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

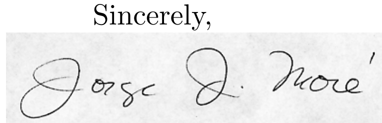
Dear Gary:

This proposal, *Reactive Channelization in Large-Scale Solid Mantle Flow*, is being submitted in response to the **Program Announcement LAB 05-16** and represents a collaboration between the following institutions:

- Argonne National Laboratory
- Columbia University

The role played by each institution is described in the section on *Consortium Arrangements*. Marc Spiegelman of Columbia University 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	**56121**

4. WORK PACKAGE TITLE:	4a. WORK PROPOSAL TITLE:
Mathematical, Information, and Computational Sciences	Reactive Channelization in Large-Scale Solid Mantle Flow

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	Smith, B. F.

8. HEADQUARTERS/OPERATIONS OFC PROGRAM MANAGER: Johnson, G. M. 301-903-5800	11. HEADQUARTERS ORGANIZATION: Office of Science	14. DOE ORG. CODE: 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
Reactive Channelization in Large-Scale Solid Mantle Flow

Quantitative characterization of geologic processes is crucial in several important Department of Energy activities. For example, the Office of Science's Program in Chemical Sciences, Geosciences and Biosciences includes "reactive fluid flow studies to understand contaminant remediation; seismic imaging for reservoir definition; and coupled hydrologic-thermal-mechanical-reactive transport modeling to predict repository performance." These programs will benefit from a better understanding of the inherently multiscale nature of geoscience systems. Accurately simulating magma dynamics in mantle convection will provide new techniques for subsurface problems and other reactive coupled fluid/solid systems. For the magma problem, the porosity and permeability become dynamic variables because of both mass-transfer (melting/reactions) and mechanical deformation (compaction/dilation/shear). This time dependence leads to the spontaneous formation of multiscale features such as hierarchical channel networks and localized melt-rich shear bands that can lead to singularities in properties such as permeability or strength. Because the overall deformation of the solid (i.e., mantle convection) is governed by elliptic equations, however, they are sensitive to both the largest scales and local singularities. Standard techniques such as upscaling or hierarchical models with strong separation of scales are not obviously appropriate for these problems. We will develop mathematical and computational tools to explore the coupled dynamics in the convecting mantle models. In addition, we will continue and expand ANL's hosting and mentoring of Columbia's applied mathematics students and the lecture series the ANL staff presents several times yearly at Columbia.

19. CONTRACTOR WORK PROPOSAL MANAGER:		20. OPERATIONS OFFICE REVIEW OFFICIAL:	
	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

BUD-11B (1-05)
Page 2

WORK PROPOSAL REQUIREMENTS FOR OPERATING/EQUIPMENT OBLIGATIONS AND COSTS

CONTRACTOR NAME	WORK PROPOSAL NO.	REVISION NO.	CONTRACTOR NO.	DATE PREPARED
University of Chicago/ANL			56121	03-28-05

22. STAFFING (in staff years)	PRIOR YEARS	FY 2005	FY 2006		FY 2007		FY 2008	FY 2009	TOTAL TO COMPLETE
			ESTIMATE	REVISED	REQUEST	AUTHORIZED			
a. SCIENTIFIC				1.5	1.5		1.5		
b. OTHER DIRECT				0.0	0.0		0.0		
c. TECHNICAL SERVICES*				0.0	0.0		0.0		
d. TOTAL DIRECT				1.5	1.5		1.5		
23. OBLIGATIONS AND COSTS (in thousands)									
a. TOTAL OBLIGATIONS				275	285		300		
b. TOTAL COSTS				275	285		300		
24. EQUIPMENT (in thousands)									
a. EQUIPMENT OBLIGATIONS				0	0		0		
b. EQUIPMENT COSTS				0	0		0		

25. MILESTONE SCHEDULE (Tasks)	FY 2007 DOLLARS		PROPOSED SCHEDULE	AUTHORIZED SCHEDULE
	PROPOSED	AUTHORIZED		

26. REPORTING REQUIREMENTS

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:
Reactive Channelization in Large-scale Solid Mantle Flow

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 $ 860,000.00

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 Barry Smith
TITLE Principal Investigator
ADDRESS Argonne National Laboratory
9700 S. Cass Avenue
Building 221
Argonne, Illinois 60439
PHONE NUMBER 630-252-9174

* Barry Smith (Electronically submitted)

SIGNATURE OF PRINCIPAL INVESTIGATOR/ PROGRAM DIRECTOR
(please type in full name if electronically submitted)
Date March 22, 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 22, 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).

NOTICE FOR HANDLING PROPOSALS

PRIVACY ACT STATEMENT

Contents

Reactive Channelization in Large-scale Solid Mantle Flow

A proposal to DOE University and Laboratory Program Announcements
DE-FG01 05ER-16/LAB 05-16

Marc Spiegelman (PI)

Dept. of Applied Physics and Applied Mathematics
Dept. of Earth and Environmental Sciences
Columbia University
New York, NY 10027
email: `mspieg@ldeo.columbia.edu`
phone: (845) 365-8425
fax: (845) 365-8150

Co-Investigators: Richard Katz, Matthew Knepley, and Barry Smith

Abstract

Quantitative characterization of geologic processes is crucial in several important Department of Energy activities. For example, the Office of Science's Program in Chemical Sciences, Geosciences and Biosciences includes "reactive fluid flow studies to understand contaminant remediation; seismic imaging for reservoir definition; and coupled hydrologic-thermal-mechanical-reactive transport modeling to predict repository performance."

These programs will benefit from a better understanding of the inherently multiscale nature of geoscience systems. Accurately simulating magma dynamics in mantle convection will provide new techniques for subsurface problems and other reactive coupled fluid/solid systems. For the magma problem, the porosity and permeability become dynamic variables due to both mass-transfer (melting/reactions) and mechanical deformation (compaction/dilation/shear). This time dependence is expressed as the spontaneous emergence of multiscale features such as hierarchical channel networks and localized melt-rich shear bands that can, in turn, lead to singularities in properties such as permeability or strength. Because the overall deformation of the solid (*i.e.*, mantle convection) is governed by elliptic equations, it is sensitive to both the largest scales and to these emergent, local singularities. Standard techniques such as upscaling or hierarchical models with strong separation of scales may not be appropriate for these problems. We will *develop mathematical and computational tools to explore the coupled dynamics in the convecting mantle models.*

In addition, we will continue and expand *ANL's hosting and mentoring of Columbia's applied mathematics students and the lecture series the ANL staff presents several times yearly at Columbia.*

Executive Summary

Quantitative characterization of geologic processes is crucial in several important Department of Energy activities. First, Office of Science's Chemical Sciences, Geosciences and Biosciences Program supports research on "mineral-fluid interactions; rock, fluid, and fracture physical properties;... The activity contributes to the solution of problems in multiple DOE mission areas, including reactive fluid flow studies to understand contaminant remediation; seismic imaging for reservoir definition; and coupled hydrologic-thermal-mechanical-reactive transport modeling to predict repository performance" [49]. Second, at the DOE's Office of Environmental Management billions of dollars are devoted to "cleaning up and keeping clean the soil and water at and around its former nuclear weapons sites." [48]. Another example is DOE's Fossil Energy program that funds research in oil and gas exploration, production and reservoir life extension [18].

Geoscience processes involving the interaction of fluids and solids are an important class of problems with significant societal, scientific and mathematical challenges. These problems are only a subset of a larger class of problems of fluid flow in *deformable* permeable media, however, where deformation introduces additional challenges that are not obviously addressable with current techniques. Perhaps the most dramatic of these applications is the flow of molten rock (magma) in the Earth's convecting mantle. This class of problems demonstrates a rich range of behavior arising from the coupling of reactive fluid flow with large scale deformation of a heterogeneous solid. In the partial differential equations that describe coupled magma/mantle flow, porosity and permeability are dynamic variables that change due to both mass-transfer (melting/reactions) and mechanical deformation (compaction/dilation/shear). This time-dependence leads to the emergence of multiscale features such as hierarchical channel networks and localized melt-rich shear bands that can generate singularities in properties such as permeability or strength. Unlike cascading turbulence in low-viscosity fluid, the overall flow of the solid (*i.e.* mantle convection) is governed by elliptic equations that are sensitive to both the largest scales and local singularities.

The key feature of these systems is that the structures at small and large scales are strongly coupled. For example, the large scale solid-flow can lead to the time-dependent development of small scale weak, fluid-rich channels that significantly change the large scale solid flow. Thus standard techniques such as upscaling or hierarchical models with strong separation of scales may not be appropriate for these problems. The purpose of this proposal is to develop and explore mathematical and computational tools to handle these problems and explore the implications of these coupled models.

All of this behavior is described within a single, tractable set of PDE's that have already been solved at their respective scales. All of the basic models have been implemented within the PETSc framework, providing significant flexibility for exploration of both novel solution techniques as well as efficiency for performing the fine-scale numerical experiments against which we can validate and explore various upscaling and multiscale techniques. Operating at a high level of abstraction, these codes will allow a wide range of coupling strategies, as well as provide an infrastructure for scalable, multilevel algorithms.

We will consider several different models of coupling from simple embeddings of approximate solutions for partially molten regions in intermediate scale mantle dynamics to fully multiscale codes that resolve several orders of magnitude from fine scale channel networks ($\sim 1 - 1000$m) to the size of partial molten regions (~ 100km) to whole mantle convection ($\sim 3000 - 10,000$km). The principal thrust of the research is to develop and explore general techniques for this problem but also to test the fundamental scientific hypothesis that for solid-earth dynamics, the accurate inclusion of small scale coupled fluid/solid flow could significantly improve our understanding of the dynamics of the planet.

The Department of Applied Physics and Applied Mathematics at Columbia University and the Mathematics and Computer Science Division at Argonne National Laboratory already have a successful small-scale student exchange program. In additional, several ANL scientific staff, including those on this proposal, have been lecturing at Columbia. This proposal will allow us to expand this university-laboratory interaction with more student training at ANL and the development of a full set of lectures and notes to introduce the Columbia students to issues in multiscale mathematics and high performance computing at the national laboratories. In conjunction with the Computational Infrastructure for Geodynamics, we also plan to propose a CIG sponsored open workshop on multiscale mathematics and computation in solid-earth sciences.

1 Background and Significance of Proposed Work

1.1 Significance

Quantitative characterization of geologic processes is crucial in several important Department of Energy activities. First, in the Office of Science's Basic Energy Sciences Program core research activities in Chemical Sciences, Geosciences and Biosciences roughly $20 million is spent on "mineral-fluid interactions; rock, fluid, and fracture physical properties;... The activity contributes to the solution of problems in multiple DOE mission areas, including reactive fluid flow studies to understand contaminant remediation; seismic imaging for reservoir definition; and coupled hydrologic-thermal-mechanical-reactive transport modeling to predict repository performance." [49]. Second, in DOE's Office of Environmental Management several billion dollars is devoted to "cleaning up and keeping clean the soil and water at and around its former nuclear weapons sites." [48]. Finally DOE's Fossil Energy program devotes roughly $40 million per year to oil and gas exploration and production and reservoir life extension [18].

All of these problems will benefit from a better understanding of how to handle the inherently multi-scale nature of natural, heterogeneous systems. Understanding the behavior of the most dynamic of these problems (i.e. magma dynamics in the convecting mantle) will provide new techniques for both subsurface problems as well as more general issues in the behavior of reactive coupled fluid/solid systems.

1.2 Earth Science Background

A large class of problems in Earth Science can be described by the flow of low-viscosity, reactive fluids through deformable permeable media. Some of the usual examples of these problems include the flow of oil, gas and water in the subsurface and contaminant transport and remediation. All of these problems are beset with multi-scale issues from understanding the behavior of fluid/solid interaction from the pore scale to the basin scale (e.g. see [19]). The most dramatic of these problems, however, involve the flow of partially molten rock (magma) in the Earth's convecting mantle. Due to the additional freedom of high temperatures, large mass transfer and large-scale solid deformation, these problems introduce an additional set of challenges for solving complex fluid/solid systems from the grain scale to the size of the planet. In particular, unlike most porous media problems where the porosity/permeability is a static field, in these problems the porosity and permeability are dynamic and develop emergent, time-dependent multi-scale structures such as cascading channels that require new techniques for efficient solution. Developing these techniques will be a major goal of the proposed research. To understand the challenges however, it is worth briefly reviewing our current understanding and modeling capability in magma dynamics.

At the largest scale, magma-dynamics is an essential component of global mantle convection and its surface manifestation as plate tectonics. Partially molten regions where both liquid rock (magma) coexists with its solid source are principally restricted to the upper ~ 200 km of the mantle in the vicinity of plate boundaries where plates are diverging (mid-ocean ridges) and converging (subduction zones) (see Figures F.1 and F.2) While these partially molten regions are small compared to the scale of mantle dynamics, they may control the dynamics of plate boundaries (where over 90% of both earthquakes and volcanoes occur). In particular, they may provide the weakening mechanism that allows for large-scale tectonic plates ($\sim 3000 - 10,000$km diameter) separated by narrow weak zones [67, 68]. The existence of large plates with weak boundaries dominates the structure of convection in the planet. Because of the extremely high viscosities of mantle materials $10^{18} - 10^{26}$ Pa s, mantle flow fields are governed by elliptic Stoke's equations where the presence or absence of small weak regions such as faults or plate boundaries can radically change the large-scale flow. Thus developing accurate and consistent models of large-scale mantle dynamics requires resolving small-scale features at the plate boundaries.

Within the partially molten regions, however, there is also likely to be a considerable range of structures due to the coupling between reactive fluid flow and the deformation of the solid matrix. Previous work (reviewed below) based on a system of PDE's for flow in deformable porous media (e.g. [45, 51, 52]) demonstrate that partially molten regions can be highly time dependent and develop a host of spontaneously forming features. Such features include non-linear traveling porosity waves (e.g. [51, 7, 8, 73]) on scales of 1-10km; hierarchical channel networks created by corrosive reactive flow (e.g. [2, 40, 60, 59]) with channel spacings from 0.01–100 m [38, 12]; and mechanically driven shear-bands and melt channels [32, 56, 58] observed in experiments and likely to occur on similar scales (see Figures F.4–F.6).

All of these mechanisms are likely to be active in partially molten regions and may strongly affect the bulk response of these systems and their observable consequences. The scientific challenge is to understand the interactions between these different mechanism within the partially molten regions and the interaction of these partially molten regions with plate tectonics and global mantle convection. Fortunately, this problem is tractable as all of this disparate behavior is governed by a single system of PDE's that have been solved at their individual scales. Thus this system provides a useful test case for developing multi-scale techniques for time-dependent problems with emergent heterogeneous structures.

1.3 Mathematics Background

The equations for magma migration were derived independently by several authors [45, 51, 52, 23] and are discussed in detail by [54, 55, 57] with modifications by [10]. Following McKenzie [45], the equations for conservation of mass, momentum and energy (enthalpy) of a two-phase system of melt in a viscously deformable solid matrix can be written

$$\frac{\partial \rho_f \phi}{\partial t} + \boldsymbol{\nabla}\cdot [\rho_f \phi \mathbf{v}] = \Gamma, \tag{1.1}$$

$$\frac{\partial \rho_s (1-\phi)}{\partial t} + \boldsymbol{\nabla}\cdot [\rho_s (1-\phi) \mathbf{V}] = -\Gamma, \tag{1.2}$$

$$\phi\,(\mathbf{v} - \mathbf{V}) = -\frac{k_\phi}{\mu}\left[\boldsymbol{\nabla} P - \rho_f \mathbf{g}\right], \tag{1.3}$$

$$\boldsymbol{\nabla} P = \boldsymbol{\nabla}\cdot \left[\eta(\boldsymbol{\nabla}\mathbf{V} + \boldsymbol{\nabla}\mathbf{V}^T)\right] + \boldsymbol{\nabla}\left[(\zeta - 2\eta/3)\boldsymbol{\nabla}\cdot \mathbf{V}\right] + \bar{\rho}\mathbf{g}, \tag{1.4}$$

$$\frac{D_{\bar{\mathbf{v}}} T}{Dt} = \frac{T}{\bar{\rho} c_P}\left(\rho_s \alpha \bar{\mathbf{v}} \cdot \mathbf{g} - \Delta s \Gamma\right) + \kappa \nabla^2 T + H \tag{1.5}$$

where ϕ is the volume fraction of melt (porosity); ρ_f and ρ_s are the melt and solid densities; $\bar{\rho}(\phi, T)$ is the mean density of the two-phase mixture that includes both thermal and melt buoyancy; $\mathbf{v}$ and $\mathbf{V}$ are the melt and solid velocities; Γ is the total rate of mass transfer from solid to liquid; k_ϕ is the permeability, which is a nonlinear function of porosity; μ is the melt viscosity; P is the fluid pressure; $\mathbf{g}$ is the acceleration due to gravity; η is the solid shear viscosity and ζ is the bulk viscosity that resists volume changes of the matrix. Also, T is temperature, Δs is the difference in specific entropy between the solid and fluid phases, α and c_P are the thermal expansivity and specific heat, both of which are assumed to be the same for melt and solid; κ is the thermal diffusivity and H are heat sources (e.g. radioactive decay or viscous heating). Temperature is advected by a combination of fluid and solid flow, represented by the velocity field

$$\bar{\mathbf{v}} = \frac{\rho_f \phi \mathbf{v} + \rho_s (1-\phi)\mathbf{V}}{\rho_f \phi + \rho_s (1-\phi)} \tag{1.6}$$

Equations (1.1) and (1.2) conserve mass for the melt and solid, respectively, and allow mass transfer between the phases at rate Γ. Equation (1.3) governs the separation of melt from solid in a porous medium and is an extension of Darcy's law. Equation (1.4) governs stress balance and deformation of the creeping, porous solid matrix which is modeled as a highly viscous, compressible fluid. Finally, Equation (1.5) represents the conservation of enthalpy and governs temperature changes due to transport, melting and adiabatic and dissipative effects. Aharonov [2] and Spiegelman et. al [60, 59] extend the formulation to chemically reactive flows. Constitutive equations (e.g. for rheology and permeability) and PDEs representing conservation of composition (see below) are added to close the equations with respect to the melting rate Γ.

The important feature of these equations is that there is a coupling between solid deformation and fluid transport that allows the porosity ϕ to evolve in space and time. This coupling arises from dynamic pressure gradients due to viscous deformation of the solid phase as well as non-linear feedback between the porosity, temperature and the macroscopic constitutive relationships for permeability (e.g. $k_\phi \propto \phi^n$) and solid viscosities (e.g. $\eta \propto \exp(-\alpha/\phi)$) [50, 30, 29].

While these equations seem somewhat complicated, they were designed to be a reasonably tractable set of conservation equations for fluid flow in a solid matrix that reduces to the equations for incompressible thermal convection of the mantle in the limit $\phi \to 0$. Inspection of Eqs. (1.1)–(1.5) shows that, for $\phi = 0$, $k_\phi = 0$ and no melting ($\Gamma = 0$), these equations reduce to those for incompressible Stoke's flow for the solid phase and a single-phase advection-diffusion equation for temperature (e.g. see Figure F.2).

For regions with non-zero porosity, however, these equations have been shown to display a rich variety of behavior from non-linear porosity waves to mechanically driven localization instabilities. Thus these equations allow for consistent solution of both large-scale mantle convection and small-scale magma dynamics. The goal is to explore efficient mathematical and computational techniques to develop consistent multi-scale models of mantle convection with embedded partially molten regions to understand the interactions of these processes across scales. We can already solve many of these problems in two spatial dimensions and time at their respective scales (see next section). The challenge is to develop efficient methods to move to 3-D global models to explore global dynamics.

1.4 Computational Methods

All of the basic computational models for the problems demonstrated in Figures F.2–F.6 have been implemented using PETSc (Portable, Extensible Toolkit for Scientific computation) [6]. PETSc is the most widely used scalable package for the solution of algebraic equations arising from the discretization of partial differential equations, and will form the basis of all future simulations. It supports not only the standard sparse, parallel algebraic operations, but also mesh manipulation, structured parallel communication, and multilevel preconditioning techniques.

Moreover, it is an open platform for development of PDE codes, contributed to by more than twenty researchers in the past year. Thus, results obtained from one project are immediately available to the wider field of users. One example of this is our previous joint work on a method of characteristics algorithm [63] for the solitary wave problem. It is well known that chemical diffusivities are extremely low in magma and effectively zero in solid mantle, making numerical diffusion in most advection schemes problematic. In order to eliminate excessive dissipation, we developed a parallel characteristic integrator for structured meshes based upon the PETSc `DA` and `VecScatter` components. This code was then refactored into a generic PETSc module applicable to any field with velocity distribution lying on a compatible mesh. This reuse, and the feedback it facilitates, will be even more important in the rapidly developing field of multi-scale mathematics.

PETSc was designed to incorporate the power of modern object oriented design while still remaining comfortable for engineers and scientists. It uses a library level parallelism programing model that does not require explicit MPI programing but has the performance, cost, and portability advantages of distributed memory models.

2 Preliminary Studies Relevant to the Proposed Work

Most of the physics described by the governing equations 1.1-1.5 has been considered at its own inherent length and time scales, neglecting interactions with processes at other scales. The majority of this work has focused on single-phase systems (no porosity or melting), including global mantle convection calculations [65, 13, 66, 72] and regional models of mantle flow and thermal structure [24, 42, 43, 71, 39, 16, 25, 70, 28, 17, 9, 11, 27]. We have developed regional flow models of both mid-ocean ridges and subduction zones using PETSc [44] and used this code to model a recently reported set of observations of globally consistent asymmetry in the mid-ocean ridge system [15]. We succeeded in quantifying the effect of ridge migration above a static asthenospheric mantle on the asymmetry in melting beneath ridges [37]. Example calculations of ridge and subduction-related mantle flow and viscosity are shown in Figure F.2.

Some work has been done to consistently compute the flow of magma in regional mantle convection models [61, 62, 5, 14], however these studies have invariably relied on simplified versions of the mantle dynamics equations that, to make the problems tractable, suppress the emergence of small scale features. Other studies of magma dynamics have instead considered highly simplified behavior of the solid matrix, limiting the possibilities for comparison with observations of the Earth. The latter category of studies has shown, however, that self-organized patterns emerge at length-scales (determined by the physical parameters) that are much larger than the grain-scale and much smaller than the typical scales of mantle convection. These patterns are non-linear waves of porosity, stress-induced formation of high porosity shear bands and high-porosity reactive dissolution channels. We have modeled these phenomena extensively and describe our work and results in three sections below.

Since their earliest derivation, it has been clear that the intrinsic length-scale in these problems is the *compaction length* [45]

$$\delta = \sqrt{\frac{k_\phi(\zeta + 4\eta/3)}{\mu}}$$

which depends on the permeability and the ratio of solid and melt viscosities. Estimates of the compaction length for natural systems range from $10^2 - 10^4$m although at the extremely small grain-sizes used in laboratory experiments, the compaction length can be reduced to the sample size of $\sim 1 - 2$mm. Moreover, for systems where the permeability $k_\phi \to 0$ and the bulk-viscosity ζ remains bounded, then the compaction length can go to zero and the equations can develop singularities. Physically, the compaction length is the length scale over which variations in flux are propagated by stresses in the solid [53, 54]. Flux variations much larger than the compaction length propagate as non-linear porosity waves, while systems smaller than the compaction length are dominated by viscous stresses and can develop flow localization instabilities. However, because the compaction length itself can vary over orders of magnitude due to feedbacks between porosity, permeability and solid viscosity, these features can arise and interact at a large range of scales.

2.1 Magmatic Porosity Waves

For systems much larger than the compaction length (i.e. loosely coupled systems), variations in melt flux can propagate through the deformable matrix as non-linear porosity waves. In particular, these equations have been shown to admit solitary wave solutions in 1-,2- and 3-dimensions. Figure F.3 shows numerical solutions for the evolution of dispersive non-linear porosity waves in 1-D [54] and 3-D [73]. These solutions have been benchmarked against analytic solutions for solitary waves and have shown to be accurate and stable as long as the smallest compaction length in the system is well resolved [54]. The waves themselves, however are an order of magnitude bigger than this smallest compaction length leading to significant resolution issues, particularly since the waves are dispersive and often eventually fill space (see Figure F.3a). The evolution and stability of the solitary waves are discussed by several authors (e.g. [51, 52, 8, 7]) and they are shown to be a natural consequence of the non-linearity of permeability with porosity and the ability of the solid matrix to deform viscously. Surprisingly, viscous dissipation actually gives rise to a dispersive system of PDE's. Heuristics for wave formation and amplitude are given by Spiegelman [53, 54] who suggests that magmatic systems can be strongly time dependent and spontaneously generate small scale evolving structure. Outstanding questions exist regarding whether these waves will be stable in the presence of other localization phenomena. This is one of the questions that the work proposed here will be able to address.

2.2 Shear Instabilities and Emergent Banded Porosity Networks

At scales smaller than the compaction length, viscous stresses in the solid dominate the flow of fluid and can lead to a host of localization instabilities. One such instability arises in systems undergoing shear where the solid viscosity is a decreasing function of porosity. This instability was first discussed by Stevenson [64] for pure shear and extended to simple shear by Spiegelman [56]. Experimental studies have confirmed both the rheological prerequisite [35, 31] and the existence of this instability [32]. In the experiments, a uniform mixture of solid grains of mantle rock and mantle derived melt are held at high temperature and pressure and subjected to about 300% simple shear deformation. The experiments are then quenched and sectioned. Figure F.4a shows a sectioned experiment. As predicted [64], melt has localized into bands of high porosity between regions of compacted, low porosity rock. Figure F.4b shows numerical solutions of Eqs. (1.1)–(1.4) appropriate for lab-scale samples [58]. The important non-linearity in this problem is that the shear viscosity η is a decreasing function of porosity. Thus higher porosity regions are weak and can dilate when sheared. This dilation produces lower pressures in the weak regions which draws in more fluid making the regions weaker in a positive feedback. Spiegelman [56] presents a linear stability analysis for this system and shows that all plane-wave perturbations with wavelengths shorter than the compaction length and oriented at shallow angles should grow when the viscosity is porosity weakening. This analysis, however, does not predict a preferred wave-length and only suggests that lower angled bands are favored. Numerical results are qualitatively similar to the lab experiments producing large amplitude melt bands surrounded by very small porosity regions [58]. These solutions suggest that the preferred spacing is a non-linear effect caused by larger melt bands preferentially compacting smaller ones; however, the angle of the melt-bands in simulations is generally too high ($\approx 45°$)

Because of the lower matrix viscosity in high porosity regions, matrix shear deformation is localized on the bands. When scaled up to mantle conditions, these features probably appear with a length-scale of hundreds of meters to kilometers. The incorporation of shear band calculations into regional and global convective flow models may have important consequences for the modeled permeability structure and paths of magma flow. It will also have feedbacks on the pattern of large-scale solid convection by modifying the matrix viscosity structure. To solve these problems consistently and answer these questions, however, will require solutions that can incorporate small scale shear bands into large scale mantle flow.

2.3 Reactive Infiltration Instability and Channelization of Magma Flux

Another important localization mechanism that arises naturally from the mantle dynamics equations is the reactive infiltration instability [2, 41, 1, 60, 46]. The analysis of this instability was motivated by observations of reactive dissolution (melting) channels in exposed sections of mantle rock that were once beneath mid-ocean ridges [40, 26, 12, 69]. An example of such an exposure from Oman, called an Ophiolite, is shown in Figure F.5c.

Most of the work on reactive flow, including our own, has been in an effort to understand magma genesis and transport in mid-ocean ridge environments [60, 59, 21]. Figure F.5a and b show results from a calculation of melt rising under buoyancy through a non-deforming matrix that has increasing solubility with height. A channelized pattern of melt flux emerges and dominates the porosity structure of the problem with important consequences for the chemistry of "erupted" lavas [59].

While much attention has focused on modeling melting and melt transport at mid-ocean ridges, subduction zones are host to most of the subaerial volcanoes on Earth and present a significant challenge in terms of understanding the sources of magma that feed them. Figure F.1 shows, in schematic cross-section, how volatile elements carried to depth by the subducting slab are released into the mantle by metamorphic reactions and percolate upward, triggering melting. This melting process can be modeled as the reactive infiltration of a corrosive, aqueous fluid into a soluble mantle matrix [36]. Progressive dissolution of rock by the fluid as it rises through the mantle leads to enrichment in silicate components until the fluid becomes magma. A sharp thermal gradient above the subducting slab (Figure F.2) translates to a sharp gradient in the reactive dissolution rate and necessitates finer meshes for computational models relative to those required for mid-ocean ridges.

As with our computational models of reactive flow beneath mid-ocean ridges, we have neglected matrix deformation because of the longer length-scales that it introduces. And as in earlier calculations of reactive flow, the reactive infiltration instability leads to the emergence of channelized melt flow. A time-series of porosity (color) and temperature (contours) from a representative calculation is shown in Figure F.6. There is an important difference between this calculation and those relevant to mid-ocean ridges: the fluid solubility of rock increases from the slab to the core of the wedge and then decreases again with height, unlike the linear, monotonic-increasing solubility profile of ridge simulations. The effect of this long wavelength solubility variation (which results from the vertical temperature profile of a subduction zone) is clearly visible in Figure F.6; closely spaced channels coalesce into bundles that occur at with much larger spacing. The channel bundles transport a significant amount of heat to the base of the upper thermal boundary layer, where they widen into magma storage zones. Although preliminary, these results seem to be consistent with the spacing of volcanoes along subduction zones such as the Pacific Northwest of the USA. We are exploring hypotheses for the mechanism of channel coalescence.

Due to the already significant cost of reactive flow simulations in a non-deforming mantle matrix and the small length-scales involved in this problem (channel spacing and widths are less than one compaction length), simulations coupling reactive melting to large-scale mantle flow beneath ridges have not been constructed. However, having developed the simpler models for scalability in the PETSc framework, extensions to two dimensional models of combined magma/mantle flow at mid-ocean ridges may now be feasible. If so, they would provide a stronger basis for comparison of physical and chemical predictions with observations of the Earth. Such an effort is expected to be complicated by the interaction of high porosity channels with plate-driven shear deformation. As with the induced porosity banding shown in Figure F.4, matrix shear is expected to localize on the narrow, weak channels, reorganizing large-scale mantle flow and leading to effects at length-scales much longer than the compaction length.

2.4 Scalable Implementations

We have constructed parallel simulations both of reactive flow at the scale of mantle melt channels, and mantle subduction at the ridge and arc scale [36]. These codes were designed using the PETSc object framework, and thus can be easily combined. They utilize a uniform code management scheme, build environment, and profiling architecture. They have been run with good parallel efficiency on hundreds of processes using the ANL Jazz cluster [44], drastically reducing the turnaround time for the results in Figure F.2 for example.

Moreover, we are actively involved in the NSF Computational Infrastructure for Geodynamics (CIG) [22] which supports the development of community codes, as well as open source code management tools, build environments, and application frameworks. This initiative has assumed support for the CitComS code for whole earth mantle dyanmics [47] which we intend to couple to our ridge and arc models to examine the effects of weak boundary regions on the stability of the global flow pattern. This integration will again be facilitated by the high level reorganization of the CitComS code along the lines laid out for PDE simulations by CIG researchers and PETSc itself. The CitComS code, and other codes currently being refactored, will provide a general software framework for geodynamics models which will heavily leverage current DOE software initiatives, such as the TOPS SciDAC project.

3 Proposed Research and Education

3.1 Motivating Questions

The previous section has demonstrated that the equations for magma/mantle dynamics govern a rich array of behavior from scales of a few meters to the plate boundary scale to the scale of whole mantle convection. Each of the model problems illustrated by Figures F.2–F.6 was designed to isolate, resolve and understand one component of this behavior. Outstanding scientific and mathematical questions remain as to the effect of interactions between scales on the system as a whole, as well as on the testable geochemical and geophysical predictions that these models make. The principal scientific questions concern the interaction and coupling of small-scale and large scale dynamics. In particular:

- **What is the interaction between well resolved magmatic regions and larger scale convective solid mantle flow beneath ridges and subduction zones?** i.e. how does the inclusion of small scale processes such as mechanical and reactive localization instabilities change the *observable* large scale behavior of these systems.
- **How does the inclusion of multi-scale magmatic plate-boundary models affect and change the behavior of global mantle convection and plate tectonics?**

To address these problems requires efficient multi-scale methods that can handle a fine-scale problem that is time-dependent, evolves with the large scale dynamics, is often highly anisotropic (channelized) and pervasive in space. These problems are inherently difficult. However, we currently have the tools to solve at least the full 2-D fine grid problem and use that to validate more complex (but potentially more efficient) methods. The long-term goal is to develop efficient 3-D calculations but this requires us to address specific mathematical and computational questions such as

- **How well do standard techniques for multiscale solution apply to the magma dynamics problem?** Can we recover the large scale behavior using techniques such as
  - Multi-resolution mesh techniques (unstructured meshes, block-structured AMR, overset grids).
  - Upscaling techniques (e.g. Oversampled FEM, Variational Multiscale analysis, homogenization [34, 3, 4, 33])

- The heterogeneous multiscale method (HMM) [20].

- **Can we develop *efficient* methods using these techniques?** Because these problems don't necessarily demonstrate a clear separation of spatial or temporal scales, open questions exist as to how much leverage multi-resolution or upscaling techniques will buy for this kind of problem. For example, some upscaling techniques require at least an approximate solve of fine-scale complexity. Given that the fine scale is constantly evolving, how much is gained from these methods?

- **Can algorithms such as algebraic multigrid be used to form appropriate coarse grid operators that produce the correct large scale behavior without needing to completely solve for the fine grid solution?**

- **Alternatively can we use upscaling techniques in multi-level schemes to accelerate the fine-scale problem?** i.e. can these ideas be used to develop improved coarse grid operators for structured or algebraic multi-grid methods?

- **What are the appropriate error estimators for these techniques?**

3.2 Proposed Research

To begin answering these questions we will explore techniques and models with different levels of multi-scale coupling. We begin with the problem of embedding partially molten regions into large scale mantle convection, then consider the full multi-scale problem of the interaction of emergent small-scale features with the large scale flow. For each of these problems we will explore a range of existing techniques to gauge their utility and at the same time develop better physical insight into the relative importance of scale interaction in these problems.

We will couple our large scale ridge and arc models to the smaller scale reactive flow, initially in two dimensions moving then to three. This coupling need not be of the block-box type since velocity and temperature fields may be defined over the entire region whereas the domain of the partially molten porous region may be substantially restricted in space. This coupling will require mesh adaptivity but we have the ability to use either overset grids or adaptive unstructured grids, depending on the problem configuration. Furthermore, we are developing finite element technology which will allow higher order elements to be used in this scenario, enabling finer resolution and faster convergence. It seems unlikely that the standard upscaling techniques that rely on fine scale calculation, as in the case of porous media, will be effective here since we may not amortize the calculation over many solves owing to the dependence of the fine structure on the evolving dynamics. Also, the presence of highly anisotropic features, such as channels, may pose problems for existing methods.

This coupling also has an obvious extension to global mantle convection models, and this work has begun in the context of CIG (Computational Infrastructure for Geodynamics). Within, this project, the existing CitComS spherical mantle convection code from Caltech is being modularized and refactored in order to support more flexible coupling at the ridge/arc scale. We will advance the preliminary work already done [47] and thus produce a model reaching from magmatic channels to the Earth as a whole.

In PETSc, the consistent use of encapsulation and abstraction opens the door to easy experimentation with hierarchical methods. Both the PDE and its approximate solution are program entities in their own right. Thus models can be manipulated in much the same way that PETSc handles vectors and matrices, allowing flexible combination of different solutions resulting from the same equations evaluated at different limits and/or scales. PETSc can manage, for example, coupling of reactive magmatic flow with regional models of mantle convection in arcs or ridges or, as another example, coupling of these regional scale arc or ridge models to a global mantle convection flow. The ability to manipulate equations and solutions easily will allow us to focus on the mathematics of coupling and convergence to an accurate global solution, rather than the underlying mechanics of software.

The existing PETSc multilevel framework will be used to build optimal preconditioners for each physical regime. These can then be easily combined in a coupled code to produce a single, scalable preconditioner. Large scale parallelism affords us the opportunity to validate any upscaling or multiscale simplification with the full, direct simulation of the entire coupled problem in two dimensions using the existing codes. In three dimensions, a full fine grid simulation will not be available, and we will have to rely on small studies of local problems or more global error estimates to validate our conclusions. PETSc will also provide the ability to adapt both the mesh and the element to changing physics and flow regimes.

Furthermore, all software constructed during the course of this project will follow the PETSc model for portable, extensible, scalable scientific software. The various algorithms, such as interscale coupling, will be refactored and appear as modules applicable to any PETSc code, as is already the case for our method of characteristics module mentioned in section 1.4. The release of our new coupling schemes as independent PETSc modules will allow rapid experimentation and feedback from other multiscale efforts.

3.3 Proposed Timeline

- **Year 1** The focus will be on getting the full, fine scale two dimensional code running scalably on hundreds of processors; this code is needed in the later years to validate the multiscaling techniques.
  - Columbia - Build two dimensional coupled fluid/solid simulations for arcs and ridges by using finite volumes and overset static grids.
  - ANL - Prepare the software libraries for solid/fluid flow in two and three dimensions using finite element/finite volume methods with variable order elements and general three dimensional meshes.
- **Year 2** Develop and validate the two dimensional multiscale methods against the fine

scale code developed in the first year.

  - Columbia - Validate the two dimensional multiscale models and write the three dimensional regional models, including arcs and ridges using the elements and mesh libraries developed during the first year.
  - ANL -Develop the software libraries for the multiscale methods in three dimensions.

- **Year 3** We will now be ready to run large scale three dimensional simulations using the multiscale libraries to incorporate the fine scale effects without needing to resolve the entire fine scale.
  - Columbia - Integrate the three dimensional regional models into the global mantle convection CIG framework.
  - ANL - Complete the software libraries and begin testing them against other application area models, such as those in fusion.

3.4 Educational Initiatives

This proposal will promote several important educational objectives. First it will provide significant training and education for the next generation of applied mathematician that can work effectively at the interface between mathematics and its applications. This project will provide important opportunities for several graduate students. The first GRA at Columbia is Gideon Simpson, who is currently a second year graduate student at Columbia in Applied Mathematics. Gideon comes with a pure math background from Cornell and is possibly the strongest applied analyst at Columbia in the past 10 years. While Gideon's background and training is in mathematics, he has an impressive ability to understand and interpret the physical earth science arguments as easily as the mathematics. He is particularly interested in analysis of the non-linear wave problems as well as analysis of variational multi-scale techniques. Gideon is jointly supervised by Spiegelman and Prof. Michael Weinstein (Columbia APAM) who brings expertise in analysis of non-linear PDE's. Gideon has been currently supported by an NSF IGERT 2 year fellowship for the Columbia joint program in Applied Mathematics and Earth Sciences, but requires additional support for the remainder of his Ph.D. The second graduate student is Ethan Coon (also a recent IGERT fellow) and now the recipient of the DOE CSGF fellowship. Ethan also comes from a pure math background but also has expertise in computation and solid mechanics. His Ph.D. research concerns extending the magma dynamics formulation to more complex solid rheologies such as visco-elastic, elastic-plastic to extend the theory to crustal systems such as sedimentary basins and faulting systems. Ethan will not require any direct support from this proposal but will be an integral component of all aspects of multi-scale mathematics as it pertains to coupled fluid/solid flow. In addition to Gideon and Ethan, Martin Collier is a Spiegelman student in Earth and Environmental sciences who will be investigating the chemical consequences of mid-ocean ridge models and will benefit significantly from any improvements in ridge models. All of these students, and others will benefit greatly from interaction with the Argonne group and other students at Argonne. Both the IGERT fellowship and CSGF have opportunities for summer internships and we expect that these will be coordinated with Argonne. Richard Katz already developed much of his work during a CSGF summer practicum at Argonne and he expects to continue his close collaboration with Knepley and Smith.

The second principal educational activity will be workshops and classes to discuss and propagate experiences in multi-scale mathematics and computation. In particular, both Spiegelman and Knepley are involved with the CIG project (Computational Infrastructure for Geodynamics) who sponsors workshops of interest to both the earth science and computational science community (CIG is currently sponsoring three workshops this summer on lithospheric deformation, mantle convection and computational seismology which Spiegelman and Knepley will attend). We propose to develop an open CIG workshop on multi-scale mathematics in solid-earth science and leverage ours, and others, experiences with multi-scale problems in either summer 06, or 07. In addition to formal workshops and education, Smith and Knepley have already been active guest lecturers for David Keye's courses in scalable computation and PETSc at Columbia, as well as for the recent DD16 meeting on domain decomposition. Both Smith and Knepley plan to continue this close collaboration with Columbia.

3.5 Consortium Arrangements

This initiative offers an excellent opportunity to expand the already fruitful collaboration between ANL and Columbia. Argonne researchers bring a wealth of knowledge and experience in scientific computation, iterative methods, parallel computing, and software management. This will complement the strong geophysical research at LDEO and mathematical work at APAM. The synergy with ANL will enhance the already expanding effort in scientific computing at APAM. ANL will also provide much needed computer resources in the form of the 5 TFlop Jazz cluster and newly minted 6 TFlop Blue Gene system, and a development infrastructure tailored to producing and supporting valuable community codes and libraries. ANL has already mentored and hosted APAM students with great success and we hope to expand this in the future. ANL staff members are frequent speakers at APAM; we plan to present a regular lecture series.

References

[1] E. Aharonov, M. Spiegelman, and P. Kelemen, *Three-dimensional flow and reaction in porous media: implications for the earth's mantle and sedimentary basins*, J. Geophys. Res., 102 (1997), pp. 14821–14833.

[2] E. Aharonov, J. Whitehead, P. Kelemen, and M. Spiegelman, *Channeling instability of upwelling melt in the mantle*, J. Geophys. Res., 100 (1995), pp. 20433–20450.

[3] T. Arbogast, *An overview of subgrid upscaling for elliptic problems in mixed form*, in Current trends in scientific computing (Xi'an, 2002), vol. 329 of Contemp. Math., Amer. Math. Soc., Providence, RI, 2003, pp. 21–32.

[4] ——, *Analysis of a two-scale, locally conservative subgrid upscaling for elliptic problems*, SIAM J. Numer. Anal., 42 (2004), pp. 576–598 (electronic).

[5] L. Baker, C. Hall, P. Asimow, P. Smith, and M. Gurnis, *Subduction dynamics and mass transfer: A synthesis model*, in EOS Trans. Amer. Geophys. Union, vol. 85, 2004. Fall Meet. Suppl., Abstract V12A-08.

[6] S. Balay, K. Buschelman, V. Eijkhout, W. D. Gropp, D. Kaushik, M. G. Knepley, L. C. McInnes, B. F. Smith, and H. Zhang, *PETSc Web page*. `http://www.mcs.anl.gov/petsc`.

[7] V. Barcilon and O. Lovera, *Solitary waves in magma dynamics*, J. Fluid Mech., 204 (1989), pp. 121–133.

[8] V. Barcilon and F. M. Richter, *Non-linear waves in compacting media*, J. Fluid Mech., 164 (1986), pp. 429–448.

[9] T. Becker, C. Faccenna, R. O'Connell, and D. Giardini, *The development of slabs in the upper mantle: insights from numerical and laboratory experiments*, J. Geophys. Res., 104 (1999), pp. 15207–15226.

[10] D. Bercovici, Y. Ricard, and G. Schubert, *A two-phase model for compaction and damage 1. general theory*, J. Geophys. Res.-Solid Earth, 106 (2001), pp. 8887–8906.

[11] M. Billen and M. Gurnis, *A low viscosity wedge in subduction zones*, Earth Plan. Sci. Lett., 193 (2001), pp. 227–236.

[12] M. Braun and P. Kelemen, *Dunite distribution in the Oman ophiolite: Implications for melt flux through porous dunite conduits*, Geochem. Geophys. Geosys., 3 (2002).

[13] H. Bunge, M. Richards, and J. Baumgardner, *A sensitivity study of three-dimensional spherical mantle convection at 10(8) rayleigh number: effects of depth-dependent viscosity, heating mode, and an endothermic phase change*, J. Geophys. Res., 102 (1997), pp. 11991–12007.

[14] A. Cagniocle, E. Parmentier, and L. Elkins-Tanton, *The effect of solid mantle flow above a subducting plate on melting and fluid migration*, in EOS Trans. Amer. Geophys. Union, vol. 85, 2004. Fall Meet. Suppl., Abstract V12A-03.

[15] S. Carbotte, C. Small, and K. Donnelly, *The influence of ridge migration on the magmatic segmentation of mid-ocean ridges*, Nature, 429 (2004), pp. 743–746.

[16] J. Conder, D. Wiens, and J. Morris, *On the decompression melting structure at volcanic arcs and back-arc spreading centers*, Geophys. Res. Letts., 29 (2002).

[17] C. Currie, K. Wang, R. Hyndman, and J. He, *The thermal effects of steady-state slab-driven mantle flow above a subducting plate: the Cascadia subduction zone and backarc*, Earth Plan. Sci. Lett., 223 (2004), pp. 35–48.

[18] O. o. F. E. Department of Energy, *Doe's fossil energy budget - fiscal year 2006*. `http://www.fossil.energy.gov/aboutus/budget/06/FY2006_Budget_.html`, 2006.

[19] J. Dolbow, M. A. Khaleel, and J. Mitchell, *Multiscale mathematics initiative: A roadmap*, tech. rep., U.S. Department of Energy, 2004.

[20] W. E and B. Engquist, *The heterogeneous multi-scale method*, in Proceedings of ICCM 2001, 2001.

[21] Y. Fang and M. Spiegelman, *Consequences of adiabatic decompression melting on magmatic channeling instabilities*, EOS Trans. Amer. Geophys. Union, 85 (2004). Fall Meet. Suppl., Abstract V21A-0595.

[22] C. I. for Geodynamics, *Computational infrastructure for geodynamics*. `http://www.geodynamics.org/`.

[23] A. Fowler, *A mathematical model of magma transport in the asthenosphere*, Geophys. Astrophys. Fluid Dyn., 33 (1985), pp. 63–96.

[24] Y. Furukawa, *Magmatic processes under arcs and formation of the volcanic front*, J. Geophys. Res., 98 (1993), pp. 8309–8319.

[25] T. Gerya and D. Yuen, *Rayleigh-taylor instabilities from hydration and melting propel 'cold plumes' at subduction zones*, Earth Plan. Sci. Lett., 212 (2003), pp. 47–62.

[26] M. Godard, J. Bodinier, and G. Vasseur, *Effects of mineralogical reactions on trace-element redistributions in mantle rocks during percolation processes - a chromatographic approach*, Earth Plan. Sci. Lett., 133 (1995), pp. 449–461.

[27] M. Gurnis, C. Hall, and L. Lavier, *Evolving force balance during incipient subduction*, Geochem. Geophys. Geosys., 5 (2004).

[28] M. Gutscher and S. Peacock, *Thermal models of flat subduction and the rupture zone of great subduction earthquakes*, J. Geophys. Res., 108 (2003).

[29] G. Hirth and D. Kohlstedt, *Experimental constraints on the dynamics of the partially molten upper mantle 2. deformation in the dislocation creep regime*, J. Geophys. Res., 100 (1995), pp. 15441–15052.

[30] ——, *Experimental constraints on the dynamics of the partially molten upper mantle: Deformation in the diffusion creep regime*, J. Geophys. Res., 100 (1995), pp. 1981–2002.

[31] G. Hirth and D. Kohlstedt, *Rheology of the upper mantle and the mantle wedge: A view from the experimentalists*, in The Subduction Factory, J. Eiler, ed., AGU Geophysical Monograph, AGU, 2003.

[32] B. Holtzman, N. Groebner, M. Zimmerman, S. Ginsberg, and D. Kohlstedt, *Stress-driven melt segregation in partially molten rocks*, Geochem. Geophys. Geosyst., 4 (2003). Art. No. 8607.

[33] U. Hornung, ed., *Homogenization and porous media*, vol. 6 of Interdisciplinary Applied Mathematics, Springer-Verlag, New York, 1997.

[34] T. Y. Hou and X.-H. Wu, *A multiscale finite element method for elliptic problems in composite materials and porous media*, J. Comput. Phys., 134 (1997), pp. 169–189.

[35] S. Karato and P. Wu, *Rheology of the upper mantle: A synthesis*, Science, 260 (1993), pp. 771–778.

[36] R. Katz and M. Spiegelman, *Progress towards an integrated computational model of magma genesis and transport in subduction zones*, in EOS Trans. Amer. Geophys. Union, vol. 85, 2004. Fall Meet. Suppl., Abstract V12A-04.

[37] R. Katz, M. Spiegelman, and S. Carbotte, *Ridge migration, asthenospheric flow and the origin of magmatic segmentation in the global mid-ocean ridge system*, Geophys. Res. Letts., 31 (2004).

[38] P. Kelemen, M. Braun, and G. Hirth, *Spatial distribution of melt conduits in the mantle beneath oceanic spreading ridges: Observations from the Ingalls and Oman ophiolites*, Geochem. Geophys. Geosys., 1 (2000). Paper 1999GC000012.

[39] P. Kelemen, M. Parmentier, J. Rilling, L. Mehl, and B. Hacker, *Thermal convection of the mantle wedge*, Geochim. Cosmochim. Acta, 66 (2002), pp. A389–A389.

[40] P. Kelemen, N. Shimizu, and V. Salters, *Extraction of mid-ocean-ridge basalt from the upwelling mantle by focused flow of melt in dunite channels*, Nature, 375 (1995), pp. 747–753.

[41] P. Kelemen, J. Whitehead, E. Aharonov, and K. Jordahl, *Experiments on flow focusing in soluble porous-media, with applications to melt extraction from the mantle*, J. Geophys. Res., 100 (1995), pp. 475–496.

[42] C. Kincaid and I. Sacks, *Thermal and dynamical evolution of the upper mantle in subduction zones*, J. Geophys. Res., 102 (1997), pp. 12295–12315.

[43] S. King, *Subduction zones: observations and geodynamic models*, Phys. Earth Planet. In., 127 (2001), pp. 9–24.

[44] M. Knepley, R. Katz, and B. Smith, *Numerical Solution of Partial Differential Equations*, Springer-Verlag, 2004, ch. Developing a Geodynamics Simulation with PETSc.

[45] D. McKenzie, *The generation and compaction of partially molten rock*, J. Petrol., 25 (1984), pp. 713–765.

[46] L. Montési, P. Kelemen, and M. Spiegelman, *Formation of inclined melt channels beneath mid-ocean ridges*, in EGS - AGU - EUG Joint Assembly Meet. Prog., 2003. Abstract 00224.

[47] L. Moresi, M. Gurnis, and S. Zhong, *Plate tectonics and convection in the earth's mantle: toward a numerical simulation*, Computing in Science & Engineering, 2 (2000), pp. 22–33.

[48] D. of Energy, *Department of Energy, environmental management*. `http://www.em.doe.gov/`.

[49] ——, *Basic energy sciences - fy 2006 congressional budget*. `http://www.sc.doe.gov/bes/archives/budget/BES_FY2006budget.pdf`, 2006.

[50] J. Renner, K. Visckupic, G. Hirth, and B. Evans, *Melt extraction from partially molten peridotites*, Geochem. Geophys. Geosyst., 4 (2003). 8606, doi:10.1029/2002GC000369.

[51] D. Scott and D. Stevenson, *Magma solitons*, Geophys. Res. Lett., 11 (1984), pp. 1161–1164.

[52] ——, *Magma ascent by porous flow*, J. Geophys. Res., 91 (1986), pp. 9283–9296.

[53] M. Spiegelman, *Flow in deformable porous media. Part 1. Simple analysis*, J. Fluid Mech., 247 (1993), pp. 17–38.

[54] M. Spiegelman, *Flow in deformable porous media. part 2. Numerical analysis—The relationship between shock waves and solitary waves*, J. Fluid Mech., 247 (1993), pp. 39–63.

[55] M. Spiegelman, *Physics of melt extraction: theory, implications, and applications*, Phil. Trans. R. Soc. London A, 342 (1993), pp. 23–41.

[56] ——, *Linear analysis of melt band formation by simple shear*, Geochem. Geophys. Geosys., 4 (2003). article 8615, doi:10.1029/2002GC000499.

[57] M. Spiegelman and T. Elliott, *Consequences of melt transport for uranium series disequilibrium in young lavas*, Earth Plan. Sci. Lett., 118 (1993), pp. 1–20.

[58] M. Spiegelman, R. Katz, and M. Jung, *Getting on the band wagon: analysis of melt localization instabilities due to mechanical shear*, EOS Trans. Amer. Geophys. Union, 85 (2004). Fall 2004 Meeting Suppl: V24-A02.

[59] M. Spiegelman and P. Kelemen, *Extreme chemical variability as a consequence of channelized melt transport*, Geochem. Geophys. Geosys., 4 (2003).

[60] M. Spiegelman, P. Kelemen, and E. Aharonov, *Causes and consequences of flow organization during melt transport: the reaction infiltration instability in compactible media*, J. Geophys. Res., 106 (2001), pp. 2061–2077.

[61] M. Spiegelman and D. McKenzie, *Simple 2-D models for melt extraction at mid-ocean ridges and island arcs*, Earth Plan. Sci. Lett., 83 (1987), pp. 137–152.

[62] M. Spiegelman and J. Reynolds, *Geochemistry in motion: Combined theoretical and observational evidence for convergent melt flow beneath the EPR*, Nature, 402 (1997), pp. 282–285.

[63] A. Staniforth and J. Cote, *Semi-Lagrangian advection schemes for atmospheric models - a review*, Monthly Weather Review, 119 (1991), pp. 2206–2223.

[64] D. Stevenson, *Spontaneous small-scale melt segregation in partial melts undergoing deformation*, Geophys. Res. Lett., 16 (1989), pp. 1067–1070.

[65] P. Tackley, *Effects of strongly variable viscosity on three-dimensional compressible convection in planetary mantles*, J. Geophys. Res., 101 (1996), pp. 3311–3332.

[66] ——, *Self-consistent generation of tectonic plates in three-dimensional mantle convection*, Earth Plan. Sci. Lett., 157 (1998), pp. 9–22.

[67] P. J. Tackley, *Mantle convection and plate tectonics: Toward an integrated physical and chemical theory*, Science, 288 (2000), pp. 2002–2007.

[68] ——, *Self-consistent generation of tectonic plates in time-dependent, three-dimensional mantle convection simulations, part 2: Strain weakening and asthenosphere*, Geochem. Geophys. Geosys., 1 (2000). Paper number 2000GC000043.

[69] E. Takazawa, T. Okayasu, and K. Satoh, *Geochemistry and origin of the basal lherzolites from the northern Oman ophiolite (northern Fizh block)*, Geochem. Geophys. Geosys., 4 (2003).

[70] P. van Keken, *The structure and dynamics of the mantle wedge*, Earth Plan. Sci. Lett., 215 (2003), pp. 323–338.

[71] P. van Keken, B. Kiefer, and S. Peacock, *High-resolution models of subduction zones: implications for mineral dehydration reactions and the transport of water into the deep mantle*, Geochem. Geophys. Geosys., 3 (2002).

[72] P. Van keken and S. Zhong, *Mixing in a 3d spherical model of present-day mantle convection*, Earth Plan. Sci. Lett., 171 (1999), pp. 533–547.

[73] C. Wiggins and M. Spiegelman, *Magma migration and magmatic solitary waves in 3-D*, Geophys. Res. Letts., 22 (1995), pp. 1289–1292.

A Budget and Budget Explanation

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. Barry Smith					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.			Funds Requested	Funds Granted
		CAL	ACAD	SUMR	by Applpicant	by DOE
1.	5 Barry Smith, PI	3.00			$50,385	
2.	4 Matthew Knepley, Co-PI	3.00			$37,041	
3.						
4.						
5.						
6. ( )	OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7.	(2) TOTAL SENIOR PERSONNEL (1-6)	6.00			$87,426	
B.	OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (1)	POST DOCTORAL ASSOCIATES	12.00			$92,064	
2. ( )	OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. (1)	GRADUATE STUDENTS				$10,848	
4. (1)	UNDERGRADUATE STUDENTS				$5,424	
5. ( )	SECRETARIAL - CLERICAL					
6. ( )	OTHER					
	TOTAL SALARIES AND WAGES (A+B)				$195,762	
C.	FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
	TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$195,762	
D.	PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
	TOTAL PERMANENT EQUIPMENT					
E.	TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$4,000	
	2. FOREIGN					
	TOTAL TRAVEL				$4,000	
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				$5,462	
	2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
	3. CONSULTANT SERVICES					
	4. COMPUTER (ADPE) SERVICES					
	5. SUBCONTRACTS					
	6. OTHER					
	TOTAL OTHER DIRECT COSTS				$5,462	
H.	TOTAL DIRECT COSTS (A THROUGH G)				$205,224	
I.	INDIRECT COSTS (SPECIFY RATE AND BASE)					
	TOTAL INDIRECT COSTS				$69,776	
J.	TOTAL DIRECT AND INDIRECT COSTS (H+I)				$275,000	
K.	AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L.	TOTAL COST OF PROJECT (J+K)				$275,000	

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. Barry Smith				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. CAL	ACAD	SUMR	Funds Requested by Applpicant	Funds Granted by DOE
1. 5 Barry Smith, PI	3.00			$52,231	
2. 4 Matthew Knepley, Co-PI	3.00			$38,398	
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (2) TOTAL SENIOR PERSONNEL (1-6)	6.00			$90,629	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (1) POST DOCTORAL ASSOCIATES	12.00			$95,508	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. (1) GRADUATE STUDENTS				$11,245	
4. (1) UNDERGRADUATE STUDENTS				$5,623	
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$203,005	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$203,005	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$4,160	
2. FOREIGN					
TOTAL TRAVEL				$4,160	
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				$5,521	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS				$5,521	
H. TOTAL DIRECT COSTS (A THROUGH G)				$212,687	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS				$72,313	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$285,000	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$285,000	

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:** 3 of 4	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Dr. Barry Smith				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.			Funds Requested by Applicant	Funds Granted by DOE
	CAL	ACAD	SUMR		
1. 5 Barry Smith, PI	3.00			54,141	
2. 4 Matthew Knepley, Co-PI	3.00			39,802	
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (2) TOTAL SENIOR PERSONNEL (1-6)	6.00			$93,944	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (1) POST DOCTORAL ASSOCIATES	12.00			$99,069	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. (1) GRADUATE STUDENTS				$11,656	
4. (1) UNDERGRADUATE STUDENTS				$5,828	
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$210,497	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$210,497	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$4,326	
2. FOREIGN					
TOTAL TRAVEL				$4,326	
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				$9,057	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS				$9,057	
H. TOTAL DIRECT COSTS (A THROUGH G)				$223,881	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS				$76,119	
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	

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. Barry Smith				Requested Duration: 3-Year Total	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.			Funds Requested	Funds Granted
	CAL	ACAD	SUMR	by Applpicant	by DOE
1. Barry Smith, PI	9.00			$156,757	
2. Matthew Knepley, Co-PI	9.00			$115,242	
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (2) TOTAL SENIOR PERSONNEL (1-6)	18.00			$271,999	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (1) POST DOCTORAL ASSOCIATES	36.00			$286,642	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. (1) GRADUATE STUDENTS				$33,749	
4. (1) UNDERGRADUATE STUDENTS				$16,875	
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$609,264	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$609,264	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$12,486	
2. FOREIGN					
TOTAL TRAVEL				$12,486	
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				$20,040	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS				$20,040	
H. TOTAL DIRECT COSTS (A THROUGH G)				$641,791	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS				$218,209	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$860,000	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$860,000	

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. Barry Smith		
The PI's effort charged per year to this proposal is :		3.00	man-months
Senior Personnel support includes:	Matthew Knepley, Co-PI	3.00	man-months
Post doctoral appointees' effort charged per year to this proposal is :		12.00	man-months
Graduate Students	Semester = 3 month appointment	3.00	man-months
Undergraduate Students	Semester = 3 month appointment	3.00	man-months

E Travel

Domestic: $1K per trip/escalate 4.0% per yr.
Projecting 1-trip per staff member per year to present results/status to collaborative instituitions.
Projecting 1-trip per staff member per year to present results at Conference.-TBD

G Other Direct Costs

1. Materials and Supplies:
Software, low-end computers (<$5k), computer supplies/ peripherals, and misc supplies.

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 Budget Page (See reverse for Instructions)	OMB Control No. 1910-1400 OMB Burden Disclosure Statement on Reverse

ORGANIZATION The Trustees of Columbia Univeristy in the City of New York				**Budget Page No:** Year 1	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Marc Spiegelman				Requested Duratior 12 (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	SUMF	by Applpicant	by DOE
1. Prof. Marc Spiegelman, P.I.	0.00	0.00	2.00	$21,067	
2.	0.00			$0	
3.					
4.					
5.					
6. (0) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. ( ) TOTAL SENIOR PERSONNEL (1-6)	0.00	0.00	2.00	$21,067	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (1) POST DOCTORAL ASSOCIATES	12.00			$45,000	
2.(0) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. (1) GRADUATE STUDENTS GRA				$24,750	
4. (0) UNDERGRADUATE STUDENTS					
5. (0) SECRETARIAL - CLERICAL	0.00				
6. (0) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$90,817	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS) 26.40%				$17,442	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$108,258	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.) Computer /Lap Top					
TOTAL PERMANENT EQUIPMENT				$3,000	
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$5,000	
2. FOREIGN				$0	
TOTAL TRAVEL				$5,000	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL				$0	
4. OTHER (fully explain on justification page)				$0	
TOTAL PARTICIPANTS ( ) TOTAL COST				$0	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				$1,000	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				$3,000	
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES				$0	
5. SUBCONTRACTS				$0	
6. OTHER tutition fee/1 GRA 05-06				$15,724	
TOTAL OTHER DIRECT COSTS				$19,724	
H. TOTAL DIRECT COSTS (A THROUGH G)				$135,982	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) 61.00% ICR on campus of 117258 = 71,528					
TOTAL INDIRECT COSTS				$71,528	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$207,509	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES				$0	
L. TOTAL COST OF PROJECT (J+K)				$207,509	

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

GANIZATION The Trustees of Columbia Univeristy in the City of New York				Budget Page No: Year 2	
INCIPAL INVESTIGATOR/PROJECT DIRECTOR Marc Spiegelman				Requested Duratior 12 (Months)	
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	SUMF	by Applpicant	by DOE
Prof. Marc Spiegelman, P.I.	0.00	0.00	2.00	$21,699	
				$0	
				$0	
				$0	
			0.00	$0	
0) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
(1) TOTAL SENIOR PERSONNEL (1-6)	0.00	0.00	2.00	$21,699	
OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1) POST DOCTORAL ASSOCIATES				$46,350	
0) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				$0	
1) GRADUATE STUDENTS GRA				$25,493	
0) UNDERGRADUATE STUDENTS				$0	
0) SECRETARIAL - CLERICAL				$0	
0) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$93,541	
FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS) 26.40%				$17,965	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$111,506	
PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$5,000	
2. FOREIGN				$0	
TOTAL TRAVEL				$5,000	
TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL				$0	
4. OTHER (fully explain on justification page)				$0	
TOTAL PARTICIPANTS ( ) TOTAL COST				$0	
OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				$1,030	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				$3,090	
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES				$0	
5. SUBCONTRACTS					
6. OTHER Tuition fee/1 GRA 06/07				$16,196	
TOTAL OTHER DIRECT COSTS				$20,316	
TOTAL DIRECT COSTS (A THROUGH G)				$136,822	
INDIRECT COSTS (SPECIFY RATE AND BASE) 61.00% ICR on campus of 120626 = 73,582					
TOTAL INDIRECT COSTS				$73,582	
TOTAL DIRECT AND INDIRECT COSTS (H+I)				$210,404	
AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES				$0	
TOTAL COST OF PROJECT (J+K)				$210,404	

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 Columbia Univeristy in the City of New York				**Budget Page No:** Year 3	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Marc Spiegelman				Requested Duratior 12 (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. Prof. Marc Spiegelman, P.I.	0.00	0.00	2.00	$22,350	
2.	0.00	0.00	0.00	$0	
3.				$0	
4.				$0	
5.				$0	
6. (0) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (1) TOTAL SENIOR PERSONNEL (1-6)	0.00	0.00	2.00	$22,350	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (1) POST DOCTORAL ASSOCIATES				$47,741	
2.(0) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				$0	
3. (1) GRADUATE STUDENTS GRA				$26,257	
4. (0) UNDERGRADUATE STUDENTS				$0	
5. (0) SECRETARIAL - CLERICAL				$0	
6. (0) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$96,347	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS) 26.40%				$18,504	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$114,851	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT				$0	
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$5,000	
2. FOREIGN				$0	
TOTAL TRAVEL				$5,000	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL				$0	
4. OTHER (fully explain on justification page)				$0	
TOTAL PARTICIPANTS ( ) TOTAL COST				$0	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				$1,061	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				$3,183	
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER TutionFees 1 GRA 07/08				$16,682	
TOTAL OTHER DIRECT COSTS				$20,926	
H. TOTAL DIRECT COSTS (A THROUGH G)				$140,777	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) 61.00% ICR on campus of 124095 = 75,698					
TOTAL INDIRECT COSTS				$75,698	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$216,475	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES				$0	
L. TOTAL COST OF PROJECT (J+K)				$216,475	

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 Columbia Univeristy in the City of New York				Budget Page No: Cumulative	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Marc Spiegelman				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.			Funds Requested by Applpicant	Funds Granted by DOE
	CAL	ACAD	SUMR		
1. Prof. March Spiegelman, P.I.	0.00	0.00	6.00	$65,115	
2.				$0	
3.					
4.					
5.					
6. (0) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (1) TOTAL SENIOR PERSONNEL (1-6)	0.00	0.00	6.00	$65,115	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (1) POST DOCTORAL ASSOCIATES				$94,091	
2.(0) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				$0	
3. (1) GRADUATE STUDENTS GRA				$76,500	
4. (0) UNDERGRADUATE STUDENTS				$0	
5. (0) SECRETARIAL - CLERICAL				$0	
6. (0) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$235,705	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS) 26.4%.				$53,910	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$289,615	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT				$3,000	
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$15,000	
2. FOREIGN				$0	
TOTAL TRAVEL				$15,000	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL				$0	
4. OTHER (fully explain on justification page)				$0	
TOTAL PARTICIPANTS ( ) TOTAL COST				$0	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				$3,091	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				$9,273	
3. CONSULTANT SERVICES				$0	
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS				$0	
6. OTHER tuition fees 02-05/1 students cumulative				$48,602	
TOTAL OTHER DIRECT COSTS				$60,966	
H. TOTAL DIRECT COSTS (A THROUGH G)				$413,581	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) 61.00% ICR on campus of 361979 = 220,807					
TOTAL INDIRECT COSTS				$220,807	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$634,388	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES				$0	
L. TOTAL COST OF PROJECT (J+K)				$634,388	

BUDGET EXPLANATION PAGE

FOR COMPLETING
DOE F 4620.1 (Budget Page)
This Budget Explanation describes the 3 year Cumulative part for Columbia University for Inclusion in the proposal
A full year-by-year Explanation is included in the Columbia IIPS submission

SECTION

A. Senior Personnel **Cum 3 years**

Name	Position	Hours/Time	Project Dollars
			$65,115
Marc Spiegelman P.I.	**Prof.**	**2 months/year**	

List any personnel, funds for salary, and the number of person months on Budget Page.

B. Other Personnel

$170,590

Name	Position	Hours/Time
Richard Katz	Post-Doctoral Res. Sci.	12 months/year
Gideon Simpson	Graduate Res Assistant	20/hrs week

List any personnel, funds for salary, and the number of person months on Budget Page.
Must be listed individually on budget page, their rate of pay and % as well as length of time working on the project. Also include a written narrative that fully justifies the need for requested personnel

Salaries/Wages are based upon University/Company established rates/salaries which are comparable to others doing similar research effort both within and outside the University/Private Industry.

C. ☑ **Fringe Benefits**

$53,910

Must include the current fringe benefit rate established for your organization as well as the total cost or a list of cost and type for each individual employed on the project.

☐ Fringe Benefit rate(s) based upon an approved rate from _______________ (Approved by Federal Agency rate DCAA, DHHS, etc. …)

If Fringe Benefit rate is not approved, attach backup documentation to support the basis of your estimate.

D. Equipment **List each item, its cost and reason it is needed for the project**

$3,000

Computer laptop (year 1) Just year 1

Justification
Provide laptop to new GRA

☐ Cost estimates are based upon quotes from vendors or catalog series.
☐ Cost estimates are based on past experience of purchases of similar or like items.

Cost estimate is based upon Similar Past Purchases (Powerbook G4 15")

E. Travel

$5,000

Destination/Number of Individuals	Lodging/Subsistence	Cost Estimate	From		To	
NYC/Chicago collab, 3 person	1,000/person	$3000/year	From	TBD	To	
AGU San Fran or SIAM CS&E (TBD) 2 person	1,000/person	$2000/year	From	12/5/2005	To	12/9/05
			From		To	

List each trip's destination, dates, estimated costs including transportation and subsistence, number of staff traveling and the purpose of the travel and how it related to the project personnel

☐ Travel cost estimates are based upon quotes from vendors or catalog series

F. Trainee/Participant Costs

$0

Names

☒

Dates From ______ to ______ Location ______

Number of Participants ______ Cost for each Participant $ ______

Educational projects that intend to support trainees (pre-college, college, graduate and post graduate) must list each trainee cost that includes stipend levels and amounts, cost of tuition for each trainee, cost of any travel (provide the same information as needed under the regular travel category, Item E), and costs for any related training expenses. Participant costs are those costs associated with conferences, workshops, symposia or institutes and breakout items should indicate the number of participants, cost for each participant, purpose of the conference, dates and places of meetings and any related administrative expenses.

Trainee cost estimates are based upon past experience of support of similar number of trainees on similar projects.
Participant cost estimates are based upon past experience of support of similar number of participants attending similar conferences/workshops/symposia.

G. Other Direct Costs

$60,966

1. Materials and Supplies: indicate types required and estimate of cost.
2. Publication Costs/Documentation/Dissemination: Estimate cost of preparing and publishing project results.
3. Consultant Services: Indicate name. Daily compensation, number of days service required and justify.
4. Computer (ADP) Services: Include justification based upon established computer service rates at the proposing institution. Purchase of equipment falls under section D above.
5. Subcontracts: Include a budget and justify details.
6. Other: Itemize and justify details. Under this item list tuition remission for students employed to work on this project listed under the personnel category. (Do not include tuition remission if this costs is included under fringe benefit category).

Cost estimates are based upon past experience of purchase of similar or like items.
Cost estimates are based upon quotes/past experience of purchase of similar computer services.
☒ Subcontract/Consultant cost estimates are based upon previous experience/quotes for similar or like services.
☒ Other Direct Cost estimate is based upon ______

H. Total Direct Costs

$413,581

I. Indirect Costs

$220,807

Indirect Cost rate(s) is based upon approved rate from ______ (Federal Agency Approved rate, DCAA, DHHS, etc…)

Please attach a copy of rate approval letter (if not submitted previously). If Indirect Cost rate(s) is not approved, attach backup documentation to support the basis of your estimate (Tax records, copies of accounting information, etc,…)

J. Total Direct and Indirect Costs

$634,388

☒

☒

K. Amount of Cost Sharing

$

List the amount of proposed Cost Sharing and also provide the basis of the cost sharing. This will include the estimate of cost and copies of documentation you based the estimate on.

L. Total Cost of Project **$634,388**

RENEWAL AWARDS

ESTIMATE OF UNOBLIGATED BALANCES

- ☐ I estimate that **all** funds will be obligated before the end date of the *previous* project period.
- ☐ I estimate that **$ ____________** funds will remain to be carried forward into the next project period.

3 Year Cumulative 07/01/05-06/30/2008:

Personnel on DOE Grant "Reactive Channelization in Large-scale Solid Mantle flow"

Prof. Marc Spiegelman : Is Principal Investigator and Project Director. Has extensive experience in mathematics and computation of coupled fluid/solid flows with applications to magma dynamics. Will supervise Post-docs and GRA's.

Richard Katz: Post Doctoral Research Scientist (Currently DOE CSGF Fellow, expected Ph.D, 9/2005). Has extensive experience in high-performance computing for solid-earth dynamics. Has developed the majority of Solid-Earth/magma codes within the PETSc framework. Maintains close collaboration with Co-PI's Smith and Knepely and PETSc ANL group.

Graduate Research Assistant: Gideon Simpson. Applied Mathematician with expertise in analysis of PDE's and homogenization. Co-supervised by Michael I Weinstein (Columbia Applied Mathematics). Will work on analysis of solitary waves and variational multi-scale methods for magma dynamics.

Travel Justification:
Domestic: (2 to Fall AGU San Francisco, Dec 2005, Dec 2007, 2 to SIAM CS&E (TBD) 2006)
$2,000/year
New York to Chicago Collaborative meetings: 1 trip/person @ $1000/trip $3,000/year
Total $5,000/year

Materials &Supplies:

Limited purchases of software, and office supplies, telephone: research related toll calls, Services: Xeroxing, mailings, and printing. $1000/escalate 3%/year

Publications: $3000/escalate 3%/year (AGU/JGR Solid-Earth, Page charges plus color publication charges, 2-3 publications)

Tuition remission, Columbia University: Year 1, $15,724; Year 2, $16,196 GRA; Year 3, $16,682

B Current and Pending Support of Investigators

MATTHEW G. KNEPLEY

Current Support

Project Name	Sponsor	FY05	Date	Effort
Terascale Optimal PDE	DOE MICS	$884K	10/01/04-	
Simulation Center	SciDAC		09/30/05	50%
Computational Infrastructure	NSF	$140K	10/01/05	
for Geodynamics		(ANL)	09/30/08	50%

Pending Support

Project Name	Sponsor	FY05	Date	Effort
Reactive Channelization in	DOE MICS	$450K	07/01/05-	
Large-Scale Solid Mantle Flow			06/30/08	50%

Notes

1. Effort will be adjusted if the pending proposals are funded.

2. Unless otherwise noted, FY05 budget data is for the entire project.

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
3/11/05

MARC SPIEGELMAN

A Supporting Agency	B Project Title	C Award Amount	D Period Covered Award	E Man-Month Acad. Sum. Cal.	F Location
A. Current Support					
NSF DGE 02-21041	IGERT: A JOINT GRADUATE PROGRAM IN APPLIED MATHEMATICS AND THE EARTH & ENVIRONMENTAL SCIENCES. (POLVANI, L., PI; PHONG, D., SPIEGELMAN, M., LALL, U., DE LA PENA, V., CO-PI)	1,554,710	12/15/02 11/30/04	N/C	CU
NSF EAR 04-41230	25TH INTERNATIONAL CONFERENCE ON MATHEMATICAL GEOPHYSICS. (SPIEGELMAN, M., PI)	10,000	8/15/04 7/31/05	N/C	LDEO
ONR N00014-03-1-0140	2D AND 3D MODELING OF THE STRATIGRAPHIC SEQUENCES AT THE ADRIATIC AND RHONE CONTINENTAL MARGINS (STECKLER, M.; w/SPIEGELMAN, M.)	292,351	10/15/02 9/30/05	4	LDEO
NSF OCE 01-37108	COLLABORATIVE RESEARCH: GEOCHEMICAL CONSEQUENCES OF MELT CHANNELING: EXPLORING A NEW CLASS OF MODELS FOR GEOCHEMICAL VARIABILITY. (SPIEGELMAN, M., PI)	240,307	3/1/02 2/28/05	1/1/1 summer	LDEO/APAM
B. Pending Support					
NSF #11128	UNDERSTANDING MAGMA GENESIS IN SUBDUCTION ZONES: NEW MODELS FOR REACTIVE HYDOUS MELTING AND TRANSPORT. (SPIEGELMAN, M., PI)	102,664	9/1/05 8/30/06	0.5 summer	LDEO
NSF #10976	RIDGE 2000 POSTDOC: DYNAMICS OF COUPLED TECTONIC HYDROTHERMAL SYSTEMS AT MID-OCEAN RIDGES; A DAMAGE RHEOLOGY APPROACH. (SPIEGELMAN, M., PI (ADVISOR))	131,170	3/1/05 2/28/07	N/C	LDEO
NSF DMS 0530853	CMG RESEARCH: ANALYTICAL AND COMPUTATIONAL STUDIES OF MAGMA DYNAMICS (WEINSTEIN, MI, PI, SPIEGELMAN, M CO-PI)	316,627	9/1/05 8/31/08	1/1/1 summer	CU/APAM
DOE This Proposal	REACTIVE CHANNELIZATION IN LARGE-SCALE MANTLE FLOW (SPIEGELMAN, PI; SMITH, B, CO-PI; KNEPLEY, M CO-PI)	630,583	7/1/05 6/30/08	2/2/2 summer	CU/APAM
C. Outstanding Increments					
NSF DGE 02-21041	YEAR 3, 4 & 5: IGERT: A JOINT GRADUATE PROGRAM IN APPLIED MATHEMATICS AND THE EARTH & ENVIRONMENTAL SCIENCES. (POLVANI, L., PI; PHONG, D., SPIEGELMAN, M., LALL, U., DE LA PENA, V., CO-PI)	1,624,216	12/1/04 11/30/07	N/C	CU

D. Proposals Planned to be Submitted in Near Future:
NONE

E. Transfer of Support:
NONE

F. Other Agencies to Which Proposal Has Been/Will be Submitted:
NONE

C Biographical Sketches

Biographical Sketch: Richard F. Katz

Department of Earth and Environmental Science
Lamont Doherty Earth Observatory
of Columbia University
Palisades, New York 10964

Phone: 845-365-8462
Fax: 845-365-8150
Web: `www.ldeo.columbia.edu/~katz`
E-mail: `katz@ldeo.columbia.edu`

Professional Preparation

2000 - B.A. Science of Earth Systems, Cornell University.

2003 - Summer practicum participant, Division of Mathematics & Computer Science, Argonne National Lab.

2004 - M.Phil. Geodynamics, Columbia University.

2005 - (Expected) Ph.D. Geodynamics, Columbia University.

Honors

Outstanding Student Paper Award, Meeting of the American Geophysical Union, Fall 2001 and Spring 2003.

Department of Energy Computational Science Graduate Fellowship, 2001-present.

National Science Foundation Graduate Research Fellowship (declined).

Graduated *Cum Laude* and member of Phi Beta Kappa, Cornell University, 2000.

Publications Related to the Proposed Research

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

Katz, R. F. and M. Spiegelmam, Progress towards an integrated computational model of magma genesis and transport in subduction zones. *Eos Trans. AGU*, 85(47), Fall Meet. Suppl., Abstract V12A-04, 2004.

Katz, R.F., M. Spiegelman and S. Carbotte, Ridge migration, asthenospheric flow and the origin of magmatic segmentation in the global mid-ocean ridge system, *Geophys. Res. Lttrs.* 31(15):L15605, 2004.

Synergistic Activities

Instructor for Environmental Science for Decision Makers—Quantitative Analysis Section, School of International Policy and Affairs. Responsible for design of class, 1 weekly lecture, writing and grading problem sets, office hours.

Collaborators

Matthew Knepley (Argonne), Charles Langmuir (Harvard), Craig Manning (UCLA), Barry Smith (Argonne), Marc Spiegelman (Columbia)

Biographical Sketch: Matthew G. Knepley

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

Phone: 630-252-1870
Fax: 630-252-5986
E-mail: knepley@mcs.anl.gov

Professional Preparation

1994 - B.S. Mathematical Physics, Case Western Reserve University.

1996 - M.S. Computer Science, University of Minnesota.

2000 - Ph. D. Computer Science, Purdue University.

Appointment

Assistant Scientist, Argonne National Laboratory, 2004 –

Honor Societies

Sigma Xi (1993)

Phi Beta Kappa (1994)

Golden Key (1994)

Upsilon Pi Epsilon (2000)

Publications Related to the Proposed Research

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

S. Balay, K. Buschelman, V. Eijkhout and W. Gropp, D. Kaushik, M. Knepley, L. McInnes, B. Smith, and H. Zhang, *PETSc 2.0 Users Manual*, Argonne National Laboratory Report, 2005.

Robert C. Kirby, Matthew G. Knepley, and L. Ridgway Scott, *Optimal Evaluation of Finite Element Matrices*, Technical Report TR2004-04, Department of Computer Science, University of Chicago, 2004.

Matthew G. Knepley, Ahmed H. Sameh, and Vivek Sarin, *Design of Large Scale Parallel Simulations*, Proceedings of Parallel Computational Fluid Dynamics '99, David Keyes, et.al., Ed., Elsevier North-Holland, 1999.

Matthew G. Knepley and Vivek Sarin, *Algorithm Development for Large Scale Computing*, Proceedings of the SIAM Workshop on Object-Oriented Methods for Interoperable Scientific and Engineering Computing, October 1998.

Matthew G. Knepley and Denis Vanderstraeten, *Parallel Building Blocks for Finite Element Simulations*, Proceedings of Parallel Computational Fluid Dynamics '97, R. Emerson, et.al., Ed., Elsevier North-Holland, pp. 281–287, 1998.

Synergistic Activities

My work on PETSc (Portable, Extensible Toolkit for Scientific computation) (`www.mcs.anl.gov/petsc`) has been to extend it with packages that support meshing, finite element discretization, and an abstract language for PDEs.

Collaborators

Robert Kirby (University of Chicago), David Keyes (Columbia), Barry Smith (Argonne), Mike Gurnis (Caltech), Michael Aivasiz (Caltech), Marc Spiegelman (Columbia), Richard Katz (Columbia), L. Ridgway Scott (University of Chicago)

Biographical Sketch: 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

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

S. Balay, K. Buschelman, V. Eijkhout and W. Gropp, D. Kaushik, M. Knepley, L. McInnes, B. Smith, and H. Zhang, *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), Matthew Knepley (Argonne), Lois McInnes (Argonne), Boyana Norris (Argonne), Marc Spiegelman (Columbia) Xianzhu Tang (LANL)

Biographical Sketch: Marc Spiegelman

Dept. of Applied Physics and Applied Mathematics
Dept. of Earth and Environmental Sciences
Columbia University
New York, NY 10027

Phone: 212-854-4918
Phone: 845-365-8425
Fax: 845-365-8150
E-mail: `mspieg@ldeo.columbia.edu`

Professional Preparation

1985 - B.S. Earth Science, Harvard University.

1989 - Ph.D. Geophysics, Cambridge University, U.K.

1989–1991 - Lamont Postdoctoral research Fellowship, LDEO/Columbia.

Appointment

Assoc. Prof. Columbia University: Joint DAPAM/DEES, 2000–

Research Scientist LDEO/Adj. Assoc. Prof DEES, 1997–1999

Storke-Doherty Lecturer LDEO/DEES, 1993–1997

Assoc. Res. Scientist LDEO, 1991–1993

Honors

2003 SEAS Alumni Teaching Award

2002 DEES Outstanding Teaching Award

1998 DEES Outstanding Teaching Award

1993 First Storke-Doherty Lecturer, LDEO

1992 Storke Research Award, LDGO

1988 Lamont Post-doctoral Fellowship

1985 Marshall Scholarship

Publications Related to the Proposed Research

Katz, R., M. Spiegelman, and S. Carbotte [**2004**]. Ridge migration, asthenospheric flow and the origin of magmatic segmentation in the global mid-ocean ridge system. *Geophys. Res. Lett.*, **31**(15). Art. No. L15605.

Spiegelman, M. [**2003**]. Linear analysis of melt band formation by simple shear. *Geochem. Geophys. Geosyst.*, **4**(9). Article 8615, doi:10.1029/2002GC000499.

Spiegelman, M. and P. B. Kelemen [**2003a**]. Extreme chemical variability as a consequence of channelized melt transport. *Geochem. Geophys. Geosyst.*, **4**(7). Article 1055, doi:10.1029/2002GC000336.

SPIEGELMAN, M., P. B. KELEMEN, and E. AHARONOV [**2001**]. Causes and consequences of flow organization during melt transport: The reaction infiltration instability in compactible media. *J. Geophys. Res.*, **106**(B2):2061–2077.

WIGGINS, C. and M. SPIEGELMAN [**May 15 1995**]. Magma migration and magmatic solitary waves in 3-D. *Geophys. Res. Lett.*, **22**(10):1289–1292.

SPIEGELMAN, M. [**1993**]. Flow in deformable porous media. part 1. Simple analysis. *J. Fluid Mech.*, **247**:17–38.

SPIEGELMAN, M. [**1993a**]. Flow in deformable porous media. part 2. Numerical analysis—The relationship between shock waves and solitary waves. *J. Fluid Mech.*, **247**:39–63.

Synergistic Activities

CIG Executive committee: Vice-Chair 2004–present
CIG Organizing committee: 2003–2004
Secretary: IUGG Committee on Mathematical Geophysics - 2000–present
Contributor McNair Cities Project – 2004: project to enhance materials and earth science education in NYC high schools.
LDEO OpenHouse: –demonstrate basic fluid mechanics and rheology to the public.

Collaborators

Einat Aharonov (Weizmann, Israel) Tim Elliott (University of Bristol, U.K.), Richard Katz (Columbia), Peter Kelemen (Columbia/LDEO), David Keyes (Columbia), Matthew Knepley (Argonne), Craig Manning (UCLA), Dan McKenzie (University of Cambridge, U.K.), Lorenzo Povani (Columbia), Michael I Weinstein (Columbia)

D Description of Facilities and Resources

Argonne National Laboratory

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 a 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.

E Letters of Intent from Collaborators

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 22, 2005

Dear Marc,

It is my great pleasure to continue our collaboration with your new proposal: Reactive Channelization in Large-scale Solid Mantle Flow. With your expertise in geodynamics and our experiences developing and implementing innovative numerical algorithms I think we have a great opporunity to develop a much more quantative understanding of channalization.

I expect to devote my time in this work to assisting with developing the appropriate fine level discretizations, coarse graining process and numerical solvers.

Sincerely,

Barry Smith

ARGONNE NATIONAL LABORATORY

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

Telephone: (630) 252-1870
Faxphone: (630) 252-5986
Email: knepley@mcs.anl.gov

March 25, 2005

Dear Marc,

It is my great pleasure to continue our collaboration with your new proposal: Reactive Channelization in Large-scale Solid Mantle Flow.

I am excited to start developing novel coupling algorithms between the various physical regimes and problem scales. I expect to manage the development process as well, in conjunction with my role in the NSF CIG project.

Sincerely,

Matthew G. Knepley
Assistant Scientist

COLUMBIA UNIVERSITY
IN THE CITY OF NEW YORK
LAMONT-DOHERTY EARTH OBSERVATORY

March 23, 2005

Dear Marc,

I look forward to a continuing collaboration with you under your new proposal: Reactive Channelization in Large-scale Solid Mantle Flow. We have developed a suite of research codes that give us a strong base on which to build simulations of magma/mantle dynamics. By working closely with Barry Smith and Matt Knepley of Argonne National Laboratory we will be able to develop and employ sophisticated computational tools that are critical for further progress in addressing the multiscale nature of these problems.

I expect to devote my time in this work to developing application codes that leverage computational tools for problems of magma migration in the convecting mantle and to exploration and interpretation of the results.

Sincerely,

Richard F. Katz

P.O. Box 1000 61 Route 9W Palisades, NY 10964-8000 USA 845-365-2900 http://www.ldeo.columbia.edu

F Figures

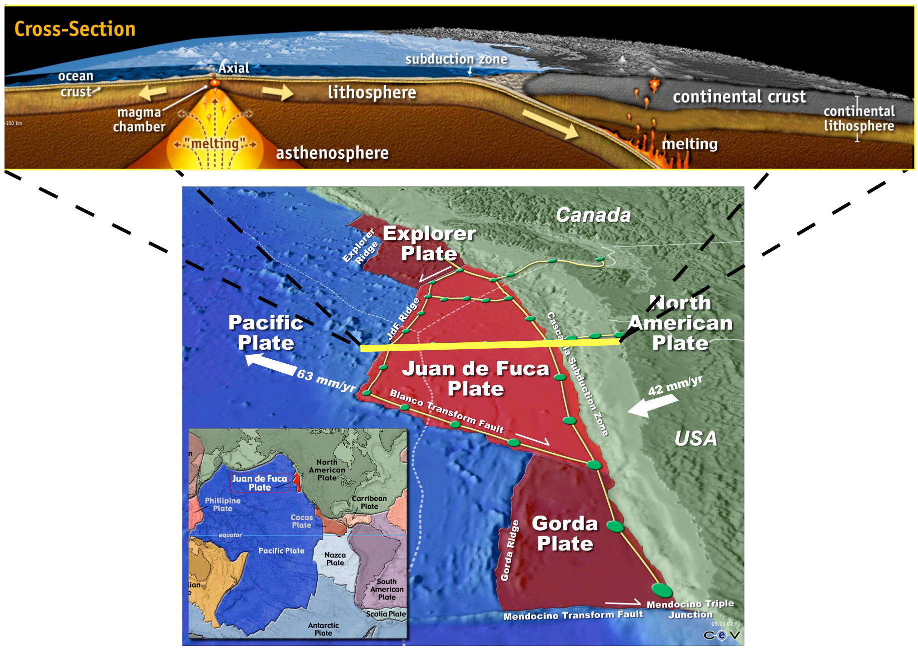


Figure F.1: The distribution of global tectonic plates and the structure of partially molten magmatic regions at plate boundaries. The inset map shows the global distribution of plates with emphasis on the Juan de Fuca plate off the pacific northwest coast. Cross-section at top shows a vertical slice through the plates highlighting both mid-ocean ridge spreading centers and the subduction zones of the pacific northwest (compare with actual quantitative calculations in Figure F.2). Images provided courtesy of the NEPTUNE Project (www.neptune.washington.edu) and produced by CEV. The NEPTUNE Project is designed to implement a real-time cabled sea-floor observatory (green dotted line) to observe the dynamics of the Juan de Fuca Plate and the water column above it.

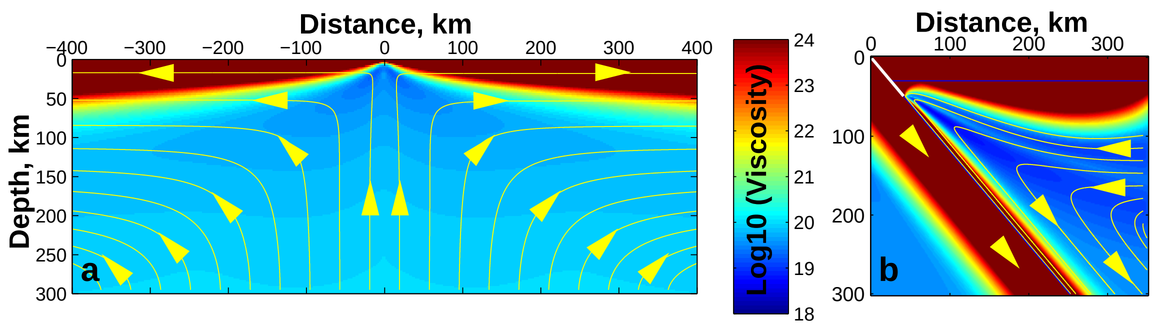


Figure F.2: Results from numerical solution of the mantle dynamics equations (1.1)–(1.6) in the limit of no porosity and melting ($\phi = \Gamma = 0$) showing quantitative models for solid flow and thermal structure beneath mid-ocean ridges and subduction zones (compare with cartoons in Figure F.1). Colors show the log of the viscosity, η which is a non-linear function of temperature, pressure and stress; streamlines show the solid flow field, $\mathbf{V}$. Buoyancy is neglected and thus flow is passively driven by the boundary conditions. Panel **a** shows 2-D simulation results perpendicular to a mid-ocean ridge. The lithospheric plates are cold and thus highly viscous and move rigidly away from the spreading center. Hot, lower viscosity solid mantle rises beneath the ridge and is accreted onto the lithospheric plates. Panel **b** shows a 2D simulation of a subduction zone. Flow is driven by the kinematically prescribed subducting lithosphere that enters the domain in the upper left corner and descends at 50° from vertical.

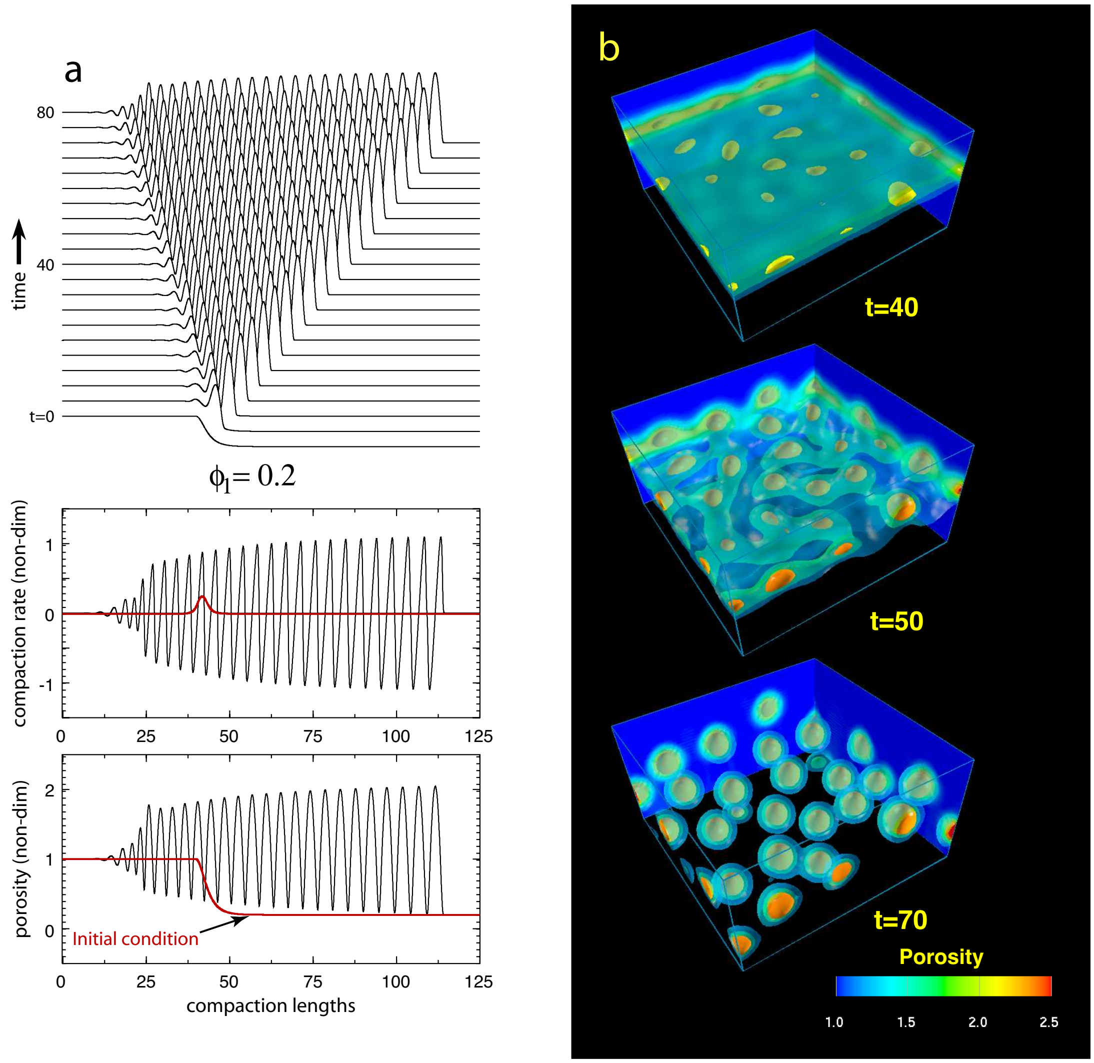


Figure F.3: Development of non-linear porosity waves in magma dynamics. (**a**) Solitary waves in 1-D showing the dispersion of an initial step in flux into a rank ordered train of non-linear waves (In this figure, gravity moves fluid from left to right). In the absence of viscous volume changes, this initial condition would simply generate a single Burger's shock [53]. Accurate solution of solitary waves require resolving the smallest compaction length in the system (i.e. the region preceding the waves). Because the system is dispersive, however, these regions move and eventually fill space. (**b**) Instability of a 1-D porosity wave to 3-D spherically symmetric solitary waves [73]. 3-D calculations use a combination of semi-lagrangian advection schemes (e.g.[63]) and geometric multi-grid to produce efficient algorithms that scale as $O(N)$.

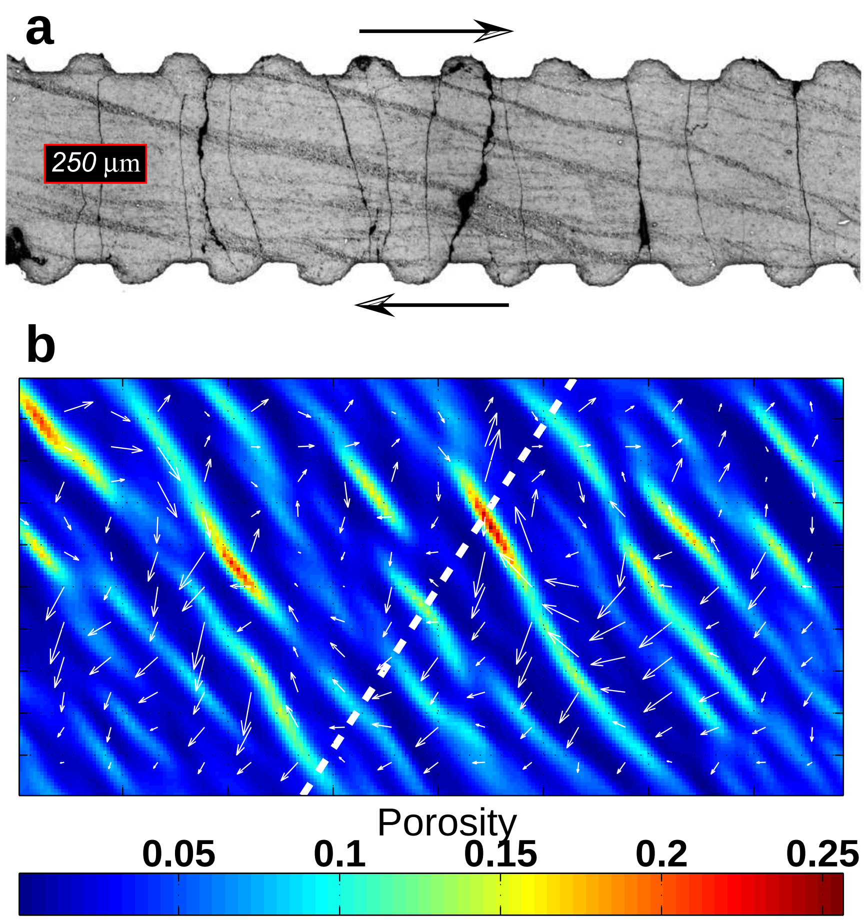


Figure F.4: Porosity banding in experiments (**a**) and simulations (**b**). (**a**) Experimental results from [32] showing the localization of melt into high porosity bands produced through a feedback between porosity and solid shear viscosity. The bands appear as dark colored, low angle stripes in **a** (the vertical black lines are decompression cracks, an experimental artifact). The bands form from a homogeneous initial state by strains of ~ 1 and persist at low angles to the shear plane ($\sim$ 15–30°) to large strains. The spacing of the bands is somewhat variable but the largest bands are separated by many grains yet are on scales smaller than the estimated compaction length of the sample (here about the width of the sample). (**b**) Numerical solutions of Eqs. (1.1)–(1.4) neglecting melting and gravity ($\Gamma = 0$ and $\mathbf{g} = 0$) which is appropriate for lab-scale samples [58]. In these calculations, the solid shear viscosity is a decreasing function of porosity (here $\eta \propto \exp(-\alpha\phi)$ with $\alpha = 30$ [32]). Thus shear across weak regions, causes the pressure to drop, drawing in more melt in a positive feedback. The initial condition is constant porosity plus a small amount of Gaussian white-noise. The dotted line in panel **b** is a strain marker that was initially vertical. This instability is expected to occur at roughly the same scale as (and indeed interact with) the Reaction-Infiltration Instability shown in Figures F.5 and F.6. Work is currently under way to understand the physics of this mechanical instability in greater detail by modeling experiments.

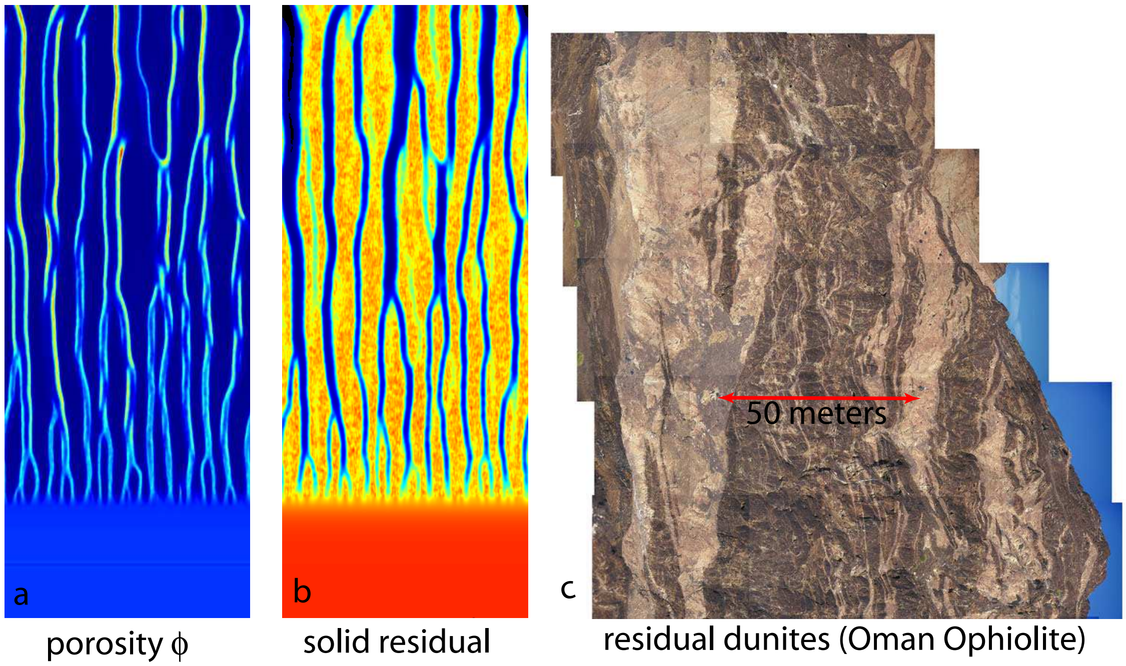


Figure F.5: Panels **a** and **b** show results from a 2D simulation of anhydrous reactive melting and melt transport beneath a mid-ocean ridge [60, 59]. The solid matrix is deforming by volumetric compaction with no shear. High permeability channels are visible in the porosity field (panel **a**). Most of the fluid flux and hence the reactive dissolution is concentrated in these channels. The colors in the solid residual (panel **b**) represent the degree to which the reactive phase has been stripped from the solid matrix. Panel **c** shows a photomosaic of an outcropping of mantle rock, called an Ophiolite, that was once below the sea-floor at a mid-ocean ridge [38, 12]. The variations in darkness results from variations in the fraction of Orthopyroxene, a dark-colored mantle mineral that is soluble in upwelling magma. Dissolution channels are light colored and correspond to the blue channels in panel **b**. The mosaic has been rotated to align the upward direction at the time the dissolution channels formed with vertical on the page.

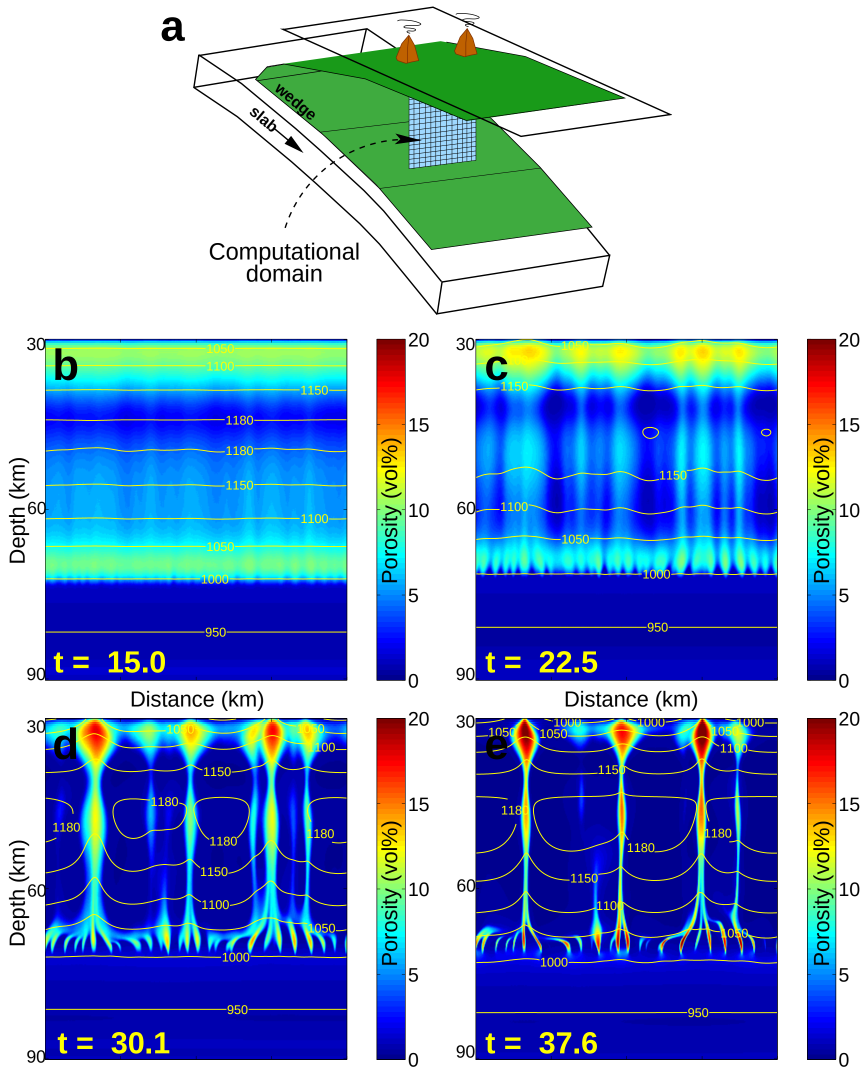


Figure F.6: (**a**) A schematic diagram of the position and orientation of the computational domain relative to the subducting slab, mantle wedge and arc volcanos. (**b-e**) Porosity (color) and temperature (contours) at four non-dimensional times in a hydrous reactive melting simulation. Temperature increases above the bottom of the domain into the wedge core and then decreases with height toward the surface. Channels form and immediately begin to coalesce into bundles that tighten with time. These channel bundles carry a large flux of melt and are able to significantly perturb the temperature field. Freezing melt near the top boundary lowers the permeability and confines outflow to narrow, high flux gaps. Below these gaps, melt pools in high porosity zones. We are exploring hypotheses for the mechanism of coalescence.