# Direct Simulation of Fluid Particle Motions

Look at flows of particle-laden fluids like

- Sedimentation
- Fluidized beds
- Slurry flows driven by pressure to shear in simple and complex geometries

The fluid satisfies its equations (Navier-Stokes, Oldroyd B, etc)

Particles are moved by forces computed from the fluid motion according to the equations of dynamics of rigid solids

Fluid and solid equations are solved together by simulation.

No approximations are made; the solutions are as exact as numerical methods allow.

Competitors for direct simulation:

- Two-fluid models (can be viewed as coming from ensemble averaging)
- Molecular dynamics
- Lattice-Bolzman model

# What is the Challenge?

Probably the NSF knew what the challenge was from the start but we didn't; it took us a time to understand this and what an exciting challenge it really is.

The challenge is to make good marriage of computational fluid dynamics and computer science.

It never worked before; it may not work. It's a moderate risk, high reward effort. Our direct simulation competitors don't do it.

Tezduyar's group
Trygvasson's group
We have no viscoelastic competitors

If we are successful, we will develop the Microsoft of particle movers.

# People Working on the Grand Challenge

We have CFD people and CS people working together. The group we have assembled is large. Not all of the people working on the grant are paid by the grant:

**MINNESOTA:**

Dan Joseph (PI)
Ahmed Sameh (Co PI) CS
Peter Huang (G) CFD
Todd Hesla (G) CFD
Walter Wang (G) CFD
Nicolas Devaux (PD) CFD
F. Hecht, INRIA, Pirroneau, Paris
Pierre Saramito (PD) CFD
Matt Knepley (G) CS
Vivek Sarin (G) CS
Michael Oettli (PD) CS
Vipin Kumar (P) CS
George Karypys (G) CS
Serguei Maliasov (PD) CFD

**UNIVERSITY OF PENNSYLVANIA:**

Howard Hu (Co PI) CFD
Neelash Patankar (G) CFD
Ming Yu Zhu (G) CFD

**HOUSTON:**

Roland Glowinski (Co PI) CFD
T.Y. Pan (Prof) CFD
Bertrand Maury (P. Doc) CFD
Yuri Kuznetsov (Prof) CFD

**STANFORD:**

Gene Golub (Co PI) CS
Dave Burgess (P Doc) CS
Denis Vanderstraaten (P Doc) CS

Sameh, Kneply, Sarin are going to Purdue.
Burgess goes to New Zealand.
Adam Huang became a software engineer.

# Achievements:

We developed three codes; two of them are based on unstructured grids.

**1.** Howard's code (Partflow)
**2.** Bertrand's code

One of the codes is on a fixed grid using fictitious (Glowinski) or embedded (Golub) domains.

**3.** Developed as a particle mover by Glowinski and Pan using ideas of Hesla.

**(1)** Partflow works for Newtonian and viscoelastic sedimentation and shear flow.

Partflow is the only code worldwide to move particles in a viscoelastic fluid.

We have a serial and parallel version of Partflow and are comparing them.

We have the first 3D results for Partflow for spheres sedimenting in Newtonian fluid

## *Achievements, cont.*

**(2)** Bertrand can simulate the sedimentation of 1000 2D spheres in a Newtonian fluid. The code is serial and has some great new features. We have to make a parallel version and a viscoelastic version.

**(3)** The particle mover based on fictitious or embedded domains may turn out to be the best of all, since it computes on a fixed grid.

**(4)** In an earlier version of Partflow, Howard published a simulation of 400 spheres in sedimenting and shear flows of a Newtonian fluid (*Int. J. Multiphase Flow*). Unilever asked Howard to simulate carrots falling in soup, etc. They have given Howard a contract in which they pay for a post doc. We are moving Nicolas into this so we can get some good work from Nicolas without GC money.

**(5)** There is a huge demand in different industries for the codes that we are developing. We could discuss this if there is time and interest.

# Marriage of CFD and CS

We are working to make an effective team of people from different institutions to work as one. We also have to deal with the fact that CFD and CS people don't speak a common language (I think this is the main obstacle).

### 1. Communications Between Different Institutions

- I have tried to ignore institutions and to move people from different institutions to where they are needed

  Nicolas → Howard
  Matt → Howard
  Denis → Minnesota
  Bertrand → Minnesota

- Group meetings and working groups. We have had 2 meetings at Minnesota and 1 at Stanford. The meetings are expensive and not always focused. We need to have meetings, but not too many. Working groups are excellent because they focus.

- Telephone. I do a lot of managing by telephone, using the squeaky wheel principle. The post docs and grad students rarely use the phone.

## *Marriage of CFD and CS, cont.*

- E-mail. We have a fantastic team of grad students and post docs working on Howard's code and other versions.

  Howard Hu
  Matt Knepley
  Dave Burgess
  Denis Vanderstraaten
  Bertrand Maury

  These people work together all the time through e-mail. Probably we couldn't manage long distance communication well without it.

- WWW. We started to use this, but it has fallen out of favor partly because of security and partly because we want to keep our errors private.

## *Marriage of CFD and CS, cont.*

### 2. Communication Between CS and CFD

To an extent there are different communities with different languages. To use CS results, the CFD must be translated into the language of well-characterized matrices.

In our case we had to translate the CFD into modules that can be understood by computer scientists. There is nothing easy about this; either the CFD have to learn how to do things in a CS way or the computer scientists have actually to understand and be able to code the CFD.

We have to thank Matt Knepley for working closely with Howard to understand all the CFD issues and then to rewrite parts of the code for CS. Matt, Howard, Denis, Dave, and Peter have been now working hard to make the 2D codes parallel to benchmark improvements in efficiency.

Bertrand Maury, on his own has developed a solver based on characteristics, a novel way of refining unstructured grids and some applications of USAWA preconditioning from Gene Golub's work. He can move 1000 spheres in 2D in a serial node.

# Problems to Solve

1. Parallel preconditioners not designed for everything

2. Collision Strategies
   - “elastic” collision with coefficient of restitution
   - lubrication theory (maybe Patera’s NIP elements work)
   - Bertrand Maury’s engineering solution

3. Remesh criteria for unstructured grids

4. Numerical methods for avoiding Hadamard instability

5. Relation of 2D and 3D simulations

# Next Year

Fully parallel 2D Newtonian and Viscoelastic CS efficient packages. More than 1000 particles. High volume concentrations. Non-spherical particles.

3D movers based on unstructured grids. These problems may have more than $10^6$ nodes and matrix based on 2D algorithms may not carry over.

Particle movers using imbedded domains (fixed mesh) are maybe 1 year behind.

Build flow loops.