WORKSHOP REPORT

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Edited and Summaries by: Katie Cooper, Claire Currie, Lorraine Hwang, Louise Kellogg, Eric Mittelstaedt

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Introduction

The Computational Infrastructure for Geodynamics' (CIG) long-term tectonics community partnered with EarthScope for the first CIG-EarthScope Institute for Lithospheric Modeling workshop, held in Tempe, Arizona at the EarthScope National Office on the ASU campus. This working meeting focused on geodynamic modeling of lithosphere dynamics, data integration, and the software tools that facilitate this work.

The participants in this workshop identified science drivers and challenges, and used them to establish use cases. Use cases are specific examples of scientific or technical problems or questions, with identified goals, key users, scope, and outcomes. The use cases will facilitate the development of a list of functional specifications, scientific goals, and end-user criteria that will improve current and future development of lithosphere modeling software as well as enhance use of EarthScope-related observations of lithospheric structure and deformation.

The workshop combined researcher and developer presentations on new advances in lithosphere research and modeling tools, posters, and work in small breakout groups to identify science drivers, observational efforts, and computational developments that are advancing our understanding of lithospheric deformation. 46 geoscientists and computer scientists participated, including 16 early-career and 9 international participants. Telepresence was successfully incorporated with participants from Australia and Europe. In-depth discussions between end-users and developers helped address the needs and goals of both groups and how these can be integrated into the EarthCube framework.

This meeting report summarizes the science drivers, challenges, and frontiers of numerical modeling identified at the workshop. We then identify the next steps to be taken over the short term (1-2 years), intermediate term (2-4 years), and long term (beyond) incorporating our vision for the community. The appendices include the use cases and an index of codes in current use by the community.

Our goal out of these discussions is to develop a white paper that will outline a 5-10 yr roadmap for the long-term tectonics community including major scientific goals, numerical advances, and benchmarks.

SCIENCE DRIVERS

The primary goal of the long-term tectonics modeling community is to address scientific questions related to lithosphere dynamics through the use of numerical models and assimilation of data. During this meeting, community members identified several scientific problems currently at the forefront of long-term tectonics.

- Melting and Melt Transport

  The process of melting and the movement of melt from the Earth's interior to the surface is a complex problem that integrates thermodynamics, chemistry, and physics. Current theory addresses the flow of small melt fractions (<~20%) of melt in a viscous, two-phase medium, but there is still debate about their proper formulation. Numerically, these equations are successfully employed in 2D simulations, but they are computationally difficult to solve in 3D, limiting our understanding of melt movement. Beyond transport of melt in viscous materials, there is no theory to adequately describe melt transport across the solidus and through the lithosphere. Several questions remain about the transport of melt and its effect on the material through which it passes: How does lithosphere control melt delivery to the surface? What is the long-term effect of melt on the deformation and strength of the lithosphere? Where does melt stop, accumulate, and then start moving again through the Earth? How and why do magma chambers form?

- Strain localization and de-localization

  Deformation of the Earth occurs on nearly all length- and time-scales. Within the ductile and brittle regimes, this deformation generally occurs in either localized features such as faults and rift zones (e.g., fast-spreading mid-ocean ridges), or across distributed areas (e.g., diffuse deformation). Understanding what controls the localization and de-localization of strain in the Earth is an outstanding question in long-term tectonics.

- Surface Processes
  Erosion of the Earth's surface through, for example, rainfall, the development of river systems, and mass wasting events, both drive and are driven by interactions with processes both beneath and above the Earth's surface. Coupling simulations of long-term tectonics and surface processes will allow workers to address the feedbacks between evolution of topography, the atmosphere, and surface processes with mantle/crustal dynamics.

- Mantle-Lithosphere Interaction
  Mantle-lithosphere interactions take many forms, including shear between the moving plates and underlying mantle, and the formation of dynamic topography due to buoyancy driven motions in the mantle. The strength of the coupling between the viscous mantle and the more rigid overlying lithosphere is a long-standing question in geodynamics. A strong coupling leads to models of bent plume conduits and the spreading of plume material that is a balance between shearing associated with plate motions and buoyancy-driven self-spreading. However, disagreement between plate motions (e.g., GPS-derived velocities) and indicators of deep mantle flow (e.g., anisotropy) suggest that the mantle and

lithosphere may be de-coupled. What is the level of coupling between the mantle and lithosphere?

Viscous motions of the deep mantle driven by lateral variations in buoyancy as well as changes in surface loads on the lithosphere can cause changes to surface topography. How can observations of dynamic topography inform our understanding of the mantle?

- Incorporating Results from Seismology

  How do we convert seismic tomography to physical parameters such as density/temperature, etc. and back?

  What properties of melt (e.g. temperature, hydration etc.) can be inferred?

- Earthquake Cycle

  At the large scale, earthquakes and the earthquake cycle are driven by plate tectonics. Understanding earthquake recurrence requires understanding the complexity of lithospheric coupling, complex and evolving fault geometries, non-linear and time-varying rheologies, and a mix of continuum materials and discontinuous boundaries. In many locations, regional geodetic and earthquake slip rates differ (as revealed by PBO continuous GPS and other EarthScope data). What are the important boundary conditions driving the earthquake cycle? How do the longer and processes of lithospheric and evolution influence the shorter term observations of the earthquake cycle? What is the role of lithosphere -asthenosphere coupling in the generation of large earthquakes?

- Plate Boundary Evolution

  Plate boundaries are the most dynamic locations on the planet. At these locations, there are often large variations in rheological behavior, volcanism, fluid flow, and deformation. Due to these complexities, our understanding of plate boundary zones is limited. What controls the evolution of plate boundaries, including processes such as mountain building, orogenic collapse, subduction, rifting, volcanism, fault localization, large-scale deformation, and spatial stress transfer?

- Incorporation of Earth-like Behaviors in Numerical Models
  Several aspects of long-term tectonics push the boundaries of current numerical method research. This includes incorporation of large strains, complex rheologies, large viscosity jumps, and the coupling of multiple physics into a single model. These problems are driving development of new numerical tools for simulating long-term tectonics.

CHALLENGES

During break out sessions, attendees were asked to each identify challenges that they encounter in their research efforts. Several common themes emerged from this discussion ranging from the lack of well-developed theories to the practicality of sharing codes. Specific challenges are listed below.

Theoretical Challenges

- Develop a better understanding of the underlying physics and how to incorporate this into a numerical model: The physics involved in many fundamental processes that govern lithosphere dynamics is still not well understood. For example, there is currently no well-developed theory for how melt travels from the upper mantle (across the solidus) to the surface and therefore it is unclear how to best model two-phase flow.
- Coupling between processes operating across a wide range of temporal and spatial scales: the Earth experiences deformation ranging from micro- to macro- scale processes as well as at near instantaneous rates to processes that occur over millions to billions of years. How and whether it is important to couple these processes still remains unclear.
- Key material properties are not well constrained, such as rock rheology and thermal parameters (including their pressure and temperature dependence). More experimental and field studies of rock properties are needed, as well as an assessment of how experimental results can be extrapolated to geological time/space scales.

Computational/Numerical Challenges

- Modeling of lithosphere dynamics requires the ability to model systems with large magnitude variations in material properties occurring over short spatial scales (e.g., viscosity). It is also necessary to maintain discrete boundaries between different materials as the model evolves.
- Models must be able to handle large magnitude deformation of materials with complex, non-linear rheologies. A particular challenge is how to incorporate faulting. Faults and shear zones should spontaneously emerge based on the physical processes, rather than being artificially imposed.
- Lithosphere deformation occurs over a range of spatial and temporal scales. Recent work uses multi-scale models to capture this variability, but coupling of models with different space/time resolution remains a challenge.
- The extension of models from 2D to 3D is not straightforward. High computational costs are involved in modeling a three-dimensional domain at high resolution over long periods of time.
- Feedbacks between surface processes and lithosphere dynamics can be explored with numerical models, but a challenge is how to couple computer codes that were developed separately to study each system.
- Various parameter sensitivities exist within numerical models of which users (and developers) may not be aware. Inadvertent perturbations to the system can then cause

unexpected and unwanted changes in the model outputs. We need methods or tools to test and quantify parameter sensitivity.

Data Incorporation Challenges

- There is a wealth of datasets that provide information about long term and large-scale deformation processes, especially in the advent of EarthScope. However, implementing joint interpretation and/or joint inversions of multiple datasets (and often, quite large datasets) remains a difficult process.
- We agree that data integration and data assimilation moves numerical modeling from the realm of theoretical possibilities toward better representation of Earth processes. However, it remains unclear and challenging as to how to best accomplish this goal; opportunities associated with EarthCube may facilitate progress.
- In addition, the integration and assimilation of data into numerical models also introduces the need to better treat and quantify uncertainty within our simulations. The datasets themselves include level of uncertainties - how do we include and propagate these uncertainties into the models?

Educational/Outreach/Image Challenges:

- Many existing or previously used numerical codes are inaccessible and not easily usable for new users. However, we do not want new users to treat any numerical code as a black box; even with good instruction the underlying physics and the capabilities and limitations of each code must be understood. New users should realize and appreciate that running a model and understanding a model are not the same.
- There are inherent challenges in the practicality of sharing codes. There is often missing documentation that can step a user from installation of the code to the implementation of a working model. Furthermore, there is also often missing information about built-in modules as well as commenting within the code. Developers encounter disincentives to code sharing, ranging from lack of credit for the effort involved, to concerns about misuse of codes.
- While we wish to integrate more data and geological complexity into models, our ability to communicate across communities (such as geochemists, field geologists, geomorphologists) is often limited. Bridging across the various communities is difficult when we don’t attend common meetings (or sessions within the meetings) or read common scientific journals.
- Finally, we are suffering from an image problem - numerical modeling, as a research field, is not as attractive to incoming researchers as it was in the past. How do we make modeling sexy *again* to ensure that we continue to train experts who are capable of advancing the field?

NEXT STEPS

SHORT TERM (1-2 years)

- Identify selected analytical cases to be used as a basis for accuracy benchmarks (verification)
    - establish and disseminate a repository of such cases.
- Begin work on a community benchmark(s) of available and in-development codes (e.g., the computational use case developed at this workshop).
- Begin development of tutorials
- Invite initial donations to CIG for benchmarking and testing.
- Establish partnerships between CIG and EarthScope.

INTERMEDIATE TERM (2-4 years)

- Develop educational use case and tools.
- Establish a set of community benchmarks that are the standard for all future code efforts.
- Investigate the applicability of using cloud or grid computing for both educational and research efforts
- Investigate the applicability of including virtual machines in tutorials.
- Improve and increase access to computing resources for the research community.

LONG TERM (beyond)

- Converge on community best practices for LTT modeling.
- Create a user-oriented framework for evaluation of community codes - matching computational and scientific methods, capabilities, and resources to science needs.

ONGOING

- Regular, dedicated meetings to promote interaction amongst the LTT community. Meetings will also help raise awareness in the LTT and larger community about the philosophy, best practices, and methods of numerical modeling and code development.

APPENDIX A: Use Cases

The Feynman Algorithm, according to Murray Gell-Mann:
1. *Write down the problem*
2. *Think real hard.*
3. *Write down the solution.*

As part of the workshop, participants as groups were asked to brainstorm on use cases for the long-term tectonics community. Below summarizes these into 10 categorizes. Five of these were selected for further elaboration in separate breakout groups (Part II). Education was a theme throughout and was developed separately by conference organizers.

Part I. Use Case Summary

A. NUMERICAL

1. Verification and Uncertainty Quantification

Goal: Grid convergence and a posterior PDF (probability distribution function).

2. Code Verification

Goal: Measure the numerical error in a way that a geodynamicist understand.

Description: The developer provides code verification, analytics, and manufactured solution, and therefore provides a meaningful measure of the numerical error.

B. TWO-PHASE FLOW

1. Solve the Two-phase Flow Equations in 3D (in the mantle)

Goal: Write a code that will solve, in 3D, the equations of melting and two-phase flow. The code should be flexible enough to allow inclusion of feedbacks on viscosity, temperature, and other physics. The code/model should be able to model melt accumulation to high melt fraction (up through disaggregation).

2. Transport of Melt from the Asthenosphere to the Surface

Goal: We need a new theory to explain the transport of melt beyond the viscous mantle and into the ductile and brittle crust. There is no satisfactory theory to do this at the moment. The next step would be to determine the correct numerical implementation of this physics-based theory.

3. Coupling Solid State Flow and Melt and Fluid Transport in Subduction Zones and Characterizing the Surface Expression of Volcanism.

Goal: Tracking the chemistry of melt and fluids through the subduction system from the slab to the mantle wedge, and then how the chemical signature is filtered through the overlying lithosphere. An additional component of this is to validate the models using the geophysical expressions of melt and fluid in the wedge (e.g., seismic attenuation, magnetotellurics).

4. Modeling the Interaction between the Outer Rise Bending Faults and Hydration of the Subducting Slab.

Goal: Modeling two-phase flow in a faulted plate. Understanding the effects of metamorphic reactions on crack propagation. Does the previous work on this have elasticity, two-phase flow, reaction driven cracking?

5. Melt in Extensional Systems Interaction Between Faulting and Magmatism in 3D

C. STRAIN LOCALIZATION

1. Implementation of Strain Localization

Goal: Capture the physics of strain localization and how to best implement that in numerical schemes. Fault systems and shear strain; localized vs. distributed deformation [not magmatism - not yet anyway].

2. Implementation of Strain Localization 2

Goals: Capture the physics of strain localization driven by melt freezing/transport/emplacement. Why do wide rift zones form vs. narrow rift zones vs. wide-to-narrow rift transitions? [aside from mechanical strain localization]. Are continents too strong to break without magmatism? Chicken & egg - magmatism need decompression need rifting, but rifting seems to need melt to establish breakup.

D. EDUCATION

1. Build Model Intuition. As an educator, I would like tools that help me to demonstrate to students how different model parameters and rheologies affect tectonic processes and that allow students to explore model space for educational purposes.

2. Develop capability in the community to fully and accurately use numerical models. As a researcher and as an educator, I want my graduate students to be effective, knowledgeable users of codes that are accessible and not treated as a black box.

E. SOFTWARE

1. Keep Software Limitations from Limiting Our Science

Goal: Stop this from happening: “I would like to do <this>, but I can’t because the code doesn’t exist or the code I have can’t do it.”

2. Efficient Multigrid

Goal: As an impatient scientist, I would like robust textbook multigrid efficiency.

3. Provenance

Goal: Mandated open code and model availability (as source and in executable form with all dependencies fulfilled) and documentation to enable reproducible science.

F. DATA INTEGRATION & JOINT INVERSION

1. Data and Model Integration

Goal: Integration of data with models of lithospheric evolution:

surface deformation data from

- Plate Boundary Observations (GPS and strain),
- InSAR,
- geological and geomorphological observations,
- inferred structural characteristics from seismology (velocity, anisotropy etc.) and,
- inferred structural characteristics from and MT (conductivity).

2. Joint Inversion for Physical Properties of Earth's Crust and Mantle

Goal: Derive estimates or bounds on a range of physical properties, including T, composition, pressure. water content, partial melt content, etc. from seismic velocity and potentially other inputs. Are there clever approaches along the lines of adjoint inversion for seismic waveforms (velocity structure) or an approach to compute probability density functions based on ability to predict observations?

G. LARGE SCALE DEFORMATION & SURFACE PROCESSES

1. Evolution of Fault systems in Large-Scale Regional Plate Boundaries

Goal: To handle topological changes in plate simulations.

2. 4D Lithosphere Modeling with Coupled Processes

Goal: A usable 4D lithosphere-scale model that incorporates reasonable surface processes asthenospheric flow. The goal is to develop a modeling capability to explore the impact of surface and asthenospheric processes on the deformational, magmatic, pressure-temperature-time, and topographic evolution of the lithosphere.

3. Coupling Long-term Tectonic Models with Surface Processes During Mountain Building.

Goal: Coupling simulations of surface processes to simulations of 3D tectonic evolution to explore the connections between tectonic deformation, surface processes, and deep mantle flow during the formation and collapse of orogens.

4. Oceanic plate boundary evolution, structure, and melt chemistry

Goal: As a researcher I would like to understand the mantle controls on oceanic plate boundary motion/relocation, segmentation, lithospheric structure, crust formation, and melt chemistry.

5. Long-term Orogenic Studies with 3D Variations in Climate, Surface Properties, and Lithosphere Properties.

6. 2D modeling with Erosion and Rifting.

How does that affect the crustal flow and the stresses in the system?

H. EARTHQUAKE DYNAMICS

1. Fluid-solid Interactions Impact on Induced Seismicity

Goal: Development of physics and numerical models which enable us to better understand induced seismicity.

2. Model Postseismic Deformation with a Seamless Transition Between Local (halfspace/layered space) and global spherical 3D Earth

Goal: Currently modeling tools exist to model coseismic and postseismic deformation for a half-space, for a layered space, a layered sphere, and some software allows extension to 3D. Each approach or tool requires different inputs, is valid and efficient within certain limits, but problems for large earthquakes cross over these boundaries

b. Earthquake Cycle Model Driven by Plate Tectonics

Goal: Earthquake hazard forecast. Simulating earthquake cycles driven by boundary conditions of plate motions. Long-term goal is scaling up to earthquake hazards at the plate boundary scale. Enabling to do probabilistic and deterministic earthquake problems at the same time. Incorporating viscoelasticity, plasticity, afterslip, 3D heterogeneity in properties. Do this on a spherical earth, big picture problems. For example, a Japan, Chile, or Alaska (size 9.0 or greater) earthquake where the rupture size is > 1000 km and the curvature of the earth is important.

I. MANTLE INTERACTIONS

1. The Surface Manifestations of Mantle Plumes

Goal: Relate deep mantle dynamics to surface expressions of mantle plumes. Can we understand the deep mantle dynamics from the surface expressions of mantle plume tracks?

Description: Model the volcanic flux and volcano spacing of an age-progressive hotspot track. Use chemical tracers as a constraint. Benchmarks for Stoke's sphere, variable viscosity, free surface. Is there an analytical solution for a buoyancy source with free surface? Have CIG manage and make available these solutions.

J. BENCHMARKS

See I1.

a. Critical wedge

Goal: Develop a plastic critical wedge model.

Description: Plastic material with Mohr-Coulomb failure on top of a frictional surface; analytical solution for the surface slope. Provide guidance on the type of codes and mesh/techniques that are able to solve this problem. Include non-associated plasticity and/or weakening to produce localized fault.

Part II: Selected Use Cases - In Detail

A. EDUCATION

A. Use Case Name: Develop a Workforce Capable of Using Long-term Tectonics Numerical Modeling

B. Point of contact:

C. Goal I: **Build Model Intuition.** As an educator, I would like tools that help me to demonstrate to students how different model parameters and rheologies affect tectonic processes (rift behavior and evolution, mountain building, strain localization). I also want interfaces that allow students to explore model space for educational purposes (example: an online isostasy calculator). Simple geophysical simulation tools are needed that allow students to explore key processes and observations.

Goal II: **Develop capability in the community to fully and accurately use numerical models.** As a researcher and as an educator, I want my graduate students to be effective, knowledgeable users of codes that are accessible and not treated as a black box. To accomplish this, I want tutorials, documentation, cookbooks, and other tools for engaging and instructing early-career scientists in the effective use of numerical modeling and integration of EarthScope data into models.

D. Users: University instructors, graduate students, researchers, postdocs, CIG and EarthScope staff.

E. Scope:

- Development of high-quality tutorials that introduce students to modeling techniques at the beginning and (eventually) level
- Tutorials and documentation for specific codes
- Accessible software (such as pre-packaged virtual machines)
- Accessible pre- and post-processing tools

F. Primary Scenario Summary

Students in the geoscience domain are typically not taught much about modeling, and less about computation, as part of their formal education. In order to be effective, responsible, knowledgeable users and user-developers of computational and modeling tools, students require education in the use of models, assimilation of data, and training in the use of modeling software tools.

Educators also need tools for use in their own classrooms to demonstrate (and allow students to explore) physical processes and data.

1. Physics

2. Precondition

- Well-documented codes, with clear definitions of input files and outputs.
- Cookbooks that build from simple cases to more complex.
- Tools for mesh generation and visualization
- Students who are prepared to learn
- Access to computing
- Access to datasets

3. Key Interfaces/Inputs

- Gridding tools
- Sample input files

4. Key Outputs

B. EARTHQUAKE CYCLE

A. Use Case Name: Earthquake Cycle Model Driven by Plate Tectonics

B. Point of contact: Brad Aagaard

C. Goal:

Earthquake cycle modeling driven by plate tectonics with spherical geometry

Applications:

- Earthquake rupture forecasts and earthquake hazard maps
- Optimize instrumentation siting

D. Users:

Researcher in earthquake physics, geodesy, earthquake probabilities/forecasting.

General Public and Policy makers are likely consumers of model outputs.

E. Scope

In scope:

- 3-D rheology - elasticity, fluid flow, heat flow, damage etc.
- complex fault geometry,
- time scale of single earthquakes to hundreds of earthquake cycles,
- spatial scales of single earthquake to fault systems and plate boundaries,
- changes in permeability, pore pressure
- spherical earth

Out of scope:

- changes in relative fault geometry (fault evolution)
- changes in fault roughness (may need to be reconsidered in future, with respect to evolution of fluid pressure during individual events, etc.)

F. Primary Scenario Summary

Simulating earthquake cycles driven by boundary conditions of plate motions.

Long-term goal is scaling up to earthquake hazards at the plate boundary scale. Enabling probabilistic and deterministic earthquake hazard assessments at the same time. Incorporation of viscoelasticity, plasticity, afterslip, 3D heterogeneity in properties. Need to be able to do this on scales up to a spherical earth to handle large subduction zone earthquakes; for example, M 9+ Tohoku, Chile, Alaska earthquakes where the rupture size is > 1000 km and the curvature of the earth is important.

0. Benchmarks

Sources of uncertainty:

1. Physical Model (e.g., slip distribution, fault geometry, elastic/viscoelastic model, contribution from unmodeled processes)

2. Measurement uncertainty (note that this often involves assumption of a physical model, as in the fitting of a secular trend to geodetic data)

3. Computational uncertainty

Verification

- Rheologies
- non-dislocation deformation, perhaps Mogi-style inflation sources to explore role of fluids
- Single event elasticity
    - Postseismic relaxation
- Spontaneous rupture
    - Nucleation
- Earthquake cycle
    - Interseismic loading to nucleation to postseismic deformation
- Multiple earthquake cycles
    - Single fault
    - Multiple fault
- Performance/Scalability
- Data assimilation

Validation:

- comparisons/predictions against data (big events: watch reference frame issues and data resolution in mind)

1. Physics

- Bulk rheologies
    - Type of rheology (elasticity, viscoelasticity, viscoelastoplasticity, damage rheology)
    - 3-D spatial variation of rheology parameters
    - Role of fluids (poroelasticity, anthropogenic extraction/injection)
- Faults
    - Type of rheology (rate-state friction, melting, thermal pressurization)
    - Spatial variation of rheology parameters
    - Role of fluids (changes permeability and porosity)
    - Shear zones in lower crust
    - Evolution of small scale fault geometry (roughness)
- Fields of interest
    - Displacement, fault slip
    - Strain (plastic strain, viscous strain, total strain)
    - Stress
    - Fluid pressure
    - Temperature

2. Precondition

Self-consistent numerically

3. Key Interfaces/Inputs

- Geometry of fault system
- Topography (non-evolving)
- Initial stress/ state of lithosphere
- Elastic structure -- half-space, layered space or sphere, 3D
- Viscous/viscoelastic structure -- as above
- Ability to impose slip or drive it from other variable/state

4. Key Outputs

- displacement and strain as a function of time
- including dynamic displacements due to seismic waves
- including deformation field and time history for tsunami inputs
- including predicted observables to feed into inversions or comparison
- Fields (time histories)
    - Displacement, fault slip
    - Strain (plastic strain, viscous strain, total strain)
    - Stress
    - Fluid pressure
    - Temperature

5. Numerical Methods

- Selection of appropriate computational method, user specific but with automatic selection option given desired numerical accuracy (for certain problems)
    - analytical solution
    - semi-analytical solution
    - numerical (mode summation, etc)
    - finite element
- Finite-element issues
    - Unstructured meshes (if using complex interior surfaces)
    - Adaptive mesh refinement
    - Remeshing
- Slip on interior interfaces (faults)
- Homogenization of small scale processes

H. Milestones

(A proposed set by Jeff Freymueller)

Elastic problem -- integrate local (Okada) to global scale

Consistent interface with existing codes (e.g., RELAX, PyLith)

Integrate elastic and basic viscoelastic capabilities

Full integration with earthquake cycle simulation

I. Extensions

Other influences (forces) to seismic cycle: volcanism, glacial (un)loading, anthropogenic signals (bias interpretations of data as purely tectonic)

Coupling to tsunamis; dynamic triggering

Inversion of everything (fault slip, bulk rheology parameters, fluid pressure, etc.)

Workflow tool to guide simulation pathways based on observations, inputs, outputs, and physics.

Suite of tools:

Separate tools may be required for each of these cases, but many parts of codes are in common, and all aspects from shortest to longest term need to be mutually consistent. Could work from a common library of code to a large degree.

Tools should be extensible such that new physical processes should be easily integrated.

- coseismic -- static and dynamic displacements
- postseismic -- single earthquake postseismic response
- multi-cycle models -- stress accumulation and release over multiple earthquake cycles
- long-term earthquake simulation -- multi-fault, multi-cycle in a 3D viscoelastic earth

C. MANTLE PLUME-LITHOSPHERE INTERACTION

A. Use Case Name: The Surface Manifestations of Mantle Plumes
B. Point of contact: Audrey Huerta
C. Goal:
Explore the deformation, stresses, and topography of a plume on the lithosphere over long-term evolution.
Relate deep mantle dynamics to surface expressions of mantle plumes. Can we understand the deep mantle dynamics from the surface expressions of mantle plume tracks?

D. Users:
Researchers, educational, App (iphone) users, students - classroom demonstrations, teaching tool.

E. Scope
Explore the deformation, stresses, and topography of a plume on the lithosphere over long-term evolution.
Understand possible termination.

F. Primary Scenario Summary
Model the volcanic flux and volcano spacing of an age-progressive hotspot track. Use chemical tracers as a constraint. Benchmarks for Stoke's sphere, variable viscosity, free surface. Is there an analytical solution for a buoyancy source with free surface? Have CIG manage and make available these solutions.

0. Benchmark

- fully elastic case

1. Physics
3D stokes ball impeding on an elastic plate and viscoelastic plastic plate.

2. Precondition

- Have a user interface that an undergrad can use (App)
- Code is flexible enough to modify.
- Variable flux boundary condition at bottom
- Variable of plate velocity
- Isostatic stress boundary condition: vertical
- Temperature plate: adiabatic
- High thermal conductivity in mantle (to avoid cooling of the model)?
    - Model convective cells?
- Viscosity gradient: lithosphere and asthenosphere boundary

3. Key Interfaces/Inputs

- Rheology: Non-newtonian (flexibility: laws and constants), fully elastic, plasticity

- Lithospheric types: ocean vs. continental lithospheric, thickness, layered
- Vary degree of thermochemical buoyancy
- Upper mantle winds
- Plate motions & physical coupling of mantle and lithosphere
- Temperature contrast
- Size of plume
    - Diameter
    - Flux (as input at “bottom of box”)
- Sedimentation - explanation of cycle uplift
- 2D/3D, 3D sphere
- Termination - how does plumes stop?

4. Key Outputs

- Evolution of topography
- Deformation
- Gravity
- Plume dynamics
- User selection of outputs
- Evolution of stress and strain
- Spatial and temporal variable velocities

5. Numerical Methods

6. Extension

- faulting

D. TWO-PHASE FLOW USE CASE

A. Use Case Name: Two Phase Flow

B. Point of contact: Eric Mittelstaedt: emittelstaedt@uidaho.edu

C. Goal:

1. We want to understand where melt stops, accumulates, and keeps going.

2. How does magma affect the long-term deformation and chemistry of the lithosphere?

D. Users:

Research scientists and graduate students

E. Scope

Out of scope:

1. 2nd order phases
2. Detailed chemical structure of the crust
3. Eruption dynamics

F. Primary Scenario Summary

To simulate 2 phase flow from melt generation through interaction with the lithosphere and eventual eruption at a volcanic edifice in three dimensions and constrained by observations.

1. How is the lithosphere affected by magma?
    - a. deformation?
    - b. chemistry?
2. How does the lithosphere control where magma goes
    - a. Where does it go at the base of the lithosphere?
    - b. Where does it go in the crust? (Detailed models of the crust.)
    - c. where does it go at the surface?

0. Benchmark

Verification:

- starting point: existing tests for 2 phase flow models by Spiegelman
- elastic end member case: how well do you simulate surface deformation of magma
- injection (dikes, Mogi sources - including thermal effects)
- simple darcy flow: compaction column problem with density stratification
- channel flow within a slot (non-linear)
- Stokes sphere
- non-linear corner flow solutions
- instantaneous Stephan problem for injection of dikes

Validation:

- formations of shear bands and melt bands - comparison to experiments

1. Physics

a. buoyancy - variations in buoyancy (melt composition, stratification of the lithosphere)

b. rheology - brittle failure, ductile deformation (tensile cracking, diking)
c. compressibility
d. thermodynamics of melting and freezing
e. transport - porous flow, etc.
f. energy equation
g. chemistry of melt-rock reaction

2. Precondition

Questions to answer first:

- What equations you are going to use, which formulation?
- What are the boundary conditions?
- What pre-existing structure you want should be included?
- Determine what observables exist to constrain your models

Needs:

- A database of material properties and thermodynamic properties
- A melting and reaction model
- Constraints on volumes, distribution, and timing of deformation, magmatism
- New theory to handle continuum that includes liquid and solid

3. Key Interfaces/Inputs

Data needed:

- MT data
- chemistry: volatile outputs, source (isotopes), proxies for melting (traces), phases (mineralogy)
- geodetic data
- seismicity
- seismic structure of the crust and mantle

4. Key Outputs

Model outputs:

- Surface deformation
- Final melt distribution in space and time
- Chemistry of melt products - volcanics, intrusives
- Evolving strength of the lithosphere

5. [Numerical Methods] time permitting

Methods required:

- One code to simulate the solid and the liquid phases from small melt fractions through complete disaggregation and subsequent propagation.
- Code to simulate chemical communication between phases

E. STRAIN LOCALIZATION

A. Use Case Name: Strain Localization

B. Point of contact: Jean-Arthur Olive & Katie Cooper

C. Goal:

Develop a robust implementation of strain localization with a meaningful set of benchmarks and a means of verification.

Robust = convergence, reliability

D. Users:

Researchers

E. Scope

In Scope:

Why do we want strain localization? Behavior of the deforming system with localizations. What is the appropriate weakening term - need to track some state variable(s) (strain, strain rate, etc.).

Out of Scope:

Fault physics - physical parameters that control dynamic faulting (rate-state friction)

F. Primary Scenario Summary

To model compression, extension and lateral shear in the lithosphere that allows for localization of strain with some accommodation outside of faults ; understanding how localization influences lithospheric stress state. Deformation is driven either by velocity boundary conditions or coupling to mantle convection.

Observables:

natural fault dips, fabrics, rates of subsidence, topography

<u>Brittle Layer and Free Surface Overlying a Low-viscosity Layer</u>

Apply different kinematic side BCs (extension, compression) and compare modes of strain localization:

- within the standard “effective viscosity“ framework with strain weakening, systematically investigate the effect of changing cohesion vs. friction, the kinematics of weakening
- try to implement weakening mechanisms that involve different physics and have inherent length scales (i.e. can be resolved and converge) and compare them - observables and derived quantities include topography, strain/stress fields, velocity field, fabrics, known shape of natural faults
- compare different numerical implementations of the same physics (where yield stress criterion is implemented, solvers…)
- then relax initial assumptions (kinematic BCs, free surface, compression / extension rates)

0. Benchmark

Code Verification: manufactured solution test accuracy of code

Shear band orientation (use Hafner solution and test orientation of slip lines, initial stage with analytics.

Analogue (sand box, gels, etc.) experiments for large strain

Performance:

- Accuracy
- Speed
- Memory footprint
- Multi-processing scalability

1. Physics

Viscoplastic behavior with elasticity

Strain weakening with state variable (state variable = damage, temperature)

Strain rate hardening to make length scales arise

2. Precondition

User Skill Level: high

Initial & Boundary Conditions: lithospheric deformation problem; do we need to seed the deformation (either a “weak” spot or numerical noise depending on the geologic problem at hand)?; free surface

Methods: Existing numerical code that can solve a non-linear problem that has flexibility to change/implement different rheologies

3. Key Interfaces/Inputs

Ideally, it can interface with fluid interaction, melts, and surface processes, but it can also be a stand-alone self-contained model.

4. Key Outputs

Key outputs include: maps of strain rate, accumulated strain, stress state in lithosphere, topography, visual deformation, and temperatures.

One critical point is that results MUST be mesh independent.

5. Numerical Methods

We are undecided as whether it is more appropriate to use finite difference vs. finite element methods. However, we do agree that the most pragmatic choice is to use Material Point Markers (aka Particle in Cell).

F. COMPUTATIONAL SCIENCE

A. Use Case Name(s):
- Code and Model Verification
- Benchmarking
- Uncertainty Quantification

B. Points of contact:
- Dave May
- Jed Brown
- Margarete Jadamec

C. Goal:
- Would like to use numerical models and take responsible measures of quality control.
- Ensure that numerical code(s) used and model results published are sound numerically and can be reproduced.
- As a responsible scientist, I would like grid convergence and a posterior PDF (probability distribution function).

D. Users:
- researchers
- code developers
- computational scientists
- those responsible for disseminating codes

E. Scope
- Analytic Solutions for Comparison,
- Methods of Manufactured of Solutions (general guidelines for their construction)
- Encourage atmosphere of Code Transparency/Some level of Documentation/Sufficient Supplemental Material to enable Reproducibility (e.g. supplementary material in a published paper, solver tolerances, version of software used, provide any software patches, post-processing tools)
- We assume the Physics has been defined *a priori*, and focus on code and model verification

F. Primary Scenario Summary

As codes are developed, they must be validated and verified/benchmarked. Our focus is on incorporating best practices for verification and benchmarking into the code development and testing framework; also to provide tools for computing errors if these are unable to be provided directly by the methodology being tested.

0. Benchmark
- Comparison to analytical solutions

- Comparison to semi-analytic solutions
- Method of Manufactured Solutions (MMS): to enable comparison among codes and to verify and validate numerical approximations to strongly nonlinear problems. (Notes here refer to equations on board - guidelines for choosing phi, and make sure is resolved by your grid so you plot f so make sure it is smooth, have K(x) be arctan for whatever best represents jumps or the non-linear feature your code will make; axes f (vert) versus x (horiz); will require small code modification to enable/implement the MMS.)
- Comparison to analogue experiments where relevant
- We are not focusing on inter-code comparison

1. Physics

- Physics independent (assumes physics is understood previously).

2. Preconditions

- Reading guidelines for establishing order of accuracy which CIG will provide.
- Reading the description of each solution provided.
- Performing a series of numerical experiments on different mesh resolutions/timestep, etc.

3. Key Interfaces/Inputs

- Create Repository that works through example of Methods of Manufactured Solutions
  so, Users can use this to test code implements/benchmarks that don't have an analytic solution.
  First- construct and have these solutions.
  Second- show what users should do with these solutions to show the method is working.
- Suggested Requirement - any code that is accepting and posting code to CIG should show can pass these tests.
- Benchmarks are used in different ways -
  When using analytic solution - guidelines to demonstrate order of accuracy, as well as fit
- Example procedure determine order of accuracy using analytic and the Methods of Manufactured Solutions (MMS) are described here:

Duretz, T., May, D. A., Gerya, T. V., & Tackley, P. J. (2011). Discretization errors and free surface stabilization in the finite difference and marker-in-cell method for applied geodynamics: A numerical study. *Geochemistry, Geophysics, Geosystems*, *12*(7).

Burstedde, C., Stadler, G., Alisic, L., Wilcox, L. C., Tan, E., Gurnis, M., & Ghattas, O. (2013). Large-scale adaptive mantle convection simulation. *Geophysical Journal International*, *192*(3), 889-906.

See also the benchmark cases for Underworld (steady state incompressible, variable viscosity Stokes flow). These are stand alone C functions defining analytic solutions derived in a classical way. All these examples are for linear viscous problems.

4. Key Outputs

- Examples of how to implement MMS so users/developers can verify code implementations. Necessary for problems for which no known analytic solutions have been defined.
- Repository of analytic benchmarks.
- Explanation of what should be computed for meaningful measure of error.
- Expectations would be users/developers should demonstrated methodology converges and the accuracy of their discretisation has been quantified.

5. Numerical Methods

- Not relevant here. Possibly symbolic algebra tools (e.g. sympy, maple).

G. Extensions

- Education associated with numerical analysis. e.g. explaining to the Earth science community (non-math specialists) how to formally demonstrate that their chosen discretisation solves the intended set of PDEs and that the methodology is convergent (verification). This procedure adds rigor and user confidence in the methods used in Earth sciences.
- These procedures can also be used to develop suitable stopping conditions for linearized and non-linear problems.

APPENDIX B - LIST OF CODES & SOFTWARE PACKAGES IN USE

Commercial

Abaqus

ArcGIS

COMSOL Multiphysics (FE)

Matlab

Academic

ASPECT (FE, AMR, Trilinos, PETSc)

CitcomS/CU (multigrid, PETS)

CUBIT

ELEFANT (ALE, Q1P0 FE, marker in cell, MUMPS)

Ellipsis

FLAC

Gale (ALE, FE)

GMT

HIPSTER – Highly Parallel Stokes with Exotic Rheologies (FD, Marker-in-cell, PETSc)

IDL

i2elvis/i3elvis (FD, marker in cell, mulitgrid solvers in 3d, direct solvers in 2d)

LAYER

Matplotlib

Paraview

pTatin3d (ALE, Q2P1, PETSc)

Pylith (FE)

SNACRelax

SOPALE (FE, ALE)

STRCH (FEM)

Underworld (ALE, FE)

Appendix C: List of Workshop Participants

Brad	Aagaard	*US Geological Survey*
Ramon	Arrowsmith	*Arizona State University*
Emma	Baker	*University of Idaho*
Mark	Behn	*WHOI*
Jed	Brown	*Argonne National Laboratory/CU Boulder*
W. Roger	Buck	*Lamont-Doherty Earth Observatory of Columbia University*
Eunseo	Choi	*Center for Earthquake Research and Information, University of Memphis*
Catherine	Cooper	*Washington State University*
Claire	Currie	*University of Alberta*
Lucy	Flesch	*Purdue University*
Jeff	Freymueller	*University of Alaska Fairbanks*
Ed	Garnero	*Arizona State University*
Ronni	Grapenthin	*Berkeley Seismo Lab, UC Berkeley*
Dennis	Harry	*Colorado State University*
Christopher	Havlin	*Brown University*
Audrey	Huerta	*Central Washington University*
Lorraine	Hwang	*University of California, Davis*
Margarete	Jadamec	*Department of Geological Sciences, Brown University*
Boris	Kaus	*Johannes Gutenberg University Mainz*
Anna	Kelbert	*Oregon State University*
Louise	Kellogg	*University of California, Davis*
Fansheng	Kong	*Missouri University of Science & Technology*
Laetitia	le Pourhiet	*University Pierre and Marie Curie*
Mingming	Li	*Arizona State University*
Lijun	Liu	*University of Illinois at Urbana-Champaign*
Rowena	Lohman	*Cornell University*
Gayatri	Marliyani	*Arizona State University*
David	May	*ETH Zurich*
Allen	McNamara	*Arizona State University*
Eric	Mittelstaedt	*University of Idaho*
Laurent	Montesi	*University of Maryland*
Louis	Moresi	*Monash University*
Thomas	Morrow	*University of Idaho*
James	Ni	*New Mexico State University*
Jean-Arthur	Olive	*MIT / WHOI Joint Program in Oceanography*
Felipe	Orellana	*University of California, Berkeley*
Chris	Rollins	*California Institute of Technology*
Brandon	Schmandt	*University of New Mexico*
Johnny	Seales	*University of Houston*
Stathis	Stiros	*Dept. of Civil Engineering, Patras Univeristy, Patras, Greece*
Gerya	Taras	*Swiss Federal Institute of Technology (ETH-Zurich)*
Cedric	Thieulot	*Univ of Utrecht*
Xiaopeng	Tong	*University of California San Diego*
Jolante	van Wijk	*New Mexico Tech*
Guangliang	Wu	*The University of Texas at Austin*
Jiyang	Ye	*Geological Sciences Department, University of Missouri - Columbia*