

A Project Summary

The proposal in this document was funded as a grand challenge HPCC grant and is presently being implemented. Now we want to integrate Pierre Saramito and his group into our effort. He has developed efficient numerical methods by which he circumvents the ubiquitous failure of viscoelastic simulations when the Deborah number (an elasticity parameter) is large and we want to integrate his techniques into our codes. The proposal in this document is as it was originally, though it has now been funded, so that referees can evaluate the grand challenge effort generally and see the value added by bringing in Saramito. The rationale for the NSF-CNRS joint effort is presented in section 2.1 on the “French research team”; it is the only new material which has been added.

The grand challenge proposed is to develop highly efficient methods for computing the three-dimensional motions of large numbers of particles in solid-liquid flows, under the action of the hydrodynamic forces and torques exerted by the suspending fluid, and to use these methods to elucidate the fundamental dynamics of particulate flows and solve problems of engineering interest. The goal is to develop high-performance, state-of-the-art software packages called *particle movers*, capable of simulating the motion of thousands of particles in 2-D and hundreds in 3-D domains, in both Newtonian fluids, governed by the Navier-Stokes equations, and in several popular models of viscoelastic fluids. Such simulations will be *extremely* computationally intensive. It is therefore imperative to develop the most efficient possible computational schemes, and to implement them on parallel machines, using state-of-the-art parallel algorithms.

To meet this challenge, we propose to develop two different computational schemes for simulating solid-liquid flows on parallel computers. The first is a generalization of the standard Galerkin finite element method in which both the fluid and particle equations of motion are incorporated into a *single* variational equation, containing both the fluid and particle velocities as primitive unknowns. The hydrodynamic forces and torques on the particles are eliminated in the formulation, so need not be computed as separate quantities. The computation is performed on an unstructured body-fitted grid, and an arbitrary Lagrangian-Eulerian moving mesh technique has been adopted to deal with the motion of the particles.

In the second approach, an *embedding method*, the fluid flow is computed as if the space occupied by the particles were filled with fluid. The no-slip boundary condition on the particle boundaries is enforced as a *constraint* using Lagrange multipliers. This allows a fixed grid to be used, eliminating the need for remeshing, a definite advantage in parallel implementations.

Both approaches have been initiated by us, for quite different kinds of applications. At present, one scheme does not fit all applications. Perhaps ultimately, a “best” universal scheme for moving particles may evolve, but it is not presently prudent to make a bet.

A crucial computational issue to be addressed is the efficient solution of the various algebraic systems which arise in the schemes. These systems can be extremely large for 3-D problems, and their solution can consume up to 95% of the CPU time of the entire simulation. It is therefore imperative to use efficient iterative solution methods, with matrix-free preconditioners, and to implement them on parallel architectures.

We plan to develop a library of parallel numerical algorithms to solve these systems. This parallel library will consist of algorithms for solving nonlinear algebraic equations using variants of Newton’s method, preconditioned iterative solvers for sparse symmetric indefinite and nonsymmetric linear systems, and rapid elliptic and Stokes solvers on uniform grids. This library will be used for rapid prototyping of simulation codes for the application problems referred to above.

The library will be augmented with a collection of kernels to allow it to be efficiently portable across either the massive parallelism of the Cray T3-D or its successors, or cluster-based parallelism such as that of several interconnected SGI Power-Challenge workstations. Both architectures exhibit two-level parallelism that is ideally suited for schemes such as the embedding method on a fixed grid.

The new schemes will be used to study the microstructural (pair interaction) effects which produce clusters and anisotropic structures in particulate flows, to produce statistical analyses of particulate flows (mean values, fluctuation levels and spectral properties), to derive engineering correlations of the kind usually obtained from experiments, and to provide clues and closure data for the development of two-phase flow models and a standard against which to judge the performance of such models. They will also be used to solve practical problems of industrial interest such as sedimentation, fluidization and slurry transport of solid

particles in Newtonian and viscoelastic fluids.

Finally, the results of all numerical simulations will be compared with experiments from the literature or experiments to be done in the Minnesota laboratory, or with field data from industry—especially from our industrial sponsors. The project will therefore advance the science of solid-liquid flow using all the available tools: theory, experiments, and numerical simulation.

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C Project Description

Part I

Introduction

1 Project Overview

The current popularity of computational fluid dynamics is rooted in the perception that information implicit in the equations of fluid motion can be extracted without approximation. A similar potential for solid-liquid flows, and multiphase flows generally, has yet to be fully exploited. To extract information implicit in the equations of motion for solid-liquid flows, it is necessary to numerically solve the coupled system of differential equations consisting of the equations of fluid motion, and the equations of rigid-body motion (governing the particle motions), together with suitable initial and boundary conditions. These equations are coupled through the no-slip boundary condition on the particle surfaces, and through the hydrodynamic forces and torques exerted by the fluid on the particles.

Developing highly efficient computational schemes for solving this coupled system of equations in two and three dimensions, both for Newtonian fluids (governed by the Navier-Stokes equations) and for the family of viscoelastic fluids (with Oldroyd B principal parts) most frequently studied in the rheology literature, represents a grand challenge in computational mechanics.

The goal is to develop high-performance, state-of-the-art software packages called *particle movers*, capable of simulating the motion of 1000 particles in two-dimensional simulations in Newtonian fluids in regular and complex geometries, 100 spheres in similar circumstances in three dimensions, and 100 particles in viscoelastic fluids. Such simulations will be *extremely* computationally intensive. It is therefore imperative to develop the most efficient possible computational schemes, and to implement them on parallel machines, using state-of-the-art parallel algorithms.

We propose to develop two different finite element schemes to meet this challenge. The first is a generalization of the standard Galerkin finite element method in which both the fluid and particle equations of motion are incorporated into a *single* variational equation, in which both the fluid and particle velocities appear as primitive unknowns. The hydrodynamic forces and torques on the particles are eliminated in the formulation, so need not be computed as separate quantities. The computation is performed on an unstructured body-fitted grid, and an arbitrary Lagrangian-Eulerian moving mesh technique has been adopted to deal with the motion of the particles. This scheme is discussed further in Section 6.

In the second approach, an *embedding method*, the fluid flow is computed as if the space occupied by the particles were filled with fluid. The no-slip boundary condition on the particle boundaries is enforced as a *constraint* using Lagrange multipliers. This allows a fixed grid to be used, eliminating the need for remeshing, a definite advantage in parallel implementations. This scheme is discussed further in Section 7.

A crucial computational issue to be addressed is the efficient solution of the various algebraic systems which arise in the schemes. These systems can be extremely large for 3-D problems, and their solution can consume up to 95% of the CPU time of the entire simulation. It is therefore imperative to use efficient iterative solution methods, with matrix-free preconditioners, and to implement them on parallel architectures.

We plan to develop a library of parallel numerical algorithms to solve these systems. This parallel library will consist of algorithms for solving nonlinear algebraic equations using variants of Newton's method, preconditioned iterative solvers for sparse symmetric indefinite and nonsymmetric linear systems, and rapid elliptic and Stokes solvers on uniform grids. This library will be used for rapid prototyping of simulation codes for the application problems referred to above. These issues are discussed further in Section 8.

The library will be augmented with a collection of kernels to allow it to be efficiently portable across either the massive parallelism of the Cray T3-D or its successors, or cluster-based parallelism such as that of several interconnected SGI Power-Challenge workstations. Both architectures exhibit two-level parallelism

that is ideally suited for schemes such as the embedding method on a fixed grid.

The codes will also be placed in the public domain, in modules designed to encourage the widest audience of potential users. The number of potential users of public-domain software for workstations is large and continually increasing as workstations get cheaper and more powerful.

The number of potential applications for such codes is extremely large. We propose to use them to address several fundamental issues in the dynamics of solid-liquid flows, and also to study a number of problems of practical engineering interest. In the category of fundamental dynamics, we propose to reveal the local rearrangement mechanisms responsible for the clusters and anisotropic microstructures observed in particulate flows, produce statistical analyses of solid-liquid flows—mean values, fluctuation levels and spectral properties, derive engineering correlations of the kind usually obtained from experiments, and provide clues and closure data for the development of two-phase flow models and a standard against which to judge the performance of such models. These issues are discussed further in Section 3.

Among the industrial applications we propose to address are sedimentation, fluidization, slurry transport of solid particles in Newtonian and viscoelastic fluids and hydraulic fracturing of hydrocarbon reservoirs. These applications are discussed further in Section 4.

All simulation results will be compared with experimental data. The literature contains a large volume of experimental data. The results from simulations of actual industrial processes will be compared with actual field data whenever possible. At the moment, we are thinking of advancing our understanding of the lubricated transport of slurries, the bubbling of fluidized beds and particle placements by proppant in fractured oil reservoirs. The existing data are incomplete; we therefore plan to carry out our own experiments, under the conditions assumed in the simulations. Probably most of the experiments will be carried out in Joseph's lab using funding from other grants. The present idea is to construct equipment with controlled and continuous inputs of particles and fluids to examine slurry transport in pipes in horizontal, tilted and vertical flow.

The comparison of simulations with experiments is essential when the suspending fluid is viscoelastic because the constitutive equation for the fluid used in the experiments is never known exactly; it may be adequate for some flows and not for others. This is to be contrasted with the situation for Newtonian fluids, where a single constitutive equation applies in all the usual situations. It is therefore *extremely* important to develop particle movers for the viscoelastic fluids which are actually used in the fracturing industry and in other applications.

2 Research Teams

2.1 U.S. Research Team

The team we have assembled to meet this Grand Challenge is multidisciplinary. The various individuals shared a common interest in the challenge presented by moving many particles in direct simulation before we even knew about the Grand Challenge Initiative of the National Science Foundation.

Joseph is an engineer specializing in experiments and theory. Hu was Joseph's student; as part of his Ph.D. thesis he developed a finite element package using unstructured grids to simulate the motion of spheres and ellipses in two dimensions under the action of hydrodynamic forces obtained from the Navier-Stokes equations [44, 45]. Many results about particulate flows have been obtained by interrogating simulations based on this package. Recently, Hu [42] has developed a meshing routine for periodic domains and an iterative solver which allows him to move 400 particles in a direct simulation in two dimensions (see Figure 6). Glowinski is a mathematician who specializes in computational mechanics. Glowinski, Joseph, their students, and postdocs [26, 33] are presently in an active collaboration in the computation of hydrodynamic forces on spheres and spheroids in Newtonian and non-Newtonian fluids in three dimensions using the method of embedded domains on a fixed grid on which the no-slip condition at the boundary of the particles is enforced by a Lagrange multiplier method. We plan to develop this method into a high performance software package for moving particles in fluids.

Golub and Sameh are specialists in numerical linear algebra and in state-of-the-art approaches to the development of parallel numerical algorithms. Golub, *et al.* created (see [15]) the embedded domain method which was later developed by Glowinski, *et al.* [32, 33] for solving elliptic problems in conjunction with domain decomposition. Golub and Sameh are also experts on the development of parallel algorithms for the indefinite

linear systems that arise from the generalized Stokes problem, a by-product of the θ decomposition of the Navier-Stokes equation; θ codes were introduced by Glowinski and are being used by students in Joseph's group for direct simulation of particulate flows [41].

The activities of the team will be coordinated in Minneapolis by Joseph and Sameh. Tri-annual meetings are planned in Minneapolis, Stanford and Houston. We plan to communicate frequently on the Internet and transfer codes, results and manuscripts electronically. We also plan to hold regular user workshops with our industrial collaborators (see Section 4.1).

2.2 French Research Team

The U.S. team wants to incorporate methods and ideas recently developed by Pierre Saramito for the numerical simulation of the flow of viscoelastic fluids. In his paper [90] Saramito presents a new and efficient method for computing flows of a viscoelastic fluid based on two independent concepts. First, he does a time-dependent scheme that allows operator splitting and is order two in time. This σ method was introduced by one of our Co-PIs, (Glowinski) but is here used for viscoelastic flows. This method should work well for our particle movers which are time dependent and need high accuracy in time. Saramitos' method combines the incompressible Raviart-Thomas element, the discontinuous Lesaint-Raviart element, and a finite volume element which satisfies mass conservation exactly, and optimizes cost in terms of the total number of degrees of freedom versus mesh size. When applied to the benchmark 4 to 1 contraction problem for an Oldroyd B fluid, Saramitos' package is 5 times faster than the GMRES method which is presently used by us for particle movers.

In a more recent work [89], Saramito computed solutions to 4 to 1 contraction benchmark for values of the Deborah number 10 times larger than ever before. It would be irresponsible for us not to seek such a strong improvement in efficiency in our viscoelastic direct simulations.

The U.S. team would like Saramito to adapt his method to the particle movers we use for viscoelastic fluids using unstructured grids. These codes work well for tests of particles in two-dimensional simulations, but they are rather slow. We believe that Saramito can help us to greatly increase the speed of computation. Saramito, for his part, wants to do direct simulation, and the laboratory of Piau in Grenoble would like to promote this collaboration.

Saramito will work with French students in Grenoble on direct simulation, but they all need instruction in our methods. The purpose of the four visits to Grenoble which we have proposed is to provide the French team with the hands-on instruction they need to make their methods compatible with our codes, to learn how they do their work in their computing environment, and to help bring our separate teams in close personal collaboration.

Part II

Applications

3 Fundamental Dynamics

3.1 Studies of Local Rearrangement Mechanisms

The clusters and anisotropic microstructures observed in solid-liquid flows, such as those shown in Figure 1, are the result of particle migrations produced by particle-particle and particle-wall interactions. These local rearrangement mechanisms mediated by things like hydrodynamic forces at stagnation and separation points, wake interactions, vortex shedding, and turning couples on long bodies [46] (and on pairs of spherical bodies in momentary contact). Direct simulation may be the only theoretical tool available for studying all these nonlinear and geometrically complicated phenomena.

There are striking differences in the observed microstructures between Newtonian and viscoelastic particulate flows, which are not well understood. Results from direct simulations bearing on cooperative effects associated with these microstructures have as yet to be obtained for viscoelastic fluids. Simulations to date

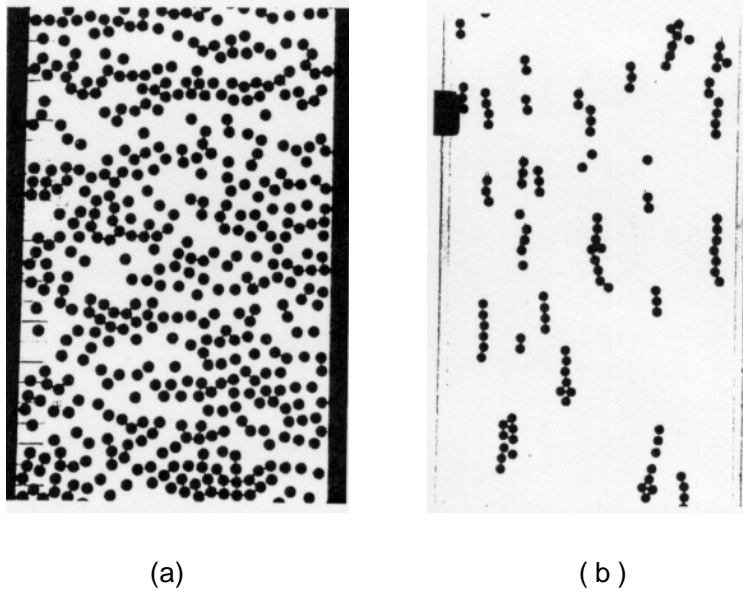


Figure 1: Flow-induced anisotropy of fluidized suspensions: (a) Particles across the stream are induced by drafting, kissing and tumbling in water; (b) Chain of spheres settle in a polyox solution.

using embedded domains [26, 55] indicate that these differences are associated with the sign of the pressure due to normal stresses.

3.1.1 Particle-Particle Interactions

Particle pair interactions are fundamental mechanisms which enter strongly into all practical applications of particulate flows. They are due to inertia and normal stresses and they appear to be maximally different in Newtonian and viscoelastic liquids [58, 57, 55]. The principal interactions between neighboring spheres can be described as *drafting, kissing and tumbling* [27, 56, 52] in Newtonian liquids (Figure 2) and as *drafting, kissing and chaining* [58, 57, 65] in viscoelastic liquids (Figure 1b). The drafting and kissing mechanisms involved are distinctly different, despite appearances.

In Newtonian liquids, when one falling sphere enters the wake of another, it experiences reduced drag, *drafts* downward toward the leading sphere, and *kisses* it. The two kissing spheres momentarily form a single long body aligned parallel to the stream. But the parallel orientation for a falling long body is unstable: hydrodynamic turning couples tend to rotate it to the broadside-on orientation (perpendicular to the stream). The pair of kissing spheres therefore *tumbles* to a side-by-side configuration. Two touching spheres falling side-by-side are pushed apart until a stable separation distance between centers across the stream is established [58]; they then fall together without further lateral migrations (see Figure 3a).

This local rearrangement mechanism implies that globally, the only stable configuration is one in which the most probable orientation between any pair of neighboring spheres is across the stream. The consequence of this microstructural property is a flow-induced anisotropy, which leads ubiquitously to lines of spheres across the stream; these are always in evidence in two-dimensional fluidized beds of finite size spheres, as shown in Figure 1a. Though they are less stable, planes of spheres in three-dimensional beds can also be found [60].

In viscoelastic liquids, on the other hand, two spheres falling side-by-side will be pushed apart if their initial separation exceeds a critical value [80]. However, if their initial separation is small enough, they will attract (“draft”), kiss, turn and chain [58], as shown in Figure 3b. One might say that we get dispersion in the Newtonian liquid and aggregation in the viscoelastic liquid.

This chaining of falling spheres, shown in Figure 1b, is not well understood. It seems to be related to the reversal of pressure due to normal stresses; there is a tension between chained spheres. The exact mechanism

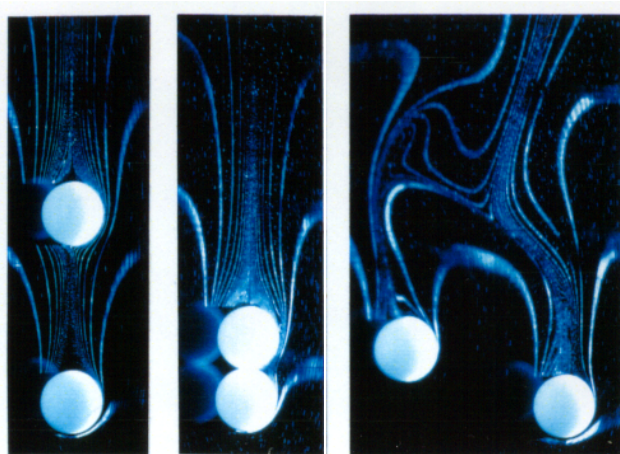


Figure 2: Drafting, kissing and tumbling.

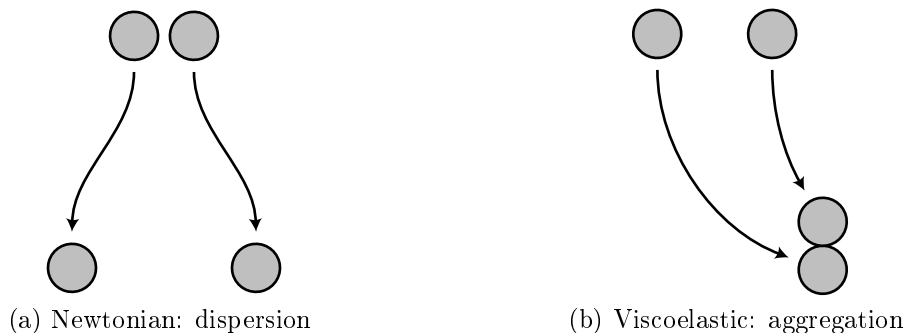


Figure 3: Side-by-side sphere-sphere interactions.

needs to be clarified.

3.1.2 Particle-Wall Interactions

Particle-wall interactions also produce anisotropic microstructures in particulate flows, such as clear zones near walls, and the like. If a sphere is launched near a vertical wall in a Newtonian liquid, it will be pushed away from the wall to an equilibrium distance at which lateral migrations stop (see Figure 4a).

If the same sphere is launched near a vertical wall in a viscoelastic liquid, it will be sucked all the way to the wall (see Figure 4b), and will rotate anomalously as it falls [58] (see Figure 5). This is very strange since the sphere appears to touch the wall where the friction would make it rotate in the other sense [66].

3.2 Statistical Analysis

Statistical analysis of simulations is yet another window in which to view the fundamentals of solid-liquid flows. The time-averaged particle (or bubble) dynamics in a periodic or infinite domain can be described in terms of the number density, velocity current, and force correlations, and their Fourier transforms. The number density correlation gives the relative arrangement and motion of the particles; the velocity current correlation gives the propagation velocities of the dominant modes; and the force correlation gives the form of the forcing term driving the particle system. For a numerical solution, the above distributions can be easily obtained by recording the particles' (or bubbles') coordinates, velocities and forces at regular time intervals [93].



Figure 4: Particle-wall interactions.

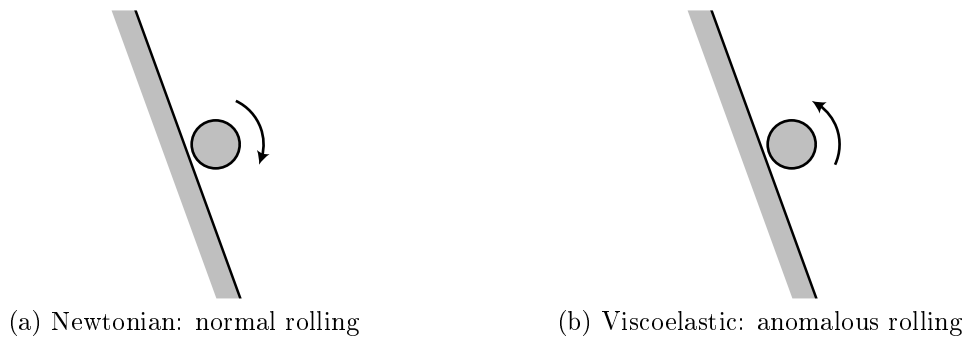


Figure 5: Anomalous rolling of spheres down an inclined plane.

3.3 Empirical Correlations

One of the great engineering opportunities of the present day is the use of direct numerical simulations to construct empirical correlations, of the kind usually generated from experiments. We can hope to construct correlations similar to that of Richardson and Zaki [79] for fluidized suspensions, and to the friction factor vs. Reynolds number correlation for slurries. There are many other possibilities. However, engineering practice would not admit such numerically generated correlations without first verifying that they work in benchmark cases; therefore, experiments *must* be considered.

3.4 Two-Fluid Modeling

In the past, solid-liquid flows were studied using continuum modeling. When done rigorously, using spatial, temporal or ensemble averaging [1, 18, 59, 71, 109, 110, 111], this leads to “two-fluid” models in which one of the two fluids is the solids phase [18, 49, 96]. The equations are formally correct, but the terms of interactions must be modeled, and models which work for one flow may not work for another. Direct simulations can provide clues for modeling the interaction terms and a standard to judge the performance of modeling assumptions.

4 Industrial Problems

Particulate flows of solids in fluids are widely used for different purposes in different industries. The practical applications often involve more than the hydrodynamics of particle laden flows; heat transfer, chemical reactions, gas-liquid-solid flows, phase changes and other complications must be addressed in practical ap-

plications. Particle movers in direct simulations open the door to a much more realistic treatment of these complicating features than the multiphase flow modeling which was used in the past.

Among the practical applications without complicating features, many are suitable for direct simulation; sedimenting and fluidized suspensions, lubricated transport and hydraulic fracturing of hydrocarbon reservoirs span this field and present grand challenges for particle movers.

4.1 Industrial Collaborators

We have formed an industrial collaborators group to help us focus our research on relevant problems. At present, we have obtained moral support and cash commitments from Schlumberger-Cambridge and Dowell-Schlumberger (Tulsa), from Shell in Houston, and from Intevep, S. A. (see Part V for cost sharing details and Section I of the overall proposal for letters of support.) We plan to hold regular workshops with our collaborators and to enter into actual collaborations in both simulations and experiments.

4.2 Sedimentation Columns and Fluidized Beds

In sedimentation columns and fluidized beds, the fluidized particles are held up by a stream of air or liquid under a balance of weight and drag [1, 52, 79, 81, 93]. The benefits which accrue to fluidizations are that both the transport of heat and the promotion of chemical reactions can be greatly enhanced by bringing over fresh fluid to the particles; this is an excellent way to dry grains, to coat particulates or promote the combustion of coal. The use of catalyst particles in a fluidized bed to promote the conversion of light crudes to gasoline (catalyst cracking) is a multi-billion dollar technology at the foundation of the refining business.

Fluidized beds may bubble, offsetting the advantages of mixing by substantial bypass of particle contact by the fluid. Introducing spouts can improve the mixing, and draft tubes can improve the stability helping to avoid bubble formation. A detailed understanding of the fluid dynamics of bubbling with a potential for evaluating the continuum approaches taken in the past can be achieved by particle movers in direct simulation [42, 92]. It may be hopeless to analyze spouted beds with a draft tube in any way other than direct simulation.

4.3 Lubricated Transport

Lubricated transport of viscous materials is another application area with grand challenges. Nature's gift is that lubricated flows are stable; the low viscosity constituent migrates to the walls, where the shearing is greatest [51, 60, 54]. This effect produces a lubricated flow, greatly reducing the cost of transport. The tendency for solid-liquid mixtures in pipes to segregate into solid-rich core regions surrounded by solid-poor liquid regions near the pipe wall gives rise to lubrication; coal slurries in water are one example. The problem here is to determine the nature of forces which push particles away from the wall and to examine the different ways in which the holdup of the solids may develop. Flow charts depending on the liquid and solid input are unknown, even from experiments, but are required for understanding when and how to exploit the tendency to lubricate.

Lubricated transport of viscous materials will be the topic of an IUTAM symposium to be held in Trinidad and Tobago in January 1997. The symposium is being organized by D. Joseph and Harold Ramkissoon. Water lubricated transport of heavy crudes is perhaps the most studied [51, 60, 74] and best developed of applications of lubricated transport to technology.

4.4 Hydraulic Fracturing

A third rich area of application of solid-liquid flow in which the fluids rheology plays a crucial role is the fracturing industry [72]. Hydraulic fracturing is a process often used to increase the productivity of a hydrocarbon well. A slurry of sand in a highly viscous, usually elastic, fluid is pumped into the well to be stimulated, at sufficient pressure to exceed the horizontal stresses in the rock at reservoir depth. This opens a vertical fracture, some hundreds of feet long, tens of feet high, and perhaps an inch in width, penetrating from the well bore far into the pay zone. When the pumping pressure is removed, the sand acts to prop the fracture open. Productivity is enhanced because the sand-filled fracture offers a higher-conductivity path for fluids to enter the well than through the bulk reservoir rock, and because the area of contact for flow out

from the productive formation is increased. It follows that a successful stimulation job requires that there be a continuous sand-filled path from great distances in the reservoir to the well, and that the sand is placed within productive, rather than non-productive, formations.

It has been suspected for some time [72], and experiments have demonstrated [61, 97], that the suspended sand does not remain uniformly distributed during pumping of these slurries. It is found that under the flow conditions expected within the fracture during pumping, the sand particles migrate rapidly towards the center plane of the fracture, leaving a clear fluid layer at the fracture walls. This clear layer lubricates the motion of the slurry, and so increases the rate of gravity driven, settling and density currents. The net result of these processes is to cause sand to accumulate at the bottom of the fracture and good vertical filling to be lost [102]. This in turn reduces well productivity, and can also interfere with the fracture growth process by blocking downward extension.

It is sometimes suggested that migration of sand occurs while the slurry is being pumped down the tubing to reservoir depth. This may cause preferential injection of solids-rich fluid at the bottom of the reservoir and of solids-poor fluid at the top. While it is not known if this process actually occurs, if it did, the consequences to final fracture productivity would be similar to those described above.

The phenomenon of proppant migration is not currently controlled or exploited in the fracturing industry. One reason for this is that the relationship between migration and fluid properties is not understood (there is some indication from experiments [61, 97] and single particle theories [57, 64], that the combination of fluid elasticity and non-uniform shear flow are necessary for rapid migration). It is therefore not possible confidently to design fluids which, for example, suppress migration.

The results of a careful theoretical and experimental investigation of the phenomenon of migration during flow of moderately-concentrated suspensions of heavy particles in viscoelastic fluids, in particular the identification of the fluid properties and flow conditions responsible for migration, and of those which can be controlled to suppress it, would benefit the hydrocarbon industry by permitting the development of more effective fracturing fluid systems.

Proppant settling in fracturing fluids is also a problem area in fracturing technology. The settling of particles within the fracture after pumping has stopped, but before the fracture closes, also impacts final fracture productivity; loosely speaking, the more settling, the more non-uniform the coverage of the productive formation and the lower the productivity. Settling rates are influenced in a poorly understood way by suspending fluid viscoelasticity.

The current trend in the industry is towards the use of fracturing fluids with lower concentrations of polymer; this brings cost savings and productivity and environmental benefits through the use of less material. However, there is a lower limit on polymer concentrations set, among other factors, by the need to ensure good particle carrying and suspending properties. A better understanding of the fluid properties controlling static settling of solids in viscoelastic fluids could permit further reductions in polymer concentration to be achieved.

Part III

Computational Methods

Two separate lines of code development have been pursued by the principal investigators to date, a generalized ALE Galerkin finite element method and an embedding method. Both approaches have been initiated by us, for quite different kinds of applications. At present, one scheme does not fit all applications. Perhaps ultimately, a “best” universal scheme for moving particles may evolve, but it is not presently prudent to make a bet.

An important issue to be addressed in developing the computational schemes is the modeling of particle-particle and particle-wall collisions, with proper account taken of the frictional forces between the particles (or between a particle and the wall) at the moment of contact. This is an open problem.

In experiments, particles are observed to touch one another and the retaining walls. In slow flows, the contact is usually gentle, so rebound and friction are probably not important. In faster flows, however, collisions are much more vigorous, so it is imperative to develop a satisfactory theoretical and computational model for them. There is no solution to this fundamental problem in the literature. The best current codes

refine the mesh as the particles approach, but this can only be carried so far. These codes do seem to reproduce the local dynamics correctly, even though collisions are not well represented.

A crucial computational issue to be addressed is the efficient solution of the various algebraic systems which arise in the schemes. These systems can be extremely large for 3-D problems, and their solution can consume up to 95% of the CPU time of the entire simulation. It is therefore imperative to use efficient iterative solution methods, with matrix-free preconditioners, and to implement them on parallel architectures.

5 Existing Literature

Recent computational approaches to solid-liquid flows, possibly inspired by molecular dynamics, are cellular automata [63, 107] and the lattice Boltzmann method [63, 62, 70, 112]. These models can handle huge numbers of particles. However, they replace the equations of motion with computer rules and do not deal with stagnation and separation points, wakes, turning couples, drafting, kissing and tumbling, etc. The interesting results produced by these methods are not yet sufficiently reliable to be used in engineering practice.

It is possible to simplify the flow description considerably by ignoring viscous effects completely (inviscid, potential flow) or by ignoring inertia completely (Stokes flow). Potential flow simulations do lead to cross-stream arrays [87, 88, 94], but the wakes needed for the drafting part of the fundamental rearrangement mechanism in a fluidized suspension are absent.

Brady, *et al.* [10, 9] have created good techniques for dealing with the motion of many particles in Stokes flow. These simulations are appropriate for colloids at very small Reynolds number and they appear to successfully capture the hydrodynamic interactions. On the other hand, the inertial mechanisms which turn long bodies broadside on and control the lateral migration of particles do not exist in Stokes flow.

Direct simulations of many particles at finite Reynolds numbers have only just begun. Unverdi and Tryggvason [101, 100] introduced a front tracking/finite difference method for computing the unsteady motion of drops and bubbles. In their work, the drop surface is tracked by separate computational points that are moved on a fixed grid by interpolating their velocity from the grid. These points form a front that is used to keep the density and viscosity stratification sharp and to calculate surface tension forces. Esmaili (and Tryggvason) [21] have computed the rise of 16 bubbles in three dimensions and 144 and 324 two-dimensional bubbles in a doubly periodic domain at a Reynolds number near 2. These simulations have not been adapted to solid particles and rigid walls, but they do give rise to drafting, kissing and tumbling as in the case of sedimenting solid spheres.

Johnson [50] (and Tezduyar) did a three-dimensional simulation using a space-time finite element method advocated by Hughes [48] and Tezduyar, *et al.* [6, 98] of the sedimentation of five solid spheres in a tube at a Reynolds number of 100. Their simulation gives rise to drafting, kissing and tumbling into a plane perpendicular to the fall.

The Minnesota group has done direct simulations of initial value problems for the two-dimensional motion of circular and elliptical particles in sedimenting, Couette and Poiseuille flows of a Newtonian fluid at particle Reynolds numbers in the hundreds [22, 23, 24, 26, 25, 44, 43, 46, 53]. Recently, Hu has simulated the motion of 400 circular particles in sedimenting and shear flows at particle Reynolds numbers in the hundreds [42] (see Figure 6). The first direct simulation of the initial value problem for the two-dimensional motion of circular and elliptical particles settling in a viscoelastic fluid (Oldroyd B) has recently been done by the Minnesota group.

6 Generalized ALE Galerkin Finite Element Method

A generalized Galerkin finite element scheme which incorporates both the fluid and particle equations of motion into a *single* coupled variational equation has been developed by Joseph's group and Hu in [41, 42] for Newtonian fluids in 2-D and 3-D domains. The formulation can be easily extended to viscoelastic fluids. The hydrodynamic forces and torques acting on the particles are eliminated in deriving the combined variational equation, so need not be computed explicitly.

An arbitrary Lagrangian-Eulerian (ALE) moving mesh technique has been adopted to deal with the motion of the particles (see, for example, [40, 47, 73]). In our implementation, the nodes on the particle

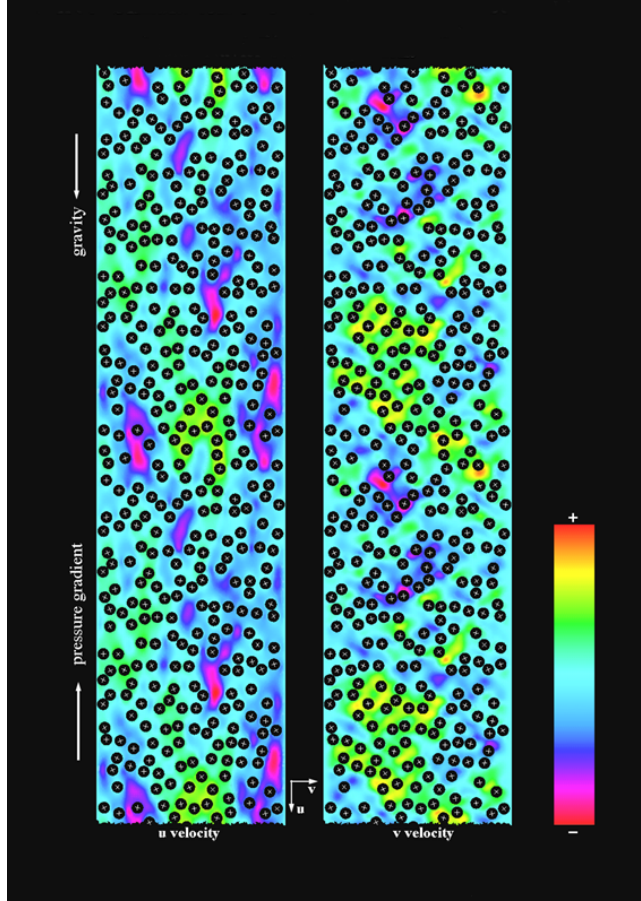


Figure 6: Direct simulation (after Hu [42]) of 400 particles in a periodic flow of a Newtonian fluid in a channel (30% solids fraction): the pressure gradient pushes the flow up against gravity; the x component u of the velocity is color coded on the left and the y component v on the right. The particles-across-the-stream alignment (see Figure 1a) is evident.

surface are assumed to move with the particle. The nodes in the interior of the fluid are computed using Laplace’s equation, to guarantee a smoothly varying distribution of nodes. At each time step, the grid is updated according to the motion of the particles and checked for element degeneration. If unacceptable element distortion is detected, a new finite element grid is generated and the flow fields are projected from the old grid to the new grid.

Initially, the particles are positioned randomly in the fluid, with zero velocity. The fluid is either at rest or flowing steadily around the particles. The particles are then released and the motion of the combined fluid/particle system is computed using the procedure described in [44, 42]. In this scheme, the positions of the particles and grid nodes are updated explicitly, while the velocities of the fluid and the solid particles are determined implicitly.

This generalized ALE Galerkin finite element formulation gives rise to a set of nonlinear algebraic equations which is solved via a quasi-Newton scheme; the resulting linear system is shown in (2). For 3-D domains with large numbers of particles, these systems will be *extremely* large, requiring iterative solvers and matrix-free preconditioning strategies. This issue is further discussed in Section 8.

Extending this approach to 3-D domains will also require a robust 3-D mesh generator and an associated projection scheme for moving the mesh. We plan to develop a parallel automatic grid generator based on the GHS-3D generator developed at INRIA, France (see [30, 29]). In work to date, it is assumed that the particles do not collide, but that there is always a thin layer of fluid between approaching particles, and between particles and retaining walls. The grid generator must therefore possess a local refinement capability

to handle grid in these thin layers, which is essential to correctly model the “particle collision” process.

Finally, in computing flows with large numbers of particles, it is often desirable to use periodic boundary conditions in one or more directions because it is a perfectly absorbing boundary condition, because particles near a periodic boundary can interact with particles near the opposite periodic boundary rather than with a solid wall, so that the same local physics applies uniformly to all particles, and because no mathematical approximation is involved.

At the periodic boundaries particles frequently leave the computational domain and enter at the opposite periodic boundary. We will design the grid generator to handle any number of pairs of periodic boundaries without introducing artificial cuts.

The above approach will be further extended to viscoelastic fluids. In this case, the constitutive equation relating the stress to the strain rate is more complicated. Various constitutive models (with Oldroyd B principal parts) will be considered, including those in which the viscosity function and the relaxation time may depend on the shear rate. While the general plan of the computational scheme will be essentially identical to that for Newtonian fluids, the computation of the fluid flow will need special attention. In particular, we will need very effective linear and nonlinear system solvers, because the problem will become dramatically larger (due to the larger number of flow variables) and more ill-conditioned (due the strong coupling of the velocity, pressure and stress fields), and because of the existence of thin stress boundary layers.

Over the last ten years, several numerical schemes have been developed for handling viscoelastic flows in simple two-dimensional geometries (see for example [2, 7, 17, 69, 77]). To prevent numerical instability due to convection dominance in the constitutive equations, we plan to develop an elastic-viscous split stress Galerkin least-squares (EVSS-GLS) finite element formulation [48]. In the GLS formulation, grid-dependent terms are added to the standard Galerkin equations. These terms are functions of the residuals of the governing equations evaluated element-wise, and are designed to enhance the stability of the Galerkin method without degrading its consistency and accuracy. The GLS formulation has yet to be applied to simulation of viscoelastic flows.

7 Embedding Methods

We also propose to investigate the simulation of particle motions using a class of methods based on the principle of *embedded* or *fictitious* domains. There are several ways to design high-performance particle movers by generalizing the application of this principle to the problem of fluid flow around fixed obstacles. Though particle movers based on embedding methods have yet to be developed, they appear to be natural and show great promise for development into very fast high-performance particle movers. Ultimately, embedding methods may be even more powerful than methods based on efficient remeshing of unstructured grids.

Embedding methods, or fictitious domain methods were introduced by Golub, *et al.* in [15], and developed by Glowinski, *et al.* in [26, 32, 33]. The idea is to embed an irregular computational domain into a larger, simpler domain, and to specify simple boundary conditions on its boundary. Thus, since the larger domain admits a *uniform* grid, we can use fast elliptic and fast Stokes solvers when applying these methods to the time-dependent Navier-Stokes problem, for example. Fictitious domain methods have been applied to linear and nonlinear 2-D and 3-D elliptic and parabolic problems [32], to the 2-D Navier-Stokes problem [33], and to the 3-D Navier-Stokes problem [26]. It is also suitable for flow-related shape optimization problems.

To apply the fictitious domain approach to the problem of fluid flow around fixed obstacles, we may take, for the larger simpler domain, the fluid domain *plus the interiors of the obstacles*. That is, the fluid flow is computed *as if the obstacles were filled with fluid*. The no-slip boundary condition on the obstacle boundaries is enforced as a *constraint equation* using well chosen source terms which are either associated with singularities distributed on the obstacle boundaries (as in [26, 32, 33, 34, 75]), or with body forces distributed inside the obstacles (as in [8]). In the approach developed in [32, 33, 34], the unknown distributions of singularities are *Lagrange multipliers* associated with the boundary conditions on the obstacle boundaries. It is therefore natural to apply powerful variational principles to both the spatial discretization by finite elements and to iterative solution methods.

Recent results (see [31]) show that fictitious domain methods can be successfully applied to the Navier-Stokes flow around *moving* obstacles (i.e., particles) when the motion of these obstacles is *prescribed in advance* (oscillating airfoil in a channel).

In [15], the interface between the actual and simpler domains was consistent with the same mesh used for both domains. In more recent publications [32, 33, 34], it was shown that this consistency is unnecessary. In particular, it was shown that if the actual boundary conditions on the interface are enforced using Lagrange multipliers, it is important to have the discrete multiplier space be associated with the intrinsic geometry of the original (irregular) domain and not with the mesh of the larger simpler domain. This may be somewhat complicated to implement on parallel architectures, but once done, the scheme can easily be applied to problems with moving boundaries, such as the surfaces of moving particles.

Fictitious domain methods can accommodate *fixed* grids—indeed, *uniform* fixed grids—a definite advantage in dealing with moving obstacles, despite the advances achieved with moving grids, since we can use fast elliptic and fast Stokes solvers when applying such methods to the time-dependent Navier-Stokes problem. Based on boundary layer thickness considerations and on the large number of particles assumed to fill the flow domain, we can expect that a fine uniform grid will need to be used at large Reynolds numbers.

In order to apply fictitious domain methods to the problem of simulating the flow of a fluid with *free* particles (i.e., obstacles with *unprescribed* motion), the hydrodynamic forces and torques exerted by the fluid on the particles must be accurately evaluated. Once this has been accomplished, solving the coupled equations of fluid and particle motion will be fairly easy through approximate time stepping methods using, for example, operator splitting techniques, such as the θ -scheme introduced in [14].

The θ -scheme is a particularly good time stepping method. In fact, recent evaluations and comparisons done at the University of Heidelberg under the supervision of R. Rannacher (one of the leading world experts on the approximation of the unsteady Navier-Stokes equations) show that the Glowinski θ -scheme offers the best compromise for accuracy, stability, robustness and ease of implementation; see [99]. The θ -scheme is well suited to fictitious domain methods, as shown in [33, 31]. It is also well suited to the simulation of viscoelastic flow, which is one of our main objectives (see [14]). Research team members have been using the θ -scheme extensively in both Houston and Minneapolis.

Coupling the θ -scheme for the flow simulation to the time-discretization scheme for the equations of particle motion will be easy once the hydrodynamic forces and the contact forces between particles are known.

The major computational task in fictitious domain methods, coupled with operator splitting, is the solution of symmetric indefinite systems of the form

$$\begin{pmatrix} A & B \\ B^T & 0 \end{pmatrix} \begin{pmatrix} u \\ p \end{pmatrix} = \begin{pmatrix} f \\ g \end{pmatrix} \quad (1)$$

in each time step. Here, both A and B are sparse matrices with A being symmetric positive definite and B of maximal column rank. Iterative schemes for solving such indefinite systems will be discussed in Section 8.

8 Linear System Solvers

Both of the proposed computational schemes require the solution of large systems of linear and nonlinear algebraic equations. For 3-D simulations involving a large number of particles, these systems can be *extremely* large—perhaps $n \times n$, where $n \sim 10^6$. In simulations conducted by research team members, up to 95% of the computational time of the entire simulation is consumed by the linear system solver alone.

In both the generalized ALE Galerkin scheme and the embedding scheme, we must solve large sparse linear systems for which direct methods based on Gaussian elimination are too expensive in terms of both time and storage cost. For this class of problems, iterative methods must be used, possibly in conjunction with direct methods when we consider preconditioning strategies. Important building blocks in the library of parallel system solvers to be developed for this project are preconditioned iterative schemes for solving indefinite linear systems of the form (1).

Such systems may be solved using a variety of iterative schemes (see, for example, [4, 5, 11, 19, 20, 28, 67, 68, 78, 91, 106, 108]). Of particular interest is the family of the Uzawa schemes and their variations [3, 36, 76]. Also, for the case of nonsymmetric matrices A , one may resort to Krylov subspace methods such as GMRES [83, 82, 104, 105], CGS and variations [95, 103], among others. The main drawback of those nonsymmetric iterative solvers is lack of robustness without effective preconditioners. Developing effective preconditioners that are also suitable for parallel computers will be one important focus of this research. Row projection

schemes, accelerated via the conjugate gradient algorithm, provide a robust alternative to Krylov subspace methods [12, 13]. More work needs to be done to increase the rate of convergence, however.

In the embedding scheme, outlined above, using the θ -method together with a uniform grid results in matrices A that are both structured and symmetric positive definite. In such a case, an important part of the library will be the rapid elliptic solvers developed mainly by Golub in [16], as well as [84, 85], in addition to the parallel conjugate gradient algorithm with a variety of preconditioners [39]. For the ALE Galerkin formulation, however, the matrix A is nonsymmetric. Specifically, the linear systems that need to be solved in this case are of the form

$$\begin{pmatrix} A & B & C \\ B^T & 0 & 0 \\ D & E & G \end{pmatrix} \begin{pmatrix} u \\ p \\ U \end{pmatrix} = \begin{pmatrix} f \\ g \\ h \end{pmatrix} \quad (2)$$

in which C , D , E and G are sparse matrices with G being symmetric positive definite, u and p represent the velocity and pressure of the fluid, and U represents the velocities of the particles.

We plan to develop tools for rapid prototyping of parallel preconditioned solvers for both types of systems. Since the size of such linear systems can be extremely large when handling 3-D problems (n is of order 10^6), we propose to study preconditioners that do not require explicit storage of coefficient matrices. In other words, we need to find preconditioners that do not depend on obtaining approximate factorization of the systems involved. Moreover, we will develop iterative solvers which share the property of direct solvers in the sense that once they are used for solving either (1) or (2) with one right-hand side then they can be used at a much less cost for another right-hand side, assuming of course that the matrix of coefficients does not change, or changes slowly, from one time step to another.

Another motivation for considering multiple right-hand sides is efficiency in conducting parametric studies.

8.1 Preconditioners

One approach to preconditioning without using approximate factorization of the linear system under consideration, is the use of an inner iterative process to affect the preconditioning step. For reasons of efficiency, this is only done approximately. The question then arises as to how the accuracy of the inner iteration affects the convergence of the outer iteration. For Chebyshev outer iterations, this question has been studied in detail by Golub and his collaborators [37]. Using a conjugate gradient-type method as the outer iteration in combination with an inner iteration method remains an open problem.

At each step of the conjugate gradient method, for example, it is necessary to solve a system of the form

$$Mz = r,$$

where M is the preconditioner and r is the residual. The matrix M is often suggested by the application at hand—e.g., domain decomposition. Or if A is real positive, it may be desirable to choose $M = (A + A^T)/2$. In any event it is not possible to solve for z exactly. Instead, we solve the system

$$Mz = r + q,$$

in which q is the residual vector for the inner iteration. We generally iterate until $\|q\| < \tau\|r\|$. This seems like a good rule since we expect $\|r\|$ to be approaching zero.

The convergence theory for the conjugate gradient method (CG) as well as GMRES heavily depends upon orthogonality of various vectors. When this is violated, there is no proof of convergence. We have tried many examples and we have noted there is a barrier for τ such that if τ exceeds some value the CG method stalls or diverges. We have observed that for τ sufficiently small, the method will converge. We need to investigate this situation analytically. This is an unsolved problem whose solution will have great impact in the use of the CG method.

A related inner iteration scheme is one in which the outer iteration provides information about the eigenvectors of the troublesome eigenvalues while the inner iteration solves the projected linear system in which the projector deflates those eigenvalues. These projectors become more effective as the outer iterations proceed.

In a recent paper [38], we have considered the solution of the system (1), in which A is real positive, using as preconditioner the symmetric indefinite matrix

$$\begin{pmatrix} D & B \\ B^T & 0 \end{pmatrix}$$

in which the matrix D is real, symmetric and positive definite. In other words, one can use an iterative Stokes solver to precondition the Navier-Stokes equations.

Finally, another approach for matrix-free preconditioning is via Newton's iteration for obtaining the inverse of a matrix. Choosing an initial approximation for the inverse that commutes with the matrix in question leads to a recursive function for the successive approximation of the solution vector. This approach is still in the experimental stage, and further investigation is needed to explore its numerical stability and suitability for parallelism [86].

8.2 Multiple Right-Hand Sides

The efficient handling of multiple right-hand sides proves to be a challenge to most iterative methods because one of their main advantages is that not much information needs to be stored and therefore very little information is saved from the solution of one system which can be reused for the solution of subsequent systems.

Consider the situation where we have two right-hand sides b and c . Our goal is to solve the second system $Ax = c$ using information gathered from the first system $Ax = b$. Here we consider the case where A is an $n \times n$ symmetric matrix but the basic ideas apply to more general situations. Consider using the Lanczos method for solving the linear systems since it is well known that the conjugate gradient method is mathematically equivalent to the Lanczos method. Our idea is easier to express in the Lanczos framework, but we expect to be able to derive a conjugate gradient and GMRES version as well.

In applying the Lanczos method to the first system, we generate a $k \times k$ tridiagonal matrix $T = Q^T A Q$, where Q is an orthonormal matrix of $k \ll n$ columns. If we assume, without loss of generality, that the initial guess is $x = 0$, then the first column of Q is $q_1 = b/\|b\|$. The question now is: how do we generate the factorization of A corresponding to c , with $q_2 = c/\|c\|$, without computing further matrix-vector products? This question has been addressed successfully and the resulting algorithm is still in the early stage of development [35], and will be explored further in this proposed study and extended to other iterative schemes for nonsymmetric systems.

Part IV

Concluding Statement

The goal of this grand challenge proposal is to make a massive advance in the study of fluid-solid flows by direct simulations of the underlying equations of motion of the fluid and solid without approximation. We propose to move a hundred or more particles in direct simulations by developing the most efficient numerical algorithms at the edge of what is currently possible. We hope to provide useful software in the public domain as a tool to do the science and engineering associated with the widest possible variety of applications of particulate flows; slurry transport, hydraulic fracturing and fluidized beds are examples we shall treat. Many of the important applications require that we develop particle movers for viscoelastic as well as Newtonian fluids.

The codes are meant to be used for understanding the role of particle interactions in determining the gross properties, the particle distribution and velocity, and the anisotropic structures which develop in particulate flow. The marked differences in the flow properties of particles in Newtonian and viscoelastic fluids are important in many applications but are not yet well enough understood. We intend to develop algorithms to produce mean and fluctuation levels, power spectra, probability and other statistical measures for particulate flow.

Another goal of direct simulation is to aid in the closure of two-phase flow models and to provide a standard to judge the performance of such models. We will also derive engineering correlations from our

simulations; for example, formulas relating the average superficial velocity to the average solids fraction in a fluidized suspension and the mass flow vs. pressure gradient for slurries. We recognize that there are important applications of particulates in turbulent flow which we cannot address in this challenge. Even without turbulence, there are practically an unlimited number of results which could be obtained from intelligent interrogation of direct simulations.

The process of building efficient codes using state-of-the-art parallel algorithms, and the applications of the simulations to real scientific and technological problems should have a profound effect on the education and career direction of all students involved in the work. Even more, our efforts in this direction should create a computing environment and culture at several institutions which will impact many students beyond the group directly involved. All in all, we believe that the activities involved in this grand challenge will have a significant effect on the future education of students in computing and in the applications of computing.

To accomplish our goals, we have formed a multidisciplinary group of qualified professionals with different skills relevant to the multifaceted nature of the grand challenge goals. It is our hope that this group can develop the synergism necessary to produce excellent collective works well beyond what we might hope to produce as separate individuals.

Part V
Results from Prior NSF Support

D Bibliography

- [1] T. B. Anderson and R. Jackson. A Fluid Mechanical Description of Fluidized Beds, *Ind. Eng. Chem. Fund.* **6**, 52–58 (1964).
- [2] M. R. Apelian, R. C. Armstrong, and R. A. Brown. Impact of the Constitutive Equation and Singularity on the Calculation of Stick-Slip Flow: The Modified Upper-Convected Maxwell Model (MUCM), *J. Non-Newt. Fluid Mech.* **27**, 299–321 (1988).
- [3] K. J. Arrow, L. Hurwicz, and H. Uzawa. *Studies in Linear and Non-Linear Programming*, Stanford University Press (1958).
- [4] O. Axelsson. Preconditioning of Indefinite Problems by Regularization, *SIAM J. Num. Anal.* **16**, 58–69 (1979).
- [5] R. Bank, B. Welfert, and H. Yserentant. A Class of Iterative Methods for Solving Saddle Point Problems, *Numer. Math.* **56**, 645–666 (1990).
- [6] M. Behr and T. E. Tezduyar. Finite Element Solution Strategies for Large-Scale Flow Simulations, *Comp. Meth. Appl. Mech. Eng.* **112**, 3–24 (1994).
- [7] A. N. Beris, R. C. Armstrong, and R. A. Brown. Spectral/Finite-Element Calculations of the Flow of a Maxwell Fluid between Eccentric Rotating Cylinders, *J. Non-Newt. Fluid Mech.* **22**, 129–167 (1987).
- [8] F. Bertrand, P. A. Tanguy, and F. Thibault. A New Finite Element Method for Viscous Flow Problems in Enclosures Containing Moving Parts, SIAM Annual Meeting, San Diego (1994).
- [9] J. F. Brady. Stokesian Dynamics Simulation of Particulate Flows, in *Particulate Two-Phase Flow*, (M. C. Roco, ed.), pp. 912–950. Butterworth-Heinemann (1993).
- [10] J. F. Brady and G. Bossis. Stokesian Dynamics, *Ann. Rev. Fluid Mech.* **20**, 111–157 (1988).
- [11] J. Bramble and J. Pasciak. A Preconditioning Technique for Indefinite Systems Resulting from Mixed Approximations of Elliptic Problems, *Math. Comp.* **50**, 1–17 (1988).
- [12] R. Bramley and A. H. Sameh. Domain Decomposition for Parallel Row Projection Algorithms, *Appl. Num. Math.* **8**, 303–315 (1991).
- [13] R. Bramley and A. H. Sameh. Row Projection Methods for Large Nonsymmetric Linear Systems, *SIAM J. Sci. Stat. Comp.* **13**, 168–193 (1992).
- [14] M. O. Bristeau, R. Glowinski, and J. Periaux. Numerical Methods for the Navier-Stokes Equations, *Comp. Phys. Rep.* **6**, 73–187 (1987).
- [15] B. L. Buzbee, F. W. Dorr, J. A. George, and G. H. Golub. The Direct Solution of the Discrete Poisson Equation on Irregular Regions, *SIAM J. Num. Anal.* **8**, 722–736 (1971).
- [16] B. L. Buzbee, G. H. Golub, and C. W. Nielson. On Direct Methods for Solving Poisson’s Equation, *SIAM J. Num. Anal.* **7**, 627–656 (1970).
- [17] F. Debae, V. Legat, and M. J. Crochet. Practical Evaluation of Four Mixed Finite Element Methods for Viscoelastic Flow, *J. Rheol.* **38**, 421–442 (1994).
- [18] D. A. Drew. Mathematical Modeling of Two-Phase Flow, *Ann. Rev. Fluid Mech.* **15**, 261–291 (1983).
- [19] N. Dyn and W. Ferguson. The Numerical Solution of Equality-Constrained Quadratic Programming Problems, *Math. Comp.* **41**, 165–170 (1983).

- [20] H. Elman and D. Silvester. Fast Nonsymmetric Iterations and Preconditioning for Navier-Stokes Equations, *CS-TR 3283* and *UIACS-TR 94-66*, University of Maryland (1994).
- [21] A. Esmaeeli. *Numerical Simulations of Bubbly Flows*. PhD thesis, University of Michigan. Advisor: G. Tryggvason (1995).
- [22] J. Feng, H. H. Hu, and D. D. Joseph. Direct Simulation of Initial Value Problems for the Motion of Solid Bodies in a Newtonian Fluid. Part 1: Sedimentation, *J. Fluid Mech.* **261**, 95–134 (1994).
- [23] J. Feng, H. H. Hu, and D. D. Joseph. Direct Simulation of Initial Value Problems for the Motion of Solid Bodies in a Newtonian Fluid. Part 2: Couette and Poiseuille Flows, *J. Fluid Mech.* **277**, 271–301 (1994).
- [24] J. Feng, P. Y. Huang, and D. D. Joseph. Dynamic Simulation of the Motion of Capsules in Pipelines, *J. Fluid Mech.* **282**, 233–245 (1995).
- [25] J. Feng and D. D. Joseph. The Unsteady Motion of Solid Particles in Creeping Flows, submitted to *J. Fluid Mech.* (1995).
- [26] J. Feng, D. D. Joseph, R. Glowinski, and T.-W. Pan. A Three-Dimensional Computation of the Force and Moment on an Ellipsoid Settling Slowly through a Viscoelastic Fluid, *J. Fluid Mech.* **283**, 1–16 (1995).
- [27] A. Fortes, D. D. Joseph, and T. S. Lundgren. Nonlinear Mechanics of Fluidization of Beds of Spherical Particles, *J. Fluid Mech.* **177**, 467–483 (1987).
- [28] M. Fortin and R. Glowinski. Augmented Lagrangian Methods: Applications to the Numerical Solution of Boundary-Value Problems, North-Holland (1983).
- [29] P. L. George. Automatic Mesh Generation: Application to Finite Element Methods, John Wiley and Sons (1991).
- [30] P. L. George, F. Hecht, and E. Saltel. Automatic Mesh Generator with Specified Boundary, *Comp. Meth. Appl. Mech. Eng.* **92**, 269–288 (1991).
- [31] R. Glowinski, A. J. Kearsley, T.-W. Pan, and J. Periaux. Fictitious Domain Method for Viscous Flow Simulation, to appear in *CFD Rev.* (1995).
- [32] R. Glowinski, T.-W. Pan, and J. Periaux. A Fictitious Domain Method for Dirichlet Problems and Applications, *Comp. Meth. Appl. Mech. Eng.* **111**, 283–303 (1994).
- [33] R. Glowinski, T.-W. Pan, and J. Periaux. A Fictitious Domain Method for External Incompressible Viscous Flow Modeled by Navier-Stokes Equations, *Comp. Meth. Appl. Mech. Eng.* **112**, 133–148 (1994).
- [34] R. Glowinski, T.-W. Pan, and J. Periaux. Fictitious Domain/Domain Decomposition Methods for Partial Differential Equations, to appear in *Japan J. Ind. Appl. Math.* (1995).
- [35] G. H. Golub. Iterative Schemes for Multiple Right Hand Sides, in preparation (1995).
- [36] G. H. Golub and H. Elman. Inexact and Preconditioned Uzawa Algorithms for Saddle Point Problems, *SIAM J. Num. Anal.* **31**, 1645–1661 (1994).
- [37] G. H. Golub and M. Overton. The Convergence of Inexact Chebyshev and Richardson Iterative Methods for Solving Linear Systems, *Numer. Math.* **53**, 571–593 (1988).
- [38] G. H. Golub and A. Wathen. An Iteration for Indefinite Systems and Its Application to the Navier-Stokes Equations, to appear (1995).
- [39] A. Gupta, V. Kumar, and A. H. Sameh. Performance and Scalability of Preconditioned Conjugate Gradient Methods on Parallel Computers, *IEEE Trans. Parallel Distrib. Syst.* **6**, 455–469 (1995).

- [40] P. Hansbo. The Characteristic Streamline Diffusion Method for the Time-Dependent Incompressible Navier-Stokes Equations, *Comp. Meth. Appl. Mech. Eng.* **99**, 171–186 (1992).
- [41] T. I. Hesla, P. Singh, and D. D. Joseph. The Dynamical Simulation of Two-Dimensional Fluid/Particle Systems, in preparation (1995).
- [42] H. H. Hu. Direct Simulation of Flow of Fluid-Solid Mixtures, to appear in *Int. J. Multiphase Flow* (1995).
- [43] H. H. Hu. Motion of a Circular Cylinder in a Viscous Liquid Between Parallel Plates, to appear in *Theor. Comp. Fluid Dyn.* (1995).
- [44] H. H. Hu, D. D. Joseph, and M. J. Crochet. Direct Simulation of Fluid Particle Motions, *Theor. Comp. Fluid Dyn.* **3**, 285 (1992).
- [45] H. H. Hu, D. D. Joseph, and A. Fortes. Experiments and Direct Simulations of Fluid Particle Motion, *Int. Vid. J. Eng. Res.* **2**, 17 (1992).
- [46] P. Y. Huang, J. Feng, and D. D. Joseph. The Turning Couples on an Elliptic Particle Settling in a Vertical Channel, *J. Fluid Mech.* **271**, 1–16 (1994).
- [47] A. Huerta and W. K. Liu. Viscous Flow with Large Free Surface Motion, *Comp. Meth. Appl. Mech. Eng.* **69**, 227–324 (1988).
- [48] T. J. R. Hughes, L. P. Franca, and G. M. Hulbert. A New Finite Element Formulation for Computational Fluid Dynamics. VIII: The Galerkin/Least-Squares Method for Advective-Diffusive Equations, *Comp. Meth. Appl. Mech. Eng.* **73**, 173–189 (1989).
- [49] M. Ishii. Thermo-Fluid Dynamic Theory of Two Phase Flows, Eyrolles (1975).
- [50] A. A. Johnson. *Mesh Generation and Update Strategies for Parallel Computation of Flow Problems with Moving Boundaries and Interfaces*. PhD thesis, University of Minnesota. Advisor: T. Tezduyar (1994).
- [51] D. D. Joseph. Separation in Flowing Fluids, *Nature* **348**, 487 (1990).
- [52] D. D. Joseph. Finite Size Effects in Fluidized Suspension Experiments, in *Particulate Two-Phase Flow*, (M. C. Roco, ed.), pp. 300–324. Butterworth-Heinemann (1993).
- [53] D. D. Joseph, Interrogation of Numerical Simulation for Modeling of Flow Induced Microstructure, in *Liquid-Solid Flows 1994* **189**, 31–40, American Society of Mechanical Engineers (1994).
- [54] D. D. Joseph. Lubricated Pipelining, to appear in *Ann. Rev. Fluid Mech.* (1997).
- [55] D. D. Joseph and J. Feng. The Negative Wake in a Second Order Fluid, accepted for publication in *J. Non-Newt. Fluid Mech.* (1995).
- [56] D. D. Joseph, A. Fortes, T. S. Lundgren, and P. Singh. Nonlinear Mechanics of Fluidization of Beds of Spheres, Cylinders and Disks in Water, in *Advances in Multiphase Flow and Related Problems*, (G. Papanicolau, ed.), pp. 101–122. SIAM (1987).
- [57] D. D. Joseph and Y. J. Liu, Motion of Particles Settling in a Viscoelastic Liquid, in *Proceedings of the Second International Congress on Multiphase Flow*, (A. Serizawa, T. Fukano, and J. Bataille, eds.), 3–7 (1995).
- [58] D. D. Joseph, Y. J. Liu, M. Poletto, and J. Feng. Aggregation and Dispersion of Spheres Falling in Viscoelastic Liquids, *J. Non-Newt. Fluid Mech.* **54**, 45–86 (1994).
- [59] D. D. Joseph and T. S. Lundgren. Ensemble Averaged and Mixture Theory Equations for Incompressible Fluid-Particle Suspensions, *Int. J. Multiphase Flow* **16**, 35–42 (1990).
- [60] D. D. Joseph and Y. Y. Renardy. Fundamentals of Two-Fluid Dynamics. Part II: Lubricated Transport, Drops and Miscible Liquids, volume 4 of “Interdisciplinary Applied Mathematics,” Springer (1992).

- [61] A. Karnis and S. G. Mason. Particle Motions in Sheared Suspensions. XIX: Viscoelastic Media, *Trans. Soc. Rheol.* **10**, 571–592 (1966).
- [62] A. J. C. Ladd. Numerical Simulations of Particulate Suspensions via a Discretized Boltzmann Equation, *J. Fluid Mech.* **271**, 285–339 (1994).
- [63] A. J. C. Ladd, M. E. Colvin, and D. Frenkel. Application of Lattice-Gas Cellular Automata to the Brownian Motion of Solids in Suspension, *Phys. Rev. Lett.* **60**, 975–978 (1988).
- [64] L. G. Leal. Particle Motions in a Viscous Fluid, *Ann. Rev. Fluid Mech.* **12**, 435 (1980).
- [65] Y. J. Liu and D. D. Joseph. Sedimentation of Particles in Polymer Solution, *J. Fluid Mech.* **48**, 225–235 (1993).
- [66] Y. J. Liu, J. Nelson, J. Feng, and D. D. Joseph. Anomalous Rolling of Spheres down an Inclined Plane, *J. Non-Newt. Fluid Mech.* **50**, 305–329 (1993).
- [67] F. G. Lou. Some New Results for Solving Linear Systems Arising from Computational Fluid Dynamics Problems, *CSR D Report 1201*, University of Illinois, Urbana-Champaign (1992).
- [68] F. G. Lou, A. H. Sameh, and V. Sarin. An Augmentation Method for Solving Saddle-Point Problems, *UMSI 95/29* (1995).
- [69] J. M. Marchal and M. J. Crochet. A New Mixed Finite Element for Calculating Viscoelastic Flow, *J. Non-Newt. Fluid Mech.* **26**, 77–114 (1987).
- [70] G. McNamara and G. Zanetti. Use of the Boltzmann Equation to Simulate Lattice-Gas Automata, *Phys. Rev. Lett.* **61**, 2332–2335 (1988).
- [71] R. I. Nigmatulin. Spatial Averaging in the Mechanics of Heterogeneous and Dispersed Systems, *Int. J. Multiphase Flow* **5**, 353–385 (1979).
- [72] K. G. Nolte. Fluid Flow Considerations in Hydraulic Fracturing, *SPE 18537* (1988). See also Errata submitted July 1992 for SPE 18537, available from SPE Book Order Department.
- [73] T. Nomura and T. J. R. Hughes. An Arbitrary Lagrangian-Eulerian Finite Element Method for Interaction of Fluid and a Rigid Body, *Comp. Meth. Appl. Mech. Eng.* **95**, 115–138 (1992).
- [74] R. V. A. Oliemans and G. Ooms. Core-Annular Flow of Oil and Water through a Pipeline, in *Multiphase Science and Technology*, (G. F. Hewitt, J. M. Delhaye, and N. Zuber, eds.), volume 2, pp. 427–476. Hemisphere Publishing Corp., Washington, D.C. (1986).
- [75] C. S. Peskin and D. M. McQueen. A Three-Dimensional Computational Method for Blood Flow in the Heart I. Immersed Elastic Fibers in a Viscous Incompressible Fluid, *J. Comp. Phys.* **81**, 372–405 (1989).
- [76] W. Queck. The Convergence Factor of Preconditioned Algorithms of the Arrow-Harwics Type, *SIAM J. Num. Anal.* **26**, 1016–1030 (1989).
- [77] D. Rajagopalan, R. A. Brown, and R. C. Armstrong. Finite Element Methods for Calculation of Steady, Viscoelastic Flow Using Constitutive Equations with a Newtonian Viscosity, *J. Non-Newt. Fluid Mech.* **22**, 129–167 (1987).
- [78] A. Ramage and A. J. Wathen. Iterative Solution Techniques for the Stokes and Navier-Stokes Equations, *Int. J. Num. Meth. Fluids* **19**, 67–83 (1994).
- [79] J. F. Richardson and W. N. Zaki. Sedimentation and Fluidization: Part I, *Trans. Instn. Chem. Engrs.* **32**, 35–53 (1954).
- [80] M. J. Riddle, C. Narvaez, and R. B. Bird. Interactions Between Two Spheres Falling Along Their Line of Centers in a Viscoelastic Liquid, *J. Non-Newt. Fluid Mech.* **2**, 23–35 (1977).

- [81] Particulate Two-Phase Flow, (M. C. Roco, ed.), Butterworth-Heinemann (1993).
- [82] Y. Saad. A Flexible Inner-Outer Preconditioned GMRES Algorithm, *SIAM J. Sci. Comp.* **14**, 461–469 (1993).
- [83] Y. Saad and M. Schultz. GMRES: A Generalized Minimal Residual Algorithm for Solving Nonsymmetric Linear Systems, *SIAM J. Sci. Stat. Comp.* **7**, 856–869 (1986).
- [84] A. H. Sameh, On Two Numerical Algorithms for Multiprocessors, in *Proc. of NATO Adv. Res. Workshop on High-Speed Comp. (Series F: Computer and Systems Sciences)* **7**, 311–328 (1983).
- [85] A. H. Sameh. A Fast Poisson Solver for Multiprocessors, in *Elliptic Problem Solvers II*, (G. Birkhoff and A. Schoenstadt, eds.), pp. 175–186. Academic Press (1984).
- [86] A. H. Sameh and D. Su. A Parallel Newton-Based Iteration for Solving Systems of Linear Equations, in preparation (1995).
- [87] A. S. Sangani and A. K. Didwania. Dynamic Simulations of Flows of Bubbly Liquids at Large Reynolds Numbers, *J. Fluid Mech.* **250**, 307–337 (1993).
- [88] A. S. Sangani and A. Prosperetti. Numerical Simulation of the Motion of Particles at Large Reynolds Numbers, in *Particulate Two-Phase Flow*, (M. C. Roco, ed.), pp. 971–998. Butterworth-Heinemann (1993).
- [89] P. Saramito. Numerical simulation of viscoelastic fluid flows using incompressible finite element method and a σ method, *Math. Modeling and Numerical Anal.* **28**, 1–35 (1994).
- [90] P. Saramito. Efficient simulation of nonlinear viscoelastic fluid flows, *J. Non-Newt. Fluid Mech.* **60**, 199–223 (1995).
- [91] D. Silvester and A. Wathen. Fast Iterative Solution of Stabilised Stokes Systems. Part II: Using General Block Preconditioners, *SIAM J. Num. Anal.* **31**, 1352–1367 (1994).
- [92] P. Singh, P. H. Caussignac, A. Fortes, D. D. Joseph, and T. S. Lundgren. Stability of Periodic Arrays of Cylinders Across the Stream by Direct Simulation, *J. Fluid Mech.* **205**, 553–571 (1989).
- [93] P. Singh and D. D. Joseph. Dynamics of Fluidized Suspensions of Spheres of Finite Size, *Int. J. Multiphase Flow* **21**, 1–26 (1995).
- [94] P. Smereka. On the Motion of Bubbles in a Periodic Box, *J. Fluid Mech.* **254**, 79–112 (1993).
- [95] P. Sonneveld. CGS, a Fast Lanczos-Type Solver for Nonsymmetric Linear Systems, *SIAM J. Sci. Stat. Comp.* **10**, 36–52 (1989).
- [96] S. L. Soo. Fluid Dynamics of Multiphase Systems, Blaisdell Publishing Co., Waltham, MA (1967).
- [97] A. Tehrani, P. S. Hammond, and A. T. Unwin. Experimental Study of Particle Migration in Suspensions Undergoing Poiseuille Flow, Presentation given at the Society of Rheology 66th Annual Meeting (1994).
- [98] T. E. Tezduyar, J. Liou, D. K. Ganjoo, M. Behr, and R. Glowinski. Unsteady Incompressible Flow Computations with the Finite-Element Method, in *Finite Elements in Fluids*, (T. J. Chung, ed.), volume 8, pp. 177–209. Hemisphere Publishing Corp., Washington, D.C. (1992).
- [99] S. Turek. Comparative Study of Some Time Stepping Techniques for the Incompressible Navier-Stokes Equations: From Fully Implicit Nonlinear Schemes to Semi-Implicit Projection Schemes, to appear in *J. Num. Meth. Fluids* (1995).
- [100] S. O. Unverdi and G. Tryggvason. Computations of Multi-Fluid Flows, *Physica D* **60**, 70–83 (1992).
- [101] S. O. Unverdi and G. Tryggvason. A Front-Tracking Method for Viscous, Incompressible, Multi-Fluid Flows, *J. Comp. Phys.* **100**, 25–37 (1992).

- [102] A. T. Unwin and P. S. Hammond. Computer Simulations of Proppant Transport in a Hydraulic Fracture, *SPE* 29649. Presented at the Society of Petroleum Engineers Western Region Meeting (1995).
- [103] H. van der Vorst. BI-CGSTAB: A Fast and Smoothly Converging Variant of BI-CG for the Solution of Nonsymmetric Linear Systems, *SIAM J. Sci. Stat. Comp.* **13**, 631–644 (1992).
- [104] H. van der Vorst and C. Vuik. GMRESR: A Family of Nested GMRES Methods, to appear in *Num. Lin. Alg. with Appl.* (1995).
- [105] C. Vuik and H. van der Vorst. A Comparison of Some GMRES-Like Methods, *Lin. Alg. and Its Appl.* **160**, 131–162 (1992).
- [106] A. Wathen and D. Silvester. Fast Iterative Solution of Stabilised Stokes Systems. Part I: Using Simple Diagonal Preconditioners, *SIAM J. Num. Anal.* **30**, 630–649 (1993).
- [107] S. Wolfram. Cellular Automaton Fluids 1: Basic Theory, *J. Stat. Phys.* **45**, 471–526 (1986).
- [108] H. Yserentant. Preconditioning Indefinite Discretization Matrices, *Numer. Math.* **54**, 719–734 (1988).
- [109] D. Z. Zhang and A. Prosperetti. Averaged Equations for Inviscid Disperse Two-Phase Flow, *J. Fluid Mech.* **267**, 185–219 (1994).
- [110] D. Z. Zhang and A. Prosperetti. Ensemble Phase-Averaged Equations for Bubbly Flows, *Phys. Fluids* **6**, 2956–2970 (1994).
- [111] D. Z. Zhang and A. Prosperetti. Effective Equations for Disperse Two-Phase Flows and Their Closure in the Dilute Limit, submitted to *J. Fluid Mech.* (1995).
- [112] D. P. Ziegler. Boundary Conditions for Lattice Boltzmann Simulations, *J. Stat. Phys.* **71**, 1171–1177 (1993).

VI. Results from Prior NSF Support (D.D. Joseph)

1. NSF Award, CTS 9213979, for \$365,000 from 10/30/92 to 2/29/96.
2. Project title: Studies of Two-Phase Flows of Liquids and Solids.
3. Summary of prior results:

Of 36 papers we published since 1993, the 25 listed below are related to the present proposal. They cover four topics: (i) experiments on the settling of particles in viscous and viscoelastic fluids [3,4,6,17,18,19,22]; (ii) direct simulation of the motion of particles in a viscous liquid [1,7,10,11,13,14,16,23]; (iii) two-phase flow modeling of solid-liquid flow [17,18,22] and (iv) studies of lubricated transport of hydrocarbons and remedial strategies against fouling [2,5,9,12,15,16,20,21,24,25].

The experiments (i) showed that the overall flow-induced anisotropy in Newtonian and viscoelastic liquids is determined by pair interactions due to wakes and turning couples on long bodies. This leads to characteristic pair interactions between particles which are maximally different in Newtonian and non-Newtonian fluids, with across-the-stream arrangements in Newtonian fluids and along-the-stream arrangements in viscoelastic fluids (see figure 2). The experiments are described in our research summary. From our direct simulations (ii) (also described in the research summary), we showed how the pressures at stagnation and separation points cause lateral migrations of particles and produce couples that control the orientation of long bodies in Newtonian and viscoelastic fluids. In modeling fluidized suspensions (iii), we proposed that the solids area fraction rather than the volume fraction is the fundamental variable controlling the dynamics and stability. A construction [17] was given relating the volume and area solids fraction and some predictions about the zeros of the area fraction were confirmed in experiments [18]. Our proposal can be fully tested by the direct simulations proposed here. The experiment in [22] showed that the values of the effective density and viscosity are close to the average density of the mixture and to the viscosity of the mixture predicted by correlation suggested by Thomas when the test particles are of the same size as the suspended particles, but not too much smaller.

In the study of the fluid dynamics of core flows (iv), we correlated all the available data on friction factors and hold-up for core flow and have shown good agreements between experimental data and $k-\epsilon$ models in turbulent flow. We analyzed the stability of eccentric core annular flow and we showed that there is no linear mechanism for centering the flow when the density is matched. The modes of instability of the eccentric core annular flow are a combination of an asymmetric mode and a first mode of azimuthal variation and it resembles cork screw waves seen in experiments. We completed the first direct numerical simulation of axisymmetric core flow, and we verified that the pressure at the front of the wave steepens the wave there while the backside is smoothed by low pressures. The steepening can be regarded as a shock up by inertia and it shows that dynamics work against the formation of long waves usually assumed in analyses. We found that there is a threshold Reynolds number below which the total force corresponding to the pressure is negative, positive above, and we conjectured, therefore, that inertia is required to center a density matched core and to levitate the core off the wall when the density is not matched [24].

Another category of study treats the problem of fouling pipe walls with oil, with undesirable increases in pressure gradients and even blocking. We found an apparent remedy for this using cement-lined pipes; over 140 cements were tested [20,21]. The best cements require hydration in sodium meta-silicate; a calcium silicate gel is formed at the surface which is extraordinarily hydrophilic and resists spotting by oil. A patented for the method of preventing fouling pipe walls for lubricated transport was obtained for cement linings (U.S. Patent No. 5,385,175).

We also considered problems of the lubricated transport of concentrated emulsions [25]. We found that concentrated emulsions of crude oil do lubricate when the pipe material is hydrophilic. In the case of very concentrated, say, 80/20, bimodal dispersions of oil in water, we showed that there is a crisis at a certain shear wherein the large drop fraction is broken into small drops by direct contact as in comminution of rocks. On the other side, we showed that bitumen drop coalescence in concentrated emulsion is, in fact, not coalescence but is a local inversion in which water appears to be the large drop. The fluid motion concentrates further an already concentrated dispersion, testing the maximum packing fraction locally. The way to total inversion is locally, in patches.

Our laboratory setting is a human resource center. It serves as a hub of activities for graduate and undergraduate students and also a kind of social center. The undergraduates are supported by programs from the University (Undergraduate Research Opportunities) and from the NSF program on Research Experiences

for Undergraduates (REU). Thirteen undergraduate students, four of whom are women, have worked for us in these programs in the past five years; three students are currently working in the lab. All of these undergraduates have gone on to careers in science and engineering. These undergraduate programs are visible in the undergraduate community as opportunity programs for highly qualified students. Graduate students who participated in the research of this prior NSF grant are M. Arney, R. Bai, C. Christodoulou, K.P. Chen, J. Feng, T. Hall, H. Hu, P. Huang, A. Huang, T. Liao, J. Liu, G. Ribeiro and H. Vinagre.

Publications

1. Direct simulation of fluid-particle motions (with H. Hu and M. Crochet), AHPCRC preprint 91-43, *Journal of Theoretical and Computational Fluid Dynamics* **3**, 285-306 (1992).
2. Friction factor and holdup studies for lubricated pipelining (with M.S. Arney, R. Bai, E. Guevara, and K. Liu). *Int. J. Multiphase Flow* **19**(6), 1061-1076 (1993).
3. Orientation of long bodies falling in a viscoelastic liquid (with Y.J. Liu). *J. Rheol.* **37**(6), 961-984 (Nov/Dec 1993).
4. Anomalous rolling of spheres down an inclined plane (with Y.J. Liu, J. Nelson and J. Feng). *J. Non-Newtonian Fluid Mech.* **50**, 305-329 (1993).
5. A note on the net force and moment on a drop due to surface forces (with T. Hesla and A.Y. Huang) *J. Colloid & Interface Science* **158**, 255-257 (1993).
6. Sedimentation of particles in polymer solutions (with Y.J. Liu) *J. Fluid Mech.* **225**, 565-595 (1993).
7. Direct simulation of initial value problems for the motion of solid bodies in a Newtonian fluid (with J. Feng and H. Hu). *J. Fluid Mech.* **261**, 95-134 (1993).
8. Aggregation and dispersion of spheres falling in viscoelastic liquids (with Y.J. Liu, M. Poletto and J. Feng). *J. Non-Newtonian Fluid Mech* **54**, 45-86 (1994).
9. Friction factor and holdup studies for lubricated pipelining. Part II: laminar and $k-\epsilon$ models of eccentric core flow (with A. Huang and C. Christodoulou). *Intl. J. of Multiphase Flow* **20**(3), 481-491 (1994).
10. The turning couples on a elliptic particle settling in a vertical channel (with P.Y. Huang and J. Feng). *J. Fluid Mech.* **271**, 1-16 (1994).
11. Direct simulation of initial value problems for the motion of solid bodies in a newtonian fluid. part 2: couette and poiseuille flows (with J. Feng and H. Hu). *J. Fluid Mech* **277**, 271-301 (1994).
12. Parallel pipelining (with H. Hu, R. Bai, T.Y. Liao and A. Huang). Accepted for publication in *J. Fluids Eng.* (1994).
13. Interrogation of numerical simulations for modeling of flow induced microstructures. *ASME FED* **189** (Liquid-Solid Flows), 31-40 (1994).
14. A three-dimensional computation of the force and moment on an ellipsoid settling slowly through a viscoelastic fluid (with J. Feng, R. Glowsinski and T.W. Pan). *J. Fluid Mech.* **283**, 1-16 (1995).
15. Stability of eccentric core-annular flow (with A. Huang). *J. Fluid Mech.* **282**, 233-245 (1995).
16. Dynamic simulation of the motion of capsules in pipelines (with J. Feng). *J. Fluid Mech.* **286**, 201-207 (1995).
17. Dynamics of fluidized suspensions of spheres of finite size (with P. Singh). *International Journal of Multiphase Flow* **21**, 1-26 (1995).
18. Propagation of voidage wave in a two-dimensional liquid-fluidized bed (with M. Poletto and R. Bai). To appear in *Int. J. Multiphase Flow* **39**, 323-344 (1995).
19. Motions of particles settling in a viscoelastic fluid. To appear in Proceedings of the Second International Conference on Multiphase Flow, Kyoto, Japan, April 3-7, 1995.
20. Adhesion of crude oil to wet ceramics (with G. Ribeiro, M. Arney, M. Rivera and T. Hall). Submitted to *Canadian J. Chem. Eng.* (1995).
21. Cement-lined pipe for water lubricated transport of hydrocarbons (with M. Arney, G. Ribeiro, E. Guevarra and R. Bai). To appear in *Int. J. Multiphase Flow* (1995).
22. The effective density and viscosity of a suspension (with M. Poletto). *J. Rheology* **39**(2), 323-343 (1995).

23. The unsteady motion of solid particles in creeping flows (with J. Feng). Submitted to *J. Fluid Mech.* (1995).
24. Direct simulation of interfacial waves in a high viscosity ratio of axisymmetric core annular flow (with R. Bai and K. Kelkar). Submitted to *J. Fluid Mech.* (1995).
25. Flow characteristics of concentrated emulsions of very viscous oil in water (with G. Núñez, Maria Briceo and Clara Mata). In preparation.

C. Project Description

D. Bibliography

E. Biographical Sketches

F. Summary Proposal Budget

G. Current and Pending Support

J. Appendix

**I. Special Information/
Supplementary Documentation**

H. Facilities, Equipment and Other Resources