldsymbol{\omega}\,d\mathbf{y} + \boldsymbol{U_0}(\mathbf{x},t), \tag{15}$$

where $\boldsymbol{U_0}(\mathbf{x}, t)$ is the solution of the homogeneous Equation 14, and $\mathbf{K}(\mathbf{z})$ denotes the Biot-Savart kernel for the Poisson equation.

The Navier-Stokes equations can be expressed in a Lagrangian formulation, leading to a set of equivalent ODEs as:

$$\frac{d\mathbf{x}_p}{dt} = \mathbf{u}(\mathbf{x}_p, t) \tag{16}$$

$$\frac{d\boldsymbol{\omega}_p}{dt} = \left[\nabla \mathbf{u}(\mathbf{x}_p, t)\right] \boldsymbol{\omega}_p + \nu\ \Delta\boldsymbol{\omega}(\mathbf{x}_p), \tag{17}$$

where $\mathbf{x}_p$, $\boldsymbol{\omega}_p$ denote the locations and the vorticity carried by the fluid elements. The equations need to be supplied with initial and far-field conditions along with the no-slip condition in the presence of solid boundaries.

The essence of the VMs we describe herein is based on the work of Krasny (1986) and it amounts to the regularization of the convecting velocity field and the systematic removal of spurious vortical structures.

VMs are based on this Lagrangian description and use vorticity-carrying particles with a finite core size ε so the vortex-blob approximation is given by

$$\boldsymbol{\omega}_\varepsilon^h(\mathbf{x}) = \sum_p v_p \boldsymbol{\omega}_p \zeta_\varepsilon(\mathbf{x} - \mathbf{x}_p), \tag{18}$$

where $\mathbf{x}_p$, v_p, and $\boldsymbol{\omega}_p$, respectively, represent the locations, volumes, and vorticity of the particles. In VMs, the field is recovered at every location of the domain only if one considers the collective behavior of all computational elements. In addition, when particles overlap, the scales of the physical quantities that are resolved are determined by the particle core rather than the interparticle distance. This observation differentiates particle methods from schemes such as finite differences. Viscous effects are simulated using the method of PSE (Equation 11). Flows with solid boundaries are treated using a fractional step algorithm (Chorin 1973), solving in turn the inviscid and viscous parts of the equations. The enforcement of kinematic boundary conditions (such as no-through flow at solid boundaries) can be achieved by boundary integral methods whereas enforcement of viscous boundary conditions (such as no-slip) is translated into a vorticity flux boundary condition (Cottet & Poncet 2004, Koumoutsakos et al. 1994) complementing the viscous part of the equations. This boundary condition is enforced using an integral formulation, resulting in an explicit modification of the particle weights near the boundary. It can be formulated by adding a forcing term to the vorticity equation, amounting to an immersed boundary method (see article by Mittal & Iaccarino in this volume).

The vortex-blob method can be summarized by the following system of ODEs for the particle locations and vorticities

$$\frac{d\mathbf{x}_p}{dt} = \sum_{q=1}^{N} v_q\ K_\varepsilon(\mathbf{x}_p - \mathbf{x}_q) \times \boldsymbol{\omega}_q + \boldsymbol{U_0}(\mathbf{x}_p, t) \tag{19}$$

$$\frac{d\boldsymbol{\omega}_p}{dt} = \left[\sum_{q=1}^{N} v_q \, \nabla K_\varepsilon(\mathbf{x}_p - \mathbf{x}_q) \times \boldsymbol{\omega}_q\right] \boldsymbol{\omega}_p \tag{20}$$

$$+ \frac{\nu}{\varepsilon^2} \sum_{q=1}^{N} v_q \, [\boldsymbol{\omega}_q - \boldsymbol{\omega}_p] \, \eta_\varepsilon(|\mathbf{x}_p - \mathbf{x}_q|) + \boldsymbol{F}(\mathbf{x}_p), \tag{21}$$

where the term $\boldsymbol{F}(\mathbf{x}_p)$ accounts for the generation of vorticity at solid boundaries. Based on these discretizations, particle methods are unconditionally linearly stable. Nonlinear stability imposes that particle trajectories do not cross, which results in a time-step constraint of the type

$$\Delta t \leq C \|\nabla \mathbf{u}\|_\infty^{-1}, \tag{22}$$

where the coefficient C depends on the particular numerical scheme. The stability properties of VMs make them a suitable candidate for the Heterogeneous Multiscale Methods (HMM) framework introduced by E & Engquist (2003).

In the past, VMs were used extensively for simulations of engineering applications, such as unsteady bluff body flows, with reasonable agreement between computational and experimental results (see Sarpkaya 1989 for a thorough review). This agreement can be explained by analyzing the error (Leonard 1985) introduced by smooth VMs, indicating that computations with vortex particles implicitly realize some kind of turbulence modeling (Cottet 1996). Ignoring viscous effects, smooth VMs amount to solving a mollified form of the Euler equations:

$$\frac{\partial \overline{\boldsymbol{\omega}}}{\partial t} + \boldsymbol{\nabla} \cdot \overline{\mathbf{u}_\varepsilon \boldsymbol{\omega}} - \overline{(\boldsymbol{\omega} \cdot \nabla)\mathbf{u}_\varepsilon} = 0, \tag{23}$$

where the overbars denote mollification with a smooth kernel. When compared to the Euler equation for the fields $\mathbf{u}_\varepsilon$ and $\boldsymbol{\omega}_\varepsilon$, this equation involves a truncation error with a component proportional to $\nabla \cdot ([\nabla \mathbf{u}_\varepsilon] \nabla \boldsymbol{\omega})$, contributing to enstrophy transfer between different scales. This term is responsible for the emergence of microstructures in calculations using VMs, because unlike grid-based methods, their dynamics is not constrained to any minimal scale beyond the initialization stage. To remove the backscatter, a natural scheme is to formulate the error term as an integral operator amounting to anisotropic diffusion and to adjust accordingly the particle weights to compensate for this term. Alternatively, regularization of the particle locations can compensate for this error.

In the last two decades we have seen a number of theoretical developments and benchmark flow simulations using VMs. Direct Numerical Simulations (DNS) of the flow past an impulsively started cylinder (Figure 1) for a range of Reynolds numbers (Koumoutsakos & Leonard 1995) have demonstrated that VMs can automatically adapt computational elements in regions of the flow where increased resolution is necessary to capture unsteady separation phenomena. The results obtained by VMs for this flow are in excellent agreement with experimental and analytical studies. Comparisons in terms of the drag coefficient for this flow for

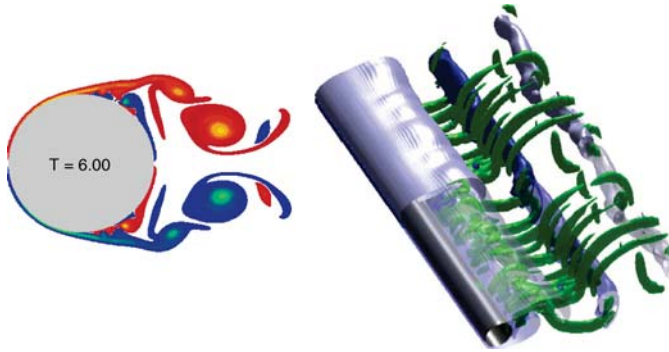

Figure 1 Left: Vorticity at T = 6.0 for flow past a two-dimensional impulsively started cylinder of Re = 9500 using the Vortex Method with a Fast Multipole Method (courtesy of Koumoutsakos & Leonard 1995). Right: Three-dimensional flow past a cylinder at Re = 300 that was computed using a vortex-in-cell method. Iso-surfaces of spanwise and transverse vorticity are shown (courtesy of Cottet et al. 2004).

Re = 1000, with high-order finite difference methods (Anderson & Reider 1996), show that VMs compare favorably in terms of the number of computational elements for the same accuracy. Comparisons with spectral element methods (Fischer 1997) for Re = 9500 reveal that the results obtained with VMs can be obtained by spectral element methods, albeit only when using additional elements in critical parts of the flow. These parts of the flow are not always known a priori and for grid-based methods suitable criteria need to be devised to add computational elements in critical regions depending on the physics of the flow. VMs have the advantage that computational elements are inherently linked to the physics they represent and thus no such additional criteria are necessary. Simulations using VMs of flow past a sphere (Ploumhans et al. 2002) and a 3D cylinder (Figure 1) (Cottet & Poncet 2004) have shown the same advantages for 3D flows.

The use of VMs is particularly advantageous for simulations of controlled flows involving unsteady boundary motions as the Lagrangian formulation of the convective transport term enables large time steps. In Eulerian-based methods, because finer resolution is necessary to capture the vortical structures near the boundaries, smaller time steps are necessary to obey the transport Courant-Friedrichs-Levy (CFL) condition as the near wall elements experience large velocities induced by the motion of the boundary (Poncet 2004).

Simulations of homogeneous turbulence show that energy spectra obtained using VMs are in excellent agreement with those predicted by spectral element methods (see Figure 2) (Cottet et al. 2002). These simulations indicate that although VMs are less efficient than spectral methods, their computational cost is not prohibitive for simulations of homogeneous turbulence.

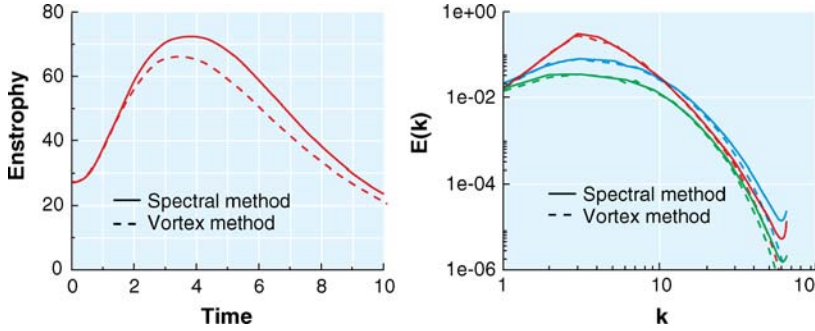

Figure 2 Comparison of Vortex and Spectral methods of the evolution of enstrophy and energy spectrum in simulation of homogenous isotropic turbulence courtesy of Cottet et al. (2002).

The adaptivity and robustness of VMs has enabled simulations of reacting flows (Ghoniem & Oppenheim 1984, Knio & Ghoniem 1992) and flows in porous media (Zimmerman et al. 2001). In the latter case, a comparison with grid-based methods shows that Lagrangian particle methods perform better than several finite difference methods in capturing highly anisotropic diffusion phenomena while accurately transporting scalar fields. Simulations of particle-laden flows (see Figure 3) (Walther & Koumoutsakos 2001) reveal flow structures and flow instabilities that were predicted experimentally but had not been obtained before by grid-based methods, possibly due to the absence of adaptivity and the dissipation induced by the discretization of the nonlinear transport term. The method has been extended to compressible flows (Eldredge et al. 2001), but its relevant advantages in this field are a subject of ongoing investigations.

It has been well known since the works of Krasny in the 1980s (Krasny 1986) that particle methods are well suited for interface capturing. Level sets present today the standard framework to capture interfaces (Osher & Fedkiw 2001) and a particle level set formulation has been implemented (Enright et al. 2002) to remedy some problems involved in the evolution of a level set on a fixed grid. Recently, a novel particle level set method for capturing interfaces was proposed (Hieber & Koumoutsakos 2004). In this method, the level set equation is solved in a Lagrangian frame using particles that carry the level set information. A key aspect of the method involves a consistent remeshing procedure for the regularization of the particle locations. This Lagrangian description of the level set method is inherently adaptive and exact in the case of solid body motions. Comparisons on a set of benchmark problems with existing level set formulations demonstrates that the proposed particle-level set method achieves superior results using a reduced number of computational elements.

A detailed description of particle methods with an emphasis on VMs and some of their applications can be found in the monograph by Cottet & Koumoutsakos (2000).

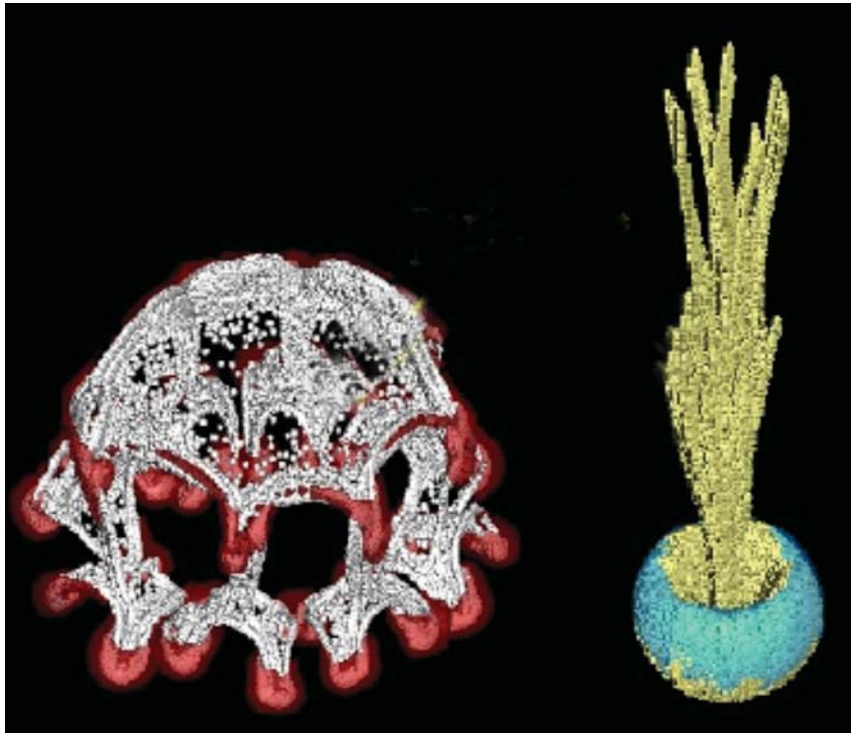

Figure 3 Simulation of particle-laden flow. Vorticity isosurfaces (*red* and *blue*) and solid particles (*white* and *yellow*) for a drop of solid particles falling in a fluid with zero (*left*) and nonzero (*right*) initial vorticity field (Walther & Koumoutsakos 2001).

2.3. Smooth Particle Hydrodynamics

The method of SPH was introduced by Lucy in the late 1970s and was further developed by Monaghan (see Monaghan 1988 and references therein) for grid-free astrophysics simulations.

In SPH, function approximations are consistent with Equation 4 and particle weights are selected as $w_p^{SPH} = f(\mathbf{x}_p)\, v_q = f(\mathbf{x}_p) m_p/\rho(\mathbf{x}_p)$ by invoking the continuity equation and implicitly bypassing the requirement for an exact calculation of the volume associated with each particle. In SPH, the key requirements for the particle kernel are positivity and local support, and the scheme relies in the conservative approximation of derivative operators using

$$D^\beta f(\boldsymbol{x}_p) = \sum_q^N \left(f_q - f_p\right) v_q D^\beta W(\boldsymbol{x}_p - \boldsymbol{x}_q, h), \tag{24}$$

where $W(\boldsymbol{x}_p - \boldsymbol{x}_q, h)$ is used instead of the mollifier kernel $\zeta_\varepsilon$employed in VMs, with the interparticle distance h taking the role of the mollifier core size. Using

Equation 24, the continuity and momentum equation can be expressed in the SPH formulation as

$$\frac{d\mathbf{x}_p}{dt} = \mathbf{u}_p$$

$$\frac{d\rho_p}{dt} = \sum_q v_q \left(\mathbf{u}_q - \mathbf{u}_p\right) \cdot \nabla W(\mathbf{x}_p - \mathbf{x}_q, h)$$

$$\frac{d\mathbf{u}_p}{dt} = \frac{1}{\rho_p} \sum_q v_q \left(\underline{\underline{\tau}}_q - \underline{\underline{\tau}}_p\right) \cdot \nabla W(\mathbf{x}_p - \mathbf{x}_q, h) + \mathbf{F}, \qquad (25)$$

where $\underline{\underline{\tau}}$ denotes the stress tensor of the flow and $\mathbf{F}$ corresponds to external force fields experienced by the particles. A closure relationship is necessary to express the stress tensor as a function of known variables. In the past 20 years many simulations using SPH have been conducted, extending its application range from gas dynamics in astrophysics to Newtonian and viscoelastic flows (see Ellero et al. 2002, Monaghan 1985b and references therein).

Several open questions remain regarding the enforcement of boundary conditions and the consistency of the method in situations of highly distorted particle configurations. The particle distortion leads to errors in the approximation of derivative operators (Belytschko et al. 1996). Flow simulations using SPH involve an implicit subgrid-scale modeling (although currently no analysis exists for this), and suitable corrections are necessary to enhance the accuracy of the method. Several techniques [such as artificial viscosity (Gingold & Monaghan 1983) and dynamic conditions (Ellero et al. 2002)] have been proposed to compensate for this problem. Inspired by techniques in VMs, the introduction of regularization of particle distortion in SPH via remeshing (Chaniotis et al. 2002) has led to second-order accuracy, but this detracts from the characterization of the method as grid-free.

Recent work has focused on the relationship between SPH and particle methods developed for solving boundary value problems. These so-called meshless methods, in order to be distinguished from schemes like finite differences and finite elements where node connectivity is important, are Galerkin-type methods. They compute the approximations of derivative operators by solving systems of equations to construct conservative, particle-based, discrete mollifier kernels. Works by Duarte & Oden (1996), and Belytschko et al. (1996) provide a unifying framework for methods such as Moving Least Squares, Reproducing Kernel Particle Methods, and Element-Free Galerkin, and discuss their relationship with SPH. We refer to review articles by Belytschko, and more recently by Babuska et al. (2002), on the developments of these methods and their formulation as Partition of Unity Methods. Meshless methods have been mostly implemented in Galerkin formulations of solid mechanics problems, but their developments carry a number of concepts, such as multiscale particle representations and formulation of accurate boundary conditions, that should be further explored to increase the capabilities of Lagrangian particle methods for flow simulations.

3. GRIDS AND PARTICLES

Particle methods are often defined as grid-free methods, making them an attractive alternative to mesh-based methods for flows past complex and deforming boundaries. However, the adaptivity provided by the Lagrangian description can introduce errors and particle methods have to be conjoined with a grid to provide consistent, efficient, and accurate simulations. The grid does not detract from the adaptive character of the method and serves as a tool to restore regularity in the particle locations via remeshing while it simultaneously enables systematic multiresolution particle simulations (Bergdorf et al. 2004), allows fast-velocity evaluations (Harlow 1964), and facilitates hybrid particle mesh methods capable of handling different numerical methods and different equations in various parts of the domain (Cottet 1990).

3.1. Remeshing for Particle Distortion

Particle methods, when applied to the Lagrangian formulation of convection-diffusion equations, enjoy an automatic adaptivity of the computational elements as dictated by the flow map. This adaptation comes at the expense of the regularity of the particle distribution because particles adapt to the gradients of the flow field. The numerical analysis of VMs shows that the truncation error of the method is amplified exponentially in time, at a rate given by the first-order derivatives of the flow that are precisely related to the amount of flow strain. In practice, particle distortion can result in the creation and evolution of spurious vortical structures due to the inaccurate resolution of areas of high shear and to inaccurate approximations of the related derivative operators.

To remedy this situation, location processing techniques reinitialize the distorted particle field onto a regularized set of particles and simultaneously accurately transport the particle quantities. The resulting problem of extracting information on a regular grid from a set of scattered points has a long history in the fields of interpolation (Schoenberg 1946) and statistics (see Cleveland & Loader 1996 and references therein). To facilitate the analysis we restrict our attention to a 1D equispaced regular grid with unit mesh size onto which we interpolate quantities (q_n) from scattered particle locations (x_n):

$$Q(x) = \sum_n q_n \, W(x - x_n). \tag{26}$$

The properties of the interpolation formulas can be analyzed through their behavior in the Fourier space (Schoenberg 1946). The characteristic function $g(k)$ of the interpolating function W(x) is defined as

$$g(k) = \int_{-\infty}^{+\infty} W(x)\, e^{-ikx}\, dx.$$

When W decays fast at infinity, g is a smooth function and the interpolation formula Equation 26 is of degree m if the following two conditions hold simultaneously: (a) $g(k) - 1$ has a zero of order m at $k = 0$ and (b) $g(k)$ has zeros of order m at all $k = 2\pi n$, $(n \neq 0)$. These requirements translated back in the physical space are nothing but the moment properties of the interpolant

$$\int W(y)\,dy = 1; \quad \int y^{\alpha} W(y)\,dy = 0, \quad \text{if} \quad 1 \leq |\alpha| \leq m-1.$$

This is reminiscent of the conditions for accurate function particle approximations using moment conserving kernels. In fact, the interpolation accuracy (Hockney & Eastwood 1988) can be described by splitting the interpolation error into a convolution and sampling error reminiscent of the smoothing/quadrature error for function approximations. Hence, good interpolation schemes are those that are band-limited in the physical space and are simultaneously close approximations of the ideal low-pass filter in the transformed space. Monaghan (1985b) presents a systematic way of increasing the accuracy of interpolating functions, such as B-splines, while maintaining their smoothness properties using extrapolation. He constructs interpolation formulas such that, if $m = 3$ or $m = 4$, the interpolation will be exact for quadratic functions, and the interpolation will be third- or fourth-order accurate. One widely used formula involves the so-called M_4' function

$$M_4'(x) = \begin{cases} 0 & \text{if} \quad |\mathrm{x}| > 2 \\ \frac{1}{2}(2 - |x|)^2(1 - |x|) & \text{if} \quad 1 \leq |\mathrm{x}| \leq 2 \\ 1 - \frac{5x^2}{2} + \frac{3|x|^3}{2} & \text{if} \quad |\mathrm{x}| \leq 1. \end{cases} \tag{27}$$

Interpolations in higher dimensions can be achieved by tensorial products of these formulas. However, these tensorial products require particle remeshing on a regular grid. For non-grid-conforming boundaries, remeshing introduces particles onto areas that are outside the flow domain and violates the flow boundary conditions. Remedies such as one-sided interpolation have been proposed and a working solution can be obtained (Cottet & Poncet 2004, Ploumhans et al. 2002) by eliminating particles outside the domain and adjusting accordingly the modification of particle strengths by re-enforcing the boundary conditions in a fractional step algorithm. Alternatively, weight processing schemes attempt to explicity (Beale 1986) or implicitly (Strain 1997) modify the particle weights in order to maintain the accuracy of the calculation, but they result in rather costly calculations.

3.1.1. HYBRID METHODS Hybrid methods involve combinations of mesh-based schemes and particle methods in an effort to combine computational advantages of each method. The first such method involves the Particle in Cell algorithm pioneered by Harlow (1964), in which a particle description replaces the nonlinear advection terms and mesh-based methods can be used to take advantage of the efficiency of Eulerian schemes to deal with elliptic or hyperbolic problems.

Lagrangian-Eulerian domain decomposition methods use high-order grid methods and VMs in different parts of the domain (Cottet 1990, Ould-Salihi 2000) and can even be combined with different formulations of the governing equations. A finite difference scheme (along with a velocity-pressure formulation) can be implemented near solid boundaries, and VMs (in a velocity-vorticity formulation) can be implemented in the wake to provide the flow solver with accurate far-field conditions. In this approach Eulerian methods handle the wall boundary conditions and can be complemented with immersed boundary methods (Mittal & Iaccarino 2005) to handle complex geometries. A rigorous framework for particle-based immersed boundary methods has been developed based on a unified formulation of the equations for flow-structure interaction (Cottet 2002). Simulations involving this formulation are a subject of ongoing investigations.

4. MULTIRESOLUTION PARTICLE METHODS

The accuracy of smooth particle methods with overlapping cores is determined by the core size ε of the mollifier. For computational efficiency this core size needs to be spatially variable to adequately discretize gradients in different parts of the flow, such as the boundary layer and the wake of bluff body flows. Because particles must overlap spatially, varying cores imply a corresponding adaptation for the spacing of the particles. This can be achieved by remeshing the particle locations on a spatially varying mesh by

- remeshing on a regular grid corresponding to variable size particles by using a global (adaptive or nonadaptive) mapping and by
- remeshing by combining local mappings in a domain decomposition framework.

In VMs, Hou (1990) first introduced a variable-size VM for the 2D Euler equations by defining a function $\varepsilon(\mathbf{x}) << 1$ for the vortex particles so that

$$\omega_\varepsilon^h(\mathbf{x}) = \sum_p v_p \omega_p \zeta_{\varepsilon(\mathbf{x}_p)}(\mathbf{x} - \mathbf{x}_p^h). \tag{28}$$

This leads to a spatially varying mollified velocity kernel for the advancement of vortex particles

$$\mathbf{u}^h(\mathbf{x}) = \sum_p v_p \omega_p \mathbf{K}_{\varepsilon(\mathbf{x}_p)}(\mathbf{x} - \mathbf{x}_p^h). \tag{29}$$

The convergence of the method was proven for the Euler equations under the assumption that there is a positive, bounded, smooth function F such that $\varepsilon(\mathbf{x}) = \varepsilon F(\mathbf{x})$.

The straightforward extension of this method to viscous flows by the modification of the kernel in Equation 11 leads to an inconsistent approximation. To avoid this inconsistency, we need to assume a mapping from the physical coordinates,

with variable-size blobs, to a coordinate system where blobs have a uniform size, as presented by Cottet et al. (2000). The algorithm involves the mapping of a domain $\hat{\Omega}$ with uniform blobs, to a domain Ω, where we wish to use variable blob sizes through a mapping denoted by $\mathbf{F}$:

$$\mathbf{x} = \mathbf{F}(\hat{\mathbf{x}});\ \hat{\mathbf{x}} = \mathbf{G}(\mathbf{x});\ \boldsymbol{\omega}(\mathbf{x}) = \hat{\boldsymbol{\omega}}(\hat{\mathbf{x}}).$$

If $J = \det[a_{ij}] = \det[\frac{\partial G_i}{\partial x_j}]$ denotes the Jacobian determinant of the inverse mapping $\mathbf{G}$, we can express the Laplacian operator in the variable core domain, in terms of gradient operators in the uniform domain, as:

$$\Delta_{\mathbf{x}}\boldsymbol{\omega} = J \operatorname{div}_{\hat{\mathbf{x}}}[\mathrm{B}\nabla_{\hat{\mathbf{x}}}\hat{\boldsymbol{\omega}}], \tag{30}$$

where B is the matrix with entries $b_{jk} = J^{-1}\sum_i a_{ki}a_{ji}$.

Integral approximations for the differential operator in the mapped coordinates, in the righthand side of Equation 30, can be derived by using Equation 12 with $\psi_{ij} = x_i x_j \theta(|\mathbf{x}|)$, where the spherically symmetric kernel θ is normalized such that $\int x_i^4 \theta(\mathbf{x})\, d\mathbf{x} = d+2$, where d denotes the dimension of the problem. The PSE scheme for the Navier-Stokes equation that follows from these formulas is given as

$$\frac{d\boldsymbol{\omega}_p}{dt} = \nu\varepsilon^{-4} J(\mathbf{x}_p) \sum_{q,i,j} \hat{v}_q (\hat{x}_p^i - \hat{x}_q^i)(\hat{x}_p^j - \hat{x}_q^j)\theta^{\varepsilon}(\hat{\mathbf{x}}_p - \hat{\mathbf{x}}_q)$$
$$\times \left[b_{ij} - \frac{1}{d+2}\sum_i b_{ii}\delta_{ij} \right] \left(\frac{\hat{\mathbf{x}}_p + \hat{\mathbf{x}}_q}{2} \right) (\boldsymbol{\omega}_q - \boldsymbol{\omega}_p). \tag{31}$$

The scheme is conservative because the volumes of the particles in the physical and mapped spaces are related through $v_p J(\mathbf{x}_p) = \hat{v}_p$.

The PSE scheme in Equation 31 relies on the explicit knowledge of a global invertible mapping in the computational domain. This is easily accomplished for flows in geometries such as channels and cylinders where such mappings can be derived. However, for more complex geometries or geometries involving several bodies such mappings are not available. Similar to r-adaptive mesh-based methods (Ceniceros & Hou 2001), it is desirable to require enhanced resolution for vortex particles in areas of high shear. One way to achieve this is to construct adaptive maps. Bergdorf et al. (2004) introduced global adaptive mappings through a particle approximation of a differential and continuous map

$$\mathbf{x}(\hat{\mathbf{x}}, t) = \boldsymbol{F}(\hat{\mathbf{x}}, t) = \sum_{j=1}^{M} \boldsymbol{\mu}_j(t)\, \varphi_j(\hat{\mathbf{x}})\,. \tag{32}$$

The parameters in the map that are changed in the process of adaptation are the node values $\{\boldsymbol{\mu}_j\}_{j=1}^M$. Using a map, as described in Equation 32, makes it impossible to leap back and forth from physical to reference space. However, its differentiability enables casting the governing equations into reference space and

solving the problem there without needing the inverse map. The adaptivity of the map presents us with an extra degree of freedom because complementing the convection of the particles with velocity **u** in physical space, particles are adapted by the convection/adaptation of the map with a specified velocity

$$\frac{d\boldsymbol{\mu}_i}{dt} = \mathcal{U}(\hat{\boldsymbol{x}}, t). \tag{33}$$

The method was implemented successfully for 1D (Burger's equation) and 2D (inviscid axisymmetrization of an elliptical vortex) problems (Figure 5). Using a suitable map velocity that implies that the core size in the physical space is being deformed in the same way the volume is deformed by the flow, the adaptive particle overlap maintains enhanced resolution in areas of high gradients where the particles are compressed. This multiresolution VM amounts to specifying rules for deformation of the particle shapes proportional to the spatially varying spacing of the particles.

A more versatile technique to achieve multiresolution in particle methods involves the combination of several local mappings with variable blobs associated to each mapping linked through domain decomposition techniques (Bergdorf et al. 2004, Cottet et al. 2000). In a domain decomposition algorithm involving particle solvers, interface conditions must be supplied to compute particle velocities and to update particle strengths. Given a vorticity field, determining the velocity amounts to solving a Poisson equation, and the Schwarz alternating method is a natural way to enforce the right interface conditions. In a vortex code, the method iterates between the boundary source terms that must be added to the Biot-Savart law in each subdomain. The fact that variable blobs, corresponding to different mappings, are implemented does not introduce any difficulty, provided the overlapping zone has a width exceeding the blob sizes in this area.

Once the velocities are evaluated on each subdomain, particle locations and circulations must be updated. Because VMs are based on explicit time discretization of the vorticity convection-diffusion equation, the vorticity transfer from one domain to another is simply achieved by interpolating the particle strengths in the overlapping zone.

The essence of the algorithm is independent of the dimension and the geometry of the domain. To illustrate the algorithm, let us consider the example sketched in Figure 4. In this example, Ω_1 and Ω_2 are two domains with nonuniform grid spacing, overlapping with a domain Ω_3 with uniform spacing. During the remeshing step, starting from a distorted particle configuration in the buffer zone,

- particles of type 1 and 2 are remeshed onto particles of type 3, using the cartesian mapping;
- similarly, particles of type 3 are remeshed onto particles of type 1 and 2 with polar mappings;
- and particles are advanced and exchange vorticity in each sub domain via PSE to account for diffusion.

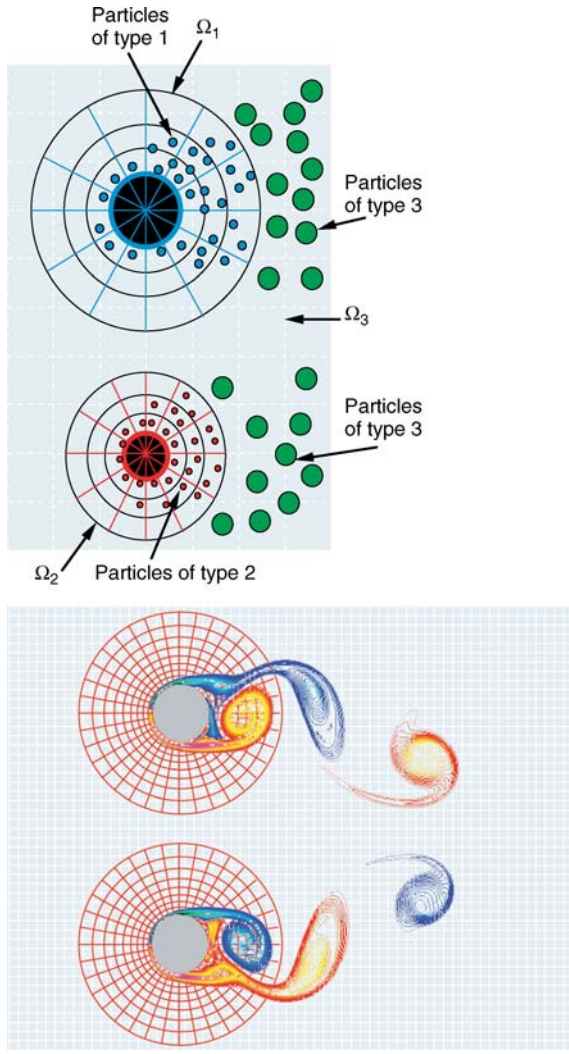

Figure 4 Domain Decomposition for flow past two circular cylinders.

At the end of these steps, the vorticity has been updated in all three domains. Provided that the overlapping width exceeds the core radius of the PSE kernel, this procedure allows a consistent transfer of vorticity through diffusion.

In variable blob methods remeshing must be applied in the mapped coordinates and at a frequency that prevents particles in low-resolution areas to travel too far in the high-resolution areas between two remeshing steps. Note that the remeshing of particle methods provides a flexible method for multiresolution representations

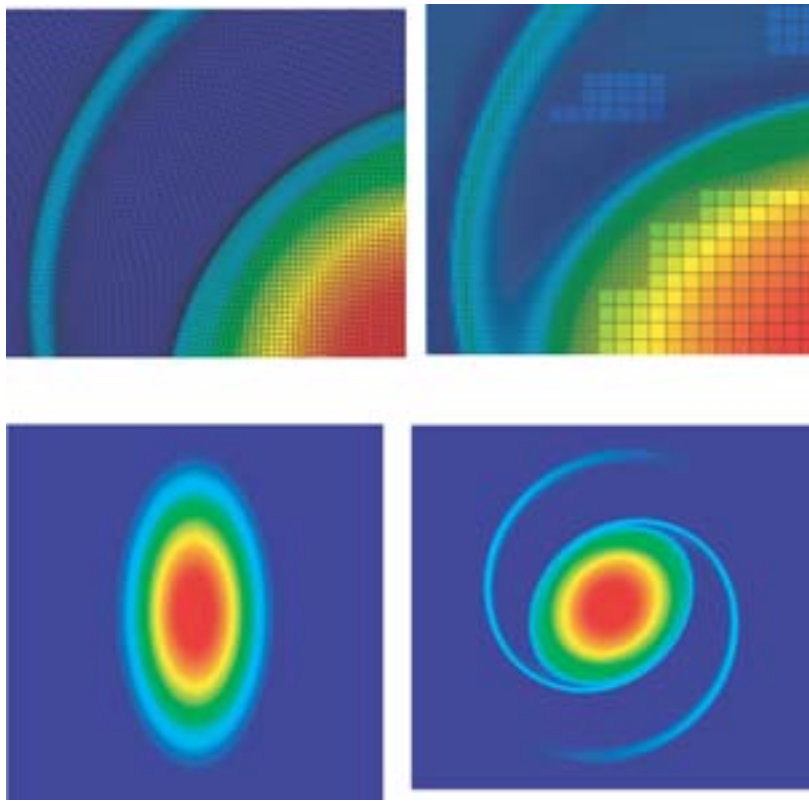

Figure 5 Inviscid simulation of an elliptical vortex. (*Bottom left*) Initial condition. (*Bottom right*) Vorticity field at T = 1.5. (*Top right*) Close-up of vorticity distribution as computed by an Adaptive Vortex Method based on Adaptive Mesh Refinement (AMR). (*Top left*) Close-up of vorticity distribution as computed by an r-adaptive Vortex Method based on Adaptive Global Mappings (AGM). (Courtesy of Bergdorf et al. 2004.)

because it is compatible with hierarchical mesh refinement (Guskov et al. 2002). When the mesh nodes are translated into particles this provides a flexible multiresolution representation with no particular restrictions on the connectivity of the computational elements.

Besides multiresolution particle methods, as described above, a recent work by Hou (2004) discusses the application of particle-based methods in multiscale modeling of incompressible flows using ideas from homogenization along with a formulation for the Lagrangian transport of small scales. The extension of concepts first developed for grid-based methods, such as homogenization, to particle methods may offer a promising avenue for constructing adaptive and consistent multiscale formulations.

5. PARTICLE METHODS FOR DISCRETE SYSTEMS

Discrete models such as molecular dynamics (MD) and dissipative particle dynamics (DPD) can describe flows for which the macroscale description through the Navier-Stokes equations is not adequate. In addition, they can complement macroscale descriptions by providing a suitable description of fluctuating hydrodynamics and by elucidating phenomena such as the validity of the no-slip condition for which only empirical evidence exists. In these methods there is a direct correspondence between the computational particles and the structures (molecules, fluid particles) that model the behavior of the system.

5.1. Molecular Dynamics and Fluids

MD simulations are used to model fluids (gas, liquid) characterized by the time and length scales of molecular motion. MD amounts to computing the trajectories of particles interacting through classical simplified force fields.

The simulation of fluids in MD dates back to the inception of the method in the mid-1950s works of Fermi et al. (1955) and Alder & Wainwright (1957), in which the phase diagram of a hard sphere system was investigated. In 1971, Rahman & Stillinger (1971) reported the first simulations of liquid water. Over the years, the development of suitable force fields propelled the current method to become one of the key interdisciplinary computational tools for investigating large molecular systems. Please see the book by Schlick (2002) for a comprehensive description.

Today, MD simulations are increasingly popular in the field of fluid mechanics and in the last decade several review articles have appeared, starting with the work of Koplik & Banavar (1995), who discussed the formulation of continuum flow deductions from atomistic simulations. Micci et al. (2001) reviewed nanoscale flow phenomena related to atomization and sprays.

Today, with increased computational powers, computations involving flows of complex fluids such as water are becoming routine. MD simulations of water have elucidated a number of issues associated with fluid mechanics of wetting and hydrophobicity (Figure 6) at the nanoscale (Walther et al. 2004), water transport through carbon nanotubes (Hummer et al. 2001), and, particularly, with the validity of the no-slip boundary condition for water flows in various nanoscale geometries (Sokhan et al. 2002). Recent MD studies (Walther et al. 2004) of water flows past carbon nanotubes reveal that the validity of the no-slip boundary condition at the nanoscale depends not only on the fluid and surface material properties but also on the particular geometric configuration. Extensive reviews of nanoscale fluid mechanics can be found in Maruyama (2001) and Koumoutsakos et al. (2004).

5.1.1. MOLECULAR DYNAMICS: FORCE FIELDS AND POTENTIALS The potential energy function or force field provides a description of the relative energy or forces of the ensemble for any geometric arrangement of its constituent atoms. This description includes energy for bending, stretching, and vibrations of the molecules,

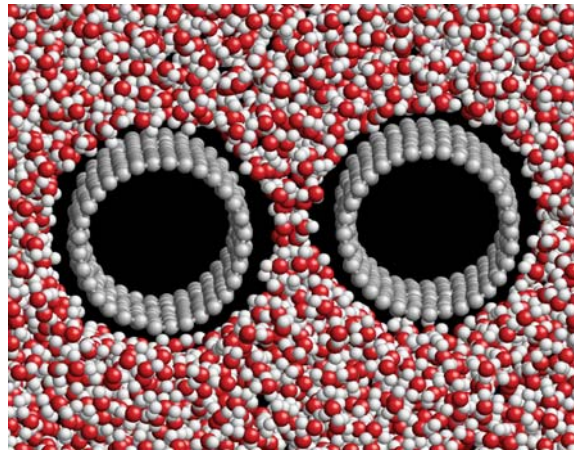

Figure 6 Hydrophobic hydration of carbon nanotubes in water (from Walther et al. 2001).

and nonbonded interaction energies between the molecules. Classical force fields are usually built up by the superposition of simple potential energy expressions. Mostly pair potentials $V(r_{ij})$ are used, but in systems where bonds are determining the structure, multibody contributions $V(r_{ij}, r_{ik})$, and $V(r_{ij}, r_{ik}, r_{il})$ may also enter the expression, thus

$$U = \sum_{i,j} V(r_{ij}) + \sum_{i,j,k} V(r_{ij}, r_{ik}) + \sum_{i,j,k,l} V(r_{ij}, r_{ik}, r_{i,l}), \tag{34}$$

where $r_{ij} = |r_i - r_j|$ is the distance between i-th and j-th atoms. The contribution to the interaction potential can be ordered in two classes: intramolecular and intermolecular contributions. Whereas the former describe interactions that arise in bonded systems, the latter are usually pair terms between distant atoms modeling electrostatics and Van der Waals interactions.

The study of nonequilibrium processes or dynamic problems, such as fluid flows in nanoscale geometries, is usually performed by nonequilibrium molecular dynamics (NEMD). NEMD is based on the introduction of a flux in thermodynamic properties of the system (Allen & Tildesley 1987). Cummings & Evans (1992) review NEMD with regard to the computation of transport coefficients of fluids from the knowledge of pair interactions between molecules. Ryckaert et al. (1989) compare the performance of NEMD with Green-Kubo approaches to evaluate the shear viscosity of simple fluids. Tuckerman et al. (1997) present a modified NEMD approach to ensure energy conservation.

5.1.2. BOUNDARY CONDITIONS FOR MOLECULAR DYNAMICS In multiscale simulations, the MD part of the flow has to interface mesoscopic and macroscale models

through suitable boundary conditions. For situations involving the simulation of a solvent, the small volume of the computational box in which solvent and other molecules of interest are contained can introduce undesirable boundary effects if the boundaries are modeled as simple walls. To circumvent this problem, the system may be placed in vacuum (Allen & Tildesley 1987) or a periodic system may be assumed. However, periodic boundary conditions imposed on small systems may introduce artifacts in systems that are not inherently periodic.

Stochastic boundary conditions enable reduction of the size of the system by partitioning the system into two zones with different functionality: a reaction zone and a reservoir zone. The reservoir zone is excluded from MD calculations and is replaced by random forces whose mean corresponds to the temperature and pressure in the system. The reservoir zone is further subdivided into a reaction zone and a buffer zone. The stochastic forces are only applied to atoms of the buffer zone. Please see Brunger et al. (1984) and Berkowitz & McCammon (1982) for the application of stochastic boundary conditions to a water model.

6. CONTINUUM-MOLECULAR SIMULATIONS

Nanoscale flows are often part of larger-scale systems (for example, when nanofluidic channels are interfacing microfluidic domains), and in simulations we are confronted with an inherently multiscale problem. The simulation of such flows is challenging because one needs to suitably couple the nanoscale systems with larger spatial and time scales. The macroscale flows determine the external conditions that influence the nanoscale system, which in turn influences the larger scales by modifying its boundary conditions.

Hybrid computational techniques attempt to overcome these problems using, for the molecular part of the flow, Direct Simulation Monte Carlo (DSMC) for dilute gases or MD for liquids, coupled with a relevant continuum description (Flekkøy et al. 2000, Hadjiconstantinou 1999a, Hadjiconstantinou & Patera 1997, Li et al. 1999, Sun et al. 2004, Werder et al. 2004). An alternative is coarse-grained, mesoscopic particle models of complex fluids, such as DPD, which do not involve any explicit coupling of the continuum and the atomistic description.

6.1. Dissipative Particle Dynamics

The initial formulation of the DPD model was given by Hoogerbrugge & Koelman (1992) and was intended to provide a mesoscale model that enables the simulation of complex fluids such as colloidal suspensions, emulsions, polymers, and multiphase flows. It is based on the notion of fluid particles representing a collection of atoms or molecules that constitute the fluid. These fluid particles interact pairwise through three types of forces,

$$\mathbf{f}_i = \sum_{j \neq i} \left[\mathbf{F}^C(\mathbf{r}_{ij}) + \mathbf{F}^D(\mathbf{r}_{ij}, \mathbf{u}_{ij}) + \mathbf{F}^R(\mathbf{r}_{ij}) \right], \tag{35}$$

where $\mathbf{F}^C$ represents a conservative force derived from a soft repulsive potential and $\mathbf{F}^D$ is a dissipative force depending on the relative particle velocity $\mathbf{u}_{ij}$ to model friction whereas the stochastic force $\mathbf{F}^R$ models the effect of the suppressed degrees of freedom in the form of thermal fluctuations.

DPD simulations of complex fluids offer advantages in two respects when compared to MD. First, the conservative pairwise forces between the DPD particles are soft repulsive, which makes it possible to extend simulations to longer timescales, whereas coarse graining in the particle representation allows studies of larger systems. Second, a special "DPD thermostat" for the canonical ensemble is implemented in terms of dissipative as well as random pairwise forces such that the momentum is locally conserved, which results in the emergence of hydrodynamic flow effects on the macroscopic scale. Today, one can reach simulation times of the order of 100 ns with molecular dynamics, whereas one can routinely study phenomena on the microsecond scale with DPD. A drawback of the DPD method is that its thermodynamic behavior is determined by the conservative forces and is therefore an output of the model and not an input (Serrano & Espanol 2001). Espanol & Revenga (2003) recently introduced the smoothed dissipative particle dynamics method (SDPD) starting from a formulation of SPH. In these simulations every particle has an associated position, velocity, constant mass, entropy and, in addition, two extensive variables, a volume and an internal energy. The interpolant used in the SDPD formulation fulfills the second law of thermodynamics explicitly and thus enables the consistent introduction of thermal fluctuations through the use of the dissipation-fluctuation theorem.

DPD is particularly well suited for simulations of polymers and surfactant systems and the reader is referred to recent reviews on mesoscale simulations of complex fluids using DPD (Glotzer & Paul 2002, Kremer & Müller-Plathe 2002, Warren 1998).

6.2. Multiscaling: Linking Macroscopic to Atomistic Scales

The Navier-Stokes equations are based on classical Newtonian mechanics and rely on the continuum approximation as well as on the assumption of thermodynamic (quasi-) equilibrium. The continuum approximation relies on the formulation of local flow properties such as density, velocity, and stress as averages over fluid elements. Thermodynamic (quasi-) equilibrium postulates that when equilibrium is achieved within small volumes for certain fluid properties, their gradients vary linearly between these volumes, hence the stress is linearly related to the strain and the heat flux is linearly related to the temperature gradient. For dilute gas flows the conditions under which the above assumptions hold are well characterized by the degree of rarefaction of the fluid measured in terms of the Knudsen number, $Kn = \lambda/L$, where λ is the mean-free path and L a characteristic macroscopic length (Bird 1994). A flow with $Kn < 0.01$ is in the continuum regime and can be well described by the Navier-Stokes with no-slip boundary conditions. For $0.01 < Kn < 0.1$, the slip-flow regime, the Navier-Stokes equations can still be used

along with tangential slip-velocity boundary conditions. In the transition regime, for $0.1 < Kn < 10$, the constitutive equation for the stress tensor starts to lose its validity and higher-order corrections such as the Burnett or Woods equations along with higher-order slip models at the boundary are needed. At even larger Knudsen numbers ($Kn > 10$), the continuum assumption fails completely and atomistic descriptions such as DSMC of the gas flow are needed (Bird 1994). Note that as the considered system size L shrinks, the thermodynamic equilibrium assumptions fails before the continuum approximation does (Karniadakis & Beskok 2002).

For liquid flow, the situation is more complicated because the molecules that constitute a liquid are essentially always in a collision state and, thus, the concepts of a mean-free path and Knudsen number are not useful. There is no well established molecular-based theory for liquids, such as for dilute gases. Therefore, one must resort to experiments or to a computational analysis using MD, where fluids are modelled as what they really are—a collection of strongly interacting molecules.

6.3. Hybrid Atomistic-Continuum Computations

O'Connell & Thompson (1995) described an early attempt to extend the length scales accessible in molecular dynamics simulations through the combination with a continuum descriptions. In their simulations, they applied constrained dynamics in an overlap (X) between the particle (P) and continuum (C) regions to ensure stress continuity across the P – C interface. O'Connell & Thompson applied this algorithm to an impulsively started Couette flow where the P – C interface was parallel to the walls. This ensured that there was no net mass flux across the MD-continuum interface. Hadjiconstantinou (Hadjiconstantinou 1999, Hadjiconstantinou & Patera 1997) pointed out that this scheme decouples length but not time scales and therefore suggested an iterative procedure based on the Schwarz alternating method to alleviate this problem. In this iteration, the continuum solution in C provides boundary conditions for a subsequent atomistic solution in P and vice versa until the solution converges in the overlap region X. The Schwarz method is inherently bound to steady-state problems; however, for cases with the hydrodynamic time scale much larger than the molecular time scale, a series of quasi-steady Schwarz iterations can be used to treat transient problems (Hadjiconstantinou & Patera 1997). A hybrid formulation of the moving contact line problem served as a test problem. Flekkøy et al. (2000) presented a hybrid model which, in contrast to earlier hybrid schemes (Hadjiconstantinou 1999, O'Connell & Thompson 1995), is explicitly based on direct flux exchange between the particle and the continuum region. The main difficulty in the approach of Flekkøy et al. arises in the imposition of the flux boundary condition from the continuum region on the particle region. The fluxes exhibit significant oscillations that do not enable fast convergence of the iterative scheme. The scheme was tested for a 2D Lennard-Jones fluid coupled to a continuum region described by the compressible Navier-Stokes equations. The first test was a Couette shear flow parallel

to the P – C interface, and the second test involved a Poiseuille flow where the flow direction was perpendicular to the P – C interface. They obtained results on velocity profiles comparable with those obtained by full-scale MD simulations. Wagner et al. (2002) extended this work to include the energy equation and applied the technique to flow in a channel. Garcia et al. (1999) proposed a coupling of a DSMC solver embedded within an adaptive compressible Navier-Stokes solver to study gas flows. They successfully tested their scheme on systems such as an impulsively started piston and flow past a sphere.

Li et al. (1998) introduced a method called thermodynamic field estimator to extract continous fields from particle data based on the concept of maximum likelihood inference. This so-called thermodynamic field estimator method is subsequently used as detector in a feedback loop implemented to impose boundary conditions in hybrid schemes of the Schwarz iteration type (Li et al. 1999). The desired boundary condition is obtained by resetting the particle velocities in a buffer region, such as to minimize $\sum_i |\mathbf{v}_i' - \mathbf{v}_i|^2$, where $\mathbf{v}_i$ and $\mathbf{v}_i'$ denote the particle velocities before and after the transformation. An additional buffer layer is introduced in between the action region and the overlap region to relax the effect of the artificial disturbance.

6.3.1. DOMAIN DECOMPOSITION ALGORITHMS Recently, Hadjiconstantinou et al. (2003) derived an estimate for the number of independent samples needed in molecular systems to obtain a fractional error E_q in a quantity q that is measured in a domain of volume V. The study quantified the fact that the cost in terms of sampling time to measure fluxes (such as the momentum flux) is orders of magnitude larger than the cost for densities. Based on this observation which favors the use of a density-based scheme over flux-based schemes, Werder et al. (2004) proposed a hybrid multiscale algorithm for simulating dense fluids using argon molecules to describe the molecular system. The algorithm uses the alternating Schwarz method (cf., Hadjiconstantinou 1999), and couples a MD and continuum fluid dynamics system by interfacing the molecular system with a finite volume mesh covering the continuum computational domain (Figure 7). In contrast to Hadjiconstantinou's work (1999), the scheme is not limited to the use of periodic systems in the molecular part, but enables more general boundary conditions. These boundary conditions are implemented by a combination of specular walls, a potential of mean force (Werder et al. 2004), and a particle insertion algorithm (Delgado-Buscalioni & Coveney 2003).

Using the flow of argon past a carbon nanotube as a test case, the mehod converges in a few iterations, and the drag coefficient is within 30% of the continuum Stokes-Oseen flow past a circular cylinder for the associated Reynolds number.

In blending MD and continuum simulations it is necessary that a reasonable equilibration is achieved in the MD part to lead to a convergent algorithm. This imposes length and time limitations on the MD computations in order to obtain reasonable average quantities in the interface with the continuum (Werder et al. 2004). One possibility to overcome this problem is to add a mesoscopic domain between the molecular and macro domains that can accomodate in a systematic

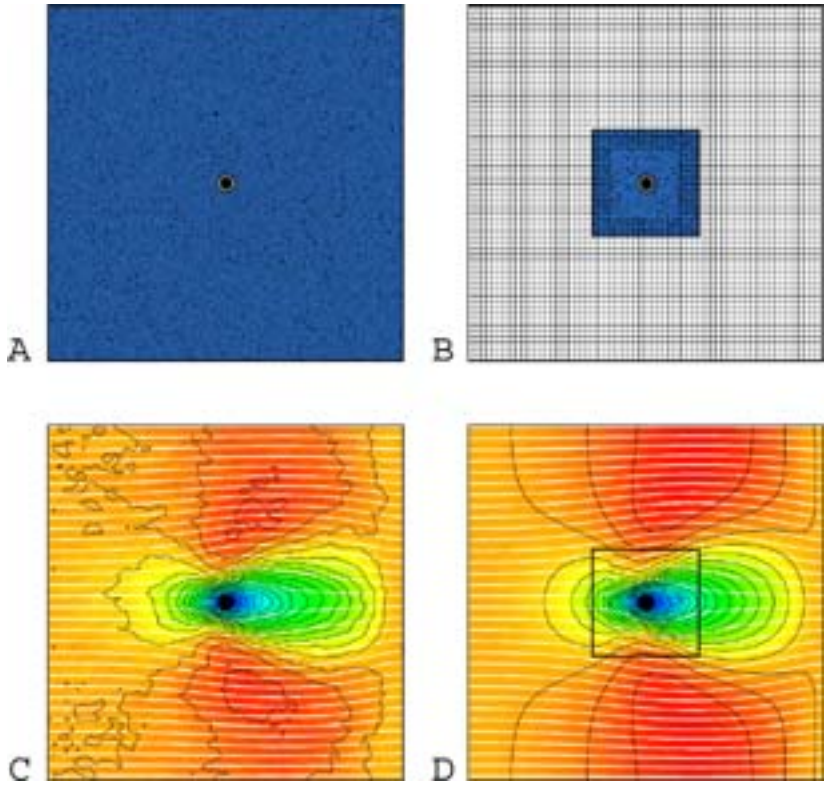

Figure 7 (*a*) Computational domain for the reference solution of the flow of argon around a carbon nanotube using a purely atomistic description. (*b*) Hybrid atomistic/continuum computational domain. Both computational domains have an extent of 30 nm $\times$ 30 nm. (*c*) Velocity field for the reference solution averaged over 4 ns. The white lines are streamlines, and the black lines are contours of the speed $|\mathbf{u}|$. (*d*) Velocity field of the hybrid solution after 50 iterations. The black square denotes the location of the atomistic domain. The solution in the atomistic domain is averaged over 10 iterations. (Courtesy of Werder et al. 2004.)

manner the fluctuations of the molecular system while simultaneously leading to a consistent approximation of the macroscale system. Ongoing studies involve the master equation approach introduced by Breuer & Petruccione (1992) for fluid dynamics. In this approach the fluid is regarded as a stochastic dynamical system. The velocity of the fluid is related to a stochastic process governed by an appropriate master equation (van Kampen 1981) acting in a discrete phase space. The master equation is constructed in such a way that the average of the velocity field obeys the underlying Navier-Stokes equations (Breuer & Petruccione 1995). Using the master equation formalism presents several advantages because boundary conditions are easy to implement, the method is robust with respect to initial conditions, and it is easily parallelizable. Because the interfacing conditions

with the macroscale involve velocity or vorticity boundary conditions, it provides a natural complement to macroscale simulations using vortex particle methods.

7. FAST PARTICLE METHODS

Particle methods constitute an N-body problem with a computational cost that scales as $\mathcal{O}(N^2)$ for N particles. Although short-range forces can be calculated using cutoffs, the most time-consuming aspect in particle simulations is accurately evaluating the long-range interactions associated with the field equations. A mesh can be used to solve the field equations (such as the Poisson equation) that pervade the whole space. There are efficient algorithms to reduce the computational cost, ranging from simple sorting as first implemented by Verlet (1998) to accurate fast summation techniques such as Ewald summation (Ewald 1921), the Particle-Mesh Ewald (PME) method (Darden et al. 1993), and the particle-particle particle-mesh technique (P^3M) (Hockney et al. 1973) to account for particles in close proximity in terms of the grid spacing. The nominal cost of Ewald summation requires $\mathcal{O}(N^{1.5})$ operations, the PME and P^3M techniques scale as $\mathcal{O}(N \log N)$.

In the last 20 years several mesh-free techniques based on the concept of multipole expansions have been introduced that circumvent the need for simulating periodic systems and have minimal numerical dissipation. Examples of such methods include the Barnes-Hut algorithm (Barnes & Hut 1986), the Fast Multipole Method (FMM) (Greengard & Rokhlin 1988), and the Poisson Integral Method (PIM) (Anderson 1992). These methods employ clustering of particles and use expansions of the potentials around the cluster centers with a limited number of terms to calculate their far-field influence onto other particles. These techniques rely on tree data structures to achieve computational efficiency. The tree allows a spatial grouping of the particles, and the interactions of well-separated particles is computed using their center of mass or multipole expansions for the Barnes-Hut and FMM algorithms, respectively. Another advantage of using tree-data structures is that it allows one to incorporate variable time steps (Mathiowetz et al. 1999) to integrate the particle trajectories. For a comprehensive review of the treatment of long-range electrostatics in MD simulations, see Sagui & Darden's work (1999).

8. SUMMARY AND OUTLOOK

In this review we outline advances in multiresolution particle methods for simulating continuous systems as well as methodologies for interfacing particle methods describing molecular systems with the continuum. We try to identify the key characteristics of these methods and, where possible, highlight their advantages and drawbacks compared to other numerical schemes.

Particle methods for continuum flows offer an accurate, stable, and versatile method to describe incompressible flow phenomena. In the last decade, a number of benchmark simulations using VMs have demonstrated that the method is capable of efficient DNS of turbulent, unsteady separated and interfacial flows. In

addition, a number of open issues are subjects of ongoing research, including the development of accurate techniques for handling boundary conditions in the continuum and atomistic scale as well as in the interface between the two descriptions. In microscale flows as well as in high Re number flows the use of atomistic models to describe the near wall part of the flow may be critical in developing consistent and accurate boundary conditions for the macroscale Navier-Stokes equations that describe the bulk of the flow.

Multiresolution particle methods for continuum flows complement the inherent adaptive character of the method, making it a powerful alternative to grid-based methods. In conjuction with research on efficient techniques for spatially varying particle methods, ongoing research involves the incorporation of adaptive time integrators and the systematic implementation of particle methods in a rigorous framework to handle practical flow problems with a very high number of scales that are not separable. The extension of concepts first developed for grid-based methods, such as homogenization, to particle methods may offer a promising avenue for constructing adaptive and consistent multiscale formulations. In the future we may wish to distinguish multiscale simulations by the number of and the separability of the scales involved. In these simulations a systematic analysis with rigorous error control is necessary. Particle methods offer a unique and unifying framework to formulate multiscale flow phenomena and may serve as a starting point for several seemingly diverse physical systems in a seamless, interdisciplinary fashion. This framework would exploit the remarkable and unique features of particle methods, namely that unlike other numerical methods, such as finite differences and finite elements, they are fundamentally linked to the physics they aim to reproduce.

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LITERATURE CITED

Alder BJ, Wainwright TE. 1957. Phase transition for a hard sphere system. *J. Chem. Phys.* 27(5):1208–9

Allen MP, Tildesley DJ. 1987. *Computer Simulation of Liquids*. Oxford: Clarendon

Anderson CR. 1992. An implementation of the fast multipole method without multipoles. *SIAM J. Sci. Stat. Comput.* 13(4):923–47

Anderson CR, Reider MB. 1996. A high order explicit method for the computation of flow about a circular cylinder. *J. Comput. Phys.* 125:207–24

Babuska I, Banerjee U, Osborn J. 2002. Meshless and generalized finite element methods: a survey of some major results. In *Meshfree Methods for Partial Differential Equations*, M Griebel, ed. pp. 1–20. Berlin: Springer Verlag

Barnes J, Hut P. 1986. A hierarchical *O*(*N* log *N*) force-calculation algorithm. *Nature* 324(4):446–49

Beale JT. 1986. A convergent 3-D vortex method with grid-free stretching. *Math. Comput.* 46:401–24

Belytschko T, Krongauz Y, Organ D, Fleming M, Krysl P. 1996. Meshless methods: an overview and recent developments. *Comp. Meth. Appl. Mech. & Eng.* 139(1–4):3–47

Bergdorf M, Cottet GH, Koumoutsakos P. 2004. Multilevel adaptive particle methods for convection-diffusion equations. *Multiscale Model. Simul.* In press

Berkowitz M, McCammon JA. 1982. Molecular-dynamics with stochastic boundary-conditions. *Chem. Phys. Lett.* 90(3):215–17

Bird GA. 1994. *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*. Oxford: Clarendon

Breuer HP, Petruccione F. 1992. A stochastic approach to computational fluid dynamics. *Continuum Mech. Thermodyn.* 4:247–67

Breuer HP, Petruccione F. 1995. How to build master equations for complex systems. *Continuum Mech. Thermodyn.* 7:439–73

Brünger A, Brooks CL, Karplus M. 1984. Stochastic boundary conditions for molecular dynamics simulations of ST2 water. *Chem. Phys. Lett.* 105(5):495–500

Ceniceros HD, Hou TY. 2001. An efficient dynamically adaptive mesh for potentially singular solutions. *J. Comput. Phys.* 172(2):609–39

Chaniotis AK, Poulikakos D, Koumoutsakos P. 2002. Remeshed smooth particle hydrodynamics for the simulation of viscous and heat conducting flows. *J. Comput. Phys.* 182:67–90

Chorin AJ. 1973. Numerical study of slightly viscous flow. *J. Fluid Mech.* 57(Part 4):785–96

Cleveland W, Loader C. 1996. Smoothing by local regression: principles and methods. In *Statistical Theory and Computational Aspects of Smoothing*, W Haerdle, GE Schimek, ed. pp.10–49. Berlin: Springer

Cottet GH. 1990. A particle-grid superposition method for the Navier-Stokes equations. *J. Comput. Phys.* 89:301–18

Cottet GH. 1996. Artificial viscosity models for vortex and particle methods. *J. Comput. Phys.* 127:299–308

Cottet GH. 2002. A particle model for fluid-structure interaction. *C.R. Acad. Sci. Paris Ser. I* 335:833–38

Cottet GH, Koumoutsakos P. 2000. *Vortex Methods – Theory and Practice* . New York: Cambridge Univ. Press

Cottet GH, Koumoutsakos P, Salihi MLO. 2000. Vortex methods with spatially varying cores. *J. Comput. Phys.* 162(1):164–85

Cottet GH, Michaux B, Ossia S, VanderLinden G. 2002. A comparison of spectral and vortex methods in three-dimensional incompressible flows. *J. Comput. Phys.* 175:702–12

Cottet GH, Poncet P. 2004. Advances in direct numerical simulations of 3D wall-bounded flows by Vortex-in-Cell methods. *J. Comput. Phys.* 193(1):136–58

Cummings PT, Evans DJ. 1992. Nonequilibrium molecular dynamics approaches to transport properties and non-Newtonian fluidy rheology. *Ind. Eng. Chem. Res.* 31:1237–52

Darden T, York D, Pedersen L. 1993. Particle mesh Ewald: An $N \cdot \log N$ method for Ewald sums in large systems. *J. Chem. Phys.* 98(12):10089–92

Degond P, Mas-Gallic S. 1989a. The weighted particle method for convection-diffusion equations. Part 1: The case of an isotropic viscosity. *Math. Comput.* 53(188):485–507

Degond P, Mas-Gallic S. 1989b. The weighted particle method for convection-diffusion equations. Part 2: The anisotropic case. *Math. Comput.* 53(188):509–25

Delgado-Buscalioni R, Coveney PV. 2003. Continuum-particle hybrid coupling for mass, momentum, and energy transfers in unsteady flow. *Phys. Rev. E* 67:046704–1–046704–13

Duarte CA, Oden JT. 1996. An *h-p* adaptive method using clouds. *Comp. Meth. Appl. Mech. Eng.* 139(1-4):237–62

E W, Engquist B. 2003. The heterogeneous multiscale methods. *Commun. Math. Sci.* 1(1):87–132

Eldredge J, Colonius T, Leonard A. 2001. A vortex particle method for compressible flows. *AIAA Pap.* 2641:1–9

Eldredge JD, Leonard A, Colonius T. 2002. A general deterministic treatment of derivatives in particle methods. *J. Comput. Phys.* 180(2):686–709

Ellero M, Kröger M, Hess S. 2002. Viscoelastic flows studied by smoothed particle dynamics. *J. Non-Newton. Fluid Mech.* 105(1):35–51

Enright D, Fedkiw R, Ferziger J, Ian M. 2002. A hybrid particle level set method for improved interface capturing. *J. Comput. Phys.* 183:83–116

Espanol P, Revenga M. 2003. Smoothed dissipative particle dynamics. *Phys. Rev. E* 67(4):026705–1–026705–12

Ewald PP. 1921. Die Berechnung Optischer und Elektrostatische Gitterpotentiale. *Annalen der Physik* 64:253–87

Fermi E, Pasta J, Ulam S. 1955. Studies in nonlinear problems. *Los Alamos Rep. LA-1940*

Fischer P. 1997. An overlapping Schwarz method for spectral element solution of the incompressible Navier-Stokes equations. *J. Comput. Phys.* 133:84–101

Flekkøy EG, Wagner G, Feder J. 2000. Hybrid model for combined particle and continuum dynamics. *Europhys. Lett.* 52(3):271–76

Garcia AL, Bell JB, Crutchfield WY, Alder BJ. 1999. Adaptive mesh and algorithm refinement using direct simulation Monte Carlo. *J. Comput. Phys.* 154:134–55

Ghoniem AF, Oppenheim AK. 1984. Numerical solution for the problem of flame propagation by the random element method. *AIAA J.* 22(10):1429–35

Gingold RA, Monaghan JJ. 1983. Shock simulation by the particle method sph. *J. Comput. Phys.* 52(2):374–89

Glotzer SC, Paul W. 2002. Molecular and mesoscale simulation methods for polymer materials. *Annu. Rev. Mater. Res.* 32:401–36

Greengard L, Rokhlin V. 1988. The rapid evaluation of potential fields in three dimensions. *Lect. Notes Math.* 1360:121–41

Guskov I, Khodakovsky A, Schröder P, Sweldens W. 2002. Hybrid meshes: multiresolution using regular and irregular refinement. In *Proc. 18th Ann. Symp. Comput. Geom.*, pp. 264–72. Barcelona: ACM

Hadjiconstantinou NG. 1999a. Combining atomistic and continuum simulations of contact line motion. *Phys. Rev. E* 59(2):2475–78

Hadjiconstantinou NG. 1999. Hybrid atomistic-continuum formulations and the moving contact-line problem. *J. Comput. Phys.* 154:245–65

Hadjiconstantinou NG, Garcia AL, Bazant MZ, He G. 2003. Statistical error in particle simluations of hydrodynamic phenomena. *J. Comput. Phys.* 187:274–97

Hadjiconstantinou NG, Patera AT. 1997. Heterogeneous atomistic-continuum representations for dense fluid systems. *Int. J. Mod. Phy. C* 8(4):967–76

Harlow FH. 1964. Particle-in-cell computing method for fluid dynamics. *Methods Comput. Phys.* 3:319–43

Hieber SE, Koumoutsakos P. 2004. A Langrangian particle level set method. *J. Comput. Phys.* Submitted

Hockney RW, Eastwood JW. 1988. *Computer Simulation Using Particles*. 2nd ed. Bristol, PA: Inst. Phys. Publ.

Hockney RW, Goel SP, Eastwood JW. 1973. A 10000 particle molecular dynamics model with long-range forces. *Chem. Phys. Lett.* 21:589–91

Hoogerbrugge PJ, Koelman JMVA. 1992. Simulating microscopic hydrodynamics phenomena with dissipative particle dynamics. *Europhys. Lett.* 19(3):155–60

Hou TY. 1990. Convergence of a variable blob vortex method for the Euler and Navier-Stokes equations. *SIAM J. Numer. Anal.* 27:1387–404

Hou TY. 2004. Multiscale modeling and computation of incompressible flow. In *Applied Mathematics Entering the 21st Century: Invited Talks from the ICIAM 2003 Congress,* ed. JM Hill, R Moore. SIAM Publ.

Hummer G, Rasaiah JC, Noworyta JP. 2001. Water conduction through the hydrophobic channel of a carbon nanotube. *Nature* 414:188–90

Karniadakis GE, Beskok A. 2002. *Micro Flows. Fundamentals and Simulation*. New York: Springer-Verlag

Knio OM, Ghoniem AF. 1992. The three-dimensional structure of periodic vorticity layers under non-symmetrical conditions. *J. Fluid Mech.* 243:353–92

Koplik J, Banavar JR. 1995. Corner flow in the sliding plate problem. *Phys. Fluids* 7(12):3118–25

Koumoutsakos P, Leonard A. 1995. High-resolution simulation of the flow around an impulsively started cylinder using vortex methods. *J. Fluid Mech.* 296:1–38

Koumoutsakos P, Leonard A, Pépin F. 1994. Boundary conditions for viscous vortex methods. *J. Comput. Phys.* 113(1):52–61

Koumoutsakos P, Zimmerli U, Werder T, Walther JH. 2004. Nanoscale fluid mechanics. In *The Handbook of Nanotechnology. Nanometer Structures. Theory, Modeling, and Simulation.* pp. 319–93

Krasny R. 1986. A study of singularity formation in a vortex sheet by the point vortex approximation. *J.Fluid Mech.* 167:65–93

Kremer K, Müller-Plathe F. 2002. Multiscale simulation in polymer science. *Mol. Sim.* 28: 729–50

Leonard A. 1985. Computing three-dimensional incompressible flows with vortex elements. *Annu. Rev. Fluid Mech.* 17:523–59

Li J, Liao D, Yip S. 1998. Coupling continuum to molecular-dynamics simulation: reflecting particle method and the field estimator. *Phys. Rev. E* 57(6):7259–67

Li J, Liao D, Yip S. 1999. Nearly exact solution for coupled continuum/MD fluid simulation. *J. Comput.-Aided Mat. Design* 6:95–102

Maruyama S. 2001. Molecular dynamics methods for microscale heat transfer. In *Advances in Numerical Heat Transfer*, Vol. 2, ed. WJ Minkowycz, EME Sparrow, pp. 189–226. New York: Taylor and Francis

Mathiowetz AM, Jain A, Karasawa N, Goddard WA III. 1994. Protein simulations using techniques for very large systems—the cell multipole method for nonbond interactions and the Newton-Euler inverse mass operator method for internal coordinate dynamics. *Proteins* 20(3):227–47

Micci MM, Kaltz TL, Long LN. 2001. Molecular dynamics simulations of atomization and spray phenomena. *Atomization Sprays/* 11(4):351–63

Mittal R, Iaccarino G. 2005. Immersed boundary methods for viscous flow. *Annu. Rev. Fluid Mech.* 37. In press

Monaghan JJ. 1985a. Extrapolating B splines for interpolation. *J. Comput. Phys.* 60(2): 253–62

Monaghan JJ. 1985b. Particle methods for hydrodynamics. *Comp. Phys. Rep./* 3:71–123

Monaghan JJ. 1988. An introduction to SPH. *Comp. Phys. Commun.* 48(1):89–96

O'Connell ST, Thompson PA. 1995. Molecular dynamics-continuum hybrid computations: a tool for studying complex fluid flow. *Phys. Rev. E* 52(6):R5792–95

Osher S, Fedkiw RP. 2001. Level set methods: an overview and some recent results. *J. Comput. Phys.* 169(2):463–502

Ould-Salihi ML, Cottet GH, El Hamraoui M. 2000. Blending finite-difference and vortex methods for incompressible flow computations. *SIAM J. Sci. Comput.* 22(5):1655–74

Ploumhans P, Winckelmans GS, Salmon JK, Leonard A, Warren MS. 2002. Simulation of three-dimensional bluff body flows: applications to the sphere at $Re = 300$, 500 and 1000. *J. Comput. Phys.* 178:427–63

Poncet P. 2004. Topological aspects of the three-dimensional wake behind rotary oscillating circular cylinder. *J. Fluid Mech.* In press

Rahman A, Stillinger FH. 1971. Molecular dynamics study of liquid water. *J. Chem. Phys.* 55(7):3336–59

Raviart PA. 1986. Particle approximation of first-order systems. *J. Comput. Math.* 4(1):50–61

Rosenhead L. 1930. The spread of vorticity in

the wake behind a cylinder. *Proc. R. Soc. A* 127(A):590–12

Ryckaert JP, Bellemans A, Ciccotti G, Paolini GV. 1989. Evaluation of transport coefficients of simple fluids by molecular dynamics: comparison of Green-Kubo and nonequilibrium approaches for shear viscosity. *Phys. Rev. A* 39(1):259–67

Sagui C, Darden TD. 1999. Molecular dynamics simulations of biomolecules: long-range electrostatic effects. *Annu. Rev. Biophys. Biomol. Struc.* 28:155–79

Sarpkaya T. 1989. Computational methods with vortices—the 1988 Freeman scholar lecture. *J. Fluids Eng.* 111:5–52

Schlick T. 2002. Molecular modeling and simulation, Vol. 21. In *Interdisciplinary Applied Mathematics*. New York: Springer-Verlag

Schoenberg IJ. 1946. Contribution to the problem of approximation of equidistant data by analytic functions. *Q. Appl. Math.* 4:45–99, 112–41

Serrano M, Espanol P. 2001. Thermodynamically consistent mesoscopic fluid particle model. *Phys. Rev. E* 64:046115–1–046115–18

Sokhan VP, Nicholson D, Quirke N. 2002. Fluid flow in nanopores: accurate boundary conditions for carbon nanotubes. *J. Chem. Phys.* 117(18):8531–39

Strain J. 1997. Fast adaptive 2D vortex methods. *J. Comput. Phys.* 132:108–22

Sun QH, Boyd ID, Candler GV. 2004. A hybrid continuum/particle approach for modeling subsonic, rarefield gas flow. *J. Comput. Phys.* 194(1):256–77

Tuckerman ME, Mundy CJ, Balasubramanian S, Klein ML. 1997. Modified nonequilibrium molecular dynamics for fluid flows with energy conservation. *J. Chem. Phys.* 106(13):5615–21

van Kampen NG. 1981. *Stochastic Processes in Physics and Chemistry* . Amsterdam: North-Holland

Verlet L. 1968. Computer experiments on classical fluids. ii. Equilibrium correlation functions. *Phys. Rev.* 165(1):201–14

Wagner G, Flekkøy E, Feder J, Jossang T. 2002. Coupling molecular dynamics and continuum dynamics. *Comp. Phys. Commun.* 147:670–73

Walther JH, Jaffe RL, Kotsalis EM, Werder T, Halicioglu T, Koumoutsakos P. 2004. Hydrophobic hydration of C_{60} and carbon nanotubes in water. *Carbon* 42(5–6)1185–94

Walther JH, Koumoutsakos P. 2001. Three-dimensional particle methods for particle laden flows with two-way coupling. *J. Comput. Phys.* 167:39–71

Walther JH, Werder T, Jaffe RL, Koumoutsakos P. 2004. Hydrodynamic properties of carbon nanotubes. *Phys. Rev. E* 69:062201–1–062201–4

Warren PB. 1998. Dissipative particle dynamics. *Curr. Opin. Colloid Inter. Sci.* 3:620–29

Werder T, Walther JH, Koumoutsakos P. 2004. Hybrid atomistic-continuum method for the simulation of dense fluid flow. *J. Comput. Phys.* Accepted

Zimmermann S, Koumoutsakos P, Kinzelbach W. 2001. Simulation of pollutant transport using a particle method. *J. Comput. Phys.* 173:322–47

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