ILLUMINATING EARTH'S INTERIOR THROUGH ADVANCED COMPUTING

Today's computational strategies for modeling Earth's interior structure and dynamics come from high-performance computing systems in the US and others such as the Japanese Earth Simulator. Modeling efforts currently underway focus on problems such as geodynamo and earthquake modeling.

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Our solid Earth undergoes constant change from motions within its core to the surface. Solid Earth is the physical planet we live on, not the oceans or atmosphere. Motions near Earth's center affect the geodynamo, which generates the Earth's magnetic field. Convection within Earth's mantle drives plate tectonics at the surface (lithosphere), creating earthquakes and volcanoes and modifying land surfaces. The solid Earth is extremely heterogeneous, with complex interactions occurring on timescales of seconds to millions of years and spatial scales ranging from microscopic to global. Computing various solid Earth system components consumes weeks to years on powerful desktop workstations, making supercomputers the only means of achieving the necessary time and space resolutions.

Space-based measurement and observational technologies are revolutionizing our understanding of the solid Earth and revealing subtle changes that occur on regional and global scales. Understanding these complex processes requires large global data sets and sophisticated computational models coupled with the necessary associated computational infrastructure.[1] Subfields of solid Earth research that must use computational resources include earthquake dynamics, volcanoes, tectonics, geodynamo, mantle dynamics, surface processes, landscape evolution, gravity, magnetic fields, cryosphere and ice modeling, and hydrology.

In this article, we'll discuss how the rapidly increasing availability of data and a more robust and pervasive computational infrastructure could combine to give us new opportunities to understand this complex system.

The Solid Earth as a Complex System

The Earth is complex, nonlinear, and self-organizing, making it difficult to determine the underlying physics. Space-based data provide a synoptic global and regional view of the system. Numerical simulations also allow us to study the system's otherwise unobservable physics as well as to speed up time to study the long-term processes. The large data volumes and simulations make it possible to search for patterns too subtle to detect otherwise. Advances in computational science and numerical simulations integrated with large data sets now let us address several questions related to understanding the complex solid Earth system:

- How can we use space-based data sets to study strongly correlated solid Earth systems?
- What can numerical simulations reveal about the physical processes that characterize these systems?
- How do interactions in these systems lead to space–time correlations and patterns?
- What are the important feedback loops that mode-lock the system behavior—that is, cause the system to be in a nearly periodic state in which the same patterns of activity are repeatedly seen, in the same order, and at the same time intervals?
- How do processes on a multiplicity of different scales interact to produce the emergent structures that we observe?
- Do the strong correlations provide the capability to forecast any system's behavior?

Even with the most advanced observational systems, we can't take complete temporal samples of geophysical phenomena because solid Earth processes can take up to hundreds of thousands of years. Therefore, while we continue to make observations, we must perform simulations by inserting observational data into computational models that include constraint and validation processes.

Because solid Earth processes occur on many different spatial and temporal scales, it is often convenient to use model hierarchies rather than focus on a single or limited set of scales. Increasing interoperability and distributed Web-based computing help us with this system-level science.

Integrating Science and Computing

A major problem facing scientists today is that scientific data is increasing faster than computational power. This disparity challenges analysis and modeling. Programs such as Earthscope, an integrated program to apply modern observational, analytical, and telecommunications technologies to investigate the structure and evolution of the North American continent and the physical processes controlling earthquakes and volcanic eruptions, will add tremendous amounts of seismic and geodetic data, on the order of nearly 5 Tbytes per year. New space-based missions will generate 10 to 20 Tbytes per week.

Improved algorithms are simplifying processing and approximating complex phenomena so that researchers can handle the large data volumes as well as identify data sets' dominant physical processes. Pattern recognition is another approach we are applying to identify subtle features in large data sets. The scientific legacy and long-term value of new data and modeling results will depend on the ability to handle complex queries over data sets from multiple instruments and multiple missions.

Web-Enabled Computational Approaches

Members of the solid Earth community, primarily those who focus on modeling crustal deformation and earthquake processes, are developing the International Solid Earth Research Virtual Observatory (iSERVO; www.servogrid.org), which will let investigators seamlessly merge multiple data sets and models and create new queries. The iSERVO framework will archive simulation data with analysis and animation tools and the original simulation code. Observational data—which is heterogeneous and distributed in nature—will be accessible through cooperative federated databases.[2] iSERVO will include tools for visualization, data mining, and pattern recognition, along with data fusion in a Web services (portal-based) problem-solving environment (PSE) (see Figure 1).[3] The PSE will provide for model and algorithm development, together with testing, visualization, and data assimilation to address multiscale modeling challenges.

Problems developed within the PSE will be scalable to workstations or supercomputers depending on the problem's size. Algorithms within the framework will include partial differential equation (PDE) solvers, adaptive mesh generators, inversion tools, fast spherical harmonic transforms, wavelet analysis, particle dynamics, ray tracing and visualization preparation, and image processing and spectral analysis. The PSE will provide a mechanism to facilitate teams of scientists (within and across disciplines) and IT specialists on framework design and development.

iSERVO uses Web services to describe the interfaces and communication protocols. Web services are the constituent parts of an XML-based distributed-service system. Standard XML schemas define

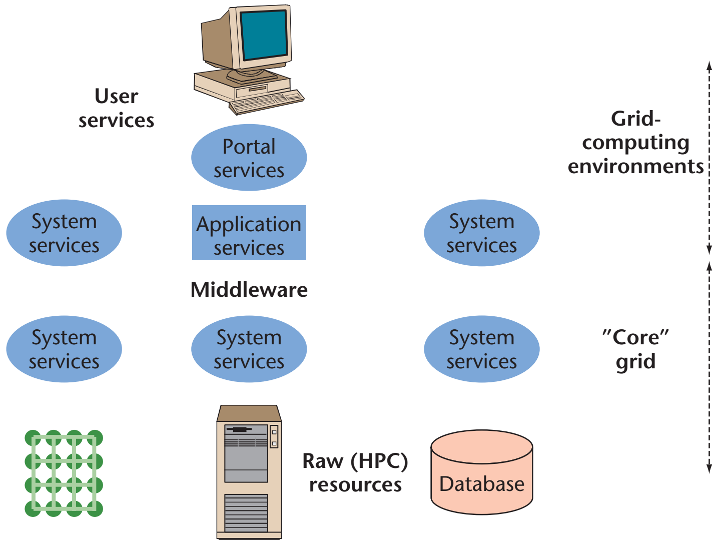

Figure 1. High-level architecture of a planned system showing Grids, portals, and Grid-computing environments. This three-tiered approach isolates the user from the computational resources, which include distributed processors and databases.

implementation-independent representations of the service's invocation interface (the Web Service Definition Language, WSDL), and the messages (using SOAP) exchanged between two applications. XML-based repositories provide interfaces to services. Numerous other services can supplement these basic capabilities, including message-level security and dynamic invocation frameworks that simplify client deployment. In principle, we can implement clients and services in any programming language (such as Java, C++, or Python), obtaining interoperability through XML's neutrality.

One of the basic attributes of Web services is their loose integration; you do not have to use SOAP as the remote-method invocation procedure, although there are times when this is desirable. For example, several protocols are available for file transfer, each of which focuses on reliability, performance, or some other aspect. We can describe these services in WSDL, with WSDL ports binding to appropriate protocol implementations, or, perhaps, to several similar implementations. In such cases, negotiation must occur between client and service.

Our approach to Web services divides them into two major categories: core and application. Core services include general tasks such as file transfer and job submission. Application services consist of metadata and core services needed to create instances of scientific application codes. Application services can be bound to the particular host computers and core services needed to accomplish a particular task.

Two very important investigations are currently underway under the auspices of the Global Grid Forum (www.gridforum.org). The first is merging Grid-computing technologies and Web services (that is, Grid Web services). Web services are often static pages on which each interaction (such as download contents) is independent. The Grid and the Web's e-commerce applications require dynamic content and interactions that form a session, with information preserved between interactions; such stateful services and mechanisms to begin and end sessions are being standardized. A further major activity is a survey of requirements and tools needed to orchestrate multiple independent (Grid) Web services into aggregate services. Our goal is to provide interfaces through which users transparently access a heterogeneous collection of independently operated and geographically dispersed databases, as if they were a large virtual database.[2]

Five main challenges are associated with developing a metaquery facility for earthquake science databases:

- Define a basic collection of concepts and interrelationships to describe and classify information units exported by participating information providers (a *geophysics meta-ontology*), to provide for a linkage mechanism among the database collections.
- Develop a *metaquery mediator* engine to let users formulate complex metaqueries.
- Develop methods to translate metaqueries into simpler derived queries addressed to the component databases.
- Develop methods to collect and integrate the results of derived queries, to present a user with a coherent reply that addresses the initial metaquery.
- Develop generic software engineering methodologies that facilitate simple and dynamic system extensions, modifications, and enhancements.

Today, the preceding computational methods are producing realistic earthquake fault systems simulations. One example is the QuakeSim project (see "The QuakeSim Project" sidebar) in which we describe three computationally intensive solid Earth applications that benefit from high-performance computing and improved computational infrastructure. Geodynamo calculations are extremely computationally intensive, requiring leading-edge high-performance computers. Models of earthquake processes also benefit from high-per-

The QuakeSim Project

Funded by a NASA Computational Technologies contract to Caltech's Jet Propulsion Lab in Pasadena, California, the QuakeSim project (http://quakesim.jpl.nasa.gov) is part of an effort to construct general earthquake models (GEMs). The project focuses on three modeling areas, Virtual California, GeoFEST, and PARK, each targeted for improved performance through design changes that make them efficient high-performance parallel codes. The project also focuses on the development of Web-based computing, interoperability, and Web services to make large-scale simulations feasible (see Figure 4 in the main text).

Virtual California[1] is a collection of codes that simulate the dynamics of stress evolution on a complex fault system such as the San Andreas fault system in California. It uses computational representations of elastic Green's functions, or stress transfer coefficients, that can be easily computed for rectangular three-dimensional fault segments together with friction laws that are parametrizations of laboratory experiments to construct dynamical models solved by cellular automaton methods.

GeoFEST is a discrete finite-element code package that models earthquake fault surfaces and the associated elastic and viscoelastic material rheologies, as well as other nonlinear rheologies. GeoFEST handily computes stresses, strains, and displacements at arbitrary points within the modeled Earth, including spatial heterogeneity in material properties. Coupled with an adaptive mesh generator that constructs a mesh based on geometric and mechanical properties of the crustal structure, the GeoFEST system makes it possible to efficiently model time-dependent deformation of interacting fault systems embedded in a heterogeneous Earth structure.

PARK is a boundary-element-based code for studying unstable slip at the Parkfield segment of the San Andreas or at other faults. It aims to capture instability; thus, it represents a fault's slip at many scales and captures the developing seismic slip details over an extraordinary range of timescales (subseconds to decades). This is the first earthquake-simulation code to seek enhanced scalability and speed by employing a multipole technique. This problem requires massive parallel computing to support many small-slip patch elements to cover the nucleation scale that initiates the instability.

You can find the current library of GEM codes at www.servogrid.org, a sample of 1,000 years of synthetic InSAR surface deformation—output from a Virtual California computation—at http://pat.jpl.nasa.gov/public/RIVA/images.html.mpeg, and a sample computation of Interferometric Synthetic Aperture Radar surface deformation from a model of the 17 February 1995 Northridge earthquake at http://pat.jpl.nasa.gov/public/RIVA/images.html.

Reference

1. J. Rundle, D.L. Turcotte, and W. Klein, eds., *GeoComplexity and the Physics of Earthquakes*, AGU Geophysical Monograph, 2000.

formance computing, and require an improved computational infrastructure to integrate the multiple spatial and timescales.

Geodynamo

Earth's fluid outer core is in convection, driven by gravitational energy released from the planet's slow cooling. The convective flow generates and maintains the core's magnetic field, the geodynamo; however, we do not understand the details of how that dynamo works. Hydromagnetics, or the dynamics of an electrically conducting fluid in a magnetic field, and geodynamo numerical modeling place extraordinary demands on currently available computational resources. Recent calculations have consumed months to years of supercomputer CPU time.

Over the past 150 years, the main (axial dipole, or magnetic dipole positioned at Earth's center and aligned with the rotational axis) component of Earth's magnetic field has decayed by nearly 10 percent. This decay rate is 10 times faster than if the dynamo were not operating, indicating that it is destroying part of the dipole field. This suggests that we may be entering a geomagnetic polarity reversal. Such reversals occur, on average, about once every 500,000 years. Today, the region most affected is the South Atlantic Ocean, where the field at Earth's surface is about 35 percent weaker than we would expect (see Figure 2). This localized field weakness and the decay in Earth's overall magnetic field above its surface could have serious implications for low Earth-orbiting satellite operations as they allow greater radiation exposure.

The anomaly has increased significantly over the last 100 years. Satellite observations coupled with numerical models will help determine how much longer the anomaly will continue to grow, and how deep it will become.

Because modeling the geodynamo requires solving computationally intensive coupled magnetohydrodynamics (the dynamics of an electrically

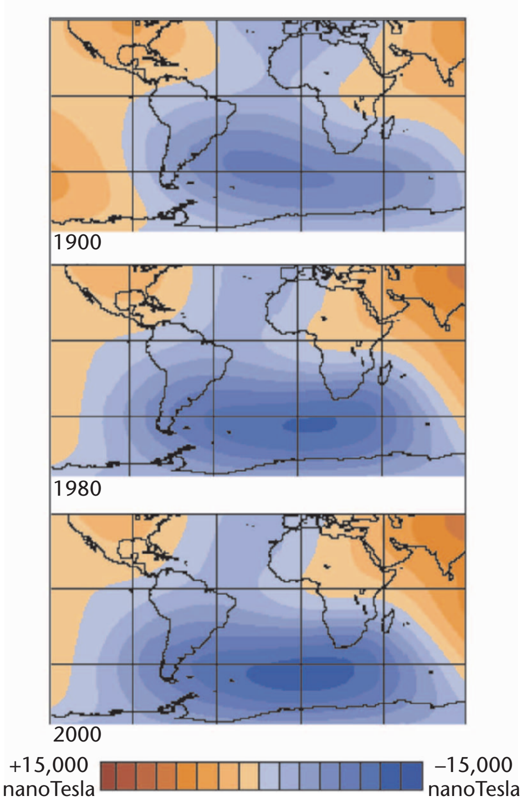

Figure 2. South Atlantic Magnetic Anomaly strength at an altitude of 500 kilometers.

conducting fluid in a magnetic field) equations, it could benefit from massive computational Grids. Current models, running on 64 nodes of the Earth Simulator (see "The Japan Earth Simulator for Solid Earth Studies" sidebar) optimize a spectral code and obtain a performance of 0.16 second per time step for 256 degrees of spherical harmonics. The increased resolution is letting us develop more realistic convection models and understand the implementation of lateral heterogeneity of electrical conductivity in the mantle's base.[4]

Earthquakes

The Kobe, Japan, earthquake on 16 January 1995 was a magnitude 6.9 event and produced an estimated US$147 billion loss. Despite an active earthquake-prediction program in Japan, this event was a complete surprise. Similar scenarios are possible in Los Angeles, San Francisco, Seattle, and other urban centers around the Pacific plate boundary. If the 1906 San Francisco earthquake were to happen today, it would be a US$500 billion event. Ground- and space-based observations coupled with computer models might unlock the secrets of earthquake forecasting.

During the past decade, space-based geodetic measurements coupled with numerical models have begun to transform our understanding of earthquake processes. While seismology measures earthquakes and the seismic waves they generate, surface deformation measurements let us view the strain associated with the entire earthquake cycle.

Large amounts of strain occur before, during, and after earthquakes, and a significant portion of this strain can be *aseismic*—that is, not producing seismic waves. Recent measurements of this "quiet" strain show that intermediate and large earthquakes can transfer stress and activate nearby or distant faults. Although data are sparse, observations indicate that the shallow part of the Sierra Madre fault located along the northern boundary of the Los Angeles basin exhibited "fault creep" for several years following the Northridge earthquake in Southern California.[5] In the past few years, "quiet earthquakes" with durations as long as two weeks occur on deep portions of the subduction zones in Japan and in the pacific northwest of the US and Canada.[6] It is becoming clear that we must study earthquakes in the context of regional fault systems and that one earthquake can "turn on" or "turn off" an earthquake on another fault located within the same region.[7] We need simulations to model this long- and short-term behavior.

Turning all these data into assessments and forecasts requires modeling and pattern extraction. For forecasting, we require a dynamic model that can span scales larger than a finite-element code, and hence, high-performance computers. In principle, boundary-element methods can fulfill computational forecasting needs. Substantial testing and development remain, however, to come up with new methods that fully model complex system behavior such as thermoporoelastic equations, which take into account temperature differences and fluid transport, nonlinear elastic models, or evolving models.

Figure 3 shows the results when we couple a Northridge thrust–fault system with finite-element regional models. With 100,000 unknowns and 4,000 time steps, a simulation takes an estimated eight hours on a high-end workstation. Modeling the Southern California system requires 4 million unknowns and 12,800 processor hours for 1-kilometer (km) resolution; 0.5-km resolution would take 100,000 processor hours (400 hours, or 17 days) on a dedicated 256-processor machine.

We can estimate the floating-point operations count for a regional simulation that couples finite elements with boundary elements (most of the cost is in the regional interactions). For example, with 80 regions covered at 10 per day, 10^5 fault segments

The Japan Earth Simulator for Solid Earth Studies

In 1998, Japan launched a joint Earth science and computer science project to develop large-scale computer simulations based on physical models and data. The project has two main parts: development of a high-performance, massively parallel processing computer system, called the Earth Simulator, and multiscale–multiphysics parallel computing software systems for solid Earth dynamics numerical simulation. The Earth Simulator is a 40-Tflop massively parallel processing system with 5,120 CPUs and 10 Tbytes of memory. The Solid Earth Simulator processing system consists of three subsystems corresponding to core–mantle dynamics, intermediate-term regional simulation of crustal activity, and short-term local simulation of earthquake generation and strong motion. The core–mantle dynamics group developed 3D computer simulation models to understand the dynamic processes of three coupled convective systems in the fluid outer core, the subsolidus mantle, and the outermost solid shell. The crustal activity group developed a realistic computer simulation model for the entire process of earthquake-generation cycles in and around Japan. The earthquake rupture–strong-motion group developed computer simulation models for dynamics rupture on an interacting complex fault system and radiation and propagation of seismic waves in a realistic 3D heterogeneous medium.

International collaborations that bridge computer science and solid Earth science are carried out largely through the Asia–Pacific Economic Cooperation (APEC) Cooperation on Earthquake Simulations (ACES). ACES aims to develop realistic supercomputer simulation models for the complete earthquake-generation process to provide a virtual laboratory to probe earthquake behavior and offer a new opportunity to understand the earthquake nucleation process and precursory phenomena. The project represents a grand scientific challenge because of the complexity of phenomena and range of scales from microscopic to global involved in the earthquake-generation process. It is a coordinated international effort linking complementary nationally based programs, centers, and research teams.

per region with 10^{10} interactions, 100 operations per interaction, 1,000 update steps for data-driven corrections (including recent history), and 0.1 computational efficiency, the requirement is a sustained 1 Tflop.

For detailed forecasting based on seismicity, we can use methods in which the patterns of seismicity are expanded in a series of eigenpattern vectors using time-dependent coefficients. For each region, the 10^5 fault patches imply 10^{15} operations using arguments similar to those already outlined. Direct methods indicate the need for a sustained 0.1-Tflop performance. We can use these pattern rates for daily updates to an earthquake hazard map via vector-oriented input; the process probably wouldn't require more than 0.1 Tflops. End-to-end processing and modeling from a mission such as Interferometric Synthetic Aperture Radar (InSAR) for earthquake forecasting comes to about 2 Tflops sustained, which equates to about 10^4 Pflops per year.

This combination of data and modeling will give us knowledge of fault systems' emergent behavior, and pattern-recognition techniques applied to seismicity data will reveal anomalies that correlate with observations of surface deformation. These techniques[8,9] show promise for forecasting locations of future earthquakes greater than magnitude 5 (see Figure 4). An enlargement (lower left) of the Northridge region forecast shows a seismic anomaly with the same distribution as the observed surface deformation following the Northridge earthquake. Numbered arrows indicate earthquakes above magnitude 5 that have occurred since the forecast was made.

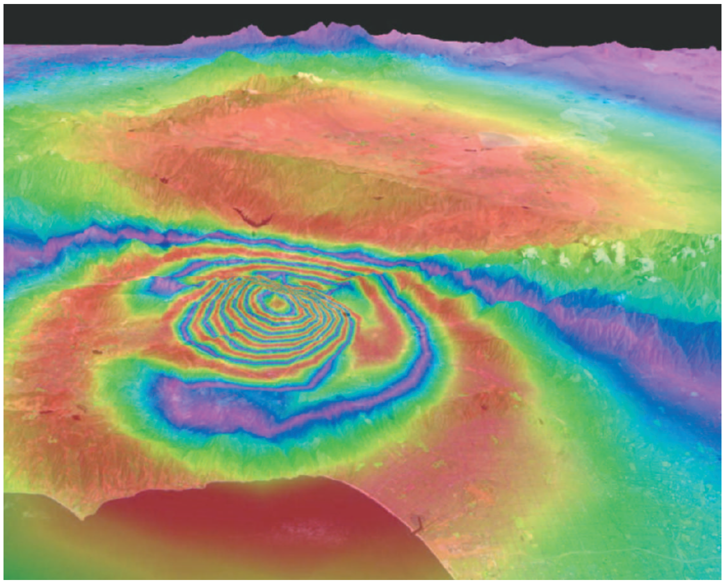

Figure 3. A Northridge earthquake-class simulation. The image is a simulated synthetic aperture radar interferogram for the decades after the Northridge earthquake (details at http://quakesim.jpl.nasa.gov). Color cycles represent 5.6 centimeters (one wavelength) of deformation and are equivalent to contours of uplift related to the earthquake.

Combining multiple data types—such as InSAR

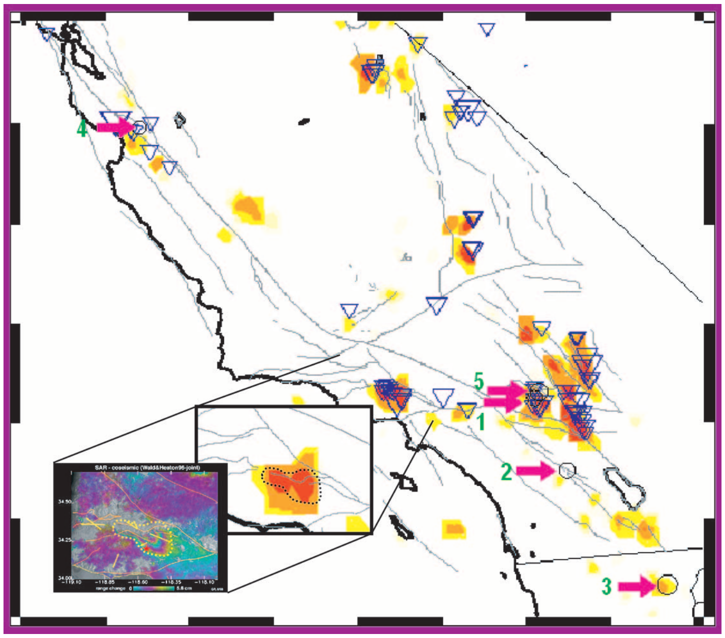

Figure 4. Probability density functions based on seismicity in southern California. Lower left: postseismic surface deformation observed with Interferometric Synthetic Apterture Radar (InSAR) from the European remote-sensing satellite, ERS-1. Right small panel: anomaly identified from seismic data. (Seismic anomaly plot courtesy of Kristy Tiampo, University of Colorado, and John Rundle, University of California, Davis. See text for arrows and numbers 1 through 5.)

and seismicity—is a powerful technique for understanding and forecasting earthquake fault behavior. We also need to better understand chemical and physical processes in fault zones. The San Andreas Observatory at Depth (SAFOD; www.earthscope.org) drilling project will collect new, unprecedented data in this arena. While predicting the time, location, and size of a particular earthquake remains elusive for now, more-accurate earthquake forecasts appear within reach. It is apparent, however, that to effectively monitor and forecast earthquake behavior, data and models must exist within a computational framework that allows for accessibility and implementation.

As solid Earth data sets grow more extensive, researchers will discover a variety of new phenomena. Anticipating a flood of new data, we must develop advanced knowledge-discovery computing technologies for new and realistic computational simulations, data mining, visualization, and pattern-analysis techniques. The solid Earth community is rapidly developing approaches based on boundary-element and finite-element models. Pattern-recognition techniques are exploiting methods based on principal component analysis and hidden Markov methods.[10] Computational methods will be based on Web services, federated database services, and novel Grid-computing methodologies. We anticipate a fusion of computational and mission-oriented sciences that will enable remarkable new discoveries for solid Earth dynamics. CiSE

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