

Interrogations of Direct Numerical Simulation of Solid-Liquid Flows

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Abstract

In direct simulation the fluid motion is resolved numerically and the forces which move the particles are computed rather than modeled. This procedure opens new windows for understanding and modeling. Numerical methods are discussed based on body fitted moving unstructured grids and another on a fixed grid in which the portions of the fluid occupied by solids are forced to move as a rigid body by a distribution of Lagrange multipliers. Animation of the fluidization of 1204 spheres in 3D will be compared with experiments and the concept of fluidization of slurries in conduits by lift rather than drag will be framed in animation by direct simulation. Correlation for lift-off of single particles and the bed height of slurries fluidized by lift are obtained by processing data from numerical experiments.

I. Introduction

The current popularity of computational fluid dynamics is rooted in the perception that information implicit in the equations of motion can be extracted without approximation using direct numerical simulation (DNS).

▪ What is DNS?

Direct numerical simulation of solid-liquid flows is a way of solving the initial value problem for the motion of particles in fluids exactly, without approximation. The particles are moved by Newton's laws under the action of hydrodynamic forces computed from the numerical solution of the fluid equations.

To perform a direct simulation in the above sense, therefore, one must simultaneously integrate the Navier-Stokes equations (governing the motion of the fluid) and the equations of rigid-body motion (governing the motion of the particles). These equations are coupled through the no-slip condition on the particle boundaries, and through the hydrodynamic forces and torques that appear in the equations of rigid-body motion.

These hydrodynamic forces and torques must of course be those arising from the computed motion of the fluid, and so are not known in advance, but only as the integration proceeds. It is crucial that no approximation of these forces and torques be made--other than that due to the numerical discretization itself--so that the overall simulation will yield a solution of the exact coupled initial value problem--up to the numerical truncation error.

Our goal is to do direct numerical solutions with many thousands of particles in three dimensions, with large volume fractions, for the various kinds of suspensions and slurries that model the practical particulate flows arising in applications like fluidized beds, slurry transport, transport of drill cuttings for oil production, and proppant sands in reservoir stimulations. In this article, we present the results of a simulation of the fluidization of 1204 spheres and other simulations for targeted applications.

The hope is that the direct simulation of the motions of thousands of particles will, in many cases, allow the large numbers of experiments used in deriving engineering correlations to be replaced by cheaper, safer numerical experiments in which flow, material, and process-control parameters can be altered with a computer command. With DNS you can turn physical factors on or off to isolate effects, which is something that cannot be done in experiments. There are also opportunities for the application of direct simulation to the diagnosis of industrial problems involving flowing particulates, to the establishment of benchmark standards for two-phase flow models (see Chapter VI), and to approximate numerical methods that track particles.

▪ Approximate Methods

The signal feature of approximate numerical methods which track particles is that the forces that the fluid exerts on the particle are modeled rather than computed as in DNS. Many excellent numerical studies of particulate flows of many particles which are not direct simulations in the above sense have appeared in recent years. These approximate methods include simulations based on potential flow, Stokes flow, and point-particle approximations. They all simplify the computation by ignoring some possibly important effects like viscosity and wakes in the case of potential flow; inertial forces which produce lateral migration and across-the-stream orientations in the case of Stokes flow; and the effects of stagnation and separation points in the case of point-particle approximations.

Particle tracking methods take into account the particles and the fluid motion to understand particulate flow. Particle tracking methods move the particles by Newton's equations for rigid bodies using forces that are modeled from single particle analysis or from empirical correlation rather than from forces which are obtained by direct computation from the fluid motion. This kind of simulation is called Lagrangian because the particles are tracked. The fluid motion in particle tracking methods are computed from field equations, like the Navier-Stokes defined at every point of the field including points occupied by the particles. This kind of computation from continuum partial differential equations on a field is called Eulerian; hence, particle tracking methods are Eulerian-Lagrangian. The particle tracking can have a one way coupling in which the fluid motion is computed without particles, and a two-way coupling in which some effects of the particle motion on the fluid motion are recognized. In most cases the two-way coupling is introduced by momentum exchange terms representing the force of the particles on the fluid. A more general coupling was introduced by Andrews and O'Rourke 1996 and Snider, O'Rourke and Andrews 1998. They presented a scheme that considers the particle phase both as a continuum and a discrete phase. Inter-particle stresses are calculated by treating the particle as a continuum phase, as in the fluid phase equations of a two-fluid model. This way, they can track the motion of the particles and at the same time model the inter-particle stress. In their scheme the viscosity of the fluid in the fluid phase is neglected. The method can handle particulate loading ranging from dense to dilute, and particles of different size and materials. The particles are grouped into parcels. The motion of the parcels is tracked by the Lagrangian approach. The number of parcels in a computational cell are used to calculate the solid phase volume fraction on the Eulerian grid. Patankar and Joseph 1999, 2001 have extended this kind of particle-in-cell method to account for fluid phase viscosity and other effects.

The problem of particles in turbulent flows has been treated using turbulent flow models for the fluid with one-way coupling and two-way coupling with momentum exchange applicable to

dilute mixtures. These kind of turbulent flow models have been discussed by McLaughlin 1994 in a comprehensive review paper. Some of these turbulent flow models are conventionally called DNS; they are not DNS for particulate flow in that the forces on the particles are modeled and not computed from the fluid motion.

Another method used to compute solid-liquid is the Lattice Boltzmann method (LBM). This is an unconventional computational approach that constructs simplified kinetic models for the motion of discrete fluid particles. The LBM is inspired by Boltzmann's equation which give rise to the Navier-Stokes equations at 2nd order in Chapman-Enskog expansion and to Burnett equations, which do not agree with experiments at 3rd order. The LBM gives rise to equations for a compressible fluid, which are Navier-Stokes-like but not Navier-Stokes equations (see Qian, d'Humieres and Lallemand 1992, Ladd 1994, How, Zou, Chen, Doolen and Cogley 1995, Chen and Doolen 1998). The LBM may give rise to good approximations of isochoric flow when the pressure gradients are not too large. For large pressure gradients the fluid will compress. The LBM gives rise to particulate flows that are close to those computed by DNS (see Ladd 1997; Aidun, Lu and Ding 1995, and Qi 1999). The good results achieved by LBM probably arise from the fact that the forces on particles for this method are computed rather than modeled.

▪ Data Structure for Applications of DNS

DNS generates huge amounts of data. It is necessary to post-process the data to get useful results. The way the data is generated and processed is determined by the application; to interrogate the data efficiently it is necessary to create a *data structure for post processing*. The problem of setting up a data structure for the interrogation of results of simulations is a way of determining the way that numerical simulations ought to be applied; it connects the computational world to the applications.

The literature of DNS is by now fairly extensive. This literature is listed chronologically in chapter IV. This same literature, together with the paper abstracts and animations of computer simulations, can be found on our web page http://www.aem.umn.edu/Solid-Liquid_Flows.

II. Equations of Motion

The equations to be solved in the case of a Newtonian fluid are as follows. In the fluid we have

$$\nabla \cdot \mathbf{u} = 0 \quad (\text{II.1})$$

and

$$\rho_f \left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right) = \rho_f \mathbf{g} - \nabla p + \eta \nabla^2 \mathbf{u}. \quad (\text{II.2})$$

For simplicity of presentation we consider spherical particles. The mass center of the spheres are at $\mathbf{X}(t)$. The particles equations of motion are

$$\begin{aligned} M \frac{d\mathbf{U}}{dt} &= M\mathbf{g} + \mathbf{F}[\mathbf{u}], & I \frac{d\boldsymbol{\omega}}{dt} &= \boldsymbol{\mathcal{T}}[\mathbf{u}] \\ \frac{d\mathbf{X}}{dt} &= \mathbf{U}, & \frac{d\boldsymbol{\theta}}{dt} &= \boldsymbol{\omega}, \end{aligned} \quad (\text{II.3})$$

where $\mathbf{F}[\mathbf{u}]$ is the force and $\boldsymbol{\mathcal{T}}[\mathbf{u}]$ the torque on the particle. The fluid velocity is the same as the particle velocity at the surface of the particle

$$\mathbf{u} = \mathbf{U} + \boldsymbol{\omega} \wedge \mathbf{r}. \quad (\text{II.4})$$

The fluid force $\mathbf{F}[\mathbf{u}]$ acting on the boundary of the particle is the integral over the body surface of the traction

$$\boldsymbol{\sigma} \cdot \mathbf{n} = -p\mathbf{n} + 2\eta \mathbf{D}[\mathbf{u}] \cdot \mathbf{n} \quad (\text{II.5})$$

where

$$\mathbf{D}[\mathbf{u}] = \frac{1}{2} (\nabla \mathbf{u} + \nabla \mathbf{u}^T)$$

is the rate of strain and \mathbf{n} is the outward normal and $\boldsymbol{\mathcal{T}}[\mathbf{u}]$ is the integral of the moment of the traction vector.

▪ Weak Solution for the Total Momentum

Numerical solutions of the Navier-Stokes are expressed first in terms of a weak solution, which is in integral form and must be satisfied for all test functions in a certain space. The test functions are chosen to convert weak solutions to a matrix in which solutions are obtained at nodal points. In our work we use a special weak solution in which the fluid and particle equations of motion are combined into a *single weak equation of motion*, which governs the evolution of the *total momentum* of the system—fluid plus particles; the force $\mathbf{F}[\mathbf{u}]$ and torque $\boldsymbol{\mathcal{T}}[\mathbf{u}]$ cancel and do not need to be computed.

Find \mathbf{u} , p , \mathbf{U} , $\boldsymbol{\omega}$ and satisfying

$$\int_{fluid} \rho_f \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} - \mathbf{g} \right) \cdot \mathbf{v} d\mathbf{x} - \int_{fluid} p \nabla \cdot \mathbf{v} d\mathbf{x} + \int_{fluid} 2\eta \mathbf{D}[\mathbf{u}] : \mathbf{D}[\mathbf{v}] d\mathbf{x} \quad (\text{II.6})$$

$$+ M \left(\frac{d\mathbf{U}}{dt} - \mathbf{g} \right) \cdot \mathbf{V} + I \frac{d\boldsymbol{\omega}}{dt} \cdot \boldsymbol{\xi} = 0 \quad \text{for all } \mathbf{v}, \mathbf{V}, \boldsymbol{\xi},$$

$$\int_{fluid} q \nabla \cdot \mathbf{u} d\mathbf{x} = 0 \quad \text{for all } q, \quad (\text{II.7})$$

where \mathbf{u} and \mathbf{v} are both required to satisfy the no-slip condition on the particle boundary:

$$\mathbf{u} = \mathbf{U} + \boldsymbol{\omega} \wedge \mathbf{r} \quad \mathbf{v} = \mathbf{V} + \boldsymbol{\xi} \wedge \mathbf{r}. \quad (\text{II.8})$$

The function spaces for the functions and test functions are described in papers where they are used.

The combined equation of motion (II.6), (II.7) and (II.8) in which hydrodynamic forces and torques are completely eliminated was introduced by Hesla 1991 and implemented first by Hu 1996.

The same type of methods can be used for viscoelastic liquids; of course the equations for the fluid motion are then different. For the Oldroyd-B fluids we have

$$\rho_f \frac{d\mathbf{u}}{dt} = -\nabla p + \text{div } \boldsymbol{\tau} \quad (\text{II.9})$$

$$\lambda_1 \overset{\nabla}{\boldsymbol{\tau}} + \boldsymbol{\tau} = 2\eta(\mathbf{D}[\mathbf{u}] + \lambda_2 \overset{\nabla}{\mathbf{D}}[\mathbf{u}]) \quad (\text{II.10})$$

where

$$\overset{\nabla}{(o)} = \frac{\partial(o)}{\partial t} + (\mathbf{u} \cdot \nabla)(o) - \nabla \mathbf{u} \cdot (o) - (o) \cdot \nabla \mathbf{u}^T \quad (\text{II.11})$$

is called the ‘‘upper convected derivative.’’ Here λ_1 , is a relaxation time and λ_2 is a retardation time. Newtonian fluids are recovered in the asymptotic limit $\lambda_2 \rightarrow \lambda_1$, $0 \leq \lambda_2 \leq \lambda_1$. It is convenient for simulation to write

$$\boldsymbol{\tau} = \boldsymbol{\tau}_E + 2\eta \mathbf{D}[\mathbf{u}] \quad (\text{II.12})$$

where

$$\boldsymbol{\tau}_E + \lambda_1 \overset{\nabla}{\boldsymbol{\tau}}_E = 2\eta_E \mathbf{D}[\mathbf{u}]. \quad (\text{II.13})$$

This leads to a formulation (III.1) of the problem in terms of the configuration tensor

$$\mathbf{A} = \boldsymbol{\tau}_E + \left(\frac{\eta_E}{\lambda_1} \right) \mathbf{1}.$$

III. Numerical Packages for Moving Particles in Direct Numerical Simulation

We developed two different kinds of numerical packages, called “particle movers,” one based on body fitted moving unstructured grids and another based on fixed structured grids over which bodies move by a method involving a system of Lagrange multipliers. Several different versions of each kind of code have been developed and tried on a variety of applications.

▪ ALE Particle Mover

Direct simulation of the motion of solid particles in fluids can be said to have started in the paper of Hu, Joseph and Crochet 1992a. The first method Hu *et al* 1992a uses an implicit update of the particle translational and angular velocities on unstructured grids (see figure III.1) to prevent numerical instability. This is achieved by alternately computing the hydrodynamic force and torque, then updating the particle translational and angular velocities using the equations of rigid-body motion, and iterating until the translational and angular velocities converge. The combined equations of motion (II.6, 7, 8) were used in Hu’s improved ALE scheme Hu 1996a, 2000 and Hu, Patankar and Zhu 2000.

The ALE particle mover uses a generalization of the standard Galerkin finite-element method on an unstructured body-fitted mesh, together with an Arbitrary Lagrangian-Eulerian (ALE) moving mesh technique to deal with the movement of particles (see, for example Hansbo 1992, Huerta and Liu 1988, Nomura and Hughes 1992). In our implementation, the nodes on a particle surface are assumed to move with the particle. The movement of the nodes in the interior of the fluid is computed using a modified Laplace’s equation, to ensure that they are smoothly distributed. At each time step, the grid is updated according to the motion of the particles. A new grid is generated whenever the elements of the mesh get too distorted, and the flow fields are projected onto the new grid.

The weak formulation of the ALE particle mover is based on (II.6, 7 and 8). These equations are reduced to algebraic equations by finite element methods on the unstructured grid like that in figure III.1. The strong form of these equations are the original equations (II.1 through 5) from which the weak form was derived.

Two versions of the ALE method are the integrated method introduced by H. Hu 1996a, and a splitting method implemented by H. Choi 2000. In the integrated method one solves for the velocity and pressure at the same time; in the splitting method one solves sequentially separate equations for the velocity and pressure.

The splitting method leads to a smaller system of equations than the integrated method; however, the divergence free condition is not enforced at every sequential step so that the velocity field which emerges from a divergence free step does not satisfy the momentum equation exactly; hence small time steps are required to solve the momentum equations with negligible error.

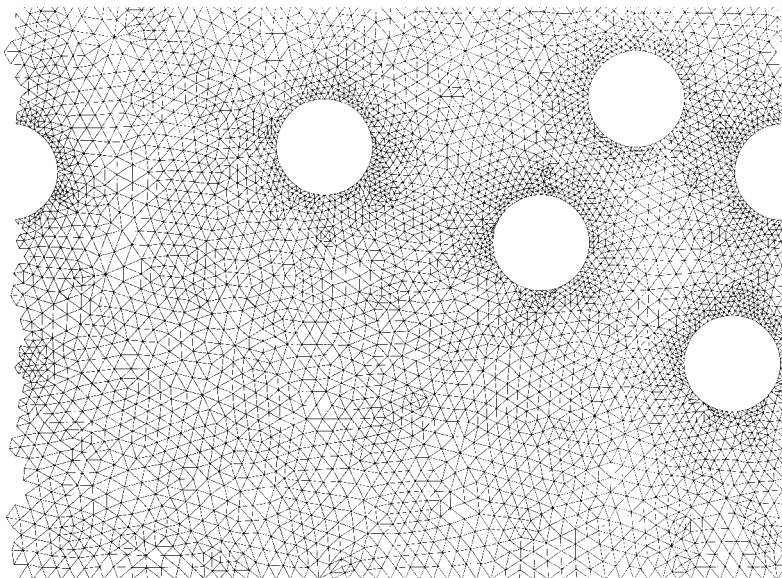


Figure III.1 Unstructured grid for the ALE method on a periodic domain.

The splitting method generates a symmetric saddle point matrix and leads to a symmetric positive definite pressure equation. The pressure gradient is solved by a conjugate gradient method without preconditioning because the matrixes involved are a composition of diagonally dominant matrices and other matrices conveniently formed with diagonal preconditioners. The methods run matrix-free of assembly of a global matrix.

▪ A Projected Particle Mover

Matt Knepley developed a variation of the ALE particle mover, Knepley, Sarin, Sameh 1998, in which the entire simulation is performed matrix-free in the space constrained to be discretely incompressible. Apart from the elegance of this approach, it simplifies the model by treating the particles and fluid in a decoupled fashion, and by eliminating pressure. The parallel multilevel preconditioner due to Sarin and Sameh 1998a, is used to obtain an explicit basis, P_v , for the discrete constrained divergence-free space. After elimination of pressure unknowns, a Krylov subspace method such as GMRES is used to solve the reduced system $P_v^T \tilde{A} P_v x = b$, where \tilde{A} is the constrained Jacobian for velocity unknowns. In contrast to the ALE particle mover discussed earlier, the linear systems in this method are positive-definite, and exhibit favorable convergence properties on account of the well-conditioned basis P_v . The algorithm has demonstrated very good scalability and efficiency for particle benchmarks on the SGI Origin 2000.

▪ DLM Particle Mover

The DLM particle mover uses a new Distributed-Lagrange-Multiplier-based fictitious-domain method. The basic idea is to imagine that fluid fills the space inside as well as outside the particle boundaries. The fluid-flow problem is then posed on a larger domain (the “fictitious domain”). This larger domain is simpler, allowing a simple regular mesh to be used. This in turn allows specialized fast solution techniques. The larger domain is also time-independent, so the *same* mesh can be used for the entire simulation, eliminating the need for repeated remeshing and projection (see figure III.2). This is a great advantage, since for three-dimensional particulate

flow the automatic generation of unstructured body-fitted meshes in the region outside a large number of closely spaced particles is a difficult problem. In addition, the entire computation is performed matrix-free, resulting in significant savings.

The velocity on each particle boundary must be constrained to match the rigid-body motion of the particle. In fact, in order to obtain a combined weak formulation with the hydrodynamic forces and torques eliminated, the velocity *inside* the particle boundary must also be a rigid-body motion. This constraint is enforced using a distributed Lagrange multiplier, which represents the additional body force per unit volume needed to maintain the rigid-body motion inside the particle boundary, much like the pressure in incompressible fluid flow whose gradient is the force required to maintain the constraint of incompressibility.

The scheme uses an operator-splitting technique for discretization in time. (Operator-splitting schemes have been used for solving the Navier-Stokes equations by many authors, starting, to our knowledge, with Chorin, 1967, 1968, and 1973, and Teman, 1997.) The linearly constrained quadratic minimization problems which arise from this splitting are solved using conjugate-gradient algorithms, yielding a method that is robust, stable, and easy to implement. For further details, see Glowinski, Pan, Hesla, Joseph and P eriaux 1999. The *immersed boundary method* of Peskin and his collaborators, Peskin 1997, 1981, Peskin and McQueen 1980, on the simulation of incompressible viscous flow in regions with elastic moving boundaries also uses a fictitious-domain method, but without Lagrange-multipliers.

The rigid motion constraint has been implemented in two ways leading to two codes, DLM1 and DLM2. The first implementation DLM1 Glowinski, Pan, Hesla and Joseph 1999 requires that the fluid at the places $P(t)$ occupied by the solid take on a rigid body velocity

$$\text{DLM1 } \mathbf{u}(\mathbf{x}, t) = \mathbf{U} + \boldsymbol{\omega} \wedge \mathbf{r}, \quad \mathbf{x} \in P(t)$$

where \mathbf{U} is the velocity of the mass center and $\boldsymbol{\omega} \wedge \mathbf{r}$ is the rotation around the mass center. The second implementation DLM2 Patankar, Singh, Joseph, Glowinski and Pan 2000 is stress-like, rigid motion on $P(t)$ is enforced by requiring that the rate of strain vanish there

$$\text{DLM2 } \mathbf{D}[\mathbf{u}] = 0, \quad x \in P(t)$$

where $\mathbf{D}[\mathbf{u}]$ is the symmetric part of $\nabla \mathbf{u}$.

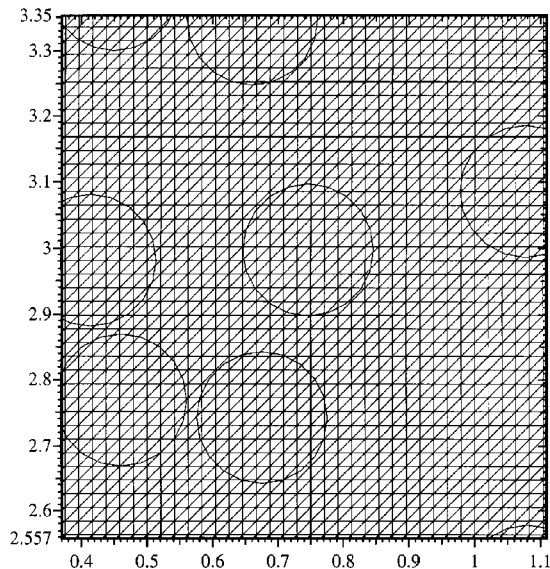


Figure III.2 Fixed triangular grid used in DLM computation. The same grid covers the fluid and solid. The fluid in the circles is bordered by Lagrange multipliers to move as a rigid body.

▪ Parallel Implementation

The DLM particle mover uses an operator-splitting technique consisting of three steps. In the first step, a saddle-point problem is solved using an Uzawa/conjugate-gradient algorithm, preconditioned by the discrete analogue of the Laplacian operator with homogeneous Neumann boundary conditions on the pressure mesh; such an algorithm is described in Turek 1996. The second step requires the solution of a non-linear discrete advection-diffusion problem that is solved by the algorithm discussed in Glowinski 1984. The third step solves another saddle-point problem using an Uzawa/conjugate-gradient algorithm.

The DLM approach uses uniform grids for two and three-dimensional domains, and relies on matrix-free operations on the velocity and pressure unknowns in the domain. This simplifies the distribution of data on parallel architectures and ensures excellent load balance (see Pan, Sarin, Glowinski, Sameh and Périaux 1999). The basic computational kernels, vector operations such as additions and dot products and matrix-free matrix-vector products, yield excellent scalability on distributed shared memory computers such as the SGI Origin 2000.

The main challenge in parallelization is posed by the solution of the Laplacian for the pressure mesh that functions as a preconditioner for the Uzawa algorithm. Fast solvers based on cyclic reduction for elliptic problems on uniform grids are overkill since the solution is required only to modest accuracy. A multilevel parallel elliptic solver, Sarin and Sameh 1998b, has been incorporated into the DLM algorithm. This has yielded speedup of over 10 for the preconditioning step on a 16 processor Origin.

The parallel DLM particle mover has been used to simulate the expansion of a fluidized bed discussed in chapter VII. Even though there is a serial component of the code, we have observed an overall speedup of 10 on the SGI Origin 2000 at NCSA, using 16 processors. In addition, this represents an impressive eight-fold increase in speed over the best serial implementation.

▪ Viscoelastic DLM Particle Mover

The ALE particle mover has been implemented for the popular Oldroyd-B constitutive model, which can be written in the form

$$\begin{aligned} \rho_f \left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right) &= -\nabla p + \nabla \cdot (2\eta \mathbf{D} + \mathbf{A}), \\ \nabla \cdot \mathbf{u} &= 0, \\ \lambda_1 \left(\frac{\partial \mathbf{A}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{A} - \mathbf{A} \cdot \nabla \mathbf{u} - \nabla \mathbf{u}^T \cdot \mathbf{A} \right) + \mathbf{A} &= \frac{\eta_E}{\lambda_1} \mathbf{1} \end{aligned} \quad (\text{III.1})$$

where \mathbf{D} is the rate-of-strain tensor, $\mathbf{A} = \boldsymbol{\tau}_E + (\eta_E / \lambda_1) \mathbf{1}$ is the configuration tensor, $\boldsymbol{\tau}_E$ is the elastic stress, η_E is the elastic viscosity, and λ_1 is the relaxation time. These equations are to be solved subject to appropriate boundary conditions.

The system (III.1) is classified mathematically as being of *composite* type, Joseph 1990a: The solution can have large gradients normal to the characteristic surfaces, which for this system are tangent to the streamlines. A numerical error in resolving these sharp gradients can cause one or more of the principal values of \mathbf{A} , which are always positive in the continuous problem, to become negative. This can cause a catastrophic amplification of short waves—a Hadamard instability, Singh and Leal 1993.

This Hadamard instability can be prevented by ensuring that \mathbf{A} remains positive-definite using a method introduced by Singh in Singh and Leal 1993, Singh and Leal 1994. The method has two key elements: a third-order upwinding scheme for discretizing the convection term in (II.10) and a time-dependent solution algorithm which explicitly forces the principal values of \mathbf{A} to be positive. The combination of these two elements ensures that the scheme will remain stable even at relatively large Deborah numbers. The equations are discretized in time using a second-order operator-splitting technique that decouples the constitutive equation from the incompressibility constraint. Singh, Joseph, Hesla, Glowinski and Pan 2000 have combined Singh's with the DLM method.

▪ Computation domains for pipe flows of slurries

In studying slurries and other pipe flows it is necessary to set the computational problem on a finite domain. It would be desirable to pose the problem as it is in nature using the end conditions. The problem posed this way requires knowledge of end conditions and the details of the motion may not determine the motion in the pipe, especially in long pipes. This same problem occurs in analysis of pipe flows in which a constant pressure gradient is prescribed as the ratio of the pressure drop Δp over the length L of pipe. The prescription of that constant pressure gradient is the only way in which the pressure drop is acknowledged. In analytical studies, the remaining nonconstant part of the pressure gradient can be posed in a suitable class of functions, say periodic in x . We could write

$$p(x, y, z, t) = Px + \Pi(x, y, z, t) \quad (\text{III.2})$$

where P is the constant pressure gradient and $\pi(x, y, z, t)$ is periodic with an assigned period in x . There are possibly different ways to choose this period and they are not equivalent. This is exactly where we are in simulation. We decompose the pressure as in (III.2), then we require that π and the velocity and other quantities are periodic in x with an assigned period. The assignment of the period is made decisively by the construction of a periodic mesh like the one shown in figure III.1. Clearly anything we compute on this mesh will have the assigned periodicity. The choice of periodicity and the selection of the period does cloud the relevance of computed to observed results and needs further study.

Simulations of single particle lift to equilibrium were also performed in a computational domain, which moves in the x -direction and is such that the particle is always at its center. The inflow and outflow boundaries are located at a specified distance from the center of the particle. A fully developed parabolic velocity profile $u(y) = \bar{p}y(W - y)/2\eta$ corresponding to the applied pressure gradient is imposed at the inflow and outflow boundaries.

▪ Collision Strategies

It is not possible to simulate the motion of even a moderately dense suspension of particles without a strategy to handle cases in which particles touch. In unstructured-grid methods, frequent near-collisions force large numbers of mesh points into the narrow gap between close particles and the mesh distorts rapidly, requiring an expensive high frequency of remeshing and projection. A “collision strategy” is a method for preventing near collisions while still conserving mass and momentum.

Four collision strategies are presently being used. They all define a security zone around the particle such that when the gap between particles is smaller than the security zone a repelling force is activated. A repelling force can be thought to represent surface roughness, for example. The repelling force pushes the particle out of the security zone into the region in which fluid forces computed numerically govern. The strategies differ in the nature of the repelling force and how it is computed. It is necessary to compare these different strategies.

A collision strategy for the ALE particle mover used by Hu 2000 chooses the repelling force so that the particles are forced just to the edge of the security zone. Another strategy for the ALE particle mover, due to Maury and Glowinski 1997, uses the lubrication force of Kim and Karrila 1991, to separate touching particles and it is also the only strategy that requires touching particles to transfer tangential as well as normal momentum. Maury and Glowinski developed his theory for smooth bodies of arbitrary shape.

A yet different collision strategy has been implemented for the DLM particle mover, Glowinski, Pan, Hesla and Joseph 1999. As in the other methods a security zone is defined. An explicit formula, linear in the distance of penetration into the security zone, is used to keep the particles apart. This repelling force may be tuned with a “stiffness” parameter.

Johnson and Tezduyar 1996, implemented a collision strategy based on the physics of inelastic collisions in which a security zone is defined by structured layers of elements around the particles. They model their strategy as an inelastic collision of elastic bodies with no fluid present and use the coefficient of restitution as a fitting parameter. The collision strategy is activated when the structured layers touch.

All of these strategies keep the particles farther apart than they ought to be, resulting in too high void fractions. To have real collision of smooth rigid particles it is necessary for the film between particles to rupture and film rupture requires physics and mathematics beyond the Navier-Stokes equations. Without film rupture physics, the best that can be expected from simulation is a strategy that allows for the action of lubrication forces to within the tolerance of the mesh.

This kind of "security zone free" scheme has been devised and implemented by Singh, Hesla and Joseph 2002. They modify the DLM method to allow the particles to come arbitrarily close to each other and even slightly overlap. When conflicting rigid body constraints from two different particles are applicable on a velocity node, the constraint from the particle that is closer to that node is used and the other constraint is dropped. An elastic repulsive force is applied when the particles overlap. The particles are allowed to overlap as much as one hundredth of the velocity element size.

The modified DLM method was applied for both Newtonian and viscoelastic liquids. Excellent results for particles in close approach and validation against analytical results were achieved.

A. Addendum to Chapter III (Addendum A). Experiments on particle collisions in viscous liquids; Stokes number

The physics of collisions is thought to correlate with the Stokes number

$$\text{Stk} = \frac{mv_0}{6\pi a^2 \mu} = \frac{1}{9} \frac{\rho_p}{\rho_f} \text{Re}$$

here defined for a sphere of radius a , where v_0 is the velocity of the sphere and $m = \frac{4}{3} \pi a^3 \rho_p$ is its mass and $\text{Re} = \frac{2av_0}{\nu_f}$ is the Reynolds number. The effects of particle

momentum mv_0 , collisions and rebound after collision are more important when Stk is larger. In simulations, collisions which trigger an elastic repulsive force require this selection of a coefficient of restitution, which is the ratio of the velocity before and after impact. G. Joseph et al 2001, 2004, in the laboratory of Melanie Hunt, have done experiments which clarify this point:

- G. G. JOSEPH, R. ZENIT, M. L. HUNT AND A. M. ROSENWINKEL. PARTICLE-WALL COLLISIONS IN A VISCOUS FLUID, *J. FLUID MECH.* **433**, 329-346 (2001).
- G. G. JOSEPH AND M. L. HUNT. OBLIQUE PARTICLE-WALL COLLISIONS IN A LIQUID. *J. FLUID MECH.* **510**, 71-93 (2004).

(Prior literature on this topic can be found in the reference list of these two papers). They find that

- For a particle colliding with a wall in a viscous fluid, the coefficient of restitution (the ratio of the velocity just prior to and after impact) depends on the impact Stokes number (defined from the Reynolds number and the density ratio) and weakly on the elastic properties of the material.
- There exists a critical value for the Stokes number below which rebound does not occur. This value is higher than the value predicted from hydrodynamics for zero impact velocity.
- The slowdown of a particle prior to impact as it approaches a wall can be computed from hydrodynamic theory to a good approximation
- Oblique collisions in a fluid obey the same laws as oblique collisions in a dry system. However, the effective coefficient of friction at the point of contact is drastically reduced due to lubrication effects.

Stated in another way, these experiments have shown that the elastic properties of the particles and walls do not have a significant effect on the measured coefficients of restitution. For a particle colliding with a wall in the normal direction, a deceleration was observed due to the presence of the wall at Stokes numbers lower than approximately 70, with rebound ceasing at approximately 10. The distance from the wall at which the particle commences to decelerate increases with decreasing Stokes number. For Stokes

numbers above 70, there is no apparent deceleration and above about 2000, the fluid effects can be neglected. For numerical studies of solids in liquids, the forces arising from lubrication are vastly more important than those arising from elasticity.

IV. Weak and Strong Formulations of the DLM Method

The weak and strong forms of the equations for the DLM method are more interesting because the Lagrange multiplier field must be introduced. There are two ways to represent the rigid motion of a fluid in portions of the space occupied by solids; one way is to impose the condition that the velocity is given by the velocity of the mass center plus a rigid rotation, and the other is that on those portions of space, the rate of strain tensor vanishes. This gives rise to two versions of the DLM method: a body force formulation and a stress formulation.

▪ Body Force Formulation of DLM Method; Weak Solution

Find \mathbf{u} , p , $\boldsymbol{\lambda}$, \mathbf{U} and $\boldsymbol{\omega}$ satisfying

$$\int_{\Omega} \rho_f \left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} - \mathbf{g} \right) \cdot \mathbf{v} \, d\mathbf{x} \\ - \int_{\Omega} p \nabla \cdot \mathbf{v} \, d\mathbf{x} + \int_{\Omega} 2\eta \mathbf{D}[\mathbf{u}] : \mathbf{D}[\mathbf{v}] \, d\mathbf{x} \\ + \left(1 - \frac{\rho_f}{\rho_s} \right) \left(M \left(\frac{d\mathbf{U}}{dt} - \mathbf{g} \right) \cdot \mathbf{V} + \frac{d(I\boldsymbol{\omega} \cdot \boldsymbol{\xi})}{dt} \right)$$

, $\mathbf{H}_1(\Omega)$, p

$$= \int_{\Omega_s} \boldsymbol{\lambda} \cdot (\mathbf{v} - (\mathbf{V} + \boldsymbol{\xi} \wedge \mathbf{r})) \, d\mathbf{x} \quad , \quad \text{for all } \mathbf{u}, \mathbf{v} \text{ in } \mathbf{H}_1(\Omega), p \text{ and } \boldsymbol{\lambda} \text{ in } \mathbf{L}_2(\Omega), \mathbf{U}, \boldsymbol{\omega}, \mathbf{V}, \boldsymbol{\xi} \text{ in } \mathbf{R}^3 \quad (\text{IV.1})$$

$$\int_{\Omega_s} \mathbf{q} \nabla \cdot \mathbf{u} \, d\mathbf{x} = 0, \quad \mathbf{q} \in \mathbf{H}_1(\Omega) \quad (\text{IV.2})$$

$$\int_{\Omega_s} \boldsymbol{\mu} \cdot (\mathbf{u} - (\mathbf{U} + \boldsymbol{\omega} \wedge \mathbf{r})) \, d\mathbf{x}, \quad \boldsymbol{\mu} \in \mathbf{L}_2(\Omega) \quad (\text{IV.3})$$

Here $\boldsymbol{\lambda}(\mathbf{x}, t)$ is the Lagrange multiplier field, \mathbf{u} , p , $\boldsymbol{\lambda}$, \mathbf{U} and $\boldsymbol{\omega}$ are the unknown velocity, pressure, $\mathbf{U}(t)$ and $\boldsymbol{\omega}(t)$ are the velocity and angular velocity; $\mathbf{v}, \mathbf{V}, \boldsymbol{\xi}$ and $\boldsymbol{\mu}$ are the test functions, Ω_s is the domain occupied by solids, and $\Omega = \Omega_f \cup \Omega_s$ is the domain occupied by both fluid and solid, the entire domain shown as triangles in figure III.2.

▪ Body Force Formulation of DLM: Strong Solutions

Using standard methods of the calculus of variations, we obtain the strong form of the DLM equations of motion and constraint in fluids and solids. We get the Navier-Stokes over the whole

domain Ω but the Lagrange multiplier field appears only on the solid. We find that $\text{div } \mathbf{u} = 0$ on fluid and solid and

$$\rho_f \frac{d\mathbf{u}}{dt} = \rho_f \mathbf{g} + \nabla \cdot \boldsymbol{\sigma} + \lambda \delta(\Omega_s) \quad (\text{IV.4})$$

where $\delta(\Omega_s)$ is one when $\mathbf{x} \in \Omega_s$ and zero otherwise and $\boldsymbol{\sigma} = -p\mathbf{1} + 2\eta\mathbf{D}[\mathbf{u}]$ is the stress. Here $\lambda - a^2\nabla^2\lambda$ is a body force. The solid is in rigid motion

$$\mathbf{u} = \mathbf{U} + \boldsymbol{\omega} \wedge \mathbf{r} \quad (\text{IV.5})$$

λ satisfies a natural boundary condition

$$(\mathbf{n} \cdot \nabla)\lambda = \mathbf{n} \cdot (\boldsymbol{\sigma}_s - \boldsymbol{\sigma}_f) \quad (\text{IV.6})$$

evaluating (IV.4) in Ω_f , we find

$$\begin{aligned} \text{div } \mathbf{u} &= 0, \\ \rho_f \frac{d\mathbf{u}}{dt} &= \rho_f \mathbf{g} - \nabla p + \eta \nabla^2 \mathbf{u} \end{aligned} \quad (\text{IV.7})$$

in Ω_f and from (IV.5), using no-slip, we get

$$\mathbf{u} = \mathbf{U} + \boldsymbol{\omega} \wedge \mathbf{r} \quad \text{on } \partial\Omega_f. \quad (\text{IV.8})$$

Equation (IV.7) and (IV.8) are a Dirichlet problem when \mathbf{U} and $\boldsymbol{\omega}$ are given and the boundary of the particles defining $\partial\Omega_f$ are known; if all these “given” were known as a function of time we could solve any initial value problem in Ω_f without reference to $\lambda(\mathbf{x}, t)$.

Using (IV.5) to evaluate (IV.4) on the solids Ω_s we get

$$\rho_f \left(\frac{d\mathbf{U}}{dt} + \frac{d\boldsymbol{\omega}}{dt} \wedge \mathbf{r} + \boldsymbol{\omega} \wedge (\boldsymbol{\omega} \wedge \mathbf{r}) - \mathbf{g} \right) = \lambda. \quad (\text{IV.9})$$

Since there is no divergence constraint for λ we may put the pressure p in the solid to zero and, of course, $\mathbf{D}[\mathbf{u}] = 0$ on rigid motions, and

$$(\mathbf{n} \cdot \nabla)\lambda = p\mathbf{n} - 2\eta\mathbf{D}[\mathbf{u}] \cdot \mathbf{n} \quad (\text{IV.10})$$

where p and \mathbf{u} are the values of these fields in the fluid on the $\partial\Omega_f$ of the solids. Once the fluid flow associated with (IV.7,8) is solved, the right side of (IV.10) is known and the linear equation (IV.9) may be solved for λ . The λ field is selected to make the fluid on the domain Ω_s occupied by solids move as a rigid body.

In the weak solution, the position of $\Omega_s(t)$ are updated using Newton's equations (II.3) rigid bodies. The form of the equations (II.3) is specialized for spheres; for arbitrary shape Newton's equations of motion are more complicated.

▪ Stress Formulation of DLM: Weak Solutions

Patankar, Singh, Joseph, Glowinski and Pan 2000 have introduced a new formulation of the distributed Lagrange multiplier/fictitious domain method for particulate flows. In this formulation the deformation rate tensor in the fluid occupied by solids is constrained to be zero. The Lagrange multiplier field λ turns out to be a velocity and the mathematics gives rise to a stress like equation for λ in which the particle phase pressure may be put to zero.

The new formulation starts with the observation that on a rigid solid

$$\mathbf{D}[\mathbf{u}] = 0 \quad (\text{IV.11})$$

and a partial differential equation equivalent to (IV.11) is

$$\nabla \cdot \mathbf{D}[\mathbf{u}] = 0 \text{ in } \Omega_s \text{ and } \mathbf{D}[\mathbf{u}] \cdot \mathbf{n} = 0 \text{ on } \partial\Omega_s. \quad (\text{IV.12})$$

The combined form of the total momentum equation is formulated as follows:

Find $\mathbf{u}, p, \lambda, \mathbf{U}$ and $\boldsymbol{\omega}$ satisfying

$$\begin{aligned} \int_{\Omega} \rho_f \left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} - \mathbf{g} \right) \cdot \mathbf{v} \, d\mathbf{x} + \int_{\Omega} 2\eta \mathbf{D}[\mathbf{u}] : \mathbf{D}[\mathbf{v}] \, d\mathbf{x} - \int_{\Omega} p (\nabla \cdot \mathbf{v}) \, d\mathbf{x} + \int_{\Omega} q (\nabla \cdot \mathbf{u}) \, d\mathbf{x} \\ + \int_{\Omega_s} (\rho_s - \rho_f) \left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} - \mathbf{g} \right) \cdot \mathbf{v} \, d\mathbf{x} + \int_{\Omega_s} \mathbf{D}[\lambda] : \mathbf{D}[\mathbf{v}] \, d\mathbf{x} + \int_{\Omega_s} \mathbf{D}[\mathbf{u}] : \mathbf{D}[\mathbf{u}] \, d\mathbf{x} = 0 \quad (\text{IV.13}) \end{aligned}$$

and

$$\begin{aligned} M\mathbf{U} &= \int_{\Omega_s} \rho_s \mathbf{u} \, d\mathbf{x} \\ \mathbf{I}\boldsymbol{\omega} &= \int_{\Omega_s} \mathbf{r} \times \rho_s \mathbf{u} \, d\mathbf{x}. \quad (\text{IV.14}) \end{aligned}$$

▪ Stress Formulation of DLM: Strong Solutions

The strong form for (IV.13) may be found by the usual method of the calculus of variations. In Ω_f , we have $\text{div } \mathbf{u}=0$,

$$\rho_f \frac{d\mathbf{u}}{dt} = -\nabla p + \eta \nabla^2 \mathbf{u} + \rho_f \mathbf{g}. \quad (\text{IV.15})$$

In Ω_s , $\text{div } \mathbf{u}=0$, $\mathbf{D}[\mathbf{u}]=0$ and

$$\rho_s \frac{d\mathbf{u}}{dt} = -\nabla p + \eta \nabla^2 \mathbf{u} + \rho_s \mathbf{g} + \nabla \cdot \mathbf{D}[\boldsymbol{\lambda}]. \quad (\text{IV.16})$$

The velocity and stress traction vectors are continuous across $\partial\Omega_s = \partial\Omega_f$

$$\left. \begin{aligned} \mathbf{n} \cdot (-p_f \mathbf{1} + p_s \mathbf{1} + 2\eta \mathbf{D}[\mathbf{u}_f - \mathbf{u}_s]) &= \mathbf{n} \cdot \mathbf{D}[\boldsymbol{\lambda}], \\ \mathbf{u}_f &= \mathbf{u}_s. \end{aligned} \right\} \quad (\text{IV.17})$$

Noting next that (IV.5) holds in Ω_s and on $\partial\Omega_s$, we arrive again at the Dirichlet problem (IV.7) and (IV.8) for the Navier-Stokes equation in Ω_f . After putting $\mathbf{u} = \mathbf{U} + \boldsymbol{\omega} \wedge \mathbf{r}$ into (IV.16) and evaluating (IV.17), we get

$$\nabla \cdot (\mathbf{D}[\boldsymbol{\lambda}]) = \rho_s \left(\frac{d\mathbf{U}}{dt} + \frac{d\boldsymbol{\omega}}{dt} \wedge \mathbf{r} + \boldsymbol{\omega} \wedge (\boldsymbol{\omega} \wedge \mathbf{r}) - \mathbf{g} \right) \quad (\text{IV.18})$$

$$\mathbf{n} \cdot \mathbf{D}[\boldsymbol{\lambda}]_s = \mathbf{n} \cdot (-p\mathbf{1} + 2\eta \mathbf{D}[\mathbf{u}])_f. \quad (\text{IV.19})$$

This is a linear Dirichlet problem for $\boldsymbol{\lambda}$ when $\mathbf{U}(t)$, $\boldsymbol{\omega}(t)$ and the position of $\bar{\mathbf{X}}$ and $\boldsymbol{\theta}$ of the particles. This data determines \mathbf{u} and p in Ω_f through (IV.15) (or (VI.7)) and (IV.8).

$\mathbf{D}[\boldsymbol{\lambda}]$ is the rate of strain for the Lagrange multiplier velocity field $\boldsymbol{\lambda}$ in 3D and three equations (IV.18). It is *not* required that $\text{div } \boldsymbol{\lambda} = 0$; in general $\text{div } \boldsymbol{\lambda} \neq 0$. Hence a ‘‘pressure’’ field is not associated with $\boldsymbol{\lambda}$ field. We might frame this result for two-fluid models of solid-liquid flow which states the particle phase pressure vanishes.

B. Addendum to Chapter IV (Addendum B). Weak form of the body force formulation when the Lagrange multiplier is eliminated

Using equation (IV.9) and (IV.10), we may eliminate λ in the weak solution.

$$\begin{aligned} & \int_{\Omega_s} \lambda \bullet (\mathbf{v} - (\mathbf{V} + \boldsymbol{\xi} \wedge \mathbf{r})) dx \\ &= \rho_f \int_{\Omega_s} (\dot{\mathbf{U}} + \dot{\boldsymbol{\omega}} \wedge \mathbf{r} + \boldsymbol{\omega} \wedge (\boldsymbol{\omega} \wedge \mathbf{r}) - \mathbf{g}) \bullet (\mathbf{v} - (\mathbf{V} + \boldsymbol{\xi} \wedge \mathbf{r})) dx \end{aligned} \quad (\text{IV.20})$$

where

$$\dot{\mathbf{U}} = \frac{d\mathbf{U}}{dt}, \quad \dot{\boldsymbol{\omega}} = \frac{d\boldsymbol{\omega}}{dt}.$$

Noting now that $\Omega = \Omega/\Omega_s \cup \Omega_s$, where $\Omega/\Omega_s = \Omega_f$ is the part of Ω occupied by the fluid alone, we may write (IV.1), using (IV.20) as

$$\begin{aligned} & \int_{\Omega_f} \{ \rho_f \left[\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \bullet \nabla) \mathbf{u} - \mathbf{g} \right] \bullet \mathbf{v} + 2\eta \mathbf{D}[\mathbf{u}] : \mathbf{D}[\mathbf{v}] - p \nabla \bullet \mathbf{v} \} dx \\ &+ \int_{\Omega_s} \rho_f \left[\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \bullet \nabla) \mathbf{u} - \dot{\mathbf{U}} - \dot{\boldsymbol{\omega}} \wedge \mathbf{r} - \boldsymbol{\omega} \wedge (\boldsymbol{\omega} \wedge \mathbf{r}) \right] \bullet \mathbf{v} dx \\ &+ (1 - \frac{\rho_f}{\rho_s}) \left[M (\dot{\mathbf{U}} - \mathbf{g}) \bullet \mathbf{V} + \frac{d}{dt} (\mathbf{I} \boldsymbol{\omega}) \bullet \boldsymbol{\xi} \right] \\ &+ \rho_f \int_{\Omega_s} [\dot{\mathbf{U}} + \dot{\boldsymbol{\omega}} \wedge \mathbf{r} + \boldsymbol{\omega} \wedge (\boldsymbol{\omega} \wedge \mathbf{r}) - \mathbf{g}] \bullet (\mathbf{V} + \boldsymbol{\xi} \wedge \mathbf{r}) dx = 0, \end{aligned} \quad (\text{IV.21})$$

where

$$\mathbf{I} = \rho_s \int_{\Omega_s} [r^2 \mathbf{1} - \mathbf{r} \otimes \mathbf{r}] dx$$

is the moment of inertia tensor.

The position vector \mathbf{r} is measured from the mass center of the particle. Since ρ_s is uniform, the volume and mass centers are identical and

I'm indebted to Todd Hesla for his help with the reduction of the weak to strong solution and some of the calculations leading to (IV.25).

$$\int_{\Omega_s} \mathbf{r} dx = 0 \quad (\text{IV.22})$$

where $\mathbf{r} = \mathbf{x} - \mathbf{X}(t)$ and \mathbf{X} is the center of mass.

Using (IV.22), we may simplify and rewrite the last term of (IV.21) as

$$\rho_f (\dot{\mathbf{U}} - \mathbf{g}) \cdot \mathbf{V} \int_{\Omega_s} dx + \rho_f \int_{\Omega} [\dot{\boldsymbol{\omega}} \wedge \mathbf{r} + \boldsymbol{\omega} \wedge (\boldsymbol{\omega} \wedge \mathbf{r})] (\boldsymbol{\xi} \wedge \mathbf{r}) dx .$$

Noting next that $M = \rho_s \int_{\Omega_s} dx$, the terms proportional to \mathbf{V} in (IV.21) are

$$M[\dot{\mathbf{U}} - \mathbf{g}] \cdot \mathbf{V}$$

and the terms proportional to $\boldsymbol{\xi}$ become

$$\left(1 - \frac{\rho_f}{\rho_s}\right) \frac{d}{dt} (\mathbf{I}\boldsymbol{\omega}) \cdot \boldsymbol{\xi} + \rho_f \int_{\Omega} [\dot{\boldsymbol{\omega}} \wedge \mathbf{r} + \boldsymbol{\omega} \wedge (\boldsymbol{\omega} \wedge \mathbf{r})] (\boldsymbol{\xi} \wedge \mathbf{r}) dx$$

which, after applying well known vector identities, becomes

$$\left(1 - \frac{\rho_f}{\rho_s}\right) \frac{d}{dt} (\mathbf{I}\boldsymbol{\omega}) \cdot \boldsymbol{\xi} + \rho_f \int_{\Omega_s} [\mathbf{r}^2 \dot{\boldsymbol{\omega}} - (\mathbf{r} \cdot \dot{\boldsymbol{\omega}}) \mathbf{r} + \boldsymbol{\omega} \cdot \mathbf{r} (\mathbf{r} \wedge \boldsymbol{\omega})] \cdot \boldsymbol{\xi} dx$$

or

$$\left(1 - \frac{\rho_f}{\rho_s}\right) \frac{d}{dt} (\mathbf{I}\boldsymbol{\omega}) \cdot \boldsymbol{\xi} + \frac{\rho_f}{\rho_s} (\mathbf{I}\dot{\boldsymbol{\omega}}) \cdot \boldsymbol{\xi} + \frac{\rho_f}{\rho_s} \boldsymbol{\omega} \wedge (\mathbf{I}\boldsymbol{\omega}) \cdot \boldsymbol{\xi} . \quad (\text{IV.23})$$

We note next that

$$\frac{d}{dt} (\mathbf{I}\boldsymbol{\omega}) = \mathbf{I}\dot{\boldsymbol{\omega}} + \rho_s \int_{\Omega_s} [\boldsymbol{\omega} (\mathbf{r} \cdot \frac{d\mathbf{r}}{dt}) - (\boldsymbol{\omega} \cdot \frac{d\mathbf{r}}{dt}) \mathbf{r} - (\boldsymbol{\omega} \cdot \mathbf{r}) \frac{d\mathbf{r}}{dt}] dx .$$

Since

$$\frac{d\mathbf{r}}{dt} = \left[\frac{\partial}{\partial t} + (\mathbf{U} + \boldsymbol{\omega} \wedge \mathbf{r}) \cdot \nabla \right] [\mathbf{x} - \mathbf{X}(t)] = -\dot{\mathbf{X}} + \mathbf{U} + \boldsymbol{\omega} \wedge \mathbf{r} = \boldsymbol{\omega} \wedge \mathbf{r} ,$$

this reduces to

$$\frac{d}{dt}(\mathbf{I}\boldsymbol{\omega}) = \mathbf{I}\dot{\boldsymbol{\omega}} + \boldsymbol{\omega} \wedge (\mathbf{I}\boldsymbol{\omega}) . \quad (\text{IV.24})$$

After inserting (IV.24) into (IV.23), all of the terms except $\boldsymbol{\xi} \bullet d(\mathbf{I}\boldsymbol{\omega})/dt$ vanish. The terms proportional to \mathbf{V} and $\boldsymbol{\xi}$ in (IV.21) therefore simplify drastically to

$$M[\dot{\mathbf{U}} - \mathbf{g}] \bullet \mathbf{V} + \frac{d}{dt}(\mathbf{I}\boldsymbol{\omega}) \bullet \boldsymbol{\xi} .$$

The reformulated statement of the weak form of our solid liquid system is obtained after eliminating $\boldsymbol{\lambda}$ from (IV.1) by the method just given. The combined momentum formulation, fluid plus solid, is

$$\begin{aligned} & \int_{\Omega_f} \rho_f \left[\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \bullet \nabla) \mathbf{u} - \mathbf{g} \right] \bullet \mathbf{v} dx + \int_{\Omega_f} \{ 2\eta \mathbf{D}[\mathbf{u}] : \mathbf{D}[\mathbf{v}] - p \nabla \bullet \mathbf{v} \} dx \\ & + \int_{\Omega_s} \rho \left[\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \bullet \nabla) \mathbf{u} - \dot{\mathbf{U}} - \dot{\boldsymbol{\omega}} \wedge \mathbf{r} - \boldsymbol{\omega} \wedge (\boldsymbol{\omega} \wedge \mathbf{r}) \right] \bullet \mathbf{v} dx \\ & + M(\dot{\mathbf{U}} - \mathbf{g}) \bullet \mathbf{V} + \frac{d}{dt}(\mathbf{I}\boldsymbol{\omega}) \bullet \boldsymbol{\xi} = 0 , \end{aligned} \quad (\text{IV.25})$$

where the test functions $\mathbf{v} \in \mathbf{H}^1(\Omega)^3$ and $\mathbf{V} \in R^3$ and $\boldsymbol{\xi} \in R^3$ are vectors. The integral on Ω_s guarantees that the momentum on of the patches of fluid Ω_s on places occupied by the solids is for a rigid body motion. The fluid is weakly solenoidal

$$\int_{\Omega} q \nabla \bullet \mathbf{u} dx = 0 , \quad q \in L^2(\Omega)$$

and the condition

$$\int_{\Omega_s} \boldsymbol{\mu} \bullet [\mathbf{u} - (\mathbf{U} + (\boldsymbol{\omega} \wedge \mathbf{r}))] dx = 0 , \quad \boldsymbol{\mu} \in \mathbf{H}^1(\Omega)^3$$

guarantees that the fluid moves as a rigid body.

C. Addendum to Chapter IV (Addendum C). Recent Developments in Direct Numerical Methods for Solid-Liquid flows

The method of direct simulation of solid-liquid flow has become very popular since the first edition of this book in 2002. Here, I am going to give a short synopsis of some of the main developments since 2002. These may be characterized as

- (1) Extensions of DLM to different element bases
- (2) Fast DLM methods based on quick generation of rigid body motions by “averaging” fluid motions
- (3) Explicit methods avoiding Poisson equations for the pressure using an equation of state for weak compressibility

My book is not a source for the computational methods used to implement direct simulation. These methods are described in papers cited throughout the book. For good thorough reviews of the technical CFD issues confronting researchers, I recommend the following papers. The ALE method and applications is treated by

- H. HU, N. A. PATANKAR AND M. Y. ZHU. DIRECT NUMERICAL SIMULATIONS OF FLUID-SOLID SYSTEMS USING THE ARBITRARY LAGRANGIAN-EULERIAN TECHNIQUE. *J. COMP. PHYSICS*, **169**, 427-462 (2001)

The DLM method and applications is treated by

- R. GLOWINSKI. FINITE ELEMENT METHODS FOR INCOMPRESSIBLE VISCOUS FLOW. IN PART 3 *HANDBOOK OF NUMERICAL ANALYSIS*, **IX**, NORTH-HOLLAND, AMSTERDAM (2003) (ED. P. G. CIARLET AND J. L. LIONS).

Fast computation methods are discussed in

- N. SHARMA AND N. PATANKAR. A FAST COMPUTATION TECHNIQUE FOR THE DIRECT NUMERICAL SIMULATION OF RIGID PARTICULATE FLOW. *J. COMP. PHYS.* (2004).
- N. PATANKAR. A FORMULATION FOR FAST COMPUTATION OF RIGID PARTICULATE FLOW. *CENTER FOR TURBULENCE RESEARCH ANNUAL REPORT*, STANFORD 185-196 (2001).

(1) Extension of DLM to different element bases

Even more recent advances in the DLM method are given in the papers listed below.

Extension of DLM calculations from finite element to spectral element bases were carried out and applied by

- S. DONG, D. LIU, M. MAXEY, G. KARNIADAKIS. SPECTRAL DISTRIBUTED LAGRANGE MULTIPLIER METHOD: ALGORITHM AND BENCHMARK TESTS. *J. COMP. PHYSICS*, **195**, 695-717 (2004).

Abstract: We extend the formulation of the distributed Lagrange multiplier (DLM) approach for particulate flows to high-order methods within the spectral/*hp* element framework. We implement the rigid-body motion constraint inside the particle via a penalty method. The high-order DLM method demonstrates spectral convergence rate, i.e. discretization errors decrease exponentially as the order of spectral polynomials increases. We provide detailed comparisons between the spectral DLM method, direct numerical simulations, and the force coupling method for a number of 2D and 3D benchmark flow problems. We also validate the spectral DLM

method with available experimental data for a transient problem. The new DLM method can potentially be very effective in many-moving body problems, where a smaller number of grid points is required in comparison with low-order methods.

Extension of DLM calculations from finite element to finite-difference bases were carried out and applied by

- Z. YU, N. PHAN-THIEN AND R. TANNER. DYNAMIC SIMULATION OF SPHERE MOTION IN A VERTICAL TUBE. *J. FLUID MECH*, **518**, 61-93 (2004).

They did a very thorough study and obtained results in uniformly good agreement with experiments. This paper treats sedimentation of a single sphere in tube flow. The migration problem was considered by Yang et al (2005) for a neutrally buoyant using both ALE and DLM methods (see addendum). Their results agree with those of Yu, where they overlap. Yu et al 2004 gave correlations for their results like those proposed earlier in various papers from our group but they get all their results from unconstrained rather than constrained simulations used to generate correlations in the work of Yang et al. The two papers mentioned here were done independently. The stress formulation of the DLM method in strong form has been implemented in the animation work of

- M. CARLSON, P. MUCHA AND G. TURK. RIGID FLUID: ANIMATING THE INTERPLAY BETWEEN RIGID BODIES AND FLUID. *CONFERENCE PROCEEDINGS ACM TRANSACTIONS ON GRAPHICS*, **23**, 377-384 (2004).

Abstract: We present the *Rigid Fluid* method, a technique for animating the interplay between rigid bodies and viscous incompressible fluid with free surfaces. We use distributed Lagrange multipliers to ensure two-way coupling that generates realistic motion for both the solid objects and the fluid as they interact with one another. We call our method the *rigid fluid* method because the simulator treats the rigid objects as if they were made of fluid. The rigidity of such an object is maintained by identifying the region of the velocity field that is inside the object and constraining those velocities to be rigid body motion. The rigid fluid method is straightforward to implement, incurs very little computational overhead, and can be added as a bridge between current fluid simulators and rigid body solvers. Many solid objects of different densities (*e.g.*, wood or lead) can be combined in the same animation.

The goal of their work focuses on computer generated animation. Their research follows most closely the DLM work of Patankar et al 2000 and especially of the fast method of Patankar 2001. They program the equations in strong form using finite differences rather than finite elements. They apply their formula to several rigid bodies and not just to spheres and their animations include free surfaces which are computed using the method of level sets. Their paper is well organized and easy to follow.

(2) Fast DLM methods

N. Patankar 2001, introduced a fast method for producing rigid motions on the places Ω_s occupied by solids. His method is motivated by the Lagrange multiplier formulation and can be expressed in this frame. However, in the actual implementation the multipliers are not seen. Roughly, the computation proceeds as if there were no rigid bodies. Then the places Ω_s occupied by these bodies are identified and on them we can assure that $\mathbf{D}[\mathbf{u}] = 0$ if the velocity $\mathbf{u} = \mathbf{v}$ of the mass center of the rigid body and angular velocity $\boldsymbol{\omega}$ of the body around its mass center is selected as averages satisfying the principles of conservation of linear and angular momentum

$$M\mathbf{v} = \int_{\Omega_s} \rho_p \mathbf{u} \cdot d\Omega_s$$

and

$$\mathbf{I}\boldsymbol{\omega} = \int_{\Omega_s} \mathbf{x} \times \rho_p \mathbf{u} \cdot d\Omega_s .$$

The rigid motion $\mathbf{u}_r = \mathbf{v} + \mathbf{x} \times \boldsymbol{\omega}$ does not match the fluid velocity at every point on Ω_s but this discontinuity is corrected in Patankar's scheme and the correction is smeared on the length scale of the grid size.

A different fast method for the body force formulation of DLM has been given by

- R. GLOWINSKI, T. PAN, T. HESLA, D. JOSEPH AND J. PÉRIAUX. A FICTITIOUS DOMAIN APPROACH TO THE DIRECT NUMERICAL SIMULATION OF INCOMPRESSIBLE VISCOUS FLOW PAST MOVING RIGID BODIES: APPLICATION TO PARTICLE FLOW. *J. COMP. PHYSICS*, **169**, 363-426 (2001).

A misprint in the fast method equations (7.33) and (7.34) in this paper was corrected in Glowinski (2003). (see pages 724-726)

A comparison of the stress based DLM fast algorithm of Sharma and Patankar (2004) and the body force based DLM fast algorithm of Glowinski et al (2001, 2003) is given in the paper of Sharma and Patankar.

(3) **Explicit methods avoiding Poisson equations for the pressure using an equation of state for weak compressibility**

A Poisson equation for the pressure

$$\nabla^2 p = -div[(\mathbf{u} \bullet \nabla)\mathbf{u}]$$

arises from the Navier-Stokes equations for incompressible fluids for which $div(\mathbf{u}) = 0$. This is an elliptic problem and it generates difficulties for efficient computation which do not arise when the pressure is given by an equation of state. One method of dealing with this problem is to introduce an equation of state for weak compressibility perturbing compressibility. The method of pseudo-compressibility, associated with the names of A. Chorin and R. Temam, is well known to CFD experts, but it has not been applied to DNS of particulate flow. The MacCormack scheme is an explicit method for compressible fluids. It is essentially a predictor-corrector scheme, similar to a second order Runge-Kutta method commonly used to solve ordinary differential equations. It is very easy to program and it runs fast and well, is widely used and is widely respected.

- R. W. MACCORMACK "THE EFFECT OF VISCOSITY IN HYPERVELOCITY IMPACT CRATERING." *AIAA PAPER 69-354*, CINCINNATI, OHIO (1969).

Some progress has been made to adapting this scheme to particulate flow in weakly compressible fluids.

- H. HU AND A. PERRIN. SIMULATIONS OF PARTICULATE FLOWS USING EXPLICIT MACCORMACK SCHEME. IUTAM SYMPOSIUM ON “COMPUTATIONAL APPROACHES TO DISPERSED MULTIPHASE FLOW” ARGONNE NATIONAL LABORATORY, ARGONNE OCT 4-7 (2004).

Abstract: Most incompressible flow solvers are implicit. Large systems of equations are constructed and solved, demanding large amounts of memory and special schemes for parallelization. We can evade these difficulties by solving flow problems based on small Mach number compressible Navier-Stokes equations with explicit finite-differences on a fixed, uniform grid at each time step. This explicit scheme eliminates the Poisson equation for pressure by relating pressure to density through an equation of state, then updating density with the compressible continuity equation. The sound speed in the media imposes a constraint on the time step for the simulation. We find empirically that for moderate Reynolds numbers (up to 200 based on the particle size), the CFL condition (based on the sound speed) applies.

Advantages similar to the MacCormack scheme are enjoyed by the Lattice Boltzmann method. This method can be described as a Galerkin approximate method based on the Bhatnager, Gross, Krook 1954 (BGK) approximation for the Boltzmann equation. The LBE method is a pseudocompressible method. Using a method of multiple scales, the continuum equations implied by this method derived; these equations are compressible, they have an equation of state and they are **not** the compressible Navier-Stokes equations, but are Navier-Stokes like.

See equations (89) in

- R. R. NOURGALIEV, T. N. DINH, T. G. THEOFANOUS AND D. D. JOSEPH 2003. THE LATTICE BOLTZMANN EQUATION METHOD: THEORETICAL INTERPRETATION, NUMERICS AND IMPLICATIONS. *INTERNATIONAL JOURNAL OF MULTIPHASE FLOW* **29**, 117-169 (2003).

The LBE method sometimes gives good results for solid-liquid flow because the particles move under computed rather than modeled forces.

(4) Hybrid methods

A hybrid method is a numerical method which makes use of results from mathematical analysis. J. Brady’s Stokesian dynamic simulations of particulate flow embed analytical results from lubrication theory for near collisions of particles with “Stokeslet” representations for far field effects. (See Brady 1993 for a recent review).

Another hybrid method is implemented in Physalis proposed by

- A. PROSPERETTI AND H. N. OGUZ. PHYSALIS: A NEW $O(N)$ FOR THE NUMERICAL SIMULATION OF DISPERSE SYSTEMS: POTENTIAL FLOW OF SPHERES. *J. COMP. PHYS.* **167**, 196-216 (2001).

Z. Zhang and A. Prosperetti have recently reported the results of simulations of sedimentation of 1024 spheres in a periodic domain at Reynolds numbers of about 40 (Nov. 21-23, 2004 MEETING OF DFD OF APS IN SEATTLE, WASHINGTON)

Physalis uses an analytical solution in the neighborhood of each particle and matches this solution to the external field calculated numerically. For the sedimentation problem the Stokes flow solution is used in the neighborhood of each sphere; locally because of no slip, the fluid velocity is nearly zero in the frame of the moving particle. A boundary

layer would reduce the size of the Stokes flow layer at high global values of Re , but the use of an analytical solution probably needs fewer mesh points on the sphere than a direct method at any Re . It may be difficult to use this method on solids whose shape does not allow a convenient analytical representation.

(5) Colloids and nanoparticles

Brady's (1993) Stokesian dynamic method has been applied successfully to many colloid problems at low global values of Re .

A promising new method which is not restricted to Stokes flow or to random forces has been proposed by

- N. SHARMA AND N. PATANKAR. DIRECT NUMERICAL SIMULATION OF THE BROWNIAN MOTION OF PARTICLES USING THE FLUCTUATING HYDRODYNAMIC EQUATIONS. *J. COMP. PHYS.* **201**, 466-486 (2004).

Abstract: In this paper, we present a direct numerical simulation scheme for the Brownian motion of particles. Solving the fluctuating hydrodynamic equations coupled with the particle equations of motion result in the Brownian motion of the particles. There is no need to add a random force term in the particle equations. The particles acquire random motion through the hydrodynamic force acting on its surface from the surrounding fluctuating fluid. The random stress in the fluid equations is easy to calculate unlike the random terms in the conventional Brownian dynamics type approaches. We present a three-dimensional implementation along with validation.