ARGONNE NATIONAL LABORATORY

Mathematics and Computer Science Division

9700 South Cass Avenue, Argonne, Illinois 60439-4844

Telephone 630-252-7238
FAX 630-252-5986
more@mcs.anl.gov

March 27, 2005

Dr. Gary Johnson
Office of Advanced Scientific Computing Research
U.S. Department of Energy
SC-31 Germantown Building
1000 Independence Ave., SW
Washington, DC 20585

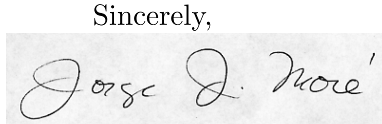
Dear Gary:

This proposal, *A Multiscale Computational Framework for Dense Particulate Flows*, is being submitted in response to the **Program Announcement LAB 05-16** and represents a collaboration between the following institutions:

- Argonne National Laboratory
- Oak Ridge National Laboratory
- Princeton University

The role played by each institution is described in the section on *Consortium Arrangements*. Paul Fischer of Argonne is the lead for this proposal.

Sincerely,



Jorge J. Moré
Senior Scientist
Director, Laboratory for Advanced Numerical Software

BUD-11A (1-02)
Page 1

U. S. DEPARTMENT OF ENERGY
FIELD WORK PROPOSAL

1. WORK PACKAGE NO.:	1a. WORK PROPOSAL NO.:	2. REVISION NO.:	3. DATE PREPARED	3a. CONTRACTOR NO.:
ANL			03-28-05	56113

4. WORK PACKAGE TITLE:	4a. WORK PROPOSAL TITLE:
Mathematical, Information, and Computational Sciences	A Multiscale Computational Framework for Dense Particulate Flows

5. BUDGET & REPORTING CODE:	6. WORK PROPOSAL TERM: Begin: End:	7. IS THIS WORK PACKAGE INCLUDED IN THE INST. PLAN?	7a. PRINCIPAL INVESTIGATORS:
KJ-01-01-01	07/01/05-06/30/08	☐ YES ☐ NO	Fischer, P. F.

8. HEADQUARTERS/OPERATIONS OFC PROGRAM MANAGER:	11. HEADQUARTERS ORGANIZATION:	14. DOE ORG. CODE:
Johnson, G. M. 301-903-5800	Office of Science	SC
9. OPERATIONS OFFICE WORK PROPOSAL REVIEWER:	12. OPERATIONS OFFICE: Chicago	15. DOE ORG. CODE: CH
10. CONTRACTOR WORK PROPOSAL MANAGER: Stevens, R. L. 630-252-3378	13. CONTRACTOR NAME: University of Chicago/ANL	16. CODE: 12

17. IS THIS PROPOSAL TO DO WORK THAT INCLUDES A SECURITY INTEREST? ☐ YES ☒ NO

18. WORK PROPOSAL DESCRIPTION (Approach, anticipated benefit in 200 words or less):

Program Announcement LAB 05-16
A Multiscale Computational Framework for Dense Particulate Flows

Applications-level extensions of the equation-free multiscale approach are proposed to aid in the prediction of dense particulate flow, a phenomenon that has eluded a consistent macroscale desciption. Several DOE science and engineering applications are targeted, including prepation of powders for compaction, which is relevant to nanoparticle processing and to processing of nuclear fuel, the motion of fuel pebbles in pebble bed reactors, and thermal convection in pebble bed reactors. Tasks include extension of the equation-free method to nonuniform meshes, the definition of microscale boundary conditions compatible with the method and the physics, and the development of efficient coarse-to-fine lifting (initialization) strategies for each application. Several young scientists will be trained in both multiscale analytical and computational techniques via hands-on experience as well as by course material that will be developed as part of the project.

19. CONTRACTOR WORK PROPOSAL MANAGER:		20. OPERATIONS OFFICE REVIEW OFFICIAL:	
[signature]	03-28-05		03-28-05
SIGNATURE	DATE	SIGNATURE	DATE

21. DETAIL ATTACHMENTS: (See instructions.) Task Proposals Attached.

☐ a. Facility requirements	☐ d. Background	☐ g. Future accomplishments	☐ j. Explanation of milestones
☐ b. Publications	☐ e. Approach	☐ h. Relationships to other projects	☐ k. Human or Animal Subjects Activities
☐ c. Purpose	☐ f. Technical progress	☐ i. Environmental assessment	☐ l. Other

DOE F 4650.2
Rev. (10-03)
(All Other Editions Are Obsolete)

Department of Energy
Office of Science (SC)

Face Page

OMB Control No.
1910-1400
(OMB Burden Disclosure Statement on Back)

TITLE OF PROPOSED RESEARCH:
A Multiscale Computational Framework for Dense Particulate Flows

1. CATALOG OF FEDERAL DOMESTIC ASSISTANCE #
81.049

2. CONGRESSIONAL DISTRICT:
Applicant Organization's District: 13th
Project Site's District: 13th

3A. I.R.S. ENTITY IDENTIFICATION OR SSN:
36-2177138

3B. DUNS Number:
02-003-2538

4. AREA OF RESEARCH OR ANNOUNCEMENT TITLE/#:

Program Announcement LAB 05-16

5. HAS THIS RESEARCH PROPOSAL BEEN SUBMITTED TO ANY OTHER FEDERAL AGENCY?
☐ YES ☑ NO

PLEASE LIST

6. DOE/OER PROGRAM STAFF CONTACT (if known):
Dr. Gary Johnson

7. TYPE OF APPLICATION:
☑ New ☐ Renewal
☐ Continuation ☐ Revision
☐ Supplement

8. ORGANIZATION TYPE:
☐ Local Govt. ☐ State Govt.
☑ Non-Profit ☐ Hospital
☐ Indian Tribal Govt. ☐ Individual
☐ Other ☐ Inst. of Higher Educ.
☐ For-Profit
☐ Small Business ☐ Disadvan. Business
☐ Women-Owned ☐ 8(a)

9. CURRENT DOE AWARD # (IF APPLICABLE):
Not Applicable

10. WILL THIS RESEARCH INVOLVE:
10A. Human Subjects ☑ No ☐ If yes
Exemption No. ______ or
IRB Approval Date ______
Assurance of Compliance No: ______
10B. Vertebrate Animals ☑ No ☐ If yes
IACUC Approval Date ______ or
Animal Welfare Assurance No: ______

11. AMOUNT REQUESTED FROM DOE FOR ENTIRE PROJECT PERIOD $ 2,553,340.00

12. DURATION OF ENTIRE PROJECT PERIOD:
07/01/05 to 06/30/08
MM/DD/YY MM/DD/YY

13. REQUESTED AWARD START DATE
07/01/05
MM/DD/YY

14. IS APPLICANT DELINQUENT ON ANY FEDERAL DEBT?
☐ Yes (attach an explanation) ☑ No

15. PRINCIPAL INVESTIGATOR/PROGRAM DIRECTOR
NAME Paul F. Fischer
TITLE Principal Investigator
ADDRESS Argonne National Laboratory
9700 S. Cass Avenue
Building 221
Argonne, Illinois 60439
PHONE NUMBER 630-252-6018

* Paul F. Fischer (Electronically submitted)

SIGNATURE OF PRINCIPAL INVESTIGATOR/ PROGRAM DIRECTOR
(please type in full name if electronically submitted)
Date March 28, 2005

PI/PD ASSURANCE: I agree to accept responsibility for the scientific conduct of the project and to provide the required progress reports if an award is made as a result of this submission. Willful provision of false information is a criminal offense. (U.S. Code, Title 18, Section 1001).

16. ORGANIZATION'S NAME Argonne National Laboratory
ADDRESS 9700 S. Cass Avenue
Building 221
Argonne, IL 60439

CERTIFYING REPRESENTATIVE'S
NAME Rick L. Stevens
TITLE Director, Mathematics and Computer Science Division
PHONE NUMBER 630-252-3378

SIGNATURE OF ORGANIZATION'S CERTIFYING REPRESENTATIVE
(please type in full name if electronically submitted)
Date March 28, 2005

CERTIFICATION and ACCEPTANCE: I certify that the statements herein are true and complete to the best of my knowledge, and accept the obligation to comply with DOE terms and conditions if an award is made as the result of this submission. A willfully false certification is a criminal offense. (U.S. Code, Title 18, Section 1001).

A Multiscale Computational Framework for Dense Particulate Flows
Argonne National Laboratory
Principal Investigator - Paul Fischer

		Year 1		Year 2		Year 3		Total
National Laboratories								
Argonne National Laboratory- MCS	$	500,000	$	500,000	$	500,000	$	1,500,000
Oak Ridge National Laboratory	$	100,000	$	100,000	$	100,000	$	300,000
Total National Laboratories	**$**	**600,000**	**$**	**600,000**	**$**	**600,000**	**$**	**1,800,000**
Universities								
Princeton University	$	282,305	$	231,157	$	239,878	$	753,340
Total Proposal	**$**	**882,305**	**$**	**831,157**	**$**	**839,878**	**$**	**2,553,340**

Contents

A Multiscale Computational Framework for Dense Particulate Flows

Paul F. Fischer (Principal Investigator)

Mathematics and Computer Science Division
Argonne National Laboratory
9700 S. Cass Avenue
Argonne, IL 60439
phone: 630-252-6018
fax: 630-252-5986
fischer@mcs.anl.gov

Co-PIs: Mihai Anitescu, Yannis Kevrekidis, Gary Leaf, Sreekanth Pannala, Barry Smith, and Sankaran Sundaresan

Abstract

Applications-level extensions of the Equation-Free Multiscale approach are proposed to aid in the prediction of dense particulate flow, which is a phenomenon that has eluded a consistent macroscale desciption. Several DOE and Office of Science applications are targeted, including prepation of powders for compaction, which is relevant to nanoparticle processing and to processing of nuclear fuel; the motion of fuel pebbles in pebble bed reactors; and thermal convection in pebble bed reactors. Until this point equation free methods have demonstrated mainly a proof of concept and the extensions proposed here are essential for its migration to applications of interest to DOE. The topics addressed in this proposal are: extension of the equation-free method to nonuniform meshes, the definition of microscale boundary conditions compatible with the method and the physics, the development of efficient coarse-to-fine lifting (initialization) strategies for each application, and the development of high-order methods. Several young scientists will be trained both in multiscale analytical and computational techniques via hands on experience as well as by course material that will be developed as part of the project.

Project Summary

We propose to implement and extend the equation-free multiscale analysis approach through its application to a class of physical phenomena whose consistent description has so far eluded scientific modeling: dense granular flow. This applications area was chosen because it exemplifies the class of problems for which micro-macroscale closures are believed to exist but are not known and because of its relevance to industrial processing and to the DOE and Office of Science missions.

The equation free approach is a multiscale computational framework that uses only the microscale description of a physical phenomenon to efficiently predict temporal evolution or equilibrium behavior at the macroscale. The appeal of the method is that it makes no other assumption about the solution or about the model other than that the macro scale observables can be faithfully represented on a relatively uniform macro scale mesh, an assumption relying on scale separation in the the physics of the problem and the model used for its description. The method is a concurrent multiscale approach that has been validated by reproducing the successes of past explicit homogenization approaches and has been shown able, in principle, to perform many of the system-level tasks (e.g., time evolution, eigenvalue prediction, and bifurcation analysis) that are needed from a modern computationally based predictive tool.

In order to successfully validate and extend the method, we propose to systematically test the critical implementation assumptions that have been taken for granted up to this point in order to provide the proof of concept. Among these issues are the selection and implementation of physics-inspired boundary conditions compatible with the method, the extension to nonuniform meshes, the derivation of higher order methods, and the selection of appropriate macroscopic observables through data analysis.

We will study the applications of our analysis and simulation technology to a topic for which it holds real promise, namely, the predictive modeling of a class physical phenomena for which no consistent macro scale model has been defined to date: dense particulate flows. Such flows are essential in engineering science and materials processing and in two instances, which will be covered in our work, are of critical interest to two energy oriented applications. Those applications are the macro scale thermal hydraulic behavior of the very high temperature nuclear reactor and the preparing of powder and particulate matter for further processing, such as compaction. This latter area is relevant to processing of nanomaterials and of nuclear fuel.

The proposed work contains a mixture of mathematical analysis, modeling, scientific computations and phenomena prediction. Several young scientists will be trained both in multiscale analytical and computational techniques via hands-on experience with the details of the project as well as by course material that will be developed from the successes of this work.

1 Background

The proposed research aims at bridging traditional, continuum level numerical analysis and scientific computation with modern, physics-based microscopic simulators. Using particulate flow problems that are relevant to the DOE Mission as a scaffold, we propose to explore both practical and theoretical issues that arise when the problem is approached through the equation-free computational framework. The research aspires to significantly expand the scope and applicability of equation-free multiscale algorithms and the theory underpinning them and to address important science and engineering questions in the area of dense particulate flows.

1.1 The Equation-Free Multiscale Method

Continuum evolution equations (ordinary and partial differential equations) constitute the models of choice for a large variety of physical and engineering processes. Scientific computation algorithms built on the numerical analysis of methods for the solution of such continuum equations are the workhorse of contemporary scientific modeling. These continuum equations are mostly conservation laws (mass, momentum, energy, charge, chemical species etc.) complemented by appropriate closures. In contemporary scientific modeling, however, the closures required to write these continuum equations in closed form are not available, and the only modeling tools are simulation algorithms at an atomistic or stochastic level (molecular dynamics, kinetic Monte Carlo, agent based). The scale gap between the level at which modeling tools are available and the level at which engineering questions are asked and design answers are required is simply too large to bridge through brute force simulation.

Our work aims at enabling engineering modeling of *effectively simple* multiscale problems: problems for which a closure for the coarse-grained, macroscopic, systems level, engineering behavior conceptually exists but is not available in closed form. If the stumbling block for modeling is the lack of closed form coarse-grained equations, we know that it is possible to circumvent it: we can create a bridge between direct microscopic simulation and macroscopic numerical analysis by using the micro-simulator as a *computational experiment* that can be initialized at will. The equation-free approach to complex, multiscale modeling uses traditional continuum numerical analysis to, effectively, design the most economical amount of computational experiments with the fine scale code, in order to solve the engineering problem at hand.

The use of an inner simulator as an experiment starts to appear in contemporary numerical analysis in the last twenty years; so co-called timestepper based methods, like the Recursive Projection Method of Shroff and Keller [106] appear in the late 80's–early 90's, and their combination with matrix free iterative linear algebra dates from that time also. The idea of using a microscopic, fine scale simulator instead of a continuum one appears to be a relatively new idea, and the development of a systematic framework based on it lies at the heart of our proposed research. More than anything else, the approach is a computational enabling technology: it links existing tools from different disciplines (numerical analysis, detailed physics and chemistry-based simulation, and systems theory) in new ways, allowing us to face problems inaccessible by brute force simulation. New mathematics, underpinning the new combinations of existing tools, arise in a natural way – if the only description of a numerical method available is in an input-output form, how to design experiments that will estimate the bounds and stability criteria usually obtained through formulas ? Finally, it is important to state that the macroscopic variables (observables) used in equation-free computation do not have to be the traditional fields (concentration, momentum, temperature); they can be order parameters arising from data analysis, thus creating a link between data mining, image processing and feature extraction algorithms with scientific computer modeling. This is a particularly promising research direction that we propose to explore throughout the project.

1.1.1 Significance of Research to DOE Applications

Our development of the equation-free multiscale approach will focus on four test problems in the area of dense particulate flow, namely, spouted beds, dense-phase pneumatic conveying, granular flows, and turbulent heat transfer in fixed packed beds. All of these problems feature a microscale set by the size of the particulates that is much smaller than the macroscale variable representation of relevance to engineering design and analysis. The first two test problems feature strongly coupled particle and fluid motions. In the third problem, the granular flow is assumed to be decoupled from the fluid flow, and in the fourth problem, the fluid is assumed to move through a fixed bed of particles. These problems were chosen because they exemplify the class of problems for which micro-macroscale closures are believed to exist but are not known and because of their relevance to industrial processing and to the DOE Mission.

Fluidized beds, spouted beds, dense phase conveying and other dense particulate flow technologies are essential for a wide variety of applications in chemical, fossil and petrochemical industries. These processes are directly related to energy production and consumption. Fundamental understanding of gas-solid flow in the dense regime is critical to strengthening national energy security and of great relevance to DOE and Office of Science (OS). We list here a few of the DOE related applications for each of our model problem areas:

Spouted beds: Spouted beds are used for coating nuclear fuel particles with carbon and silicon carbide to contain the fission products in a nuclear reactor. The coated particles are compacted using resin to make pebbles for the pebble bed reactors (or hexagonal blocks for the prismatic design). The quality and strength of the coatings is very important as the coater layers are the first and last defense against the gaseous fission products.

Dense phase conveying: Fluidization and pneumatic conveying in vertical, horizontal or inclined ducts are common operations in particle handling. The former is widely encountered in chemical reactors, while the latter is frequently employed to transport particles from one location to another in a plant (e.g., coal).

Granular flows: In recent years, with the advent of nanotechnology and nanosized particles and powders, there is tremendous interest within DOE OS to process granular and particulate matter. Nanomaterials have wonderful catalytic properties but are difficult to handle because of their cohesive nature and their health affects are uncertain as they can easily be airborne and enter our respiratory and blood system.

Granular flow is also important in the design and operation of the *Pebble Bed Reactor* (PBR), which consists of a large silo filled with $> 10^5$ graphite coated nuclear fuel pebbles. During operation, the tennis-ball-sized pebbles are extracted from the bottom of the vessel at the rate of 2 per minute, analyzed, and recirculated through the top of the reactor if they are deemed to have enough fissionable material or are replaced by new pebbles if not. Understanding the migration of the pebbles is important to predicting the fuel and thermal loading in the bed, and the statistics of the void distributions have important consequences for the passage of the high pressure He coolant.

Turbulent heat transfer in fixed beds: Flow in fixed beds arises in many industrial and geophysical applications. Here, we focus on high-Reynolds number flow and heat transfer in configurations similar to the PBR. The nuclear reactions in the PBR produce heat that is subsequently extracted by helium flow, which is blown through the pebbles and reactor walls and exits the reactor vessel at very high output temperature (1000 C). Therefore the physics of the pebble bed nuclear reactor consists of very slow granular flow for the fluid motion, and very fast cooling flow. Uniformity of the temperature distribution at the outlet, hot streaks, and pressure losses at the sidewalls are all issues that affect reactor efficiency.

1.1.2 Broader Significance of Research: Education

We will ensure dissemination of multiscale research through presentations at conferences (e.g., APS, AIChE, SIAM) and workshops, seminars presented at universities and industries, scholarly articles written and published in a timely manner, and results posted on our research group web sites. The simulation tools developed in the course of the proposed study will be made available to the research community. The proposed research will also provide an excellent vehicle for training PhD students and post-doctoral fellows in multiscale analysis techniques.

One of the PIs (IGK) teaches periodically a graduate chemical engineering/applied mathematics course where multi-scale methods, and the equation-free method in particular, is discussed; examples from the proposed research will be integrated into this course. The PIs will work together and create a module on multi-scale methods applied to particulate flow problems; this module, consisting of lecture notes, PowerPoint slides and movies, will be made available to the broad community through our web sites. At Princeton, all the undergraduate students in Chemical Engineering do a year-long senior thesis. The PIs will design and offer senior thesis and summer REU projects related to this research program.

Princeton University is committed to expanding the diversity of its student body and this commitment is affirmed in the Strategic Plan launched by the School of Engineering & Applied Science (SEAS) in May 2004. Under this plan, SEAS will work aggressively to recruit (and retain) under-represented minorities into its student body and faculty. SEAS has launched recently a student exchange program with Smith college, see http://www.princeton.edu/pr/news/05/q1/0105-smith.htm. The PIs will work with the university in pushing forward these initiatives. SEAS also organizes science and engineering expos for local middle school students every year. The PIs have participated in these activities and will continue to do so in the future. As the SEAS associate dean for academic affairs for six years (1997-2003), SS played an active in fostering many (scholarly) student organizations including Graduate Women in Science & Engineering (GWISE). Today, GWISE is a thriving student organization http://www.princeton.edu/∼gwise/.

1.2 Challenges and Methodologies for Dense Particulate Flows

Dense particulate flows are encountered in a variety of process industries—manufacturing of bulk and specialty chemicals, petroleum refining, coal handling, gasification and combustion, etc. [12, 20, 43, 62, 123, 25, 35, 32, 61, 112].

The interstitial fluid flow couples with the dense particulate flow and dictates the overall flow characteristics in many devices used in these industries, such as fluidized beds, circulating fluidized beds, spouted beds, moving bed reactors and dense phase conveying. Size distribution and cohesive interaction between particles are very common, and they are central to proper interpretation of many problems concerning flow, mixing and segregation [22, 98, 92]. In most problems of practical interest, the number of particles involved is very large (tens to hundreds of millions), and hence, solving for the motion of each and every particle in the assembly is computationally expensive or simply unaffordable. This consideration has driven the development of continuum models through ensemble-averaging of the equations governing the motion of the individual particles as a practical alternative to probe macroscopic flow characteristics [43, 61, 28, 105, 76, 64]. In this approach, the particle phase is treated as a continuum, and locally-averaged quantities, such as the volume fraction, mean velocity, and mean-squared fluctuating velocity of the particle phase, appear as dependent variables. Derivation of the general form of the averaged equations and associated constitutive models has been the subject of much research, but such theories are invariably limited to a small subset of cases of practical importance. For example, the current kinetic theory of granular materials applies only for spherical, non-cohesive and weakly dissipative particles and, the ability to handle particle size distribution is still evolving [46, 57]. Validated continuum models that capture cohesive interactions between the particles remain elusive. As a result, mathematical analyses of large-scale dense particulate flows have lagged behind applications. In the research using the equation-free coarse-grained approach proposed here, we will develop the mathematical and computational tools needed to analyze the macroscale flow characteristics in dense particulate flows; more specifically, we will address the mathematical issues associated with wrapping coarse integration and fixed point analysis tools around particle-level simulators. The approach will be used to analyze a class of dense particulate flow problems of significant practical interest.

1.2.1 Challenges in dense granular flows

Particulate materials manifest vastly different rheological behavior under rapid shear flow conditions and slow, quasi-static deformation. In rapid shear flow, the particles interact primary through binary inelastic collisions, with both the shear and normal stresses manifesting a strong (typically second-order) dependence on shear rate [20]. Continuum models for flow in this regime deduced by adapting the kinetic theory of dense gases to particles are discussed and analyzed extensively in the literature (e.g., see [76, 63, 43]).

At the other end of the spectrum in rheology, namely under quasi-static flow conditions, where the particles in a dense assembly make enduring contact with their neighbors, the shear stress is essentially independent of shear rate [2]. Bead-pack calculations with frictional spheres [45] suggest that Lade-Duncan [71] form of yield surfaces capture the general features of granular plasticity. However, predictive models that connect particle-level information to continuum rheological description are unavailable.

The transitional regime connecting the quasi-static and rapid flow regime is only beginning to be explored at a fundamental level [104, 21, 118]. Most dense particulate flows – chute flow, fluidized beds, spouted beds, dense phase pneumatic conveying, rotary mixers, bin discharge – involve all three regimes occurring simultaneously at different spatial locations. Reliable continuum models spanning all three regimes, with particle properties (such as radius, density, coefficients of restitution and friction) as inputs are essential for accurate modeling of all of these flows – such models are unavailable even for the simple case of non-cohesive, uniformly sized particles. Flows encountered in practice are more complex. Size distribution and cohesive interaction between particles are very common, and they are central to proper interpretation of many problems concerning flow, mixing and segregation [22, 98, 92].

At present, the Discrete element method (DEM), where one follows the motion of individual particles using classical equations of motion, is virtually the only available tool to simulate most real flows; these discrete particles may be the real particles involved in the flow, or fictitious particles representing a collection of real particles. When dealing with large scale flows involving large numbers of particles, the time and length scales associated with the flow span many orders of magnitude. DEM simulations resolve details at the level of the individual particles and these occur on a very fast time scale. Macroscopic quantities of interest, occur over coarser length and time scales, and are often captured through a suitable set of lower order moments of the particle distribution. However, closed continuum equations in terms of these lower-order moments are not explicitly available over most of the flow regimes. The equation-free multiscale approach proposed here aspires to tackle precisely this type of complex problems. We believe that this approach will impact our ability to simulate, understand, design and control each class of dense particulate flow mentioned above.

1.2.2 Discrete Element Method Simulations

The Discrete Element Method (DEM) was introduced nearly three decades ago [27] and has been used to model and understand many different granular flows: hopper flows [23], [93], charging and discharging of silos/bins [59]-[58], chute flow [51], [70], avalanches [20], flow and mixing in rotating drums [81], [19] and vibrated layers [11], [129], etc.. In DEM simulations, the trajectory of every particle is computed by Newton's equations of motion, allowing for external body force and interaction between particles and between particles and system boundary. In the so-called spring-dashpot model by Cundall and Strack [27], the interaction in the normal direction is modeled by a spring and a damper. Particles are allowed to overlap and the contact force in the normal direction is determined by the extent of overlap (through a Hertzian or Hookean spring model [32]) and the normal component of their relative velocity. In the tangential direction, the interaction is modeled by a spring and a slider, and the total tangential force is limited by the Coulomb frictional force. The model parameters can readily be expressed in terms of the Young's modulus and Poisson's ratio of the material, and the coefficients of friction and restitution. In general, DEM simulations allow the particles to be considerably softer than they really are and, as a result the particles overlap more in the computer simulations than they do in real experiments. This is necessary to keep the computational cost manageable, as the time step required to accurately resolve the particle-particle contact decreases with the spring stiffness; however, this does not cause any noticeable inaccuracy for a wide range of problems [53]. There are other variants on the particle interaction model, where instead of a damper, one uses different stiffness constants depending on whether the overlapping particles are moving toward or away from each other [124]. Rapaport [55], [96], and [95] has accelerated the DEM calculations through the extension of traditional molecular dynamics through the introduction of Lennard-Jones type of potential to handle the interaction between the soft particles. Other contributions to the normal force, such as van der Waals attraction, electrostatic force and capillary force, can be added to the force model readily [11], [69], [77], [116], and [132].

Another variant of DEM developed to prevent the excessive particle overlap problem is one where the nonsmooth contact and friction laws are enforced by hard constraints [86, 87, 111, 8]. This improvement comes at the cost of solving a linear complementarity problem [24] whose cost per time step is larger than the one of a linear system, but can take larger time steps than spring-dashpot models without loss of stability. Such methods have been proven to converge to weak formulations of the nonsmooth dynamics problem [110]. These methods have been applied with success to predict the complex force distribution pattern in two dimensional granular systems, but the difficulty in solving the underlying linear complementarity problem has not made them to date the algorithm of choice for large scale simulations.

The DEM method has also been coupled to fluid phase for simulating gas-solid flows where the role of gas cannot be neglected. In this case, the local-average gas velocity and pressure fields are found by solving locally-averaged equations of motion for the gas phase, while the particle motion is tracked using DEM and the interphase drag term is computed through known correlations. This approach has been used by several researchers [131, 125, 117, 18] and has been applied to several gas-solid flows in fluidized beds [131, 125], spouted beds [117, 102] and pneumatic transport [115, 130]. In particular, DEM is coupled with an open-source DOE funded multiphase flow simulation suite called MFIX [113, 114] for cohesionless [15] and cohesive [125] particles. Even with recent advances in computational capabilities, the number of particles in the simulation studies are generally limited to a hundred thousand or less [102, 60], and occasional studies [20, 18] consider as high as a million 2D discs. Actual systems typically have millions or hundreds of millions of particles and the current multiscale approach will enable simulation of such large systems.

1.3 Challenges and Methodologies for Turbulent Packed-Bed Flows

Turbulent flow in packed beds arises in many industrial applications such as thermal conversion of solid fuels, drying grains, catalysis, and so forth. It is also the principal mechanism for energy extraction from pebble bed reactors that are being investigated as one of two very high temperature reactor (VHTR) configurations under consideration by the DOE. The VHTRs use high temperature helium as the working medium and are designed to be intrinsically safe, efficient, and environmentally acceptable. In the pebble bed reactor (PBR), the core comprises hundreds of thousands of tennis-ball-sized fuel pebbles randomly packed in a silo that is several meters across and roughly ten meters high. A cost-saving feature of the PBR is that it operates continuously, without shutting down for fuel replacement. This is achieved by steadily extracting pebbles from the bottom of the bed (at a rate of ≈ 2 per minute), inspecting them, and returning them to service or discarding, according to indicated level of fissionable material.

The principal energy-transfer mechanism in the PBR is through turbulent heat transfer from the pebbles to the He, which then passes into an exit plenum and onto an intermediate heat exchanger or directly to a power turbine. Thermal-hydraulic analysis and validation are key components of VHTR research and represent a truly multiscale problem. The temperature distribution in the VHTR strongly affects the local power output, through feedback to the neutronics, and the mechanical loading, through thermal expansion of the graphite-fuel matrix or graphite-fuel pebbles.

Heat-transfer analysis of the PBR configuration is particularly challenging because of its geometric complexity and range of scales. The flow domain for convective heat transfer in the PBR comprises the void regions between the pebbles and interior to the reactor walls. At the void scale, the Reynolds number is $Re_v \approx 70{,}000$, which means that the flow is fully turbulent and induces a broad range of subvoid scales. At the mesoscale, void-to-void correlations can result in extensive channels through which gas can easily flow. At the macro- (reactor) scale, there are roughly a million voids.

Most macroscopic simulations of porous media flow are based on homogenization models involving a Stokes flow assumption (Darcy's law) that is appropriate for low Reynolds number flows, or nonlinear corrections that give a pressure drop that is quadratic in $\mathbf{u}$ [34]. These, however, have limitations in finite beds and are unable to capture any of the high-order moments in the statistical description of the particle distribution [82, 54]. For example, models that are based solely on a void fraction representation risk missing effects of channels, which arise when voids become aligned (e.g., as in the case of a hexagonally close-packed lattice) and which are known to alter bulk flow properties [97]. On average, the bed is expected to be nearly close-packed, with a void fraction of $\approx .31$, which implies that momentum transfer may be largely localized through screening effects (i.e., subharmonics larger than the void scale will be cut off) [67, 54, 89].

The fundamental heat transfer questions that need to be addressed include

- the expected mean and variation of temperature distribution,
- the amount of horizontal dispersion/diffusion in the bed,
- the amount of bypass flow expected at the sidewalls,
- the prevalence of hot streaks (which also relates to fuel distribution),
- the uniformity of the exit temperature, and
- the expected pressure drop as a function of void fraction.

All of these questions are intimately tied to the statistics of the bed packing, which is dynamic because of pebble recycling and thermal-mechanical loading. Particle distributions from granular flow simulations, to be carried as part of this proposed effort, will indicate which detailed microscale and mesoscale simulations to undertake and also dictate the statistical void-distribution in the heterogeneous macroscopic model (e.g., What is the void fraction as a function of the reactor length z? What is the distribution of channels and how to best characterize it ?")

Detailed analysis of single-phase flow through packed beds has received renewed attention through the ability to carry out direct numerical, large eddy, and Reynolds-averaged simulations in such configurations and with the need for more highly optimized designs. Detailed simulations can provide input to determining parameters for closure (upscaling) models or, as we propose here, by being performed in appropriately coupled "patches" in the patch-dynamics setting of the equation-free coarse-grained simulation.

2 Preliminary Results

The equation-free (EF) approach to complex systems modeling combines many existing elements of scientific computation, applied mathematics and numerical analysis. Novel aspects have more to do with the way these existing elements (model reduction, design of experiments, estimation and filtering, matrix-free iterative linear algebra, data mining, numerical analysis) are integrated in a coherent computational framework and connected with state-of-the-art microscopic/atomistic simulation codes. The first paper on the approach appeared in *PNAS* in August of 2000 [121] and showed how to use matrix-free iterative linear algebra techniques to implement coarse-grained bifurcation analysis of an inner fine-scale (in that case, a Lattice-Boltzmann) dynamic simulator. Most of the elements of equation-free computation are already present in that first paper (1) the use of the inner simulator as a computational experiment, short bursts of which are used to estimate important quantities on demand; (2) the lifting and restriction operations, from macroscopic observables to consistent microscopic realizations and back; (3) the design of experiments templated on a continuum numerical method (fixed point and bifurcation computation); and (4) the extensive use of matrix-free iterative linear algebra (in that case, through the Recursive Projection Method of Shroff and Keller). The wide scope of the approach was briefly discussed in that paper. The same year, the first application of EF methods to Partial Differential Equation simulation (the gaptooth scheme) is presented by Kevrekidis in a plenary lecture of the CAST division of the AIChE, using again a Lattice Boltzmann inner simulation code in small, coupled spatial domains. The next important step in EF method development took place in late 2000; upon retirement from the Directorship of NEC Institute, C. W. Gear started collaborating with Kevrekidis on equation-free acceleration of direct simulation methods; projective integration and telescopic projective integration algorithms are among the first results of that collaboration, making the point that most continuum numerical algorithms (and not only fixed point, stability and continuation algorithms) can be integrated in an equation-free framework. Later it has been demonstrated that additional computational tasks (like the design of stabilizing and optimal controllers, optimization, as well as the computation of traveling and self-similar solutions) are also naturally integrated in the EF framework.

Method development and new applications go hand in hand after this important first year. In Spring of 2001 a paper is submitted to Nonlinearity, demonstrating the EF implementation of homogenization, or effective medium techniques (the application was a reaction-diffusion traveling problem in porous media). There follows the study of kinetic Monte Carlo simulations of chemical reactions; EF wrappers are constructed around both stochastic simulation algorithms (the Gillespie SSA) as well as lattice gas models of heterogeneous catalytic reactions. The first application to the coarse integration, stability and bifurcation analysis and control for stochastic differential equations involves a Brownian Dynamics study of nematic liquid crystal rheology that appears in J. Chem. Phys. [107]. On the computational biology side, a collaboration with Hans Othmer in Minnesota leads to EF studies of chemotaxis; a collaboration with Simon Levin at Princeton leads to the EF exploration of evolutionary epidemiological models; and the collaboration with Dr. G. Hummer at NIH leads to the wrapping of EF methods around molecular dynamics codes, studying in particular the effective free energy and kinetics of alanine dipeptide folding in water. A collaboration starts with the numerical analysis group at Leuven, in Belgium, which leads to a sequence of papers on the numerical analysis of gaptooth and patch dynamics methods for PDEs (patch dynamics is the combination of gaptooth with projective integration). The use of these algorithms in control and optimization applications is pursued at Princeton through a sequence of postdocs that go on to academic positions (Theodoropoulos at UMIST, Siettos at NTU Athens, Armaou at Penn State).

The first EF study of multiphase flows (an inner Lattice Boltzmann, outer Navier-Stokes level study of bubble flow) is published in 2001 and 2004 in collaboration with S. Sundaresan [119, 120]; the collaboration continues currently with the EF study of fluidized beds and granular mixing. EF modeling of dislocation motion in a field of diffusing impurities (with D. Srolovitz) and the acceleration of equilibrium GCMC simulations of micelle aggregation and breakup (with Panagiotopoulos) expand the range of applications. Gas dynamics studies (with Nicolas Hadjiconstantinou at MIT), effective descriptions of discrete systems (with O. Runborg and J. Moeller in Sweden) and coarse molecular dynamics studies of water interaction with carbon nanotubes (with G. Hummer) have also been completed.

As the applications expand, two "manifesto-type" publications appear about the equation-free framework. One appears in 2003, in Comm. Math. Sci., while the second, briefer one appears as an invited Perspective article in the AIChE Journal in 2004 [40, 65]. An important application (the construction of EF wrappers for existing, legacy dynamics codes) is explored through a collaboration with Imperial College (and the commercial software gPROMS) [108]. Along the same lines, the development of EF-wrappers around traditional Navier-Stokes codes is pursued with G. Karniadakis at Brown, and the equation-free approach to uncertainty quantification, circumventing the derivation and implementation of Stochastic Galerkin algorithms is also completed (with R. Ghanem and D. Xiu, to appear in 2005). New applications include the EF study of coupled oscillator dynamics, homogenization in truly random media (with D. Xiu), the effective bifurcation analysis of agent-based models in economics (a new class of applications, opening a window towards certain environmental and social science problems) and model studies of passive particle dispersion in model turbulent flows.

Two important recent developments are worth mentioning: The first is the use of equation-free methods to study coarse renormalization problems (i.e., locating macroscopically self-similar solutions directly from microscopic level codes); examples include molecular diffusion, gravitational star collapse problems (with D. Merritt), cell aggregation problems (with H. Othmer), studies of glassy dynamics (with P. Kevrekidis) and certain SPDE computational turbulence models (with V. Yakhot). The second is the onset of a collaboration, through the last year, with Professor R. Coifman and his group at Yale [88]; they have been developing data mining techniques based on graph diffusion, which hold the promise to data-driven identification of good macroscopic observables (order parameters) for the description of complex problems. This provides the appropriate variables with which to do equation-free computation; we can think of it as the "variable free" component of an "equation free–variable free" modeling approach to complex systems. Among the continuing theoretical, computational and example-driven equation-free research, this new possibility of combining equation-free with "variable-free" computations seems to be the most exciting prospect for the coming years.

2.1 Discrete Element Method Simulations

Coupling DEM with a computational fluid dynamics (CFD) code MFIX (described in the earlier section) has now been achieved and it offers a powerful way to understand gas-solid flow dynamics by accounting accurately for the interactions between the two phases. This code will be used as the microscopic time-stepper-type simulator for the equation-free coarse-grained analysis of the test problems involving spouted bed and dense phase pneumatic conveying applications.

In this microscopic simulator, each particle trajectory in the solid phase is computed using the discrete element method while the gas phase is handled through locally-averaged continuum equations. Thus, the simulator does not resolve the flow around each particle, but accounts for the fluid-particle interaction through a drag force correlation which is treated as model input. The inter-particle collisions are handled through a DEM soft sphere model [mentioned earlier]. Though a number of techniques for coupling the two phases have been published in the literature [131, 128, 72], not all ensure that interaction forces are equal and opposite between the phases. When mass, momentum and energy are exchanged, these must be reciprocal to ensure conservation; in this simulator a sequential and iterative procedure has been used for coupling the gas and particle phase calculations in a consistent manner.

Generally, a fairly large time step is used for solving the gas using semi-implicit backward Euler method. After every gas-phase time step, several tens of DEM sub-steps are taken and, the local volume fraction and local-average particle velocity are computed at the end of the sub-steps. The gas phase velocity and pressure fields are then updated, and the whole procedure is repeated until the desired time interval is covered. This code has already been used successfully to analyze test problems by Boyalakuntla [15] and Boyalakuntla and Murthy [17, 16]. Team members at ORNL have subjected this code to a number of test calculations, and compared the results with those published by Tsuji et al. [131] and Xu and Yu [128], but the details of this validation are not included here. In addition, the DEM part of the code has been opensourced for more than a year with constant validation by independent users and continuous improvements. The feasibility of performing coarse-grained equation-free analysis of dense particulate flows was recently explored by the Princeton group - collaborators in this proposal [83]. In this study, we considered a fluidized bed of uniformly sized particles where the coarse structure was restricted to be only 1D in space. While bubble-like voids form spontaneously in real 2D and 3D fluidized beds [112], simulations of very narrow beds, where lateral structures are not allowed to develop, yield 1D traveling waves (instead of bubbles). In this idealized example, the local-averaged equations of motion for the gas can be simplified considerably and the effect of the gas on particles can be explicitly brought into the equations governing the motion of the particles through additional terms involving coarse-grained variables; in effect, we are solving only the linear and angular momentum equations for the particles, and the gas phase effects are introduced almost trivially [83]. We used this "3D DEM and 1D gas" model to simulate the dynamics of a deep fluidized bed of uniformly sized particles, allowing for van der Waals interaction between them [98] and imposing periodic boundary conditions in the two horizontal directions for the DEM solver, and observed the expected formation of a train of upward traveling, 1D waves. In a fluidized bed of finite height, these wavetrains were not regular, but the dominant wavelength and the average particle volume fraction could be identified readily [84]. We then performed DEM simulations of a single wave unit in this wavetrain by considering a fully periodic box (in all three directions) whose vertical height was commensurate with this dominant wavelength and choosing the average particle volume fraction in this box to be the same as that in the wavetrains. These clean simulations involving about 1,400 particles led to well-defined traveling wave solutions. The evolution of the 1D (vertical) structure of the coarse-grained macroscopic variables (such as particle volume fraction, local average velocity, mean-squared velocity fluctuations, stresses transmitted through contact, etc.) following an initial perturbation of the uniformly fluidized state was then analyzed both with and without the application of coarse projective integration. We chose this idealized test problem for three reasons:

(a) One-dimensional traveling waves, which arise in this simple problem, represent the first stage in the bifurcation hierarchy leading to bubbles in fluidized suspensions and there is interest in understanding how inter-particle forces affect this first stage structure [112];

(b) Because these waves could be computed without the use of coarse projective integration at affordable computational cost, one can examine the accuracy of coarse projective integration in dense particulate flows through this test problem; and

(c) The coarse-grained macroscopic variables in this problem, if viewed from the laboratory frame, remain time-dependent even when the traveling wave is fully developed; however, when viewed from a frame of reference traveling with the wave (a.k.a. co-traveling frame), their spatial variation becomes independent of time in the fully developed state. Thus, by transforming to a co-traveling frame (through the template transformation method of Rowley and Marsden [78], one can examine the feasibility of directly computing the fully developed state by combining the coarse-grained computational method with a matrix-free fixed-point algorithm. We note that closed-form continuum equations for dense assemblies of particles with van der Waals interaction are not available and DEM simulations are the only means of calculating the structure of these 1D waves and the evolution of more complex structures when larger domains are considered.

We briefly note that by simply using the local-average values of particle volume fraction, particle velocity and gas velocity as coarse-grained variables, one can indeed successfully apply the coarse projective integration scheme. We tackled this test example by first performing full-fledged "3D DEM and 1D gas" simulations with a microscopic particle configuration which was consistent with the desired small initial disturbance to the homogeneous state. The results of this simulation were treated as the reference ("control") for assessing all the other simulations described below. By using the usual local averaging procedure–this is equivalent to the restriction operation in equation-free analysis–we computed the profiles of particle volume fraction, particle phase velocity in the vertical direction, the mean-squared fluctuating velocity of the particles in the three directions (and the various components of the stress due to contact and van der Waals interactions at an arbitrary intermediate time during the evolution of the wave in the "control" simulation. We then performed the so-called lifting operation using only the volume fraction, mean particle velocity, and mean-squared fluctuating velocity profiles at this time as inputs, thus creating a few of the infinitely many possible microscopic configurations. For each of these microscopic configurations, we followed the subsequent transient, determined how the locally-averaged quantities evolved with time and compared them with the results from the control simulation. Excellent correspondence was achieved indicating that the stresses due to contact and van der Waals interactions need not be considered as separate coarse variables and that they get slaved to other coarse variables quickly. Further calculations revealed that it suffices to consider only the volume fraction

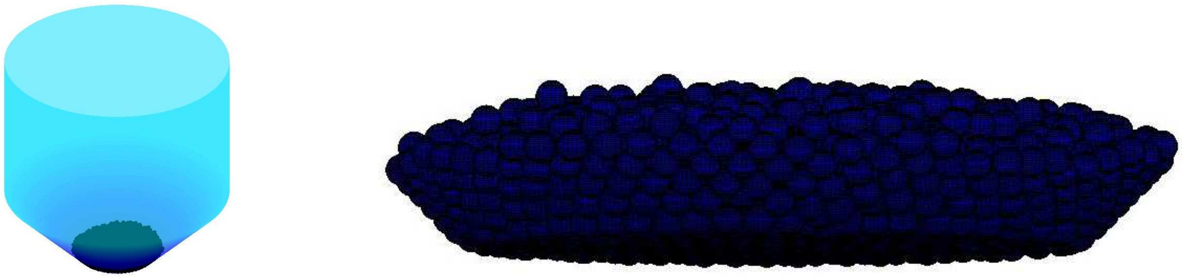


Figure 1: Simulation of 2000 hard spheres in a pebble bed.

and velocity as the coarse variables, and the fluctuating velocities become slaved to these two coarse variables as well.

During the course of this analysis, we had to address several practical issues concerning the lifting step–namely, how microscopic configurations which were consistent with specified volume fraction and vertical velocity profiles could be generated. We found that, for this example, starting with a box packed with particles and removing particles judiciously was the easiest way to generate microscopic configurations corresponding to a desired volume fraction profile. We were also able to ascertain that coarse projective integration steps are indeed possible in our computations of the evolution of the wave structure. By analyzing the temporal evolution of the coarse variables of the control simulation in the co-traveling frame, we took a small projective step, performed the lifting operation to reinitialize the DEM solver, and repeated the procedure. This simple example was chosen as proof of concept. As the full problem could be computed easily, improved speed or efficiency afforded by the coarse-grained computational method was not a real issue in this test problem–to realize these benefits, we must consider very large scale problems. This analysis, however, has achieved its main purpose–namely, demonstration of the feasibility of the restriction and lifting operations and coarse projective integration (which are essential elements of coarse-grained computational method) in one dense particulate flow problem.

The Argonne group has been investigating the the numerical properties and the correct formulation of linear complementarity based time stepping schemes for multirigid body dynamics with contact and friction, which are essentially equivalent to DEM with hard constraints. These problems solve a linear complementarity problem at every step [24]. Previous studies have included the consistent formulation of such methods, [8, 10], extensions to stiff cases, [9], efficient constraint stabilization [7, 5], as well as iterative solution of the subproblem [6, 4].

Recently, we have formulated a class of such methods where the subproblem that needs to be solved at every step is a quadratic program, with potentially much lower complexity than the one of the linear complementarity problem that was used by previous methods [3]. In the same reference, we proved that our formulation is convergent in a weak sense, that is that it converges to a measure differential inclusion, similar to the result for the more complex linear complementarity problem [110]. We have applied this method to simulate the settled fuel pebble configuration after following a randomized loading protocol. We present the final configuration for 2000 pebbles in Figure 1. Efforts are currently under way to extend the capabilities of our approach.

2.2 Turbulent Flow in Fixed Beds

Accurate microscale computations are a critical component of the proposed multiscale analysis approach. Contrary to most turbulent hydraulic flows, the PBR flow passages are highly curved, lack any single extensive direction, and feature fully separated flow almost everywhere, which severely limits the utility of models that have built-in assumptions from boundary layer theory. Turbulent flow in the pebble-bed void space is consequently not well characterized and has only recently become accessible to direct and large-eddy simulations. Recent studies have employed lattice-Boltzmann methods (LBM) to analyze transitional flow in periodic crystalline and random arrays but these were limited to Reynolds numbers of a few hundred [54]. Reynolds numbers of 2000 were obtained by coupling the LBM with a Smagorinsky eddy-diffusivity to perform large-eddy simulation (LES) [97].

Our microscale simulations will be based on the ANL-developed spectral element code, Nek5000, which is designed specifically for DNS and LES of high-Reynolds number flows in complex domains. The spectral element method (SEM) is essentially a high-order finite element approach, save that expansions within each element are taken to be high-order (typ., N=8–16) tensor-product polynomial (locally spectral) expansions. The high-order approximations yield minimal numerical dissipation and dispersion and, hence, provide excellent transport properties [47]. The tensor-product bases provide significant reductions in memory and operation costs over standard p-type finite elements and are central to achieving an efficient high-order implementation. Nek5000 employs third-order semi-implicit timestepping, recently developed spectral element multigrid methods [36, 75], dealiased treatment of

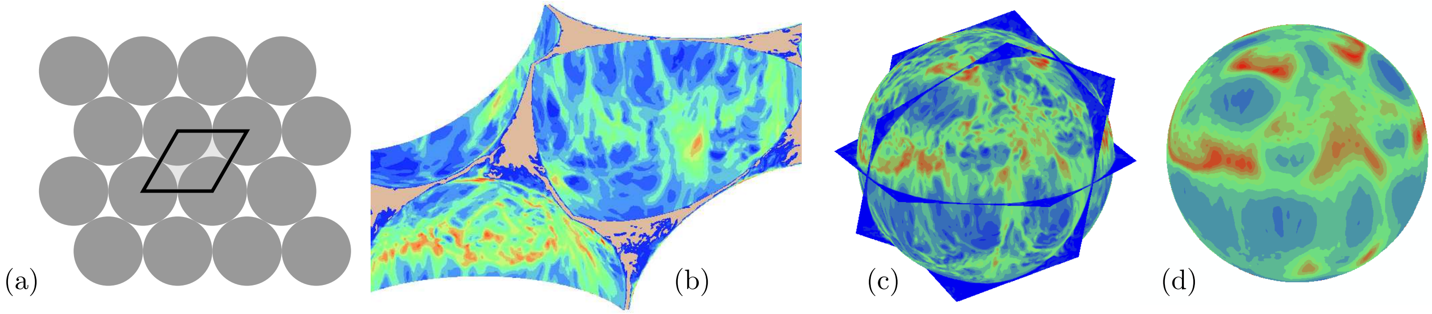


Figure 2: Temperature distributions for microdomain thermal simulations of the PBR: (a) cross section of an fcc latice with embedded unit-period cell; (b) computational domain showing instantaneous distribution on pebble and periodic boundaries; (c) sphere-centric view of (b); (d) time-averaged temperature distribution.

nonlinearities, stabilaztion for convection-dominated flows [37], and scales to 1000s of processors. The algorithmic quality and scalability of Nek5000 was recognized with the 1999 Gordon Bell award for high-performance computing [122].

We have undertaken a series of direct numerical simulations of heat transfer in a unit periodic cell of an fcc lattice at Reynolds numbers ranging from Re_v=0 to 3800. The $Re_v = 3800$ case employed a mesh of 1536 elements of order N=11 (approx. 2 million gridpoints). A mean velocity and mean thermal gradient were imposed using generalizations of the Green's function techniques developed in our earlier work on simulation of heat transfer in grooved channels (e.g., [50, 48, 49]). Because the timestepping is semi-implicit, one can precompute auxiliary solutions to the linear unsteady Stokes problem associated with a fixed mean pressure gradient, and then add the correct multiple of this solution to enforce a fixed flow rate at each step. A similar procedure is used to impose mean temperature gradients [42, 91] in the energy equation. (This mean+periodic decomposition is the central mechanism through which the macroscale coupling proposed in Section 3.5 will be imposed.)

Figure 2 shows the computational domain and instantaneous and time-averaged temperature distributions on a single pebble subject to a unit thermal flux at the surface for $Re_v = 3800$. The simulations provide the local pressure drop, the rate of thermal mixing, and the local extrema of the time-averaged temperature distributions. Starting from a fully developed flow field, averages were computed over 7000 timesteps with $\Delta t = .0001$, corresponding to roughly 5 flow-through times, which required 42 hours on a 64-node (2.4 GHz Intel Xeon) Linux cluster. Earlier simulations indicate that approximately 20 flow-through times are required to obtain converged statistics. We anticipate that spatially converged validation runs, to be carried out on ANL's 2048-processor Blue Gene/L platform, will require approximately 5–10 million gridpoints. These DNS studies will be used to validate LES microscale simulations proposed in Section 3.5.

3 Technical Approach

The central effort of our work consists of the development and implementation of equation-free "wrappers" around the fine scale simulation codes briefly described above; the purpose of these wrappers is to perform scientific computation for the unavailable in closed form macroscopic equations describing the coarse-grained behavior of the fine scale simulation codes. We envision that the work will advance our understanding and ability to predictively model dense particulate flows. At the same time, we expect to gain experience with equation-free computation, study its mathematical underpinnings, and extend it in several important directions.

3.1 General Approach

The EF-framework is designed for problems that are "effectively simple": problems for which we believe that macroscopic (averaged, population level, coarse-grained, effective) evolution equations exist conceptually, yet are not available in closed form. The only available model comes as a "fine scale" (atomistic, stochastic, agent-based) simulator; running this over macroscopic space and time scales is typically prohibitively expensive. The equation-free approach circumvents the explicit derivation of closures leading to coarse-grained models; instead, it uses the fine scale simulator as an experiment that can be initialized and run at will. The basic idea is to operate at two levels: (a) design and execution of appropriately initialized short-time numerical experiments with "the best available" microscopic model, followed by (b) use of the numerical results of such microscopic computations to estimate coarse quantities (residuals, action of Jacobians) required in numerical computations of the unavailable macroscopic equations.

The computational methodology consists of the following basic steps: (a) Choose the statistics of interest for describing the long-term behavior of the system and an appropriate representation for them. For example, in a gas simulation at the particle level, the statistics would probably be density and momentum (zeroth and first moment of the particle distribution over velocities) and we might choose to discretize them in a computational domain via finite elements. We call this the macroscopic description, $\mathbf{u}$. These choices suggest possible restriction operators, $\mathbf{M}$, from the microscopic-level description $\mathbf{U}$, to the macroscopic description: $\mathbf{u} = \mathbf{MU}$; (b) Choose an appropriate lifting operator, μ, from the macroscopic description, $\mathbf{u}$, to one or more consistent microscopic descriptions, $\mathbf{U}$. For example, in a gas simulation using pressure etc., as the macroscopic-level variables, μ could make random particle assignments consistent with the macroscopic statistics. $\mu\mathbf{M} = \mathbf{I}$, i.e., lifting from the macroscopic to the microscopic and then restricting (projecting) down again should have no effect, except roundoff. (c) Start with a macroscopic condition (e.g. concentration profile) $\mathbf{u}(t_0)$; (d) Transform it through lifting to one -or more- fine, consistent microscopic realizations $\mathbf{U}(t_0) = \mu\mathbf{u}(t_0)$; (e) Evolve this(ese) realization(s) using the microscopic simulator for the desired short macroscopic time T, generating the value(s) $\mathbf{U}(T)$. (f) Obtain the restriction(s) $\mathbf{u}(T) = \mathbf{MU}(T)$ (and average over them).

This procedure constitutes the coarse time-stepper, or coarse time-T map. If this map is accurate enough, we showed above how to use it in a two-tier procedure to perform Coarse Projective Integration [39, 38, 41]. Repeating steps (e-f) over several time steps and obtaining several $\mathbf{U}(t_i)$ as well as their restrictions $\mathbf{u}(t_i) = \mathbf{MU}(t_i)$, $i = 1, 2, \ldots, k+1$, using the chord approximating these successive time-stepper output points to estimate the derivative—the right-hand-side of the equations we do not have—we can then use this derivative in another, outer integrator scheme (such as forward Euler) to produce estimates of the macroscopic state much later in time $\mathbf{u}(t_{k+1+m})$ and go back to step (d). The procedure is illustrated in Fig. 3(a).

In coarse projective integration we exploit the smoothness in time of the unavailable macroscopic equation in order to project (jump) to the future. In the case of macroscopically (spatially or otherwise) distributed systems, one can exploit smoothness of the unavailable macroscopic equation in space in order to perform the microscopic simulations only over small, but appropriately coupled, computational boxes ("teeth"). The procedure is: (a) Coarse variable selection (same as above, but now the variable $\mathbf{u}(x)$ depends on the *coarse space* x. We have chosen for simplicity to consider only one space dimension.) (b) Choice of lifting operator (same as above, but now we lift entire profiles of $\mathbf{u}(x)$ to profiles of $\mathbf{U}(y)$, where y is microscopic space corresponding to the macroscopic space x. This lifting involves therefore not only the variables, but the space descriptions too. The basic idea is that a coarse point in x corresponds to an interval (a *box* or *tooth* in y). (c) Prescribe a macroscopic initial profile $\mathbf{u}(x, t_0)$ the "coarse field." In particular, consider the values $\mathbf{u}_i(t_0)$ at a number of macro-mesh points; the macroscopic profile arises from interpolation of these values of the coarse field. (d) Lift the "mesh points" x_i and the values $\mathbf{u}_i(t_0)$ to profiles $\mathbf{U}_i(y_i)$ in microscopic domains (teeth) y_i corresponding to the coarse mesh points x_i. These profiles should be conditioned on the values $\mathbf{u}_i$, and it is a good idea that they are also conditioned on certain boundary conditions motivated by the coarse field (e.g., be consistent with coarse slopes at the boundaries of the teeth that are computed from the coarse field). (e) Evolve the microscopic dynamics in each of these boxes for a short time T based on the microscopic description, and through ensembles that enforce the coarsely inspired boundary conditions and thus generate $\mathbf{U}_i(y_i, T)$ (f) Obtain the restriction from each patch to coarse variables $\mathbf{u}_i(T) = \mathbf{MU}_i(y_i, T)$. (g) Interpolate between these to obtain the new coarse-field $\mathbf{u}(x, T)$.

Up to this point, we have the gaptooth scheme: a scheme that computes in small domains (the teeth) which communicate over the gaps between them through coarse-field-motivated boundary conditions. We can now proceed by combining the gaptooth scheme with Projective Integration ideas to (h) Repeat the process (lift within the teeth, compute new boundary conditions, evolve microscopically, restrict to macroscopic variables and interpolate) for a few steps, and then (i) Project coarse fields *long* into the future. For a projective forward Euler this would involve the chord between two successive coarse fields to estimate the right-hand-side of the unavailable coarse equation, and then an Euler projection of the coarse field long into the future. (j) Repeat the entire procedure starting with the lifting (d) above. This leads to the *patch dynamics* procedure illustrated in Fig. 3(b): a computational framework in which simulations using the microscopic description over short times and small computational domains (patches in space-time) can be used to advance the macroscopic dynamics over long times and large computational domains. Initializing microscopic computations conditioned on macroscopic variables is an important component of coarse projective integration; similarly, imposing macroscopically motivated boundary conditions to microscopic computations is an important element of gaptooth and patch dynamics.

3.2 Patch Dynamics

There is a natural progression in the coarse-graining of space and time within the equation-free framework. *Projective integration* embodies the coarse-graining of time only; bursts of *full space* microscopic simulations are performed, and the time derivatives of the corresponding fields are estimated from these bursts and passed on to traditional numerical integration algorithms. *The gap-tooth scheme* represents the coarse-graining of space only; simulations are performed in macroscopically small domains ("teeth", surrounded by empty "gaps") for all time. Yet these "teeth" are alloweed periodically to communicate with each other through effective smoothness boundary conditions. These approaches will be tested and validated on the way to the main tool we propose to explore, which embodies their combination, by coarse-graining both space and time: *patch dynamics*.

The patch dynamics approach, where projective integration is used for time evolution and the spatial domain is covered only by a microdomains, is the approach of choice for the proposed research in dense granular flows, since it has clear potential for substantial computational savings. For very dense granular flows projective steps may be appropriate for some parts of the domain, while different projective steps or "full time" gaptooth may be appropriate for other parts of the domain; this will give rise to multirate schemes.

3.2.1 Patch dynamics for the simulation of dense particulate flow

For the full-fledged patch dynamics problem, the objective of our research will be to predict the macro scale behavior of macroscopic observables of the particulate flow, such as particle density and velocity, coarse-grained flow velocity and temperature fields. In the microdomains, the physics will be described by a molecular dynamics-level simulation of the particles coupled with a fluid flow described by our flow solvers. In order to transport information between the scales two critical steps need to be resolved. We use macro scale moments in order to generate a statistical distribution of particles, and subsequently construct ensembles of particles consistent with that distribution.

Aspects of the latter step have been recently resolved for non sticky particles in two dimensions even for relatively high packing fractions of 0.54 in the work of Torquato [99] by use of stochastic optimization, in effect a simulated annealing approach applied to the appropriate energy functional. For sticky particles, however, the results of the stochastic optimization problem do not result in a medium reconstruction of reasonable accuracy. In this work, we will expect to take advantage of the stochastic optimization approach where appropriate, and extend it to three dimensions; we will also investigate alternative approaches that can provide better medium reconstruction for sticky particles.

The problem of distance constraint reconstruction was recently approached successfully by a smoothing and continuation approach [85] and a semidefinite programming relaxation approach, [14]. Given the similarity between the stochastic medium reconstruction problem and the distance reconstruction problem we propose to investigate extensions of those approaches to the reconstruction of dense particulate media.

The reverse question, i.e. the question of estimating macro scale quantities from particular given microscale distributions, is also significant. In some cases it may be as simple as the computation of a few moments of a given distribution. When, however, smooth fields need to be extracted from many replica simulations with relatively small numbers of particles, efficient filtering and estimation techniques need to be used; the Thermodynamic Field Estimator of Yip and coworkers [73], and in general- maximum likelihood estimation techniques for stochastic systems need to be explored and implemented [1]. The resulting estimation procedure will be used to extract the macro scale information at the end of each microscale simulation step.

In the same way that *lifting* (constructing distributions consistent on a number of their statistics) often involves the solution of an optimization problem, the estimation part of restriction may also give rise to an optimization problem when maximum likelihood estimates are involved. We also plan to explore the number of basis functions required to successfully represent the estimated fields given the number of data points and replica simulations available.

In a separate step, the estimation tools will be used to assess the suitability of the algorithm-relevant parameters that introduced by our approach. Such parameters include (a) the size of the meaningful computational domain ("tooth") (b) the size of the appropriate buffers that may be needed to alleviate computationally intensive boundary

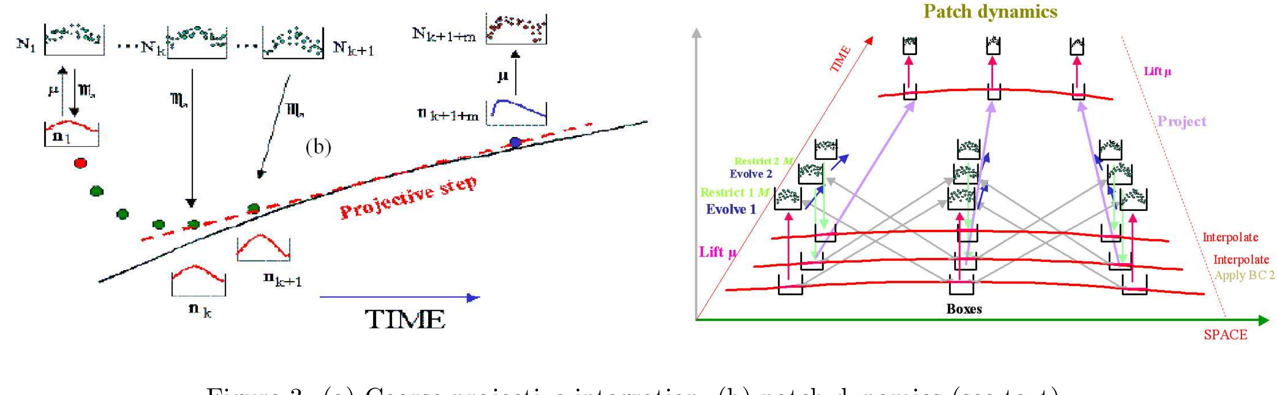


Figure 3: (a) Coarse projective integration; (b) patch dynamics (see text).

conditions and (c)the time over which the detailed simulation can proceed before macroscopic reinterpolation and temporal projection steps can be taken.

3.2.2 Algorithmic improvements to the equation free method

To enable the equation free approach to perform system-level tasks, several of the assumptions that were used in its development and its proof of concept simulations will need to be tested and validated. The main assumption is the fundamental one that accurate deterministic predictions can be performed (i.e., equations can successfully close) at the level of the relevant coarse grained observables on a macro-scale mesh (as a result of separation of time and concomitant space scales).

Perhaps a crucial point in our investigation is the definition of the appropriate tooth boundary conditions. In the first published particle-based simulation using the gap tooth method, particles were teleported across computational domains (teeth) with appropriate weights to ensure effective flux smoothness. That approach is relatively easy to implement in the situation where the mean collision length is reasonably larger than the size of the particle. The latter assumption clearly does not hold for dense particulate flows, and in that case the teleportation approach needs to either be abandoned or extended.

For high particle density it appears unavoidable that we will consider the "meaningful" computational microdomain surrounded by a buffer region; this region effectively implements effective smoothness, and its particles are not considered when the relevant statistics is extracted at every macro-interpolation or projection step. We already know that it is possible to trade "goodness" of boundary conditions with buffer size; we will investigate the possible extension of the optimal particle controller [73] to our case.

In addition to buffer-mediated imposition of effective smoothness, we will still explore remedies to the teleportation procedure (e.g. teleportation between buffer regions followed by a quick, off-line equilibration before the actual simulation is resumed); in this direction we will explore the current statistical mechanical literature on non-equilibrium ensembles for dense particle systems.

Macroscopic boundary conditions need also be imposed at the edges of teeth adjacent to macrodomain boundaries; these may be simple to implement microscopically (e.g. periodic, no flux) or may necessitate more complex approaches (e.g. immersed boundary methods for flexible boundaries).

3.2.3 Analytical and equation-free numerical analysis investigations

We will study the convergence of the methods defined here for the usual test cases of partial differential equations with highly oscillatory diffusion coefficients. As a first step, we will extend the analysis in [44] to the case of nonuniform meshes and more than one dimensions. In that paper the error has been shown to consist of several components; we expect the qualitative nature of these components to persist in higher dimensions. We expect to prove convergence of the scheme for nonuniform meshes and explore the multiscale behavior of the error (its composition from terms depending on the macro-scheme discretization and terms involving the micro/macro scale ratios).

It is interesting that the coarse timestepper computational technology, which underpins our computations, can also be used to perform certain equation free numerical analysis tasks. Matrix-free methods can be used to estimate, for example, the stability of the numerical scheme itself (through its damping factors, the eigenvalues of the scheme linearization); such computations have been demonstrated in [44].

Furthermore, since the scheme parameters (buffer size, type of boundary conditions, microscopic evolution time before estimation) are naturally part of the scheme timestepper, matrix free eigenanalysis can be used to track the dependence of these damping factors on the scheme parameters (analogous to the dependence of traditional PDE damping factors on the mesh spacing and time step).

3.3 Dense Particulate Flows

In this proposal, we consider application of equation-free coarse-grained approach to two test problems involving coupled fluid-solid phase motions. These deal with the hydrodynamics of spouted beds and dense phase pneumatic conveying in horizontal ducts. These are representative of complex flow patterns that one encounters in many gas-particle handling devices, and have direct relevance to energy-related industries.

Spouted Beds. Spouted beds have been long used for various applications including coating particles [79]. Spouted beds have been applied to coat nuclear fuel particles starting in 1970s, when there was renewed interest in the nuclear power due to the world-wide energy crisis and various countries including US have started looking at alternate safer nuclear power plants. It was proposed to coat the nuclear particles (around 500 μm) with amorphous carbon, pyrolytic carbon and Silicon Carbide (SiC) called the TRISO particle. The coated particles are then compacted using resin to form pebbles which go into a reactor like pebble bed reactor. The coatings need to have extremely high quality with failures less than 1 in 10^4 or less to ensure in-reactor retention of fission products (fuel performance). Germans

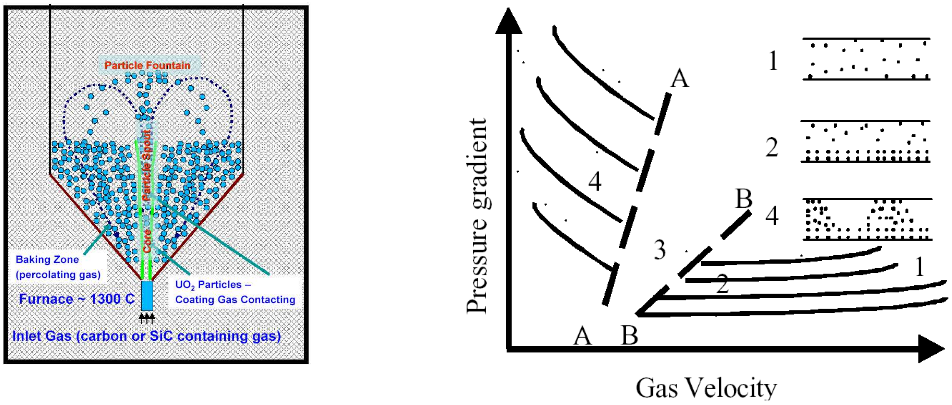


Figure 4: (a) Schematic of spouted bed. (b) Schematic of dense-phase conveying characteristics for granular particles: (1) dilute phase transport; (2) conveying in layers; (3) unstable zone; (4) slug flow. Solid lines show lines of constant solids flux and broken lines demarcate the regime of unstable operation. AA - dense-phase slugging boundary; BB - dilute phase boundary.

produced some of the best fuel through several decades of trial-and-error experimental process [52]. The US had an active fuel coating program but the coating quality never met the required quality [90]. The nuclear fuel coating has been revived recently and controlled experiments along with developed multiphase flow modeling tools are targeted to produce high quality coated particles [94]. Spouted beds represent excellent examples where all the regimes of particulate flows can be found in a single device.

Figure 4(a) shows a typical schematic of spouted beds. In the core region, the loading of particles is small (a few volume percent); the particles (from the annular region) are picked up by the gas entering at the bottom and carried up. At the top of the bed, a fountain of particles transfers them from the core to the annular region. In the annular region, a dense assembly of particles descends slowly, and at the boundary separating the core and annular regions, complex interaction occurs between the particles. The overall flow characteristics are strongly influenced by the dense phase flow in the annular region, where reliable closed-form continuum models are unavailable. Accurate estimates of stresses experienced by the particles in the bed, especially in the annular region, are important in the nuclear fuel coating process. The particle failures (e.g. fracture) occurs in the stress annular zone and this is critical in ensuring the quality of the coated particles. DEM simulations coupled with local average treatment of the gas phase can provide the sort of detailed information on flow and stress characteristics desired in the design of the nuclear fuel coating process and other spouted bed applications.

Dense phase conveying. Fluidization and pneumatic conveying in vertical, horizontal or inclined ducts are common operations in particle handling. The former is widely encountered in chemical reactors, while the latter is frequently employed to transport particles from one location to another in a plant. In both instances, spatial and temporal nonuniformities readily occur. The details of these nonuniformities depend on the material properties of the particles and the fluid, the geometry of the vessel/duct and throughput. A variety of flow regimes have been observed and documented in the literature for fluidization as well as pneumatic conveying (e.g., see[29, 35]). Here we consider dense phase pneumatic conveying in horizontal ducts as a model problem. Fine powders that fluidize easily and do not deaerate quickly (typically Geldart Type A powders) are generally easy to transport in dense-phase mode [126]. In contrast, larger particles deaerate easily and this leads to very different performance characteristics in the dense phase transport regime [126, 127, 29]. In particular, low-velocity slug flow can be achieved as one of the regimes (see Fig. 4(b)), where particle damage can be minimized. Simplified analysis of pressure drop across and velocity of steady, fully developed slugs can be found in the literature [68, 30]. One of the striking features seen in Fig. 4(b) is the regime of unstable transport obtained at intermediate conditions. In this regime, flow occurs with very large excursions in gas pressure and the stresses exerted on the duct by the moving slugs. The flow alternates between fast-moving unstable slugs and dilute phase transport with increasing levels of deposition. Which of these two modes dominates depends on the location of the operating condition inside the unstable regime - the unstable slugs dominate close to the dense-phase slugging boundary, while they are less frequent near the dilute-phase boundary. One of the important challenges in the field of dense phase conveying is to predict the two boundaries of the unstable region, for specified gas, particles and duct (i.e., diameter, length, configuration and material of construction). In order to do this, we need a better understanding of how the particles inside the slugs move and transmit stresses to the wall. Only then will we be able to identify the mechanism driving this instability and the stability boundaries. As closed-form continuum equations are unavailable, discrete element simulation of the particles taking into consideration the interstitial fluid flow is the possible way to handle dense phase conveying problems. However, even if we limit our attention to a single propagating slug (say, by focusing our attention on a portion of the pipe and impose periodic boundary conditions in the axial direction), the number of particles involved is very large and complete solution of the problem via DEM quickly becomes intractable.

Coarse Stationary States. In a DEM simulation (e.g., of the two problems mentioned above), the solution is always unsteady as the velocities of the individual particles would never attain steady values. However, in the two examples that we have chosen to examine in our proposed research, coarse steady (stationary) states can be identified at least over a range of operating conditions. In the spouted bed, at a macroscopic level, a coarse steady state with a core-annular distribution of particles, superimposed by high frequency pulsations has been observed in experiments [101, 100]. In steady state dense phase conveying, at the macro-scale, a train of particle-rich slugs travel through the duct (see inset 4 in Fig. 4(b)); one can readily isolate one such slug, by considering a length of the duct (representative of the typical repeat length between the slugs) and imposing periodic boundary conditions at the boundaries. One then obtains at the macroscale a (nearly) steady traveling wave, so that a coarse steady state does exist for this flow problem if one views the solution in a frame traveling with the wave. If closed-form coarse-grained equations were available, one can compute this traveling wave and examine its stability characteristics, but they are unavailable.

These two test problems afford coarse steady states in the laboratory and traveling frames, respectively. Both involve very large numbers of particles and brute-force DEM simulations, coupled with averaging of the data to extract the coarse steady states, are neither feasible nor desirable from practical viewpoint. On the other hand, the same simulation approach, when enhanced by the equation-free coarse-grained approach outlined in this proposal, not only becomes more feasible, but also efficient approach to learn about the macro-scale characteristics of these flows. Coarse integration, fixed point calculation and bifurcation analysis are methodologies that can be applied to these problems to expose not only the flow and stress characteristics, but also shed more light on the mechanism through which dense phase conveying gives way to the unstable conveying regime illustrated in Fig. 4(b).

Approach. Oak Ridge National Laboratory will lead the effort on the spouted bed analysis, and the Princeton group will focus on the dense phase conveying example. Both these groups will work closely with each other, assisting each other on the code implementation issues that are common to gas-particle flows, and with the Argonne group on the methodological issues, such as efficient lifting and restriction, boundary condition implementation in the gaptooth/patch dynamics approach and fixed point iterations.

In both examples, we will first tackle implementation of the multiscale approach in simpler quasi-two-dimensional problems, and then build to fully three-dimensional problems. Quasi-two-dimensional problems will be constructed by considering a thin section of the domain in the third direction and imposing periodic boundary conditions in that direction. For example, a fully 3D spouted bed would assume the form of a conical hopper, while in 2D, it would be a wedge shaped hopper. The results of the fully three-dimensional DEM simulations in the wedge shaped spouted bed would be averaged over the third direction, so that the coarse analysis is only two-dimensional. This would dramatically decrease the number of particles to be considered in the analysis and allow us to test and develop the ideas using simpler cases. In the dense phase conveying, we would first consider a thin section in the horizontal direction perpendicular to the flow and impose periodic boundary conditions (or real wall boundary conditions) in that direction. This would once again reduce the coarse analysis to quasi-2D. In both examples, we would subsequently change the periodic boundary condition in the third, neutral direction to real wall boundary conditions to understand how introduction of particle-boundary interactions introduces complexities in both the multiscale methodology and the flow characteristics.

We will further break the quasi-2D analysis into simpler problems to allow us to test the different aspects of the coarse-grained approach. We will begin by considering relatively small units with only a modest number of particles, so that the entire flow can be solved with brute-force approach. This would allow us to ascertain that the gas-particle flow codes are working properly, and also gather “true” solutions which can be used to test the success or failure of the multi-scale approach. We will then consider only coarse projective integration considering the full domain and sort out the associated implementation issues. This will be followed by implementation of fixed point iterations for the coarse-grained variables to accelerate convergence to the steady (or traveling) solutions, thus mitigating the need for fully resolved simulations over long time horizons. We will then implement 1D gaptooth method on these problems with gaps and teeth only in the main flow direction (and spanning the entire region in the other two directions), performing integration over the full time horizon. We will then add coarse projective integration to this 1D gaptooth method, thus obtaining a proper example of patch dynamics. We will then extend the analysis to two dimensional patches. The extension of these efforts to fully 3D problems will proceed along similar lines. At each stage in the analysis, we will devote appropriate level of effort to understand and expose the underlying physical phenomena in these test flow problems.

3.4 Hard Sphere Computations

We will use the equation free algorithms for dense particulate flow developed and implemented in this proposal to simulate the motion of fuel pebbles in VHTR. To that end, we will develop our hard particle based method to a level that it would be usable as a microsimulator. Given that VHTR has no more than 500,000 pebbles, we expect that we will be able to capture the motion of the pebbles once our simulator can handle about 100,000 pebbles distributed in microdomains or microdomains with buffers. To solve the optimization problem associated with the lifting step at every microsimulation interval [3], we will use a conjugate gradient projection technique in the dual space (the force space) in which the problem has the structure of a bound constrained optimization problem that can be fairly efficiently solved by this technique [74]. In addition, such methods can be hot-started with the dual solution from the previous step, which is likely to enhance their efficiency in this regime where the configuration is in very slow motion overall.

We will use this setup to characterize the long-term behavior the pebble bed motion. In particular, our simulation will help us characterize the void distribution, which is essential for predicting the behavior of the cooling flow. The high safety standards for VHTR results in the need to quantify the occurance of potentially dangerous phenomena, that are unique to such granular medium.

1. **Quaking** Even in mass flow discharge (i.e. one where there are no permanent, stagnant shoulders), discharge is likely to occur via quaking - a well known stick-slip phenomenon in silos. The quaking sets up structural vibrations which can be very dangerous for the life of the structure.

2. **Slip Planes** The discharge in a such unit will occur by forming dynamic slip planes - which can provide short-cut pathways for the helium to flow through. This can promote hot streaking, which may occur even without such slip-plane induced channeling.

3. **Local Crystallization** Unlike most engineering systems, where one has a particle size distribution, this system is likely to be very tightly monodisperse. This can favor local crystallization, which promotes locking and can lead to patches of low porosity, hot streaking and rigidity against particle rearrangement.

4. **Arching** Plugging by mechanical arch may be a concern when particle withdrawing happens by narrow orifices.

3.5 Turbulent Flow in Fixed Beds

We will consider the extension of the equation-free method (EFM) to the problem of high-Reynolds number convective transport in *fixed beds* that are either rigid or evolve on a timescale much longer than the relevant fluid dynamics and heat transfer timescales. To fix ideas, we have in mind as an example fluid flow in a pebble bed reactor of size $L \approx 10m$ containing $\approx 300{,}000$ spheres of diameter $D = .06m$ subject to blow-down flow of high pressure He at ≈ 100 m/s. The corresponding Reynolds number at the void scale ($\approx .3$ D) is $Re_D \approx 70{,}000$. The bed evolution timescale is $\approx 100s$, the global thermal relaxation timescale is $\approx 10^4 s$, the local thermal relaxation timescale is $\approx$ 1–10 s, and the local fluid time scale is $\approx 10^{-3}$ s. There are several macroscopic feedback mechanisms that are important to reactor analysis, including temperature-induced variations in thermal (neutron) output and temperature induced variations in fluid density that, in turn, affect the fluid velocity. Ultimately, one would like to be able to faithfully simulate the forward and feedback physics over the domain scale, L, and transient thermal scales of 10^4–10^5 s. The macroscopic variables of interest are (coarse-grained) pressure, velocity, and temperature fields.

While there are several distinct spatial scales in this problem, the discrepancy between the fluid and bed evolution timescales implies that the spectrum of the fluid turbulence is truncated at the void-scale by the quasi-static bed. This screening effect precludes large scale coherent fluid motion and results in a clear scale separation that would not exist in open turbulent flow [67]. Our multiscale analysis will thus combine microdomain simulations of turbulent heat transfer at the void scale, using large eddy simulation (LES), with macroscopic evolution at the domain scale, using the lift-run-restrict procedure of the EFM. In the sequel, we outline the proposed EFM procedure for thermal transport and then discuss required extensions for the hydrodynamics.

The thermal transport problem is of the form $T_t = \mathcal{L}(T)$, where $\mathcal{L}$ is the spatial component of the linear convection-diffusion operator with prescribed time-dependent velocity field in $\mathbb{R}^d$, d=2 or 3. The macro-domain Ω_L is populated with gridpoints $\mathbf{x}_i$ having a characteristic spacing $H \gg \epsilon := D$ and we assume that there exists a interpolation operator that will provide a smoothly varying macro-variable $T_c^n(\mathbf{x})$, $\mathbf{x} \in \Omega_L$, given nodal point values $T_{c,i}^n := T_c^n(\mathbf{x}_i)$. We surround each point $\mathbf{x}_i$ with a domain Ω_i of size h, $\epsilon < h \ll H$, and populate it with a statistically relevant solid phase.[1] The discrete macro-variables $T_{c,i}^n$ represent averages of temperature over the ith microdomain at the macro time-level, t^n. Starting with an assumed initial condition $T_c^n(\mathbf{x})$, macroscale evolution of T_c proceeds by lifting (interpolating) T_c^n to all points in each microdomain, running independent computations on the microdomains

[1] Solid phase distributions will be obtained from particulate flow simulations described in Section 3.4.

to evolve $\mathcal{L}(T)|_{\Omega_i}$ to a statistically quasi-steady state, and computing T_c^{n+1} via an explicit step using a kth-order backward difference update. For example, with k=1, one computes $T_{c,i}^{n+1} = T_{c,i}^n + \Delta t \mathcal{L}_{c,i}^n$, where $\mathcal{L}_{c,i}^n$ is a space-time average that represents the macroscopic spatiotemporal behavior of $\mathcal{L}(T)$ on $\Omega_i \times [t^{n+1} - t_R, t^{n+1}]$. Here, t_R is a relaxation (healing) time that avoids incorporation of nonphysical transients in the estimate of $\mathcal{L}$. In a like manner, one can restrict the spatial integration to a subdomain interior to Ω_i in order to avoid spurious numerical boundary layers near $\partial\Omega_i$, as suggested by Hou [56] and Samaey et al. [103].

To simplify the microscale turbulence computations, we assume that each microdomain is self-periodic, that is, that we can topologically connect points where flow is leaving the domain with corresponding points where flow is entering the domain *with the same velocity.* (Schemes for generating "random" particle distributions in periodic cells are described in, e.g., [26, 80].) Communication of boundary information at each macroscale time level is accomplished via the splitting $T(\mathbf{x}, t) = T_i'(\mathbf{x}, t) + T_c(\mathbf{x}, t^n)$, $\mathbf{x} \in \Omega_i$, where T_i' represents the local fluctuation and is periodic on Ω_i. This decomposition is recommended in the heterogeneous multiscale method of Enguist and E [33] and is commonly used in heat transfer analysis of periodic domains [50, 42, 91]. Note that if T_c is linear in $\mathbf{x}$ then $\mathcal{L}(T_c)$ is constant and, hence, periodic in space—there will be no spurious boundary layers. For higher degree polynomials, $\mathcal{L}(T_c)$ will in general be discontinuous, resulting in boundary layers near $\partial\Omega_i$, and the restricted sampling strategy suggested above should be used when constructing $\mathcal{L}_{c,i}^n$.

The linear convection-diffusion problem presents no particular difficulties and will serve as a starting point for developing our computational framework. Somewhat more challenging is the computation of the hydrodynamic velocity field. The difficulty here stems primarily from incompressibility rather than nonlinearity. Two ingredients are required to ensure global mass conservation at t^{n+1}. The first is a consistent projection operator that can produce a divergence-free field at the macroscale. This operator can be developed by deriving the interpolating macro-basis from any consistent finite-element space that satisfies the inf-sup condition for appropriate velocity-pressure pairs. The second ingredient is a mechanism to inject macroscale mass-conservation into the micro-computations. It is this second ingredient, in fact, that defines the macro-microscale interaction: the flow in each periodic microcell will be driven be a local mean (macroscopic) pressure gradient of arbitrary orientation. Because healing will be required after each pressure projection update, it makes sense to solve the macroscopic pressure system at the end of each microstep. This approach is relatively inexpensive given the relative number of degrees of freedom at the macro- and microscales and is consistent with the physics of the pressure propagation, which represents the fastest scales in the system. As in the thermal problem, projective integration of the mean velocity is used once the dynamics of the microcell computations have settled onto a slow manifold. We use appropriately restricted spatiotemporal averaging to estimate the mean behavior, step $\mathbf{u}_c$ forward in time, project onto a divergence-free space, and repeat, starting with the microcell computation. We note that there are nominally two "short" timescales associated with the microdomain simulations, namely, the healing time associated with the start of a new macrostep and the turbulent fluctuation time. In Section 2.2, we noted that roughly 20 flow-through times were required to obtain converged statistics in a unit periodic cell at $Re_v = 3800$. We can expect, however, that the *spatio*-temporal mean will converge more rapidly, which will result in significant computational savings for the macroscale evolution.

At first glance, it appears a bit incongruous to expect projective integration to play any role in a system that is macroscopically equilibrated (here, by the macro-pressure) at every microstep. However, properly implemented, we expect projective integration to pick out the macroscale evolution of the velocity through finite differences, and allow the large temporal jumps that will reduce the overall cost of computing the macro velocity field. By enforcing the mass balance, the mean velocity field will evolve on a slow and, in this case, divergence-free manifold.

Further cost reductions. Even with the patch-dynamics framework to reduce the computational costs, it is clear that reactor-scale computations will be beyond the reach of all but the largest of present-day platforms. For example, a coarse $10 \times 10 \times 10$ array of vertices would require performing 1000 microdomain LES runs. While this is certainly daunting, it is not out of the question for problems of national interest and it will certainly be a tractable computation within a few years. The key is to develop and refine the methodology now and, in the process, develop an understanding of how it can be improved and economized.

We will pursue several strategies to validate the framework and to test it in restricted domains that are large enough to exhibit macroscale physics. As a starting point, we will consider two dimensional Navier-Stokes simulations in dense random arrays of non-touching cylinders. This approach will allow us to compare against benchmarks in which we directly compute *all scales of motion*. While the nature of two- and three-dimensional turbulence is quite different, there is nothing intrinsically three-dimensional about the EFM. Having an accurate full-scale benchmark will greatly accelerate the development of the framework. As a next step, we note that it is relatively inexpensive to piggyback multiple heat transfer problems with a single hydrodynamics computation. We can thus develop the three-dimensional heat transfer analysis at a significant macroscale by associating, say, tens of thermal "patches" to a single fluids patch. Macro-variability will arise through imposition of domain-scale boundary conditions on the macro-temperature. As a next step, we envision computations comprising multiple three-dimensional microsimulations coupled in a two-dimensional axisymmetric slice of the reactor. All macro-boundary conditions would be correct, save that periodicity would be imposed in the azimuthal direction. This 3D/2D approach could then be extended to a full three-dimensional wedge, as is common practice in reactor analysis. Of course, several of these optimization strategies may be combined.

Extensions to the Method. Several extensions of our current technology will be required to realize a useful implementation of the EFM. These include:

Micro-scale wall boundary conditions. Accurate assessment of flow near the walls is central to analysis of the PBR. In addition to standard periodic cells, we will develop "wall cells" that are periodic in two of the cardinal directions. It is likely that these cells will need to be augmented with a richer set of moments for the macroscale velocity (i.e., something other than just the mean) in order to support macroscale gradients in the wall normal direction. This should be a straightforward extension of the Green's function technique mentioned in Section 2.2.

Heterogeneous void distributions. It is important to understand the role and expected frequency of channels and other statistically significant void configurations on the PBR performance. As data becomes available from the hard sphere simulations described in Section 3.4, we will analyze the most prevalent configurations.

Influence of thermal expansion. Our incompressible model is adequate for the microscale computations but will need to be extended in the macroscale because the helium exhibits significant expansion as it moves through the reactor. To account for this thermal dilation, we will implement an anelastic velocity-pressure formulation of our macroscale finite element framework that imposes mass conservation.

Coupling to VHTR Design. The ANL and INEEL teams will work closely throughout this project to ensure maximum benefit and insight is gained from the simulations in relationship to the INEEL very high temperature reactor (VHTR) design and analysis needs. The INEEL group is already working with several of the ANL team members on development of a fully-integrated reactor design code that couples solid mechanics, fluid mechanics, thermal and neutronics transport. The proposed multiscale research will have an opportunity to significantly influence and the integrated-code project and the two projects will benefit from the opportunity for cross-validation, which constitutes a significant fraction of code-development effort.

3.6 Multiscale Software Infrastructure

A key component of our multiscale development effort will be to provide a natural computational framework in which one can readily formulate multiple microsimulations that are coupled only by an external driver (the macrosimulator). This is a natural fit with our experience in domain decomposition techniques and with experimental high-performance computer architecture such as the Teragrid, which features multiple loosely connected Linux clusters.

One of the co-PIs (BFS) has devoted a significant portion of his career to developing, implementing and applying scalable algebraic solvers for PDEs. Some of this work is exemplified in the Portable, Extensible Toolkit for Scientific computation (PETSc) [13]. PETSc has been used in dozens of diverse application areas [109], including particulate flows [66].

PETSc has access to virtually all major algorithms for linear system solves including parallel multigrid. PETSc also has a family of parallel higher order, explicit Runge-Kutta methods. All of these algorithms are implemented in a *data structure neutral* manner and may be used recursively (for example, an ODE integrator calls another ODE integrator within the "right hand side function evaluation"). This is crucial in the proposed work when using the the "equation free" representations in modern multiscale paradigms. We plan to use PETSc as the building block for any necessary code development needed to accomplish the proposed work, however we will not be developing PETSc under the proposed work.

In our development of PETSc we have learned a great deal about mapping mathematical abstractions into software abstractions. This is not as trivial as it may appear at first. Many obvious solutions lead to inefficient computations and/or unusable software. The unusability often comes from 1) too many abstractions (so no one can keep them all straight) and/or 2) abstractions that are simply too abstract to be accepted by scientists and engineers. Thus it is a balancing act powered by 1) a clear mathematical understanding of the algorithms, their generality and applicability, and 2) a practical understanding of how the algorithms will be used in code. Refining the abstractions is an iterative process requiring constant refactoring of the algorithms, software and mathematical understanding.

Multigrid algorithms, though in some ways very different than patch dynamics do share common features. PETSc, and earlier MadPack [31], are the only two packages we are aware of that feature a completely abstract multigrid framework that encompasses not only standard flexibility such as V and W cycles, full multigrid, Cascadic multigrid, etc but provide complete extensibility for generation of the interpolation/restriction and coarse grid correction, as well as a simple, but powerful way of composing smoothers. Using the same software infrastructure

PETSc also has some support for Full Approximation Scheme (FAS) (nonlinear multigrid); the support for FAS corresponds more closely to the needs of equation-free and related algorithms given the nonlinear "local micro-scale" calculations that arise in the multi-scale mathematical paradigms.

The design of the current infrastructure will be the starting point for a flexible, general purpose approach to software for multiscale dense particulate flows. Particular features that have a correspondence between multigrid methods and multiscale mathematical methods are the "lifting" of the equation free approach (termed "reconstruction" in the HMM of E and Engquist [33]) (corresponds to interpolation or prolongation in multigrid) and the compression or restriction (corresponds to multigrid's restriction (also called projection)).

4 Milestones

We list here the intermediate milestones for development and validation of the equation-free multiscale computational framework. For the spouted bed (SB) and dense phase conveying (DPC) problems, only the milestones for quasi-2D systems are listed. The same chain of activities will be followed for the fully-3D systems in parallel with the 2D analysis, but lagging behind the timeline indicated there by two quarters. Thus, the final two quarters of SB/DPC project will be devoted entirely to 3D systems. Below, we denote the turbulent heat transfer and hard-sphere simulation efforts effort by THT and HS, respectively.

Year 1

SB/DPC Demonstrate successful functioning of the microscopic simulator using small domains and only about 10,000 particles.

SB/DPC Perform full simulations using systems large enough to contain about 100,000 particles to generate "computational data" to benchmark the success of the coarse-grained approaches listed below.

SB/DPC Demonstrate the feasibility of coarse projective integration.

SB/DPC Demonstrate the feasibility of computing the macroscopic steady states through fixed point iteration of the coarse-grained variables evolved through the DEM simulators. Also demonstrate the ability to perform coarse stability analysis.

HS Development of stochastic optimization techniques for random medium reconstruction, investigation of three dimensional techniques and techniques for sticky particles.

HS Investigation of maximum likelihood estimation techniques for stochastic particle systems.

HS Investigate gradient projection techniques in the dual space for efficient constraint-based hard particle simulators.

HS Extend the capability of the hard particle approach to the 100,000 particle level.

THT Complete unit-periodic microsimulation benchmark

THT Develop "wall-cells" to support single inhomogeneous boundary conditions

THT Develop 2D patch-dynamics framework

THT Develop support for single-hydro/multiple-thermal patches

Year 2

SB/DPC Using these tools, expose relevant physical processes and phenomena occurring in these flows.

SB/DPC Demonstrate and validate gaptooth method on these problems with gaps and teeth only in the main flow direction (and spanning the entire region in the other two directions), performing integration over the full time horizon.

SB/DPC Demonstrate patch dynamics approach by combining coarse projective integration and 1D gaptooth.

SB/DPC Extend the gaptooth method to two dimensions.

HS Deployment of random medium reconstruction and estimation techniques for use with the equation free method.

HS Coupling of the hard particle simulator to the equation free framework.

HS Validate and tune the equation free methods using short direct numerical simulations.

THT Extend microsimulations to LES of multisphere cells

THT Develop "3D-macro/2D-micro" patch dynamics

Year 3

- **SB/DPC** Extend spouted bed and dense-phase conveying to patch dynamics
- **HS** Investigate distance function related optimization techniques to solve the random medium reconstruction problem
- **HS** Assess the possibility of quaking, local crystallization, arching of the granular (pebble) flow in VHTR.
- **HS** Quantify the pebble flow interaction with the thermohydraulics of VHTR.
- **THT** Incorporate thermal dilation into macroscale hydrodynamics
- **THT** Full 3D patch dynamics demonstration

5 Consortium Arrangements

This multi-institution proposal involves personnel from Argonne (Paul Fischer (PI), Mihai Anitescu, Gary Leaf, and Barry Smith), Oak Ridge (Sreekanth Pannala), and Idaho (Hans Gougar) National Laboratories, and from Princeton University (Ioannis Kevrekidis and Sankaran Sundaresan). All personnel will be involved in developing the overarching multiscale methodology for the general problem of particulate flows, with specific attention to one or more of the three targeted applications: dense particulate flows, granular flow simulations, and fluid flow and convection in fixed beds.

Argonne will lead the effort on formulating and implementing the the equation-free method with hard particle methods, and applying it to granular flow simulations (Anitescu) and convection in fixed beds (Fischer, Leaf, Smith). Argonne will collaborate with Kevrekidis to complete the analytical and numerical analytical work (Fischer, Smith, Anitescu) and formulating and solving the optimal reconstruction and estimation problems (Anitescu). These problems are directly relevant to pebble bed reactor design and we will be working closely with the VHTR analysis group of Gougar at INEEL to ensure the validity of our approach and relevance of the results. The INEEL group has extensive experience in reactor design and porous media flows and will act as consultants on the project. We have budgeted travel funds for two extended ANL/INEEL visitor exchanges per year. Smith, who is one of the principal drivers of PETSc, will play a major role in designing and helping to implement the algorithms we develop in the course of the research.

Oak Ridge will lead the effort on the spouted bed analysis, and the Princeton group will focus on the dense phase conveying example. Both these groups will work closely with each other, assisting each other on the code implementation issues that are common to gas-particle flows, and with the Argonne group on the methodological issues, such as efficient lifting and restriction, boundary condition implementation in the gaptooth/patch dynamics approach and fixed point iterations.

Kevrekidis will provide expertise in the development, implementation, analysis and application of the equation-free method. The emphasis of his participation in the project will be on the multiscale computation and numerical analysis issues arising in the dense particulate flow systems. He and Sundaresan will work together to address issues of lifting and restriction, the efficient implementation of macro-inspired boundary conditions, and the adaptive selection of timesteps, meshes, and macroscopic observables.

Sundaresan will assist with the soft-particle DEM simulations both with and without interstitial gas effects, help develop appropriate lifting and restriction algorithms that are integral parts of the coarse-grained equation-free multi-scale approach, physically interpret the results obtained in the model problems examined in the project, and identify and extract closures for the coarse-grained equations, wherever appropriate. Sundaresan will assist with the physical interpretation and validation of the numerical simulation of the granular flow motion of the fuel pebbles in VHTR.

Pannala will focus on extensions of the multiscale framework to soft particles simulated through the Discrete Element Method (DEM), inclusion of boundary effects, and development of alternate forms of contact forces to reduce computational expense within DEM methodology.

Educational aspects of the project will be pursued through employment of summer students and post-docs at the labs and course development at Princeton. Equation-free and timestepper-based methods already constitute parts of an elective graduate course taught at Princeton. Pannala will play an active role in the education component of the project through training of Ph.D. students involved in the research at the Joint Institute of Computational Science (JICS). JICS is a joint institute between University of Tennessee at Knoxville and ORNL.

References

[1] Y. Ait-Sahalia, *Maximum-likelihood estimation of discretely-sampled diffusions: A closed-form approximation approach*, Econometrica **70** (2002), 223–262.

[2] R. Albert, M. A. Pfeifer, P. Schiffer, and A.-L. Barabási, *Slow drag in a granular medium*, Phys. Rev. Lett. **82** (1999), 205–208.

[3] Mihai Anitescu, *Optimization-based simulation of nonsmooth dynamics*, (2004), to appear.

[4] Mihai Anitescu and Gary D. Hart, *Solving nonconvex problems of multibody dynamics with joints, contact and small friction by sequential convex relaxation*, Mechanics Based Design of Machines and Structures **31(3)** (2003), 335–356.

[5] ______, *A constraint-stabilized time-stepping approach for rigid multibody dynamics with joints, contact and friction*, International Journal for Numerical Methods in Engineering **60(14)** (2004), 2335–2371.

[6] ______, *A fixed-point iteration approach for multibody dynamics with contact and friction*, Mathematical Programming, Series B **101(1)** (2004), no. ANL/MCS-P985-0802, 3–32.

[7] Mihai Anitescu, Andrew Miller, and Gary D. Hart, *Constraint stabilization for time-stepping approaches for rigid multibody dynamics with joints, contact and friction*, Proceedings of the 2003 ASME International Design Engineering Technical Conferences, no. DETC/VIB-48432, American Society for Mechanical Engineering, 2003, Chicago.

[8] Mihai Anitescu and Florian A. Potra, *Formulating dynamic multi-rigid-body contact problems with friction as solvable linear complementarity problems*, Nonlinear Dynamics **14** (1997), 231–247.

[9] ______, *Time-stepping schemes for stiff multi-rigid-body dynamics with contact and friction*, International Journal for Numerical Methods in Engineering **55(7)** (2002), 753–784.

[10] Mihai Anitescu, Florian A. Potra, and David Stewart, *Time-stepping for three-dimensional rigid-body dynamics*, Computer Methods in Applied Mechanics and Engineering **177** (1999), 183–197.

[11] A.J P. A. Langstonand A. J. Matchett B. N. Asmar and J. K. Walters, *Validation tests on a distinct element model of vibrating cohesive particle systems*, Comput. Chem. Eng. **26** (2002), 785–802.

[12] R. A. Bagnold, *The physics of blown sand and desert dunes*, Methuen & Co., London, 1954.

[13] Satish Balay, Kris Buschelman, Victor Eijkhout, William D. Gropp, Dinesh Kaushik, Matthew G. Knepley, Lois Curfman McInnes, Barry F. Smith, and Hong Zhang, *PETSc users manual*, Tech. Report ANL-95/11 - Revision 2.2.0, Argonne National Laboratory, August 2004.

[14] P Biswas and Yinyu Ye, *Semidefinite programming for ad hoc wireless sensor network localization*, Proceedings of Third International Workshop on Information Theory, 2004.

[15] D. Boyalakuntla, *Simulation of granular and gas-solid flows using discrete element method*, Ph.D. thesis, Carnegie Mellon University, 2003.

[16] D. S. Boyalakuntla and J. Y. Murthy, *Discrete element simulation of bubbling fluidized bed with a binary particle size distribution*, AIChE Annual Meeting, San Francisco, CA, Nov. 2003.

[17] ______, *Effect of drag correlations on fluidized bed simulations*, AIChE Annual Meeting, San Francisco, CA, Nov. 2003.

[18] P. W. Clearly C. S. Campbell and M. Hopkins, *Large-scale landslide simulations – global deformation, velocities and basal friction*, J. Geo. Res. – Solid Earth **100** (1995), no. B5, 8267–8283.

[19] M. Moakher F. J. Muzzio C. Wightman and O. Walton, *Simulation of flow and mixing of particles in a rotating and rocking cylinder*, AIChE J. **44** (1998), 1266–1276.

[20] C. S. Campbell, *Rapid granular flows*, Annual Rev. Fluid Mech. **22** (1990), 57–92.

[21] ______, *Granular shear flows at the elastic limit*, J. Fluid Mech. **465** (2002), 261–291.

[22] A. Castellanos, J. M. Valverde, A. T. Pérez, A. Ramos, and P. K. Watson, *Flow regimes in fine cohesive powders*, Phys. Rev. Lett. **82** (1999), 1156–1159.

[23] P. W. Cleary and M. L. Sawley, *Dem modelling of industrial granular flows: 3d case studies and the effect of particle shape on hopper discharge.*, Appl. Math. Model. **26** (2002), 89–111.

[24] Richard W. Cottle, Jong-Shi Pan, and Richard E. Stone, *The linear complementarity problem*, Academic Press, Boston, 1992.

[25] C. Crowe, M. Sommerfeld, and Y. Tsuji, *Multiphase flows with droplets and particles*, CRC Press, 1997.

[26] M. Cruz, *A parallel Monte-Carlo partial-differential-equation procedure for the analysis of multicomponent random media*, Ph.D. thesis, Massachusetts Institute of Technology, 1993, Cambridge, MA.

[27] P. A. Cundall and O. D. L. Strack, *A discrete numerical model for granular assemblies*, Geotechique **29** (1979), 47–65.

[28] J. S. Curtis and B. van Wachem, *Modeling particle-laden flows: A research outlook*, AIChE J. **50** (2004), 2638–2645.

[29] S. V. Dhodapkar and G. E. Klinzing, *Pressure fluctuations in pneumatic conveying systems*, Powder Technol. **74** (1993), 179–195.

[30] S. V. Dhodapkar, S. I. Plasynski, and G. E. Klinzing, *Plug flow movement of solids*, Powder Technol. **81** (1994), 3–7.

[31] C. C. Douglas, *Madpack: A family of abstract multigrid or multilevel solvers*, Comput. Appl. Math. **14** (1995), 3–20.

[32] J. Duran, *Sands, powders, and grains: An introduction to the physics of granular materials*, (2000).

[33] W. E and B. Engquist, *The heterogeneous multiscale methods*, Comm. Math. Sci. **1** (2003), 88–134.

[34] S. Ergun, *Flow through packed columns*, Chem. Eng. Prog. **48** (1952), 89–94.

[35] L.-S. Fan and C. Zhu, *Principles of gas-solid flows*, Cambridge University Press, Cambridge, 1998.

[36] P.F. Fischer and J.W. Lottes, *Hybrid schwarz-multigrid methods for the spectral element method: Extensions to navier-stokes*, Domain Decomposition Methods in Science and Engineering Series (R. Kornhuber, R. Hoppe, J. Priaux, O. Pironneau, O. Widlund, and J. Xu, eds.), Springer, 2004.

[37] P.F. Fischer and J.S. Mullen, *Filter-based stabilization of spectral element methods*, Comptes rendus de l'Académie des sciences, Série I- Analyse numérique **332** (2001), 265–270.

[38] C. W. Gear, C. Theodoropoulos, and I. G. Kevrekidis, *Coarse integration/bifurcation analysis via microscopic simulators: Micro-galerkin methods*, Comp. Chem. Engr. **26** (2002), 941.

[39] C.W. Gear, *Projective methods for distributions*, NEC Tech. Rep.

[40] C.W. Gear, J. M. Hyman, P. G. Kevrekidis, O. Runborg, and K. Theodoropoulos, *Equation-free coarse-grained multiscale computation: enabling microscopic simulators to perform system-level tasks*, Comm. Math. Sciences **1** (2003), 715–762.

[41] C.W. Gear and I. G. Kevrekidis, *Projective methods for stiff differential equations problems with gaps in their eigenvalue spectrum*, SIAM J. Sci. Comput. **24** (2003), 1091.

[42] N.K. Ghaddar, G.E. Karniadakis, and A.T. Patera, *A conservative isoparametric spectral element method for forced convection: Application to fully developed flow in periodic geometries*, Numer. Heat Transfer **9** (1986), 277–300.

[43] D. Gidaspow, *Multiphase flow and fluidization: Continuum and kinetic theory description*, Academic Press, Boston, 1994.

[44] Iannis G. Kevrekidis Giovanni Samaey and D. Roose.

[45] J. D. Goddard and A. K. Didwania, *Computations of dilatancy and yield surfaces for assemblies of rigid frictional spheres*, Q. Jl. Mech. Appl. Math. **51** (1998), 15–43.

[46] I. Goldhirsh, *Rapid granular flows*, Annu. Rev. Fluid Mech. **35** (2003), 267–293.

[47] D. Gottlieb and S.A. Orszag, *Numerical analysis of spectral methods: Theory and applications*, SIAM-CBMS, Philadelphia, 1977.

[48] M. Greiner, R.J. Faulkner, V.T. Van, H.M. Tufo, and P.F. Fischer, *Simulations of three-dimensional flow and augmented heat transfer in a symmetrically grooved channel*, J. Heat Transfer. **122** (2000), 653–660.

[49] M. Greiner, P.F. Fischer, H.M. Tufo, and R.A. Wirtz, *Three dimensional simulations of enhanced heat transfer in a flat passage downstream from a grooved channel*, J. Heat Transfer **124** (2002), 169–176.

[50] M. Greiner, G. Spencer, and P. Fischer, *Direct numerical simulation of three-dimensional flow and augmented heat transfer in a grooved channel*, ASME J. of Heat Transfer **120** (1998), 717–723.

[51] D. M. Hanes and O. R. Walton, *Simulations and physical measurements of glass spheres flowing down a bumpy incline*, Powder Tech **109** (2000), no. 1-3, 133–144.

[52] W. Heit, *Sic in nuclear technology*, Gmelin Handbook of Inorganic Chemistry, Silicon Suppl. **B3** (1986), 478–500.

[53] H. J. Herrmann and S. Luding, *Review article: Modeling granular media with the computer*, Continuum Mechanics and Thermodynamics **10** (1998), 189–231.

[54] R.J. Hill, D.L. Koch, and A.J.C. Ladd, *Moderate-reynolds-number flows in ordered and random arrays of spheres*, J. Fluid Mech.

[55] Rapaport D. C. Hirshfeld, D., *Molecular dynamics studies of grain segregation in sheared flow*, Phys. Rev. E 56 **2012** (1997).

[56] T. Y. Hou.

[57] L. Huilin, H. Yurong, D. Gidaspow, Y. Lidan, and Q. Yukun, *Size segregation of binary mixture of solids in bubbling fluidized beds*, Powder Tech. **134** (2003), 86–97.

[58] J. Y. Ooi J. M. F. G. Holst, J. M. Rotter and G. H. Rong, *Numerical modeling of silo filling. ii: Discrete element analyses*, J. of Eng. Mech **125** (1999), no. 1, 104–110.

[59] J. Y. Ooi J. M. Rotter, J. M. F. G. Holst and A. M. Sanadt, *Silo pressure predictions using discrete-element and finite-element analyses*, Phil. Trans. Roy. Soc. Lond. A **356** (1998), 2685–2712.

[60] L. E. Silbert J. W. Landry, G. S. Grest and S. J. Plimpton, *Confined granular packings: Structure, stress, and forces*, Phys Rev E 67 **4** (2003).

[61] R. Jackson, *The dynamics of fluidized particles*, Cambridge University Press, Cambridge, 2000.

[62] H. M. Jaeger, S. R. Nagel, and R. P. Behringer, *Granular solids, liquids, and gases*, Rev. Mod. Phys. **68** (1996), 1259–1273.

[63] J. T. Jenkins and F. Mancini, *Kinetic theory for binary mixtures of smooth, nearly elastic spheres*, Phys. Fluids A **1** (1989), 2050–2057.

[64] J. T. Jenkins and M. W. Richman, *Grad's 13-moment system for a dense gas of inelastic spheres*, Arch. Ration. Mech. Anal. **87** (1985), 355–377.

[65] I.G. Kevrekidis, C. William Gear, and G. Hummer, *Equation-free: the computer-assisted analysis of complex, multiscale systems*, A.I.Ch.E. J. **50** (2004), 1346–1354.

[66] Matthew Knepley, Ahmed H. Sameh, and Vivek Sarin, *Parallel simulation of particulate flows*, pp. 226–237, 1998.

[67] D. L. Koch, R. J. Hill, and A. S. Sangani, *Brinkman screening and the covariance of the fluid velocity in fixed beds*, Physics of Fluids **10** (1998), 3035–3037.

[68] K. Konrad, D. Harrison, R. M. Nedderman, and J. F. Davidson, *Prediction of the pressure drop for horizontal dense phase pneumatic conveying of particles*, Proceedings of the 5th Int. Conf. Pneumatic Transport of Solids in Pipes (London, Pneumotransport), vol. 5, 1980, pp. 225–244.

[69] K. Kuwagi and M. Horio, *A numerical study on agglomerate formation in a fluidized bed of fine cohesive particles*, Chem. Eng. Sci. **57** (2002), 4737–4744.

[70] J. W. Landry L. E. Silbert and G. S. Grest, *Granular flow down a rough inclined plane: Transition between thin and thick piles*, Phys. of Fluids **15** (2003), no. 1, 1–10.

[71] P. V. Lade and J. M. Duncan, *Elastoplastic stress-strain theory for cohesionless soil*, J. Geotech. Eng. Div. ASCE **101** (1975), 1037–1053.

[72] J. Li and J. A. M. Kuipers, *Gas-particle interactions in dense gas-fluidized beds*, Chem. Eng. Sci. **58** (2003), 711–718.

[73] Ju Li, S Yiao, and Sidney Yip.

[74] Chih-Jen Lin and Jorge More, *Newton's method for large bound-constrained optimization problems*, SIAM Journal on Optimization **9** (1999), no. 4, 1100–1127.

[75] J. W. Lottes and P. F. Fischer, *Hybrid multigrid/Schwarz algorithms for the spectral element method*, J. Sci. Comput. **(to appear)** (2004).

[76] C. K. K. Lun, S. B. Savage, D. H. Heffery, and N. Chepurniy, *Kinetic theories for granular flow: Inelastic particles in couette flow and slightly inelastic particles in a general flow field*, J. Fluid Mech. **140** (1984), 223–256.

[77] M. Nguyen P. Stewart M. J. Rhodes, X. S. Wang and K. Liffman, *Onset of cohesive behaviour in gas fluidized beds: A numerical study using dem simulation*, Chem. Eng. Sci. **56** (2001), 4433–4438.

[78] A. Marsden, O. Vasilyev, and P. Moin, *Constuction of commutative filters for LES on unstructured meshes*, Tech. Report CTR Ann. Res. Briefs, Stanford Univ., 2000.

[79] K. E. Mathur and N. Epstein, *Spouted beds*, Academic Press, New York, USA, 1974.

[80] B. Maury, *A many-body lubrication model*, Comptes rendus de l'Académie des sciences, Série I- Analyse numérique **325** (1997), 1053–1058.

[81] J. J. McCarthy, *Micro-modeling of cohesive mixing processes*, Powder Technol. **138** (2003), 63–67.

[82] A. Montillet, *Flow through a finited packed bed of spheres: a note on the limit of the applicability of the forchheimer-type equation*, J. Fluids End. **126** (2004), 139–143.

[83] S. J. Moon, I. G. Kevrekidis, and S. Sundaresan, *Molecular dynamics-based simulation of vibrated gas fluidized bed*, AIChE Annual Meeting, Austin, TX, Nov. 2004.

[84] S. J. Moon, S. Sundaresan, and I. G. Kevrekidis, *Equation-free, coarse grained approach to vibrated gas fluidized bed*, AIChE Annual Meeting, Austin, TX, Nov. 2004.

[85] Jorge More and Zhijun Wu, *Global continuation for distance geometry problem*, SIAM Journal on Optimization **7** (1997), no. 3, 814–836.

[86] Jean J. Moreau and Michel Jean, *Numerical treatment of contact and friction: The contact dynamics method*, Proceedings of the Third Biennial Joint Conference on Engineering Systems and Analysis (Montpellier, France), July 1996, p. to appear.

[87] Jean Jacques Moreau, *Numerical aspects of the sweeping process*, Computer methods in applied mechanics and engineering **177** (1999), 329 –349.

[88] B. Nadler, S. Lafon, R. C. Coifman, and I. G. Kevrekidis, *Diffusion maps, spectral clustering and the reaction coordinates of dynamical systems*, Appl. Comp. Harm. Anal.

[89] D.A. Nield, *Alternative models of turbulence in a porous medum, and related matters*, Trans. ASME **123** (2001), 928–934.

[90] R. Noren and R. Develasco, *Evolution of coating gas distributors*, Tech. Report PC- 000345, General Atomics report, 1992.

[91] S.V. Patankar, C.H. Liu, and E.M. Sparrow, *Fully developed flow and heat transfer in ducts having streamwise-periodic variations of cross-sectional area*, J. Heat Transfer **99** (1977), 180–186.

[92] F. Podczeck, *Particle-particle adhesion in pharmaceutical powder handling*, Imperial College Press, London, 1998.

[93] A. V. Potapov and C. S. Campbell, *Computer simulation of hopper flow*, Phys. of Fluids **8** (1996), no. 11, 2884–2894.

[94] J. McLaughlin J. Kelly C. S. Daw S. Pannala R. Lowden, J. Hunn and C. E. A. Finney, *Coated particle fuel for advanced gas reactors*, Annual Meeting of the American Ceramic Society, Indianapolis, Indiana, 2004.

[95] D. C. Rapaport, *Simulational studies of axial granular segregation in a rotating cylinder*, Phys. Rev. E 65 (2002).

[96] ———, *The art of molecular dynamics simulation*, 2nd edn. (2004).

[97] A. M. Reynolds, *Effects of periodicity on flow and dispersion through closely packed fixed beds of spheres*, Phys. Rev. E. **65** (2002), 026308.

[98] K. Rietema, *The dynamics of fine powders*, Elsevier Applied Science, London and New York, 1991.

[99] Mark D. Rintoul and Salvatore Torquato, *Reconstruction of the structure of dispersions*, Journal of Colloid and Interface Science **186** (1997), no. 2, 467–476.

[100] C. E. A. Finney D. Boyalakuntla D. Bruns S. Pannala, C. S. Daw and J. Zhou, *Simulating the dynamics of spouted beds using eulerian-eulerian formulation*, Tech. report, Under Preparation.

[101] ———, *Ornl fy04 process modeling summary report for the advanced gas reactor fuel development and qualification program*, Tech. Report Technical Report ORNL/CF-04/11, Oak Ridge National Laboratory, 2004.

[102] X. S. Wang S. Takeuchi and M. J. Rhodes, *Discrete element study of particle circulation in a 3-d spouted bed*, Chem. Eng. Sci. **60** (2005), 1267–1276.

[103] G. Samaey, I.G. Kevrekidis, and D. Roose, *Patch dynamics with buffers for homogenization problems*, J. Comput. Phys. **submitted** (2004).

[104] S. B. Savage, *Analyses of slow high-concentration flows of granular materials*, J. Fluid Mech. **377** (1998), 1–26.

[105] S. B. Savage and S. McKeown, *Shear stresses developed during rapid shear of concentrated suspensions of large spherical particles between concentric cylinders*, J. Fluid Mech. **127** (1983), 453–472.

[106] G. M. Shroff and H. B. Keller, *Stabilization of unstable procedures: a recursive projection method*, SIAM J. Numer. Anal. **30** (1993), 1099–1120.

[107] C. Siettos, M. D. Graham, and I. G. Kevrekidis, *Coarse brownian dynamics for nematic liquid crystals: Bifurcation, projective integration and control via stochastic simulation*, J. Chem. Phys. **118** (2003), 10149–10157.

[108] C. Siettos, C. C. Pantelides, and I. G. Kevrekidis, *Enabling dynamic process simulators to perform alternative tasks: A time-stepper based toolkit for computer-aided analysis*, Ind. Eng. Chem. Res. **42** (2003), 6795–6801.

[109] B. Smith et al., *Scientific Applications Using PETSc*, http://www.mcs.anl.gov/petsc/petsc-as/publications.

[110] David E. Stewart, *Convergence of a time-stepping scheme for rigid body dynamics and resolution of Painleve's problems*, Archive Rational Mechanics and Analysis **145(3)** (1998), 215–260.

[111] David E. Stewart and Jeffrey C. Trinkle, *An implicit time-stepping scheme for rigid-body dynamics with inelastic collisions and Coulomb friction*, International Journal for Numerical Methods in Engineering **39** (1996), 2673–2691.

[112] S. Sundaresan, *Instabilities in fluidized beds*, Annu. Rev. Fluid Mech. **35** (2003), 63–88.

[113] M. Syamlal, *Mfix documentation: Numerical technique*, Tech. Report Tech. Rep. DOE/MC31346-5824 (DE98002029), Morgantown Energy Technology Center, Morgantown, West Virginia, 1998.

[114] Rogers W. Syamlal, M. and T. J. O'Brien, *Mfix documentation: Theory guide*, Tech. Report Tech. Rep. DOE/METC-94/1004 (DE9400087), Morgantown Energy Technology Center, Morgantown, West Virginia, 1993.

[115] Y. Tsuji T. Kawaguchi, T. Tanaka, *Numerical analysis of density wave in dense gas-solid flows in a vertical pipe*, Progress of Theoretical Physics Supplement **138** (2000), 696–701.

[116] H. Kamiya T. Mikami and M. Horio, *Numerical simulation of cohesive powder behavior in a fluidized bed*, Chem. Eng. Sci. **53** (1998), 1927–1940.

[117] T. Charinpanitkul T. Kawaguchi T. Tanaka Y. Tsuji T. Swasdisevi, W. Tanthapanichakoon, *Investigation of fluid and coarse-particle dynamics in a two-dimensional spouted bed*, Chem. Eng. & Tech **27** (2004), no. 9, 971–981.

[118] G. I. Tardos, *A fluid mechanics approach to slow, frictional powder flows*, Powder Technol. **92** (1997), 61–74.

[119] C. Theodoropoulos, S. Sankaranarayanan, S. Sundaresan, and I.G. Kevrekidis, *Coarse bifurcation studies of bubble flow microscopic simulations*, 3rd Pan-Hellenic Conference in Chemical Engineering, 2001, pp. 221–224.

[120] ———, *Coarse bifurcation studies of bubble flow lattice boltzmann simulations*, Chem. Eng. Sci. **59** (2004), 2357–2362.

[121] K. Theodoropoulos, Y.-H. Qian, and I.G. Kevrekidis, *Coarse stability and bifurcation analysis using timesteppers: a reaction diffusion example*, Proc. Natl. Acad. Sci. **97** (2000), 9840–9843.

[122] H.M. Tufo and P.F. Fischer, *Terascale spectral element algorithms and implementations*, Proc. of the ACM/IEEE SC99 Conf. on High Performance Networking and Computing (IEEE Computer Soc.), 1999, p. CDROM.

[123] P. B. Umbanhowar, F. Melo, and H. L. Swinney, *Localized excitations in a vertically vibrated granular layer*, Nature **382** (1996), 793–796.

[124] O. R. Walton and R. L. Braun, *Viscosity, granular temperature, and stress calculations for shearing assemblies of inelastic, frictional disks*, J. of Rheology **30** (1986), 949–980.

[125] M. Weber, *Simulation of cohesive particle flows in granular and gas-solid systems*, Ph.D. thesis, University of Colorado, 2004.

[126] P. W. Wypych, *5th Int. Conf. On Bulk Materials Storage, Handling and Transportation, Newcastle, 10-12 july 1995*, IEAust Proc., vol. 1, 1995, pp. 47–56.

[127] ———, *Chemeca 97, Rotorua, New Zealand, 29 Sept.–1 Oct. 1997, SCENZ, Particle Technology Workshop Preprints, IPENZ*, 1997, pp. 129–138.

[128] B. H. Xu and A. B. Yu, *Numerical simulation of the gas-particle flow in a fluidized bed by combining discrete particle method with computational fluid dynamics*, Chem. Eng. Sci. **52** (1997), 2785–2809.

[129] T. Yasukawa Y. Tatemoto, Y. Mawatari and K. Noda, *Numerical simulation of particle motion in vibrated fluidized bed*, Chem. Eng. Sci. **59** (2004), 437–447.

[130] T. Ishida Y. Tsuji, T. Tanaka, *Lagrangian numerical-simulation of plug flow of cohesionless particles in a horizontal pipe*, Powder Technology **71** (1992), no. 3, 239–250.

[131] T. Kawaguchi Y. Tsuji and T. Tanaka, *Discrete particle simulation of two-dimensional fluidized bed*, Powder Technol. **77** (1993), 79–87.

[132] S. H. Liu Y. Wang and D. A. Sun, *Numerical study of soil collapse behavior by discrete element modelling*, Comput. Geotech. **30** (2003), 399–408.

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy

Budget Page

(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION
The University of Chicago, Operator of Argonne National Laboratory

Budget Page No: 1 of 4

PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR
Dr. Paul Fischer

Requested Duration: 12 (Months)
Year 1 of 3

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested by Applpicant	Funds Granted by DOE
1. 5 Paul Fischer, PI	3.00			$50,385	
2. 5 Mihai Anitescu, Computer Scientist	1.80			$30,231	
3. 5 Gary Leaf, Mathematician	1.80			$30,231	
4. 5 Barry Smith, Computer Scientist	1.80			$30,231	
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (4) TOTAL SENIOR PERSONNEL (1-6)	8.40			$141,078	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (2) POST DOCTORAL ASSOCIATES	24.00			$184,128	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. (2) GRADUATE STUDENTS				$21,696	
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$346,902	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$346,902	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$10,000	
2. FOREIGN					
TOTAL TRAVEL				$10,000	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				$11,232	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER				$5,000	
TOTAL OTHER DIRECT COSTS				$16,232	
H. TOTAL DIRECT COSTS (A THROUGH G)				$373,134	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS				$126,866	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$500,000	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$500,000	

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy

Budget Page

(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION The University of Chicago, Operator of Argonne National Laboratory				Budget Page No:	2 of 4
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Dr. Paul Fischer				Requested Duration: 12 (Months) Year 2 of 3	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos.			Funds Requested by Applpicant	Funds Granted by DOE
	CAL	ACAD	SUMR		
1. 5 Paul Fischer, PI	3.00			$52,231	
2. 5 Mihai Anitescu, Computer Scientist	1.80			$31,339	
3. 5 Gary Leaf, Mathematician	1.80			$31,339	
4. 5 Barry Smith, Computer Scientist	1.80			$31,339	
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (4) TOTAL SENIOR PERSONNEL (1-6)	8.40			$146,247	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (2) POST DOCTORAL ASSOCIATES	24.00			$191,016	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. (2) GRADUATE STUDENTS				$22,490	
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$359,754	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$359,754	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$10,400	
2. FOREIGN					
TOTAL TRAVEL				$10,400	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				$14,174	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS				$14,174	
H. TOTAL DIRECT COSTS (A THROUGH G)				$384,328	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS				$130,672	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$515,000	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$515,000	

DOE F 4620.1	**U.S. Department of Energy**	OMB Control No.
(04-93)	**Budget Page**	1910-1400
All Other Editions Are Obsolete	(See reverse for Instructions)	OMB Burden Disclosure Statement on Reverse

ORGANIZATION The University of Chicago, Operator of Argonne National Laboratory				**Budget Page No:**	3 of 4
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Dr. Paul Fischer				Requested Duration: 12 (Months) Year 3 of 3	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested by Applpicant	Funds Granted by DOE
1. 5 Paul Fischer, PI	3.00			54,141	
2. 5 Mihai Anitescu, Computer Scientist	1.80			32,485	
3. 5 Gary Leaf, Mathematician	1.80			32,485	
4. 5 Barry Smith, Computer Scientist	1.80			32,485	
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (4) TOTAL SENIOR PERSONNEL (1-6)	8.40			$151,595	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (2) POST DOCTORAL ASSOCIATES	24.00			$198,139	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. (2) GRADUATE STUDENTS				$23,312	
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$373,046	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$373,046	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$10,816	
2. FOREIGN					
TOTAL TRAVEL				$10,816	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				$11,660	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS				$11,660	
H. TOTAL DIRECT COSTS (A THROUGH G)				$395,522	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS				$134,478	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$530,000	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$530,000	

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy
Budget Page
(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION
The University of Chicago, Operator of Argonne National Laboratory

Budget Page No: 4 of 4

PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR
Dr. Paul Fischer

Requested Duration: 36 (Months)
3-Year Total

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested by Applpicant	Funds Granted by DOE
1. Paul Fischer, PI	9.00			$156,757	
2. Mihai Anitescu, Computer Scientist	5.40			$94,054	
3. Gary Leaf, Mathematician	5.40			$94,054	
4.	5.40			$94,054	
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (4) TOTAL SENIOR PERSONNEL (1-6)	25.20			$438,921	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (2) POST DOCTORAL ASSOCIATES	72.00			$573,283	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. (2) GRADUATE STUDENTS				$67,498	
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$1,079,702	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$1,079,702	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$31,216	
2. FOREIGN					
TOTAL TRAVEL				$31,216	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				$37,067	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER				$5,000	
TOTAL OTHER DIRECT COSTS				$42,067	
H. TOTAL DIRECT COSTS (A THROUGH G)				$1,152,985	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS				$392,015	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$1,545,000	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$1,545,000	

Budget Explanation

A-C Salaries and Fringe Benefits

Argonne National Laboratory is a government-owned facility operated by the University of Chicago. As a contractor for the Department of Energy, Argonne National Laboratory must comply with DOE general policies and procedures on budgeting and accounting. The Laboratory's costing procedures are based on the assumption that all costs incurred will be recovered. The costing procedures use standard rates, which are used throughout the Laboratory on a consistent basis and uniformly applied to all work supported by the Department of Energy and other federal agencies.

Standard rates are established at the beginning of the fiscal year for each research division, and are monitored and revised as necessary. All labor costs are distributed using standard rates which are developed by the laboratory's budget office for each major payroll classification within the lab. The division-wide rates are based on pay bands (salary ranges) and fringe benefits (34.5% for a regular staff and clerical, and 11% for post/pre doctoral appointees), plus a factor for divisional overhead and for paid absences. Graduate and undergraduate students costs include housing allowance and fringe benefits(7.65%). Effort is escalated each year by a rate provided by the Argonne Budget Department.

The prinicipal investigator for this proposal is:	Dr. Paul Fischer		
The PI's effort charged per year to this proposal is :		3.00	man-months
Senior Personnel support includes:	Mihai Anitescu, Computer Scientist	1.80	man-months
	Gary Leaf, Mathematician	1.80	man-months
	Barry Smith, Computer Scientist	1.80	man-months
Post doctoral appointees' effort charged per year to this proposal is :		24.00	man-months
Graduate Students	Semester = 3 month appointment	6.00	man-months

E Travel

Domestic: $1K per trip/escalate 4.0% per yr.
Projecting 1-trip(s) per staff member per year to present results/status to collaborative instituitions.
Projecting 1 to 2 -trips per staff member per year to present results to conferences-TBD
Projecting 2 trips for INEEL collaborators to visit Argonne.

G Other Direct Costs

1. Materials and Supplies:
Software, low-end computers (<$5k), computer supplies/ peripherals, and misc supplies.
6. Other:
Relocation expenses related to hiring of two new post-docs.

I Indirect Costs

Standard rates are also developed for Laboratory General and Administrative (G&A) expense. The procedures for distributing Laboratory G&A and program expense is applied on the basis of the total cost of the work performed. The following indirect rates are provisional and have been estimated for each fiscal year budget period:

PBCS Program Expenses @ 3.3%
Laboratory G&A:
Common Support @ 25.50%
Equipment/Subcontracts@ 6.2%
G&A Burden @ 4.034%

Argonne' s indirect rates are continuously reviewed and audited by
Cognizant Federal Agency:
Martin Straka
Department of Energy-Chicago Operations Office
9800 South Cass Avenue
Argonne, Illinois 60439
630-252-7724

DOE F 4620.1 (04-93) All Other Editions Are Obsolete	**U.S. Department of Energy**	OMB Control No. 1910-1400 OMB Burden Disclosure Statement on Reverse

Budget Page

(See reverse for Instructions)

ORGANIZATION Oak Ridge National Laboratory (Year 1)				**Budget Page No:**	Year 1
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR				Requested Duration:	(Months)
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos.			Funds Requested by Applpicant	Funds Granted by DOE
	CAL	ACAD	SUMR		
1. Pannala, Sreekanth	1.4				
2.					
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. ( ) TOTAL SENIOR PERSONNEL (1-6)	1.4			$12,269	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (0.5) POST DOCTORAL ASSOCIATES				$50,000	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$62,269	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$4,306	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$66,575	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
TOTAL TRAVEL					
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER-Oranization burden costs associated with personnel				$18,270	
TOTAL OTHER DIRECT COSTS				$18,270	
H. TOTAL DIRECT COSTS (A THROUGH G)				$84,845	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS				$15,155	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$100,000	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$100,000	

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy

Budget Page

(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION Oak Ridge National Laboratory (Year 2)				**Budget Page No:**	Year 2
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR				Requested Duration:	(Months)
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested by Applpicant	Funds Granted by DOE
1. Pannala, Sreekanth	1.3				
2.					
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. ( ) TOTAL SENIOR PERSONNEL (1-6)	1.3			$12,271	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (0.5) POST DOCTORAL ASSOCIATES				$50,000	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$62,271	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$4,307	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$66,578	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
TOTAL TRAVEL					
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER-Oranization burden costs associated with personnel				$18,231	
TOTAL OTHER DIRECT COSTS				$18,231	
H. TOTAL DIRECT COSTS (A THROUGH G)				$84,809	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS				$15,191	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$100,000	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$100,000	

DOE F 4620.1 (04-93) *All Other Editions Are Obsolete*	**U.S. Department of Energy** **Budget Page** (See reverse for Instructions)	OMB Control No. 1910-1400 OMB Burden Disclosure Statement on Reverse

ORGANIZATION Oak Ridge National Laboratory (Year 3)				**Budget Page No:** Year 3	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR				Requested Duration: (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos.			Funds Requested	Funds Granted
	CAL	ACAD	SUMR	by Applpicant	by DOE
1. Pannala, Sreekanth	1.3				
2.					
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. ( ) TOTAL SENIOR PERSONNEL (1-6)	1.3			$12,360	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (0.5) POST DOCTORAL ASSOCIATES				$50,000	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$62,360	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$4,338	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$66,698	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
TOTAL TRAVEL					
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER-Oranization burden costs associated with personnel				$18,112	
TOTAL OTHER DIRECT COSTS				$18,112	
H. TOTAL DIRECT COSTS (A THROUGH G)				$84,810	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS				$15,190	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$100,000	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$100,000	

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy

Budget Page

(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION Oak Ridge National Laboratory [Summary]				Budget Page No:	Summary
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR				Requested Duration:	36 (Months)
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested by Applpicant	Funds Granted by DOE
1. Pannala, Sreekanth	4.0				
2.					
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. ( ) TOTAL SENIOR PERSONNEL (1-6)	4.0			36,900	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (0.5) POST DOCTORAL ASSOCIATES				150,000	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				186,900	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				12,951	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				199,851	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
TOTAL TRAVEL					
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER-Oranization burden costs associated with personnel				54,613	
TOTAL OTHER DIRECT COSTS				54,613	
H. TOTAL DIRECT COSTS (A THROUGH G)				254,464	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS				45,536	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				300,000	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				300,000	

ORNL Budget Explanation

Budget Pages

Cost estimates presented in the ``budget pages" of this proposal have been reclassified in order to be comparable to proposals submitted by other research institutions. At the Oak Ridge National Laboratory (ORNL), costs are collected and reported in accordance with approved Department of Energy (DOE) accounting guidelines. Although costs have been reclassified in this proposal, integrity has been maintained in total and between direct versus indirect costs.

A. (1-7) Senior Personnel

The ORNL's cost accounting system utilizes wage pools based upon salary ranges. For purposes of this budget, the wage pool cost estimate is divided by the fringe benefits rate. The labor component is being reported in Item A and the fringe component is being reported in Item C.

The list of senior personnel participating in this project is as follows:
Dr. Sreekanth Pannala will be working on extending the multiscale framework to soft particles modeled by Discrete Element Method and publishing the code and data online for other researchers to develop closure relationships.

B.1 Post-Doctoral Associates

Post-BS subcontractors, who work on the ORNL site, are assessed a $1,030 per month organization burden charge. This charge recovers the division's costs associated with working on-site (primarily space and utilities). This is being reported in Item G.6.

Dr. Dhanunjay Boyalakuntla will be working on extending the multiscale framework to soft particles modeled by Discrete Element Method.

C. Fringe Benefits

Fringe Benefits for ORNL employees are estimated to be 36.9% of labor costs for each year. Included in fringe benefits is labor burden.

G.6 Other - Organization Burden Administration

Use of cost collection centers in ORNL R&D divisions is the approved method for collection and distribution of organization burden costs. These accounts are established to collect costs associated with an R&D division. The types of costs which can be charged to organization burden cost collection centers are unfunded paid hours; division administration; and general materials/service costs, including, but not limited to telecommunications, space, utilities, word processing, and copying which are not directly attributable or chargeable to R&D projects. Division Administration costs include: *(i)* managerial, technical, and administrative oversight; and *(ii)* support personnel such as facilities and operations, environmental, safety, and health, finance and budget, quality, and health physics provided for the general benefit of a division.

For ORNL staff, the labor and fringe components have been estimated and reported in items A - C. For Post-BS subcontractors, the subcontract costs have been reported in Item B.1. For ORNL staff and Post-BS subcontractors, the organization burden component has been estimated and is being reported in Item G.6. Inclusion of these costs is necessary to provide a full accounting of estimated cost for the project period. All cost will be collected and reported in ORNL's cost accounting system.

I. Indirect Costs

Full General & Administrative (G&A), Legacy Charge, and Management Fee are assessed on ORNL labor costs (Items A, C, and G.6), Materials and Supplies, and Equipment less than $35,000 unit value. Full G&A is estimated to be 38.1% for FY 2005, FY 2006, and FY 2007. Legacy Charge is estimated to be 2.9% each year. Management Fee is estimated to be 2.5% each year.

DOE F 4620.1

(04-93)

All Other Editions Are Obsolete

U.S. Department of Energy

Budget Page

(See reverse for Instructions)

OMB Control No.

1910-1400

OMB Burden Disclosure

Statement on Reverse

ORGANIZATION Thr Trustees of Princeton University				**Budget Page No:** Year 1	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Yannis G. Kevrekidis				Requested Duration: (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos.			Funds Requested	Funds Granted
	CAL	ACAD	SUMR	by Applpicant	by DOE
1. Kevrekidis, Yannis G Principal Investigator			1.00	17,460.00	
2. Sundaresan, Sankaran Co-PI			1.00	17,229.00	
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (2) TOTAL SENIOR PERSONNEL (1-6)			2.00	34,689.00	0.00
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (1) POST DOCTORAL ASSOCIATES				38,000.00	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. (1) GRADUATE STUDENTS				27,305.00	
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				99,994.00	0.00
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				24,607.00	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				124,601.00	0.00
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.) 32 Processor Computer Cluster					
TOTAL PERMANENT EQUIPMENT				60,000.00	
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				6,000.00	
2. FOREIGN					
TOTAL TRAVEL				6,000.00	0.00
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES				15,955.00	
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST				15,955.00	0.00
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES				0.00	
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS				0.00	0.00
H. TOTAL DIRECT COSTS (A THROUGH G)				206,556.00	0.00
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS				75,749.00	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				282,305.00	0.00
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				282,305.00	0.00

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy

Budget Page

(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION: The Trustees of Princeton University — Budget Page No: Year 2

PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR: Yannis G. Kevrekidis — Requested Duration: ____ (Months)

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested by Applplicant	Funds Granted by DOE
1. Kevrekidis, Yannis G Principal Investigator			1.00	18,159.00	
2. Sundaresan, Sankaran Co-PI			1.00	17,919.00	
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (2) TOTAL SENIOR PERSONNEL (1-6)			2.00	36,078.00	0.00
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (1) POST DOCTORAL ASSOCIATES				39,520.00	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. (1) GRADUATE STUDENTS				28,160.00	
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				103,758.00	0.00
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				26,098.00	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				129,856.00	0.00
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				6,000.00	
2. FOREIGN					
TOTAL TRAVEL				6,000.00	0.00
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES				16,505.00	
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST				16,505.00	0.00
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES				0.00	
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS				0.00	0.00
H. TOTAL DIRECT COSTS (A THROUGH G)				152,361.00	0.00
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS				78,796.00	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				231,157.00	0.00
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				231,157.00	0.00

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy

Budget Page

(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION The Trustees of Princeton University				**Budget Page No:** Year 3	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Yannis G. Kevrekidis				Requested Duration:	(Months)
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos.			Funds Requested by Applpicant	Funds Granted by DOE
	CAL	ACAD	SUMR		
1. Kevrekidis, Yannis G Principal Investigator			1.00	18,885.00	
2. Sundaresan, Sankaran Co-PI			1.00	18,635.00	
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (2) TOTAL SENIOR PERSONNEL (1-6)			2.00	37,520.00	0.00
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (3) POST DOCTORAL ASSOCIATES				41,101.00	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. (3) GRADUATE STUDENTS				28,960.00	
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				107,581.00	0.00
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				27,442.00	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				135,023.00	0.00
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				6,000.00	
2. FOREIGN					
TOTAL TRAVEL				6,000.00	0.00
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES				17,060.00	
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST				17,060.00	0.00
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES				0.00	
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS				0.00	0.00
H. TOTAL DIRECT COSTS (A THROUGH G)				158,083.00	0.00
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS				81,794.00	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				239,877.00	0.00
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				239,877.00	0.00

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy

Budget Page

(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION: The Trustees of Princeton University — **Budget Page No:** Cumulative

PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR: Yannis G. Kevrekidis — Requested Duration: ______ (Months)

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested by Applpicant	Funds Granted by DOE
1. Kevrekidis, Yannis G Principal Investigator			1.00	54,505.00	
2. Sundaresan, Sankaran Co-PI			1.00	53,783.00	
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (2) TOTAL SENIOR PERSONNEL (1-6)				108,288.00	0.00
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (3) POST DOCTORAL ASSOCIATES				118,621.00	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. (3) GRADUATE STUDENTS				84,425.00	
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				311,334.00	0.00
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				78,147.00	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				389,481.00	0.00
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.) 32 Processor Computer Cluster					
TOTAL PERMANENT EQUIPMENT				60,000.00	
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				18,000.00	
2. FOREIGN					
TOTAL TRAVEL				18,000.00	0.00
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES				49,520.00	
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST				49,520.00	0.00
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES				0.00	
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS				0.00	0.00
H. TOTAL DIRECT COSTS (A THROUGH G)				517,001.00	0.00
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS				236,339.00	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				753,340.00	0.00
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				753,340.00	0.00

Budget Justification

Iaonnis G. Kevrekidis (PI) and Sankaran Sundaresan (co-PI) will devote a substantial part of their times during the academic year to this project, for which no funding is sought. They will also devote one month of their summer to this project and funds to support them are requested. SS will be responsible for the microscopic simulator development, testing and the analysis of the physical aspect of the test examples. IGK will be responsible for all aspects of the coarse-grained, equation-free analysis. They will work together in implementation and testing of restriction and lifting schemes and boundary conditions for the cells in the Gaptooth/Patch Dynamics approach.

The division of labor between the post-doctoral fellow and the graduate student is described in the proposal. Because of the natural overlap in their efforts, there will be much interaction between them. Funds to fully support the post-doctoral fellow and the graduate student are sought. All Ph.D. students are supported fully by Princeton University during their first academic year in residence. Thus, the three year funding effectively translates to four years of support for the student.

Computational work in the research groups of Kevrekidis and Sundaresan is done on linux clusters. They have one cluster with 32 processors (900MHz Intel Pentium P3) and another with 16 processors (1.7GHz Intel Pentium P3), which are available for this project. These clusters are nearly 5 years old and they will have to be replaced soon. With this in mind, funding is sought for one 32 processor (3.4 GHz Intel Pentium P4) cluster.

A modest level of funding is sought to allow the PIs, the post-doctoral fellow and the student to travel to team meetings with collaborators and to technical conferences. We request funding for travel to two team meetings per year – the team meetings will be held at Argonne. We also request funding for travel to one conference per participant during the course of the three-year project:

<u>Six team meetings over the three-year project:</u>	
The cost of air travel (four tickets x six trips in three years):	$ 8000
Hotel accommodation for two rooms x one night x six trips:	$ 1400
Subsistence for two days x 4 people x six trips:	$ 1800
Local travel in Chicago city and Princeton (4 people x 6 trips):	$ 1800
Total expense for team meetings:	$ 13000

<u>Trip to conferences over the three-year project:</u>	
Airfare (4 tickets)	$ 1600
Conference registration (4 people)	$ 2000
Hotel accommodation for two rooms x three nights:	$ 700
Subsistence for three days x 4 people:	$ 400
Local travel in conference city and Princeton (4 people):	$ 300
Total per year:	$ 5000

Total travel budget = $18,000 for three years. Thus, the travel budget per year = $6,000.

Current and Pending Support

Investigator: **Kevrekidis, Yannis G**

Other agencies (including NSF) to which this proposal has been/will be submitted.

Support: [X] Current [ ] Pending [ ] Submission Planned in Near Future [ ] *Transfer of Support

Project Title: A System-identification Based. "closed-on-demand" Toolkit for Multiscale Simulation, Stability/bifurcation Analysis, Optimization and Control:...

Source of Support: Air Force Office of Scientific Research

Total Award Amount: $ 510,797 **Total Award Period Covered:** 01/01/03 - 12/31/05

Location of Project: Princeton University

Person-Months Per Year Committed to the Project. Cal: 0.00 Acad: 0.00 Sumr: 0.00

Support: [X] Current [ ] Pending [ ] Submission Planned in Near Future [ ] *Transfer of Support

Project Title: DARPA Subcontract Proposal Entitled, "Photonic Reagents: The Production of Cyclic Ozone

Source of Support: Temple University

Total Award Amount: $ 125,000 **Total Award Period Covered:** 12/01/04 - 11/30/05

Location of Project: Princeton University

Person-Months Per Year Committed to the Project. Cal: 0.00 Acad: 0.00 Sumr: 0.00

Support: [X] Current [ ] Pending [ ] Submission Planned in Near Future [ ] *Transfer of Support

Project Title: Equation-Free Computation Tools For Predicting Real Optimized Materials

Source of Support: Army Research Laboratory

Total Award Amount: $ 155,000 **Total Award Period Covered:** 06/21/04 - 10/20/05

Location of Project: Princeton University

Person-Months Per Year Committed to the Project. Cal: 0.00 Acad: 0.00 Sumr: 0.75

Support: [X] Current [ ] Pending [ ] Submission Planned in Near Future [ ] *Transfer of Support

Project Title: ITR/AP: Enabling Microscopic Simulators to Perform System-Level Analysis

Source of Support: National Science Foundation

Total Award Amount: $ 800,000 **Total Award Period Covered:** 08/15/02 - 07/31/05

Location of Project: Princeton University

Person-Months Per Year Committed to the Project. Cal: 0.00 Acad: 0.00 Sumr: 0.00

Current and Pending Support

Investigator: **Kevrekidis, Yannis G**

Other agencies (including NSF) to which this proposal has been/will be submitted.

Support: [X] Current [ ] Pending [ ] Submission Planned in Near Future [ ] *Transfer of Support

Project Title: MSPA-CSE: Equation-Free Modeling of Biological Self-Organization: Coarse Computational Swarming

Source of Support: National Science Foundation

Total Award Amount: $ 280,000 **Total Award Period Covered:** 09/15/04 - 08/31/08

Location of Project: Princeton University

Person-Months Per Year Committed to the Project. Cal: 0.00 Acad: 0.00 Sumr: 0.00

Support: [X] Current [ ] Pending [ ] Submission Planned in Near Future [ ] *Transfer of Support

Project Title: Pixelated Matter for Multi-Functional Composites Development

Source of Support: Defense Advanced Research Projects Agency

Total Award Amount: $ 40,000 (YGK part) **Total Award Period Covered:** 08/19/04 - 08/18/05

Location of Project: Princeton University (I.A. Aksay, PI)

Person-Months Per Year Committed to the Project. Cal: 0.00 Acad: 0.00 Sumr: 0.00

Support: [X] Current [ ] Pending [ ] Submission Planned in Near Future [ ] *Transfer of Support

Project Title: The Center for Multiscale Plasma Dynamics

Source of Support: DOE - Germantown

Total Award Amount: $ 114,732 **Total Award Period Covered:** 08/01/04 - 07/31/09

Location of Project: Princeton University

Person-Months Per Year Committed to the Project. Cal: 0.00 Acad: 0.00 Sumr: 0.00

Support: [ ] Current [X] Pending [ ] Submission Planned in Near Future [ ] *Transfer of Support

Project Title: Coarse-grained, equation-free multiscale simulation of large-scale granular and gas-particle flows

Source of Support: National Science Foundation

Total Award Amount: $ 656,758.03 **Total Award Period Covered:** 07/01/05 - 06/30/08

Location of Project: Princeton University

Person-Months Per Year Committed to the Project. Cal: 0.00 Acad: 0.00 Sumr: 1.00

Current and Pending Support

Investigator: **Kevrekidis, Yannis G** | Other agencies (including NSF) to which this proposal has been/will be submitted.

Support: [ ] Current [X] Pending [ ] Submission Planned in Near Future [ ] *Transfer of Support

Project Proposal Title: **Collaborative Research-Smoluchowski Equations: Analysis of Dynamics, Singularities and Statistics in Complex Fluid-Particle Mixtures**

Source of Support: **National Science Foundation**

Total Award Amount: $ **235,936.66** **Total Award Period Covered:** **07/01/05 - 06/30/08**

Location of Project: **Princeton University**

Person-Months Per Year Committed to the Project. **Cal: 0.00** **Acad: 0.00** **Sumr: 0.5**

Support: [ ] Current [X] Pending [ ] Submission Planned in Near Future [ ] *Transfer of Support

Project Proposal Title: **Multiscale Analysis of Dense Particulate Flows**

Source of Support: **Department of Energy**

Total Award Amount: $ **753,339** **Total Award Period Covered:** **10/01/2005 - 09/30/2008**

Location of Project: **Princeton University (S. Sundaresan, Co-PI)**

Person-Months Per Year Committed to the Project. **Cal: 0.00** **Acad: 0.00** **Sumr: 1.00**

Support: [ ] Current [X] Pending [ ] Submission Planned in Near Future [ ] *Transfer of Support

Project Proposal Title: **Predictive Multiscale Modeling of Materials for Performance Uncertainty Reduction**

Source of Support: **Department of Energy**

Total Award Amount: $ **780,000** **Total Award Period Covered:** **10/01/2005 - 09/30/2008**

Location of Project: **Princeton University (Emily Carter, Co-PI)**

Person-Months Per Year Committed to the Project. **Cal: 0.00** **Acad: 0.00** **Sumr: 1.00**

Current and Pending Support

Investigator: **Kevrekidis, Yannis G** | Other agencies (including NSF) to which this proposal has been/will be submitted.

Support: **Current** ☐ **Pending** ☐ **Submission Planned in Near Future** ☐ ***Transfer of Support**

Project Proposal Title:

Source of Support:

Total Award Amount: $ **Total Award Period Covered:**

Location of Project:

Person-Months Per Year Committed to the Project. **Cal:** **0.00** **Acad:** **0.00** **Sumr:** **0.00**

Support: **Current** ☐ **Pending** ☐ **Submission Planned in Near Future** ☐ ***Transfer of Support**

Project Proposal Title:

Source of Support:

Total Award Amount: $ **Total Award Period Covered:** **-**

Location of Project:

Person-Months Per Year Committed to the Project. **Cal:** **0.00** **Acad:** **0.00** **Sumr:** **0.00**

Current and Pending Support

PAUL FISCHER

Current Support

Project Name	Sponsor	FY05	Date	Effort
Applied Mathematics	DOE MICS	$2.7M	10/01/04- 09/30/05	60%
Terascale Simulation Tools and and Technologies Center	DOE MICS SciDAC	$351K	10/01/04- 09/30/05	20%
Computational Nanophotonics	DOE MICS	$400K	10/01/04- 09/30/05	10%
Biomechanical Mechanisms and Venous Intimal Hyperplasia	NIH (UofC)	$193K	02/01/03- 01/31/06	10%
3D Numerical Investigation of Density Currents	NSF	$100K	09/01/02- 08/31/05	12%
Collaborative Research: Large Large-Eddy Simulations of of Stratified Coastal Flows	NSF	$54K	07/01/05- 06/30/08	6%

Pending Support

Project Name	Sponsor	FY05	Date	Effort
A Multiscale Computational Framework for Dense Particulate Flows	DOE MICS	$730K	07/01/05- 06/30/08	25%
Understanding the LES Models through Sensitivity Analysis	DOE MICS	$600K	07/01/05- 06/30/08	10%
The Dynamics of Small Perturbations in Large Systems Driven Far-From-Equilibrium	DOE MICS	$625K	07/01/05- 06/30/08	10%
Laboratory Study of MHD Effects on Stability and Turbulence in Free-Surface Liquid Metal Flows	DOE OSC	$30K	07/01/05- 08/31/05	7%

Notes

1. Effort will be adjusted if the pending proposals are funded.
2. Unless otherwise noted, FY05 budget data is for the entire project.

Current and Pending Support

MIHAI ANITESCU

Current Support

Project Name	Sponsor	FY05	Date	Effort
Applied Mathematics	DOE MICS	$2.7M	10/01/04-09/30/05	100%

Pending Support

Project Name	Sponsor	FY05	Date	Effort
A Multiscale Computational Framework for Dense Particulate Flows	DOE MICS	$730K	07/01/05-06/30/08	15%
Multiscale Fusion Plasma Simulations	DOE MICS	$500K	07/01/05-06/30/08	15%
Multiscale Optimization in Materials Science via Density Theory	DOE MICS	$680K	07/01/05-06/30/08	25%

Notes

1. Effort will be adjusted if the pending proposals are funded.
2. Unless otherwise noted, FY05 budget data is for the entire project.

Current and Pending Support

GARY LEAF

Current Support

Project Name	Sponsor	FY04/05	Date	Effort
Applied Mathematics	DOE MICS	$177,000	10/01/04-09/30/05	100%

Role: PI

Pending Support

Project Name	Sponsor	FY04/05	Date	Effort
A Multiscale Computational Framework for Dense Particulate Flows	DOE MICS	$730K	07/01/05-06/30/08	15%

BARRY SMITH

Current Support

Project Name	Sponsor	FY05	Date	Effort
Applied Mathematics	DOE MICS	$2.7M	10/01/04- 09/30/05	50%
Terascale Optimal PDE Simulation Center	DOE MICS SciDAC	$884K	10/01/04- 09/30/05	50%

Pending Support

Project Name	Sponsor	FY05	Date	Effort
A Multiscale Computational Framework for Dense Particulate Flows	DOE MICS	$680K	07/01/05- 06/30/08	10%
Revisiting Fusion Plasma Simulations with Emerging Multiscale Paradigms	DOE MICS	$500K	07/01/05- 06/30/08	25%
Reactive Channelization in Large-Scale Solid Mantle Flow	DOE MICS	$450K	07/01/05- 06/30/08	10%

Notes

1. Effort will be adjusted if the pending proposals are funded.
2. Unless otherwise noted, FY05 budget data is for the entire project.

Current and Pending Support – Pannala, Sreekanth
Current:
(1) Organization or agency: DOE/Nuclear Energy
Title: Advanced Gas Reactor (AGR) Fuel Development and Qualification Program – CVD Process Model Development

1. **% Effort:** 20%
2. **Inclusive dates of the project:** Annual Renewal
3. **Annual Funding:** $ 300,000

(2) Organization or agency: DOE/Fossil Energy
Title: Computational Fluid Dynamics for Multiphase Flow

1. **% Effort:** 30%
2. **Inclusive dates of the project:** Annual Renewal
3. **Annual Funding:** $ 175,000

(3) Organization or agency: DOE/Energy Efficiency
Title: CLEERS Program coordination

1. **% Effort:** 10%
2. **Inclusive dates of the project:** Annual Renewal
3. **Annual Funding:** $ 190,000

(4) Organization or agency: DOE/ Energy Efficiency
Title: Microscale catalyst model, deactivation processes at materials microstructure level

1. **% Effort:** 10%
2. **Inclusive dates of the project:** Annual Renewal
3. **Annual Funding:** $ 85,000

Pending:
None.

Current and Pending Support

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.

Investigator: Sundaresan, Sankaran | Other agencies (including NSF) to which this proposal has been/will be submitted.

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: NIRT: Environmentally benign mixing of nanoparticles (in collaboration with NJIT, Auburn)

Source of Support: National Science Foundation

Total Award Amount: $ 300004.00 Total Award Period Covered: 07/01/05 – 06/30/08

Location of Project: Princeton University

Person-Months Per Year Committed to the Project. Cal: Acad: Sumr: 0.50

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: THIS PROPOSAL: Coarse-grained, equation-free, multi-scale simulation of large-scale granular and gas-particle flows (with Yannis Kevrekidis as co-PI)

Source of Support: National Science Foundation

Total Award Amount: $ 656758.00 Total Award Period Covered: 07/01/05 – 06/30/08

Location of Project: Princeton University

Person-Months Per Year Committed to the Project. Cal: Acad: Sumr: 1.00

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Compaction and dilation rate dependence of stresses in fluid-particle flows (collaborative research jointly with John Brady, CalTech)

Source of Support: National Science Foundation

Total Award Amount: $ 306397.00 Total Award Period Covered: 07/01/05 – 06/30/08

Location of Project: Princeton University

Person-Months Per Year Committed to the Project. Cal: Acad: Sumr: 1.00

*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.

USE ADDITIONAL SHEETS AS NECESSARY

Paul F. Fischer

Professional Preparation

B.S.	1981	Mechanical Engineering,	Cornell University	
M.S.	1982	Mechanical Engineering,	Stanford University	
Ph.D.	1989	Mechanical Engineering,	M.I.T.	Advisor: A. T. Patera
Postdoc	1990-1991	Applied Mathematics,	Caltech	Advisor: H. B. Keller

Professional Appointments

7/98-present	Mathematician, MCS Division, Argonne National Laboratory
9/00-present	Senior Fellow, Computational Institute, University of Chicago
4/03-present	Adjunct Faculty, Dept. of Mech. Eng., University of Illinois, Chicago
7/91-7/98	Assistant professor, Applied Mathematics, Brown University
6/93,8/94,8/95	Visiting Scientist, ICASE, NASA Langley
1/90-6/91	Post-doctoral Fellow, Applied Mathematics, Caltech
7/89-12/89	Post-doctoral Fellow, Fluid Mechanics Laboratory, M.I.T.
7/86-6/89	Research Assistant, Fluid Mechanics Laboratory, M.I.T.
4/83-7/86	Sr. Mechanical Engineer, Digital Equipment Corp., Shrewsbury, MA
4/82-12/82	Research Assistant, Stanford Univ./NASA Ames, Mountain View, CA

Honors

DOE INCITE Award, 2005.
Gordon Bell Prize for High-Performance Computing, 1999.
First Center for Research on Parallel Computation Prize Fellowship, Caltech, 90/91.

Ph.D. Thesis and Postdoctoral Advisees

G.W. Kruse (Brown); J.S. Mullen (Brown); H.M. Tufo (Brown); N.I. Miller (Brown); T. Iliescu (ANL); M.S. Min (ANL)

Publications

- 53 refereed articles.
- 5 publications relevant to the proposal:
  - M.O. Deville, P.F. Fischer, and E.H. Mund, *High-Order Methods for Incompressible Fluid Flow*, Cambridge University Press, 510 p. (2002).
  - J.W. Lottes and P.F. Fischer, "Hybrid Multigrid/Schwarz Algorithms for the Spectral Element Method," *J. Sci. Comp.*, accepted, (2004).
  - M. R. Paul, K-H. Chiam, M. C. Cross, and P. F. Fischer "Rayleigh-Benard Convection in Large-Aspect-Ratio Domains," *Phys. Rev. Let.* (accepted, 2004).
  - P.F. Fischer, G.W. Kruse, and F. Loth "Spectral element methods for transitional flows in complex geometries," *J. Sci. Comp.* **17** 1, pp. 81–98 (2002).
  - P.F. Fischer and J.S. Mullen, "Filter-based Stabilization of Spectral Element Methods" *Comptes Rendus de l'Académie des sciences Paris, t. 332, Série I - Analyse numérique*, p. 265–270 (2001).

- 5 other publications:
  - M. Greiner, P.F. Fischer, H.M. Tufo, and R.A. Wirtz, "Three Dimensional Simulations of Enhanced Heat Transfer in a Flat Passage Downstream from a Grooved Channel", *J. Heat Transfer.* **124** pp. 169-176 (2002).
  - H.M. Tufo and P.F. Fischer, "Fast Parallel Direct Solvers For Coarse Grid Problems," *J. Par. & Dist. Comput.*, 61 p. 151–177 (2001).
  - H. M. Tufo and P. F. Fischer, "Terascale Spectral Element Algorithms and Implementations" Gordon Bell Prize paper, *Proc. of the ACM/IEEE SC99 Conf. on High Performance Networking and Computing.* IEEE Computer Soc., CDROM (1999).
  - P. Fischer, "An overlapping Schwarz method for spectral element solution of the incompressible Navier-Stokes equations," *J. of Comp. Phys.* **133** 84–101 (1997).

– Fischer, P.F. and Patera, A.T., "Parallel Simulation of Viscous Incompressible Flows" *Ann. Rev. Fluid Mech.*, Vol 26, (1994) p.483–528.

Synergystic Activities

- With the help of several collaborators, I have made our Navier-Stokes code, Nek5000, freely available and supported at over a dozen institutions worldwide. In addition to providing a scalable high-order-accuracy simulation engine, the source distribution provides researchers with direct access to advanced parallel algorithms and implementations. Working with U. Chicago members of the Center for Magnetic Self Organization in Laboratory and Astrophysical Plasmas, we have recently extended Nek5000's capabilities to include incompressible MHD.
- I have advised 16 students at ANL over the last five years, and am currently advising one predoc and one postdoc. I am currently a thesis committee member for Ph.D. students at U. Toronto, Purdue, U. Illinois (Urbana-Champaign), and U. Illinois (Chicago).
- At Brown, I developed and taught graduate courses in parallel scientific computing, iterative methods, and computational fluid dynamics. In addition, I taught undergraduate courses in numerical analysis and scientific computing.
- Member of Editorial Board, SIAM J. Sci. Comp., 1998-2001; reviewer for J.Comp. Phys., SISC, J. Fluid Mech., J. Sci. Comp., SINUM.

Collaborators within the past 48 months

S. Balachandar (U. Ill., Urbana-Champaign), Michael Cross (Caltech), Fausto Cattaneo (U. Chicago), Jeffrey Duan (Ill. Inst. of Tech.), Frank Giraldo (NRL), Sigal Gottlieb (U. Mass.), Henry Greenside (Duke Univ.), Miles Greiner (U. Nevada), Traian Iliescu (V. Tech), Gary Leaf (Argonne), Frank Loth (U. Ill., Chicago), Misun Min (Argonne), Julie Mullen (Worcester Poly. Inst.), Tamay Ozgokmen (U. Miami), Mark Paul (V. Tech), Franco Preparata (Brown U.), Juan Restrepo (U. Arizona), Steve Thomas (NCAR), Henry Tufo (U. Colorado).

Mihai Anitescu

Mathematics and Computer Science Division
Argonne National Laboratory
Argonne, Illinois 60439

Phone: 630-252-4172
Fax: 630-252-5986
E-mail: anitescu@mcs.anl.gov

Professional Preparation

1992 - Engineer Diploma, Polytechnic University of Bucharest, Romania

1997 - Ph.D. University of Iowa

Appointments

Computer Scientist, Argonne National Laboratory, 2002 –

Adjunct Associate Professor, University of Pittsburgh, 2004 –

Editorial Board, Mathematical Programming, 2004 –

Software Editor, Optimization Methods and Software, 2004 –

Five Publications Closely Related to the Proposed Research

M. Anitescu. Optimization-based simulation of nonsmooth dynamics. Preprint ANL/MCSP1161-0504. To appear in Mathematical Programming.

M.Anitescu, F.A. Pahlevani, William J. Layton. Implicit for local effects and explicit for nonlocal effects is unconditionally stable. Preprint ANL/MCS-P1093-0903.Pdf Version. To appear in Electronic Transactions of Numerical Analysis.

M. Anitescu and G.D. Hart. A constraint-stabilized time-stepping approach for rigid multibody dynamics with joints, contact and friction. International Journal for Numerical Methods in Engineering, 60(14), 2335-2371, 2004.

M. Anitescu and G.D. Hart. A Fixed-Point Iteration Approach for Multibody Dynamics with Contact and Small Friction. Mathematical Programming, 101(1), 3–32. 2004.

M. Anitescu and Florian A. Potra Time-Stepping Schemes for Stiff Multi-Rigid-Body Dynamics with Contact and Friction. International Journal for Numerical Methods in Engineering, 55 (2002), 753–784

Five Other Publications Related to the Proposed Research

M. Anitescu On Solving Mathematical Programs with Complementarity Constraints as Nonlinear Programs. Preprint ANL/MCS-P864-1200. To appear in SIAM Journal of Optimization.

M Anitescu. Global Convergence of an Elastic Mode Approach for A Class of Mathematical Programs with Complementarity Constraints. Preprint ANL/MCS-P1143-0404. To appear in SIAM Journal of Optimization.

M. Anitescu. A Superlinearly Convergent Sequential Quadratically Constrained Quadratic Programming Algorithm for Degenerate Nonlinear Programming, SIAM Journal of Optimization 12 (2002), 949-978.

M. Anitescu. On the rate of convergence of Sequential Quadratic Programming with nondifferentiable exact penalty function in the presence of constraint degeneracy. Mathematical Programming, 92 (2002), 359-386

M. Anitescu. Degenerate Nonlinear Programming with a Quadratic Growth Condition. SIAM Journal on Optimization 10 (4) : 1116-1135, 2000.

Prizes and Awards

Silver Medal, International Mathematical Olympiad, 1986.

Wilkinson Fellow, Argonne National Laboratory, 1997.

Mentoring.

Co-advisor (at the University of Pittsburgh with William J Layton) for Faranak Pahlevani, Ph.D 2004. Currently Postdoctoral Fellow at Montana State University.

Advisor (at the University of Pittsburgh) of Gary D. Hart, Ph.D 2005 (expected).

Dan Negrut, Postdoctoral Fellow, Argonne National Laboratory. 2004-

Collaborators

Bogdan Gavrea (University of Maryland, Baltimore County) Gary D. Hart (University of Pittsburgh), William J. Layton (University of Pittsburgh), Pierre Moulin (University of Illinois), Dan Negrut (Argonne National Laboratory), Faranak Pahlevani (Montana State), Florian Potra (University of Maryland, Baltimore County), Kannan Ramchandran (Berkeley), David Stewart (University of Iowa), Paul Tseng, (University of Washington), Jeff Trinkle, (Rensselaer Polytechnic Institute), Stephen J. Wright (University of Wisconsin),

Gary K. Leaf

Professional Preparation

1961 University of Illinois, Ph.D., Mathematics

Appointments

1963–present	Mathematician, Argonne National Laboratory
1961–1963	Post Graduate National Science Foundation Fellow University of Chicago, Mathematics Department

Selected Publications

1. Thompson, C. P., G. K. Leaf, and J. Van Rosendale, "A Dynamically Adaptive Multigrid Algorithm for the Incompressible Navier-Stokes Equations–Validation and Model Problems," Applied Numerical Mathematics 9 (1992) 511-53
2. Bayliss, A., G. K. Leaf, and B. J. Matkowsky, "Pulsating and Chaotic Dynamics near the Extinction Limit," Combust. Sci. and Tech. 84 (1992), 253-27
3. Kaper, H. G., G. K. Leaf, D. M. Levine, and V. Vinokur, "Glassy Motion of an Elastic String," Phys. Rev. Lett. 71(22) (November 1993), 3713-371
4. Restrepo, J. M., and G. K. Leaf, "Wavelet-Galerkin Distetization of Hyperbolic Equations," J. of Computational Physics 122 (November 1995) 118-128
5. Gropp, W. D., H. G. Kaper, G. K. Leaf, D. M. Levine, M. Palumbo, and V. M. Vinokur, "Numerical Simulation of Vortex Dynamics in Type-II Superconductors," J. Computational Physics 123 (1996) 54-266
6. Braun, D. W., G. W. Crabtree, H. G. Kaper, A. E. Koshelev, G. K. Leaf, D. M. Levine, and V. M. Vinokur, "The Structure of a Moving Vortex Lattice," Phys. Rev. Lett. 76 (1996), pp. 831-834
7. Restrepo, J. M. and G. K. Leaf "Inner Product Computations Using Periodized Daubechies Wavelets," International J. for Numerical Methods in Engineering 40 (1997), pp. 3557-3578
8. Restrepo, J. M., G. K. Leaf, and A. Griewank, "Circumventing Storage Limitations in Variational Data Assimilation," J. of Scientific Computing 19 (1998), pp. 1586-1605
9. Jiang, J. S., S. D. Bader, H. G. Kaper, G. K. Leaf, et al., "Rotational Hysteresis of Exchange-Spring Magnets," J. Phys. D, Applied Physics, v35, p. 2339 (2002)
10. Leaf, G. K., S. Obukhov, S. Scheidl, V. M. Vinokur, "Transient Dynamics of Pinning of Domain Wall, J. Magnetism and Magnetic Materials, v. 241, p. 118 (2002)
11. Grimsditch, M., G. K. Leaf, H. G. Kaper, D. A. Karpeev, R. E. Camley, "Normal Modes of Spin Excitation in Magnetic Nanoparticles," Phys. Rev. B, v. 69 (2004)
12. Grimsditch, M., L. Giovannini, F. Montoncello, F. Nizzoli, G. K. Leaf, H. G. Kaper, "Normal Modes in Ferromagnetic Nanoparticles: A Dynamical Matrix Approach," Phys. Rev. B, v. 70 (2004)
13. Grimsditch, M., L. Giovannini, F. Montoncello, F. Nizzoli, G. K. Leaf, H. G. Kaper, D. A. Karpeev "Magnetic Normal Modes in Nano-particles," Physica B, v. 354, p. 266 (2004)

Collaborators in past 48 months

I. S. Aronson (Argonne), R. Camley (U Colorado, Colorado Springs), P. Fischer (Argonne), A. Griewank (TU Dresden), M. Grimsditch (Argonne), J. S. Jiang (Argonne), H. G. Kaper (Argonne), D. Karpeev (Argonne), M. Knepley (Argonne) J. M. Restrepo (U Arizona), B. Smith (Argonne), V. M. Vinokur (Argonne)

Barry Smith

Mathematics and Computer Science Division
Argonne National Laboratory
Argonne, Illinois 60439

Phone: 630-252-9174
Fax: 630-252-5986
E-mail: bsmith@mcs.anl.gov

Professional Preparation

1986 - B.S. Mathematics, Yale University.

1990 - Ph. D. Mathematics, Courant Institue, New York University.

Appointment

Scientist, Argonne National Laboratory, 1995 –

Honors

First Prize, Student Paper Competition, Copper Mountain Conference on Iterative Methods, April 1990.

Second Prize, Fifth Leslie Fox Prize Meeting, June 1991, international prize in numerical analysis offered every two years.

Co-winner, 1993 Householder Prize for best dissertation in numerical linear algebra during the previous three years.

SC'99 Gordon Bell prize in the special category for the paper Achieving High Sustained Performance on an Unstructure Mesh CFD Application, by Kyle Anderson, William Gropp, Dinesh Kaushik, David Keyes and Barry Smith.

Publications Related to the Proposed Research

Developing a Geodynamics Simulation with PETSc, Richard Katz, Matthew Knepley, and Barry Smith to appear in the book: **Numerical Solution of Partial Differential Equations on Parallel Computers**, A. M. Bruaset, P. Bjorstad, and A. Tveito, editors, Springer-Verlag.

S. Balay, L. Curfman McInnes, W. Gropp, and B. Smith, *PETSc 2.0 Users Manual*, Argonne National Laboratory Report, 2005.

B. Norris, S. Balay, S. Benson, L. Freitag, P. Hovland, L. McInnes and B. Smith, *Parallel Components for PDEs and Optimization: Some Issues and Experiences*, **Parallel Computing**, 28 (12) (2002) pp. 1811-1831.

W. L. Wan, T. Chan, and B. Smith, *An Energy-minimizing Interpolation for Robust Multigrid Methods*, **SIAM Journal on Scientific Computation**, Vol. 21, No. 4, pp. 1632–1649.

B. Smith, W. Gropp and P. Björstad **Domain Decomposition: Parallel Multilevel Methods for Elliptic Partial Differential Equations**, Cambridge University Press, 1996.

L. A. Freitag, W. D. Gropp, P. D. Hovland, L. C. McInnes, and B. F. Smith, *Infrastructure and Interfaces for Large-Scale Numerical Software*, **Proceedings of the 1999 Conference on Parallel and Distributed Processing Techniques and Applications (PDPTA'99)**, 1999.

T. Chan, B. Smith, and J. Zou, *Overlapping Schwarz Methods on Unstructured Meshes using Non-matching Coarse Grids*. **Numer. Math.**, Vol. 73, pp. 149–167, 1996.

Synergistic Activities

PETSc (Portable, Extensible Toolkit for Scientific computation) (www.mcs.anl.gov/petsc) is the most widely used scalable package for the solution of algebraic equations arising from the discretization of partial differential equations. The main design goals are usability, portability, performance and scalable parallelism. This has been achieved by determining abstract commonalities in the mathematical algorithms and using these to systematically seperate the various concerns of the implementations, this allows dramatic amounts of code reuse.

Collaborators

Paul Hovland (Argonne), David Keyes (Columbia), Mathew Knepley (Argonne), Lois McInnes (Argonne), Boyana Norris (Argonne), Marc Speiglman (Argonne) Xianzhu Tang (LANL)

Sreekanth Pannala

Research Staff Member
Computational Mathematics Group
Computer Science and Mathematics Division
Oak Ridge National Laboratory
(865) 691-0684
pannalas@ornl.gov
http://www.csm.ornl.gov/∼pannala

Education:

- Ph.D. in Aerospace Engineering, Georgia Institute of Technology, Atlanta, Georgia (May 2000), [On Large-eddy Simulations (LES) of Reacting Two-phase Flows]
- M.S. in Aerospace Engineering, Georgia Institute of Technology, Atlanta, Georgia (Dec. 1994), [Emphasis in CFD and Turbulence]
- B.Tech (Hons.) in Aerospace Engineering, Indian Institute of Technology, Kharagpur, India (Aug. 1993)

Research and Professional Experience:
Research Staff Member, Computational Mathematics Group, Computer Science and Mathematics Division, Oak Ridge National Laboratory (June 2001 - Present)
Post Graduate/Doctoral Research Fellow, Computer Science and Mathematics Division, ORAU/Oak Ridge National Laboratory (Mar. 1999 –May 2001)

- Loosely coupled multiscale model for simulating carbon nanotubes
- Modeling of spouted bed CVD coaters for fuel particles for advanced nuclear reactors
- Parallel multi-phase DNS and LES modeling for dense fluidized beds for applications in Chemical and Fossil industries
- Thermal radiation model for automotive applications
- Models for emission reduction components in diesel engines
- Reduced order models for simulating fludized beds

Graduate Research Assistant, Georgia Institute of Technology (Sept. 1993 – Mar. 1999)

1. Research was part of MURI (Army's Multi-Disciplinary University Research Initiative) for Intelligent Turbine Engines in developing parallel two-phase LES solvers with lagrangian droplet tracking using MPI and was a DoD HPCMO grand challenge project.

Professional Societies:
1996 ASME
1996 AIAA
2001 AIChE
2003 SIAM
2003 ACM
Publications:

- Over 30 publications (journal, conference proceedings and reports) in the fields of computational fluid dynamics of multiphase flows, high performance computing, multiscale modeling of growth of carbon nano-tubes and lower order dynamical models for fluidized beds.
- Recent Relevant Publications/Presentations:

"Pressure Based Methods for Two-Fluid Models," with A. Prosperetti and S. Sundaresan, Book chapter in Computational Methods for Multiphase Flows; Editors: A. Prosperetti and G. Tryggvason; Publisher: Cambridge University Press. (*Under Review*)
"Dynamic Interacting Bubble Simulation (DIBS): An Agent-Based Bubble Model for Reacting Fluidized Beds," with C. S. Daw and J. S. Halow, Special issue of CHAOS on "Nonlinear dynamics in spatially extended mechanical systems," CHAOS, Vol. 14(2), 2004.
"Multiscale Simulations of Carbon Nanotube Nucleation and Growth: Mesoscopic Continuum Calculations," with R. F. Wood, Special issue on SWNT Growth Mechanisms, J. Nanosci. Nanotech. 2004, Vol. 4(4), 2004.
"Monte Carlo Method for LNT Aging," with W. A. Shelton and C. S. Daw, Poster at 7th CLEERS workshop, Detroit Diesel, Detroit, June 16-17, 2004.

“Coated Particle Fuel for Advanced Gas Reactors,” R. Lowden, J. Hunn, J. McLaughlin, J. Kelly, C. S. Daw, S. Pannala, and C. E. A. Finney, Annual Meeting of the American Ceramic Society, Indianapolis, Indiana, April 21, 2004

“Simulations of Reacting Fluidized Beds Using an Agent-Based Bubble Model,” with C. S. Daw, and J. Halow, International Journal of Chemical Reactor Engineering, Vol. 1: A20, 2003. http://www.bepress.com/ijcre/vol1/A20

“Multiscale Studies of Catalyst-Assisted Carbon Nanotube Growth,” with J. C. Wells, B. Sumpter, Q. M. Zhang, J. Z. Zhang, and R. F. Wood, Artificially Structured Nanomaterials: Formation and Properties, Gatlinburg, TN, USA, October 10-13, 2003.

Yannis G. Kevrekidis
Address: Department of Chemical Engineering and PACM,
Olden St., Princeton University, Princeton, NJ 08544, USA
Telephone: (609) 258-2818, Fax:(609) 258-0211
E-mail: yannis@arnold.princeton.edu

Areas of Research Interest:
Nonlinear Dynamics of Physicochemical and Engineering Systems, Instability and Pattern Formation in PDEs, Numerical Bifurcation Theory, Numerical Methods for PDEs, System Identification and Adaptive Control, Model Reduction for Distributed Systems, Multiscale Computation.

Education:
1986 Ph.D. in Chemical Engineering, University of Minnesota, Mplis.
1986 M.A. in Mathematics, University of Minnesota, Mplis

Professional Experience:
1986–present Chemical Engineering, Princeton (Professor: 1994)
1987–present Program in Applied and Computational Mathematics, (Senior Faculty: 1993)
2002—present Mathematics (Associated Faculty)

Honors and Awards:
2005 Guggenheim Fellow
2003 J. D. Crawford Prize, SIAM / Dynamical Systems
2002 O. A. Hougen Visiting Professorship, U. of Wisconsin
1998 Alexander von Humboldt Senior Research Prize
1996 Bodossakis Foundation Award in the Applied Sciences
1994 American Institute of Chemical Engineers, Allan P. Colburn Award
1994 Stanislaw Ulam Visiting Scholarship, Center for Nonlinear Studies, Los Alamos National Lab.
1989 National Science Foundation, Presidential Young Investigator Award
1988 David and Lucile Packard Foundation, Fellowship in Science and Engineering
1999 SEAS Distinguished Teaching Award, Princeton University

Professional: Associate Editor / Editorial Board
Multiscale Modeling and Simulation (SIAM); SIAM Journal on Applied Mathematics; SIAM Journal on Numerical Analysis; Journal of Nonlinear Science (Springer Verlag); Chaos (APS); Chemical Engineering Science (Elsevier); Journal of Nonlinear Science (Springer Verlag); International Journal of Bifurcations and Chaos in Applied Sciences and Engineering (World Scientific), Reviews in Chemical Engineering (Freund);

5 Closely Related Publications:
"Coarse" stability and bifurcation analysis using time-steppers, *PNAS* **97** pp.9840-9843 (2000) with C. Theodoropoulos and Y.-H. Qian
Coarse Integration/Bifurcation Analysis via Microscopic Simulators: micro-Galerkin methods, C. W. Gear, I.G.K and C. Theodoropoulos, *Comp. Chem. Engng.* **26** pp.941-963 (2002)
Coarse bifurcation analysis of kinetic Monte Carlo simulations: a lattice gas model with lateral interactions, A. G. Makeev, D. Maroudas, A. Z. Panagiotopoulos and I.G.K., J. Chem. Phys. **117**(18) pp.8229-8240 (2002)
Coarse molecular dynamics of a peptide fragment: free energy, kinetics and long time dynamics computations, G. Hummer and I.G.Kevrekidis, J. Chem. Phys. **118**(23) pp. 10762-10773 (2003)
Equation-free coarse-grained multiscale computation: enabling microscopic simulators to perform systemlevel tasks", with C. W. Gear, J. M. Hyman, P. G. Kevrekidis, O. Runborg and K. Theodoropoulos, Comm. Math. Sciences **1** pp.715-762 (2003)

5 Other Significant Publications:
Coarse Bifurcation Studies of Bubble Flow Lattice Boltzmann Simulations, with C. Theodoropoulos, K. Sankaranarayanan and S. Sundaresan, *Chem.Eng.Sci.*, **59** pp.2357-2362 (2004).
Analysis of Drag and Virtual Mass Forces in Bubbly Suspensions using an Implicit Formulation of the LBM, with K. Sankaranarayanan, X. Shan and S. Sundaresan, *J. Fluid Mech.* **452** pp.61-96 (2002)
On the computation of inertial manifolds, *Physics Letters A* **131** 433-436 (1991), with C. Foias, M. S. Jolly, G. R. Sell and E. S. Titi
An equation-free, multiscale computational approach to uncertainty quantification for dynamical systems, D. Xiu, R. Ghanem and I. G. Kevrekidis, *IEEE CiSE* in press, (2005)
Equation-free: the computer-assisted analysis of complex, multiscale systems, with C. W. Gear and G. Hummer, *A.I.Ch.E Journal*, **50**(7), pp.1346-1354 (2004)

Ph.D. Students:
H. S. Brown (Simulation Sciences, CA), M. A. Taylor (Salomon Brothers, NY), C. E. Frouzakis (ETH, Zuerich, Switzerland), R. Rico-Martinez (Tech Celaya, Celaya, Mexico), B. Glasser (Rutgers U., NJ), A. K. Bangia (Oliver Wyman, NY), J. Anderson (ExxonMobil, NJ), M. Johnson (Entelos Inc., CA), E. Achilleos (Hyperion Inc., Cyprus), S. Shvartsman (Princeton,NJ), J. Krishnan (ISR, U Maryland, MD), X. Li (Merck).

Post Doctoral Research Associates Supervised:
R. A. Adomaitis (U. Maryland, MD), M. S. Jolly (Indiana U. IN), A. E. Deane (NASA Goddard), D. Barkley (U. Warwick, England), K. Krischer (FHI, Berlin), M. Graham (U. Wisconsin, WI), M. Baer (MPI, Dresden, Germany), N. Gicquel (Citroen, Paris, France), A. Bergeon (U. Toulouse, Toulouse, France), G. Flaetgen (FHI, Berlin, Germany), A. Armaou (Penn State U., PA)), Olof Runborg (KTH, Stockholm), C. Siettos (NTU, Athens)

Graduate and Postgraduate Advisors:
Regents' Professors R. Aris and L. D. Schmidt, Ph.D. Advisors; Professors R. P. McGehee and D. Aronson, MA advisors in Math. (U. of Minnesota)

Recent Collaborators:
E. Titi (UC Irvine), S. Sundaresan (Princeton), B. B. Peckham (U. Minn. Duluth), M. S. Jolly (Indiana U., Bloomington), T. Mountziares (SUNY Buffalo), S. Pavlou (U. Patras, Greece), G. Karniadakis (Brown U.), A. Smits (Princeton), G. Ertl and H.-H. Rotermund (FHI, Berlin, Germany), R. Imbihl U. Hannover, Germany), J. L. Hudson (U. Virginia), P. Kolodner (Lucent, NJ), C. Jacobson and A. Khibnik (UTRC, CT). K. Christodoulou (Avery, Pasadena, CA), Y.-H. Qian (Exa, MA), P. Constantin (Chicago), K. Lust (Leuven, Belgium), C. William Gear (NEC, Princeton), D. Maroudas (U. Mass, Amherst), P.G. Kevrekidis (Umass, Amherst), G. Hummer (NIDDK, NIH), S. Setayeshgar (Princeton), H. Othmer (U. of Minnesota). D. Kessler (Bar-Ilan) S. Levin (Princeton), G. Samaey (Leuven, Belgium), C. T. Kelley (NC State, USA), N. Kazantzis (WPI, USA), M. D. Graham (Madison, USA), C. Siettos (NTU, Greece), C. Rowley (Princeton, USA), J. Marsden (Caltech, USA), P. Holmes (Princeton, USA), A. Stuart (Warwick), R. Coifman (Yale, USA)

Sankaran Sundaresan

Department of Chemical Engineering,
Princeton University,
Princeton, NJ 08544
(609) 258-4583 (Tel) (609) 258-0211 (fax)

Education:
B. Tech., Chemical Engineering, Indian Institute of Tech., Madras, India, 1976.
M.S., Chemical Engineering, University of Houston, Houston, Texas, 1978.
Ph.D., Chemical Engineering, University of Houston, Houston, Texas, 1980.

Employment:
1980 - 1987 Assistant Professor of Chemical Engineering, Princeton University
1987 - 1992 Associate Professor of Chemical Engineering, Princeton University
Summer 1981 Research Engineer, E. I. DuPont de Nemours and Co., Inc. Exp. Station, Wilmington, DE.
1988 - 1989 Visiting Assoc. Professor, Materials Sci. and Engg., University of Washington, Seattle, WA.
1989 - 1995 Departmental Representative, Chemical Engineering, Princeton University
Summer 1990 Visiting Scientist, Mobil Research & Development Corporation, Paulsboro, NJ
1992 - Professor of Chemical Engineering, Princeton University
1997 - 2003 Associate Dean for Academic Affairs, School of Engineering & Applied Science, Princeton University

Courses Taught at Princeton:
Chemical Engineering Analysis Topics in Transport Phenomena
Introduction to Chemical Engineering Advanced Process Control
Chemical Engineering Laboratory Kinetics and Reactor Design
Fluid Mechanics Applied Mathematics
Kinetics and Reactor Design Fluid Mechanics
Chemical Process Control Mechanics of Granular Mat. &
Environmental Technology Two-phase Flows
Mass, Momentum and Energy Transport Introduction to Ceramics

Name of graduate advisor:Neal R. Amundson, MS and PhD advisor, 1976-80.

Names of graduate and post-graduate advisees:
K. R. Kaza, post-doctoral fellow, 1982-83; T. R. Reilly, M.S. student, 1985; J. S. Buchanan, Ph.D., 1986; G. Christensen, M.S., 1986; V. A. Burrows, Ph.D., 1986; J. K. Wong, Ph.D., 1986; E. M. Breckner, Ph.D., 1986; I. S. Metcalfe, Ph.D., 1987; N. A. Collins, Ph.D., 1988; E. W. Arnold, III, Ph.D., 1989; D.C. Dankworth, Ph.D., 1991; C. Gerardin, post-doctoral fellow, 1991-93; H. S. Brown, post-doctoral fellow, 1991-93; K. G. Anderson, Ph.D., 1995; V. V. Guliants, Ph.D., 1995; C.-Hwa Wang, Ph.D., 1996; S. Dasgupta, Ph.D., 1997; B. J. Glasser, Ph.D., 1997; M. F. Simpson, Ph.D., 1997; A. W. Akhras, Ph.D., 1998; K. Agrawal, Ph.D., 2000; A. Srivastava, Ph.D., 2002; P. Loezos, Ph.D., 2002; K. Sankaranarayanan, Ph.D., 2002; M. Al-Adel, M.S., 2002; B. Muite, M.S., 2003. A. Ten Cate, post-doctoral fellow, 2002-04;
Other Collaborators:ExxonMobil: J. A. Pita, Muralidhar, F. J. Krambeck, G. Jersey;
Princeton University Colleagues: R. Jackson, I. A. Aksay, I. G. Kevrekidis, J. B. Benziger and J. Wei;
New Jersey Institute of Technology: R. Pfeffer, R. Dave; PSRI, Inc.: S. Reddy Karri, T. M. Knowlton;
Fluent: M. Syamlal; US DOE: T. O'Brien (NETL), S. Pannala (Oak Ridge); Others: P. Nott (IISc, India), K. K. Rao (IIsc, India), M. Alam (IISc, India), J. Derksen (Delft), J. F. Brady (CalTech),

Editorial Activities
Associate Editor, *AIChE Journal,* responsible for papers on Particle Technology, Fluidization, Fluid Mechanics and Transport Phenomena.(2002 −−).
Associate Editor, *Chemical EngineeringJournal.* (1995 −−1999).
Editorial Board: *Powder Technology* (2003 –); Internal Journal of Multiphase Flow (2004 –) *Industrial & Engineering Chemistry Research* (2002 –);

Publications:Author or co-author of 105 publications, 200 conference presentations and 4 patents.

5 Selected Publications most closely related to the Proposed Project:

S. Sundaresan, "Instabilities in Fluidized Suspensions", *Annu. Rev. Fluid Mech.*, **35**, 63 – 88 (2003).
B. Glasser, I. G. Kevrekidis and S. Sundaresan, "One- and Two-dimensional Traveling Wave Solutions in Gas-Fluidized Beds", *J. Fluid Mech.* **306**, 183-221 (1996).
B. J. Glasser, I. G. Kevrekidis and S. Sundaresan, "Fully-developed Travelling Wave Solutions and Bubble Formation in Fluidized Beds", *J. Fluid Mech.* **334**, 157-188 (1997).
B. J. Glasser, S. Sundaresan and I. G. Kevrekidis, "From Bubbles to Clusters in Fluidized Beds", *Phys. Rev. Let.* **81** (9), 1849-1852 (1998).
K. Sankaranarayanan, X. Shan, I. G. Kevrekidis & S. Sundaresan, "Analysis of Drag and Virtual Mass Forces in Bubbly Suspensions using an Implicit Formulation of the Lattice Boltzmann Method", *J. Fluid Mech.,* **452**, 61 – 96 (2002).

5 Other Selected Significant Publications:

A. Srivastava, K. Agrawal, S. Sundaresan, S. B. Reddy Karri and T. M. Knowlton, "Dynamics of gas-particle flow in circulating fluidized beds", *Powder Tech.*, **100**, 173-182 (1998).
P. R. Nott, M. Alam, K. Agrawal, R. Jackson and S. Sundaresan, "The Effect of Boundaries on the Plane Couette Flow of Granular Materials: A Bifurcation Analysis", *J. Fluid Mech.* **397**, 203-229 (1999).
P. N. Loezos, P. Costamagna & S. Sundaresan, "The role of contact stresses and wall friction on fluidization", *Chem. Eng. Sci.*, **57**, 5123 – 5141 (2002).
S. Sundaresan, J. Eaton, D. L. Koch & J. M. Ottino, "Report of Study Group on Disperse Flows", *Int. J. Multiphase Flow* **29**, 1069 – 1087 (2003).
K. Agrawal, P. N. Loezos, M. Syamlal and S. Sundaresan, "The Role of Meso-scale Structures in Rapid Gassolid Flows", *J. Fluid Mech.,* **445**, 151 – 185 (2001).

Recent Awards

Richard H. Wilhelm Award in Chemical Reaction Engineering, American Institute of Chemical Engineers, 1999.
Distinguished Alumnus Award, Indian Institute of Technology-Madras, Chennai, India, 2000.

Facilities and Resources

Personnel associated with this proposal will have access to facilities at Argonne National Laboratory, and in particular to facilities associated with the Mathematics and Computer Science Division at Argonne.

Argonne National Laboratory has computing and networking facilities located in the Mathematics and Computer Science Division. These resources include major parallel computing clusters, visualization systems, advanced display environments, collaborative environments, and high-capacity network links.

As one of the five participants in the NSF's Distributed Terascale Facility, Argonne operates the TeraGrid's visualization facility. The entire TeraGrid is a 13.6 TF grid of distributed clusters using Intel McKinley processors with over 6 TB of memory and greater than 600 TB of disk space. The full machine is distributed between NCSA, SDSC, Caltech, the Pittsburgh Computer Center, and Argonne. The individual clusters are connected by a dedicated 40 Gb/s link that acts as the backbone for the machine. The Argonne component of the machine consists of 16 dual IA-64 nodes for computation, a 96 dual Pentium IV nodes with G Force Ti 4600 graphics accelerators for visualization, and 20 TB of storage.

Argonne also is a participant in the I-WIRE project, which links to the TeraGrid and StarLight, as well as linking facilities at Argonne to various research institutions in Illinois.

A second supercomputer at Argonne, which is available to researchers for production computing, is "Jazz." This Linux system, which has achieved a sustained teraflop, ranks among the 50 fastest computers in the world. Jazz has 350 compute nodes, each with a 2.4 GHz Pentium Xeon with 1.5 GB of RAM. The cluster uses Myrinet 2000 and Ethernet for interconnect and has 20 TB of on-line storage in PVFS and GFS file systems. In addition, Argonne has a cluster dedicated for computer science and open source development called "Chiba City." Chiba City has 512 Pentium-III 550MHz CPUs for computation, 32 Pentium-III 550 CPUs for visualization and 8 TB of disk. Chiba City is unique testbed that is principally used for system software development and testing

Argonne's most recent addition to its supercomputing facilities is a one-rack IBM Blue Gene/Light. The system includes a 2048-processor compute node with a peak performance of 5.7 teraflops.

Argonne has substantial visualization devices as well, each of which can be driven by the TeraGrid visualization cluster, by Chiba City, or by a number of smaller dedicated clusters. These devices include a 4-wall CAVE, the ActiveMural (an 11 million pixel large-format tiled display), and several smaller tiled displays such as the portable MicroMural, which has 3 million pixels.

Furthermore, Argonne currently supports numerous Access Grid nodes, ranging from AG nodes in continual daily use to AG2 development nodes.

The Center for Computational Sciences (CCS) at ORNL provides state-of-the-art resources for high performance computational science and computing science research (projects). The CCS offers storage resources as well as computing, networking and visualization resources. Primary CCS machines include:

- Phoenix: a Cray X1, with 512 multi-streaming vector processors and 2 TB of globally addressable memory.
- Ram: a 256-processor SGI Altix with 2 TB of shared memory. Each processor is a 1.5 GHz Intel Itanium2.
- Cheetah: a 27-node IBM p690 system, where each node has thirty-two 1.3 GHz Power4 processors. Most of the nodes have 32 GB of memory, but five of the nodes have 64 GB of memory, and two have 128 GB of memory.
- Eagle: a 184-node IBM RS/6000 SP, 176 "thin" nodes have four 375 MHz Power3-II processors and 2GB of memory while 8 "wide" nodes have two 375 MHz Power3-II processors and 2GB of memory.

More information of CCS is available at http://www.ccs.ornl.gov/user/computers.html. DOE Leadership-Class computing capability for science will be developed at Oak Ridge National Laboratory and more details are available at http://www.ccs.ornl.gov.

ARGONNE NATIONAL LABORATORY

Mathematics and Computer Science Division

9700 South Cass Avenue, Argonne, Illinois 60439-4844

Phone: +1 (630) 252-4172
Fax: +1 (630) 252-5986
email: anitescu@mcs.anl.gov
March 26, 2005

Dr. Paul Fischer,
Mathematics and Computer Science Division,
Argonne National Laboratory
9700 S Cass Avenue,
Argonne, IL 60439

Dear Paul,

I am delighted to write this letter confirming my participation for the proposed MICS multiscale project "A Multiscale Computational Framework for Dense Particulate Flow". As a participant in this project, I will work closely with yourself and the PI group in order to ensure the successfull development of the proposal. I will personally devote 15 % of my time to this project.

My role will be to help setting up the extensions of the equation free approach for the hard particle simulations, help developing the multiscale framework and the needed analytical and methodological investigations and determining appropriate computational solutions for the relevant optimization problems in stochastic media reconstruction and estimation.

Mihai Anitescu, Computer Scientist

U.S. Department of Energy The University of Chicago

ARGONNE NATIONAL LABORATORY
Mathematics and Computer Science Division
9700 South Cass Avenue, Argonne, Illinois 60439

Telephone: 630-252-7241
Fax: 630-252-5986
E-mail: leaf@mcs.anl.gov

March 24, 2005

Dr. Paul Fischer
Building 221, Room D-248
Mathematics and Computer Science Division
Argonne National Laboratory
9700 S. Cass Avenue
Argonne, IL 60439

Dear Paul,

I am happy to collaborate with you on the proposed project *A Multiscale Computational Framework for Dense Particulate Flows*. This work will build upon our studies of flow and heat transfer in packed beds. I look forward to extending our preliminary study through simulations with increased domain sizes, with increased Reynolds numbers, and with macroscale coupling.

Sincerely,

Gary K. Leaf

ARGONNE NATIONAL LABORATORY

Mathematics and Computer Science Division
9700 South Cass Avenue, Argonne, Illinois 60439-4844

Telephone: (630) 252-9174
Faxphone: (630) 252-5986
Email: bsmith@mcs.anl.gov

March 23, 2005

Dear Paul,

It is my pleasure to collaborate with you on the proposal: A Multiscale Computational Framework for Dense Particulate Flows. As you know, my expertise is in numerical algorithms and their implementation in software. I expect to play a major role in designing and helping to implement the algorithms we develop in the course of the research. We will, fortunately, be able to leverage parts of the ANL PETSc package for much of the software.

In addition, I anticpate playing an active role in the education component of the project, through the development of course material and hosting of Ph.D. students involved in the research.

Sincerely,

Barry Smith

OAK RIDGE NATIONAL LABORATORY

MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

Sreekanth Pannala, Ph. D.
MS 6367, Bldg. 6012
P.O. Box 2008
Oak Ridge, TN 37831-2008
(865) 574-3129

March 18, 2005

To:
Paul F. Fischer
Building 221, Room D-248
Mathematics and Computer Science Division
Argonne National Laboratory
9700 S. Cass Avenue
Argonne, IL 60439

Dear Paul,

I look forward to collaborating with you and your colleagues on the proposed project "A multiscale Computational Framework for Dense Particulate Flows."

I anticipate broad collaboration in the project, with specific attention to extension of the multiscale framework to soft particles simulated through Discrete Element Method (DEM), inclusion of boundary effects into the multiscale framework and alternate forms of expression of contact forces to reduce computational expense within DEM methodology.

In addition, I anticipate playing an active role in the education component of the project, through training of Ph.D. students involved in the research at the Joint Institute of Computational Science (JICS). JICS is a joint institute between University of Tennessee at Knoxville (UTK) and ORNL.

Sincerely,

(Sreekanth Pannala)

Princeton University

Sankaran Sundaresan
Professor of Chemical Engineering

Chemical Engineering Department
A 315 Engineering Quadrangle
Princeton NJ 08544
Telephone: 609-258-4583
Department FAX: 609-258-0211
EMAIL: sundar@princeton.edu

March 18, 2005

Paul F. Fischer
Building 221, Room D-248
Mathematics and Computer Science Division
Argonne National Laboratory
9700 S. Cass Avenue
Argonne, IL 60439

Dear Paul,

I look forward to collaborating with you and your colleagues on the proposed project "A Multiscale Computational Framework for Dense Particulate Flows."

As a participant in this project, I will work closely with Argonne to ensure an effective collaboration for developing the equations-free approach for dense particulate flow. I will personally devote 15% percent of my effort during the academic year and 40% of my effort during the summer month for the project.

My role on this project will be to: (a) assist with the soft-particle DEM simulations both with and without interstitial gas effects, (b) help develop appropriate lifting and restriction algorithms that are integral parts of the coarse-grained equations-free, multi-scale approach, (c) physically interpret the results obtained in the model problems examined in the project, and (d) identify and extract closures for the coarse-grained equations, wherever appropriate.

Professor Kevrekidis (Princeton) and I have worked together effectively for the past 18 years; we will coordinate our respective tasks well, and facilitate the proposed project. Over the past three years, I have also worked closely with Dr. Sreekanth Pannala on fluid-particle flow problems and the application of the multi-scale method to fluidized and spouted bed problems that we will do together is a natural extension of our prior interactions.

In addition, I anticipate playing an active role in the education component of the project, through the development of course material and through training of Ph.D. students involved in the research.

Sincerely,

Sankaran Sundaresan

Sankaran Sundaresan

Princeton University

YANNIS G. KEVREKIDIS
Professor of Chemical Engineering and
Applied and Computational Mathematics;
Associate Faculty, Mathematics

Chemical Engineering Department
A 207 Engineering Quadrangle
Princeton NJ 08544
Telephone: 609-258-2818
Department FAX: 609-258-0211
EMAIL: yannis@princeton.edu

Princeton., March 18, 2005

Paul F. Fischer
Building 221, Room D-248
Mathematics and Computer Science Division
Argonne National Laboratory
9700 S. Cass Avenue
Argonne, IL 60439

Dear Paul,

I am writing this letter to state my enthusiastic support for the proposal entitled *"A multiscale Computational Framework for Dense Particulate Flows"* that you are putting together, with Argonne as the lead institution. I am also stating my commitment to actively participate in the proposed research with you and your colleagues in this project.

My expertise is in the development of equation-free multiscale methods, ranging from projective integration and the gaptooth scheme to patch dynamics and coarse-grained stability and bifurcation analysis. I have extensive experience in the development, implementation, numerical analysis and application of the methods, and the emphasis of my participation in the project will be on the multiscale computation and numerical analysis issues that arise when the equation-free approach is applied to dense particulate systems. Furthermore, through my long and fruitful collaboration with my colleague, Prof. Sundaresan, I have extensive experience in multiphase flow modeling – we will work together in a coordinated way at Princeton. Issues of lifting and restriction, the efficient implementation of macro-inspired boundary conditions, and the adaptive selection of timesteps, meshes, and macroscopic observables are some of the tasks we will address.

We will also actively pursue educational aspects of the project. Equation-free and timestepper-based methods already constitute parts of an elective graduate course I am teaching at Princeton, and through both teaching and the training of graduate students and postdocs participating in the research I anticipate an important impact of this multiscale modeling and computational approach in graduate education at Princeton.

Sincerely,

Yannis G. Kevrekidis
Professor of Chemical Engineering and
Program in Applied and Computational Mathematics
Associate Faculty, Mathematics

March 27, 2005 CCN 200593

Paul F. Fischer
Building 221, Room D-248
Mathematics and Computer Science Division
Argonne National Laboratory
9700 S. Cass Avenue
Argonne, IL 60439

SUBJECT: Collaboration on High Fidelity Pebble-bed Modeling

Dear Paul:

I look forward to collaborating with you and your colleagues on the proposed project "A Multiscale Computational Framework for Dense Particulate Flows."

The Idaho National Laboratory seeks to coordinate and participate in the development of leading-edge nuclear reactor simulation capability. We acknowledge the significant contributions made by Argonne in high performance computing and computational fluid dynamics and thus perceive a real opportunity to advance the state of the art in pebble-bed reactor coolant flow simulation.

We will provide consultation on the relevant parameters for the pebble bed designs that are currently being considered for very-high temperature reactors. With the funds that you are providing, our participation in the project will be able to continue through personnel exchanges. In 2005, INL researcher Ray Barry will follow up Rich Martineau's 2004 visit to Argonne. In addition, we will provide access to our 230-node Linux cluster for the multiscale pebble-bed simulations.

Sincerely,

Hans D. Gougar, Manager
Fission and Fusion Systems

cc: L. Eric Greenwade
Richard C. Martineau
Kathryn A. McCarthy