EXECUTIVE SUMMARY: DEFORM & COMPRES EARTHCUBE WORKSHOP RESULTS

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Earth Cube Workshop Title:

EarthCube End-User Domain Workshop for Rock Deformation and Mineral Physics Research, Nov 12-14, 2013

Introduction:

Workshop participants addressed the current state, future challenges, needs, opportunities, and directions of cyberinfrastructure as related to research in rock deformation (DEFORM) and mineral physics (COMPRES). The workshop leveraged the high degree of compatibility that exists between the DEFORM and COMPRES communities. A key goal of the workshop was to identify scientifically transformative activities that could be facilitated by EarthCube.

A total of 76 participants gathered for 2.5 days, including 18 pre-tenure faculty, postdocs and other early career scientists. Workshop participants represented a variety of disciplines including mineral physics (36%), rock mechanics (34%), program managers from NSF/DOE/USGS (11%), cyber-science and engineering (9%), structural geology (5%), and geodynamics (5%). The agenda included 15 keynote talks, 12 lightning talks, and 24 posters presentations during an evening session. The workshop featured vigorous discussion from every participant during three plenary sessions, three breakout sessions, 8.5 hours of scheduled, free form discussion, and 9 hours of informal discussion. Outcomes of the workshop are summarized below.

SCIENCE ISSUES AND CHALLENGES

1. **Important science drivers and challenges:** Participants identified several high-priority science questions that will be the focus of interdisciplinary efforts during the next 5-15 years.

- As planets age and cool, how do their physical & chemical properties and internal structures evolve under the extreme conditions of pressure and temperature? What material transformations occur in complex, multiphase systems within planetary interiors and how do these impact key compositional and rheological boundaries such as the lithosphere asthenosphere boundary and the D’’ region at the base of Earth’s mantle?
- What processes determine where earthquakes occur to define the seismogenic zone, and how do they influence the tsunami-generating potential of seismic rupture at subduction megathrusts? What are the factors that dictate the spectrum of fault slip behaviors and the physics of slow earthquakes where self-sustained, quasi-dynamic ruptures propagate at velocities dictated by unknown processes.
- How do the physical and chemical properties of planetary materials control the dynamics and magnetic behavior of Earth and other planets?
- How can we best utilize seismological data and models from EarthScope and other sources to determine the composition, temperature, and flow fields that produce tectonic processes on Earth’s surface.

- What are the factors that determine the brittle ductile transition within Earth's lithosphere and how does the transition from seismic to aseismic slip vary with strain rate? How can we image the slip distribution of large crustal earthquakes, for example on the San Andreas fault, to illuminate the properties of the deep crust, the brittle ductile transition, and the rheology of the lithosphere?
- How do microstructures evolve at high strain and what feedbacks connect this evolution to deformation, seismic properties, and fluid transport processes in Earth's lithosphere? How do experimental results inform interpretation of field data/observations and vice versa? We need to develop robust flow laws for multi-phase materials and to advance our understanding of anisotropic viscosity for Earth materials.
- Many socioeconomic, environmental and energy applications, for example geothermal energy, carbon sequestration, and waste disposal, require a deeper understanding of geomechanical properties, mineral transformations, and fluid-rock interactions. How does the geologic evolution of shallow crustal conditions (sediment, rock, and fluid) influence the system response to anthropogenic forcing associated with energy production, CO2 storage, and waste disposal and how do these factors impact induced seismicity and earthquake hazard?

2. **Current challenges to high-impact, interdisciplinary science:** Several themes emerged as consistent challenges faced within/across the involved discipline(s).

   - Our communities lack the databases on Earth materials required to address key problems in mineral physics & rock deformation. Ready access to such data will facilitate transformational interaction across fields and promote innovative assessment of key problems. We need to establish links between future COMPRES and DEFORM databases and those on seismic, petrologic, thermodynamic, elastic, geochemical, and crystallographic properties of Earth materials.
   - Lack of reliable and sufficiently-automated data analysis software able to push the limits of quantitative information retrieval from both experimental and theoretical data sets to new limits of spatial, temporal, stress resolution and system complexity in response to revolutionary improvements in experimental technology capabilities. Data volumes and real-time signal processing are currently growing far faster than post-processing techniques, and automated methods for data analysis are needed to meet this challenge.
   - Need for workflows, data mining capabilities, intuitive data systems, and easy to use web-based tools that encourage best-practices in reproducible science and transparency in data processing and storage.
   - A key roadblock is that of how to extract scientifically useful information on rock fabric and mineral textures from images collected using a variety of methods. We need to build on recent developments in microtomography and 4D imaging
   - Need for accessible, easy to use computational tools that would enable calculation of physical, structural, thermodynamic and transport properties of Earth materials at any pressure and temperature conditions, particularly those not easily accessible through experiments.

TECHNICAL INFORMATION/ISSUES/CHALLENGES

1. **Desired tools, databases, etc. needed for pursuing key science questions with brief elaboration:**

    - Central data system for DEFORM and COMPRES science. This should include storage, visualization, and search protocols to provide community access to our data and solutions that will reduce activation energy to including data in these databases.
    - Community technical forums, including websites, focused on CI developments for both DEFORM and COMPRES. We note that COMPRES has a Technology Office at Argonne National Laboratory and a technology-oriented website maintained by COMPTECH, which could be a starting point. We need both tools to compare data from different labs, including functional fits, statistical analysis and model evaluation and a social network associated with our data system to provide a forum to interact virtually and lower barriers to interdisciplinary interaction between researchers. These tools should include a way to capture information about how users interact with the databases, and automated methods to improve the data system based on this information.
    - Central archive of experimental samples with integrated workflows, database templates, and community-wide DOI system for samples
    - Automated system for storage and evaluation of microstructural images, including rock fabric, texture evaluation and pore networks, as well as comparison of laboratory and field microstructures and shear zone texture.
    - Extending data mining capabilities/tools and interlinking existing repositories, (e.g. crystal structure and spectroscopic databases) with newly developed databases.
    - Reliable, sufficiently automated, easily accessible and well-documented software for efficient (preferably real time) processing of large volumes of experimental data and results from theoretical and numerical studies.
    - Improve accessibility of high-performance computing (HPC) by both lowering the entrance barrier and providing analytic/query tools to make the results of these calculations readily available to the wider observational and experimental Earth science communities. Collaboration/assistance from HPC staff with earth-science researchers at HPC centers.
    - Create a comprehensive reference Earth model that includes both deformation and elastic properties.

COMMUNITY NEXT STEPS

1. **List of what your community needs to do next to move forward how it can use EarthCube to achieve those goals:**

    - Develop RCN's for DEFORM and COMPRES databases, data systems, and data sharing among data sources. Develop a database prototype with functionality to link databases and record data processing with the goal of moving toward a system for reproducible science. Develop protocols for data transfer between data sources (experimental and computational) and data consumers.
    - RCN proposal for designing next generation data collection and analysis tools. Explore visualization and analysis tools that are known to other communities to see if they can be applied to our problems. An important component of this is image analysis and pattern recognition

including automated methods to identify deformation microstructures, LPO and other examples of fabric in rock and minerals.

- Utilize EC Building Blocks and other available funding mechanisms to enhance and expand the most promising existing CI solutions useful for our communities.
- Engage discussions with representatives of existing community organizations and facilities (DEFORM, IEDA, COMPRES, HPCAT, GSECARS, ANL, ALS) to take advantage of existing resources (websites, videoconferencing capabilities, technology focused personnel).
- RCN between experimentalists, seismologists, geodynamicists, geochemists, and computer infrastructure experts to develop approaches for achieving a three-dimensional reference Earth model that provides a mechanism to link geophysical observations with laboratory and theoretical studies.