COMPUTATIONAL
INFRASTRUCTURE FOR
GEODYNAMICS

Computational Infrastructure for Geodynamics
2016-2020
Part I: Project Description

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COMPUTATIONAL
INFRASTRUCTURE
for GEODYNAMICS

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PROJECT SUMMARY

Overview:

This proposal seeks funding for the Computational Infrastructure for Geodynamics (CIG) to build and sustain essential cyberinfrastructure and computational capacity for geodynamics and seismology. Over the past decade, CIG has developed and disseminated widely-used, open-source codes for research and education in computational seismology, mantle convection, magma dynamics, short- and long-term lithospheric and crustal deformation, and geodynamo modeling. CIG has changed the culture in computational geophysics research by improving scientific software development practices and has influenced the education of hundreds of geodynamicists. CIG's approach towards writing and disseminating scientific software has become indispensable to its community and has established and sustained deep ties to computational sciences.

CIG proposes to continue to build upon this foundation using community engagement to guide development for frontier research while remaining responsive to new opportunities. We seek to expand multidisciplinary science, facilitate broader access to high performance computing; assure scientific credibility through benchmarking, testing, and reproducibility, and create pathways for community members to receive credit for contributions.

Intellectual Merit :

Scientific computation is integral to solid Earth geosciences, allowing us to understand and quantify the processes that shape Earth. Computational models link observations and quantitative models describing the Earth's interior and evolution. This proposal seeks to continue developing and disseminating high quality scientific software to enable cutting edge geodynamics modeling, and to prepare a diverse workforce to address fundamental science questions. While CIG's primary mission is development of high-quality open-source software, a growing role is the education and development of geoscientists who are prepared to effectively use and advance computation in research and teaching. Workshops, hackathons, meeting special sessions, and tutorials foster emerging computational geoscientists who represent the long-term legacy of the project.

Broader Impacts :

Infrastructure: The primary impact of CIG is improved geoinformatics infrastructure to enable high-quality research and teaching in geodynamics and seismology. CIG's software development additionally influences widely-used scientific software projects, including PETSc and deal.II.

STEM education and educator development: CIG provides high-quality, in-depth, sustained training, including tutorials, workshops, online training, and team software development at hackathons, emphasizing participation by early career scientists.

Underrepresented groups in STEM: CIG has a demonstrated commitment to open participation by all in STEM, with a strong track record of involving women in both development and use of codes, and provides pathways to leadership by engaging early career scientists and members of unrepresented groups in governance and decision-making.

Partnerships: We have established partnerships with National Labs, USGS, and other US government agencies to build and enhance scientific capacity, and engage with other organizations and international partners to offer tutorials and co-host conferences.

Improved national security and well-being of individuals in society: CIG codes are used for research on hazards (earthquakes, volcanic eruptions, ice sheet modeling, global sea level changes, induced seismicity, and nuclear security) and natural resources (water, petroleum, and geothermal energy).

Public scientific literacy: CIG scientists engage the public by sharing scientific results with science centers and museums to increase public understanding of science and technology.

1 Introduction

Scientific computation has, for decades, helped us understand and quantify the processes that shape Earth, including convection in the Earth's core and mantle, plate tectonics, and the dynamics of plate boundaries with attendant mountain building, volcanism, and earthquakes. Computational models provide an essential link between observations made on the surface and our attempt to describe the Earth's interior and evolution.

The concrete incarnation of computational models is software. Historically in geodynamics, as in many other scientific disciplines, scientific software has been written by individual scientists for specific research projects. Software written in this way is not designed or documented for use by a larger community, and is rarely tested using professional software validation strategies. It may be shared with some collaborators, but their modifications are not usually folded back into a single, central version. This pattern of software development limits complexity, extensibility, scalability, interoperability, reliability, and reusability, duplicates effort, and limits the return on investment in scientific software development. Put differently, it limits our ability to explore the critical interdisciplinary challenges of coupled systems, using advanced numerical methods, on the large-scale parallel hardware available today. We will discuss many scientific challenges that require advanced software in Section 2.

Established in 2005, the Computational Infrastructure in Geodynamics (CIG) is a partnership between the scientific domains of solid-Earth science and computational science to advance geophysics and associated fields of research by developing and disseminating scientific software, using best practices for computational science. This project accelerates the understanding of the dynamics of Earth and Earth-like planets by providing innovative methods, resources, and technologies, enabling research from the core to the crust, and beyond. CIG provides leadership in computational geophysics, addresses multidisciplinary challenges in geosciences, and drives potentially transformative research. CIG encompasses a broad community whose research and pedagogy are fundamentally based in modeling and computation [1].

CIG's open-source codes are widely-used for research and education in computational seismology, mantle convection, magma dynamics, short-term and long-term lithospheric deformation, geodynamo, and ice sheet modeling for Earth and beyond. CIG has also significantly changed the culture in computational geophysics research by improving scientific software development practices, influencing the education of hundreds of early-career geodynamicists, and establishing and sustaining deep ties to the computational sciences. This approach to writing and disseminating scientific software has become indispensable to geophysics research, for example, see the EarthScope, GeoPrisms, seismology, geodynamics, and National Research Council reports ([2, p. 73], [3, p. 3-36], [4, p. 5-15], [5, p. 66], [6]). The scientific results portrayed in Figures 2, 3, 4, 6, 7, 8, and 9 exemplify the research by early career scientists made possible by CIG scientific software.

This proposal describes our vision for the future and our plans to extend the efforts of the past decade in response to the evolving needs of the scientific community. We describe the scientific justification for the proposed work in Section 2. CIG's accomplishments, experiences, and lessons learned are discussed in detail in Section 3. These closely inform the goals elucidated in Section 4 for software and infrastructure development, and in Section 5 for the education and community-building programs. We describe the many broader impacts of this effort in Section 6. CIG is shaped by a governance and management structure designed to maximize input from constituents and foster interaction with other communities, as outlined in Section 7. Section 8 describes results from prior NSF support; Section 9 defines frequently used abbreviations.

2 Science Justification

CIG enables high-quality, potentially transformative science in geodynamics through use of computation. The scientific priorities of this proposal reflect those of the geoscience research community as a whole, as identified by the broader geoscience communities [2, 7, 5, 4, 3, 6], outlined here:

1. How have the dynamics and structure of the solid Earth evolved since its earliest history?
2. What is the origin and evolution of Earth's magnetic field?
3. How do Earth's internal boundaries influence its composition, structure, kinematics, and dynamics: crust-mantle, core-mantle, lithosphere-asthenosphere and their transition zones?
4. What are the origins of continents, and the dynamics of continental-ocean margins?
5. What are the origins of and the factors controlling plate tectonics and lithospheric dynamics? What is the role of rheology in this process?
6. How do dynamical processes in Earth's crust drive structural and tectonics processes from the fault scale to mountain and basin scale?
7. How do internal processes drive the evolution of topography and surface processes?
8. What are the origins and dynamics of earthquakes: How do fault systems interact? How do seismic waves amplify and dampen as they propagate through complex Earth structure, and what are the implications for seismic hazard?
9. How do fluids and volatiles behave and migrate in Earth's crust and upper mantle?
10. How does tectonic activity interact with climate, including the cryosphere?

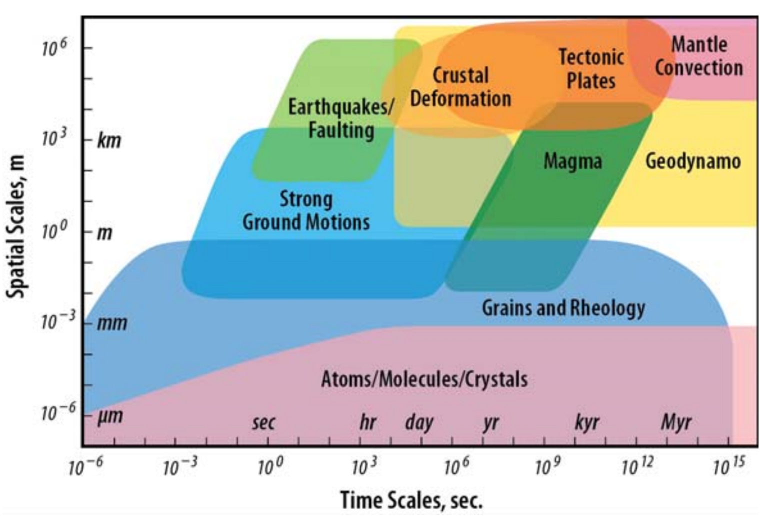

Figure 1: The range of scales of observations and computation represented by CIG-enabled geoscience. CIG is a community-driven organization that advances Earth science by developing and disseminating software for geophysics and related fields.

In community discussions of research priorities for geophysics, scientific computation consistently emerges as a requirement for understanding the behavior of Earth's complex systems and how they couple at various scales in space and time (Figure 1). Indeed, CIG is regularly cited as an example of how to advance scientific computation for the geosciences (e.g., [2, page 73]). These scientific questions require both discipline-specific codes that solve a specific set of governing equations (for continuum mechanics, magnetohydrodynamics, or elastic wave propagation, for example) and modeling coupled systems for investigating the interaction between geological systems (mantle convection with plates, coupled fluid-solid dynamics, or seismic signatures of structures regulated by geodynamics processes, for example.) These tools must also include the flexibility to apply to a wide range of processes. Here, we describe some fundamental questions in six key areas of geosciences and their interfaces that can be addressed by computational methods.

2.1 Core Dynamics

The Earth's magnetic field is generated by convection in the liquid iron alloy of the Earth's outer core. Understanding the origin and evolution of the Earth's magnetic field and dynamics of the outer core are long-standing grand challenges in geophysics that have been approached with a variety of theoretical, observational, laboratory, and computational methods. Numerical simulations have played a central role in this quest for more than 2 decades [8]. Current numerical models are capable of simulating dynamo action by rotating, convective flows that are close to laminar, but are unable to resolve strongly turbulent dynamos in fluids with properties similar to liquid metals. Hence, they have yet to answer fundamental questions about the geodynamo because of the extreme resolution required to reach fully Earth-like behavior. In particular, the flow in the outer core likely exhibits a vast range of length scales, with viscous boundary layers ~ 0.1 m in a computational domain that extends to 7×10^6 m, plus a commensurately wide range of time scales, neither captured by present-generation models. Moreover, because the flow is turbulent throughout, high resolution is required everywhere in the computational domain.

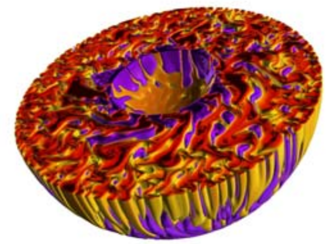

Figure 2: Temperature perturbations in a rotating Boussinesq convection, computed using Rayleigh. Hot plumes are yellow, and cool regions are violet. Visualization rendered using VAPOR (the Visualization and Analysis Platform for Ocean, Atmosphere, and Solar Researchers at the National Center for Atmospheric Research). Courtesy of N. Featherstone.

Achieving this goal requires a low viscosity (Ekman number, E) and an increase in convective vigor (Rayleigh number, Ra). Both requirements place greater demands on the numerical resolution required to represent the velocity and temperature fields in geodynamo simulations. To achieve a strong dipole with more realistic values for the magnetic Prandtl number ($Pm \approx 0.01$), simulations will require $E = 10^{-7}$ when Ra is approximately 10 to 50 times the critical value for the onset of convection. These numbers are much lower than have previously been achieved [9]. The next generation of numerical dynamos will require efficient, massively parallel computational capability to achieve the spatial and temporal resolution required to access this range. Rayleigh, a code developed by CIG, is an example of a next generation code designed with these goals in mind (Figure 2.)

2.2 Mantle Dynamics

We have learned from 2D calculations that tremendous resolution is required to resolve processes like rifting, subduction, and development of topography, especially as rheology becomes more realistic, i.e., more complex and variable. To address scientific questions such as how the mantle interacts with the core and the surface, and how Earth's dynamic history and early evolution influences its present configuration, we need very accurate, high-resolution models that can be computed for times that span the history of the Earth, while resolving heterogeneity on multiple scales. While open-source access to 3D spherical codes for researchers led to significant scientific breakthroughs, many recently published models in 3D still use 65 radial nodes to resolve the full depth of the mantle (2890 km). This resolution of almost 50 km per grid element is similar to early 3D convection models of more than two decades ago [10]. To address the stagnation in advancing grid size, CIG undertook the development of a 3D convection code with adaptive mesh refinement (AMR), in which the computational mesh in a finite element is locally refined as needed to resolve features. A preliminary experimental code, Rhea [11] demonstrated the potential of this method for mantle convection. A fully functioning adaptive mesh implementation has been realized in the code ASPECT (Advanced

Solver for Problems in Earth's ConvecTion) [12]. CIG also disseminates the well-established and widely used mantle convection codes CitComS and CitComCU [13, 14]. Because the mantle is not accessible to direct observation, the driving scientific questions require integration with observational data from mineral physics, seismology, and plate tectonics (for example [15, 16].) Researchers have also not fully characterized the physics of convection in the parameter space that requires lower resolution; models that formerly required a supercomputer can now can be run on a local small cluster or desktop, allowing researchers to explore parameter space and discover new phenomena (for example [17]). Adaptive models enable us to resolve changing, fine-scale structures, connecting mantle dynamics to plate kinematics, production and transport of melt, seismic wave propagation, mineral physics, geochemistry, deformation of the crust and lithosphere, and ice sheet evolution.

Enhanced modeling capabilities will advance understanding of phenomena such as subduction, rifting, mantle upwellings, the origins of large scale structures in the deep mantle and small scale circulation beneath the lithosphere, the long term evolution of the Earth as a planet, and the origins and scales of mantle heterogeneity. For example, it has been understood for more than a decade that variation in rheology is likely the key to strain localization and initiation of plate tectonics (see for example [18, 19], and references therein). Yet there remains debate about the driving mechanisms; one theory holds that water in the mantle is essential to plate tectonics [20], while another [21] holds that damage rheology influences subduction. Resolutions at least an order of magnitude finer than are commonly used now are needed to model the extreme gradients in rheology required to test these hypotheses.

2.3 Long-Term Tectonics

The lithosphere links the dynamics of the Earth's interior with the evolution of its surface. Lithospheric dynamics encompasses processes that span a broad spectrum of spatial and temporal scales, from localized deformation (e.g., earthquakes) to regional-scale tectonic processes (e.g., orogenesis). Computer modeling of these processes, however, is inherently difficult. Numerical methods must model a large-scale system at sufficiently high resolution to capture local-scale dynamics (e.g., fault growth). Codes must have the ability to track large-magnitude variations in material properties over a range of timescales and maintain material boundaries as the system evolves. In addition, many aspects of the underlying physics and material properties lack a complete theoretical or empirical description (e.g., rheology and strain localization, magma migration). Most material properties are non-linear, leading to complex feedback between different parts of the lithospheric system. Further, lithosphere dynamics depends strongly on the processes acting on the upper and lower boundaries of the lithosphere; thus a full description of lithosphere evolution should include surface processes (e.g., erosion, sedimentation) and coupling to the large-scale mantle convection system.

The field is primed for significant scientific advances; increases in computational power will enable high-resolution models of lithosphere dynamics, including development and evolution of plate boundaries, mountain building and basin formation, and feedback between surface processes and climate. The opportunity for improved computation is matched by enhanced images of subsurface structure from initiatives such as EarthScope and GeoPrisms, providing an opportunity for data integration techniques to provide a better understanding of coupling between mantle dynamics, lithosphere deformation and surface processes.

2.4 Crustal Dynamics

Reducing uncertainties in seismic hazard and risk assessments has the potential to transform how we mitigate risk in order to protect vulnerable populations. Current uncertainties are so large as to make it difficult to effectively target limited resources for reducing seismic risk. Earthquake rupture forecasts, such as the Uniform California Earthquake Rupture Forecast (UCERF3) [22], rely on fault slip rates inferred from geologic and geodetic models. Reconciling geologic models with relatively few sample points across hundreds to thousands of years with geodetic models with hundreds to thousands of sampling points across years to decades requires detailed models of the earthquake cycle that link crustal deformation across these wide range of scales while accounting for the 3D rheology of the crust and upper mantle along with interactions across the fault systems. The EarthScope Science Plan [5] and the Southern California Earthquake Center (SCEC) plan [23] each highlight the importance of addressing these questions with calls for integrated models of the earthquake cycle across fault systems that are consistent with deformation across temporal scales of decades to centuries.

Aqueous and magmatic fluids likely have significant roles in the rheology of fault zones as well as the lower crust and upper mantle. This is particularly true in subduction zones where both entrainment of water and dehydration of the down-going slab and other processes likely control the dynamics of fault slip, including the radiation of high frequency or low frequency energy, the presence of episodic slow-slip and tremor, and aseismic creep. Fluids also play a critical role in understanding the relationship between fluid injection and induced seismicity. Advancing the science in both of these areas will involve models that incorporate coupling between viscoelastoplastic deformation and transient fluid flow.

As models become more detailed and complex, science questions related to the earthquake cycle and induced seismicity begin to blend with those from other disciplines. Geodetic observations in polar regions capture surface deformation from many different processes occurring simultaneously, such as tidal forces, tectonics, hydrologic loads, cryospheric change, and surface loads. Understanding tectonic and/or loads associated with the cryosphere requires untangling the signals from these processes in the observations. The research questions for crustal dynamics are closely coupled with those in seismology, long term tectonics, and magma dynamics and multiphase flow.

2.5 Seismology

The seismic wavefield in the solid Earth is excited by earthquakes, and by other energetic events, including anthropogenic and volcanic explosions and fluid-solid coupling of ocean waves. The energy from these diverse sources and their interaction with the Earth produce motion across a wide range of frequencies. One of the greatest achievements in seismology of the 20th century is the ability to record ground motions from earthquakes over the broadest range of frequencies from the highest frequencies (up to 100 Hz) to the normal modes of the Earth (<10mHz). The travel time, amplitude, and frequency spectrum of seismic waves are functions of both the energy source and the geologic structures through which seismic waves propagate; thus by inverting observed seismic signals, it is possible to extract information about both the structure and the source. Forward modeling through known or inferred Earth structure can then be used to predict ground shaking, with implications for basic research and for human safety.

A great challenge to modeling the observed broadband wavefield is to reduce the uncertainties in 3D Earth structure. Seismic tomography crosses geoscience domains by providing critical constraints for investigations in core, mantle, lithospheric, and crustal dynamics. Current problems in mantle convection 2.2 use the 3D variations in Earth's internal composition and temperature, for which seismic velocities serve as a proxy. Results from imaging studies have driven modeling efforts to study regions of anomalous temperatures at the base of the lithosphere and around subducting slabs. Studies of outer core flow and the geodynamo also benefit from constraints on boundary conditions seismic imaging can provide. Better imaging of the topography of the D" layer at the core mantle boundary provides insight into the mineral physics and clues to the drivers of mantle convection. Lithospheric models from seismic imaging constrain the structure and the rheology of the crust and upper mantle for investigations of mountain building, basin formation, and plate kinematics that lead to a better understanding of crustal dynamics.

Regional and local crustal imaging use higher frequencies to improve resolution, which in turn enables identification of natural resources and seismic hazard, and better characterization of tectonic structures (see section 2.4.) Accurately assessing seismic hazard requires identifying both how faults will rupture and accurate high-resolution models of the resulting seismic wavefield (e.g., [24, 25]). This understanding is necessary to understand the entire "rupture to rafters" pathway (e.g., [26]) that is, how seismic waves are generated during an earthquake, propagate into urban areas, and shake and damage urban structures. The scientific questions associated with the fault rupture end of this process are closely connected to the research questions in crustal dynamics. On the "rafters" side, urban structures are most sensitive to ground motions from 1 Hz to above 50 Hz, frequencies that are extremely computationally challenging. Studies must span these scales in order to construct accurate, high-resolution models of Earth structure and seismic hazard.

2.6 Magma Dynamics and Multiphase Flow

The role of fluids and magmas in regional and global geodynamics and geochemistry remains one of the great unknowns in geodynamics. The presence of mobile, low-viscosity fluids significantly modifies the rheology of Earth materials, and provides fast pathways for diffusion and geochemical transport in the Earth's interior. Tectonic plate boundaries, such as mid-ocean ridges and subduction zones, are fundamentally magmatic, and magmatism may be a critical component for maintaining the weakness of plate boundaries. Melting and melt transport are fundamental processes controlling the geochemical evolution of the planet, including formation of the oceanic and continental crust. Beyond fluids and magmas in the mantle, there are a host of related problems involving the interaction of fluids in brittle crustal materials, including magmatism during crustal deformation, the role of fluids in faulting, induced seismicity, hydrofracture, and even the role of glacial melt water on glacier dynamics. Coupled fluid-solid dynamics is a scientific and computational challenge due to the complexity of the coupled multi-physics problems, including uncertainty in the fundamental conservation equations, constitutive relationships and thermodynamics of open systems, and plays an important role in crustal dynamics 2.4. A major challenge is to develop scientific software that provides flexibility to an individual scientist for composing and solving a range of models, while retaining the ability to reproduce and reuse results from successful models in other applications.

3 CIG Accomplishments

The CIG community comprises researchers interested in applications of computation to geodynamics, the study of the dynamics of the solid Earth. Participation is freely open to all, and currently involves scientists at all career stages from approximately 85 universities and government research institutions world-wide. The community is interdisciplinary and primarily includes participants from the domains of geoscience, computational science, mathematics, physics, astrophysics, planetary science, cryosphere science, and information and data sciences. The only requirement is an interest in computational geophysics and a commitment to shared open-source scientific software. Since 2010, more than 900 individuals have been involved in one or more CIG activities.

Since establishing CIG in 2005, the computational geophysics community has matured both its range of interactions and its computational capabilities. Over the past five years, CIG has developed new computational methodologies and capabilities, improved the quality of geodynamics software developed both by CIG and by individual researchers, enhanced the knowledge and capability of researchers in computational geophysics, grown and sustained our community, identified and removed barriers to using state-of-the-art scientific computing for research, and established partnerships with other organizations and international collaborators. Both membership and code repository holdings have grown, and we have improved both our software engineering practices and those used across the community. We have accomplished this by actively engaging the geodynamics community in all aspects of CIG's operation (Section 3.2). In particular, we use and disseminate software development practices that allow software projects to be independently sustainable by a broad user community.

3.1 Accomplishments

Researchers use CIG codes for research in geodynamics from the core to the crust and beyond, as detailed in the one-page research descriptions in Appendix A. Since 2010, more than 300 publications have been reported using software developed or hosted by CIG (references [101 – 413] of this proposal). An overview of significant highlights from the last five years are given below.

3.1.1 Geodynamo

In 2010, CIG hosted a scalar geodynamo code, MAG. At the time, most research in this community was done by individual scientists using their own codes. In 2012, CIG held a workshop bringing together geodynamo and solar dynamo researchers to identify state-of-the-art methods and grand challenge problems. This breakthrough event led to a long-term strategy that included: (1) improving and releasing a new donated parallel spherical harmonics code, Calypso, [27] with documentation, testing, and other standard characteristics of CIG codes; (2) developing a new code, Rayleigh, using the anelastic spherical harmonic (ASH) method that was developed for and is widely used in solar physics, and (3) defining and carrying out benchmarks to assess performance and accuracy of geodynamo codes. In response to the benchmark invitation, 14 research groups worldwide submitted their codes for testing. Performance benchmarks were run by CIG staff using CIG's Extreme Science and Engineering Discovery Environment (XSEDE) allocation on the Texas Advanced Computing Center (TACC) Stampede [28]; a manuscript is in preparation detailing both the benchmarking tests and the results. The community has also defined a small number of very large, high-resolution models needed for scientific progress, leading to the successful application for up to 319 million core hours over three years on Argonne Leadership Computing Facility's (ALCF) Mira, the world's fifth fastest computer.

3.1.2 Mantle Convection

The efforts of the community and CIG included sustaining and extending the CitCom codes [13, 14], and developing a new state-of-the-art adaptive mesh code, ASPECT [12]. CitComS (spherical shell) and CitComCU (Cartesian) are widely used around the world for mantle convection research; these codes have a range of capabilities including variable rheology, compressibility, phase transitions, and other material properties. CitComS has a remarkable scientific reach and celebrated its 20th anniversary in 2014. More than 80 papers have been published using these codes since 2010.

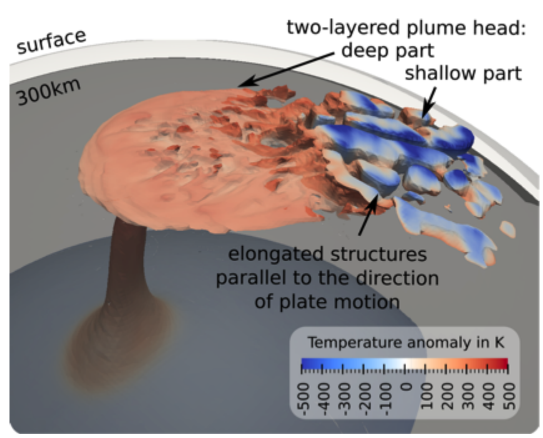

Figure 3: Low buoyancy plumes pool at 300–400 km depth forming finger-like channels when entrained in the overlying plate. ASPECT model courtesy of J. Dannberg.

ASPECT is a new parallel finite-element mantle convection code that enables refinement of the finite element grid to increase resolution in regions where higher resolution is needed; this enables running more complex, multi-scale models. ASPECT builds on a scientific software library, deal.II, which is used widely to rapidly build finite element solutions to partial differential equations for engineering and scientific applications. The use of standard libraries is one of the best practices for modern software development identified by CIG. ASPECT solves the 2D or 3D mantle convection equations (as formulated by [29].)

3.1.3 Long-Term Tectonics

Three codes are specific to long-term tectonics research: SNAC, PLASTI, and GALE. Of these, SNAC and PLASTI are donated and supported by the community. GALE, which was built on the Underworld mantle convection package [30] with support from CIG, is a parallel, 2D or 3D particle-based code used to investigate lithosphere-scale problems. Development is now complete. The code has been used to model subduction [31], rifting (e.g., [32]) and orogenic processes (e.g., [33, 34]). In addition to these domain-specific codes, the CIG codes PyLith and ASPECT, and the community developed code TerraFerma have been building capacity to address some long-term tectonics problems.

In 2014, CIG partnered with EarthScope National Office to hold the first CIG-EarthScope Institute for Lithospheric Modeling [35]. It was the first dedicated workshop in North America on modeling of lithosphere dynamics in more than a decade. The workshop demonstrated that a suite of tools is needed to meet the strong demand for a lithosphere dynamics modeling code as a single code may not suffice for the full range of scientific problems. In addition, the workshop revealed that observations need to be integrated with models, and these models should in turn link with other scales of Earth's dynamics, including mantle convection and short-term crustal dynamics [35].

3.1.4 Crustal Dynamics

In the last five years, the Short-Term Crustal Dynamics working group greatly expanded on the successes of PyLith development and training, begun in 2005. Developers added a number of important features to expand the science reach, improve PyLith's ease of use, and increase parallel scalability for larger problems. Notably, the development team implemented fault friction constitutive behavior, thereby permitting the code to be used in quasi-static and dynamic models of spontaneous fault rupture. This allows researchers to study earthquake rupture propagation, dynamic earthquake triggering, and earthquake cycle modeling. The implementation was verified using several SCEC Dynamic Rupture benchmarks [36]. The modularity of PyLith permits users to write small modules of code that can be easily integrated into the existing code to increase functionality; for example, a user-friendly interface was implemented for computing 3D static Green's functions.

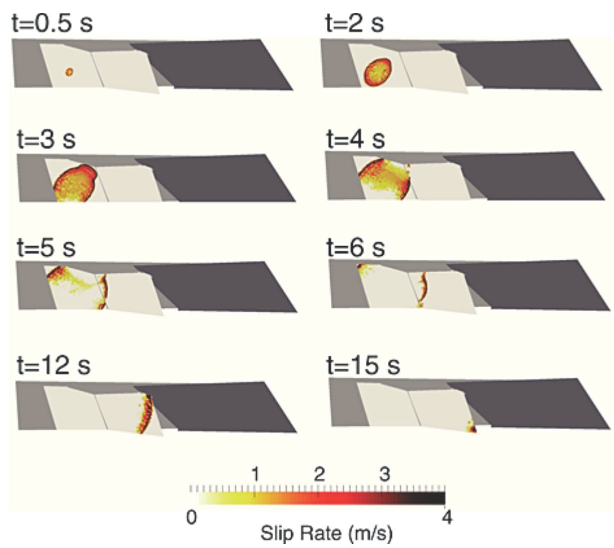

Figure 4: PyLith model of rupture across the fault system responsible for the 2010 Haiti earthquake (R. Douilly et al. 2015 [37].)

PyLith training expanded its content and increased its reach by incorporating online training. Two online tutorials (beginner and intermediate) were recorded and are available on-demand through the CIG website and YouTube channel. These expanded, targeted learning opportunities allowed users located around the world to participate in multi-day, interactive tutorials. The mix of in-person (Appendix B) and online tutorials is designed to enable participants to progress rapidly from from running small, toy examples to running simulations for research studies.

The Short-Term Crustal Dynamics working group also accepted three donated codes for hosting by CIG. RELAX is a semi-analytic viscoelastic code that provides the community with a simple, efficient code for computing the displacement and stress in a half space with gravity due to dislocations, Mogi sources, and surface tractions. It allows researchers to model nonlinear time-dependent post-seismic deformation due to power-law rheology materials in the bulk and/or rate-strengthening friction faults.Virtual Quake is a boundary element code for simulating seismicity on fault systems based on stress interactions to understand long-term statistical behavior of earthquakes. SELEN solves the "Sea Level Equation" for a spherical, layered, non-rotating Earth with Maxwell viscoelastic rheology. Sea Level Equations can be used to model the sea level variations associated with melting of late-Pleistocene ice sheets and the present-day melting of continental ice sheets. SELEN computes vertical and horizontal surface displacements, gravity variations and sea level changes on a global and regional scale.

3.1.5 Seismology

CIG seismology codes continue to lead in technical innovation. SPECFEM3D has played a leading role in benchmarking clusters and new hardware, such as the NVIDIA Tesla GPUs [38, 39]; for example, a simulation in 2013 on Blue Waters sustained 1 PF/s on 700,000 cores [40]. Ambitious efforts for global imaging with SPECFEM3D are currently underway and used on the order of 200 million CPU-hours under allocations within the Department of Energy's (DOE) Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program for leadership computing [41]. With I/O identified as a bottleneck for certain simulations and applications, the SPECFEM3D developer's group established new file formats such as HDF5-compatible ADIOS.

Capabilities for modeling wave propagation in complex structures are highlighted in research conducted with SPECFEM3D [42]. SPECFEM3D was used to perform a dynamic earthquake rupture simulation for the 2011 Tohoku earthquake [43]. Simulations of scenario earthquakes in Southern California were coupled to finite-element models of buildings, demonstrating "rupture to rafters" capabilities [26]. Adjoint seismic imaging with SPECFEM3D was demonstrated at crustal scales with earthquakes and ambient noise [44, 45, 46, 47] and expanded to upper mantle scales of Europe, where both anisotropy and attenuation were included as inversion parameters [48, 49, 50]. These efforts are part of a global wave of interest in full waveform inversion that is exploiting computational resources and massive data sets from earthquakes, ambient noise, and active sources [51, 52, 53, 54].

The Seismology working group welcomed two well-developed wave propagation codes, SW4 and AxiSEM, and a mineral physics toolbox, Burnman. SW4 is a parallelized finite-difference method code originating at Lawrence Livermore National Laboratory (LLNL) [55, 56]. The code handles models with complex geometries (including topography) and has recently been used within iterative source inversions [57]. AxiSEM is a parallel spectral-element method for 3D (an-)elastic, anisotropic, and acoustic wave propagation in spherical domains. It requires axisymmetric background models and runs within a 2D computational domain, thereby reaching all desired highest observable frequencies (up to 2 Hz) in global seismology [58, 59, 60]. Burnman [15] is a Python toolbox that allows users to calculate seismic velocity profiles for a given mineral compostion, geotherm, equation of state, or averaging scheme. These calculated seismic velocity profiles can then be compared to profiles constrained by seismology. In response to community interest, the Seismology working group is also engaged with an international team of developers encouraging development of a new normal modes code [61].

3.1.6 Magma Dynamics and Multiphase Flow

The magma dynamics community has been closely connected with the mantle convection and long term tectonics communities through workshops and software development, helping set directions for development of PETSc, ASPECT, and community codes. Software development has primarily involved the community leveraging CIG's infrastructure with other non-CIG sources of support. One code developed in this manner is TerraFERMA [62, 63] (The Transparent Finite Element Rapid Model Assembler), a software framework for model exploration, particularly for addressing coupled multi-physics problems such as magma dynamics. It leverages three advanced computational libraries – FEniCS [64], PETSc [65, 66] and SPuD [67] – that provide (1) high-level problem description, (2) composable solvers for coupled multi-physics problems, and (3) a science-neutral options handling system that allows the hierarchical management of all model options, respectively. Because all models in the framework share the same infrastructure, models become more reusable and reproducible. TerraFERMA is currently available as a developer's release [62] with full release planned for 2015 through CIG's infrastructure.

Models for coupled fluid-solid flow in subduction zones using TerraFERMA [68] show that including interaction of slab fluids with the solid rheology can drastically change the pathways of fluids and melts in the subduction system. In particular, pressure gradients induced by interaction with solid viscosity variations can drive multiple mechanisms for focusing distributed slab fluids and melts toward the sub-arc corner. This has been suggested as a mechanism to explain the small variability in location of the volcanic arc ($\sim$ 100 km above the earthquakes) with respect to the large potential variability in slab fluid sources.

While TerraFERMA aims to address the full multiphysics problem associated with melt production and transport, a complementary approach added simplified models of batch melt and porous flow transport to the mantle convection code ASPECT [69]. This enables exploration of the impact of melt in the larger convecting system.

3.2 Community

Like other scientific and engineering communities using and developing computation for research, computational geodynamics has progressed through stages towards maturity. In the five stages identified by Oberkampf and Roy [70] and by Shea et al. [71], codes are initially developed by individual researchers to solve specific research problems (Stage 1); effectiveness of the computational methods as a research tool is demonstrated through scientific publications and benchmarks (Stage 2). A decade ago, the geodynamics community recognized that a larger commitment was required to maximize the scientific return on investment (Stage 3), leading to the establishment of CIG. As this investment led to greater confidence and expanded capabilities, CIG improved the effective use of computation, through training, disseminating best practices, and facilitating access to high performance computing (Stage 4). Some areas of computational geodynamics are approaching mature capability (Stage 5) while others are still ramping up. Because computational geodynamics focuses on natural – not engineered – systems, there is continuous feedback between the stages, with mature software driving new research that eventually makes its way back into the codes (Stages 1-5). Discovery and surprise are anticipated at every stage of this process.

From an operational standpoint the community is organized into seven working groups (Geodynamo, Long-Term Tectonics, Magma Migration, Mantle Convection, Seismology, Short-Term Crustal Dynamics, and Computational Science). The working groups are led by teams of scientific experts and user-developers appointed by the Executive Committee. The Executive Committee, the primary decision-making body of the CIG, comprises seven members who are elected by representatives of member institutions on a rotating basis. The Science Steering Committee considers and recommends CIG activities, which are then considered and approved by the Executive Committee.

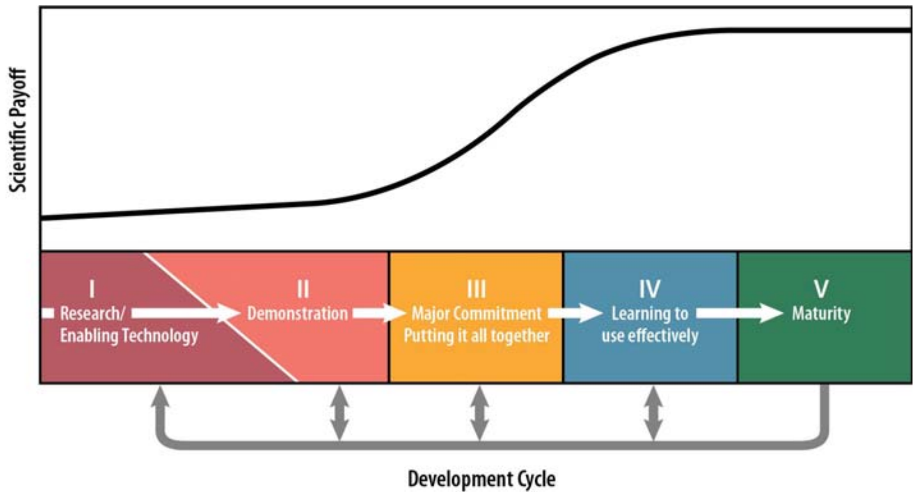

Figure 5: The five stages of scientific software development maturity, modified for geodynamics from [71, p. 12].

The CIG Headquarters is located at UC Davis and is staffed by the director, administrative staff, and a technical team. More details of the specific duties of each of these groups and the overall governance of the CIG is described in Section 7. At intervals, CIG senior leadership holds planning retreats to refine CIG's vision and goals. Our 2013 retreat resulted in a strategic planning document [1] defining CIG's mission, core values, and strategic objectives.

CIG's mission and vision [1] include building the knowledge required to use scientific software accurately and effectively through research workshops, tutorials for end users, and hackathons for user-developers (Appendix B). Since 2010, CIG has offered 19 workshops with more than 950 participants, more than 530 of whom were early career investigators. We plan to continue at this rate, using feedback from each event to set directions and improve future events. During the academic year, CIG runs monthly webinars. The series draws on experts from mathematics, computer science, and the geosciences to inform and disseminate knowledge on the tools and methodologies employed for problems in geodynamics. Webinar participants have been introduced to topics such as new software, benchmarking, numerical methods, software best practices, and scientific visualization. Webinars are recorded and are posted to our website and have been viewed more than 1500 times on YouTube.

Partnerships allow us to foster and build synergistic connections with other organizations in the geosciences and computational sciences. They help us significantly leverage our limited resources, and provide opportunities for crucial input on interdisciplinary questions. CIG collaborates with other institutions, such as the Cooperative Institute for Deep Earth Research (CIDER), EarthScope, EarthCube, Incorporated Research Institutions for Seismology (IRIS), National Aeronautics and Space Administration (NASA), United States Geological Survey (USGS), LLNL, DOE, SCEC, and XSEDE, to offer workshops and tutorials as well as provide access to resources. Some of these organizations also collaborate on and contribute to our software base.

CIG established multidisciplinary partnerships with experts in the social and library sciences and High Performance Computing (HPC) leading to two related externally-funded projects:

- The *INCITE* project is a collaboration between CIG, solar, planetary, and geodynamo experts, and computational science experts at ALCF to carry out community-defined high-resolution planetary dynamo computations [28]. Along with computing cycles, the team has access to computation, data, and visualization experts who work closely with our team.

- The *SAGA* (Software Attribution for Geoscience Applications) project brings together an interdisciplinary team from the library sciences, social sciences, computer science, and CIG to illuminate the technological and cultural barriers to effective software citation. The project seeks to provide mechanisms and tools for citation of open-source software and to effect cultural changes such that scientific software is routinely properly acknowledged and cited [72].

3.3 Technological Infrastructure

CIG promotes best practices in software development and provides the infrastructure to enhance software discoverability and usability. CIG encourages software attribution so that developers receive credit for their contributions.

3.3.1 Software Infrastructure

CIG uses and promotes use of modern software engineering practices and tools, including use of software repositories to facilitate sharing of validated open-source software, version control, documentation, and running build-and-test scripts on codes. All CIG codes have a software page on the CIG website, with links to downloads and other information.

CIG encourages researchers to donate codes that have scientific value to the geosciences for open distribution. Donated codes must be approved by the CIG Science Steering Committee and Executive Committee, and must meet CIG's Software Donation Policy. Staff work with developers to ensure all codes meet best practices before they are added to the code repository and testing framework, and the software web page is created. CIG currently hosts 31 codes (See Appendix C).

Table 1: Software developed by CIG (D_CIG) or community contributors (D_CONTRIB) or supported by community contributors (S_CONTRIB) since 2010. For a complete list of CIG codes see Appendix C.

Geodynamo	
Calypso	D_CIG
Rayleigh	D_CIG
Long-Term Tectonics	
GALE	A
Mantle Convection	
ASPECT	D_CIG
CitCom	D_CONTRIB
Seismology	
SPECFEM3D	D_CIG
SPECFEM3D_GLOBE	D_CIG
AxiSEM	D_CONTRIB
Burnman	D_CONTRIB
SW4	D_CONTRIB
Short-Term Crustal Dynamics	
PyLith	D_CIG
RELAX	D_CONTRIB
SELEN	S_CONTRIB
Virtual Quake	D_CONTRIB

We broadly categorize each code's level of activity as: developed (D), supported (S), or archived (A). *Developed* codes are leading-edge software packages that are actively being improved and enhanced. Some codes are entirely community-developed (category D_CONTRIB, e.g., RELAX, Virtual Quake, SW4), whereas others have received partial support or were primarily developed by CIG (category D_CIG; e.g., PyLith, GALE, ASPECT, SPECFEM, CitComCU, CitComS, Calypso, and Rayleigh). In practice, all codes under development rely on a mix of CIG and contributed efforts. Codes in the "D" category generally adhere to best software development practices, including regular, version-numbered releases, extensive test suites and documentation, active user and developer communities, tutorials, and a regularly updated plan for future development.

Through code development, CIG contributes to the widely-used computational science libraries PETSc [65, 66, 73] and deal.II [74, 75]. Several CIG codes rely on PETSc; development is simultaneous. For example, features are added to PETSc to support functionality in PyLith, and the new PETSc features are immediately available to the broader scientific and engineering communities.

A smaller number of codes are *supported* by the community or CIG but are no longer undergoing active development. *Archived* codes are available as stable versions but are not supported. Some archived codes remain in use (e.g., Mineos, Flexwin) but with no active development; others have been eclipsed by newer codes (e.g., LithoMop, now superseded by PyLith). Maintaining version-controlled archived codes in repositories supports reproducibility, and can reduce duplication in software development.

3.3.2 High-Performance Computing

The availability of robust scientific software increases the demand for access to high-performance computing (HPC) that uses this software for research and teaching. ASPECT, Calypso, Rayleigh, CitComS, and SPECFEM all scale well to hundreds or thousands of cores. CIG helps facilitate access by geophysics researchers to national HPC facilities by providing access to training, maintaining an allocation on the National Science Foundation (NSF)-supported XSEDE virtual research computing system system, hosting the UC Davis XSEDE Campus Champion, working with CIG groups who are interested in and ready to use leadership-class computing for their research, and representing the CIG community in discussions of HPC needs in the geosciences. CIG hosts workshops, involving partners such as national labs, IRIS, and UNAVCO (formerly the University NAVSTAR Consortium), to define the need for, and barriers to, HPC access.

CIG currently has an allocation on XSEDE's Stampede and NSF's Yellowstone. Small allocations, advice, and assistance are provided to CIG researchers who wish to carry out small-scale research tests and benchmarking in preparation for obtaining their own allocations for research. Through the CIG allocation, the community's 58 user accounts has had access to 490,000 Service Units (SUs) on Yellowstone and 3.6 million SUs on XSEDE (Stampede and Ranger).

Two CIG research groups use leadership class computing through DOE's INCITE program. The geodynamo working group leads and directs the effort to produce dynamo models at unprecedented scale and fidelity. Proposed runs for Mira (the 10-petaflops IBM Blue Gene/Q system at ALCF) will use 317 million core hours and produce a petabyte of data. The SPECFEM team is pursuing high-resolution, global adjoint tomography on Titan (Oak Ridge National Laboratory). The inversion uses waveform data from over 3,000 earthquakes world wide and will use an estimated 739 million core hours.

3.4 Lessons Learned

CIG has evolved and matured as an organization yet remains adaptable to changing needs and new opportunities. This section outlines what we have learned about the computational capabilities of our diverse scientific community, how we operate as a software ecosystem to grow and sustain these capabilities, how we have evolved to balance pragmatic requirements for sustaining infrastructure, and our aspirations for the future.

3.4.1 Software Development Modalities

CIG provides 31 codes; seven have been developed with significant direct support from CIG. These CIG-supported projects have either steadily built a user base over time (PyLith, CitCom, and SPECFEM), or experienced rapid growth (Rayleigh, Calypso, ASPECT), or sunsetted, that is, active development has ceased (GALE). The three different modalities are described here.

Sustained growth: PyLith PyLith emerged from legacy codes and has undergone steady, sustained development, accompanied by steady, sustained growth of its use for research and education. The developer–user team has several champions who define short-term and long-term goals for the code from user input, including timelines and estimates of the difficulty of each goal. Developers invest considerable effort in training, with both in-person and online tutorials and workshops. Many of the trainees return multiple times to build their skills with the codes, especially as new features are added. This training now provides a model for other CIG tutorials, and the PyLith team led development of CIG's software best practices.

Rapid growth: ASPECT Code development was initiated by CIG in 2010 in response to a need for an adaptive, flexible, modular, open code for mantle convection and lithosphere-scale modeling. The code builds on libraries, leveraging development done for engineering and other scientific applications, and uses software plug-ins to add new functionality, making it easy for others to contribute code. The code has several champions and a core user base who work closely with the lead developers to set priorities. Training is accomplished through tutorials and through hackathons, workshop-style gatherings in which user-developers work intensively with the lead developers to improve the code. Numerous hackathon participants have become expert users.

Sunset: GALE Code development was initiated in 2007 to model the complex, non-linear processes involved in lithosphere dynamics. Computational requirements for lithospheric dynamics vary widely depending on the specific scientific problem; hence the resulting code was quite complex. GALE, having branched from its predecessor and its developer base, never found a dedicated user-developer champion to sustain the code. As a result of these and other factors, the decision was made to cease further active development of GALE in 2012, after extensive discussion among the working group, Science Steering Committee, Executive Committee, and CIG staff and leadership. Stable versions of GALE (versions 1.6.1 and 2.0.1) remain available on the project website and continue to be used.

3.4.2 Best Practices

We have learned that successful scientific software development requires (at a minimum):

- Close, active partnerships and collaboration between users (domain-expert researchers) and software developers,
- Clearly identified and committed lead developer(s) or, preferably, user–developer teams,
- Well-defined scientific and computational goals that are consistently and regularly evaluated and updated,
- Use of well-defined benchmarks and testing throughout development,
- Attention throughout development to the user interface and extensibility,
- Understanding and evaluation of the complexity of dependent libraries, and
- Mitigation of complexity and management of user expectations with education, training, and support.

Community codes are most successful when a cohesive and engaged community exists in concert with a champion who assumes leadership on behalf of the community, or a broad and clear distribution of responsibilities are defined and acted upon. In practice, code champions are research professionals, professors, or research scientists with a sustained interest in the scientific use of the software. The CIG community benefits when there exists symbiosis in these roles (as with PyLith) or when development takes place across diverse communities (as with ASPECT and SPECFEM).

The CIG community's interaction with the computational science community has significantly changed how software is developed across geodynamics. Historically, geodynamics software was developed for individual research projects, without much regard to design, testing, documentation, extensibility, sustainability, or potential adoption by a larger community. In contrast, newly-developed CIG codes practice sound software development methodologies: they (i) build on widely used open-source software libraries (when available), (ii) have extensive test suites that are frequently run, (iii) use portable configuration and build systems, (iv) are extensively documented both within the code as well as in manuals and websites, and (v) use structured but human readable input formats.

CIG's Science Steering Committee articulated these principles in a set of best practices (see Section 4 and Appendix C) for software either developed by or hosted by CIG. We define three levels of expectations: a minimum set that codes donated to CIG must follow, a standard set defining the practices that should be used for codes actively developed within the CIG community, and a target set that provides goals all developers should aim for in long-term development. Expectations and practices are shared between different projects and have disseminated beyond CIG, and can increase the impact of software development for those who choose to adopt them.

Newer CIG codes are written to be extensible, e.g., the plug-in system designed into ASPECT. Using configurable components to define models as input files makes it simpler to extend a code, promotes reproducibility, and makes it possible to more aggressively incorporate contributions of the community. A sign that this is working is that our newer codes avoid the previously common situation of multiple code versions circulating in the community.

3.4.3 Training and Education

As CIG has matured and the education needs of our community evolved, we have adapted our training program to include both asynchronous and synchronous modules.

To support independent asynchronous learning, all software have manuals that include installation instructions and examples, including benchmarks, test cases, cookbooks, and tutorials, with input and output files and post-processing examples. These help build intuition and serve as starting points for research use of the codes. Video recordings of tutorials that show interactively how to use codes and lectures on introductory material, supplemented by virtual or in-person help sessions, have proven effective. Recorded beginning sessions can be used as a prerequisite to attending in-person or online synchronous advanced sessions. This expedites the transition from users getting their feet wet with toy problems to using the codes in their own research. Advanced-level training focuses on more complex topics, including new software features and broader topics such as in solvers, uncertainty quantification or mesh refinement.

Online training extends our reach and makes us more efficient in training our users. However, in-person training is still a core activity because bringing people together develops a vibrant user and developer community, enhancing learning and fostering collaboration. In-person activities, such as workshops and hackathons, blend scientific education and hands-on experience with the code. They give participants extensive time to implement their models and receive in-person support both from the developers and other researchers.

4 Software and Cyberinfrastructure for Scientific Discovery

Scientific software development often ventures into unfamiliar territory, with a considerable role for discovery and surprise. CIG both pushes both computational and scientific boundaries and vets development plans through working groups and governing committees to ensure that software development matches the science goals of the community. Throughout the process we aim to retain the nimbleness to respond to emerging opportunities. This helps us identify, acknowledge, and mitigate risks. In this section, we describe our development plans for the next five years.

4.1 Planned Development

4.1.1 Geodynamo

The geodynamo community aspires to move toward realistic Earth parameters by developing and running the Rayleigh and Calypso codes on massively parallel computers, with attention to both accuracy and performance. Currently, scientific progress in modeling the geodynamo is limited by resolution; higher resolution is required to accurately model the low viscosity of the liquid iron alloy that makes up the outer core. The geodynamo community and CIG released and support Calypso, a set of codes for magnetohydrodynamics simulation in a rotating spherical shell using spherical harmonics expansion methods, and initiated and supports development of Rayleigh, an

ASH code for magnetohydrodynamic geodynamo calculations. Development of these codes will continue including regular releases with features added as driven by the community. Initially, Calypso will implement a full-sphere model, improved Legendre transforms, support for m-folding longitudinal symmetry, and improvements to I/O. The emphasis for Rayleigh is to improve parallel efficiency, i.e., test, benchmark, and profile OpenMP implementation, create user friendly interfaces, and create output modules compatible with standard visualization software. Rayleigh will also add Cartesian geometry, implement finite-spectral elements in radius-based off-multiple Chebyshev domains, and improve sparse matrix solves through implementation of Chebyshev-tau functionality.

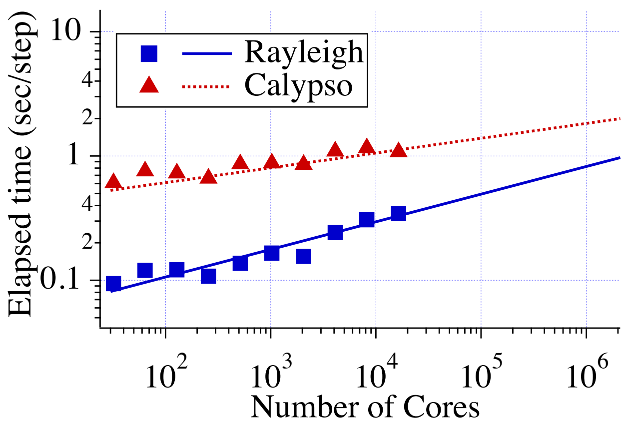

Figure 6: Weak scaling of geodynamo models on TACC Stampede up to 16,384 cores. In a weak scaling test, the total degrees of freedom (DOF) is proportional to number of processor cores. Lines are power-law fits ($t = AN_{\mathrm{cores}}{}^{p}$): where $A = 0.353$ and $p = 0.120$ (Calypso) and $A = 0.0382$ and $p = 0.222$ (Rayleigh).

The community has also determined that the large runs required to model the geodynamo over Earth's history require a newly coordinated approach. The working group applied for, and obtained, an allocation of cycles on Mira at ALCF to carry out well-defined large runs using Rayleigh, which has shown accuracy and scaling to many thousands of cores (Figure 6). ALCF is providing a significant investment of expertise to improve code performance and assist with visualization, data management, training, and other tasks necessary to success of the project. CIG will provide domain expertise, training, code development, and community coordination on this project. With technical support from ALCF, the data from these runs will be openly available to all for analysis and interpretation. This coordination of the model runs represents a new approach for the geodynamo community and will enable breakthroughs at the frontier of geodynamo modeling.

4.1.2 Mantle Convection

In the next five years, major development will focus on ASPECT, adding capabilities to enable high-resolution models of subduction, rifting, mantle plumes, deep earth dynamics and global convection, origins of plate tectonics, and early Earth history. These models require the capability to run very large models that integrate data and enable exploration of new physical regimes. Development priorities include adding new rheologies, multiphysics, topography building, accurate material interface tracking, active and passive tracers, and interoperability with other models. Performance and accuracy will continue to be improved with a redesign of the non-linear solver infrastructure, levelset formulation for accurate compositional fields, and parallel efficiency benchmarking.

Achieving higher resolution requires code benchmarking and building human capacity. Researchers must be knowledgeable about model parameterization and must fully understand the extent to which different methods can resolve subduction zones, slabs, narrow plume tails, and other features. This need can be met through well-designed benchmarking for mantle convection codes, drawing on lessons learned from previous mantle convection and recent geodynamo benchmarks, to promote understanding of the capabilities and limitations of various methods. Tutorials will train geodynamicists to use the codes and on best practices for model design (see Section 5), while hackathons will be used to develop expertise and add functionality. In addition, we will continue to support the community's use and development of the very widely used mantle convection codes CitComS and CitComCU.

Advances in software and modeling capability drive the need for access to and capability to use high performance computing sufficient to carry out these high-resolution models, some spanning substantial geologic (model) time. CIG continues its efforts to facilitate use of HPC and training.

4.1.3 Long-Term Tectonics

Long-term tectonics problems require that researchers have the ability to track discrete material boundaries and incorporate factors such as non-linear rheologies, strain localization and delocalization, metamorphic phase changes, melting and fluid transport, and surface processes. The most promising modeling approach appears to be modular codes based on a common core of numerical solvers, in which individual modules address specific aspects of lithosphere dynamics. As we have seen with ASPECT, this approach facilitates a greater involvement of individual users in the process of code development, with user-developed modules comprising a shared repository. A modular format also enables coupling with mantle convection, short-term tectonics, fluid/solid dynamics, surface, and cryosphere models.

The 2014 CIG–EarthScope Institute for Lithospheric Modeling workshop provided a community-wide view of computing capabilities and needs [35]; we continue to gather input from the community through workshops and the working group. An immediate goal for the next year is to evaluate current computational capabilities and identify existing codes that can potentially serve as the basis for next-generation long-term tectonics software. This includes evaluating potential use of ASPECT and, more generally, the deal.II libraries. ASPECT now includes plugins for viscoplasticity, topography, material tracking, and melting. The multiphysics code TerraFERMA and the short-term crustal dynamics code PyLith also provide some needed capabilities.

We will define benchmarks to compare the accuracy and performance of codes and numerical techniques, to identify the most suitable numerical approaches (e.g., solvers, discretization) for these applications and guide the development of codes and modules that address different aspects of lithosphere dynamics. Development will be driven by community requirements, both through user requests for module development and by donation of modules to CIG. Dedicated long-term tectonics workshops, in partnership with other communities such as EarthScope, GeoPrisms, and EarthCube, will engage the community and provide guidance for code development. Developing tutorials and resources will be important to empower new users of CIG software.

4.1.4 Crustal Dynamics

Research topics in crustal deformation across temporal scales of seconds to thousands of years continue to drive the software development in the Short-Term Crustal Dynamics working group. Modeling the earthquake cycle with greater fidelity holds strong promise for reducing uncertainties in earthquake rupture forecasts and seismic hazard assessments. Additionally, integrating aqueous and magmatic fluid flow into elasticity models of crustal deformation will improve our understanding of the physical processes controlling subduction zone behavior and induced seismicity. Untangling the signals from the wide variety of physical processes causing crustal deformation in polar regions requires modeling tools that can capture tectonic deformation, surface loads, and hydrologic loads. We plan to continue development of PyLith to address these needs.

Addressing the demands of these varied scales requires restructuring some of the current modules to be compatible with the Pyre framework, making use of the new prototyped multiphysics capabilities in PETSc, and providing basic kernels associated with elasticity for the bulk rheologies already implemented in PyLith as well as kernels coupling fluid flow. Implementation of coupling between elasticity and fluid flow will provide the poroelasticity functionality requested by the community as well as a template that advanced users can use to extend the multiphysics capabilities as plugins in Pyre.

To capture the dynamics of rupture propagation and radiated seismic waves at the temporal scales of microseconds to seconds, the postseismic response at the scales of minutes to years, and the interseismic deformation at scales of hundreds to thousands of years requires coupling the dynamic and quasi-static capabilities already present in PyLith. The capability to model these phenomena has been an objective for PyLith from its inception. Having delivered capabilities to investigate small slices of the earthquake cycle, we are ready to make substantial progress on coupling the two pieces. Reaching this goal will necessitate more sophisticated time-stepping algorithms, modularizing the simulation start-up, and the ability to transition from explicit to implicit solvers during the simulation.

4.1.5 Seismology

The primary challenge for CIG's seismological codes is to establish and improve computations and workflows for seismological inverse problems. SPECFEM3D has played an important role in connecting the forward simulation capabilities of wave propagation into the inverse capabilities for estimating (or "imaging") new 3D variations in Earth's structure. To undertake a simulation-based seismic imaging problem is a major challenge; a few are targeted here for continued efforts.

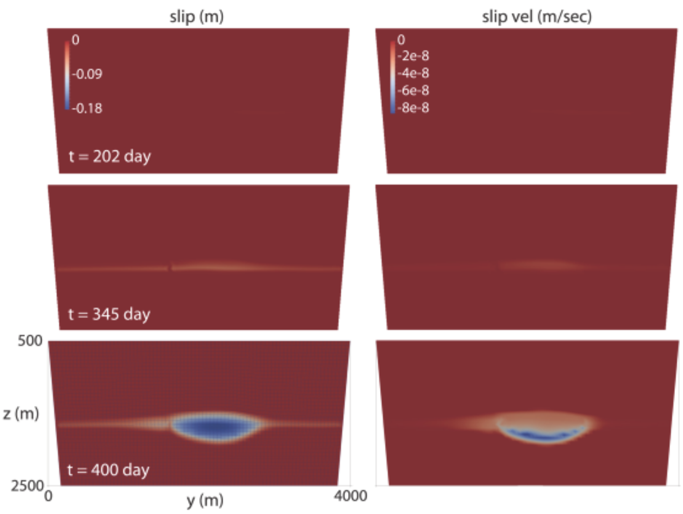

Figure 7: Model of slip magnitude (l) and slip velocity (r) on a fault plane due to CO_2 injection, modeled using PyLith by B. Jha and R. Juanes [76].

To assemble and process seismic data for usage in inversion codes requires multiple time-consuming steps using multiple software packages. Updated workflow management tools are needed to shepherd these unwieldy datas sets by improving the handling of observed and synthetic waveform data to reduce inversion workflow bottlenecks (e.g., ObsPy [77, 78]), more efficiently track the thousands of simulations on parallel systems, and calculate adjoint sources. These massive datasets present an extreme I/O challenge, driving the need to adopt the ADIOS library and further develop the Adaptable Seismic Data Format (ASDF), both of which use parallel HDF5. These large datasets are used in solving the compute intensive forward and inverse problem, requiring continual efforts to improve performance on new and existing parallel architectures including GPUs.

One unsolved implementation of the forward problem in seismology remains for global wave propagation within SPECFEM3D_GLOBE: full gravity. The full implementation removes the Cowling approximation [79]. Once implemented, this feature can be applied to the study of viscoelastic problems, such as isostatic rebound, as well as for normal-mode seismology.

Even for expert users and with streamlined workflows, handling the large data sets and the myraid of codes needed for tomographic inversions is challenging. Using these newly-developed tools and features effectively requires training. A workshop featuring workflow training, a new component for CIG, will help users close the gap in the time required from project intiation to simulation. Workshops may be held in conjunction with international and national partners (e.g. IRIS, SCEC, LLNL, the QUantitative Estimation of Earth's Seismic Sources and STructure (QUEST) or its successor program, the APEC Cooperation for Earthquake Simulation (ACES), and the Virtual

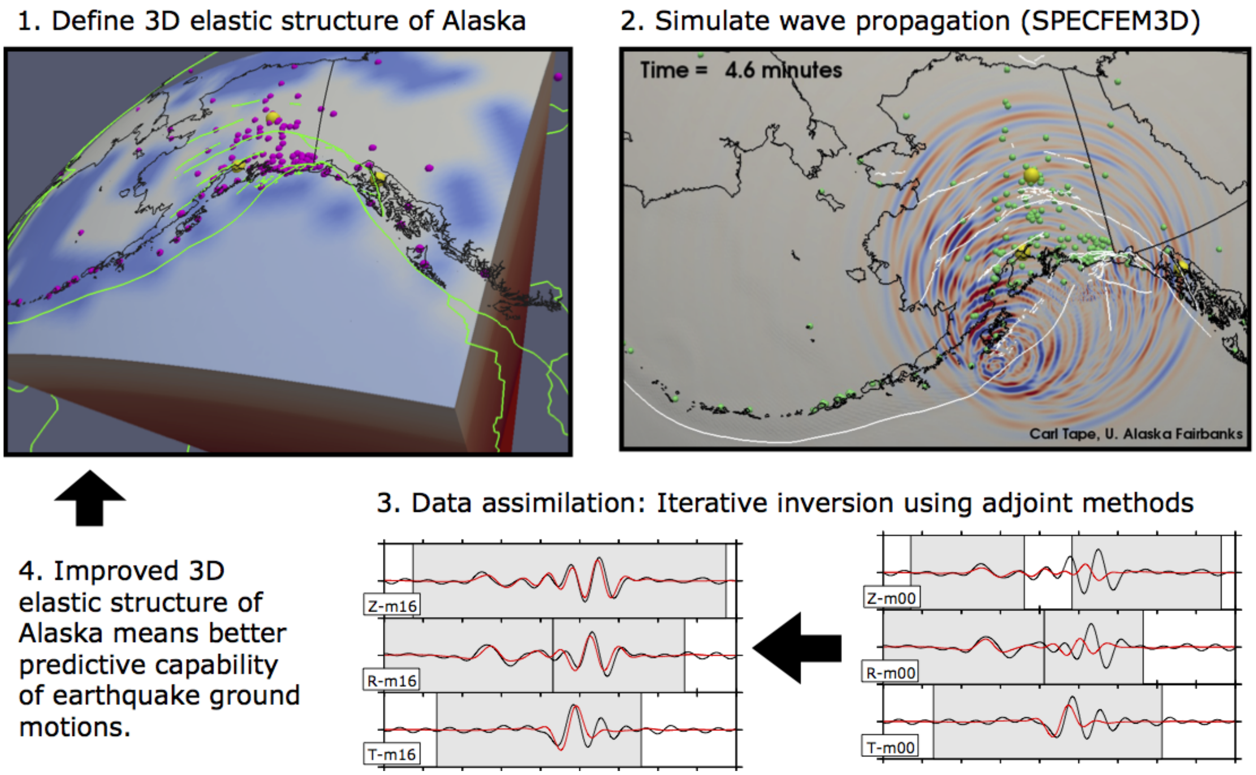

Figure 8: Data assimilation workflow for seismic imaging in Alaska. New earthquakes provide data that is used to improve the three-dimensional elastic structure model. An improved model enables better predictions of ground motion for future earthquakes (courtesy of C. Tape, [44, 80].)

Earthquake and Seismology Research Community (VERCE)).

4.1.6 Magma Dynamics and Multiphase Flow

Magma formation and dynamics require a variety of approaches. TerraFERMA, developed independently, provides a parallel framework for investigating interactions of fluids with solid deformation and other problems that involve coupling different systems. TerraFERMA v0.1.a, (Figure 9) is available as a developer's version, meaning that it is currently suited primarily for expert users and developers. CIG will assist the developers with a formal release when their initial development phase is complete; CIG's contribution would include helping with testing, documentation, benchmarking, and software best practices, providing a code release page and mailing lists for communication among users and developers.

We will support training and tutorials to develop expertise within the community of scientists interested in using this software to explore complex multi-physics problems, drawing on the tutorial cookbook, which already includes more than 50 benchmark problems in convection and magma-dynamics. A key design aspect of TerraFERMA is that each working model becomes an example problem that can be run and modified. Thus we will help the developers archive and document user-supplied examples to extend those already included with the software. This element of the code will help with computational reproducibility and improve software citability; model files used in peer-reviewed publications become part of the public record, either in the supplemental information with publications, or in a repository managed by CIG.

The lead developers have begun using this framework to explore some of the issues in developing efficient solvers for visco-plasticity, which is central to many of the problems in long-term tectonics. TerraFERMA and PyLith also share infrastructure through PETSc; the working group will evaluate and benchmark TerraFERMA and new features in PETSc such as finite element and finite volume to determine future development paths. As described below, PyLith development plans also include adding key multiphysics capabilities which will be complementary to TerraFERMA.

Development plans for ASPECT include adding plugins to enable researchers to investigate the role of magma in the dynamics of upwelling plumes and subduction zones. ASPECT is now able to run models with bulk melt generation, feedback to material parameters such as viscosity, and a Darcy flow model of the melt migration.

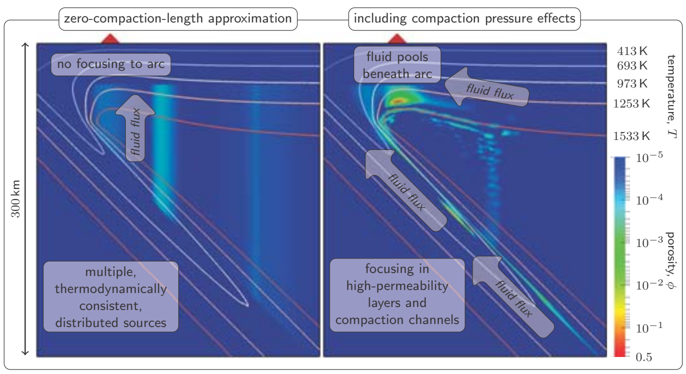

Figure 9: TerraFERMA v0.1.a calculations for coupled fluid/solid transport in subduction zones from Wilson et al. 2014 [68] showing different flow paths for fluids expected when including pressure gradients induced by flow through variable viscosity materials.

Additionally, CIG will collaborate with the developers of the widely used Melts program [81] who are developing cyberinfrastructure interfaces to thermodynamics databases so that key properties can be accessed by geodynamics models.

4.2 Crosscutting Themes

While the motivation for the CIG code development is scientific in nature, our strategy for implementation and community engagement is process-driven. We aim to create a highly efficient and synergistic program that as a whole is greater than the sum of its parts. The program is much more than a collection of scientific software. Here we describe some of the overarching crosscutting computational, software, and scienctifically motivated themes that are pervasive, create efficiencies, and knit the community together. Efforts in these broader areas benefit all of the working groups. They allow the CIG to remain flexible and responsive to opportunities that arise from individuals and from broader science and technology trends.

4.2.1 Data Integration

The Earth sciences today have a vast quality and quantity of data to inform modeling. We will extend code capabilities to use data as inputs and to create outputs that can be directly compared with data, improving input models to create an inversion scheme. Some CIG codes are already well placed in this regard. For example, the SPECFEM family of codes can compute synthetic seismograms for every major earthquake, using publicly available moment tensors and seismic velocity models, and can also compute sensitivity analyses. SPECFEM has been used for regional and global waveform inversion of seismic data with unprecedented detail.

Similarly, PyLith can use existing 3D fault models such as the SCEC community fault model [82]; both ASPECT and CitComS can use GPlates [16] data for surface velocities and have been used with a Slab 1.0-derived model [83], with a realistic Shuttle Radar Topography Mission (SRTM)-generated Synthetic Aperture Radar (SAR) topography description, and with sediment isopachs. Output from CIG codes can be compared with observations, for example crustal deformation observed by Interferometric Synthetic Aperture Radar (InSAR) and Global Positioning System (GPS), high resolution topography, Gravity Recovery and Climate Experiment (GRACE) gravity data, geochemical and petrological information, and data about evolution of the Earth's magnetic field. Many of the scientific results in Appendix A illustrate such interactions.

We will build on these approaches by developing additional modules to read and write data in formats that facilitate inverting data for models. We will strengthen partnerships with geoscience organizations that provide data, collaborating on common data formats that allow for the communication of model information between heterogenous codes (for example to make the output of a mantle convection code available as the input of a seismic code, where both are using different numerical methods on unrelated meshes). An *ad hoc* working group will advise on how the data assimilation and uncertainty quantification approaches that have been developed in other disciplines can best be adapted to the needs and often highly nonlinear and unstructured models used in geodynamics research.

4.2.2 Improved Software Interoperability

The traditional model to integrate data from one source as the input for a separate program often involved tedious manual data manipulation and multiple steps. For example, one may start with SRTM data, extract a particular region and resample at a different resolution, then convert the data into the format required by a long-term deformation code; similar steps may then be repeated for subsurface models of structure and faults.

To make data integration feasible on a regular basis, it is necessary to write data in standard and self-documenting file formats (such as the XML-based VTU format for visualization) to simplify pre- and post-processing. Some of our codes also have a framework that makes the definition of post-processing facilities within the code (e.g., for the computation of dynamic topography from the solution of a mantle convection code) simpler, thus obviating the need for further downstream processing, and enabling the use of common, science-neutral file formats already implemented in the underlying software libraries.

Using sufficiently rich file formats for input and output will also facilitate loosely coupled workflows in which two or more codes exchange data. An example would be to pass computed surface motions from a mantle convection code to a code that can simulate mountain belt formation, and to return the computed topography. While tightly coupled models are clearly superior to such loosely coupled codes, loose coupling approaches require code authors to only agree on a common file format, rather than having to understand different physics and know the details of multiple codes. Pragmatically, they are therefore more within reach. We will, however, strive to also couple different physics within individual codes, for example, adding the simulation of fluids to short-term tectonics codes, and integrating equation-of-state codes such as Burnman into geodynamics codes.

4.2.3 Reproducibility

Reproducibility is a foundation of the scientific method and increasingly journals and reviewers are asking that it be considered in evaluating scientific results [84, 85, 86]. Most recent discussion focuses on the role of reproducibility in laboratory experiments, especially the life sciences; however, open-source software like that produced by CIG is recognized as an important step towards reproducibility [87]. Assessing reproducibility in computational models has its own challenges; in particular, scientific reproducibility should not be confused with repeatability, the ability to repeat a specific computation, perhaps using virtual machines. Although repeatability has value, it is often more important to understand the implementation of the numerical method, the dependencies of the model, and model parameterizations — all elements of reproducibility.

Our software best practices were written with this in mind, and we continue to work with the community at large towards this goal through the following steps:

- Encourage developers to leverage the capabilities of version control tools for efficient development and testing. Correct use of versioning promotes contributions to open-source code and

maintains integrity and provenance of the code's master branch.
- Test and benchmark codes to ensure accuracy and stability of solutions, using both unit testing and full-scale testing with the Method of Manufactured Solutions. Archive and document solutions.
- Design codes to include output files generated at run time containing a complete set of input parameters, code version information, and the run-time environment state. This information can later be used to reproduce a computation or as a starting point for additional research.
- Archive inputs and outputs of model computations for further use by the community, using open-source tools to preserve provenance and discoverability.
- Include the topic of reproducibility in CIG training.
- Collaborate with information scientists and publishers to promote these practices and encourage development of mechanisms for archiving and attributing models.

4.2.4 High Performance Computing.

Science at the frontier pushes our modeling capabilities to larger computational resources. Facilitating deeper scientific knowledge in this manner requires that our codes scale well to large parallel computers, that developers and researchers have access to compute cycles, and that our users have the necessary expertise. CIG does not operate or directly provide high-performance computing for the geosciences; instead, we will help to meet this need by promoting benchmarking and by partnering with institutions that can provide compute cycles and expertise to our users. These partnerships with, for example, INCITE help extend geophysical models to larger and more meaningful computations, and provide training and support to our users that they are unable to receive elsewhere.

CIG's vision includes laying the scientific, computational and numerical foundations for computational modeling that moves beyond the desktop computer to strengthen the capabilities of computing at the mesoscale where most science discovery occurs, and at the leadership-class computing scale required by the largest models. Most researchers have ready access to desktop computers (the base of the pyramid of high performance computing, Figure 10), while a great deal of research takes place on small to medium-sized computing clusters (the middle layer of the HPC pyramid). CIG's activities enable pathways to leadership-class computing (the peak of the pyramid), that is, modeling using the largest computers in the world for research that requires this capability. We will achieve this goal by developing and training users on the tools of our science through a combination of tutorials, workshops, and meetings, by supporting performance benchmarks for geodynamics modeling codes, and by working with partners at national computing facilities to make CIG's codes available whenever possible.

Figure 10: The HPC pyramid.

5 Partnering with the Next Generation of Experts

5.1 Meeting the Needs of the New User

In the geosciences, most students do not acquire advanced scientific computing skills as part of their formal education. At the graduate level, computational training is most often provided via the apprenticeship model, hence students are limited by the capability of the resources around them. CIG's tutorials and training partnerships aim to fill the need with both synchronous (instructor-guided) and asynchronous (self-paced) training on topics in scientific computational methods generally, and on use of CIG codes specifically. Our goals include:

- **Best Practices.** Establish best practices in training based on our successful hybrid online and in person tutorials for PyLith, standardize training around this model, and develop additional tutorials for CIG's most extensively used software.
- **Linkages.** Expand links to other resources for general skills in topics such as software carpentry, numerical methods, and software best practices. Layer advanced education modules in geodynamics on top of these introductory materials.
- **Webinar Series.** Host a webinar series, with a theme that changes annually, to target emerging computational science topics such as uncertainty quantification and sensitivity analysis, in addition to topics in computational geophysics.
- **Online Training.** Develop online course modules and tutorials in computational science focussing on topics common to CIG science.
- **Outreach to Educators.** Provide training and collaboration opportunities for faculty from four-year colleges to work with experts in the field on specific code development projects that target educational needs.

5.2 Supporting Science at the Mesoscale

The CIG mission is not only to develop knowledgeable users but capable user–developers; geophysics domain experts for whom scientific computing is a fundamental research technique and who contribute to code development. Research and new discoveries require individuals with programming skills to implement these ideas. As our users become more adept, access to mesoscale computing and the skills that allow the implementation of larger and more sophisticated problems must be acquired. To promote this skill building, we propose:

- **Hackathons.** Continue to offer hackathons as a mechanism to train and develop a cohort of user–developers. We expect CIG's hackathons to continue to bring lead developers and up to 20 user–developers together for a week to ten days of intensive code development.
- **Access to HPC.** Engage with XSEDE and the UC Davis XSEDE Campus Champion in code development support and training. For example, CIG may host a section of *Applications of Parallel Computing*, an annual online class offered through the XSEDE partnership.
- **Creating Computing Pathways**. Promote use of preinstalled geophysics modeling software on the XSEDE Stampede supercomputer.
- **Community Allocations.** Continue to offer cycles on the XSEDE network for new users to benchmark codes and prepare research proposals.
- **Advanced Training.** Promote and support participation in training opportunities provided by the XSEDE network (e.g., XSEDE's Training, Education and Outreach Services (TEOS)) and ALCF (e.g., the Argonne Training Program on Extreme-Scale Computing (ATPESC)).
- **Mentoring.** Offer postdoctoral opportunities as a continued investment in our user–developers to prepare the next generation of experts. Promote software development as legitimate scientific contributions as both a career path and for tenure and promotions.

5.3 Supporting Science at the Crossroads

Questions geoscientists ask are complex and often require multi- or interdisciplinary insight. Computational tools allow us to push the boundaries of our science while also understanding how our science integrates with other earth systems. To create the connections within and outside our community, we propose:

- **CIG Biannual Meeting.** An all-hands meeting will combine training and science talks focusing on interdiscplinary science and common issues in tools, methods, and computing. This was recommended by the NSF midterm review panel and will be a new event for CIG. These will be held in the even-numbered years starting in 2016.

- **Specialty Workshops.** Specialty workshops will focus on a working group or special topic. We anticipate holding three of these per year (150 participants) in the odd-numbered years, alternating with the Biannual Meeting.
- **Joint Workshops and Tutorials.** We will hold joint workshops, hackathons, and offer training in collaboration with other earth science organizations, including CIDER, SCEC, USGS, NASA, IRIS, LLNL, UNAVCO, the Deep Carbon Observatory (DCO), and the European follow-on to QUEST. CIDER, for example, offers summer programs that has trained hundreds of graduate students and postdocs on the use of research tools, including CIG software. For the past several years, CIG has developed a virtual machine installation of several codes and tutorial materials used in CIDER tutorials. We will continue to offer tutorials appropriate to the theme of CIDER's annual summer programs.
- **Related Projects.** We will continue to seek augmented funding for special projects benefiting the CIG community. These may be projects with social, library, computational, applied mathematics, physical and planetary, or similar sciences. We will continue our efforts in software citation and attribution and community projects in leadership-class computing.
- **Special Sessions.** We will continue sponsoring special sessions and presenting invited talks at at other related meetings, such as Society of Industrial and Applied Mathematics (SIAM), the American Geophysical Union (AGU), EarthScope, IRIS, Geological Society of America (GSA), UNAVCO, and similar.

6 Broader Impacts of the Proposed Work

The broader impacts of this project include both activities that are accomplished directly by the CIG leadership, staff, and working groups, as well as activities by the CIG community that are enabled by our products and infrastructure.

Enhanced infrastructure for research and education: CIG's greatest impact is enhanced geoinformatics infrastructure to enable and improve high-quality research and teaching. CIG's software development primarily focuses on geodynamics and seismology, but additionally influences widely used scientific software development projects including PETSc and deal.II. We are also leading the way in the geosciences by coordinating benchmarking exercises and promoting software citation and software development best practices. The proposed work will extend and sustain the impact of this infrastructure, including enabling the community to respond to an increasing demand for open sharing of code.

Partnerships: CIG has established partnerships with national labs and other U.S. government agencies to build and enhance scientific capacity. Three of the highest impact collaborations are the long-standing collaboration between USGS and CIG on development and use of the short-term tectonics code PyLith, the more recent partnership between CIG and DOE's INCITE program on the geodynamo code Rayleigh, and the long-standing collaboration with the global community of developers of the SPECFEM family of codes. These organizations have provided substantial expertise and effort that complement CIG's effort. We also have long-standing *ad hoc* collaborations with CIDER, IRIS, UNAVCO, EarthCube, XSEDE, and others. International partnerships involve offering tutorials and co-hosting conferences with the Canadian Geophysical Union (CGU), QUEST, the Earth-Life Sciences Institute (ELSI) at the University of Tokyo – Japan, the APEC Cooperation on Earthquake Simulation, the European Geophysical Union's International Workshops on Mantle and Lithosphere Dynamics, and others.

Full participation of underrepresented groups in science, technology, engineering, and mathematics (STEM): CIG has a demonstrated strong commitment to open participation by all in STEM. We have an especially strong track record of involving women in both development and use of

CIG codes; at a recent hackathon, 9 of 23 participants were women. CIG's member institutions include minority-serving institutions and institutions in EPSCoR (Experimental Program to Stimulate Competitive Research) states. Moreover, CIG provides pathways to leadership by engaging early-career scientists and members of unrepresented groups in leadership, governing committees, working groups, and *ad hoc* committees. CIG is housed at UC Davis, which is projected to be an Hispanic Serving Institution (HSI) in 2018-19. CIG's Director has long been involved in increasing the participation of women and underrepresented groups in academia — especially at the postgraduate to faculty level — and she brings that expertise to CIG activities.

Improved STEM education and educator development: From the outset, CIG has been committed to providing high-quality training on our codes emphasizing participation by early-career scientists. In the first five years of CIG, tutorials focused on the basic mechanics of installing and using the codes. In the last five years, we identified a need for and developed more in-depth basic and advanced tutorials that introduce trainees to the underlying concepts of numerical modeling and advanced concepts. We also introduced a webinar series to provide continuing education, highlight the scientific use of CIG codes, and explore topics in software development, governance, visualization, etc.

CIG tutorials are offered through a variety of platforms, including at CIG's in-person workshops, virtual/online workshops, and through partnerships with other organizations. CIG offers tutorials at the CIDER summer programs, providing students with a virtual machine installation of ASPECT, SPECFEM, CitComS, and other codes, as appropriate to the theme of each year's program. The PyLith online and face-to-face tutorials include more than a week of lectures and hands-on 'tinker-time' for individual and collaborative work on research problems. Tutorials are recorded, are freely available online, and have a global reach. Our education plans are described in Section 5.

Improved national security and well-being of individuals in society: CIG codes are used for research on natural hazards including earthquakes, volcanic eruptions, ice sheet modeling, global sea level changes, induced seismicity, and natural resources including water, petroleum, and geothermal energy. Seismic wave propagation codes are used for nuclear security and to predict groundshaking from earthquakes to protect vital infrastructure and lives. Synergistic scientific and engineering impacts extend beyond the original core scientific disciplines of CIG. As an example, NASA scientists are using PyLith to understand feedback between lithosphere and melting ice, with implications for coastline evolution, sea level rise, and seismicity [88].

Increased public scientific literacy and public engagement with science and technology: CIG scientists regularly engage with the public to share scientific results of CIG codes, and work with science centers and museums to increase public understanding of science and technology. For example, CIG community scientists worked with the California Academy of Sciences to produce Earthquake: Life on a Dynamic Planet (Figure 11), and the Hayden Planetarium at the American Museum of Natural History to produce Seismodome: Sights and Sounds of Earthquakes and Global Seismology.

7 Project Management

7.1 Governance

CIG relies on the expertise, vision, and guidance of the community. Goals and directions are determined by community input from topical working groups and suggestions from the scientific community. A Science Steering Committee considers and recommends activities, which are then considered and approved by an Executive Committee. The Science Steering Committee and Executive Committee are charged with identifying needs across disciplines, responding to community needs and initiatives, balancing activities and use of resources, and advising on management. Governance and management, which follow a set of by-laws (Appendix D.2), are outlined below.

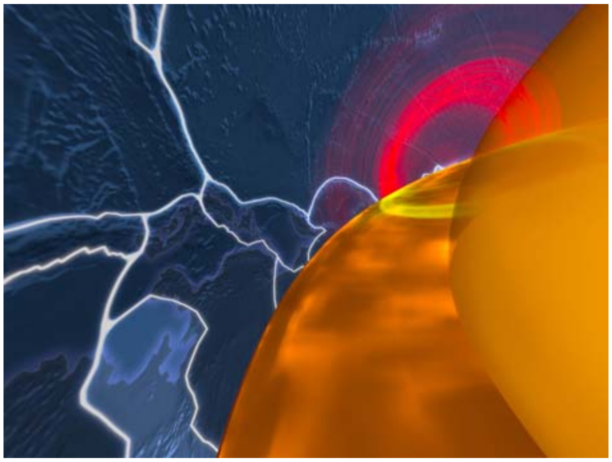

Figure 11: Scene from California Academy of Science "Earthquake" exhibit, an animation showing ground motions at the surface (red) and along a radial cross-section of Earth (yellow) for the M 7.9 1906 San Francisco earthquake computed using SPECFEM3D_GLOBE.

Membership. CIG recognizes educational and not-for-profit member institutions with a sustained commitment to CIG objectives in geodynamics and computational science. Foreign affiliate members are accepted but only United States members have voting rights. Each member institution elects one member representative to the electorate. Since 2010, CIG has grown from 51 to 72 U.S. member institutions and international affiliates.

Executive Committee. The Executive Committee is the primary decision-making body of CIG. The committee approves the annual science plan, management plan, and budget; reviews priorities for software development, with input from the electorate and the Science Steering Committee, and creates and appoints committees, such as the Nominating Committee, as needed.

Science Steering Committee. The Science Steering Committee prioritizes CIG software development from the perspective of the earth sciences and computational sciences, assesses the competing objectives and needs of all the sub-disciplines covered by CIG, and makes recommendations on the allocation of resources. The committee evaluates proposed CIG activities at least once a year – in practice more frequently – formulating a prioritized list of tasks, and developing a yearly working plan for CIG. Recommendations from the Science Steering Committee are forwarded to the Executive Committee for action.

Working groups. CIG currently has seven active working groups, appointed by the Executive Committee. They consist of active, knowledgeable, and interested researchers interested in a specific area; they are key for communication and for keeping CIG relevant and responsive to its community. The working groups suggest code development directions, workshops, tutorial topics, and other CIG activities.

Geodynamo aims to produce a series of increasingly efficient, tested, massively parallelized, well-documented community dynamo models for broad usage by the dynamo community. The working group also supports the community effort to carry out long computations on leadership-class computers by defining models and identifying tools for interpretation.

Mantle Convection promotes development and sustaining of high-quality codes for mantle convection, including codes that preceded establishment of CIG, such as CitComS, and new codes, such as ASPECT. The working group facilitates benchmark development, testing, and training.

Long-Term Tectonics aims to identify, provide, and support development of numerical tools to researchers who investigate the behavior of the lithosphere and upper mantle over time scales on the order of 10^{4-9} years.

Short-Term Crustal Dynamics provides modeling capabilities that are 1) observationally constrained and have internally consistent physics for the entire seismic cycle; 2) observationally constrained and have internally consistent physics for tectonics of magmatic systems, geothermal systems, and the cryosphere; and 3) observationally constrained by crustal deformation associated with surface loads.

Seismology promotes and informs the development of open-source seismic wave propagation codes in support of seismic source and structure studies, as well as crosscutting investigations in natural hazards, resource assessments, and planetary geophysics.

Magma Migration has the long-term goal to provide flexible multi-physics modeling capability and training for the exploration of coupled fluid-solid mechanics with an emphasis on the dynamics of magmatic plate-boundaries.

Computational Science primarily advises CIG on new developments and best practices for scientific software.

7.2 Administration

CIG headquarters is led by the CIG *Director*, who is the Principal Investigator (PI) of this proposal, and the *Associate Director*. The Director is responsible for the organization's programs and budget including: (a) devising a fair and effective process for the development of the Strategic Plan, based on proposals or work plans submitted to the Executive Committee by the Science Steering Committee, and overseeing the plan's implementation; (b) acting as the PI on proposals submitted by the core CIG facility, retaining final authority to make and implement decisions on grants awarded to the core facility and contracts; (c) ensuring that funds are properly allocated to various CIG activities; and (d) overseeing the preparation of technical reports.

The *Associate Director* leads day-to-day operations, overseeing Administrative and IT & Development teams and their coordination with the community. The Administrative team handles all tasks related to personnel, processing subawards, report preparation, accounting, executive and event support, technical writing, and education and outreach, supported by the Department of Earth and Planetary Sciences and two part-time CIG staff. The IT & Development team supports CIG's servers, website, repositories, build-and-test systems, email, help desk, compute allocations, and software support in the form of programming and development, documentation, training, and code support. System Administration is supported by part-time staff and a full-time Software Engineer. Software Development is supported by a full-time software developer, a postdoctoral researcher–developer, and a research scientist. Undergraduate research assistants support these efforts. See Appendix D.3.

7.3 Assessment

Critical success factors to fulfill CIG's mission fall into three broad categories — software, people and research. As a community committed to open-source software, CIG's impact can be quantified by repository activity, code growth, and computing cycles used for research. In the code repository, we track a variety of metrics, including downloads, code changes, lines of code, and releases over time. These numbers must be carefully interpreted because no registration is needed to download any of CIG's software. The actively developed codes have a global reach (Figure 12). To assess the scientific impact of CIG codes, we gather to the

Figure 12: Worldwide downloads of all CIG codes June 2014 – June 2015.

extent possible, scientific publications and discoveries that use CIG codes. More than 300 scientific publications have used CIG codes since 2010 (Section 8.) Scientific highlights are presented in the supplementary documents to this proposal as a series of one-page summaries of scientific results.

As a community organization, we respond to the needs of our users through governance and outreach. We track membership, governance participation, mailing lists, YouTube views, webinar attendance, and workshop participation (for the number and demographics of attendees, see Appendix B).

Finally, we regularly evaluate whether CIG has balanced its activities to reflect the needs of the community, and to identify partnerships with organizations including EarthScope, IRIS, UNAVCO, SCEC, CIDER, EarthCube, and international partners. The results of these assessments are included in our reports to CIG's governing committees and to NSF. We also disseminate this information to our constituents on the website (e.g., [89]) and in reports and newsletters. An annual business meeting, held at the AGU Fall meeting, provides opportunities for informal input, discussion, and feedback.

7.4 Managing Risk

Developing software at the scale suggested here incurs risks that need to be managed. These risks can be subdivided into technical, personnel, and community categories.

In our work, we address technical risks by building on professional IT infrastructure, including frequently backing up data, using version control systems, utilizing cloud-based repository hosting, etc. We elaborate on this in our data management plan (see the corresponding appendix to this proposal). Personnel risks are primarily the loss of critical expertise, knowledge, and community relations associated with staff members leaving CIG. We address this by assigning multiple developers to each project and assigning multiple projects to each developer, thereby duplicating expertise in our organization.

In our view, the most significant long-term risk to our goals is if CIG develops a code for which no developer community emerges. In such cases, our community as a whole may lose the ability to modify and extend this code if the primary developer leaves CIG (or if CIG as an organization ceases to exist), essentially creating a dead end for this code. To mitigate this, we have been careful to nurture user and developer communities for many of our codes. We employ a number of strategies to this end, including having sections in the manuals of our codes explaining how to extend the code and sponsoring hackathon-style workshops in which users come together not just to work on their models, but also to learn about the code and contribute to its development. The second provides important personal contact that significantly lowers the threshold to making that crucial first public contribution to a code.

An important realization in our operations has been that codes are more likely to have long-term developer communities if they have a champion who has a long-term, vested interest in the code's survival. Not coincidentally, our most successful codes are developed primarily through subcontracts to researchers and faculty at other institutions. We will continue to employ this development model.

During a 2014 strategic planning meeting, members of the Executive and Science Steering Committees developed a Strengths, Weaknesses, Opportunities, Threats (SWOT) analysis. The resulting document [1] included the identification of further risks, for example the lack of programming skills in (some of) our communities, and the current lack of ways by which contributors receive recognition for work on open-source codes. We address these and other identified risks by targeting our education and outreach activities, and, in the case of the second example, participation in an EAGER grant (see Section 8).

8 Results from Prior Support

a. EAR-0949446, $8.175M, 2/01/2010-06/30/2015 “Geoinformatics: Facility Support: Computational Infrastructure for Geodynamics (CIG)”, PI: L. Kellogg (L. Hwang, Senior Personnel). CIG provides the software cyberinfrastructure to facilitate transformative research in geodynamics by a diverse community of scientists. The computational infrastructure provided by CIG (a) is driven by community needs from 72 member institutions; (b) provides support for a virtual community that facilitates intellectual exchange and partnerships between computational scientists and earth scientists; and (c) offers specialized training and workshops for the earth science community. CIG members annually present at numerous national and international workshop and symposium and have reported more than 300 publications [101–413] as well as an unknown number of theses, dissertations, and works in progress. CIG hosts 31 open-source software packages, both donated codes and codes developed by CIG. Hosted software follows modern best practices including documentation on installation and computational methods, examples, and test cases, to support new users.

b. SMA-1448633, $299,999, 9/15/2014-9/14/2016 “EAGER: Development of software citation methodology for open-source computational science", PI: L. Kellogg, Co-PI: J. Dumit, L. Hwang, M. Smith. This award supports the Software Attribution for Geoscience Applications (SAGA) project, which identifies and addresses the technological and cultural barriers to effective software citation. It brings together diverse researchers and professionals from Social, Library and Computer Science to develop a software tool for citation of open-source software that completely describes the software environment and can be embedded into workflows that software developers and researchers will use. We have presented at the 2014 AGU [72] and have conducted interviews with scientist–developers.

c. ACI-1135588, $999,992 12/01/2011 to 11/30/2015. “CITEAM Impl: Dynamic Interdisciplinary Research Environment to Engage and Develop a CyberReady Workforce in the Geosciences, Social Sciences, and Computer Sciences,” PI: L. Kellogg, co-PIs: E. Cowgill, J. Dumit, B. Hamann, D. Sumner. This award supports mentoring and training of students in development and use of cyberinfrastructure for scientific research. Interdisciplinary teams of students jointly develop, use, and disseminate cyber-infrastructure tools and techniques using virtual reality and scientific visualization for research and education across three interdisciplinary themes: (1) Remote collaboration via immersive 3D telepresence; (2) Rapid Scientific Response to natural disasters using cyberinfrastructure and scientific visualization; (3) 3D Compare: developing the capacity to interactively manipulate and quantitatively compare digitally represented objects including 3D scans of buildings, cultural heritage sites, and archeological, geological, and paleontological samples. Students had the opportunity to collaborate internationally with visitors from Germany and Georgia on natural hazards and engineering projects, as well as with science museums on visualization products for the general public. Participants include a diverse group of women, underrepresented minorities, and first-generation college students. To date, products include at least 13 peer-reviewed publications [17, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100] and more than 20 software version releases, outreach products (videos, datasets), and meeting abstracts.

9 Glossary of abbreviations used in this document

AGU: American Geophysical Union
ALCF: Argonne Leadership Computing Facility
AMR: Adaptive Mesh Refinement
ASH: Anelastic Spherical Harmonic
ASDF: Adaptable Seismic Data Format
ASPECT: Advanced Solver for Problems in Earth's ConvecTion
ATPESC: Argonne Training Program on Extreme-Scale Computing
CGU: Canadian Geophysical Union
CIDER: Cooperative Institute for Deep Earth Research
CIG: Computational Infrastructure for Geodynamics
DOE: Department of Energy
ELSI: Earth-Life Science Institute
GRACE: Gravity Recovery and Climate Experiment
GSA: Geological Society of America
HPC: high performance computing
HSI: Hispanic Serving Institution
INCITE: Innovative & Novel Computational Impact on Theory and Experiment
IRIS: Incorporated Research Institutions for Seismology
LLNL: Lawrence Livermore National Laboratory
NASA: National Aeronautics and Space Administration
NSF: National Science Foundation
PISM: Parallel Ice Sheet Model
QUEST: QUantitative Estimation of Earth's Seismic Sources and STructure
SAR: Synthetic Aperture Radar
SCEC: Southern California Earthquake Center
SIAM: Society for Industrial and Applied Mathematics
SRTM: Shuttle Radar Topography Mission
SWOT: Strengths, Weaknesses, Opportunities, Threats
TACC: Texas Advanced Computing Center
TEOS: XSEDE's Training, Education and Outreach Services
TerraFERMA: Transparent Finite Element Rapid Model Assembler
UCERF: Uniform California Earthquake Rupture Forecast
UNAVCO: *formerly* University NAVSTAR Consortium
USGS: United States Geological Survey
VAPOR: Visualization and Analysis Platform for Ocean, Atmosphere, and Solar Researchers
VERCE: Virtual Earthquake and Seismology Research Community
XSEDE: Extreme Science and Engineering Discovery Environment

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