Budget justification for a $90,000/year supplement of the $2,000,000 three year KDI/NCC award for

"Direct numerical simulation and modeling of Solid-Liquid Flows"

The goal of the KDI/NCC proposal is to carry further the development of software packages for moving thousands of solid particles in flowing liquids in direct three-dimensional simulation, without recourse to modeling assumptions. The work divides naturally into code development using computational fluid dynamics and computer science and modeling for applications of interest to our industrial collaborators.

The KDI/NCC proposal to the NSF was for three million dollars, and it was funded at a reduced two-million dollar figure. We have adequate resources for the code development side of the work. In our grand challenge we developed two packages; one of the (ALE, developed mainly by Hu) uses a moving unstructured, body-fitting grid. The other (DLM, developed mainly by Glowinski, Pan, and Hesla) uses a fixed, regular grid and represents the particles by a field of Lagrange multipliers which enforce the constraint of rigid body motion. Recently, big advances have been made in the development of both codes; Vivek Sarin (Purdue) has implemented a parallel, multilevel preconditioner for the DLM code which is running in a matrix free mode. Sarin & T.Y. Pan (Houston) are both presently calculating the bed expansion of a fluidized bed of 1200 spheres in a channel whose side walls are slightly larger than one sphere diameter. P. Singh has got a DLM code for viscoelastic fluids up and running. H. Choi has worked a splitting which minimized communication overhead between particles and fluid for the AL E method. He, together with the post-docs in the group of Y. Saad have come up with a matrix free formulation for this code which will give order of magnitude improvements for 3D ALE simulations. Code development is in good shape.

I want the 90K supplement to build up the modeling, applications and educational aspects of our work. The supplement will be used to bridge the gap between direct numerical simulation (DNS) and applications, and to create modern graphic interfaces for the dissemination of knowledge gained from simulation and experiments of solid-liquid flows. The interfaces to be developed are video, Web and primarily CD ROM and they will take form as a course on solid-liquid mechanics. We may think of this course as inspired by the success of the "Album of Fluid Mechanics" by M. Van Dyke in the education of a generation of students and scholars of fluid mechanics. Unlike the album, our course focuses on solid-liquid flows using modern techniques of graphical display of moving rather than still images.

The largest part of the supplement is set aside for the wages of Neelesh Patankar, a skilled post-doc who is coding a Lagrangian numerical simulator which bridges the gap between DNS and "two-fluid" continuum models presently being used in field applications of many industries.

Dr. Patankar also works on the DNS side; he has implemented a new method for representing the rigid motions of particles in the DLM scheme. In this method, the fluid regions of space occupied by solids are required to have a zero rate of strain; this condition is enforced by Lagrange multipliers and it works well.

The smaller part of the supplement will be used for partial support of Prof. Antonio Fortes who will be in Minnesota for a two year leave from the University of Brasilia. Fortes was my student many years ago when he did beautiful experiments and visualizations of microstructural features of solid-liquid flows; he will be working on graphical interfaces for our course and surely also on the experimental side of the research. Since Fortes is a senior person, his wages are high. It is probable that we will need to acquire items of digital signal technology of high sensitivity like minimum distortion CCD sensors, lasers for sheet illumination and other items. In this budget we have asked only for slightly over one-half of the salary of Fortes. I will supplement this supplement with funds accumulated in my Russell Penrose chair.

Fortes and I will repeat previous experiments which illustrate the controling effects of microstructure in fluidized suspensions seeking web based and CD ROM formats for animations of the striking microstructural arrangements, like “flying birds” and chained spheres which appear on our poster which hangs on the wall of the NSF. We will also carry out new experimental research on fluidization in non-Newtonian fluids, transport of particles in foam, lift-off and resuspension of spheres in Newtonian and viscoelastic fluids and other topics which arise in the applications of our industrial partners. In each and every situation we will try to couple an experiment with numerical simulation.

Liquid-solid flows can be determined by DNS and modeled with “two-fluid” equations. These equations are completed by intelligent guessing of the form of the interaction terms between the two phases. These “two-fluid” models are very popular in industries, like the fracturing industry, which use PC bases codes to guide field operations. Marathon oil has a “two-fluid” model code for particle placement in fractures called “Gohfer”. Other “two-fluid” packages, sponsored by other oil companies, have their own advocates, but there is general agreement that none of these codes work really well. At the other extreme, DNS is as exact as numerics allow but it certainly cannot be put into a PC to guide field operations.

Between these two extremes lies a simulation method called LNS (Lagrangian numerical simulation) in which the forces on the particles are modeled rather than computed, whereas the fluid motion is computed. The continuum/continuum approach readily allows modeling of particle-particle stresses in dense particle flows using spatial gradients of particle volume fractions. However, for multimodal simulations one has to consider each particle of different size or weight as a separate phase. This requires solving extra continuity and momentum equations for each additional phase. This disadvantage can be overcome by considering the Lagrangian approach for the particle phase since it can handle a wide range of particle types. In such methods the interparticle interaction is usually resolved by Lagrangian collision calculations. Such an approach becomes unrealistic for dense particulate flows where the collision frequency is high. For this reason researchers have used the Eulerian/Lagrangian approach for dilute particulate flows. Consequently, the effect of volume fraction of the particles in the fluid continuity and momentum equations is neglected. The fluid and particle phases interact only through the momentum exchange term.

The Lagrangian numerical simulation (LNS) scheme being developed by Neelesh Patankar is an extension of the multiphase particle-in-cell (MP-PIC) method (first described in Andrews & O'Rourke, Int. J. Multiphase Flow, 22, 379-402, 1996) to include the viscous effects in the governing equation for the fluid phase. In this numerical scheme we solve for the fluid continuity and momentum equations on the Eulerian grid. However, the particle motion is governed by Newton's law thus following the Lagrangian approach. Momentum exchanges from the particle to fluid phase are modeled in the fluid momentum equation; at present the drag force opposing the drag on the particle is used for the momentum exchange. Drag, buoyant weight and interparticle (collision) stresses on the particles are presently modeled; the modification of these forces and the addition or deletion of other forces like hydrodynamic lift can be easily implemented. The effects of the volume fraction of the particles is included in the continuity and momentum equation.

The LNS method provides a numerical scheme in which the particle phase is considered both as a continuum and as a discrete phase. Interparticle stresses are calculated by treating the particles as a continuum phase. Particle properties are mapped to and from an Eulerian grid. Continuum derivatives that treat the particle phase as a fluid are evaluated to model interparticle stress and then mapped back to the individual particles. This results in a numerical scheme for multiphase flow that can handle particle loadings from dilute to dense for a wide range of particles types. The effects of volume fraction of the particles in the fluid continuity and momentum equations are accounted for. Patankar has also included the viscous stress terms in the fluid momentum equation which were ignored in the original MP-PIC method. All these features for an Eulerian/Lagrangian approach are unique and have not been reported previously.

LNS in a three dimensional complex geometry can be computationally intensive. The SIMPLER algorithm on a staggered grid used in the MP-PIC scheme is not the most efficient way to solve such complex unsteady problems. SIMPLER is a good steady state algorithm but it is not good for unsteady calculations where each time step should be solved quickly. Many industrial problems involve complex geometries for which body fitted curvilinear coordinate systems must be used. Staggered grids for velocity and pressure can require large storage space; non-staggered grids are more desirable. Keeping this in mind we have developed a new efficient three-dimensional, finite volume, time dependent LNS scheme, implementing a Chorin type pressure correction based on a fractional step scheme on a non-staggered cartesian grid. The extension to curvilinear coordinate system is in progress. Chorin type pressure correction schemes previously used have assumed constant density for the fluid phase. The effective density of the fluid phase is not constant. Our fractional step scheme accounts for varying fluid properties.

One of the test cases we have solved is for the sedimentation of particles in a tube of square cross section. There were 4X4X80 control volumes in the domain with 17280 sedimenting parcels (groups of particles). The code ran successfully until sedimentation was complete after 10000 time steps (500s). It required around 7.5s real time on an SGI cluster to complete the calculation of one time step; 4.5 MB memory was required to run these calculations. These are preliminary results and further speed-up looks feasible.

The LNS code being developed by Patankar has a commercial potential. It has many of the features of DNS but it can compute motions of a practically unlimited number of particles. LNS calculations can be done easily on work stations and we believe can be coded for PC's. The visualization of the motions of proppant particles in a fractured reservoir should be a greatly valued and new feature for understanding and control of frac jobs.

The introduction of curvilinear coordinates, the extension of LNS to viscoelastic fluids and the introduction of lift forces and validation of drag and interparticle forces by comparison with DNS are new features, made possible by KDI, which could advance the subject and impact industry.

PROPOSAL BUDGET TO: NSF Supplment YEAR I

Organization:
UNIVERSITY OF MINNESOTA - AEROSPACE ENGINEERING & MECHANICS
Principal Investigator/Project Director:

		CAL	ACAD	SUMR	FUNDS REQUESTED	TOTAL REQUESTED
A.	Senior Personnel					
	1. ( )	0.0	0.0	0.0	$0	
	2. ( )	0.0	0.0	0.0	$0	
	3. (0) Total Senior Personnel	0.0	0.0	0.0	$0	$0
B.	Other Personnel					
	1. (1) Research Assoc. 50% 12 mos.				$23,752	
	2. (1) Post Doc. Assoc. 100% 12 mos.				$30,000	
	3. ( )				$0	
	4. ( )				$0	
	5. ( )				$0	
	6. ( )				$0	
	TOTAL SALARIES AND WAGES (A+B)					$53,752
C.	FRINGE BENEFITS: Research Assoc.		13.9%		$3,302	
	Post Doc. Assoc.		13.9%		$4,170	
			0.0%		$0	
	TOTAL FRINGE BENEFITS					$7,472
	TOTAL SALARIES, WAGES AND FRINGE BENEFITS					$61,224
D.	Permanent Equipment					
	(Item and $$Amount if Over $1,000)				$0	
	TOTAL PERMANENT EQUIPMENT					$0
E.	Travel					
	1. (Domestic)				$0	
	2.				$0	
	TOTAL TRAVEL					$0
F.	PARTICIPANT SUPPORT COSTS				$0	$0
G.	Other Direct Costs					
	1. (materials and supplies)				$0	
	2. (publication costs/page charges)				$0	
	3. (consultant services)				$0	
	4. (computer [ADPE] services				$0	
	5. (subcontracts)				$0	
	6. (other)				$0	
	TOTAL OTHER DIRECT COSTS					$0
H.	TOTAL DIRECT COSTS (A through G)					$61,224
I.	Indirect Costs 47% of Total Direct Costs					$28,776
J.	TOTAL DIRECT AND INDIRECT COSTS					$90,000
K.	Less Residual Funds (renewal/continuation only)					N/A
L.	AMOUNT OF THIS REQUEST					$90,000
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PROPOSAL BUDGET TO: NSF Supplment YEAR II

Organization:
UNIVERSITY OF MINNESOTA - AEROSPACE ENGINEERING & MECHANICS
Principal Investigator/Project Director:

	CAL	ACAD	SUMR	FUNDS REQUESTED	TOTAL REQUESTED
A. Senior Personnel					
1. (0) 0	0.0	0.0	0.0	$0	
2. (0) 0	0.0	0.0	0.0	$0	
3. (0) Total Senior Personnel	0.0	0.0	0.0	$0	$0
B. Other Personnel					
1. (1) Research Assoc. 50% 12 mos.				$23,565	
2. (1) Post Doc. Assoc. 100% 12 mos.				$30,000	
3. ( )				$0	
4. ( )				$0	
5. ( )				$0	
6. ( )				$0	
TOTAL SALARIES AND WAGES (A+B)					$53,565
C. FRINGE BENEFITS: Research Assoc.		14.3%		$3,370	
Post Doc. Assoc.		14.3%		$4,290	
		0.0%		$0	
TOTAL FRINGE BENEFITS					$7,660
TOTAL SALARIES, WAGES AND FRINGE BENEFITS					$61,225
D. Permanent Equipment					
(Item and $$Amount if Over $1,000)				$0	
TOTAL PERMANENT EQUIPMENT					$0
E. Travel					
1. (Domestic)				$0	
2. (foreign)				$0	
TOTAL TRAVEL					$0
F. PARTICIPANT SUPPORT COSTS				$0	$0
G. Other Direct Costs					
1. (materials and supplies)				$0	
2. (publication costs/page charges)				$0	
3. (consultant services)				$0	
4. (computer [ADPE] services				$0	
5. (subcontracts)				$0	
6. (other)				$0	
TOTAL OTHER DIRECT COSTS					$0
H. TOTAL DIRECT COSTS (A through G)					$61,225
I. Indirect Costs 47% of Total Direct Costs					$28,775
J. TOTAL DIRECT AND INDIRECT COSTS					$90,000
K. Less Residual Funds (renewal/continuation only)					N/A
L. AMOUNT OF THIS REQUEST					$90,000

PROPOSAL BUDGET TO: NSF Supplment YEAR III

Organization:
UNIVERSITY OF MINNESOTA - AEROSPACE ENGINEERING & MECHANICS
Principal Investigator/Project Director:

		CAL	ACAD	SUMR	FUNDS REQUESTED	TOTAL REQUESTED
A.	Senior Personnel					
	1. ( )	0.0	0.0	0.0	$0	
	2. ( )	0.0	0.0	0.0	$0	
	3. (0) Total Senior Personnel	0.0	0.0	0.0	$0	$0
B.	Other Personnel					
	1. (1) Research Assoc. 50% 12 mos.				$23,565	
	2. (1) Post Doc. Assoc. 100% 12 mos.				$30,000	
	3. ( )				$0	
	4. ( )				$0	
	5. ( )				$0	
	6. ( )				$0	
	TOTAL SALARIES AND WAGES (A+B)					$53,565
C.	FRINGE BENEFITS: Research Assoc.		14.3%		$3,370	
	Post Doc. Assoc.		14.3%		$4,290	
	TOTAL FRINGE BENEFITS					$7,660
	TOTAL SALARIES, WAGES AND FRINGE BENEFITS					$61,225
D.	Permanent Equipment					
	(Item and $$Amount if Over $1,000)				$0	
	TOTAL PERMANENT EQUIPMENT					$0
E.	Travel					
	1. (Domestic)				$0	
	2. (foreign)				$0	
	TOTAL TRAVEL					$0
F.	PARTICIPANT SUPPORT COSTS				$0	$0
G.	Other Direct Costs					
	1. (materials and supplies)				$0	
	2. (publication costs/page charges)				$0	
	3. (consultant services)				$0	
	4. (computer [ADPE] services				$0	
	5. (subcontracts)				$0	
	6. (other)				$0	
	TOTAL OTHER DIRECT COSTS					$0
H.	TOTAL DIRECT COSTS (A through G)					$61,225
I.	Indirect Costs 47% of Total Direct Costs					$28,775
J.	TOTAL DIRECT AND INDIRECT COSTS					$90,000
K.	Less Residual Funds (renewal/continuation only)					N/A
L.	AMOUNT OF THIS REQUEST					$90,000
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PROPOSAL BUDGET TO: NSF Supplment SUMMARY

Organization:
UNIVERSITY OF MINNESOTA - AEROSPACE ENGINEERING & MECHANICS
Principal Investigator/Project Director:

		CAL	ACAD	SUMR	FUNDS REQUESTED	TOTAL REQUESTED
A.	Senior Personnel					
	1. ( )	0.0	0.0	0.0	$0	
	2. ( )	0.0	0.0	0.0	$0	
	3. (0) Total Senior Personnel	0.0	0.0	0.0	$0	$0
B.	Other Personnel					
	1. (1) Research Assoc.				$70,882	
	2. (1) Post Doc. Assoc.				$90,000	
	3. ( )				$0	
	4. ( )				$0	
	5. ( )				$0	
	6. ( )				$0	
	TOTAL SALARIES AND WAGES (A+B)					$160,882
C.	FRINGE BENEFITS: Research Assoc.				$10,042	
	Post Doc. Assoc.				$12,750	
					$0	
	TOTAL FRINGE BENEFITS					$22,792
	TOTAL SALARIES, WAGES AND FRINGE BENEFITS					$183,674
D.	Permanent Equipment					
	(Item and $$Amount if Over $1,000)				$0	
	TOTAL PERMANENT EQUIPMENT					$0
E.	Travel					
	1. (Domestic)				$0	
	2.				$0	
	TOTAL TRAVEL					$0
F.	PARTICIPANT SUPPORT COSTS				$0	$0
G.	Other Direct Costs					
	1. (materials and supplies)				$0	
	2. (publication costs/page charges)				$0	
	3. (consultant services)				$0	
	4. (computer [ADPE] services				$0	
	5. (subcontracts)				$0	
	6. (other)				$0	
	TOTAL OTHER DIRECT COSTS					$0
H.	TOTAL DIRECT COSTS (A through G)					$183,674
I.	Indirect Costs 47% of Total Direct Costs					$86,326
J.	TOTAL DIRECT AND INDIRECT COSTS					$270,000
K.	Less Residual Funds (renewal/continuation only)					N/A
L.	AMOUNT OF THIS REQUEST					$270,000
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