A Project Summary

This KDI/NCC proposal builds upon a prior NSF HPCC Grand Challenge award (ESC-95-27123) for the high-performance computation of the motion of solid particles in Newtonian and viscoelastic liquids; it aims to use these computations to elucidate fundamental dynamics and solve problems of engineering interest. The Grand Challenge goal was to develop software packages, called *particle movers*, capable of carrying out *direct numerical simulations* ("DNS") of the motion of thousands of particles in 2-D and hundreds in 3-D, in parallel implementation. Two state-of-the-art particle movers were developed. One of these (ALE particle mover) uses a moving unstructured, body-fitted grid, and has given rise to the first and only package which can presently move particles in viscoelastic fluids. The other (DLM particle mover) uses a fixed, regular grid, and represents the particles by a field of Lagrange multipliers which enforce the constraint of rigid-body motion. The DLM particle mover is inventive, and it appears to have great potential with respect to parallel implementation of large numbers of particles in realistic flow conditions. Both methods use a new *combined weak formulation* in which the fluid and particle equations of motion are combined into a single weak equation of motion from which the hydrodynamic forces and torques on the particles have been eliminated. These and other results achieved in the Grand Challenge project have opened new and promising lines for investigation. See the project Web site,

http://www.aem.umn.edu/Solid-Liquid_Flows

for further details.

One objective of KDI/NCC is to further develop the state-of-the-art particle movers started in the Grand Challenge project; this is incremental research, building great codes brick by brick, in which the innovation enters in the formulation of more efficient preconditioners and solvers. The handling of collisions in dense slurries is one challenging computational and physical problem suggested by the Grand Challenge work, which is intrinsic to particulate flow; it has not been faced in computational work before.

Code enhancement for the particle movers will be achieved by a major overhaul of the solvers and preconditioners. The ALE particle mover will be enhanced by implementing an operator-splitting scheme to avoid the problems created by nonlinear iteration, by a matrix-free formulation to avoid excessive memory requirements, and by multilevel and domain decomposition methods to effect better 3-D parallel performance. A viscoelastic version of the DLM particle mover will be implemented.

A second objective is to pioneer ways to convert simulation results into forms which can be used by the fracturing industry. To do this, the proposal focuses on sand transport in fractured reservoirs, a surrogate for all forms of slurry transport. The research is to be done and partly financed by partners from the oil and oil service industries in the consortium STIMLAB. The oil industry makes extensive use of models to guide field operations. DNS is a new tool for modeling forces on particles, and can even be used to generate correlations to close two-fluid models on a PC.

The research on direct numerical simulation will impact both industry and academia. DNS can change the way fracturing models are constructed and used in this multi-billion-dollar-a-year industry. New microstructural problems associated with lift-off, resuspension, and slip velocities can be expected to impact the modeling and multiphase-flow communities, and to open a new frontier for mathematicians who study the Navier-Stokes equations and the mysterious motions of particles in viscoelastic fluids. Clean mathematical problems suitable for proving theorems are generated by this work. The challenges of DNS for computer science are brand new, and the "solvers" part of the software generated to meet these challenges will be made publicly available.

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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 using direct numerical simulation ("DNS"). A similar potential for solid-liquid flows, and multiphase flows generally, has yet to be fully exploited, even though such flows are of crucial importance in a large number of industries.

Under an NSF HPCC Grand Challenge award, we have taken a major step toward the realization of this potential by developing two highly efficient parallel finite-element codes called *particle movers* for the direct numerical simulation of the motions of large numbers of solid particles in flows of Newtonian and viscoelastic fluids. One of the particle movers is based on moving unstructured meshes (Arbitrary Lagrangian-Eulerian or ALE) and the other (Distributed Lagrange Multiplier or DLM) on a structured mesh using a new method involving a distribution of Lagrange multipliers to ensure that the regions of space occupied by solids are in a rigid motion following Newton's laws. Both particle movers have been developed in parallel implementation with a present capability of moving thousands of particles in 2D simulations. Three dimensional serial computations in both codes presently are capable of moving hundreds of particles; 3D parallel implementation is expected in the next months with a fluidization calculation of the bed expansion of 1200 spheres as our target.

The DLM particle mover evolved from well-known embedding methods and its potential for applications seems to be very great since the problems of remeshing, projection and so on which plague methods based on unstructured grids have been circumvented. On the other hand, the ALE methodology is well suited for problems in irregular domains and it is at present the only code in the world which can move solid particles in a viscoelastic fluid. By comparing results from these two codes on common problems, we are able to evaluate both.

The research proposed under this KDI/NCC initiative has two goals. One is to develop state-of-the-art particle movers based on DNS; we aim to move thousands of particles in 3D slurry transport and fluidized bed calculations at the flow parameters relevant to applications. This ambitious goal can be realized by merging the best new ideas from our computer scientists with regard to parallelism, preconditioners and modular code development with new solvers and more finely tuned old solvers introduced by our CFD experts. The chances of achieving our goals have been enhanced by the momentum achieved in our Grand Challenge work in which the border which separates these two groups of experts has begun to disappear.

The second goal of our KDI/NCC research is to develop effective procedures for converting the results of DNS into forms which can be used in practical applications. Such procedures are important but not obvious. One example of how to use DNS is the expansion of a fluidized bed. We have adopted this problem as our benchmark for code comparison (Section 3.3). As you increase the fluidizing velocity the bed expands; the interest is in how the liquid fraction develops which is given by monitoring the increase of the bed height as the fluidizing velocity is increased. This information is badly needed by industries and traditionally is obtained in the form of hindered settling correlations; the most famous of these are the Richardson-Zaki correlations [75]. Now for the first time we have the opportunity to do these correlations using DNS and to compare the simulation results with highly regarded experiments that are extensively used in many industries.

Sand transport in fractured oil and gas reservoirs is another system in which the ways that DNS can impact field operations is not obvious. In this system, the effects of microstructure at the particle level scale into particle placements in the fracture at the field level. We are going to focus our research on how to use DNS on this problem, partnering with oil and gas companies in the proppant ("prop open") transport consortium STIMLAB. The people of STIMLAB are active researchers on this project; they are also supporting the work financially (see Part IV). It should not be thought that the sand transport problem is special; it is a paradigm for slurry transport generally.

2 Prior Work

Direct simulation of the motion of solid particles in fluids can be said to have started with the paper of Hu, Joseph, and Crochet [35]. Johnson and Tezduyar [41–44] developed another similar particle mover for 3-D simulations, and studied sedimentation of spheres in tubes. Other papers on direct numerical simulation of the motion of solid particles in fluids [19, 20, 23–25, 32, 33, 37, 39, 48, 64] have emerged from our Grand Challenge work, and can be found on the linked pages of our Web site. Direct simulations of the interaction of bubbles were first carried out in two and three dimensions by Unverdi and Tryggvason [93, 94].

Many authors refer to numerical codes which are faithful to the equations governing the fluid but are approximate in the way the solids are moved or in other ways as direct numerical simulations. Point particle approximations have been used for dilute suspensions, especially for turbulent flow, to advect particles following Newton's laws. In some cases the influence of the particles on the fluid flow is neglected; in other cases the force on the fluid from the particles is added to the Navier-Stokes equation. Although this approach is often referred to as “DNS,” the forces on each particle are related to its motion by semi-empirical relations and the effects of the particles on the fluid, as well as the interparticle interactions, must be modeled. Without giving here a long list of such approximations we simply point the reader to the excellent discussions and rather complete set of references in the papers [15, 28, 65, 71, 89]. In fact, it is not possible at present to do the kind of exact DNS achieved in our particle movers when the underlying fluid flow is turbulent.

We shall use the acronym LNS (Lagrangian Numerical Simulation) for all the codes in which the forces on particles are modeled rather than computed as in DNS. We have developed a particle mover based on LNS which can move tens of thousands of particles rather efficiently and has a good potential for applications. The modeling assumptions used in LNS can be evaluated and refined by direct comparison with results from DNS.

A systematic effort to marry CS (computer science) to CFD in DNS applications starts first in our Grand Challenge work. Obviously, there is a huge CS literature which can be made relevant to DNS applications, but a prior literature dedicated to these applications does not exist. The CS literature at the foundation of our computational algorithms is interwoven with descriptions of these algorithms given in Part III of this proposal.

Part II Applications of DNS

The particle movers created in our Grand Challenge project were designed to (1) simulate the remarkably different flow microstructures which arise from particle-particle and particle-wall interactions in Newtonian and viscoelastic fluids, and (2) determine the effects of these microstructures on anisotropic and other properties of flowing suspensions. These are computational studies of scale and structure; how do the effects of microstructure at the particle level scale into flow effects at the slurry level?

This KDI/NCC proposal builds on the success and remedies the shortcomings of our NSF sponsored Grand Challenge work. We were successful in simulating most of the remarkable microstructural features shown in Figures 1, 2, 3a, 3b, and 4, and in the simulation of slurry properties, examples of which are shown in Figures 5–6. A more complete and persuasive record of our achievements can be seen in the animations in our Web site.

The Grand Challenge work we did and are doing comes up short only in the sense that we know that we can build much better particle movers for greater volume fractions at realistic values of the flow parameters. Building particle movers is intrinsically incremental; it requires adding bricks to create a great edifice. Innovation here enters into the invention of new preconditioners, new solvers, new algorithms, etc., to this work.

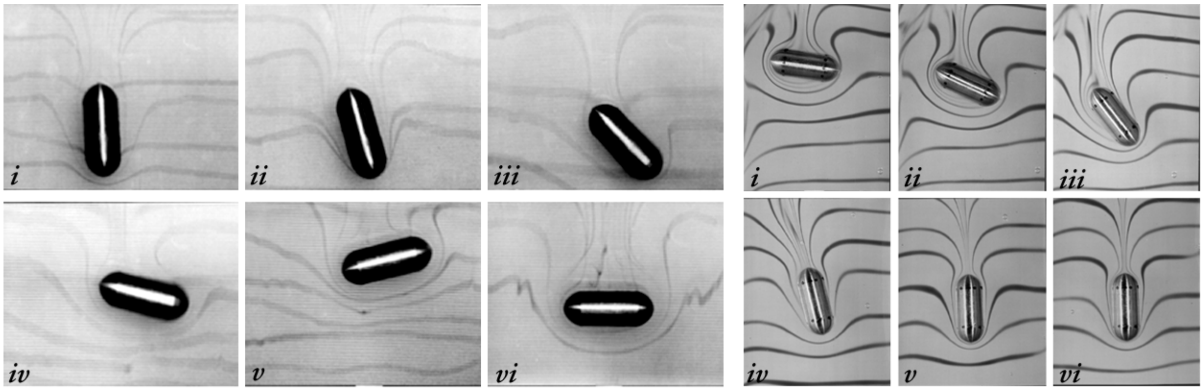
The applications side of our KDI/NCC proposal takes up the new and difficult challenge of seeking the ways to turn high-performance computations into forms which industry can recognize as adding value. To actually carry this out, we must focus, and the focus will be on sand transport in fractured oil and gas reservoirs. This focus problem is obviously of great generality, being a rather general surrogate for all forms of slurry transport. To keep our work accountable, we have partnered with the fracturing industry and committed ourselves to explicit goals.

In reading the sections which follow, the reader may note what applies to Grand Challenge work (Section 3 on work done and still in progress), and what is proposed for KDI/NCC (Section 4).

3 Fundamental Dynamics

3.1 Studies of Microstructure

There is a microstructure which is induced by the fluid dynamics of moving bodies and is governed by a very simple principle: Long bodies are stable across the stream in Newtonian fluids but along the stream in viscoelastic fluids (Figure 1). A key to understanding microstructure in flowing suspensions of spherical bodies is the stable



(a) (b)

Figure 1: Cylinders falling in (a) Newtonian fluid (glycerin), and (b) viscoelastic fluid (2% polyox in water). In glycerin, the cylinder is turned to the horizontal by inertia; in polyox, it is turned vertical by viscoelastic pressures.

orientation of long bodies and pairs of spherical bodies in momentary contact [21, 34, 38, 39, 47, 48, 50, 59, 61, 84].

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. The principal interactions between neighboring spheres can be described as *drafting*, *kissing*, and *tumbling* in Newtonian liquids (Figure 2a) and as *drafting*, *kissing*, and *chaining* in viscoelastic liquids (Figure 2b). The drafting and kissing mechanisms involved are distinctly different, despite appearances [21, 25, 34, 47, 48, 50–52, 61].

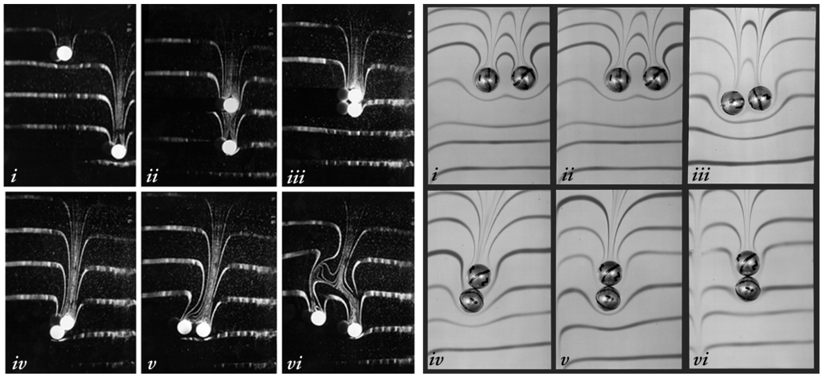
In Newtonian liquids, when one falling sphere enters the wake of another, it experiences reduced drag and *drafts* downward into *kissing* contact with the leading sphere. The two kissing spheres momentarily form a single long body aligned parallel to the stream. But the parallel orientation for a falling 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 [48, 52, 84]; they then fall together without further lateral migrations.

This local rearrangement mechanism implies that globally, the only stable configuration is the 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 [47, 84] (see Figure 3a). In viscoelastic liquids, on the other hand, two spheres falling one behind the other will be pushed apart if their initial separation exceeds a critical value. However, if their initial separation is small enough, they will attract (“draft”), kiss, turn and chain, as shown in Figure 2b. One might say that we get dispersion in a Newtonian liquid and aggregation in a viscoelastic liquid [34, 36, 47, 48, 52, 76].

Many stable arrangements—i.e., steady particulate flows—like the “birds in flight” shown in Figure 3c, and some bizarre steady arrangements of 2, 3, and 4 long cylinders (stable doublets, triplets, and quadruplets [47, 48]) are seen in thin fluidized beds. The arrangements displayed in Figures 1–3 have never been acknowledged in any two-fluid or mixture-theory model of particulate flow. **These models cannot predict such arrangements because no provision is made for the forces that turn long bodies across or along the stream; hence, two-fluid and mixture theory are silent about microstructure**. This certainly is a motivation for DNS, and suggests new challenges for mathematical analysis and two-phase flow modeling.

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. There is also an equilibrium distance for viscoelastic liquids to which spheres will always migrate; this distance is often so close to the wall that spheres appear to be sucked all the way to the wall [34, 37, 52]. These microstructural features ought ultimately to enter into understanding and control of the lubrication of slurries.

Considerable progress was made in the theoretical understanding of microstructure in our Grand Challenge work. We showed by mathematical analysis [39, 49] that the normal stresses on a rigid body in a viscoelastic fluid give rise to a “viscoelastic pressure” proportional to the square of the shear rate at the particle boundary, which is large where the velocity is large and zero at stagnation points where the pressure due to inertia is largest. Thus, the viscoelastic pressure is large where the inertial pressure is small and vice-versa, so that the turning couple on a long body has the *opposite* sign in a viscoelastic fluid than it has in a Newtonian fluid—the body aligns *parallel to* the



(a) (b)

Figure 2: (a) Spheres in Newtonian Fluids. Spheres fluidized in glycerin *draft* (*i*–*ii*), *kiss* (*iii*), and *tumble* (*iv*–*vi*). They tumble because a pair of kissing spheres acts like a long body, which is unstable when its long axis is parallel to the stream. The **forces in a Newtonian fluid are dispersive**; the tumbling spheres are pushed apart (*v*–*vi*). (b) Spheres in non-Newtonian Fluids. Spheres falling in 2% polyox in water *draft*, *kiss*, and *chain*. They chain because the **forces in a viscoelastic fluid are aggregative**. A chain of spheres acts like a long body, which is stable with its long axis vertical. The chained spheres turn just like the solid cylinder in Figure 1b(*i*–*vi*). Reversing time, we see that chaining, kissing and drafting in b(*vi*–*i*) are like drafting, kissing, and tumbling in a(*i*–*vi*)

stream. Viscoelastic pressures are compressive everywhere and tend to impel nearby bodies together (Figure 2b) whereas the stagnation point pressures act at points toward the inside of near bodies and tend to push them apart (Figure 2a). The pressures due to viscoelasticity are aggregative, gluing together the long chain of spheres in Figure 3b. The chain is stable because it is a long body aligned with the stream. The pressures of inertia are dispersive so that the array of spheres across the stream in Figure 3a are permanently separated.

Most of the microstructural features just mentioned have been simulated by the ALE particle mover developed in our Grand Challenge work. Some new arrangements are predicted. In the simulation of 5 spheres sedimenting in a tube shown in Figure 4a, 4 of the spheres fall stably in a planar array perpendicular to the stream, which fits well with the fact that the stable orientation of a long body is perpendicular to the stream. The center sphere, however, does not remain in the plane; it either escapes by dropping through the others, or oscillates back and forth across the plane of the other 4, along the center line. This is a particle-flow realization of leapfrogging vortex rings. The sedimentation of 16 spheres leads to two rings of spheres in a plane perpendicular to the stream (Figure 4b).

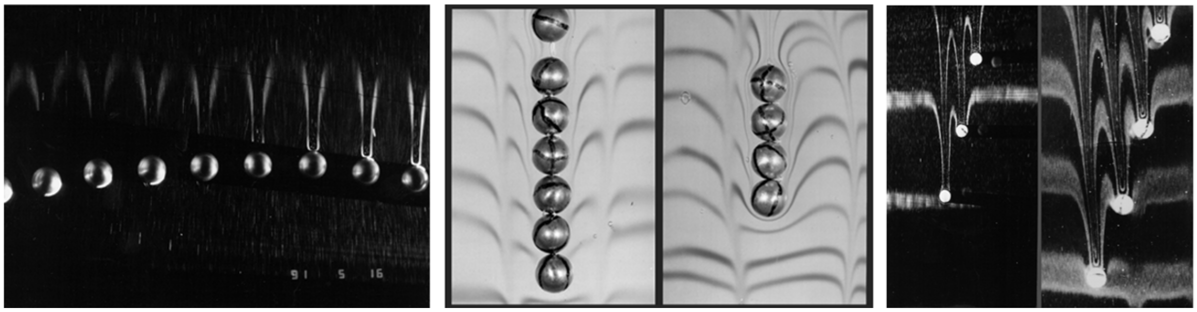
Chaining appears in our simulations, and it does not destroy the mesh between particles, even in some cases when no special collision strategy is used [17, 18, 34]. A periodic array of spheres will be sucked together to form a long chain like that in Figure 3b. Prior to this computation the cause of chaining was in dispute; many persons thought that the mechanism responsible for chaining was shear thinning rather than the normal stresses which cause chaining in our simulations.

Cross stream migration and stable orientations of elliptic particles falling through an Oldroyd B fluid in a two-dimensional channel were studied using the ALE particle mover. There are two critical numbers: the elasticity number and the velocity. For elasticity numbers below critical, the fluid is essentially Newtonian and the ellipse falls broadside-on down the channel centerline. For elasticity numbers larger than critical, the stable orientation depends on the the velocity: if the velocity is below the shear-wave speed, so that the viscoelastic Mach number is less than one, the ellipse falls down the channel centerline with its long axis parallel to the stream. For larger Mach numbers, the ellipse flips to the broadside-on orientation again [39]. (An animation may be found in our Web site.)

3.2 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.

Hesla [31] has proved that smooth rigid particles in a Newtonian fluid cannot touch—the gap between two particles cannot go to zero in a finite time. He found that the lubrication force F between spheres is proportional to $h^{-3/2}$ in 2-D, and to h^{-1} in 3-D, where h is the minimum gap between the particles [31]. He further found that the law of decrease of $h(t)$ for large t, as a sphere settles against a flat plate, is proportional to e^{-ct} in 3-D and to



(a) (b) (c)

Figure 3: Stable arrays of spheres in (a) Newtonian, and (b) viscoelastic fluids. (a) Fourteen spheres line up in a robustly stable array across the stream of a Newtonian fluid in a fluidized bed. (b) Seven and four spheres fall in a viscoelastic fluid with their long axis vertical and parallel to the stream, stably and permanently chained. (c) Spherical particles in a Newtonian fluid form like **birds in flight**. When $22 < Re < 43$, the spheres do not draft, kiss, and tumble. Three and four of them form a permanent nested wake structure in which each successive sphere is nested in the wake of the one before and rotates in a shear field there.

t^{-2} in 2-D. We are presently looking for similar asymptotic formulas for different models of viscoelastic fluids. 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.

A goal for future simulations is to develop particle movers which make no special provision for collisions or contact, relying on the equations of motion to prevent them. We are not there yet and must put in place procedures to prevent the breakdown of the mesh between particles. We aim to construct an optimal compromise between computational efficiency and faithfulness to physics.

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 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 [63], uses the lubrication force of Kim and Karrila [56] to separate touching particles and it is also the only strategy that requires touching particles to transfer tangential as well as normal momentum. Maury developed his theory for smooth bodies of arbitrary shape.

A yet different collision strategy has been implemented for the DLM particle mover [25]. 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 [44] 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. An optimal strategy for collisions is an important and difficult challenge for DNS.

3.3 Sedimentation and Fluidization

Particle collision strategies may be put to a severe test in a sedimentation column. In the sedimentation problem, we start with a crystal of close-packed particles at the top of the column; then they settle under gravity resting in a crystal of close packed particles with defects on the bottom. The defect structure ought to be related to the collision strategies used, but this has not yet been tested. Fluidization is done in the same column. The particles first form a fixed bed at the bottom; the inflow velocity is stepped up. First we find the so-called fluidizing velocity in which the fixed bed breaks up and the particles fluidize. The bed height is an increasing function of the inflow velocity; this gives the bed expansion by DNS. We have such a column in our laboratory; it is $3.2''$ wide, $0.3''$ deep and $20''$ high. In simulations and experiments we use $0.25''$ spheres so that the motion of the particles is confined basically to two dimensions though the fluid flow is in 3-D.

The sedimentation and fluidization in water of 240 particles in two and three dimensions has been designated as a benchmark problem in which we may compare ALE and DLM particle movers in both serial and parallel

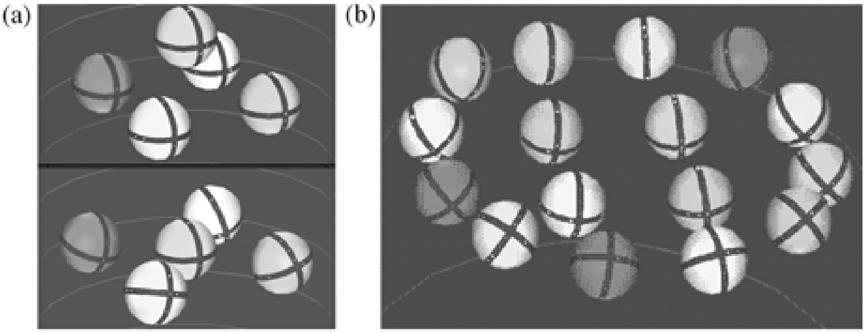


Figure 4: Planes of falling spheres across the stream in a tube computed by the ALE particle mover. (a) Five spheres ($Re = 45$); four are in a horizontal plane. The center sphere oscillates on the center line relative to the plane. (b) Sixteen spheres ($Re = 20$) in two rings in a plane across the flow.

implementation. Simulations have been carried out in two dimensions and are being done now in three. The simulations will be compared with experiments; the relation of 2-D to 3-D simulations and experiments can be assessed. Animations of these simulations from the ALE and DLM particle movers for both sedimentation and fluidization are in our Web site. A height rise or bed expansion graph for a 2-D simulation is shown in Figure 5a. It can be seen that before fluidization the bed height actually decreases because the fluid motion rearranges the particles into a more closely packed configuration with defects as shown in Figure 5b.

3.4 Mechanisms of Cross-Stream Migration

One of the uniquely useful features of DNS as compared with experiments is the ability to isolate effects. Typically in a real viscoelastic fluid the effects of viscosity, shear thinning and elasticity are all present. In simulations we may examine these effects one at a time: Newtonian, generalized Newtonian (shear thinning), Oldroyd B, and Oldroyd B with shear thinning. Results of 2-D simulation of 56 circular particles in a pressure driven spatially periodic channel flow, computed with the ALE particle mover are shown in Figure 6.

4 Slot Problems for Particle Transport in Fractured Reservoirs

We are going to focus on the problem of proppant transport in hydraulic fracturing applications. All of the features of slurry transport occur in hydraulic fracturing except that transport under turbulent conditions is not common. To understand proppant transport it is necessary to understand sedimentation, fluidization, particle migration and lubrication, lift-off and resuspension, slip coefficients, and strategies for handling contacting bodies.

4.1 Hydraulic Fracturing and Sand Transport

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.

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 [53, 66, 90]. 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 [95]. This in turn reduces well productivity and can also interfere with the fracture growth process by blocking downward extension.

The phenomenon of proppant migration is not currently controlled or exploited in the fracturing industry because the relationship between migration and fluid properties is not understood. DNS can give us this under-

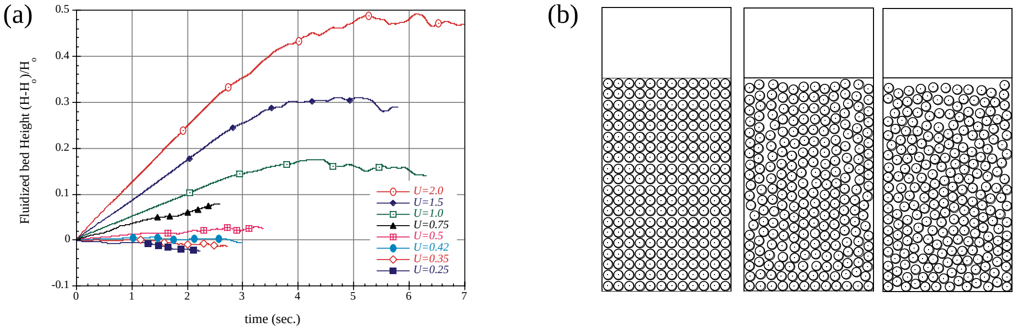


Figure 5: Fluidization of 240 particles in 2-D. (a) Height rise of a fluidized bed started from rest under the sudden increase of the inflow velocity U. The rise eventually levels off giving a unique average height for each value of U; that is, we get the bed expansion (hindered settling function) by computation. The graphs were computed using the ALE particle mover; computation of the height rise by the DLM particle mover (not shown) gives $H/H_0 - 1 = [-0.032, -0.003, 0.008, 0.032]$ for $U = [0.25, 0.35, 0.42, 0.5]$, in good agreement with ALE. (b) Particle positions at different moments, starting with a regular lattice at $t = 0$ with $U = 0.25$. The particles get rearranged into an irregular lattice with defects, in which particles pack even more closely, and the bed height decreases. The same calculation has been done for spheres in a 3-D slit column (not shown).

standing (see Figure 6). 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.

The target for this NCC proposal is the slot problem, a realistic idealization of the problem of proppant transport in a crack. A typical vertical crack may be 3 meters high, 30 meters long and 2 cm wide. The diameter of a typical sand grain is 2 mm, so that the width-diameter ratio $h(x, y, t)/d$ is about 10. The sand density is 2.4. Because of geological features related to the overburden, the preferred crack orientation is vertical. Moreover, the dimensions of the fracture are not known a priori since the crack opens and shuts in response to local changes of pressure; fracture dynamics determining the slot dimensions is coupled to proppant transport.

In a slot problem a particle laden (say 20% solids) fluid is driven by a pressure gradient and the particles settle to the bottom as they are dragged forward. Sand deposits on the bottom of the slot; a mound of sand develops and grows until the gap between the top of the slot and the mound of sand reaches an equilibrium value; this value is associated with a critical velocity. The velocity in the gap between the mound and the top of the slot increases as the gap above the mound decreases. For velocities below critical the mound gets higher and spreads laterally; for larger velocities sand will be washed out until the equilibrium height and velocity are reestablished [55]. The physical processes mentioned here are *settling* and *washout*. Washout could be by sliding and slipping; however, a more efficient transport mechanism is by *advection after resuspension* which we studied by direct simulation.

4.2 Lift-off, Resuspension, Equilibrium Height, Slip Velocities, Lift-Force Ratios

Using the ALE particle mover, we did *lift-off* and *slip-velocity* resuspension studies in Newtonian and viscoelastic fluids. A heavier particle is resting on the bottom of a channel in the presence of a shear (Poiseuille) flow at a certain critical speed. Depending on the weight and diameter of the particle, the fluid properties, and the aspect ratio of the channel, the particle rises from the wall to an equilibrium height at which the buoyant weight just balances the upward thrust of fluid forces. We found that the upward thrust (lift) is due to inertia; over 70% of the thrust is due to pressure. At equilibrium we compute the difference between the forward velocity and angular velocity of the particle and these same velocities in the fluid (at the center of the particle) when no particles are present. This gives the *slip velocity* and *angular slip velocity* which are needed for Richardson-Zaki [75] type of correlations discussed in Section 4.3.

The problem of inertial lift on a moving sphere in contact with a plane wall in shear flow has been analyzed as a perturbation of Stokes flow with inertia in [5, 58, 60]. These studies lead to specific and useful analytic results expressed in terms of translational and rotational velocity and shear rate. The lift on a stationary sphere on a wall in a shear flow varies as the fourth power of the radius and the square of the shear rate. If the shear Reynolds number is sufficiently large, the lift force exceeds the gravitational force and the sphere separates from the wall.

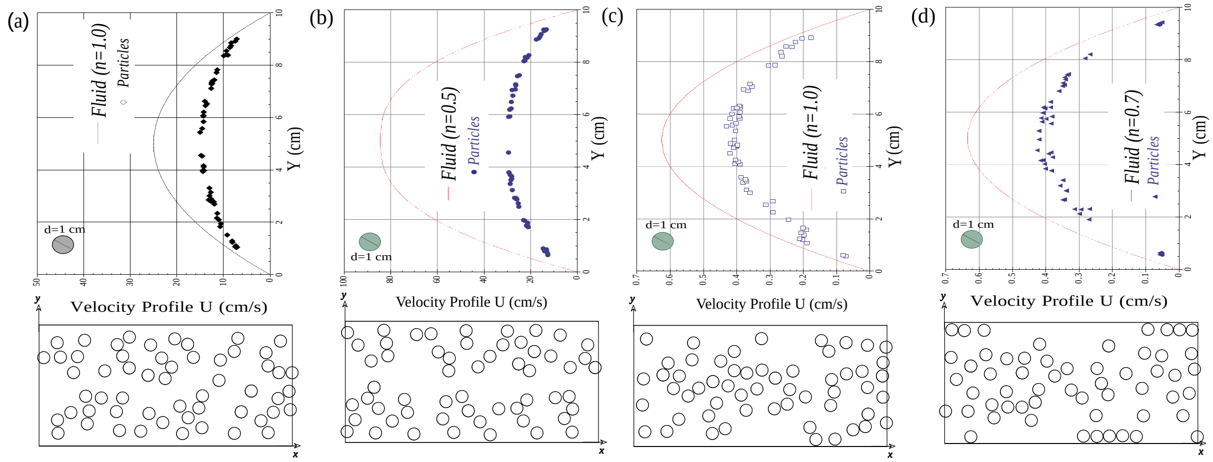


Figure 6: Cross stream migration of 56 neutrally buoyant circular particles in simulations of particle-laden Poiseuille flow using the ALE particle mover. The velocity profiles without and with particles are shown at the top of each sub-figure; underneath is a snapshot of the particle distribution. n is a power law index. (a) Newtonian fluid. The particles remain well dispersed, but a lubrication layer is evident. (b) Generalized Newtonian fluid. The particles migrate away from the center when the fluid is shear thinning. (c) Viscoelastic fluid (Oldroyd B). The particles migrate toward the center with no shear thinning. (d) Viscoelastic fluid (Oldroyd B). A clear annulus of fluid develops in the flow of an Oldroyd B fluid with shear thinning ($n = 0.7$).

The Stokes flow analysis is not valid for lift off of proppants; for these heavy particles our numerical results show lift off at shear Reynolds numbers in the hundreds. The perturbation analysis are of considerable value because they are analytic and explicit even though they are only valid well below the values characteristic of our applications. A perturbation of Stokes flow with viscoelasticity is being carried out in our group.

The rate of settling of particles is complicated by the lateral migration of particles which gives rise to lubrication layers and clumping of particles (drafting, kissing and chaining) associated with fluid microstructure. The migration of particles is greatly different in Newtonian, shear-thinning, and viscoelastic fluids and these differences are most efficiently studied using DNS validated by experiments.

The difference between the buoyant weight and inertial lift on a single suspended particle moving forward can be obtained by interrogating DNS. This difference must be modeled in problems involving settling and resuspension.

4.3 Modeling and DNS

The oil industry makes extensive use of models programmed on PCs to guide field operations. The practice is to generate commercial PC packages based on “two-fluid” equations closed by empirical correlations. We are going to work with STIMLAB on such a model, noting that now we can not only check the correlations against STIMLAB’s experiments, but can even generate the correlations themselves using DNS. We are also introducing a Lagrangian particle tracker (LNS), in which the particles obey Newton’s laws, but the fluid forces on the particles and the particles’ effects on the fluid are modeled; this modeling can be validated against DNS. LNS can run on a PC, but it has not previously been promoted for field practice.

Two-Fluid Models. Empirically based conservation models are used by the oil companies to help guide fracturing operations, but none of them works well enough for reliable guidance. The difference between the various models—and the point at which direct simulation can help—is in the correlations required to complete the model. Without going into derivations, one finds that

$$\frac{\partial}{\partial t}hc + \frac{\partial}{\partial x}hcU_{\mathrm{s}} + \frac{\partial}{\partial y}hcV_{\mathrm{s}} = 0, \tag{1}$$

$$\frac{\partial}{\partial t}h(1-c) + \frac{\partial}{\partial x}h(1-c)U_{\mathrm{l}} + \frac{\partial}{\partial y}h(1-c)V_{\mathrm{l}} + q_{\mathrm{lo}} = 0, \tag{2}$$

$$cU_{\mathrm{s}} + (1-c)U_{\mathrm{l}} = -\frac{h^2}{12\mu(c)}\frac{\partial p}{\partial x}, \tag{3}$$

$$cV_{\mathrm{s}} + (1-c)V_{\mathrm{l}} = -\frac{h^2}{12\mu(c)}\left(\frac{\partial p}{\partial y} - \rho_{\mathrm{m}} g\right). \tag{4}$$

Here $h(x,y,t)$ is the fracture width, c is an average solids fraction, $\mathbf{U}_{\mathrm{s}} = U_{\mathrm{s}}\mathbf{e}_x + V_{\mathrm{s}}\mathbf{e}_y$ and $\mathbf{U}_{\mathrm{l}} = U_{\mathrm{l}}\mathbf{e}_x + V_{\mathrm{l}}\mathbf{e}_y$ are the average solid and liquid velocities, p is the pressure, q_{lo} is the liquid leak-off into the reservoir, $\rho_{\mathrm{m}} = c\rho_{\mathrm{s}} + (1-c)\rho_{\mathrm{l}}$ is the composite or mixture density, and $\mu(c)$ is the effective viscosity of the mixture.

Equations (1)–(4) comprise four equations in the 6 unknowns U_{s}, U_{l}, V_{s}, V_{l}, c, p; two additional equations are needed to complete the mathematical system. In systems like these there is no way to proceed further without some empirical input. In fluidization and sedimentation applications, excellent results have been obtained with empirical inputs of the Richardson-Zaki type, in which the components of the slip velocity $\mathbf{U}_{\mathrm{slip}} = \mathbf{U}_{\mathrm{s}} - \mathbf{U}_{\mathrm{l}}$ are modeled by

$$U_{\mathrm{s}}(c) - U_{\mathrm{l}}(c) = K_1(c)\big(U_{\mathrm{s}}(0) - U_{\mathrm{l}}(0)\big), \tag{5}$$

$$V_{\mathrm{s}}(c) - V_{\mathrm{l}}(c) = K_2(c)V_{\mathrm{s}}(0) \tag{6}$$

where $K_1(c)$, $K_2(c)$ are to-be-determined functions of c. These equations complete the mathematical system. The quantity $V_{\mathrm{s}}(0)$ is just the terminal velocity of a settling particle, which may be obtained by equating the buoyancy force to the empirical drag formula of Dallavalle; this yields the equation

$$\frac{8}{3}\left(\frac{\rho_{\mathrm{s}}}{\rho_{\mathrm{l}}} - 1\right)ag = V_{\mathrm{s}}(0)^2\left(0.63 + \frac{4.9}{\sqrt{Re}}\right)^2\left(1 - \frac{2a}{h}\right)^{-\frac{9}{4}}, \qquad Re = \frac{2aV_{\mathrm{s}}(0)\rho_{\mathrm{l}}}{\mu(0)},$$

where a is the radius of the particle. (The last empirical factor has been introduced to account for the retarding effects of nearby walls.) The quantity $U_{\mathrm{s}}(0) - U_{\mathrm{l}}(0)$ is the slip velocity of a particle in a Poiseuille flow, and is not modeled in the two-phase flow literature. In our simulations of Poiseuille flow with a single heavy particle, the slip velocity is proportional to the pressure gradient and to the height above the bottom of the slot to which an inertially suspended particle will rise to balance its buoyant weight. DNS offers a unique opportunity to model this quantity.

To complete this theory it is necessary to determine $K_1(c)$, $K_2(c)$, and $U_{\mathrm{s}}(0) - U_{\mathrm{l}}(0)$. (In the applications, h is also unknown and is determined by coupling to the pressure through a fracture model [2, 67].) Moreover, an effective radius of the particles might be used to replace a as a fitting parameter associated with the tendency of particles to clump. It is probably incorrect to seek a set of fitting parameters and functions which would work for all different fluids, say gels and water. A more effective strategy is to divide the universe of fracturing fluids into a small number of envelopes containing fluids of roughly the same type, and to do a fitting study for each of these. The fittings required will most definitely involve backing out data from direct simulations of slot problems, as well as from STIMLAB's experiments.

Lagrangian Particle Tracker. Turning now to the second approach, we have developed a Lagrangian particle tracker (LNS) for solid-liquid flow in viscous fluids, following [88]. In this approach the fluid satisfies a two-fluid model equation in which the fluid velocity and solids fraction are unknown. The particle motion influences the fluid motion through a momentum exchange term. The fluid equations are solved in the field at each $(\mathbf{x}, t)$ point in the usual Eulerian way. On the other hand the motion of the particles is governed by a model of Newton's law for rigid particles in which an empirical form of fluid forces is used. Mapping of particle properties to an Eulerian grid and then mapping back the quantities needed to determine particle acceleration allows one to compute trajectories of the particles from dilute mixture to close pack. The motions of tens of thousands of point particles can be simulated in this way.

This method is fairly typical of many modeling approaches to particulate flows. The hope here is that microstructural properties which are not well represented by LNS average out when the suspensions are dense and the number of particles is large. Obviously such models can be used to solve slot problems but their validity should and will be checked against DNS simulations.

Part III Computational Algorithms for DNS

To extract information implicit in the equations of motion for solid-liquid flows using DNS, it is necessary to solve the coupled system of differential equations consisting of the equations of fluid motion and the equations of rigid-body motion, 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. A computational scheme for solving this coupled system of equations will be referred to as a *particle mover*.

In the Grand Challenge project, we developed two separate particle movers—the ALE particle mover and the DLM particle mover. Both use finite elements for spatial discretization; both are based on a *combined weak formulation*, introduced by Hesla in [30], in which fluid and particle equations of motion are combined into a single weak equation of motion from which the hydrodynamic forces and torques on the particles have been eliminated. This prevents a numerical instability which can arise when the equations of fluid and particle motion are integrated as a coupled system with explicitly computed force and torque (see [35]).

Both particle movers use state-of-the-art techniques of scientific computation and have been developed into highly efficient parallel codes. Under KDI/NCC, we will implement cutting-edge techniques from computer science to further increase the efficiency of our particle movers, as detailed in Sections 5.1 and 6.1.

5 ALE Particle Movers

5.1 Description

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, [29, 40, 68]). 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 governing equations are discretized in time using an implicit/explicit scheme, in which the fluid and particle velocities are determined implicitly, while the positions of the particles and grid nodes are updated explicitly. The scheme has been implemented for both Newtonian and viscoelastic fluids. For viscoelastic fluids, an elastic-viscous split stress (EVSS) scheme with mixed order interpolation functions is used to discretize the constitutive equation. For further details about this particle mover, see [32, 35].

The ALE particle mover requires the solution of a large system of nonlinear algebraic equations using Newton's method that requires the solution of a large sparse system of linear equations at each iteration. For viscoelastic fluids, this system has the form:

$$\begin{pmatrix} A & A_{I\Gamma} & B & 0 & G & 0 \\ 0 & I & 0 & 0 & 0 & P \\ B^T & B_\Gamma^T & 0 & 0 & 0 & 0 \\ H & H_\Gamma & 0 & D_1 & 0 & 0 \\ E & E_\Gamma & 0 & Q & D_2 & 0 \\ P^T A_{\Gamma I} & P^T A_\Gamma & P^T B_\Gamma & 0 & P^T G_\Gamma & D \end{pmatrix} \begin{pmatrix} u_I \\ u_\Gamma \\ p \\ \tau_N \\ \tau_E \\ U \end{pmatrix} = \begin{pmatrix} f_1 \\ 0 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \end{pmatrix} \tag{7}$$

where u_Γ denotes the velocity unknowns on the particle surface, u_I denotes the interior velocity unknowns, p are pressure unknowns, U is the particle velocity, and τ_N and τ_E are the fluid stresses. Furthermore, the projection operator P represents the no-slip boundary condition on the particle surface, and D is the symmetric and positive-definite mass matrix for the particles. The system for Newtonian fluids does not have the unknowns for fluid stresses τ_N and τ_E or the associated rows.

5.2 Solution of Linear and Nonlinear Systems

To solve the linear systems in (7) in large scale simulations of three-dimensional models, we must rely on preconditioned iterative methods implemented on parallel architectures. The two main challenges that must be addressed are that these systems are (1) extremely large—typical 3-D simulations may have millions of unknowns, and (2) ill-conditioned and indefinite, which causes serious difficulties for traditional iterative methods and general purpose preconditioners based on incomplete LU factorizations. In order to overcome these challenges, we propose to exploit parallel processing and develop preconditioning strategies specific to our problems. We will explore several solution techniques, including new methods and methods which are a continuation of work done under the Grand Challenge grant. Throughout the investigation, efforts will concentrate on developing matrix-free methods that do not require explicit storage of coefficient matrices. Next we discuss a variety of preconditioning strategies for the above linear systems.

Domain Decomposition Methods. Domain decomposition type methods [3, 4, 13, 87] are the preferred approach for solving discretized systems of partial differential equations in parallel environments. The equations are first partitioned using a general graph partitioner such as METIS [54] and the subproblems are mapped onto the processors. A preprocessing phase determines some information to prepare for the iteration phase. This preprocessing phase obtains the data to be exchanged between processors, various local data objects, and local matrices for preconditioning. Then a standard Krylov accelerator can be invoked for the solution phase. A number of libraries and packages have been developed around these principles [1, 14, 45]. PSPARSLIB is a package developed specifically for solving large sparse linear systems on distributed memory parallel computers. It provides some of the standard preconditioners such as additive and multicolored multiplicative Schwarz preconditioners. However, work done in Saad's team indicates that a technique based on global preconditioners induced by a local Schur complement preconditioner performs best [77]. The key idea of this technique is that a global preconditioner can be developed from any local preconditioning technique by using Schur complements.

Block Preconditioners. To solve the systems in (7), we first consider block preconditioning matrices obtained by neglecting G and P. This basically decouples the fluid and solid equations. This scheme was first proposed by Golub and Wathen [27, 83, 96]. Neglecting P may cause a deterioration of the convergence rate of the iteration, especially for flow problems with high Reynolds number and a large number of particles. The effect of P can be recovered by rearranging the equations or by introducing iterations. Preliminary tests reveal that the diagonal preconditioners for D, D_1, and D_2 are normally good enough. It remains to find the optimum arrangement of the systems and a suitable preconditioner for the Navier-Stokes block.

Preconditioners for Constrained Equations. Traditional preconditioners for the Navier-Stokes system work very poorly unless a fairly accurate incomplete factorization is used. The high amounts of fill-in required by these accurate IC (or ILU in the non-symmetric case) factorizations are unacceptable because of the memory requirement for large matrices. We plan to investigate a number of methods that revolve around principles first developed for solving the Stokes equation [16]. The preconditioners in [16] can be viewed as a method for preconditioning the Schur complement $B^T A^{-1} B$ with the mass matrix associated with the finite elements for the pressure variables. This induces a preconditioner for the whole matrix (7), which in turn will induce a global preconditioner in a distributed parallel programming environment. Efficient preconditioners for the Schur complement can be obtained by several means. One technique that was successfully used in the past is to overlay a regular mesh on top of the irregular one and use a fast solver for the regular problem as a preconditioner [97]. Interpolation is used each time to pass from nodes of the irregular mesh to those of the regular mesh. Another option is to use a multilevel scheme (e.g., algebraic multigrid) for the Poisson equation.

Approximate Inverse Methods. We will develop matrix-free preconditioners which do not require explicit storage of coefficient matrices. One appealing strategy is to use approximate inverse methods [9, 10]. Knowledge of the nonzero structure of the matrix can be combined with multicoloring strategies to compute sparse approximations to the inverses of the original matrix. These methods require the matrix only through matrix-vector products which can be implemented in matrix-free mode.

Parallel Balanced Scheme. An alternative to Krylov subspace methods in handling systems of the form $Ax = b$ in which A is known to be of a narrow band is a hybrid algorithm proposed by Sameh and Sarin [78]. This algorithm was motivated in part by unresolved issues in preconditioned Krylov subspace methods and limited concurrency in preconditioning. Our technique is based on a new approach described in [26] that uses projections onto subspaces spanned by block rows of the linear system. (See e.g., [62, 69, 80] for more details.) This approach can be implemented in a matrix-free setting, and is most suitable for a bandwidth that is about 1%–15% of the total number of unknowns. In this method a reduced system is generated implicitly, defined only on unknowns common to consecutive block rows, and is solved by an iterative method in which matrix-vector products are performed directly from the projections. This robust projection-type method has the desirable properties of generating a preconditioned modified system implicitly, and exhibiting concurrency both at coarse and fine levels of granularity on cluster-based parallel computers. Preliminary experiments have yielded efficiencies over 90% on parallel computers such as the SGI Origin 2000.

The linear systems involving the matrix A for three-dimensional particulate flow problems have a larger bandwidth. In such cases, the balanced scheme can be used to precondition an iterative method such as GMRES. One may extract a narrow band linear system as a preconditioner, that can be solved efficiently using the balanced scheme. Such a matrix can be extracted from the physical problem itself by accounting for the fluid flow direction that results in a dominant submatrix with a much narrower band. We plan to also formulate a general form of the balanced scheme that is not restricted to systems with narrow bandwidth.

5.3 Alternate ALE Approaches

Operator-Splitting ALE Particle Mover. We will develop a new, more efficient solver for the ALE particle mover based on an operator-splitting scheme. This decouples, at each time step, the problems related to the incompressibility, the nonlinearity, the viscoelasticity, and the particle motion. The problems to be solved at each sub-step of the splitting are therefore smaller, simpler, and often linear. These usually include several advection-diffusion problems and a generalized Stokes problem. Since they are discretized by finite-element methods on a moving, topologically unstructured mesh, these equations result in smaller and simpler algebraic systems which can be more efficiently preconditioned. The advection-diffusion problem could be linearized using the backward method of characteristics as introduced by B. A. Maury and R. Glowinski in [64].

A Projected Particle Mover. We have developed a variation of the ALE particle mover [57] 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 [81] 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.

The convergence can be improved by using a variant of the multilevel algorithm, the truncated multilevel algorithm, that requires a coarse level QR factorization, and yields a better conditioned basis P_v. We will develop scalable parallel implementations of this method and investigate its effectiveness for our problems. We will also investigate the relation of the nested iterations for the nonlinear solvers and exploit this knowledge to optimize the implementation of our solver.

6 DLM Particle Mover

6.1 Description

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. 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 A. Chorin [6–8] and R. Temam [91].) 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 [25]. The *immersed boundary method* of C. Peskin and his collaborators [72–74] on the simulation of incompressible viscous flow in regions with elastic moving boundaries also uses a fictitious-domain method, but without Lagrange-multipliers.

To date, the DLM particle mover has been implemented only for Newtonian fluids but a viscoelastic version, also based on an operator-splitting scheme, is currently under development (see Section 6.3). Operator-splitting methods, and methods such as the method of characteristics, can avoid nonlinear iterations; these iterations can create difficulties even for Navier-Stokes solvers. For viscoelastic solvers, there is reason to believe that many of the problems of divergence encountered at high Deborah numbers are associated with the nonlinear iterations commonly used. For example, P. Saramito used a θ-splitting to simulate the flow of an Oldroyd B fluid up to $De \simeq 10^2$ [79].

6.2 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 a 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 [92]. The second step requires the solution of a non-linear discrete advection-diffusion problem that is solved by the algorithm discussed in [22]. The third step solves another saddle-point problem using a 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 [70]). 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 an overkill since the solution is required only to modest accuracy. A multilevel parallel elliptic solver [82] 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. 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. At present, we are developing portable parallel code for the DLM algorithm capable of execution on a variety of architectures. We are also exploring more scalable implementations of the multilevel algorithm that will achieve optimal speedup on a larger number of processors. In addition, we plan to investigate approximations of fast elliptic solvers that may provide us with alternate parallel preconditioners.

The multilevel technique used in the DLM particle mover is a special case of the algorithm proposed in [81]. The general algorithm can be directly applied to the saddle-point problem that needs to be solved in the first step. It has been shown that such an approach can reduce the overall time for solution substantially. Furthermore, there is a clear advantage in using the multilevel algorithm to solve saddle-point problems arising from second-order time-accurate splitting methods. This approach will be investigated for the linear systems arising in the DLM algorithm.

One of the aims of this effort is to develop portable codes that may be easily optimized for any parallel architecture. This will provide us with the ability to simulate large scale problems on a wide variety of architectures, and help us keep abreast with the rapidly changing technologies of high performance computing.

6.3 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

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\boldsymbol{\nabla}\mathbf{u}\right) = -\boldsymbol{\nabla}p + \boldsymbol{\nabla}\cdot(2\mu\mathbf{D} + \mathbf{A}), \tag{8}$$

$$\boldsymbol{\nabla}\cdot\mathbf{u} = \mathbf{0}, \tag{9}$$

$$\lambda\left(\frac{\partial \mathbf{A}}{\partial t} + \mathbf{u}\cdot\boldsymbol{\nabla}\mathbf{A} - \mathbf{A}\cdot\boldsymbol{\nabla}\mathbf{u} - \boldsymbol{\nabla}\mathbf{u}^T\cdot\mathbf{A}\right) + \mathbf{A} = \frac{\eta}{\lambda}\mathbf{1} \tag{10}$$

where $\mathbf{D}$ is the rate-of-strain tensor, $\mathbf{A} = \boldsymbol{\tau}_{\mathrm{E}} + (\eta/\lambda)\mathbf{1}$ is the configuration tensor, $\boldsymbol{\tau}_{\mathrm{E}}$ is the elastic stress, η is the elastic viscosity, and λ is the relaxation time. These equations are to be solved subject to appropriate boundary conditions. The viscoelastic DLM particle mover we are developing must solve this system of equations, together with the rigid-body equations of motion for the particles.

The system (8)–(10) is classified mathematically as being of *composite* type [46]: 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 [85].

This Hadamard instability can be prevented by ensuring that $\mathbf{A}$ remains positive-definite using a method introduced by Singh in [85, 86]. The method has two key elements: a third-order upwinding scheme for discretizing the convection term in (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.

To construct a viscoelastic DLM particle mover, we will combine the viscoelastic flow solver described above, with the fictitious-domain/distributed Lagrange multiplier scheme used in the Newtonian DLM particle mover [25]. An operator-splitting method will be used to decouple the motion of particles from the viscoelastic fluid-flow problem. As in [25], rigid-body motion will be enforced weakly inside the particles using a distributed Lagrange multiplier. A second distributed Lagrange multiplier will be used to enforce the constraint $\mathbf{A} = (\eta/\lambda)\mathbf{1}$ inside the particles; the "fictitious" viscoelastic fluid inside the particles is constrained to be in the relaxed state. The decoupled viscoelastic fluid-flow problem on a fixed domain, subject to these two side constraints, will be solved using a modified version of Singh's algorithm. The particle positions will be updated using a predictor-corrector approach similar to that described in [25].

To simulate systems with a large number of particles at high volume fractions it will be necessary to develop procedures with minimal memory requirements which give accurate solutions with a small number of iterations. The regular mesh used in the DLM method allows us to use efficient solvers and to reduce the storage requirements, since only the nonzero diagonal elements of the underlying matrices need to be stored. We will extend the parallel formulation of the DLM particle mover to the viscoelastic case.

Part IV Research Team and Tasks

The multidisciplinary research team for this KDI/NCC proposal consists of experts in fluid mechanics and applications, in CFD algorithm development, in computer science, and in the engineering aspects of proppant transport in fractured reservoirs. The two goals of the proposal are to push the envelope of what is presently possible in direct numerical studies of the motion of many particles in liquids under conditions that prevail in industrial applications and to find the ways to make these DNS results useful to our partners in the oil and gas industry. This proposal brings together four of the university teams which were funded by the NSF Grand Challenge grant in 1995, together with industrial partners.

7 Applications

Our industrial partners are the 32 companies that support research on ways to stimulate the production of oil and gas from fractured reservoirs. These companies form a consortium which funds a research laboratory (STIMLAB) in Duncan, OK. The participating companies are

Acme Resin Corporation
Amoco
Aqualon Company
ARCO
BJ Services
BP Exploration
Canadian FracMaster, Ltd.
Carbo Ceramics, Inc.
Chevron
China Natl. Petro. Corp.
Conoco, Inc.
Dowell Schlumberger
Edinburgh Petro. Services, Ltd.
Gas Research Institute
Halliburton Energy Services
KELCO
Kronklijke/Shell-Exploratie
Maersk Olie Og Gas as
Marathon Oil Company
Mobil
Nowsco Well Services Ltd.
ORYX Energy Company
Pennzoil
Petrobras
Phillips Petro. Company
Produkie Laboratium (KSEPL)
Rhone-Poulenc
Santos, Ltd.
Shell
Texaco
Union Pacific Resources Co.
UNOCAL
Western Co. of No. America

The collaboration between this consortium and our multidisciplinary team is through STIMLAB. The consortium funds STIMLAB and STIMLAB funds us; they give us $20,000 per year for research and they are going to support a postdoc at $32,000 per year.

STIMLAB does experiments. They have laboratories in Duncan, OK and Edinburgh, Scotland and sales offices in many cities worldwide. They were recently absorbed by a bigger company, Core Laboratories, but they continue to operate independently. They have been collecting data on sand transport in large and small slots for fifteen years. They have a huge data bank, ripe for exploitation, which can be used for modeling and simulation. The interest of the consortium and STIMLAB in our work has drifted from experiments, which they can do themselves, to simulation, which they cannot do. I lecture at the biannual meetings of the consortium; at the last (Feb 1998) meeting they voted unanimously to support the work proposed in this KDI/NCC proposal. The consortium has assigned us 10% of their annual budget to " ... jointly with the University of Minnesota, develop pseudo-3D fluid flow correlations to predict 3D slurry transport phenomena from measured fluid properties." Joseph, Hu, Singh, and Glowinski (and their students and postdocs) will collaborate with Dr. Glenn Penny (president), Dr. Mike Conway (vice president) and Dr. D. M. Asadi (rheologist) from STIMLAB. They are going to use data from DNS on resuspension, fluidization, sedimentation, and slip velocity, together with experiments from STIMLAB, to construct LNS and two-fluid fracture-transport PC models.

8 Code Development

The group at Penn will develop a more efficient ALE particle mover by introducing block preconditioners which take full advantage of the structure of the linear systems, by developing a new solver using an operator-splitting method, and by implementing a new matrix-free formulation for solving the discretized system. They will also carry out simulations with particles of different shapes in complicated geometries.

Glowinski (Houston), together with E. J. Dean and T.-W. Pan, is going to investigate the construction of particle movers based on (1) symmetrized operator-splitting schemes in order to increase the time-discretization accuracy, (2) the treatment of the advection by the method of characteristics and the wave-equation-like approach described in [11, 12], and (3) the use of a well chosen discrete H^1 scalar product to speed up the convergence of the conjugate-gradient algorithm used to compute the distributed Lagrange multipliers in the DLM methodology.

These algorithms will be parallelized using multi-level schemes. The same methodology will be applied to the viscoelastic particle mover being developed by P. Singh [NJIT]. (Singh is a senior investigator and will work on a subcontract.) Y. Kuznetsov and his collaborators will investigate the construction of efficient parallel preconditioned conjugate-gradient algorithms to solve the very large Poisson problems required by 3-D applications when we force the incompressibility condition. They will investigate the efficient implementation of body-fitted fictitious domain methods which are in some sense intermediate between the methods developed by Hu and those developed by Dean, Glowinski, and Pan.

A. Sameh, V. Sarin, and M. Knepley propose to develop parallel algorithms for both the ALE and DLM particle movers. Further, these particle movers will be implemented so as to be modular, as well as portable across several large-scale computational platforms. Performance measurements for both particle movers will be documented and reported. In particular, they propose to (1) develop effective nested iterations, (2) develop matrix-free parallel linear-system preconditioners for both the ALE and DLM particle movers, (3) explore extensions to second-order-accurate methods such as the θ-scheme for the DLM particle mover, (4) enhance and develop extensions to 3-D viscoelastic ALE and DLM particle movers, and (5) develop scalable parallel implementations of multilevel preconditioners.

Yousef Saad's work will primarily be in the development of new iterative solvers for use in the ALE particle mover. Specific areas of focus will be (1) development of domain decomposition strategies (along with Joseph's team), (2) development of preconditioning strategies specific to constrained equations, (3) collaboration with H. Hu on preconditioners tailored to the block structure, (4) collaboration with the Houston, Penn, and Purdue teams on matrix-free preconditioners, (5) software development issues related to the global software integration of the whole project, and (6) work on a by-product library.

Part V Results from Prior NSF Support

(Please turn to next page.)

Results from Prior NSF Support: D. D. Joseph

I was supported by NSF grants nearly continuously since 1965. Here I list the grants directly relevant to liquid-solid flow since 1991: NSF/CTS 87114407, Beds of particles fluidized by liquids from 9/87 - 3/91 for $160,700; NFS/CTS 9213979, Studies of two phase flows of solids and liquids from 9/92 - 2/97 for $365,000; NSF/CTS 9527123, Direct simulation of the motion of solids in liquids (Grand Challenge) from 10/95 - 11/98 for $1,665,000; NSF/CTS 9610059, Studies of Reservoir Stimulation, drilling, transportation, emulsion stability, and bubble reactor (Goali) from 5/97 - 4/00 for $341,084.

The references listed below are all by D. D. Joseph and coauthors, who are listed after the title. The results of the other Co-PIs and senior investigators reported in papers in which Joseph is not an author, though relevant to the NSF grand challenge work, are not listed. Most of these other references can be found in the "Results . . . " sections of the Co-PIs and are cited in the project description.

The role of wakes and turning couples on long bodies in creating flow-induced microstructure lines of spherical particles across the stream and other wake stabilized architectures were first mentioned in the papers [14, 15]. I coined the words drafting, kissing and tumbling in these papers. The first directly numerical test of stability of microstructure appeared in [30]; the experimental results on microstructure induced by wakes and turning couples on long bodies are summarized in [1, 3, 20].

The first direct numerical simulation (DNS) of fluid particle motions in Newtonian fluids appears in [20] and subsequent DNS studies of microstructure are reported in [9, 12, 13, 19, 21]. The study in [12] showed that a sedimenting particle will drift to the channel center and fall without rotation at a steady terminal velocity when the Reynolds number is small, but this gives rise to a Hopf bifurcation with a periodic off-center trajectory at higher Reynolds numbers. High pressure at the front of an ellipse settling even at Reynolds in the thousands will turn the ellipse broadside-on even as it oscillates due to vortex shedding [21]. The real hydrodynamics of forces and torques on particles associated with stagnation and separation points, and with distributions of pressures and shears on the boundary of a particle size control the migration of particles and can be generally examined only through DNS [7, 13, 21]. Application of DNS to multi-particle Stokes flow [9] shows that inertia has cumulative effects on the migration of particles at long times which cannot be neglected.

Most of the major features of microstructures of particles settling in viscoelastic fluids were established in our experiments. Long bodies align with rather than across the stream; spherical particles aggregate and form chains along the stream (see figure 1 and [25–27, 29]). The observed microstructure can be interpreted as a competition between inertia and normal stresses. A theoretical interpretation of these observations was obtained by mathematical analysis in [6, 8]. Roughly speaking, the normal stresses give rise to a viscoelastic pressure, a compressive stress proportional to the square of the shear rate; the viscoelastic pressure is large near to points where the velocity is large, where the pressure due to inertia is small. This fact goes a long way in explaining why the microstructure due to viscoelasticity and inertia are so different. Some anomalous behaviors observed in experiments [10, 31] are not so well understood. **Foams** are used to carry sand in fracture to clean drilling holes and as an unwanted by-product in refining and we found that you could control and suppress foams by fluidizing particles [16, 28]; this opens a new field of study.

We studied potential flows of viscous and viscoelastic fluids. The vorticity of popular models of a viscoelastic fluid vanishes in a "Mach cone" around a cylinder moving forward at speeds greater than the speed of shear waves and greater than the speed of diffusion. (Reynolds number larger than one) in an unbounded domain [18]. Long bodies which fall this fast will flip from vertical to horizontal (broadside on) because they are then turned by potential flow at the forward face [23, 26].

Potential flows of viscous fluids differ from inviscid fluids because they support a viscous stress [24]. The study of potential flow of viscoelastic fluids turns out to be more complicated, some models give rise to a pressure function modified by extra terms [2], other models do not support potential flows in general but do support special potential flow in general. We showed that normal extension stress at a point of stagnation in potential flow of a second order fluid could change sign due to viscoelastic turning long bodies into rather than against the stream [2]. The development of a boundary layer theory for potential flow for viscoelastic fluids is an unsolved problem which must be solved before we can use potential flow theory for DNS simulation.

Our grand challenge group presented the first [4] and all the subsequent [5, 22, 23] DNS results solving initial value problems for moving solids in viscoelastic fluid without at first constraining the motion of the solids in some way; our ALE particle mover is presently a monopoly which may not last long. The perturbation study in [11] is the first application of distributed Lagrange multiplier-embedded domain methods to viscoelastic flow problems; the application of the *total momentum method*, avoiding explicit calculation of forces, led to our DLM particle mover [17].

Publications

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Results from Prior NSF Support: H. H. Hu

NSF Grant: Study of Motion of Particles in Non-Newtonian Fluids (CTS-9410022, as PI)
Amount: $100,000
Period: 7/1/94–6/30/97

NSF Grant: Direct Simulation of the Motion of Particles in Flowing Liquids (ECS-957123, Co-PI)
Amount: $234,994
Period: 10/1/95–9/30/98

The objective of the projects is to develop highly efficient numerical methods for computing motions of large numbers of particles in both Newtonian and non-Newtonian fluids, under the action of the hydrodynamic forces and moments exerted by the suspending fluid. We have developed a software (ALE particle mover) using a finite element technique based on moving unstructured body-fitted grids. The software package is able to simulate the motion of over one thousand particles in 2-D and around one hundred in 3-D domains. The developed numerical package has been used to study the micro-structural effects which produce clusters and anisotropic structures in particulate flows, to produce statistical analyses of particulate flows, 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. Specifically the results are listed below.

ALE particle mover. A finite element technique based on moving unstructured grids is developed to simulate the motion of large numbers of solid particles in a flowing liquid. A generalized Galerkin finite element formulation which incorporates both the fluid and particle equations of motion into a single variational equation is developed. The hydrodynamic forces and moments acting on the solid particles are eliminated in the formulation, so they need not be computed explicitly. An arbitrary Lagrangian-Eulerian (ALE) technique is adopted to deal with the motion of the particles. 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. The motion of the combined fluid/particle system is simulated using a procedure in which the particle and the mesh grid positions are updated explicitly, while the fluid and particle velocities are determined implicitly.

Effects of finite Reynolds number on the rheology of a suspension of neutrally buoyant solid bodies in a Newtonian fluid. We investigated the effects of inertia (finite particle Reynolds number) and fluid elasticity on the macroscopic properties of a suspension of rigid particles in a Newtonian and an Oldroyd-B fluid. The particle-fluid mixture was subjected to uniform shear flow between two parallel plates. It was seen that the suspension of particles in Newtonian fluid shear thickens. The first normal stress difference was negative and increased in magnitude as the Reynolds number was increased. It was observed that the particle contribution to the bulk stress of the suspension of rigid particles in an Oldroyd-B fluid shear thins. The first normal stress difference was positive and increased as the Reynolds number was increased. Shear thinning and the increase in the first normal stress difference was enhanced as the elasticity of the fluid was increased.

Pressure-driven flow of solid bodies in Newtonian and Oldroyd-B fluids. We studied the motion of solid particles in Newtonian and Oldroyd-B fluids subjected to a pressure gradient. We found that the ratio of the applied pressure gradient and the pressure gradient at fluidization is the most important flow parameter which helps to identify four basic flow regimes. Fluid elasticity induced stronger migration of the particles towards the center of the channel., and caused less mixing of the particles. The suspension formed prominent microstructures, such as chains, in viscoelastic fluid and cross-stream arrays in Newtonian fluids when there were few particles in the channel. For large number of particles in the channel there was greater tendency to form clusters. Inertia of the fluid and the particles enhanced the mixing and agitation in the channel.

Motion of solid particles in Couette and Poiseuille flows of viscoelastic fluids. We studied the motion of a two-dimensional circular cylinder in Couette and Poiseuille flow of an Oldroyd-B fluid and the mechanisms which cause the cylinder to migrate. The stable equilibrium position of neutrally buoyant particles varies with inertia, elasticity, shear thinning and the blockage ratio of the channel in both shear flows. Shear thinning promotes the migration of the cylinder to the wall while inertia causes the cylinder to migrate away from the wall. In a Poiseuille flow, the effect of elastic normal stresses is manifested by an attraction toward the nearby wall if the blockage is strong. If the blockage is weak, the normal stresses act through the curvature of the inflow velocity profile and generate a lateral force that points to the centerline. In both cases, the migration of particles is controlled by elastic normal stresses.

Sedimentation of elliptic particles in Oldroyd-B fluids. We show that the normal component of the extra stress on a rigid body vanishes; lateral forces and torques are determined by the pressure. Inertia turns the longside of the ellipse across the stream and elasticity turns it along the stream; tilted off-center falling is unstable. There are two critical numbers; elasticity and Mach numbers. When the elasticity number is smaller than critical the fluid is essentially Newtonian with broadside-on falling at the centerline of the channel. For larger elasticity numbers the settling turns the longside of the particle along the stream in the channel center for all velocities below a critical one, identified with a critical Mach number of order one. For larger Mach numbers the ellipse flips into broadside-on falling again. Two ellipses falling nearby, attract, line-up and straighten-out in a long chain of ellipses with longside vertical, all in a row.

Mixing of particulate flow. We studied the motion of a solid and liquid mixture within a mixer which is simplified as blades attached to an inner cylinder rotating within a cylindrical container. A collision model is implemented to improve the efficiency of the simulation. We studied the motion of both neutrally buoyant and non-neutrally buoyant solid particles suspended in a Newtonian fluid. Effects of Reynolds number, solid volume fraction and particle size are investigated.

Particle chaining in viscoelastic fluids. We studied the mechanism for particle chaining in viscoelastic fluids. We found that a long chain of particles tends to fall faster than a single particle, which causes the separation of the last particle from the chain. In Newtonian fluids, detachment will not occur if the inertial wake effects are strong enough to cause substantial drag reduction on the last particle. In a viscoelastic fluid the detachment is also restricted by the normal stress due to the elastic effects of the fluid.

Funds from these two grants were mainly used to support the education and research of two Ph.D. students (Neelesh A. Patankar and Mingyu Zhu). Dr. Neelesh A. Patankar has received his Ph.D. degree last August and currently is a Post Doctoral Research Associate at the University of Minnesota.

Publications resulting from the awards

[1] H. H. Hu, Motion of a Circular Cylinder in a Viscous Liquid between Parallel Plates, *Theoretical and Computational Fluid Dynamics* **7**, 441–455, (1995).

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Results from Prior NSF Support: R. Glowinski and T.-W. Pan

From fall 1995 to now (April 1998) R. Glowinski and T.-W. Pan have been supported by NSF under HPCC Grand Challenge Grant ECS-9527123, in order to investigate the numerical simulation of particulate flow. The methodology selected by R. Glowinski and T.-W. Pan is based on a combination of finite element methods for the space discretization, operator splitting schemes for the time discretization, and distributed Lagrange multipliers to handle the rigid body motion of particles via fictitious domain (i.e., domain embedding) techniques allowing flow calculations on a fixed finite element mesh. From this point of view, the resulting methodology has some similar ties with the immersed boundary method of Peskin (refs. [11], [13], and [12]). Using the above methodology, which is quite novel in particulate flow related investigations (to our knowledge), Glowinski and Pan have been able to simulate the flow of solid-liquid mixtures and sedimentation-fluidization phenomena for more than 1000 particles in 2-D and more than 100 in 3-D.

The Glowinski-Pan particle mover has been parallelized by Vivek Sarin; V. Sarin's results strongly suggest that with the parallel platforms to be available very soon there will be no particular difficulty in handling as many as 100,000 particles in 2-D and over 10,000 in 3-D, for Newtonian liquids at least. And in light of a recent analysis by P. Singh and R. Glowinski showing that fictitious domain/operator splitting methods are ideally suited for handling particles moving in viscoelastic liquids à la Oldroyd B or Maxwell, it is reasonable to assume that direct simulation will be possible in viscoelastic liquids of these types, with more than 10,000 particles in 2-D and 1,000 in 3-D. The methods mentioned above and the related numerical results are described in the following publications: [1], [6], [2], [8], [3], [5], [7], [9], [4].

Also, R. Glowinski has been asked by the editors of the journal *Computational Methods In Applied Mechanics and Engineering*, to write a review article on domain-embedding methods for particulate flow; he will also include a chapter on this subject in the book-sized article "Viscous Flow Simulation" he is presently writing for the *Handbook of Numerical Analysis*.

Let us also mention the NSF-supported joint work of Glowinski and B. Maury (ref. [10]) on an ALE method for particulate flow where the advection is treated by the backward method of characteristics.

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Results from Prior NSF Support: Yousef Saad

Grants CCR– 92-14116 and CCR– 96-18827.

Title: “High Performance Iterative Solvers”.
This work started out with three main goals: (1) to develop parallel preconditioners for general sparse matrices based on domain decomposition ideas; (2) to develop preconditioners based on Incomplete LU factorization with Multi-elimination (ILUM); and (3) to develop hybrid methods using approximate inverses. The two key findings so far are the following.

A generalized version of ILUM (BILUM) offers an excellent alternative to standard ILU preconditioners. BILUM *can be viewed as a multilevel (multigrid-like) technique* and seems to inherit some of the nice scaling properties of Multigrid methods. The significance of this is that we can view these methods as Algebraic Multigrid type preconditioners, thus bridging the gap between multilevel and ILU-type techniques. Another interesting viewpoint is that block versions of ILUM (BILUM) implement in effect some form of recursive domain decomposition techniques – in which Schur complements are formed recursively on ’coarser meshes’ until the resulting problem is small enough to be solved by a standard ILU approach or a direct solver. There is no real mesh, since the method is entirely algebraic, so it is very general.

These two techniques lead to numerous possibilities for parallel processing. We are very optimistic about the prospects for the applications of this new class of algorithms. They offer both the robustness and generality of frequently used preconditioners such as ILUT, and the attraction of good scalability of multilevel techniques. They are also inherently parallel. A number of Dutch mathematicians are also going in the same direction as this class of algorithm is gaining importance.

This work also emphasizes *robust* techniques. Several variations of the basic BILUM scheme have tested to obtain preconditioners that can solve harder problems [10, 11]. With these minor modifications, the method does seem fairly robust and competes very well with enhanced versions of ILUT [3].

A new approximate Schur-LU preconditioner for distributed memory computers was developed and showed excellent convergence behavior [6, 7]. The concept of distributed sparse matrices is quite natural and involves implementing data structures and pre-processing routines to prepare for communication in a distributed memory parallel computer. We have implemented such a data structure using the MPI communication library as part of the PSPARSLIB library work, a former project supported by DARPA. The library now includes this preconditioner and a few others. It is a general-purpose portable package for solving general unstructured sparse linear systems by iterative methods.

Grants DMR 92-17287 and DMR 95 25 885

Title: “Massively Parallel Algorithms for Modeling the Structure of Liquids and Liquid-Solid Interfaces,”
Principal Investigators: Professor J. R. Chelikowsky and Professor Y. Saad.

The objective of this research was to explore the use of high performance parallel computers for solving the large scale problems that arise in modeling real materials. Recent developments in high performance computing technologies have created new opportunities in the application of sophisticated electronic structure techniques to the study of these materials.

This objective required a rethinking and re-evaluation of traditional approaches. For example, the use of methods which employ Fast Fourier Transforms was avoided as these methods often present communication obstacles in parallel architectures. Instead, we focussed on new algorithms that discretize the key equations in real space, resulting in an easy implementation on multi-processor computing platforms. The key ingredients of our approach combined a higher-order finite difference method with a pseudopotential description of the electronic structure problem.

Applications of our new algorithms centered on examining technologically important electronic materials, e.g., Si, Ge, GaAs, and GaP. Key findings include predictions for the structure of neutral and charged clusters at finite temperature, and for the structural and dynamical properties of semiconductor liquids. Our work has demonstrated the feasibility and cost-effectiveness of exploiting parallel computing (massive and moderate) for examining complex systems of hundreds of atoms from first principles. The contribution of the computer science side of this project (Y. Saad) was in three areas (1) initiative in moving to real-space methods in order to avoid FFTs, (2) design and implementation of parallel algorithms, and (3) design and implementation of methods for computing eigenvalue and eigenvectors required at each self-consistent step.

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Results from Prior NSF Support: Ahmed Sameh

NSF Grant: ECS-9527123 (Purdue University)
Period: 01/01/97 - 09/30/98
Title: Direct Simulation of the Motion of Particles in Flowing Fluids

Summary of Results: We have developed innovative algorithms that have been incorporated in both ALE and DLM particle movers. Our parallel multilevel algorithm has been used to restrict ALE systems to divergence-free space [5], resulting in faster convergence for the time-consuming linear system solvers. The same algorithm has been optimized for preconditioning the linear system in the DLM approach. We have developed parallel formulations for both particle movers [5, 6], and demonstrated reasonable speedup on parallel computers such as the SGI Origin-2000. We have also investigated novel iterative algorithms [3, 7] and parallel preconditioners [2, 4, 7] that hold promise for large scale parallel simulations. We are presently engaged in integrating our iterative algorithms and preconditioners with the particle movers, and optimizing the parallel implementation of our code for particular architectures.

The project involved one postdoctoral candidate (Dr. Vivek Sarin), and one graduate research assistant (Mr. Matthew Knepley). Dr. Sarin completed his Ph.D. degree under my supervision at the University of Illinois (Urbana), and Matthew Knepley is working on his Ph.D. thesis under my supervision.

NSF Grant: CCR-9619763
Period: 02/15/97 - 01/31/99
Title: High Performance Computing for Large Dynamical Systems

Summary of Results: This study concerns the development of robust parallel algorithms for those large algebraic generalized eigenvalue problems that arise in the design and analysis of dynamical systems. We have concentrated our efforts on improving our trace minimization method, which we developed in 1980, compare it with the variety of the Jacobi-Davidson schemes for the symmetric case, and extend a concept similar to trace minimization to the nonsymmetric generalized eigenvalue problem. An improved shifting strategy for the classical Sameh-Wisniewski has been implemented [8], and our results indicate superior performance to the existing Jacobi-Davidson algorithms for the symmetric case.

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Part VI Dissemination of Results and Institutional Commitment

We are going to continue the procedures for the dissemination of academic results which were established in our Grand Challenge project. These results will ultimately be published in archival journals.

The Web is used to disseminate our research; since all the participating universities are linked in our Web site

http://www.aem.umn.edu/Solid-Liquid_Flows;

the Internet is our face to the world. In addition to explanations of our Grand Challenge effort, the biographies of our team, and the titles of the 48 papers published in the course of our grant work, we have put up many computer animations; these animations of moving particles are a particularly good theater to show the world what we do.

The applications-oriented results of our fracture/transport studies will be published in the usual multiphase flow journals, but also in journals of the oil and gas industry; in addition, these results will be disseminated to the oil companies in the STIMLAB consortium at their biannual meetings and in STIMLAB reports. The fracture results which will emerge in this KDI/NCC research are at different levels of sophistication. The engineers working on fracture jobs and their managers ought to be educated about the effects of the fluid on migration, lift-off, resuspension, and other microstructural features bearing on sand transport, at a level they will understand. We are planning a paper with STIMLAB about the aforementioned effects; this paper will be presented at SPE meetings and published in an SPE journal, and will be written for understanding at the level of the readers. Joseph is preparing a long review paper on particulate flow and DNS to be published in the *International Journal of Multiphase Flow*, for the multiphase flow community.

The main institutional commitment bearing on this proposal is allocations of computer time—particularly with regard to the SGI Origin 2000, which after experimentation with different platforms, is our platform of choice. We have used 8-processor SGI Power Challenge machines in several of our institutions, and the SGI Origin 2000 at NCSA (University of Illinois), which is the largest in the U.S. The University of Minnesota Supercomputer Institute (UMSI) has leased a 128-processor Origin 2000 with 48 gigabytes of memory, and has purchased a 256-node IBM SP2. We will have access to both machines. UMSI has already provided us with what we need locally. The problem with large machines at institutions is that they are heavily used with excessively long queues. For this reason, we are requesting funds for a dedicated machine—an 8-processor SGI Origin 2000 with 1 gigabyte of memory. This machine will be for the exclusive use of our Co-PIs. Since Minnesota (Aero and Computer Science), Houston, Purdue, and Pennsylvania all have direct ATM connections on the NSF sponsored vBNS/Internet 2 high-speed backbone project, we can have lightning-fast communications; this will speed up our development effort for parallel implementation on larger machines.

Part VII Performance Goals

Year 1

1. ALE particle mover: Preconditioners for linear systems.
    - Explore block preconditioners and domain decomposition techniques.
    - Explore preconditioners for projected ALE particle mover system.
2. ALE particle mover: Nonlinear solvers.
    - Explore relation of nested iterative method.
    - Explore alternate approaches based on method of characteristics and wave-equation.
3. DLM particle mover.
    - Develop DLM particle mover for viscoelastic fluids.
    - Develop symmetrized operator splitting schemes for DLM particle mover.
4. Develop and implement Lagrangian particle tracker.
5. Experiments and validation.
    - Study flow induced particle microstructures.
    - Benchmark flow cases with sedimentation and fluidization.
    - Investigate particle resuspension, inertia lift-off.

Year 2

1. ALE particle mover.
    - Develop alternate solver based on operator-splitting method.
    - Develop matrix-free formulations.
    - Develop parallel preconditioners based on domain decomposition and multilevel techniques.
2. DLM particle mover.
    - Develop and implement parallel formulations.
    - Implement parallel preconditioners.
    - Develop extensions to 3-D viscoelastic situations.
3. Test collision strategies.
4. Experiments and validation.
    - Study further flow-induced particle microstructures.
    - Initiate both DNS and LNS of slurry transport and hydraulic fracturing.
    - Generate correlations useful for field practice by DNS and LNS.

Year 3

1. ALE particle mover: Extensions to arbitrary shaped particles and complicated flow geometries.
2. DLM particle mover: Implement body fitted fictitious domain methods.
3. Experimentation, validation, and performance evaluation.
    - Perform additional DNSs and LNSs of slurry transport and hydraulic fracturing, and compare the results with data from STIMLAB.
    - Construct and field test a two-fluid model for fracturing transport for PCs.
    - Benchmark 3D simulation of 10,000 particles and 2D simulation of 100,000 particles in a Newtonian fluid.
    - Performance evaluation of particle movers on parallel architectures.
4. Dissemination.
    - Library development.
    - Symposium.

Part VIII Project Management Plan

The present KDI/NCC proposal brings together four of the university teams which were funded by the NSF in 1995 under a Grand Challenge grant "Direct simulation of the motion of solids in liquids" together with a new industrial partner (STIMLAB) to focus the application side of our work on sand transport in fractured oil and gas reservoirs.

Funding of the Co-PIs and one senior investigator (P. Singh, NJIT) will be through subcontracts administered through Joseph's department. Andy Wathen (Oxford) will be funded as a consultant with payment against invoice from the University of Minnesota. The participation of STIMLAB will be administered by Glenn Penny (president). They will fund the project at a level of $52,000 per year; $32,000 is for support of a postdoc.

A multidisciplinary effort as diverse as ours requires active management; direct communications between very different groups, say computer scientists and engineers, may not be possible. In our Grand Challenge work we were surprised to find that even the communication between the CFD and CS groups was not easy. These communities have distinctly different notions about how problems ought to be formulated and solved, and technical language used by each group is not always shared. Fortunately, most of the barriers were broken down in our Grand Challenge work, but it took several years. The CS workers had to learn the inside of the particle movers used in serial calculations to implement appropriate methods for parallelization and preconditioning. Vivek Sarin, a computer scientist in Sameh's group had to learn the Glowinski-Pan DLM particle mover before he could recode using his multilevel parallel preconditioner. Matt Knepley at Purdue is doing a similar reformulation of Hu's CFD code to produce modularity and other features required for improved performance. And it has taken 2 1/2 years for our CFD people to get over their skepticism about the efficacy of CS techniques. It has taken time for all four groups to establish a common momentum.

I personally keep in touch with Co-PIs and *all* of the active grad students and postdocs. I seek consensus with the Co-PIs, though I have made decisions without consensus. Generally speaking, we are a cordial group. It is necessary to encourage communication between postdocs and grad students from different institutions. If left alone these workers would tend to keep more to themselves than is good for the work. Now we have active discussions daily through E-mail and we have developed a real sense of community. The interests of our workers have to be advanced, and they need to be encouraged to write papers about their results. Unfortunately we have been too busy writing code, and a backlog of papers has developed. I enjoy mentoring and encouraging our grad students and postdocs; they are a great group and I think we have a happy team.

The management style which we evolved in the Grand Challenge features frequent and regular communication and the encouragement of open technical discussion using E-mail, telephone, and regular meetings. The project can't work without active day-to-day leadership and even a certain amount of nagging. Our management procedures are working well and I see no reason to change them.

STIM-LAB Inc.

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GLENN PENNY
President

May 5, 1998

To: Whom it may concern

From: Glenn Penny

Stim-Lab and our industrial partners strongly support the proposed work of Dr. Joseph and his research team in the development of numerical methods to model proppant transport in hydraulic fracturing applications. We have had a group of 25 to 30 industrial partners in the oil and gas industry who have supported the work of Stim-Lab for 10 years. In this period of time, a sizeable database has been created that shows the transport of proppant with various fluid types and properties vs. proppant size and concentration, reservoir temperature, velocity and fracture orientation. These observations have been incorporated into a 2D proppant transport model. The group is very interested in extending these observations to a fully 3D model of proppant transport behavior. This desire until now has more than challenged current computational methods. We have turned to Dr Joseph and his staff for the last few years to see if the modeling can be accomplished. The industrial consortium has dedicated 10% of its budget to support the work of Dr. Joseph.

The KDI/NCC proposal of Dr. Joseph represents a concerted multidisciplinary approach geared to solve the problems associated with 3D proppant transport modeling. We applaud the approach and feel that the proposed work and the guidance of the Stim-Lab industrial partners will quickly lead to a set of code that can be immediately applied in our 3D frac design models. Therefore, we heartily support the work outlined in the KDI/NCC proposal.

Sincerely.

Glenn S. Penny, Ph.D.
President

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May 11, 1998

To: William L. Garrard, Head, Department of Aerospace Engineering and Mechanics

From: Steven L. Crouch Steven L. Crouch
Associate Dean for Finance and Planning

Subject: Matching Funds for Professor Joseph's NSF Proposal

This is to confirm that the Institute of Technology will provide matching funds of $16,2000 for graduate assistant health benefits and tuition for Professor Daniel Joseph's proposal to the National Science Foundation, "Direct Numerical Simulation and Modeling of Solid-Liquid Flows." The matching funds will be provided during 1998–99 and 1999–2000, as follows:

	1998–1999	1999–2000
IT Dean's Office	$5,400	$5,400
Aerospace Engineering & Mechanics	2,700	2,700
Totals:	$8,100	$8,100

The Dean's Office will hold this commitment for six months after the provisional start date of the grant. If you do not notify us by then that the grant has been awarded, the commitment will be canceled.

C: ✓Daniel Joseph, Professor, Department of Aerospace Engineering and Mechanics
Madonna Monette, Finance Director, Institute of Technology

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[70] T.-W. Pan, V. Sarin, R. Glowinski, A. H. Sameh, and J. Périaux, A Fictitious Domain Method with Distributed Lagrange Multipilers for the Numerical Simulation of Particulate Flow and its Parallel Implementation, in *Proceedings of the 10th Parallel CFD Conference* (To appear) (1998).

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[96] A. Wathen and D. Silvester. Fast Iterative Solution of Stabilised Stokes Systems. Part I: Using Simple Diagonal Preconditioners, *SIAM J. Num. Anal. 30*(3), 630–649 (1993).

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E. Biographical Sketches

I. Senior Personnel

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EDUCATION:

1950 M.A., Sociology, U. of Chicago
1959 B.S., Mech. Engineering, Illinois Inst. of Tech.
1960 M.S., Mechanics, Illinois Inst. of Tech.
1963 Ph.D., Mechanical Engineering, Illinois Inst. of Tech.

PROFESSIONAL EMPLOYMENT

1962 Assistant Professor, Mechanical Engineering, Illinois Institute of Technology
1963 Assistant Professor, Aerospace Engineering and Mechanics, University of Minnesota
1965 Associate Professor, Aerospace Engineering and Mechanics, University of Minnesota
1968 Professor, Aerospace Engineering and Mechanics, University of Minnesota
1991 Russell J. Penrose Professor of Aerospace Eng & Mechanics, University of Minnesota
1994 Regents ’Professor, University of Minnesota

HONORS AND AWARDS

Guggenheim Fellow, 1969–70
National Academy of Engineering, 1990
G. I. Taylor Medalist, Society of Engineering Science, 1990
National Academy of Sciences, 1991
Distinguished Service Award, US Army CRDEC, 1992
G.I. Taylor Lecturer, Cambridge Phil. Soc., Jan 1992
Aris Phillips Lecturer, Yale University, April 1992
American Academy of Arts and Sciences, April 1993
Schlumberger Foundation Award, July 1993
Bingham Medalist of the Society of Rheology, October 1993
Fellow of the American Physical Society, November 1993
Timoshenko Medalist of the ASME, May 1995
Croco Lecturer, Princeton University, Mechanical Engineering, October 1995
Thomas Baron Fluid-Particle Systems Award of the AIChE and Shell. Nov. 1996
Illinois Institute of Technology Professional Achievement Award 1997

PATENTS:

Wave-speed meter (US Patent No. 4,602,502); measures wave speeds, determines the effective rigidity of a liquid.

Spinning rod interfacial tensiometer (US Pat. # 4,644,782); determines the interfacial tension between immiscible liquids.

Spinning drop tensioextensiometer (US Pat. # 5,150,607); for polymer blends, & in the oil industry where temp. is important.

Device and method for determining drag on surfaces (US Patent No. 5,301,541).

Method for preventing fouling of pipewalls for lubricated transport, (US Patent No. 5,385,175).

Method and apparatus for measuring a parameter of a multiphase flow (US Patent No. 5,646,352).

Foam suppression in a bubble column reactor by fluidizing particles, 96-247 (Patent pending).

Method for establishing self-lubricated flow of bitumen froth or heavy oil in a pipeline, (Patent pending).

Technique to promote lubrication of bitumen through the addition of colloidal particles in the water, (Patent pending).

Foam control using a fluidized bed of particles, 97-242 (Patent applied for).

Apparatus and method for determining dynamic stability of emulsions, serial no. 091030561

B. FIVE PUBLICATIONS RELEVANT TO THIS PROPOSAL

- "Aggregation and dispersion of spheres falling in viscoelastic liquids" (with Y.J. Liu, M. Poletto and J. Feng), *J. Non-Newtonian Fluid Mech*, **54**, 45-48 (1994).
- "A note on the forces that move particles in a second-order fluid" (with J. Feng). *J. Non-Newtonian Fluid Mech.*, **64** (2-3), 299-302 (1996).
- "Direct simulation of the motion of solid particles in of solid particles in Couette and Poiseuille flows of viscoelastic fluids", (with P.Y. Huang, J. Feng and H. Hu), *J. Fluid Mech.*, **343,** 73-94 (1997).
- "How bubbly mixtures foam and foam control using a fluidized bed" (with Jose Guittian), *Int. J. Multiphase Flow,* **24** (1), 1-16 (1997).
- "Direct simulation of the sedimentation of elliptic particles in Oldroyd-B Fluids" (with P. Huang & H. Hu), *J. Fluid Mech*, **362**, 297-326 (1998).

FIVE OTHER PUBLICATIONS

- "Heat waves" (with L. Preziosi), *Reviews of Modern Physics* **61**, 41-73 (1989).
- *Fundamentals of Two-Fluid Dynamics* (with Y. Renardy) Vol. 1: Mathematical Theory and Applications, Vol. II: Lubricated Transport, Drops and Miscible Liquids, Springer Interdisciplinary Applied Mathematics, Volumes 3 and 4 (1992).
- "Viscous and viscoelastic potential flow" (with T. Liao). "Trends and Perspectives in Applied Mathematics." *Applied Mathematical Sciences,* **100**, Springer-Verlag, New York (1994) and AHPCRC preprint 93-010.
- "Core-annular flows" (with R. Bai, K.P. Chen, and Y.Y. Renardy), *Annual Reviews of Fluid Mech.*, **29**, Jan (1997).
- "Cavitation and the state of stress in a flowing liquid," accepted for publication in *J. Fluid Mech.* (1997).

COLLABORATORS

Gordon Beavers (U of Minn) , C.V. Candler (Minnesota) , K.P. Chen (Arizona), Michelle Cloitre (CCNRS), R. Glowinski (Houston), H. Hu (U. of Penn.) , T.Y. Liao (Mobil), Thomas Lundgren (U of MN) , Gustavo Nunez (Intevep S.A.), T.W. Pan (Houston), Y. Renardy (Blacksburg).

TOTAL NUMBER OF GRADUATE STUDENTS SINCE 1963: 36; *POST DOCS: 36*

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DEGREES:

B.S. in Mathematics, Physics and Chemistry from Ecole Polytechnique, Paris, France, 1960
M.S. in Electrical Engineering from Ecole Nationale Superieure des Telecommunications, Paris, France, 1963
Ph.D. in Mathematics, University Paris VI, Paris, France, 1970 (Thesis Advisor: J.L. Lions)

POSITIONS:

Research Engineer, INRIA, France (1968-1970)
Professor of Applied Mathematics, University Paris VI (1970-1985 and 1992-1994)
Cullen Professor of Mathematics and Mechanical Engineering
University of Houston, (1985-present)
Scientific Director, INRIA, France (1970-85)
Chairman of the Department of Mathematics,
University Paris VI (1981-1985)
Director of CERFACS, Toulouse, France (1992-1994)
Member of the Scientific Council of Electricite de France (1990-1996)
Member of the Board of Regents, University Leonardo da Vinci,
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HONORS AND DISTINCTIONS:

Silver Medal of the City of Paris (for Research Achievement), 1980
Officer, French National Order of Merit, 1988
Knight, French Order of the Academic Palms, 1994
Invited Speaker, SIAM National Meeting, Madison, Wisconsin, 1978
Invited Speaker, International Congress of Mathematicians (45 minute lecture), Warsaw, 1983
Elected Corresponding Member, French National Academy of Sciences, 1987
Elected Member, Academia Europaea, 1988
Laureate of the Seymour Cray Prize, 1988
Sherman Fairchild Distinguished Visiting Scientist, California Institute of Technology, 1988-1989.
Laureate, Marcel Dassault Prize from the
French National Academy of Sciences, 1996.

EDITORIAL BOARDS:

R. Glowinski is a member of the editorial board of nearly thirty scientific journals and series.

SELECTED LIST OF RELATED PUBLICATIONS:

1. R. GLOWINSKI, T.W. PAN, J. PERIAUX, A fictitious domain method for external incompressible viscous flow modeled by Navier-Stokes equations, *Comp. Meth. Appl. Mech. Eng.*, **112**, (1994), pp. 133-148.
2. J. FENG, D.D. JOSEPH, R. GLOWINSKI, T.W. PAN, A three-dimensional computation of the force and torque on an ellipsoid settling slowly through a visco-elastic fluid, *J. Fluid Mech.*, **283**, (1995), pp. 1-16.
3. R. GLOWINSKI, T.W. PAN, A.J. KEARSLEY, J. PERIAUX, Numerical simulation and optimal shape for viscous flow by a fictitious domain method, *Int. J. Num. Meth. Fluids*, **20**, (1995), pp.695-711.
4. B. MAURY, R. GLOWINSKI, Fluid-particle flow: a symmetric formulation, *C.R. Acad. Sci., Paris*,**t. 324**, Serie 1, (1997), pp. 1079-1084.
5. R. GLOWINSKI, T.W. PAN, J. PERIAUX, Distributed Lagrange multiplier methods for incompressible viscous flow around moving rigid bodies, *Comp. Methods Appl. Mech. Engrg.*, **151**, (1998), pp. 181-194.

RECENT COLLABORATORS: M.O. Birsteau, G. Golub, H.H. Hu, D.D. Joseph, J.L. Lions,
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EDUCATION

Ph.D. University of Minnesota, Aerospace Engineering (June, 1992)
Thesis title: Studies in Multi–component Fluid Mechanics
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M.S. Xian Jiaotong University (China), Mechanics (November, 1986)
B.S. Zhejiang University (China), Mechanical Engineering (January, 1982)

PROFESSIONAL EMPLOYMENT

August, 1992 to Present
Assistant Professor
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November, 1987 to June, 1992
Teaching Assistant and Research Assistant
Department of Aerospace Engineering and Mechanics, University of Minnesota

HONORS AND AWARDS

The Young Scientist Multiphase Flow Breakthrough Award (1998, International Conference on Multiphase Flow). Citation "for his pioneering contributions to direct numerical simulations of particulate flow in Newtonian and viscoelastic flows in which the fluid and particle motions are determined without approximation from their respective equations of motion."

Doctoral Thesis Dissertation Fellowship, University of Minnesota (1990–1991)

B. FIVE PUBLICATIONS RELEVANT TO THIS PROPOSAL

- H.H. Hu, D.D. Joseph and M.J. Crochet, "Direct simulation of fluid particle motions", *Theoretical and Computational Fluid Dynamics* **3**, 285–306 (1992).
- H.H. Hu and D.D. Joseph, "Evolution of a liquid drop in a spinning drop tensiometer", *Journal of Colloid and Interface Science* **162**, 331–339 (1994)
- H.H. Hu, Motion of a Circular Cylinder in a Viscous Liquid between Parallel Plates, Theoretical and Computational Fluid Dynamics **7**, 441-455, (1995).
- H.H. Hu, Direct Simulation of Flows of Solid-Liquid Mixtures, International Journal of Multiphase Flow **22**, 335-352 (1996).
- N. Patankar and H.H. Hu, Numerical Simulation of Pressure-Driven Flow of Solid Bodies in Newtonian and Oldroyd-B Fluids, Journal of Fluid Mechanics (submitted, 1998)

FIVE OTHER PUBLICATIONS

- H.H. Hu and H.H. Bau, "Feedback control to delay or advance linear loss of stability in planar Poiseuille flow", *Proceedings of the Royal Society of London.* **447**, 299–312 (1994).
- 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, Journal of Fluid Mechanics **261**, 95–134 (1994).
- 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, Journal of Fluid Mechanics **277**, 271–301 (1994).
- H.H. Hu and N. Patankar, "Non-axisymmetric instability of core-annular flow", *Journal of Fluid Mechanics.* **290**, 213-224 (1995).
- P.Y. Huang, J. Feng, H. H. Hu and D. D. Joseph, Direct Simulation of the Motion of Solid Particles in Couette and Poiseuille Flows of Viscoelastic Fluids, Journal of Fluid Mechanics **343**, 73-94 (1997).

C. COLLABORATORS (48 months)

D.D. Joseph, H. H. Bau, K.I. Winey, R.J. Composto, J. Feng, P.Y. Huang

D. MASTER'S, DOCTORAL DISSERTATION AND POST DOCTORAL SUPERVISION

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Doctorat d'Etat, University of Grenoble, France , 1983; Doctorat de troisieme cycle, University of Grenoble, France, 1974.

Professional Experience

- Professor, University of Minnesota, Nov. 1990–present. Department Head since Jan. 1997.
- Senior Scientist, Research Institute for Advanced Computer Science (RIACS), Jul. 1988–Nov. 1990.
- Senior Computer Scientist, Center for Supercomputing Research and Development (CSRD) and Associate Professor, Mathematics Department, University of Illinois at Urbana-Champaign. Aug. 1986–June 1988.
- Research Scientist in Computer Science, Yale University. July 1984–Aug. 1986.
- Visiting Lecturer, Mathematics and Computer Science departments, University of California at Berkeley, Berkeley, CA. January 1981–July 1981.
- Visiting Assistant Professor, Department of Computer Science, University of Illinois at Urbana-Champaign, Urbana, Illinois. January 1980–December 1980.

Publications Related to the Research Project

- Y. Saad, Iterative Methods for Sparse Linear Systems, PWS Publishing, 1996.
- Y. Saad, "ILUM: A parallel multi-elimination ILU preconditioner for general sparse matrices", SIAM J. Scientific Computing, vol. 17, pp. 830-847 (1996).
- Peter Brown and Yousef Saad, "Hybrid Krylov methods for nonlinear systems of equations" SIAM journal on Statistical and Scientific Computing, vol. 11, pp. 450-481 (1990).
- Y. Saad, A flexible inner-outer preconditioned GMRES algorithm, SIAM Journal on Scientific and Statistical Computing, 14:461–469, 1993.
- X. C. Cai and Y. Saad, Overlapping domain decomposition algorithms for general sparse matrices, Numer. Lin. Alg. with Appl. vol. 3, pp.221-237 (1996).

Professional Activities

- Editor for IEEE J. Parallel and Distributed Computing. Jan 1996 to date.
- Editor for SIAM journal on Numerical Analysis (June 1985 – 1994)
- Editor for Journal of Numerical Linear Algebra with Applications, 1992 to date.
- Editor for the series *Algorithms and Architectures for Advanced Scientific Computing*, Manchester University Press, 1989 – 1992.
- Consultant for Scientific Computing Associates, 1985–1986
- Consultant for Kuck and Associates Inc. (KAI), 1986–1988.
- Chair and organizing committee to several international conferences.

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Professional Experience

- Head, and Samuel D. Conte Professor, Department of Computer Sciences, *Purdue University*, IN, 1997 – present
- Head, William Norris Chair and Professor, Department of Computer Science, *University of Minnesota*, Minneapolis, MN, 1993–1996.
- Director, Center for Supercomputing Research and Development, Professor, Department of Computer Science, *University of Illinois*, Urbana, IL, 1992–1993.
- Head, William Norris Chair, and Professor, Department of Computer Science, *University of Minnesota*, Minneapolis, MN, 1991–1992.
- Associate Director, Center for Supercomputing Research and Development, *University of Illinois*, Urbana, IL, 1985–1991.
- Professor, Department of Computer Science, *University of Illinois*, Urbana, IL, 1980–1991.
- Associate Professor, Department of Computer Science, *University of Illinois*, Urbana, IL, 1974–1980.
- Research Assistant Professor, Center for Advanced Computation and Department of Computer Science, *University of Illinois*, Urbana, IL, 1968–1974.

Research Interests

- Numerical Methods.
- Parallel Algorithms and Architectures.

Awards and Honors

- Phi Kappa Phi; Sigma Xi.
- Fulbright Fellow, 1963-1964.
- William Norris Chair in Large Scale Computing, 1991-1992, 1993-1996.
- Fellow of the American Association for the Advancement of Science, 1993-present.
- Distinguished Professor, Purdue University, 1997-present.

Five Publications Related to Proposed Work

- V. Sarin and A. Sameh. An Efficient Method for the Generalized Stokes Problem, (*SIAM J. Scientific Computing), Vol. 19, No. 1, pp. 206-226, 1998.*
- *A. Sameh and V. Sarin,* Hybrid Parallel Linear System Solvers*, (Proceedings of the 4-th Japan-US Symposium on Finite Element Methods in Large Scale Computational Fluid Dynamics), April 1998.*
- *V. Sarin and A. Sameh,* Multilevel Algorithms for Elliptic PDEs*, (Proceedings of the Fifth Copper Mountain Conference on Iterative Methods), April 1998.*

- *M. Knepley, A. Sameh, and V. Sarin,* Parallel Simulation of Particulate Flows, *to appear in (Proceedings of the 5-th International Symposium on Solving Irregular Structured Problems in Parallel, Lecture Notes in Computer Science, Springer-Verlag), August 1998.*
- *T. Pan, V. Sarin, R. Glowinski, A. Sameh, and J. Periaux,* A Fictitious Domain Method with Distributed Lagrange Multipilers for the Numerical Simulation of Particulate Flow and its Parallel Implementation, *to appear in (Proceedings of the 10-th Parallel CFD Conference, Elsevier), 1998.*

Five Other Publications

- G. Golub, A. Sameh, and V. Sarin, A Parallel Balanced Method for Sparse Linear Systems, Submitted to Numerical Linear Algebra with Applications, Aug 1997.
- A. Grama, V. Kumar and A. Sameh, Parallel Iterative Solvers and Preconditioners Using Approximate Hierarchical Methods, to appear in *SIAM Journal on Scientific Computing*, 1998.
- A. Gupta, V. Kumar and A. Sameh. Performance ans Scalability of Preconditioned Conjugate Gradient Methods on Parallel Computers, *IEEE Transactions on Parallel and Distributed Systems*, Vol. 6, No. 5, pp. 455-469, 1995.
- K. Gallivan, E. Gallopoulos and A. Sameh. Cedar: An Experiment in Parallel Computing, *Computer Mathematics and its Applications*, Vol. 1, No. 1, pp. 77-98, 1994.
- D. Kuck, E. Davidson, D. Lawrie, A. Sameh, et. al. The Cedar System and an Initial Performance Study, in: *Proceedings of the 20-th International Symposium on Computer Architecture*, pp. 213-223, San Diego, CA, May 16-19, 1993.

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EDUCATION

Ph.D. Aerospace Engineering (1991)
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University of Minnesota
Bachelor of Technology, Aeronautical Engineering (1985)
Indian Institute of Technology Kanpur, India

PROFESSIONAL EXPERIENCE

Assistant Professor (1996-present)
Department of Mechanical Engineering, NJIT

Technical Staff member (1995- 1996)
Los Alamos National Laboratory, Engineering Science and Applications Division

Postdoctoral Research Associate (1991-1995)
Department of Chemical Engineering, University of California Santa Barbara

Instructor
Department of Chemical Engineering, University of California Santa Barbara (1994)
Department Aerospace Engineering, University of Minnesota (1990 - 1991)

Computer Engineer (1985)
Indian Airlines, India, Maintained a real time reservation computer

Engineering Trainee (1984)
Indian Airlines, Went through a training program at the maintenance workshop of the Boeing airplanes

HONORS, AWARDS AND SCHOLARSHIPS

First prize in the Video Gallery of the 39th annual meeting of the division of fluid dynamics organized by the American Physical Society (1986)
First in class (B. Tech. 1985)
Best Project Award (B. Tech. 1985)
Represented Indian Institute of Technology on a technical exchange program to F.R.G. (1984)
Received scholarship during B. Tech (1981- 1985)

RELATED PUBLICATIONS

P. Singh and L.G. Leal, 1996 Computational Studies of the FENE Dumbbell Model with conformation dependent friction in a Co-Rotating Two-Roll Mill, *J. Non-Newtonian Fluid Mech* **67**,137-178.

P. Singh and L.G. Leal, 1995 Viscoelastic flows with comer singularities,*J. Non-Newtonian Fluid Mech* **58**, 279-313.

P. Singh and L.G. Leal, 1994 Computational studies of dumbbell model fluids in a co-rotating two-roll mill, *Joumal of Rheology* **38**, 485-517.

P. Singh and L.G. Leal, 1993. Finite element simulation of the start-up problem for a viscoelastic problem in an eccentric cylinder geometry using third-order upwind scheme. *Theoretical and Computational Fluid Mechanics* **5**, 107-137.

P. Singh, Ph. Caussignac, A. Fortes, D. D. Joseph and T. Lundgren, 1989. Stability of periodic arrays of cylinders across the stream by direct simulation, *J. Fluid Mech.* **205**, 553-57 1.

SIGNIFICANT PUBLICATIONS

P. Singh, 1998 A note of elastic scattering from assemblies of particles, *Journal of Applied Crystallography* (to appear).

B. Chaudhuri, P. Singh, M. Ramlakhan, C.Y. Wu, R. Pfeffer, and R. Dave 1997 Simulation and modeling of magnetically-assisted impaction coating (MAIC) process for dry particle coating, *World Congress of particle technology* (to appear).

P. Singh, 1996 Dynamics of an assembly of finite size Lennard-Jones spheres, *Phys. Rev. E* **53**(6)5904-5915.

P. Singh and D. D. Joseph, 1995 Dynamics of fluidized suspensions of spheres of finite size, *Intemational Joumal of Multiphase flows*, **21**,1-26.

P. Singh and D. D. Joseph, 1989. Autoregressive methods for chaos on binary sequences for Lorenz attractor, *Physics Letters A*, **135**, 247-253.

COLLABORATORS

D.D. Joseph (Thesis Advisor), T. Hesla, L.G. Leal, D.W. Mead, D. Guell, P. Lovelanti, R. Dave, D. Blackmore, R. Pfeffer, A. Rosato

CURRENT Ph.D. STUDENTS

F. Alcocer and C. Huang

CURRICULUM ACTIVITIES

Professor Singh has taught the following courses: FED 101, a freshmen course in Fundamentals of Computer Aided Design; ME304, a junior level introductory course in Fluid Mechanics; ME718, a graduate class in non-Newtonian fluid mechanics.

CURRENT RESEARCH PROJECTS

Finite element simulations of Newtonian and viscoelastic flows; iterative numerical algorithms and preconditioners; parallel computing; stability of Newtonian and viscoelastic flows; modeling and simulations of multiphase and particulate flows; and free boundary problems.

I. Senior Personnel, cont.

Tsorng-Whay Pan
Department of Mathematics, University of Houston
Houston, TX 77204
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(713) 743-3448

Education

1980	B. S., Mathematics	National Taiwan University, Taipei, R. O. C.
1990	Ph. D., Mathematics	University of Minnesota, Minneapolis

Employment

1994-present	Assistant Professor	University of Houston, Houston, TX
1990-1994	Visiting Assistant Professor	University of Houston, Houston, TX
1988-1990	Graduate Research Assistant	University of Minnesota, Minneapolis, MN
1984-1989	Graduate Teaching Assistant	University of Minnesota, Minneapolis, MN
1982-1984	Teaching Assistant	National Taiwan University, Taipei, R. O. C.

Five Publications Related to this Project

1. J. Feng, D. D. Joseph, R. Glowinski, T. W. Pan, A three-dimensional computation on the force and moment on an ellipsoid settling slowly through a viscoelastic fluid, *J. of Fluid Mech.*, **283** (1995), pp. 1-16.
2. R. Glowinski, T. Hesla, D.D. Joseph, T.-W. Pan, J. Periaux, Distributed Lagrange multiplier methods for particulate flows in *Computational Science for the 21st Century*, M-O. Bristeau, G. Etgen, W. Fitzgibbon, J.L. Lions, J. Periaux, M.F. Wheeler eds., John Wiley & Sons, Chichester, England, 1997, pp. 270-279.
3. R. Glowinski, T.-W. Pan, J. Periaux, Distributed Lagrange multiplier methods for incompressible viscous flow around moving rigid bodies, *Comp. Meth. Appl. Mech. Eng.*, **151** (1998), pp. 181-194.
4. T.-W. Pan, A Lagrange multiplier/fictitious domain/collocation method for solid-liquid flows, in *the IMA volumes in Mathematics and its Application* (to appear).
5. R. Glowinski, T.-W. Pan, T. I. Hesla, D. D. Joseph, A distributed Lagrange multiplier/fictitious domain method for particulate flows (accepted to Int. J. Multiphase Flow).

Other five significant publications

1. M. Luskin, T.-W. Pan, Nonplanar shear flows for nonaligning nematic liquid crystals, *J. of Non-Newtonian Fluid Mechanics*, **42** (1992), pp. 369-384.
2. G. Liao, T.-W. Pan, J. Su, Numerical grid generator based on Moser's deformation method, *Num. Methods for PDEs.*, **10** (1994), pp. 21-31.
3. R. Glowinski, T. -W. Pan, J. Periaux, Domain decomposition/fictitious domain methods with nonmatching grids for the Navier-Stokes equations. Parallel implementation on a KSR1 machine, in *Parallel Computational Fluid Dynamics, Implementations and Results using Parallel Computers*, A. Ecer, J. Periaux, N. Satofuka, S. Taylor eds., North-Holland, Amsterdam, 1996, pp. 617-624.
4. T.-W. Pan, On the existence of infinitely many limit points on the solution branch of planar shear flow of nematic liquid crystals, *J. Mathematical Analysis and Applications*, **208** (1997), pp. 120-140.

5. T.-W. Pan, Error Estimates for a Fictitious Domain Method with Lagrange Multiplier Treatment on the Boundary for a Dirichlet Problem, *Japan J. of Industrial and Applied Mathematics*, **15** (1998), pp. 75-85.

Collaborators: E. Dean, T. Hesla, H.H. Hu, G. Golub, D.D. Joseph, A. Sameh.

List of Advisors and Advisees:

Advisor: M. Luskin

Postdoc Advisor: R. Glowinski

Curriculum Vitae

NAME: Kuznetsov, Yuri A.
DATE OF BIRTH: August 7, 1945
PLACE OF BIRTH: Penza, Russia
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CITIZENSHIP: Russia

DEGREES: M.S. in Physics from Novosibirsk State University, Novosibirsk, Russia, 1967
Ph.D. in computational mathematics from Novosibirsk Computer Center, Academy of Sciences of the USSR, Novosibirsk, 1969 (Advisor: G.I. Marchuck)

POSITIONS:

1965-1980	Novosibirsk Computer Center,Academy of Sciences, Novosibirsk, USSR Head of a Laboratory (last held position)
1970-1980	Novosibirsk State University, USSR Associate Professor (part time)
1980-1996	Institute of Numerical Mathematics, Russian Academy of Sciences, Moscow Senior Researcher/Project director
1982-1996	Moscow Institute of Physics and Technology, USSR Professor of computational mathematics (part time)
since 1997	University of Houston, Houston, TX, Professor of Mathematics

PROFESSIONAL SOCIETIES:

American Mathematical Society (AMS)
Society for Industrial and Applied Mathematics (SIAM)
Russian Association for Scientific and Engineering Computing (ONIV)

EDITORSHIP: Numerische Mathematik (since 1992)
Numerical Linear Algebra and Applications (since 1993)
Russian Journal of Numerical Analysis and Mathematical Modelling (Managing Editor, since 1986)
East-West Journal on Numerical Mathematics (Managing Editor, since 1993)

HONORS: Invited speaker, International Congress of Mathematicians, Warsaw, 1983
Invited speaker, 3rd, 5th, 6th, 7th and 9th International Conferences on Domain Decomposition Methods

SELECTED LIST OF PUBLICATIONS:

Y.A. Kuznetsov has published more than one hundred papers, three books/monographs, and coedited proceedings of four international conferences.
The following are the five most significant publications related to the topics of the proposal:

1. Y.KUZNETSOV, Domain Decomposition Methods for Unsteady Convection-Diffusion Problems, *Computing Meth. in Appl. Sci. and Eng. Proc. of 9th Int. Conference*, R. Glowinski, A. Lichenewsky, eds., SIAM, Philadelphia, 1990, pp.211-227.

2. Y.KUZNETSOV, Overlapping Domain Decomposition Methods for Parabolic Problems. In *Domain Decomposition Methods in Sci. and Eng., Proc. of the 6th Int. Conf.*, R. Glowinski, Y. Kuznetsov, A. Quarteroni, O. Widlund, eds., AMS, Providence, 1996, pp.63-70.
3. Y. ACHDOU, Y. KUZNETSOV, O. PIRONNEAU, Substructuring Preconditioners for the Q_1 Mortar Element Method, *Num. Math.*, **79** (1995), pp. 419-449.
4. Y. KUZNETSOV, M.F. WHEELER, Optimal Order Substructuring Preconditioners for Mixed Finite Element Methods on Nonmatching Grids, *East-West J. on Numer. Math*, **3** (1995), pp. 127-143.
5. Y. KUZNETSOV, Efficient iterative Solvers for Elliptic Finite Element Problems on Nonmatching Grids, *Russian J. of Numer. Analysis and Math. Modelling*, **10** (1995), pp. 187-212.

Other publications related to the proposal are given in the list of references.

RECENT COLLABORATORS: R. Glowinski (University of Houston, Houston, TX)
O. Pironneau (University Paris VI, France)
M. Wheller (University of Texas, Austin, TX)
R. Hoppe (University of Augsburg, Germany)
P. Neittanmaki (University of Jyvaskyla, FINLAND)
O. Axelsson (University of Nijmegen, Netherlands).

Ph.D. STUDENTS:
Y.A. Kuznetsov has directed eighteen doctoral dissertations (16 in Russia and 2 in Finland).
Currently he supervises four graduate students (1 in USA, 2 in Russia, 1 in Finland).

E. Biographical Sketches, Cont.

II. Other Personnel

Vivek Sarin
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Education

- Ph.D. in Computer Science, *University of Illinois*, 1997

Professional Experience

- Research Associate, Department of Computer Science, *Purdue University*, 1997–present

Research Interests

- Numerical Computing: Numerical linear algebra, iterative methods, preconditioners for linear systems, and their application to large scale engineering problems.
- Scientific Computing: Numerical algorithms for computational fluid dynamics, electromagnetics, and biology, high performance numerical computing, and scientific visualization.
- Parallel and Distributed Computation: Parallel algorithms, advanced computer architectures, and parallel computing for large scale problems in scientific applications.

Awards

- Phi Kappa Phi
- Awarded National Talent Scholarship by the National Council for Educational Research and Training, India, 1984-1990.

Five Publications Related to Proposed Work

- V. Sarin and A. Sameh. An Efficient Method for the Generalized Stokes Problem, *SIAM J. Scientific Computing*, Vol. 19, No. 1, pp. 206-226, 1998.
- A. Sameh and V. Sarin, Hybrid Parallel Linear System Solvers, *Proceedings of the 4-th Japan-US Symposium on Finite Element Methods in Large Scale Computational Fluid Dynamics*, April 1998.
- V. Sarin and A. Sameh, Multilevel Algorithms for Elliptic PDEs, *Proceedings of the Fifth Copper Mountain Conference on Iterative Methods*, April 1998.
- M. Knepley, A. Sameh, and V. Sarin, Parallel Simulation of Particulate Flows, to appear in *Proceedings of the 5-th International Symposium on Solving Irregular Structured Problems in Parallel, Lecture Notes in Computer Science, Springer-Verlag*, August 1998.
- T. Pan, V. Sarin, R. Glowinski, A. Sameh, and J. Periaux, A Fictitious Domain Method with Distributed Lagrange Multipilers for the Numerical Simulation of Particulate Flow and its Parallel Implementation, to appear in *Proceedings of the 10-th Parallel CFD Conference, Elsevier*, 1998.

Other Publications

- G. Golub, A. Sameh, and V. Sarin, A Parallel Balanced Method for Sparse Linear Systems, Submitted to Numerical Linear Algebra with Applications, Aug 1997.
- V. Sarin, Efficient Iterative Methods for Saddle Point Problems, Ph.D. Thesis, University of Illinois, 1997.

- V. Sarin and A. Sameh, Parallel Preconditioners for Elliptic PDEs, *Proceedings of Supercomputing'96*, Pittsburg, PA.
- A. Sameh and V. Sarin, Parallel Algorithms for the Generalized Stokes Problem, *Computational Mechanics 95 - Proceedings of the International Conference on Computational Engineering Science*, Springer Verlag, 1995.
- V. Sarin and A. Sameh, A Projection Based Iterative Algorithm for Sparse Linear Systems, *Third IMACS Intl. Symp. on Iterative Methods in Scientific Computation*, July 1997.

Books

- High Performance Algorithms for Structured Matrix Problems, Volume 2 of the series *Advances in the Theory of Computation and Computational Mathematics*, edited by P. Arbenz, M. Paprzycki, A. Sameh, and V. Sarin, NOVA Science Publishers, Inc., New York (in preparation).

Andrew John WATHEN

Personal Information

Home: 12,Wyndham Way, Oxford, OX2 8DF, UK.

Work: Oxford University Computing Laboratory, Wolfson Building,
Parks Road, Oxford, OX1 3QD, UK

Birth: April 25, 1958 at Bebington, Cheshire, England

Nationality: British.

Education:

Oxford University 1977-1980
(Oriel College) B.A. (Honours) II Mathematics
Captain of College Rugby

Reading University Oct 1980-April 1984
Ph.D. in Mathematics

Employment:

Reader in Numerical Analysis, Oxford University, UK: Aug 1997 -
Fellow of New College
University Lecturer in Numerical Analysis, Oxford University: Jan 1996 - July 1997
Reader in Mathematics, Bristol University, UK: Aug 1995 - Dec 1995
Lecturer in Mathematics, Bristol University, UK: April 1985 - July 1995
Postdoctoral Research Assistant, Reading University, UK: Oct 1984 - Mar 1985.
Postdoctoral visitor, Stanford University, California: Jan-Sept 1989

Research Experience

Awarded a Leslie Fox Prize in Numerical Analysis in September 1986.

14 research grants

External Examiner for 10 PhD theses

Associate Editor, IMA Journal on Numerical Analysis

Member, Engineering and Physical Sciences Research Council Mathematics College

Selected publications relevant to research project

Golub, G.H. Wathen, A.J., 1998, ‘An iteration for indefinite systems and its application to the Navier-Stokes equations’, SIAM J. Sci. Comput. **19**(2), pp. 530-539.

Elman, H.E., Silvester, D.J. Wathen, A.J., 1997 ‘Iterative methods for problems in Computational Fluid Dynamics’, in ‘Iterative Methods in Scientific Computing’, Eds. R.H. Chan, T.F. Chan G.H. Golub, Springer-Verlag, Singapore, 271-327.

Wathen, A.J., Fischer, B. Silvester, D.J., 1995, ‘The convergence rate of the minimum residual method for the Stokes problem’, Numer. Math. **71**, 121-134.

Silvester, D.J. Wathen, A.J., 1994, ‘Fast iterative solution of stabilised Stokes systems Part II: Using general block preconditioners’, SIAM J. Numer Anal. **31**(5), 1352-1367.

Ramage, A. Wathen, A.J., 1994, ‘Iterative solution techniques for the Stokes and Navier-Stokes equations’, Int. J. Numer. Meths. Fluids **19**(1), 67-83.

Selected other publications

Silvester, D.J. Wathen, A.J., 1996, ‘Fast and robust solvers for time-discretised incompressible Navier-Stokes equations’, in ‘Numerical Analysis 1995’, Eds. D.F. Griffiths G.A. Watson, Addison Wesley Longman, Harlow, England, 154-168.

Ramage, A. Wathen, A.J., 1994, ‘On preconditioning for Finite Element equations on irregular grids’, SIAM J. Matrix Anal. Appl. **15**(3), 909-921.

Wathen, A.J. Silvester, D.J., 1993, ‘Fast iterative solution of stabilised Stokes systems Part I: Using simple diagonal preconditioners’, SIAM J. Numer. Anal. **30**(3), 630-649.

Baines, M.J. Wathen, A.J., 1988, ‘Moving Finite Element methods for evolutionary problems I: Theory’, J. Comput. Phys. **79**, 245-269.

Wathen, A.J., 1987, ‘Realistic eigenvalue bounds for the Galerkin Mass Matrix’, IMA J. Numer. Anal. **7**, 449-457.

Recent Collaborators:

Z.Z. Bai, Chinese Academy of Sciences

H.C. Elman, University of Maryland

B. Fischer, Medical University of Luebeck

G.H. Golub, Stanford University

L. Hemmingsson, Uppsalla University, Sweden

Y. Huang, Oxford University

D.D. Joseph, University of Minnesota and other members of the NSF Grand Challenge project on Particle Movers

K. Miller, Univeristy of California, Berkeley

A. Ramage, University of Strathclyde, UK

D.J. Silvester, UMIST, Manchester, UK

Persons Sponsored in last five years:

Completed PhD supervisees:

Malcolm Murphy (Oct 1993 - Nov 1997), Cable Online

Bryan Davidson (Oct 1992 - June 1995), Deutsche Morgan Grenville

Harvinder Jhass (Oct 1992 - Sept 1995), Tessella Support Services

Paul Selwood (Oct 1991 - Sept 1994), Leeds University

12 PhD students in all (5 current)

Postdoctoral research assistants:

David Kay (Nov 1996 - Dec 1999), UMIST and Oxford University

Tony Humphries (April 1993 - Mar 1996), Sussex University

Alison Ramage (Oct 1990-Sept 1993), University of Strathclyde

I was supervised by K.W. Morton (Oxford and Bath Universities) and M.J. Baines (Reading University) for my PhD and was a postdoctoral research assistant with Baines and a postdoctoral visitor with Golub.

II. Other Personnel, cont.

Michael W. Conway, Ph.D.

Doctor Conway earned a BS in Pharmacy in 1970 and a MS in Pharmacology in 1971. In 1978 he earned his Ph.D. in Organic Chemistry from the University of Oklahoma, Norman. Concurrently he spent 18 months with the Oklahoma Department of Energy as an Energy Conservation Program Manager. In 1978 Mike joined Halliburton Services, Duncan, Oklahoma, in the Fracturing Section. He was promoted to Stimulation Chemicals Research Group Supervisor and in 1985 became Group Supervisor of Engineering Applications Research. In 1987 Mike joined STIM-LAB, Inc. as Technical Manager and now is vice president.

Mike coordinates the consortium of 25 to 30 companies on the rheology and proppant transport of fracturing fluids. He worked with Marathon Oil Company on creating a proppant transport module for a 3-D frac design model.

From 1990 to 1996, under the auspices of GRI, he directed the research efforts in identifying the effects of completion and stimulation fluids on the permeability of coal. He has authored over twenty papers in various scientific disciplines and is the holder of approximately ten US patents. He is a co-author on a chapter in the "Recent Advances in Hydraulic Fracturing".

II. Other Personnel, cont.

Glenn S. Penny, Ph.D.

Doctor Penny earned a BS from Trinity University, San Antonio, Texas in 1972. In 1979 he earned a Ph.D. in Organic Chemistry from the University of Houston. He then spent six years in the industry with Halliburton Services where he held positions of Senior Chemist, Development Chemist, and Research Chemist.

He is now president of STIM-LAB, Inc. which he founded in 1985. The company offers testing expertise in the area of fracturing and acidizing such as fluid loss control, formation damage, fracture flow capacity, surfactant performance, rheology and proppant transport, matrix acidizing, fracture acidizing, and diversion. The company has laboratories in the US and the UK, with numerous representatives around the world.

He has authored numerous scientific papers and a chapter in the “Recent Advances in Hydraulic Fracturing”. He is the holder of approximately 12 US patents.

II. Other Personnel, cont.

Biographical Sketch

Mahmoud Asadi, Ph.D.

Doctor Asadi earned a BS and MS from the University of Southwestern Louisiana, Lafayette, in 1983 and 1986, respectively. He earned a Ph.D. in Petroleum Engineering in 1992 from the University of Kansas at Lawrence.

In 1992 he joined Midwest Energy & Environmental Technology Corp., Lawrence Ks, as principal investigator and project manager of various research projects. Later, 1995, he joined Structural Research and Analysis Corp., Chicago, where he was responsible for technical training, technical supports and completion of projects in the areas of linear static, heat transfer, fluid flow and engineering optimization. At the end of 1996 he became a Research Associate with the Fracturing Fluid Characterization Facility at the University of Oklahoma, Norman. At the FFCF he was primarily involved with rheological characterization of fracturing fluids, and proppant transport.

In 1997 he joined STIM-LAB, Inc. as R & D Supervisor in charge of rheology and proppant transport. He has published a number of professional papers with the SPE and other conferences.

Curriculum Vitae

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EDUCATION:
Rice University, Ph.D., 1985.
Rice University, Master of Applied Mathematical Sciences, 1979.
University of New Mexico, B.S., 1978.

POSITIONS:
Associate Professor, University of Houston, 1993-Present.
Assistant Professor, University of Houston, 1987-1993.
Visiting Assistant Professor, University of Houston, 1985-1987.
Graduate Research Assistant, Sandia National Laboratories, (Summer 1981).
Application Programmer, I.B.M. Corp., 1981.
Research Assistant, Agronne National Laboratory, (Summer 1980).

ORGANIZATIONS:
Society for Industrial and Applied Mathematics
Society for Advancement of Chicanos and Native Americans in Science

FIVE MOST RELEVANT PUBLICATIONS:

1. E. J. DEAN, R. GLOWINSKI, A wave equation approach to the numerical solution of the Navier-Stokes equations for incompressible viscous flow, C. R. Acad. Sci. paris, t.325, Série I, 1997, pp. 783-791.
2. E. J. DEAN, R. GLOWINSKI, Domain decompositions of wave problems using a mixed finite element method, submitted for the *Proceedings of the Ninth Internatinal Conference on Domain Decomposition Methods.*
3. E. J. DEAN, R. GLOWINSKI, D. A. TREVAS, An approximate factorization/least-squares solution method for a mixed finite element aproximation of the Cahn-Hilliard equation., *Japan Journal of Industrial and Applied Mathematics*, **13**, No. 3, 1996, pp. 495-518.
4. E. J. DEAN, R. GLOWINSKI, A domain decomposition method for the wave equation, in, *Les Grands Systèmes des Sciences et de la Technologie*, J. Horowitz, J. L. Lions, (eds.), Masson, Paris, 1993.
5. E. J. DEAN, Q. V. DINH, R. GLOWINSKI, J. HE, T. W. PAN, J. PERIAUX, Least squares/domain imbedding methods for Neumann problems: Applications to Fluid Dynamics, in *Fifth International Symposium on Domain Decomposition Methods for Partial Differential Equations*, D. E. Keyes, T. F. Chan, et al. (eds.), Society for Industrial and Applied Mathematics, Philadelphia, 1992, pp. 451-475.

OTHER SIGNIFICANT PUBLICATIONS:

6. M. O. BRISTEAU, E. J. DEAN, R. GLOWINSKI, V. KWOK, J. PERIAUX, Application of exact controllability to the computation of scattering waves, in *Control Problems in Industry*, I. Lasiecka and B. Morton, eds., Birkhauser, Boston, (1995), pp. 17-41.
7. E. J. DEAN, R. GLOWINSKI, Y. M. KUO, M. G. NASSER, Multiplier techniques for some dynamical systems with dry friction, *C. R. Acad. Sci. Paris*, t. 314, Series I, 1992, pp. 153-159.

8. E. J. DEAN, An inexact Newton method for nonlinear two-point boundary value problems *Journal of Optimization Theory and Applications*, **75**, No. 3, 1992, pp. 471-486.
9. E. J. DEAN, P. GUBERNATIS, Pointwise control of Burgers' equation - A numerical approach, *Computers Math. Applic.*, **22**, No. 7, 1991, pp. 93-100.
10. E. DEAN, R. GLOWINSKI, O. PIRONNEAU, Iterative solution of the stream function-vorticity formulation of the Stokes problem. Applications to the numerical simulation of imcompressible viscous flow, *Computer Methods in Applied Mechanics and Engineering*, **87**, 1991, pp. 117-155.

COLLABORATORS:
Elaine Adams, Neal Amundson, John Hardy, Edward J. Hayes, Joshua Hill, Jerome Kramer, and Ramiro Sanchez. There have been no other collaborators, in the past 48 months, other than those listed in the above publications and those collaborating in this proposal.

GRADUATE STUDENT ADVISEES:
Ping Zheng, Abdelnour Ahmed-Zaid, Thong Nguyen, Joseph Kitchen (non-thesis Master's degree students) James Jeffrey (Ph.D. student) (A total of five non-thesis Master's students and one Ph.D. student advised)

PH.D. ADVISORS:
Richard A. Tapia (Rice University), John E. Dennis, Jr. (Rice University)

POSTDOCTORAL ADVISOR:
Roland Glowinski (University of Houston)