



EarthCube

<http://earthcube.ning.com/>

**EarthCube End-User Domain Workshop for
Rock Deformation and Mineral Physics Research**
Nov 12-14, 2013, Embassy Suites Old Town Alexandria, VA
Steering Committee: Chris Marone (convenor), Jay Bass (convenor)
Przemyslaw Dera, Tom Duffy, Heather Savage, & Terry Tullis

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Agenda

TUESDAY, NOVEMBER 12

6:00 – 8:00 am	Complimentary Embassy Suites Breakfast (Atrium)	
8:00 – 8:30	Registration (Outside Lobby of Virginia Ballroom A/B)	
8:30 – 9:15	Overview of Workshop Objectives & EarthCube Program	
	Welcome & Workshop Objectives: <i>Chris Marone & Jay Bass</i>	
	EarthCube Program Overview & Governance: <i>Eva Zanzerkia, Barbara Ransom & Kim Patten</i>	
	Challenges & Action Items for EarthCube Workshops: <i>Basil Tikoff & Julie Newman</i>	
	Plenary Session 1 (Virginia Ballroom A/B) <i>Moderators: Heather Savage & Przemyslaw Dera</i>	
9:15 – 9:30	Mark Ghorso (OFM Research Inc.) Developments in Cyberinfrastructure for Geochemical & Computational Thermodynamics	
9:35 – 9:50	Padma Raghavan (Penn State Univ.) Cyberscience: Driving Innovation Through Computation & Data-Enabled Research	
10:00 – 10:25	Coffee & Discussion (Outside Lobby of Virginia Ballroom A/B)	
10:30 – 10:45	Louise Kellogg (Univ. of California, Davis) High Performance Computing Infrastructure for Geophysics	
10:50 – 11:05	David King (Exaptive Inc.) Concepts, Goals & Innovation in Database Access, Data-Mining & Reproducible Science	
11:05 – 12:15	Open Discussion	
	Scientific Challenges & Opportunities Over the Next 5-15 years	
	Identify Cybergeoscience Focus Areas & CI Road Blocks & Opportunities	
	Introduction to the Breakout Sessions	
12:15 – 1:15	Lunch & Discussion (Atrium)	Sign-up for Lightning Talks @ 5:30
	Breakout Session 1	
	Science Objectives & Questions, Road Blocks, Needs for Community Tools, Databases, & Modeling Capabilities	
1:15 – 2:15	Group A (Virginia Ballroom) Identify Use Case Scenarios for CI in COMPRES Consortium for Materials Properties Research in Earth Sciences	Group B (Carter Room) Identify Use Case Scenarios for CI in DEFORM Deformation Experimentation at the Frontier of Rock & Mineral Research
	Plenary Session 1 cont. (Virginia Ballroom A/B)	
2:15 – 3:15	Summary of Breakouts	
	Discuss, Prioritize, Embellish & Brainstorm How Best to Engage Cyber-Literate Researchers on Scientifically Transformative Activities in Our Domain?	
3:15 – 3:45	Coffee & Discussion (Outside Lobby of Virginia Ballroom A/B)	
3:45 – 4:00	Renata Wentzcovitch (Univ. of Minnesota) Virtual Laboratory for Quantum Mechanical Studies of Materials	
4:05 – 5:30	Open Discussion of Science Drivers, CI Challenges & Use Case Scenarios	
5:30 – 6:30	Lightning Talks, Intro. to Posters: 5 mins, 3 or fewer slides (sign up in advance)	
6:30 – 9:00 pm	Demos, Poster Session and Reception - Cash bar and heavy hors d'oeuvres (Mason Ballroom)	

WEDNESDAY, NOVEMBER 13, 2013

6:00 – 8:30 am	Complimentary Embassy Suites Breakfast (Atrium)		
Plenary Session 2 (Virginia Ballroom A/B) <i>Moderators: Phil Skemer & Martin Kunz</i>			
8:30 – 8:40	Dan King (DOE Geothermal Program) EarthCube Activities at DOE		
8:45 – 9:00	Kerstin Lehnert (Lamont-Doherty Earth Observatory) Geoinformatics, Scientific Data Management, & Cyberinfrastructure		
9:05 – 9:20	Jim Bowring (Coll. of Charleston) Cyberscience, Software Engineering & Automated Workflows in Geoscience: Perspectives from EARTHTIME and GeoChron		
9:30 – 9:50	Joel Cutcher-Gershenfeld (Univ. of Illinois) Social Perspectives on Multi-Disciplinary Research and CI, EarthCube Survey Results		
9:50 – 10:15	Coffee & Discussion (Outside Lobby of Virginia Ballroom A/B)		
Breakout Session 2			
10:15 – 11:15	Group A (Virginia Ballroom A) Refined Discussion of CI Needs and Commonalities for DEFORM/COMPRES Science	Group B (Virginia Ballroom B) High Performance Computing, Theory and Modeling	Group C (Carter Room) Databases, Web Based Data Access, Data Mining
11:15 – 11:25	Mini Break		
Plenary Session 2 cont. (Virginia Ballroom A/B)			
11:25 – 12:40	Summary of Breakout Results & Open Discussion		
12:40 – 1:40	Buffet Lunch & Discussion (Atrium)		
Plenary Session 2 cont. (Virginia Ballroom A/B)			
1:40 – 1:50	Brandon Dugan (Rice Univ.) Challenges & Revolutions in Hydrogeology, Geomechanics, & Cyberinfrastructure		
1:50 – 2:00	Phil Skemer (Washington Univ.) Using Microstructural Data to Link Experimental Rock Deformation, Structural Geology, & Seismology		
2:00 – 2:10	Martin Kunz (Lawrence Berkeley National Laboratory) Toward Real-Time Analysis of Large Data Volumes for Diffraction Studies		
2:10 – 2:55	Open Discussion Summary of Progress on Workshop Objectives		
2:55 – 3:20	Coffee & Discussion (Outside Lobby of Virginia Ballroom A/B)		
Breakout Session 3			
3:20 – 4:20	Group A (Virginia Ballroom) Outreach/Education/Early-Career	Group B (Carter Room) Metadata, Transducers and Instruments, Streamlining Data Collection and Access	
4:30 – 5:30	Breakout Summaries - Identify Key Workshop Outcomes		
5:30 – 7:30 pm	Complimentary Embassy Suites Evening Reception (Atrium)		

THURSDAY, NOVEMBER 14, 2013

6:00 – 8:30 am	Complimentary Embassy Suites Breakfast (Atrium)		
Plenary Session 3 (Virginia Ballroom A/B) <i>Moderators: Terry Tullis & Thomas Duffy</i>			
8:30 – 8:45	Mark Rivers (Univ. of Chicago) Novel Techniques & Connections Between High-Pressure Mineral Physics, Microtomography & Cyberinfrastructure		
8:50 – 9:05	Bob Downs (Univ. of Arizona) Future Directions in Mineralogy & Crystallography: Computational Methods for Crystal Structure & Education		
9:10 – 9:25	Harry Green (Univ. of California, Riverside) Connections Between Cyberinfrastructure & Experimental Deformation of Rocks & Minerals		
9:30 – 10:30	Summary of Progress on Workshop Goals		
10:30 – 11:00	Coffee & Discussion (Outside Lobby of Virginia Ballroom A/B)		
11:00 – 12:00	Wrap Up, Final Reports of Breakout Sessions		
12:00	Meeting Adjourns: Steering Committee meets to write workshop report DEFORM and COMPRES Cyberinfrastructure Subcommittees meet		

Overview of EarthCube Workshops

(based on information from <http://www.nsf.gov/geo/earthcube/>)

For EarthCube to achieve its potential as a new data and knowledge management system for the 21st Century, the collective needs and desires of geoscientists across the disciplines must be made known. Workshops are being held to provide information so EarthCube can be designed to help geoscientist more easily do the science they want and need to do. Its goal is to provide them with access and tools so they can take leadership roles and be more competitive in the increasingly diverse and interdisciplinary scientific world in which we live. To this end, EarthCube is funding workshops so geoscience communities can articulate and document their cyberinfrastructure needs and what it is they would like to do in the future, both within their disciplines as well as in terms of accessing data and information from other fields, geoscience or not. The science-drivers, data utilities, user-interfaces, modeling software, tools, and other needs identified in this process will help direct and shape the function and form of EarthCube. EarthCube GEO domain workshops are designed to listen to the needs of end-user groups and to understand better how data-enabled science can help them achieve their scientific goals.

Workshop Goals and Objectives:

- Educate and engage cyber-literate researchers from COMPRES and DEFORM in EarthCube
- Identify the scientific challenges and opportunities facing our communities over the next 5-15 years
- Identify cybergeoscience opportunities and objectives
- Specify the cyber-infrastructure obstacles to meeting our goals
- Compile lists of known community data and modeling resources
- Describe the data and cyber-capabilities required to meet challenges. Match obstacles with resources. List key cyberdevelopment targets and needs, and unmet needs that may develop
- Develop ideas for at least two “proof-of-concept” projects or test cases for scientifically transformative activities that could be facilitated by EarthCube

Breakout Session 1

Participants will self-identify which breakout to attend, with encouragement to hop between them. Breakout notes will be posted on-line in real time via Google Docs.

Group A: **Identify the cyber-science challenges and cyber-infrastructure opportunities facing COMPRES for the next 5-15 years.** Facilitators: Martin Kunz & Przemek Dera Scribe: Caitlin Murphy

Group B: **Identify the cyber-science challenges and cyber-infrastructure opportunities facing DEFORM for the next 5-15 years.** Facilitator: Terry Tullis & Andreas Kronenberg Scribe: Phil Skemer

Deliverables: Summary of key outcomes, outline of plan for group discussion

Breakout Session 2

Participants will self-identify which breakout to attend, with encouragement to hop between them. Breakout notes will be posted on-line in real time via Google Docs.

Group A: **Refined discussion of CI needs and commonalities for DEFORM/COMPRES Science**
Facilitators: Guoyin Shen & Heather Savage Scribe: Judi Chester

Group B: **High performance computing, theory and modeling**
Facilitators: Louise Kellogg & Bijay Karki Scribe: Jianjun Dong

Group C: **Databases, web-based data access, data mining**
Facilitators: David King & Surendra Saxena Scribe: Ashley Griffith

Deliverables: Summary of key outcomes, outline of plan for group discussion

Breakout Session 3

Participants will self-identify which breakout to attend, with encouragement to hop between them. Breakout notes will be posted on-line in real time via Google Docs.

Group A: **Outreach, education, early career**
Facilitators: Pamela Burnley & Sylvia-Monique Thomas Scribe: Nicholas van der Elst

Group B: **Metadata, transducers and instruments, streamlining data collection**
Facilitators: Vitali Prakapenka & Wen-lu Zhu Scribe: J Katherine Crispin

Deliverables: Summary of key outcomes, outline of plan for group discussion.

Instructions for Accessing Google Drive and WebEx

Our goal is to make the EarthCube workshop a very collaborative process. Towards that end, we will be asking participants to use various Google Docs during the breakout sessions to record key points and action items. In addition, we are using a conferencing system called WebEx so that participants may join the conversation virtually. Below is information for accessing these technologies.

Accessing Rock Deformation & Mineral Physics Research Shared Google Drive

Each breakout session will have a scribe (see page 3). The scribe is responsible for recording key discussion points and action items from the breakouts into existing Google Docs so that all participants (including virtual participants) will be able to view the notes and follow along in real-time. However, any participant who accesses the shared URL can also add or edit comments, so other participants may help in recording notes during these sessions. Also in Google Drive, there is a copy of the workshop agenda and notes from plenary sessions.

1. Follow this link to the shared Google Drive (you should have received this by e-mail as well):
https://drive.google.com/folderview?id=0B_VW4kvIBAzQYXZPSWFNSjlUZIE&usp=sharing
2. This link will take you to a page with the workshop agenda and a “Meeting Notes” folder. Inside the “Meeting Notes” folder are several Google Docs.
3. Click on the file you wish to access and you will see a preview of the document. Click “Open” in the bottom right corner to edit the document.
4. Once you are in a document, you will see other participants in the top right corner. You will also see multiple cursors, depending on how many people are accessing the file. Many people can be working on the document at the same time. You will see the changes in real time.

Accessing WebEx Conferencing System

WebEx allows access to participants off site. If you cannot attend all or part of the meeting, you may log on during any of the plenary sessions. You can join the group by phone or computer. You will be able to hear the presentation, ask questions, and participate in the discussion. (If you join by phone, you will not be able to see the slides.)

To join by phone (can hear audio and ask questions)

Call-in toll-free number (US/Canada): 1-855-244-8681

Call-in toll number (US/Canada): 1-650-479-3207

Call-in toll number (US/Canada)*: 1-650-479-3207

Global call-in numbers:

<https://earthcube.webex.com/earthcube/globalcallin.php?serviceType=MC&ED=253867007&tollFree=1>

Toll-free dialing restrictions: http://www.webex.com/pdf/tollfree_restrictions.pdf

Attendee access code: 222 084 51

* Call-in toll number (US/Canada) should only be used if the primary number does not work.

To join online (can hear audio, view slides, and ask questions)

Follow this link (you should have received this by e-mail as well):

<https://earthcube.webex.com/earthcube/j.php?ED=253867007&UID=1693685292&PW=NMTliYWMwMmE1&RT=MIMxMQ%3D%3D>

A password should not be required, but if it is, enter the Meeting Password: 22208451

To view in other time zones or languages, please click the link:

<https://earthcube.webex.com/earthcube/j.php?ED=253867007&UID=1693685292&PW=NMTliYWMwMmE1&ORT=MIMxMQ%3D%3D>

EXECUTIVE SUMMARY: EARTHCUBE WORKSHOP RESULTS

(C. Marone, J. Bass and workshop participants)

Earth Cube Workshop Title:

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

Introduction (field(s)/area(s) of interest and purpose, number of participants):

Workshop participants addressed the current state and future directions of cyberscience and cyberinfrastructure as related to rock deformation and mineral physics research. 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 test cases for scientifically transformative activities that could be facilitated by EarthCube.

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 (list 3 to 6).

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2. **Current challenges to high-impact, interdisciplinary science:** Several themes emerged as consistent challenges faced within/across the involved discipline(s) (list 3 to 6).

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TECHNICAL INFORMATION/ISSUES/CHALLENGES

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

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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:**

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