Modeling Collaboratory for Subduction RCN
Fluid Migration Workshop Report

May 29 – June 1, 2019
University of Minnesota – Twin Cities

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1. Introduction

The Modeling Collaboratory for Subduction Zone Science Research Coordination Network (hereafter referred to as MCS RCN) was initiated in September 2018. The MCS RCN aims to develop a community plan for building a new modeling framework for earthquake and volcano systems in subduction zones through three workshops and a series of webinars. The first of the three workshops, held May 29 – June 1, 2019 at the University of Minnesota – Twin Cities (hereafter the Workshop), was focused on the transport and migration of volatiles and melts (hereafter referred to as fluids), and this report summarizes the activities and the outcome of the Workshop.

Fluid migration was chosen as the first workshop topic because fluids are critical to both earthquakes and arc volcanism, and because quantitative modeling of fluids poses common challenges that cross disciplinary boundaries in subduction zone science. The release of fluids from the downgoing slab helps to generate silicate melts that rise to form volcanoes, crustal intrusive complexes, and mineral resources (Grove et al., 2012; Cashman and Sparks 2013; Sigurdsson et al., 2015). The presence and migration of fluids promotes localized deformation and a range of both seismic and aseismic phenomena, including megathrust earthquakes, silent slip, and forearc deformation, by affecting pore fluid pressure and forming hydrous mineral phases (Brace, 1972; Gold and Soter, 1984; Saffer and Tobin, 2011). Fluids substantially alter the constitutive behavior of Earth materials and impact the dynamics of subduction (Hirth and Kohlstedt, 2004). On a global scale, the cycling of fluids between the Earth's mantle and the surface affects the pattern of mantle convection, plate tectonics, and long-term climate (Jagoutz and Kelemen, 2015; Lee et al., 2015). For example, plate tectonics as we know it may not exist on Earth without deep water cycling (Regenauer-Lieb et al., 2001; Ni et al., 2017). Fluid migration thus occurs across the entire range of temporal and spatial scales relevant to understanding natural hazards and resources associated with subduction zones.

The key goals of the Workshop were to (1) bring diverse groups of scientists together, (2) evaluate the current state of our understanding of fluid migration processes in subduction zones, (3) identify disconnects among models and knowledge gaps among modelers, and (4) build a community plan for integrative fluid migration modeling of earthquake and volcano systems. To achieve these goals, the organizers of the Workshop, Ikuko Wada (University of Minnesota – Twin Cities) and Leif Karlstrom (University of Oregon), together with the MCS RCN program manager, Gabriel Lotto (University of Texas at Austin), invited a diverse range of scientists as session chairs, keynote speakers, and participants. The details of the Workshop organization are provided in **Section 2**.

Discussions between keynote presentations and during breakout sessions raised the following points repeatedly, which represent in our view a community consensus:

1. **We need a better understanding of processes/mechanisms that control fluid migration, particularly for megathrust activity and volcanic systems; our physical understanding of fluid migration in the subduction system as a whole is incomplete.**
2. **Current research would benefit from a multidisciplinary modeling collaboratory that identifies and resolves related challenges that exist across subduction zone science.**
3. **Interfacing scientists across disciplines to develop models is as important at this stage as interfacing models.**
4. **Community modeling resources should include approaches for model validation (and uncertainty quantification) through observations and minimum/standard sets of benchmarking exercises.**
5. **Cross-disciplinary training and knowledge exchange for students and practicing research scientists alike would be an important function of a modeling collaboratory.**

Sections 3–4 describe in more detail the Workshop outcomes associated with these points of community consensus. Additional details, including breakout session notes in raw form, are available on the Workshop website.

2. Workshop Participation and Activities

2.1. Workshop Participation

Four session themes were selected for the Workshop. For each session, a pair of session chairs were invited (**Box 1**). The session chairs are largely observationalists except for one session (Session 4), in which modeling expertise was critical for facilitating discussion. Each pair then invited three keynote speakers for their session. Note that one speaker in Session 3 was unable to attend due to a health issue. In addition, an Early Career Scientist (ECS) session was incorporated, for which two ECS chairs and three ECS keynote speakers were invited (**Box 1**).

In total, 56 participants, representing 44 different institutions, attended the Workshop in person. Broken down by career stage, 18% of participants were students, 30% early-career scientists (non-students), 34% mid-career scientists, and 18% senior scientists (**Figure 1a**). In terms of gender, 62% identified as male and 38% identified as female. To assess the scope of the participants' research areas, the organizers asked the participants to describe their area of research in their participation applications; the responses were compiled into a word cloud (**Figure 1b**; wordclouds.com). A word cloud performed on ECS participant applications revealed similar themes, but also keywords associated with funding and observations.

An additional 90 attendees (minimum ten minutes online) joined the Workshop via a live *Zoom* webinar. Webinar attendees were able to offer comments and questions during keynote talks and participate in breakout sessions via an online facilitator.

Box 1: Session Titles, Session Chairs (*in italics*), Keynote Speakers, and Keynote Titles

1. Models for fluid migration in the subducting material, along/across the subduction interface, and the mantle wedge – *Adam Simon (Univ. of Michigan) & Anne Trehu (Oregon State Univ.)*
    a. Taras Gerya (ETH Zurich): "Seismo-hydro-mechanical modeling of subduction seismicity"
    b. Rachel Lauer (Univ. of Calgary): "Regional-scale models to constrain permeability of the oceanic crust, plate boundary, and splay faults"
    c. Johannes Vrijmoed (Freie Universität Berlin): "Coupling 2D numerical models to fully quantitative automated mineralogy mapping of hydrated peridotite"
2. Models for magma transport through the crust/lithosphere – *Matt Haney (USGS) & Luca Caricchi (Univ. of Geneva)*
    a. Richard Katz (Oxford): "Magma dynamics in subduction zones: models of the production and transport of volatile-enriched melts"
    b. Janine Kavanagh (Univ. of Liverpool): "Analogue modeling of dykes and sills"
    c. Tobias Keller (Stanford Univ.): "Theory and modeling of magma transport in magmatic arcs"
3. Models for microscopic and short-time-scale mechanisms – *Patrick Fulton (Cornell Univ.) & Jessica Warren (Univ. of Delaware)*
    a. Pengcheng Fu (Lawrence Livermore National Lab): "Massively parallel simulation of fluid transport in reservoir scale: Some recent advances in LLNL's GEOS code"
    b. Victoriya Yarushina (Inst. for Energy Technology): "Micromechanics of rock deformation and macroscopic fluid transport"

4. Bridging processes and models across scales – *Laurent Montesi (Univ. of Maryland) & Carolina Lithgow-Bertelloni (UCLA)*
    a. Eric Sonnenthal (Lawrence Berkeley National Lab): "Simulating coupled reactive-transport, heat flow, and mechanical deformation using multiple-continuum approaches"
    b. Diane Arcay (Univ. of Montpellier): "Trying to bridge the gap across scales... among the mantle wedge specificities, the tip matters"
    c. Cian Wilson (Carnegie Inst. for Science): "Under the hood: Numerical challenges modeling fluid pathways across the mantle wedge"

Early Scientist Career Session – *Tianhaozhe Sun (Penn State University) & Kayla Iacovino (NASA)*
    a. Joyce Sim (Carnegie DTM): "Tectonic boundaries: A modeling perspective"
    b. Changyeol Lee (Yonsei University, South Korea): "Roles of subduction parameters and mantle temperatures in volcanism of subduction zones"
    c. Tushar Mittal (UC Berkeley): "Melt transport through the mantle lithosphere – Challenges of a dike based model"

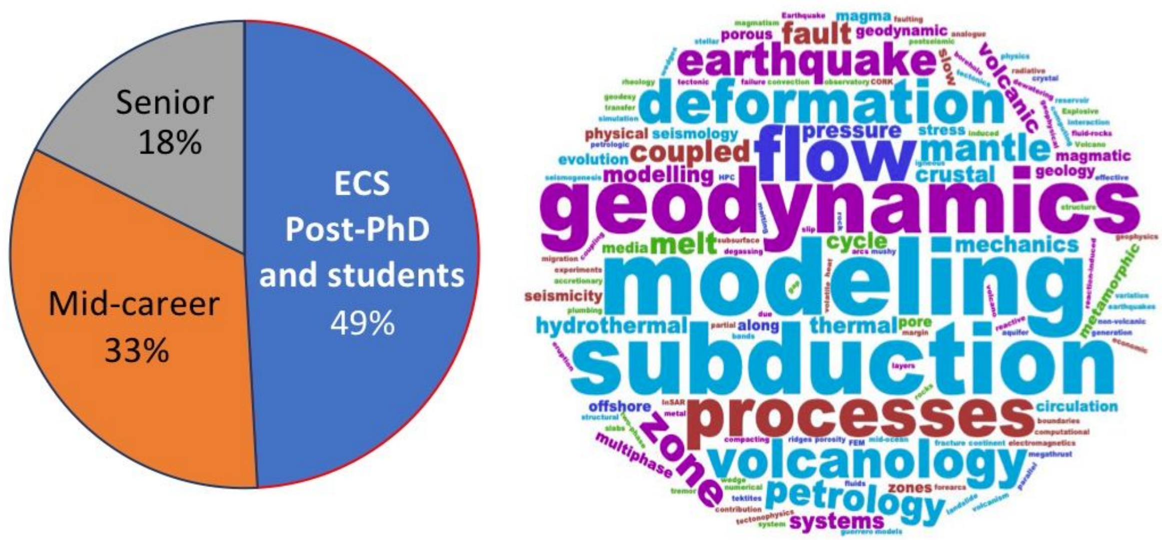

Figure 1. (a, left) Breakdown of participants by career stage and **(b, right)** a word cloud, consisting of keywords that describe the participants' research areas, indicating participation from a diverse group of researchers. The word cloud is based on the participants' response to "What are your areas of research?" in the initial workshop participation application form.

2.2. Pre-workshop Activities

Participants were asked four questions about their research prior to the Workshop in order to assess the scale and scope of modeling efforts currently underway (**Figure 2**).

1. For the conceptual or numerical model(s) of subduction-related fluid migration that you work on, what aspect do you personally view as needing the most work?
2. Indicate the range of spatial scales of your subduction fluid migration modeling efforts (including conceptual models if you work primarily on observations).
3. Indicate the range of temporal scales of your subduction fluid migration modeling efforts (including conceptual models if you work primarily on observations).

4. If you develop or use numerical models, indicate the computational expense of your typical model runs (CPU hours or similar).

Participants most often highlighted understanding and incorporating physical processes as a challenge for research. The second most common answer was constitutive relations and parameterizations that simplify models. Participants' models span an extremely large range of spatial and temporal scales, from sub-millimeter to hundreds of kilometers, and from seconds to tens of millions of years (**Figure 2**). The most typical model run-times are days and longer, although some participants could run their models in seconds.

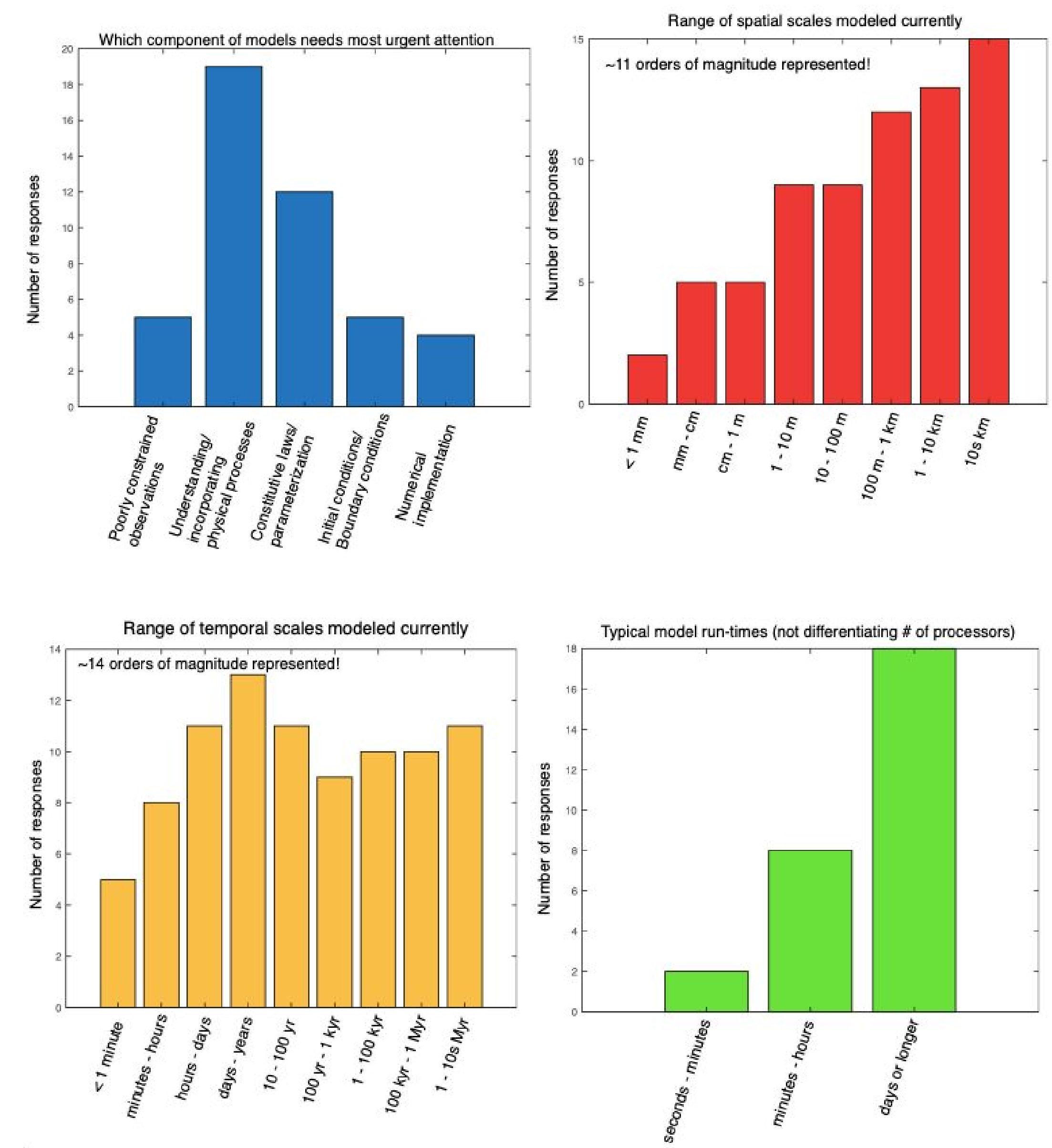

Figure 2. Participants' responses to pre-workshop questions 1–4 (see the main text).

2.3. Early Career Scientist (ECS) Session

Early-career scientists (ECSs) will be leaders in the field in the next decade, and it is prudent that a venture such as the MCS will be partially shaped by the people who will continue to use its products in the future. About half of the Workshop participants self-identified as early career scientists (**Figure 1a**). The ECS session was organized to provide a space that allowed ECS voices to be heard without being overwhelmed by established scientists. The objectives of the ECS session were also (1) to provide an opportunity for ECSs to share their experience in studying fluid migration in subduction zones and (2) to promote discussion among ECSs about key scientific questions to be addressed, current challenges, and their 10-year vision for their field, independently from the full body of participants. The session was organized by Tianhaozhe Sun at Penn State University and Kayla Iacovino at NASA. The 3.5-hour ECS session consisted of three 20-minute keynote presentations and a one-hour group discussion. The keynote speakers were asked to introduce the numerical models that they use in their research. The titles of their presentations are given in **Box 2**, and their presentation slides are available on the Workshop website.

The group discussion centered around three questions that were prepared by the session chairs. The questions and the brief summary of the ECS participants' responses are shown in **Box 3**. All questions were addressed, as well as several topics unrelated to the discussion questions. The challenge of communicating across disciplines was highlighted. Interdisciplinary studies toward solving grand challenges are seen as an important driver for modeling fluids in subduction zones, but it was noted that facilitating cross-disciplinary studies where one person's results rely on another presents non-scientific challenges, including language and culture barriers. Taking lessons from other fields (e.g., energy, exploration, engineering, and computer science) was seen as a way to bring in new tools to address both collaboration and scientific challenges. Education and inclusivity were also raised as a key issue by ECS. Workshop participants expressed interest in better formal training for numerical modeling. The outcomes of the group discussion were reported by three discussion leaders during the ECS session, and the summary of the ECS session was presented by the session chairs during the main workshop. Summary presentation slides are available on the Workshop website.

Box 2: Early Career Scientist (ECS) Session Keynote Presentations

ECS Keynote 1: Joyce Sim (Carnegie DTM): "Tectonic boundaries: A modeling perspective"
ECS Keynote 2: Changyeol Lee (Yonsei University, South Korea): "Roles of subduction parameters and mantle temperatures in volcanism of subduction zones"
ECS Keynote 3: Tushar Mittal (UC Berkeley): "Melt transport through the mantle lithosphere – Challenges of a dike based model"

Box 3: ECS Discussion Questions and Outcomes

Question 1. What are the key questions to be addressed by the field in the next 10 years?
Integration of various regimes at various spatiotemporal scales was a common theme: How can models reconcile multiscale transient phenomena? How can we better constrain spatial and temporal scales of volatile cycling, from subducting inputs to degassing, fluid fluxing, and volcanic eruption? More general overarching questions include: Why does subduction occur on Earth but not on other planets? How are fluids generated and distributed in subduction zones?
Question 2. What observational and experimental data do we need to address the key questions?
High-frequency time-series data from field observations (e.g., seismic, geodetic, fluid flow rate, pore fluid pressure) are crucial. In the laboratory, there is a need for more research on rheological properties of rocks

(viscous, brittle, plastic behaviors), and the properties of supercritical fluids at high pressures and temperatures. Obtaining these new data could be logistically challenging.

Question 3. What are the numerical challenges in multiphysics and multiscale modeling as applied to subduction zones?

How can we link physical and chemical processes within and across domains, and which equations are appropriate for which questions? Joint inversions, where one model is used to explain multiple datasets, was seen as one possible way forward for tackling these issues. Making proper use of machine learning is another potential approach for large datasets. In general, the need is emphasized for generalized models over those tailored towards explaining a particular dataset.

Question 4. How do we compare the modeling results with the observations?

The importance of iteration between models and observations was emphasized. Models may be used to constrain observations, but they may also be used as predictive tools, where a model result provides a testable hypothesis that may be investigated with observations. Obtaining rich synthetic data from models, as facilitated by the increasingly powerful computation capability, can be useful.

2.4. Themes, Keynote Presentations, and Discussions

The Workshop included four session themes, chosen to cover the range of spatial and temporal domains that fluid migration models currently address (**Figure 4**). The first session focused on fluid migration in the deeper parts of the subduction system as well as the subducting plate (e.g., Domains A–C of **Figure 4;** Session 1). The second session focused on magma transport through the crust and lithosphere (e.g., Domains D and E in **Figure 4**; Session 2). Microscopic and short-time-scale models or problems were assigned to Session 3 (e.g., Domain F in **Figure 4**) while Session 4 focused on bridging processes and models across different spatial and temporal scales. The session titles are listed in **Box 1**, and the workshop schedule is provided in **Appendix A**.

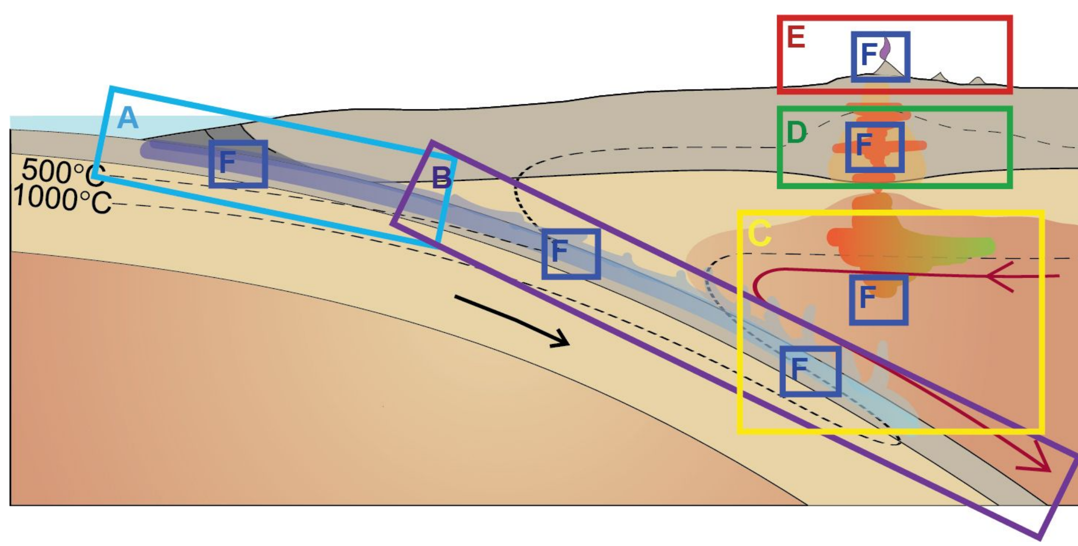

Figure 4. Schematic diagram illustrating the key components of a subduction system and domains (colored boxes with labels **A** to **F**) that are commonly investigated as an isolated system of fluid migration. Boxes **F** indicate example regions where microscopic and/or short-time-scale problems have been investigated.

Numerical modelers who are developing codes or investigating problems using data integrative models in each of the aforementioned themes were selected as keynote speakers. Each was asked to present their recent work and describe current challenges in fluid migration modeling. Because the workshop participants, including session chairs, were a mixture of observationalists and modelers, the workshop presentations and discussion covered a diverse range of approaches for studying fluid migration from grain to subduction-wide scale and from sub-second to millions of years in time scale. Discussions after keynote presentations, along with those during the breakout sessions as summarized below (**Section 2.5**), became the basis for the motivating questions described in **Section 3**.

2.5. Breakout Sessions

Three ~1.5-hour-long breakout sessions were organized. In each session, participants were divided into three groups and were asked to discuss three questions that were prepared by the organizers and session chairs. The questions and the key discussion points are given in **Box 4**. A discussion leader and a scribe were assigned to each group. The leader and/or scribe reported a summary of the group discussion in a 5-10 minute presentation during the Workshop. Breakout notes and summary presentation slides are available on the Workshop website.

Box 4: Breakout Questions and Key Discussion Points (expanded in Sections 3 and 4)

Breakout #1 (after Sessions 1 and 2):
Q1.1. Is it appropriate to model fluid migration in each subduction domain separately or is a more holistic approach necessary? What is the appropriate phenomenological temporal and spatial scales for each domain?
Combining fluid and magma transport models together into a grand model is probably not necessary or possible. A modular ("Lego brick") approach might be useful. Are the relevant physics well enough understood to develop validation tests and benchmarks? Observations that constrain models (especially at depths below the crust) are sparse. Models should strive to account for epistemic uncertainties in the physics.
Q1.2. How should the interfaces between different domains be treated given the current state of our understanding?
One potential approach for building connectivity within an integrated framework is to use outputs from one model as inputs for a second model. However, there are immense technical issues when connecting models. Parameterizations, reduced-order and sub-grid-scale models can be useful, but may require solving the fully coupled system first before defining valid approximations.
Q1.3. What are the main limitations to modeling progress for each domain (e.g., resolution/compute time/numerical methods, uncertain physics/chemistry, poor observational constraints)?
There are major uncertainties in the fluid influx entering the slab and the evolution of permeability in the crust and lithosphere. There is a need for more observations to understand fluid and deformation feedbacks in the accretionary prism. Can the top of the subducting plate be treated as a channel over long timescales but a boundary over transient timescales? May need improved numerical techniques to efficiently model high-resolution wedge dynamics in 3D where fluids become localized. Currently, there is no tractable set of equations for the full chemistry of hydrous melting. How can we develop more integrated and self-consistent models of crustal-scale magma transport?

Breakout #2 (after Session 3)
Q2.1. Which chemical and physical processes at the microscopic level dominate fluid transport?
Important issues: reactive transport, the topology of fluid connectivity and evolution of porosity/permeability, consideration of less well-studied phenomena such as cavitation in the absence of fluids for the generation of porosity. Chemical and physical processes are linked at a microscopic level, but current models are incomplete.
Q2.2. Are there common/dominant fluid migration pathways?

There is agreement on the general types of fluid migration pathways but no good understanding of the relative importance of one pathway or another. At present, it is difficult to make a quantitative prediction about dominant fluid migration pathways since each model has a set of in-built approximations and parameterizations.

Q.2.3. In what scenarios is it reasonable to simplify the description of fluid flow, and what is the right approach to validating reduced-order models?

It is appropriate to approximate certain processes as steady-state but not others. Corner flow may work for some applications, but 3-D, time-evolving subduction dynamics may be needed for others, for example. The subduction system is inherently highly nonlinear: Earthquakes and volcanic eruptions are episodic and transient expressions of quasi-steady, far-field forcing. Well-documented sensitivity tests can help to determine when to use parameterizations for multi-scale models.

Breakout #3 (after Session 4)

Q3.1. What are the essential elements (e.g., rheology, physical properties, chemical components) of fluid behavior across different domains?

A "zeroth order" model is a common goal for fluid migration. For the mantle wedge, it would need to address: What is the permeability structure of the slab and wedge? How do the physical properties of fluids and volatiles evolve? What are the feedbacks between fluids and long-term slab and wedge dynamics? The answers to these questions depend on fluid-related processes in other domains, but the relation is not consistently defined by the community.

Q3.2. What observations are currently the most significant constraints (and thus most needed) on fluid migration in each domain?

Fluid migration is constrained by seismic data, geochemistry, electrical conductivity, structures from field mapping, and petrological observations, among others. Future needs include rheology experiments that address chemical heterogeneity and reactivity; equation of state experiments for non-pure hydrothermal fluids; and analog laboratory and numerical experiments.

Q3.3. What will a modeling framework for fluid migration in subduction zones encompass in 10 years? What products or services would you like to see in a Modeling Collaboratory for Subduction Zone Science?

Useful and usable codes, with meetups for discussing, developing, and sharing codes; codes with support, documentation, and benchmarking; access to high-performance computing. There is a need for easier ways to communicate with others who are working on similar or adjacent problems, in order to share data, codes, hypotheses, and experience. Interest in a conceptual map for subduction zones that is linked to a knowledge-sharing repository. The community still disagrees about a common set of equations to solve for fluid migration, so flexibility in terms of solver frameworks is key. Workshops and summer schools to equip students and early career scientists with the best tools and to foster collaboration between researchers who wouldn't normally work together.

2.6. Lightning Talks and Poster Session

Thirteen participants each gave a one-minute lightning talk introducing their posters (**Box 5**). Lightning talk slides are available on the Workshop website. Posters were presented during a 2-hour poster session and throughout the Workshop.

Box 5: Poster Presenters and Poster Titles

Caricchi, Luca, Tom E. Sheldrake, Laura Pioli, Guy Simpson, Eniko Bali and Maurizio Petrelli: "Holuhraun-Bárðarbunga 2014-2015 (Iceland) eruption: reconstructing deep magma dynamics with cluster analysis"

Cerpa, Nestor, Ikuko Wada and Cian Wilson: "Physical controls on fluid migration in the mantle wedge"

Dunham, Eric M., Weiqiang Zhu, Kali Allison and Yuyun Yang: "Fault Valving and Pore Pressure Evolution in Simulations of Earthquake Sequences and Aseismic Slip"

Dye, Brian and **Gabriele Morra**: "Machine Learning as a Detection Tool on Infrared Images of Strombolian Eruptions atop Mount Erebus, Antarctica"

Ha, Goeun, Laurent Montési and Wenlu Zhu: "Effect of thermally controlled permeability barriers on the location of arc volcanism at subduction zones"
Hyndman, Roy: "Water in subductions zones: inputs and outputs"
Lee, Changyeol, Donghoon Seoung and Soohwan Yoo: "Roles of Subduction Parameters and Mantle Temperatures in Volcanism of Subduction Zones"
Seropian, Gilles, **Alison Rust**, Steve Sparks and Sam Mitchell: "The stability of melt lenses in magma mushes"
Sim, Shi Joyce, Marc Spiegelman, Cian Wilson and Dave Stegman: "Tectonic Boundaries: A modeling perspective"
Sun, Tianhaozhe, Demian Saffer and Susan Ellis: "Studying the coupling between deformation, pore fluid pressure, and fluid flow in subduction forearcs"
Vestrum, Zoe and **Sam Butler**: Effects of Ongoing Melting on the Formation of Shear Induced Melt Bands"
Willis, David, Peter Betts, Louis Moresi and Laurent Ailleres: "Neogene stress rotation at the transition from subduction to continental collision, Marlborough, New Zealand"
Zhan, Yan, Patricia Gregg, Hélène Le Mével and Craig Miller: "Integrating reservoir dynamics, crustal stress, and geophysical observations of the Laguna del Maule magmatic system by FEM models and data assimilation"

2.7. Synthesis Discussion

The Workshop ended with a synthesis discussion, focusing on the role and deliverables of a modeling collaboratory, in comparison with other existing and anticipated programs, such as CIG, GEOPRISMS, and SZ4D. In particular, the relation of the modeling collaboratory to SZ4D and CONVERSE was discussed in detail due to some overlap in the scope/objectives. Potential deliverables of a modeling collaboratory are further described in **Section 4**. Throughout the discussion, the need to promote and facilitate communication between scientists and modelers in different disciplines was emphasized over integration of fully developed models, given the current state of our understanding. In part this was a natural outcome of the scientifically diverse participants at the Workshop; discussion of technical issues associated with model integration would be better suited for future, modeling-specific workshops. The general consensus on the current state and future steps in advancing the research on fluid migration in subduction zones as a community is as summarized in **Section 1**. In the following section (**Section 3**), we describe some specific scientific questions that can guide the community, and therefore the future modeling collaboratory.

3. Motivation and Future Direction

As illustrated in **Figure 4**, the Workshop defined 'domains' of fluid migration in subduction zones according to classes of problems that are currently organized in scientific research and expertise. These domains are partially – but not wholly – defined by physical components of the subduction zone system: the mantle wedge and slab (Domains B and C in **Figure 4**); the megathrust seismogenic zone and accretionary prism (Domain A); and the crustal magma transport system and volcanoes (Domains D and E). Some studies focus on small-scale fluid transport phenomena that may occur in different parts of the subduction system and are not specific to a single physical location, as represented by multiple domains that are labeled F in **Figure 4**. Across domains A-F, the workshop writing committee identified three Motivating Questions (MQ) that are the focus of current research and that seem critical for an eventual integration of fluid migration modeling across subduction zones and therefore the modeling collaboratory. Each MQ contains three sub-questions and focuses on a specific spatial domain of the subduction system (**Box 6**).

Box 6: Motivating Questions (MQ)

MQ1. How do fluids affect spatio-temporal variations in seismic and aseismic tectonic activities?

MQ1a. How, where, and when are elevated pore fluid pressures generated and maintained, and how do they relate to the wide range of observed interface slip behavior?

MQ1b. What are the fundamental processes controlling short-time scale changes in pore fluid pressure, fluid flow, and effective stress on faults?

MQ1c. How does porosity and permeability evolve with matrix deformation to control fluid flow?

MQ2. How do fluids affect the spatio-temporal variations in magma ascent?

MQ2a. What processes determine the spatial distribution of magma from wedge to surface?

MQ2b. How does the rate of magma ascent vary from wedge to surface?

MQ2c. How does the petrology and geochemistry of magma relate to the dynamics of transport?

MQ3. How are fluid-related processes linked to the thermal-chemical-mechanical structure and dynamics of the subduction system?

MQ3a. How do fluid-mediated chemical reactions affect fluid migration?

MQ3b. How does fluid migration affect the large-scale thermo-mechanical structure of the mantle wedge?

MQ3c. How does the interface between two mechanically-distinct domains affect fluid migration?

MQ1. How do fluids control the spatial and temporal variations in seismic and aseismic tectonic activities?

Fluids play an important role in the enormous variety of deformation phenomena that occur in the megathrust region (Domain A in **Figure 4**). Based on the discussion during the workshop, the writing committee identified three overarching questions on the role of fluids in subduction zone seismicity, silent slip, and crustal deformation.

MQ1a. How, where, and when are elevated pore fluid pressures generated and maintained, and how do they relate to the wide range of observed slip behavior?

The development and maintenance of overpressure (pressure in excess of hydrostatic pressure) at the plate boundary require both dynamical pressurization (e.g., rock dehydration, pore compaction, thermal pressurization) and a permeability structure that maintains these pressures by impeding drainage. In the outer forearc, the region from the seismogenic zone to the brittle-ductile transition zone, the primary fluid sources are produced by a combination of 1) compaction and dewatering through tectonic burial and loading, and 2) dehydration reactions that release bound water from hydrous minerals on the incoming plate. The rate of dewatering through compaction and porosity loss is highest in the first ~3–5 km of tectonic burial (Bekins and Dreiss, 1992; Bray and Karig, 1985; Hyndman et al., 1993), decreasing with progressive burial and stiffening of the sediment framework in response to porosity reduction. As sediments are conveyed to greater depths and higher temperatures, fluid derived from dehydration reactions exceeds fluid derived from matrix compaction and porosity loss. The largest source of dehydration-derived fluid results from the transformation of smectite to illite (Bethke, 1986; Moore and Vrolijk, 1992), a reaction controlled by the temperature field and exposure time of the sediments (Pytte and Reynolds, 1989). The thermal state and convergence rate of a particular subduction zone will, therefore, determine the spatial locus of this reaction, shifting to greater depths in cooler forearcs. In deforming fluid-bearing subducted rocks, localised pressurization may also occur due to enhanced visco-plastic compaction along active faults (e.g., Dymkova and Gerya, 2013).

Direct observations of elevated pore pressure are limited to shallow boreholes in the outer forearc, although there are abundant observations from seismic reflection surveys that document high reflectivity and velocity anomalies interpreted as zones of elevated fluid pressure (e.g. Bangs et al., 2009; Park et al., 2002). The spatial correlation of these observations with the anticipated depths of clay dehydration has led some researchers to hypothesize a connection between the updip limit of seismicity and fluids sourced through dehydration (Park et al., 2002, 2010; Ranero et al., 2008; Lauer et al., 2018). Observed reflectivity may indicate an elevated fluid content from clay dehydration, which modulates fault behavior as the reaction subsides, fluids are depleted, and the associated pressure declines. However, the flow paths associated with fluids generated by dehydration are not well constrained: are they channeled along the plate interface, or is there substantial loss to the region above the plate interface (further discussed in **MQ3c**)? Recent numerical work also indicates the importance of decompaction weakening in fluid channelization (Räss et al., 2018). More quantitative estimation of spatial and temporal variations in pore pressure likely require numerical models to connect diverse observations.

Field observations and laboratory constraints on compaction and dehydration are also crucial in the modeling efforts to quantify the distributions of fluids and fluid pressures in subduction zones. Observations of porosity from active and exhumed subduction zones are used to project porosity loss and compaction sources, together with laboratory-based consolidation testing of recovered sediments, which further constrain loading behavior at depths that cannot be directly observed. The magnitude and distribution of dehydration derived sources are quantified by combining kinetic expressions (e.g. Pytte & Reynolds, 1988) with the margin thermal structure and porosity evolution (Bekins and Dreiss, 1994; Saffer et al., 2008; Lauer and Saffer, 2015). These studies reveal that fluid flux from dehydration can match or exceed that from compaction within 10–40 km from the trench, depending on the initial sediment composition and thermal structure of the forearc, though further observations are required to make site-specific predictions. Further, in order to quantify the distribution of fluid pressures, the time-evolving permeability structure that controls fluid migration pathways also needs to be taken into account, as has been done in a number of analytical and numerical modeling studies in the past several decades (Connolly & Podladchikov, 2015, Mckenzie, 1984, Räss et al., 2019, Richter & Mckenzie, 1984).

The permeability distribution exerts a primary control on flow and pressure development throughout the system. High permeability faults and fractures, as well as sandy layers in the incoming sediments, serve as drainage pathways and conduits for focused flow, whereas low permeability sediments inhibit flow and can enable the development of overpressures (e.g. Neuzil, 1995). Laboratory studies designed to explore the permeability evolution of marine sediments during progressive subduction provide important constraints for parameterizing fluid flow models, although scaling parameters from the lab sample to the regional scale remains a challenge. However, the evolution of crustal and sediment permeability during subduction remains elusive. Progress will likely require connecting laboratory-derived estimates of permeability to crustal-scale models, to better bridge the gap between geophysical observations and the fundamental processes that govern the production and movement of fluids in subduction fault systems.

MQ1b. What are the fundamental processes controlling short-time scale changes in pore fluid pressure, fluid flow, and effective stress on faults?

In addition to the long-term build-up of pressures described above, earthquakes and other fault slip behavior can immediately affect pore pressure through static and dynamic stresses. Damage-enhanced permeability also promotes fluid flow which redistributes fluid pressures and effective stress, and can potentially trigger further earthquakes, rock failure, and deformation. A variety of mechanical and chemical processes affect how permeability subsequently heals and possibly seals reservoirs.

Sustained efforts are needed to understand the magnitudes and timescales of damage and healing processes and their hydrologic effects. A variety of observational constraints exist: fault valving behavior has long been recognized in the rock record (e.g., Sibson, 1975) and transient fluid flow within subduction zones has been inferred based on geochemical and thermal constraints (e.g., Fisher and Hounslow,1990; Le Pichon et al., 1990; Blanc et al.,1991; Bekins et al., 1995; Sample, 1996; Carson and Screaton, 1998; Saffer and Tobin, 2011). Advances in our understanding so far also benefit from laboratory experiments of damage and healing effects on permeability (e.g., Elkhoury et al., 2011; Candela et al., 2014) and from borehole observatories in which transient increases in permeability in response to earthquakes have been observed along with healing over many time-scales (Elkhoury et al., 2006; Xue et al, 2013; Fulton and Brodsky, 2016) and transient fluid flow in response to earthquakes and fault slip have also been observed within large-scale subduction zone faults (Solomon et al., 2009; Fulton and Brodsky, 2016).

Other short-term transient processes of importance include the effects of fluids in the earthquake nucleation and rupture process itself. These effects include dynamic weakening through thermal pressurization in which frictional heating can rapidly increase pore pressure within the fault slip zone (e.g. Andrews, 2002), slip dilatancy which can decrease pore pressure where porosity is locally enhanced (e.g., Sleep and Blanpied, 1992; Segall and Rice, 1995), and creep-related closure of pores which can increase pore pressure through matrix compaction (e.g., Skarbek and Rempel, 2016). Transient pulses of fluid that are mediated by porosity waves may also play a role in setting the diversity of slip seen at subduction zones, such episodic tremor and slip. Insights into these processes are largely constrained by laboratory experiments (Marone et al., 1990; Di Toro et al., 2006; Omlin et al, 2017). When implemented into models, the effects are short-lived, dependent on the small-scale hydrologic and poromechanical properties, yet can strongly influence resulting slip behavior (e.g., Liu and Rice, 2005).

Given that all these processes can affect pore pressure, whether assumptions regarding relationships between pore pressure and effective stress are valid at depths throughout the seismogenic zone or for the short timescales of earthquake rupture remain open questions. For example, low porosity stiff rocks are known to have less sensitivity to pore pressure than expected with the commonly utilized Terzhaghi effective stress relationship, where effective stress is simply stress minus pore pressure (e.g., Nur and Byerlee, 1971). For these scenarios, a more complete description of the rheologically complex poro-visco-elasto-plastic matrix behavior may be required (e.g. Yarushina and Podladchikov, 2015; Gerya, 2019). Continued collaboration between modelers and experimentalists is necessary to understand how pore pressures and their transient and dynamic changes relate to effective stress, fault slip behavior, and deformation.

MQ1c. How do porosity and permeability evolve with matrix deformation to control fluid flow?

Fluid processes interact with matrix deformation processes over a vast range of spatial and temporal scales. Together they control subduction forearc geodynamics throughout and beyond the subduction earthquake cycles. In modeling subduction forearc fluid and deformation processes, different approaches can be chosen, mainly depending on (1) the timescales of the hydromechanical processes investigated and (2) the different strategies for incorporating the fluid sources and fluid-solid coupling.

To model the short-term (≤ 100s of years) fluid-related deformation associated with a single earthquake or slow slip event, simplified poroelastic models are commonly used. For example, to quantify the contribution of poroelastic rebound following a megathrust earthquake, a common strategy is to compare end-member deformation scenarios such as an "undrained" state (for immediately after the rupture when fluid flow has not initiated) and the eventual "drained" state (when a less heterogeneous fluid pressure state has been re-established), without exploring the details in the coupled evolution of fluid flow and crustal deformation (e.g., Hughes et al., 2010; Hu et al., 2014). However, numerous theoretical studies that involve poro-visco-elastic rheology also exist, including the earlier work of Connolly and Podladchikov (1998) and fully coupled hydro-mechanical models in a poro-visco-elastic matrix under shear deformation in 3-D (Räss et al., 2019). Even models that involve visco-elasto-plastic porous media are formulated (Yarushina & Podladchikov, 2015, Yarushina et al., 2015). However, more efforts are needed to integrate these models into time-evolving, tectonically constrained subduction zone simulations. To this end, comparison with studies in other tectonic settings (e.g., Jin and Zoback, 2017; Kim, 2018) may be helpful, including consideration of the hydraulic and mechanical effects of transient magmatic processes, as detailed in MQ2b. Both theoretical and experimental rheological studies of deformable porous media will also continue to be helpful (e.g. Makhnenko & Podladchikov, 2018).

To model subduction forearc compaction-driven dewatering processes over geological times, two main categories of numerical models have been used. The first consists of purely kinematic models (e.g., Bekins and Dreiss, 1992; Ellis et al., 2015; Lauer and Saffer, 2015). These models prescribe a steady-state porosity distribution in the accretionary wedge, using either simple porosity-depth relationships (e.g. Athy, 1930) or seismic velocity data and empirical velocity-porosity relationships (e.g., Hoffman and Tobin, 2004). With the steady trajectories of sediment flux also prescribed, sediment compaction and the associated dewatering can be quantified based on the conservation of fluid and solid masses, and computation of in-situ stress state is not needed. In the second category, models explicitly incorporate the mechanical loading processes (e.g., Shi and Wang, 1988; Screaton and Saffer, 2005; Gamage and Screaton, 2006; Skarbek and Saffer, 2009). In most cases, some ad hoc assumptions are made to simplify the computation of the in-situ stress state. A few studies (e.g., Rowe et al., 2012; Gao et al., 2018) employ large-scale finite element models to model the dynamically evolving subduction wedge geometry and the spatiotemporally variable in-situ stress state. Continued efforts are needed to enhance our understanding of the long-term evolution of the forearc hydro-mechanical system. Major challenges include a better understanding of the evolution of fault architecture and its control on the spatially complex drainage pattern, a better understanding of how fluid overpressure modulates fault mechanics and controls a variety of important geological processes such as basal erosion, underplating, and strain localization, and a more complete understanding of microscopic poromechanical properties that is essential in governing large-scale deformation (e.g., Nur and Byerlee, 1971).

A range of observations is required to illuminate subduction forearc hydro-mechanical processes. These include 1) measurements of the distribution and rates of fluid flow, fluid chemistry and temperature, 2) direct measurements of pore fluid pressures or inference from intrinsically related physical properties (e.g., seismic velocity and porosity data), 3) high-resolution imaging by seismic and electromagnetic techniques, 4) geodetic observations and geological field records of crustal deformation and fault-zone structures, and 5) laboratory experiments that help better understand hydraulic and mechanical properties of porous geomaterials. A modeling collaboratory could help to facilitate communication and collaboration between diverse groups of researchers focused on gathering, interpreting, and extrapolating these diverse observations. Fluid-flow modelers who work on different domains of the subduction zone may also contribute in valuable ways, for example, to better quantify the seaward fluid discharge across the mantle wedge tip or to determine the fluid input into the shallow segment where megathrust earthquakes nucleate. It is also valuable to encourage communication between modelers who study similar coupled fluid and deformation problems in other settings (e.g., soil mechanics, rock mechanics, oceanography, hydrology, or structural engineering).

MQ2. How do fluids affect the spatial and temporal variations in magma ascent?

Despite quasi-steady and spatially continuous subduction that drives melting of the mantle wedge, the processes associated with melt generation, magma ascent and storage, and volcanic eruptions are strongly unsteady in time and non-uniformly distributed in space. Identifying the origin of spatially and temporally evolving magma ascent pathways is a long-standing challenge for fluid migration modeling in subduction zones. The workshop writing committee identified three questions that could help focus future work on this topic.

MQ2a. What processes determine the spatial distribution of magma from wedge to surface?

The spatial distribution of magma in subduction zones defines a transport network consisting of structures that span at least 10 orders of magnitude in size from source region in the mantle wedge to eruption on the surface: from 10s micron-scale grain boundary melt (von Bargen and Waff, 1986) to ~100 km wide calderas being emptied in single eruptive episode (Lipman, 2007). Physical processes that control the transport structures, along with their connectivity, vary as a function of depth and can be broken into three regimes: combined aqueous fluid and slab melt transport from the subducting plate to the overlying mantle wedge (Domain B in **Figure 4**); melt generation and ascent within the wedge (Domain C in **Figure 4**); and melt transport within and through the crust (Domain D in **Figure 4**) to eruptions and surface evolution (Domain E in **Figure 4**). These divisions reflect spatially varying mechanical and chemical properties, remote forces, and mass flux within these transcrustal igneous systems.

Although observational constraints on small-scale structures in the mantle are sparse, tomographic imaging (e.g., McGary et al., 2014) suggests a spatial distribution of fluids that conforms roughly to the expected thermal and chemical structure of the wedge. Melts are generated within the wedge through a combination of decompression melting along the upward-directed corner flow streamlines and flux melting where water enters the hot core of the mantle wedge (Plank and Langmuir, 1988; Grove et al., 2012). Both processes are strongly modulated by boundary conditions at the slab and lithospheric interfaces (further discussed in **MQ3c**). Consequently, the large-scale spatial distribution of melt is expected to vary systematically across subduction zones (e.g. Syracuse and Abers, 2006) and evolve over time at a given subduction zone (Haschke et al., 2002; Chin et al., 2012). Models of two-phase flow and reactive transport suggest that melt channels arise as a natural consequence of flux melting in the wedge (Spiegelman et al., 2003). Channel networks should enhance the efficiency of melt transport and are two-way coupled to the surrounding solid-state flow through reduced (and perhaps anisotropic) bulk viscosity and advection of heat by the fluid phase. Slab interface roughness or positively buoyant fluid instabilities (at the slab interface, Gerya et al., 2004), Moho topography or fluid instabilities (at the lithosphere-asthenosphere boundary (Karlstrom et al., 2014; Yang et al. 2018) will change mantle flow patterns and subsequently affect the fine-scale structure of melt transport.

Within the deep crust and lithosphere (Domain D in **Figure 4**), the evolving spatial patterns and geometry of melt transport structures covary most strongly with host rock rheology (e.g., Keller et al., 2013), which itself is strongly modified by heat and fluids released by ascending magma. Stalling and chemical evolution of magmas are integral to magma ascent through the lithosphere, with intrusion/extrusion ratios universally greater than one (White et al., 2006). Magma storage can occur at all crustal levels but varies between arcs as a function of tectonic stress state, compositional and thermal-rheological structure (for example, the Moho), and the duration of prior magmatism (Annen, 2009). Observations from exposed crustal sections show that transport structures in a single location can encompass both magma-driven fractures (dikes with a small width/length ratio that imply elastic/brittle host material) and viscous structures (blobby bodies that exhibit an apparent power-law size distribution, Cruden et al., 2017), which provide evidence of strong temporal unsteadiness in magma transport phenomena recorded in the plutonic record (Karlstrom et al., 2017).

Such transitions between elastic and viscous transport behavior have been predicted by numerical models and laboratory experiments. Magma transport models remain modular, in the sense that models focus on an isolated magma reservoir or dike (de Silva and Gregg, 2014; Rivalta et al., 2015; Schmeidel et al., 2017; Kavanagh et al., 2018). However, ensemble models of intrusions are increasingly common (e.g., Bunger et al., 2013; Karakas et al., 2017), and crustal-scale multiphysics models that predict magma transport from Moho to surface have also been developed facilitating comparison with multiple observational constraints (e.g., George et al., 2016; Colón et al., 2017; Reuber et al., 2018a). However, insights gained from crustal-scale magma transport models are non-unique, and few models consider interactions between elements of the magma transport system that lead to spatial structuring of ascent pathways (e.g., Karlstrom et al., 2009). Although it is unknown what governs the formation or lateral extent of magma storage zones, the range of possible material behavior – granular mechanics of crystal-rich mushes (e.g. Bergantz et al., 2015) to visco-poro-elastic-plastic rheology (e.g., Liao et al., 2018) – and dissipative nature of magma ascent and cooling point to strong history effects. The magnitude (volumetric flux from the mantle) as well as the history of prior magma transport are likely controls on magmatism in the crust, and thus initial conditions are important yet often poorly known.

At shallower depths (Domain E in **Figure 4**), multiphase behavior of volatiles dissolved in magmas become a primary physical process governing ascent (Cashman et al., 2017). It is unlikely that magmas would ascend into the shallow crust or erupt from the surface without the buoyancy provided by water, CO_2, and sulfur bubbles (Gonnermann and Manga, 2007). Elastic and brittle processes in the presence of a free surface largely govern the organization of magma transport structures at shallow depth (Segall, 2010). This means that shallow magma transport is potentially sensitive to Earth surface processes, such as meteoric hydrothermal circulation (Weis, 2015), stress and strain associated with glaciers (Albino et al, 2010), and erosion. Explaining the construction/erosion (O'Hara et al., 2019), focusing, and 100s of kyr longevity of discretely spaced transport pathways represented by surface volcanic centers (Hildreth, 2007) remains a significant challenge for models of crustal magma transport.

MQ2b. How does the rate of magma ascent vary from wedge to surface?

Magma transport through the mantle wedge takes place over at least 13 orders of magnitude in time, encompassing grain boundary melting to high-speed turbulent flow during eruption, and reorganization of transport pathways over millions of years (arc front migration). Many unsteady phenomena deep in the magma transport system remain poorly constrained by data, and incompletely studied theoretically. For example, recent large-scale geodynamic models of fluid migration in the mantle wedge report fluid ascent rates, assuming porous transport only, that are slower than those estimated from geochemical analyses of arc lavas (e.g., Wilson et al., 2014; Cerpa et al., 2018). This discrepancy implies missing physics in current models, for example the amount of slab-derived fluid that is assumed to migrate into the mantle wedge, which depends on permeability contrast between the slab and the overriding mantle. Flow channelization is a clear missing ingredient, and can arise from a variety of physical mechanisms. For example, decompaction weakening is proposed to promote flow channelization (Connolly and Podladchikov, 1998, 2007; Yarushina & Podladchikov, 2015). Porosity channels and chimneys, and other feedbacks between melting, fluid flow, and porosity/permeability structure (Hewitt, 2010; Koulakov et al., 2013, Räss et al., 2018) can also lead to this behavior.

Predicting magma ascent in the mantle wedge also requires better characterization of the permeability of the partially molten mantle. Deformation and stressing of partially molten mantle material will concentrate melt into inclined bands that may lead to a highly anisotropic partially molten aggregate (Holtzman et al., 2003; Katz et al., 2006). The chemistry (and hence rheology) of fluids coevolves with transport, involving mixtures of silicate melts, water, and likely CO_2-rich fluids (Ague and Nicolescu, 2014). Serpentinization and carbonation in the mantle wedge in the colder regions near the trench will also affect the permeability structure, which may evolve to form coherent permeability barriers to melt ascent (Rondenay et al., 2010).

Melt ascent may also involve transport in mesoscale objects such as diapirs. Diapirs generated at the subduction interface, possibly involving sediments or mélange, may rise rapidly through the mantle wedge and could entrain melt generated inside the diapir (Gerya and Yuen, 2003; Behn et al, 2011; Marschall and Schumacher, 2012). Such diapir-like structure may also play a role in melt transport through the lithosphere (Cao et al., 2016; Yang et al. 2018) as long as the crust is heated enough to respond viscously to applied stresses (Rubin, 1993; Jellinek and DePaolo, 2003). However, pervasive dike structures preserved in depth sections representing all levels of crust implies that magma-driven fractures are the most efficient mechanism for crustal magma transport in arcs (Johnson and Jin, 2009; Keller et al., 2013, Kavanaugh et al., 2018) .

In the mid to upper crust, the timescale of magma ascent depends on the extent to which it stalls in magma reservoirs. Monogenetic and ultramafic eruptions (for example, kimberlites) may rise directly from the mantle to the surface through dikes in a matter of hours (Wilson and Head, 2007; Peslier et al., 2008). However, more evolved magmas ascend in a sequence of storage zones over a much longer range of times, and assembly of large silicic magma chambers that feed super-eruptions (> 500 km^3 erupted in a single episode; Lipman 2007) may require millions of years through mixing and chemical differentiation of small mafic intrusions (Miller et al., 2011). Modern geochemical tools, for example U-series disequilibria (Cooper, 2015; Rubin et al., 2017), diffusion profiles in magmatic phenocrysts (e.g., Costa et al., 2008), and melt inclusions (e.g., Humphreys et al., 2008), place constraints on pre-eruptive histories that provide a new standard for models of magma storage and eruption. The concept of large-scale 'mush zones' (Cashman et al., 2017) provides a potentially unifying framework, but this is currently challenging to model or validate. Mushes represent a nexus of challenges common to fluid migration across subduction zones: wide ranges of important time and spatial scales, complex rheologies (Bachmann and Huber, 2018), and strongly coupled physical-chemical processes. This includes magmatic/hydrothermal interactions (Weis, 2015). Phase separation of magmatic fluids from magmas can lead to ore deposit formation and influence hydrothermal features such as thermal springs and geysers (Hurwitz and Manga 2017) at the Earth's surface.

At shallow depths (upper few km), magma ascent occurs through volcanic eruptions as well as intrusions. Eruption ascent rate is dictated largely by whether or not the magma fragments (Cashman and Scheu, 2015), which governs a fundamental transition between effusive vs explosive eruptive styles. In the latter case, the ascent rate is limited by the speed of sound in the multiphase mixture of magma, gas, and crystals (Kieffer, 1989).

MQ2c. How does the petrology and geochemistry of magma relate to the dynamics of transport?

The chemistry of magmas produced in subduction zones has a first-order control on the efficiency of magma transport through the mantle wedge, through the crust, and during/after eruptions. Rheologic parameters such as viscosity and density are directly controlled by evolving magma chemistry and crystallinity, which are in turn governed by pressure, p, temperature, T, and composition, X. Upon melting, the ambient p-T-X environment changes as magmas migrate. Fractional crystallization will change bulk magma chemistry by removing crystalline phases from an evolving liquid as constrained by experimental petrology and equilibrium thermodynamics (White, 2013). Less well constrained are the chemical reactions and reactive transport that will take place between a migrating magma – or any fluid phase – and surrounding mantle (Spiegelman and Keleman, 2003) or crust (Sparks et al., 2019). Although general reactive transport conservation equations can be developed (e.g., Keller and Suckale, 2019), such models still require empirical input from equations of state and constraints on reaction kinetics for fluids and crystals at mantle p-T conditions (e.g., Facq et al., 2014; Huang and Sverjensky, 2019) or for shallow crust (Watkins et al., 2017).

Within the crust, existing experimental petrology constrains melt fraction – temperature relationships (e.g., Wolf and Wylie, 1994, Ghiorso and Sack, 1995; Bohrson et al., 2014; Gualda and Ghiorso, 2014) and are beginning to be more widely integrated into models of magma transport (e.g., Dufek and Bergantz, 2005; Gualda et al., 2018). However, rates of reactive transport in complex mush systems containing three phases (melt, crystals, bubbles), remain a significant challenge for future work (Bachmann and Huber, 2018). Moreover, there is a significant gap between box-models for magma transport (e.g., Degruyter and Huber, 2014; Tramontano et al. 2017; Liao et al., 2018; Mittal and Richards 2019) and full multiphysics treatments (e.g., Dufek and Bachmann, 2010; Colón et al., 2018; Reuber et al., 2018a) in how to treat magma mixing and phase segregation evident in erupted compositions; this gap must be overcome to make more progress connecting the petrologic record with magma ascent physics.

Key roadblocks to iterative physical-chemical modeling of fluid transport in subduction zones include: 1) integrating the vastly different spatial scales on which these processes operate; 2) better knowledge of reaction rates and equations of state for systems not at steady-state; and 3) better understanding of the efficiency of reactive processes in different flow regimes (i.e., channelized vs. porous flow). Since the reactive potential of any fluid (or, conversely, of the material a fluid is moving through) is strongly controlled by the ratio of fluid to rock, which itself depends on whether fluid flow is channelized (high fluid-to-rock ratio) or porous (low fluid-to-rock ratio). Thus, prediction of chemical reactions is strongly coupled to thermo-mechanical models of multiphase flow in deformable media (e.g., Hewitt 2010; Keller and Katz 2016).

MQ3. How are fluid-related processes linked to the thermal-chemical-mechanical structure and dynamics of the subduction system?

Understanding the migration and distribution of fluids in subduction zones requires understanding fluid interactions with the surrounding solid, which can be highly nonlinear and strongly coupled. The workshop writing committee identified three questions that focus on the potential feedback between the fluids and the surrounding solid, which determine the overall thermal-chemical-mechanical architecture of subduction zones as well as smaller-scale fluid pathways in all subduction domains (**Figure 4**).

MQ3a. How do fluid-mediated chemical reactions affect fluid migration?

The migration of fluids and melts throughout the subduction system is a reactive transport process (Manning, 2004; Danies and Kohlstedt, 1994; Spiegelman et al., 2001; Pec et al., 2015). That is, the transport of a liquid phase relative to a surrounding rock matrix generates thermal, chemical, and mechanical disequilibria, which drive phase change and chemical equilibration reactions. In turn, chemical reactions can drive volumetric changes in the fluid, exchange latent to sensible heat, and alter phase compositions. Such feedbacks affect transport phenomena that govern fluid migration, and can be highly nonlinear.

A significant fraction of fluid migration in the deeper part of the subduction system (perhaps everywhere but the crust) is dominated by porous flow of a pore liquid through a permeable, deformable, granular rock matrix. At the microscopic scale, fluid production by dehydration of subducted lithosphere likely starts as isolated pockets of fluids that become channelized as fluid volume increases (von Bargen and Waff, 1986), likely influenced by chemical heterogeneities in the matrix (Plumper et al., 2017). Effects of chemical heterogeneity can play a role in mixing and phase segregation at larger scales as well (e.g., Manga, 2010).

The equations commonly used to express the problem of two phase fluid flow (McKenzie, 1984) combine shear and compaction deformation of the rock matrix with Darcy flow of the pore liquid. The latter is driven by pressure gradients in excess of hydrostatic conditions and is modulated by the Darcy segregation coefficient, commonly given as the ratio of the matrix permeability to the liquid viscosity. The matrix permeability measures how the topology and connectedness of the two-phase aggregate allows liquid films to connect along grain boundaries (von Bargen & Waff, 1986). The liquid viscosity is mainly a function of fluid temperature and composition, notably the content of silica and volatiles in melts (Audétat and Keppler, 2004; Giordano et al., 2008; Hack and Thompson, 2011).

At least three types of reactions are pertinent. First, mineral hydration/dehydration reactions are responsible for binding water into the crust and lithosphere of the oceanic plate and releasing it as the slab becomes exposed to higher pressure and temperatures (Schmidt and Poli, 1998; Hacker et al., 2003; van Keken et al., 2011; Schmidt and Poli, 2014). Dehydration can be accompanied by substantial volume changes that, if occurring in relatively cool and stiff rock, can potentially lead to reactively induced embrittlement and hydrofracturing (which are not described by the equations of McKenzie, 1984). It remains unclear how important this effect is in enhancing permeability within the slab. A highly permeable dehydration layer in the slab would allow fluids to migrate up-dip instead of into the mantle wedge (e.g., Wilson et al., 2014). The location and mechanical conditions of slab dehydration and the ensuing pathways of hydrous fluids through the slab and into the wedge are challenging to model as they require coupling thermodynamics to mechanical models including a ductile-to-brittle rheology.

Second, phase changes are intimately linked to the thermal and chemical structure of the subduction zone. For example, the focusing of mantle melts into the lower lithosphere and crust followed by their partial crystallization upon exposure to cooler wall rock can transport sufficient sensible and latent heat to heat the locus of melt focusing by hundreds of degrees above the thermal structure predicted by steady-state models that do not account of fluid migration (e.g., Dufek and Bergantz, 2005). Melting and crystallization can lead to significant changes in permeability, as well as melt viscosity. For example, the crystallization of mafic minerals in the lower crust will leave the residual melt enriched in silica, which may entail orders of magnitude increase in viscosity (e.g., Giordano et al., 2008). Fractional crystallization and crustal assimilation within crustal magma chambers transform low-viscosity ultramafic or basaltic magmas to evolved magmas (rhyolites) with viscosity increase of 10 orders of magnitude or more.

Thirdly, dissolution/precipitation reactions are important because of their strong potential for causing flow localization (Kelemen et al., 1995; Hesse et al., 2011; Liang et al., 2011). If a liquid phase percolates along gradients in pressure, temperature, or bulk chemistry, it will become disequilibrated by that transport. Depending on whether re-equilibration reactions dissolve or precipitate minerals, the resulting reaction-transport feedback will lead to channelized flow either by reactive infiltration instability or reactive chimney formation. Localized fluids that are produced by dehydration and melting reactions will, in combination with decompaction weakening by porosity waves, also lead to flow channelization (e.g. Skarbeck and Rempel, 2016; Räss et al., 2019). Chemical reactions of viscously deformable rock also have the potential to generate porosity waves even without compaction-driven fluid pressure (Omlin et al., 2017). Such a mechanism for upper crustal fluid flow (Chakraborty, 2017) may also be applicable to fluid migration in the mantle wedge. The localization of fluid migration in turn has profound implications for the chemical and thermal evolution of the affected domain. Identifying where and on what scale flow localization takes place presents challenges due to the inherent nonlinearity and multi-scale nature of the problem.

MQ3b. How does fluid migration affect the large-scale thermo-mechanical structure of the mantle wedge?

Deformation in both the brittle and ductile regimes affects fluid migration in subduction zones. In the megathrust region, feedbacks between brittle failure and pore fluid pressure may control the seismic behavior of the slab and forearc. These processes are evaluated under **MQ1**. In volcanic systems, brittle/ductile feedbacks help control whether magma ascends or stalls within the crust, as well as the style and volumes of volcanic eruptions. These processes are evaluated under **MQ2**. The focus here is on the interplay between ductile deformation and fluid migration associated with large depths and/or high temperatures. Fluid-driven reactions can lead to mineralogical changes as discussed in **MQ3a**, which modify the mechanical properties of the slab interface and mantle wedge and potentially lead to the formation of shear zones and melt transport networks (Katz et al., 2006; Jamtveit et al., 2009; Okamoto et al., 2017). Modeling the subducting slab and mantle wedge requires thermo-mechanical models that incorporate the interplay between deformation and fluid/melt migration.

Even considered independently, ductile deformation of the solid matrix and fluid transport involve significant outstanding complexities. For ductile deformation, varying forms of solid-state flow laws and ranges of rheological parameters indicate uncertainties in the rheological behavior of Earth's material (Karato and Wu, 1993; Hirth and Kohlstedt, 2004). For fluid migration, the reactions that can occur during transport of fluid through rock are complex and poorly constrained. Few experiments have been extended to *p*-*T*-*X* conditions relevant to subduction zones, and equations of state are not available for non-pure hydrothermal fluids. As a result, only a handful of thermo-mechanical models are available that combine ductile deformation processes with fluid migration (e.g., Alevizos et al., 2014; Poulet et al., 2014; Veveakis et al., 2014). A starting point may be models that consider chemical heterogeneity and reactivity and incorporate this into the rheology, in combination with deformation and petrology experiments.

The vast majority of current two-phase fluid migration models for the mantle wedge are two-dimensional and assume solid-state mantle wedge flow that is steady in time and independent of fluid migration (Cagnioncle et al., 2007; Wilson et al., 2014; Cerpa et al., 2017). While this is unrealistic, it is a reasonable approximation to be applied to subduction zones where the slab geometry is relatively simple and uniform along the margin and the subduction direction is (sub-)normal to the margin. In these models, the choice of mantle wedge rheology is critical to fluid migration as it controls not only the transport of pore fluids directly through fluid advection and its effect on compaction pressure, but also advective heat transfer that affects the thermal structure and thus the fluid sources from dehydration reactions and partial melting. The resulting fluid distribution affects the overall rheology of the mantle. Coupling the effects of mantle rheology and fluid distribution is also an important but challenging task in future fluid migration modeling for the mantle wedge.

Recent attempts to estimate the feedback between melt migration and solid thermal state suggest that melting and melt migration have first-order impacts on the mantle wedge thermal structure due to latent heat effects and heat advection by migrating melts (e.g., Rees Jones and Katz, 2018b). This may affect the mantle flow pattern due to the strongly temperature-dependent mantle viscosity. Moreover, melt-related weakening processes have been shown to soften the aggregate strength by several orders of magnitude (e.g., Holtzman et al., 2012) and over a range of timescales (Lau and Holtzman, 2019), further affecting mantle flow. This suggests that solid and liquid flows have to be computed simultaneously, not only to better understand the conditions controlling fluid migration but also to better understand heat transfer within the subduction system and observables such as surface heat flow across the volcanic arc.

MQ3c. How does the interface between two mechanically-distinct domains affect fluid migration?

Aqueous fluids are released from the downgoing dehydrating plate (Grove et al., 2012; Schmidt and Poli, 2014), and geochemical analyses of arc lavas indicate that some of the fluids migrate into the overriding mantle wedge to trigger flux melting. However, the pathways of the fluids across the slab/mantle wedge boundary remain poorly understood. How much of the slab-derived fluids migrate into the wedge? How does melt get focused from a broad region of fluid release and melting in the wedge to a surface expression confined to a relatively narrow region (less than 100 km wide for 80% of volcanic arcs; England and Katz 2010; Karlstrom et al., 2014)?

Recent models of aqueous fluid migration show that the solid mantle grain size distribution, as well as compaction-dilatation effects, are able to partly segregate aqueous fluids towards the volcanic arc area (Cerpa et al., 2017, 2018). However, the fluid pathways depend strongly on the amount of fluids introduced to the model and their location along the base of the mantle wedge. One critical factor that controls the flux of fluids into the wedge is the permeability contrasts between the slab and the mantle. Lower permeability of the mantle wedge would discourage fluid migration into the mantle wedge and promote updip migration within the subducting material below the base of the mantle wedge until the fluids reach the mantle wedge tip, where high porosities and permeabilities allow fluid flow into the overriding mantle (Wilson et al., 2014). To quantitatively predict fluid migration around and across the interface requires a better understanding of the evolution of the permeability structure of the subducting material as well as the overriding mantle.

Within the mantle wedge, the mantle in sub-solidus solid-dominated regions is likely to deform differently from that in regions with high melt fraction (e.g., Cagnioncle et al., 2007; Green et al., 2010; Till et al., 2012; Rees Jones et al., 2018a), but the evolving spatial and temporal scales of boundaries between mechanically distinct domains are not well known. Further, the pore fluid connectivity is dependent on pressure, temperature, and the composition of fluids (Mibe et al., 1999), potentially creating a spatial divide between regions of fluid transport by solid advection where there is no fluid connectivity and porous flow migration.

In two-phase flow models for the mantle wedge, the shallow part of the mantle wedge has high viscosity due to low temperature, representing the base of the overriding lithosphere. Without the effect of brittle/plastic deformation, the high viscosity region acts as a barrier to fluid flow (e.g., Wilson et al., 2014; Cerpa et al., 2017). In these models, depending on the morphology of the viscosity barrier, fluids may simply pond in reservoirs (as has been imaged at larger scale under large igneous provinces; Ridley and Richards 2010) or they may migrate along the base of the high-viscosity region driven by buoyancy and/or overpressure. At such low-temperature conditions, brittle deformation is likely to facilitate upward fluid migration through the lithosphere (e.g., Rubin 1995), and thus the fluid transport phenomena grade into those discussed in **MQ2**. A better understanding of the mechanisms of fluid migration at this rheological transition may be important for magma transport through the lithosphere. However, the majority of mantle fluid migration models currently end at the lithosphere and thus cannot address the feedbacks that likely control volcanic arc width perpendicular to strike and volcano spacing along strike.

4. Deliverables and Implementations

The Modeling Collaboratory for Subduction Zone Science (MCS) is envisioned to provide a research environment as well as a modeling framework consisting of numerical and data integration tools. Jointly, those can form the basis of integration and analysis of a number of subduction zones, and an international platform in which scientists can collaborate and learn how to use modeling resources that are related to fluid migration and earthquake and volcano systems in general. Its long-term aim is to construct and test physical models that will advance subduction zone science, including decadal-scale forecasting and other hazard applications in data-rich observatories. We proceed to highlight several resources that an MCS should provide, from the perspective of this workshop.

4.1. Modeling Framework, Model Validation, and Benchmarking

The goal of the MCS RCN is to develop a plan for an integrative modeling framework for earthquake and volcano systems. This will not take the form of one grand model that would simulate every identified process. Instead, the MCS will aim for a modular framework (such as envisioned in **Figure 4**) in which different models can be linked in a consistent manner (e.g., resolution/accuracy), for example, in a nested hierarchical structure. Moreover, individual code building blocks should be reusable and stand on their own, such that an efficient fluid-solid solver might, for example, be used in an assembled fashion to explore regional tectonics given structural and dynamic constraints for a specific subduction zone, as well as on its own to test fundamental physical feedbacks for idealized problems. The MCS could provide a resource through which code developers can communicate efficiently and effectively with other code developers and end-users for collaboration (e.g., via an online community forum).

The majority of current models for fluid migration in subduction zones require the solution of continuum mechanics conservation laws expressed as partial differential equations, with micromechanical parameterizations of un-modeled processes and constitutive behavior (that may be separate continuum or discrete element models; e.g., Carrara et al., 2019). Unfortunately, though governing equations employed in a given model may provide an appropriate description of a particular aspect of fluid migration, the approximate solution through numerical simulation may fail to be useful in other contexts due to unmodeled physics, unrealistic parameter values, or numerical errors and instability. For example, the McKenzie (1984) equations for multiphase, multicomponent fluid flow are a widely utilized framework for exploring fluid migration in the mantle but cannot describe the full range of fluid and solid mechanics relevant to magma transport from mantle source to surface. It is likely that parameterizations and scaling laws, developed to simplify the governing equations (e.g., Reuber et al., 2018b; Keller and Suckale, 2019), will continue to play an important role in developing holistic models for lithospheric scale magma transport. The collaboratory could seek to synthesize sets of observables that can be used to test model predictions and test coarse-graining approaches.

As modelers converge toward agreement on basic governing equations and implementations by multiple groups, the MCS should take on the task of developing benchmarking exercises that ensure a standard of accuracy for numerical approximation to solutions of the underlying differential equations. For certain specific problems relevant to the MCS such benchmarks have already been proposed, for example steady-state corner flow (van Keken et al., 2008). However, we are not aware of similar benchmarking efforts for two (or more) phase flow codes required for fluid migration modeling. Current efforts in the earthquake community to benchmark dynamic rupture and earthquake cycle codes (Harris et al., 2009; Erickson et al., submitted), or the lava flow community (Cordonnier et al., 2016), provide examples that could be followed for other fluid migration problems.

4.2. Community Building and Cross-Disciplinary Training

An important function of the MCS should be community building: Long-lasting (longer than a Ph.D. cycle) buy-in from students and experts alike, as well as technical support from non-domain scientists funded by the program, is critical to the success of the MCS. One way to encourage participation is to hold regular, topically focused workshops with broad attendance, where modelers, observationalists, experimentalists, and experts from adjacent academic disciplines and industry can interact. These workshops should aim to address specific questions and should be smaller in attendance but likely longer in duration than the Workshop at UMN.

One way to organize such workshops could be to take a modular approach to fluid migration modeling in subduction zones, focusing on particular domains of fluid migration (**Figure 4** and **Section 3**) by identifying outstanding questions that require expertise from adjacent domains. For example, bringing together researchers from industry (such as ore-forming systems or hydraulic fracturing) with shallow magma transport modelers could facilitate new approaches to longstanding challenges such as dike propagation or poro-visco-elastic and thermal evolution of magma reservoirs and mushes. Likewise, bringing together mantle wedge fluid migration modelers who work on subduction zones at a geodynamic scale (large distances, long time) with modelers interested in earthquake cycles and fault rupture processes could motivate better initial and boundary conditions for earthquake models in megathrust systems.

Training workshops and webinars are also critical for the community, from students to senior scientists. The focus of such workshops might differ depending on the intended audience. For example, tutorials about existing codes or modeling approaches could deepen the quantitative toolbox of observationalists with well-tested resources. In contrast, hackathon-type or benchmarking workshops would be better suited for those actively developing codes. Community buy-in is needed at both ends of this spectrum, and there is precedent that can help guide workshop development. Participants of the Workshop particularly recognized the CIDER program and ASPECT hackathons as successful examples.

Best practices for software and workflow development should be followed, including a minimum standard for the documentation and benchmarking of all MCS tools and modeling codes. Through collaboration, the details of how two given models should be coupled (e.g., 1-way or 2-way coupling, chemical coupling) must be determined by the developers. We can benefit from lessons learned from multidisciplinary efforts such as CSDMS and CIG, e.g. as discussed by Behn et al. (2018).

The MCS can also provide support for individual PIs and the community at large to access and utilize state-of-the-art computing technologies (e.g., massively parallel CPU and GPU clusters) and workflows, possibly in collaboration with supercomputer centers at universities (e.g., TACC at the University of Texas at Austin) and government agencies (e.g., National Labs, DOE, NASA). Unifying the coding platform (e.g., C++, Python) will make code sharing more efficient. Some objectives of the MCS are complementary to those of Computational Infrastructure for Geodynamics (CIG), but the collaboratory will likely differ from CIG in that it will focus on linking different domains, processes, or models to address a set of motivating questions more so than developing and maintaining codes for specific processes. Any software and workflow development will be geared toward solving problems in subduction zone science, and assisting in the process of linking different codes and incorporating static or real-time observations into models.

The collaboratory could gradually build an online directory that identifies active research groups and their main activities. Lecture material from workshops and perhaps a compilation of currently available models/codes and their attributes (such as temporal and spatial scales, inputs and outputs, resolution, computational needs, governing equations, etc.) could also be provided. Similar to CIDER, these resources, located in a central location that implicitly has community backing, could help students and professionals alike find up-to-date resources.

Whatever the end products of the MCS are, organizing and maintaining resources – including publicity – require IT support, and perhaps software engineers tied to a modeling collaboratory endeavor. Salary for technical staff and a plan for sustaining resources past typical funding timelines should be included from the beginning. Workshop participants suggested seeking the additional expertise of a social scientist who specializes in organizational science and facilitation of effective communication, given the inherent challenges of working and developing codes among scientists from various sub-disciplines. The MCS should seek to promote an inclusive and respectful community where career stage, gender, race, sexual orientation, or disability status never pose a barrier to full participation.

4.3. Relation to SZ4D RCN and CONVERSE RCN

Following the SZ4D initiative 2017 and vision document (McGuire and Plank et al., 2017), three aligned RCN programs were funded by NSF: The MCS RCN (whose first meeting is described here); the SZ4D Umbrella RCN; and the Community Network for Volcanic Eruption Response (CONVERSE) RCN. The SZ4D Umbrella RCN is focused on the development of observatories and coordinating the collection and integration of scientific measurements in subduction zones, and is driven by fundamental scientific questions but with a strong emphasis on hazard mitigation. The CONVERSE RCN is focused on improving our ability to detect volcanic activities and respond to volcanic eruptions – it also emphasizes hazard mitigation – and its objectives drive basic scientific research on volcanic systems. The USGS report on subduction zone hazard and science (Gomberg and Ludwig, 2017) and the ERUPT report on volcanic systems (National Academies, 2017) have also been important drivers of community organization and action for the three RCNs. During the Workshop, the relationship between these three RCNs was discussed, focusing largely on the complementary nature of their goals and the need for continued coordination.

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Appendix: Workshop Schedule

Day 0 (Wednesday, May 30)

14:30	Workshop begins	Opening remarks by ECS chairs Tianhaozhe Sun and Kayla Iacovino
14:50	**Presentation 1**	*Joyce Sim*
15:15	**Presentation 2**	*Changyeol Lee*
15:40	**Presentation 3**	*Tushar Mittal*
16:00	**Breakout session**	Instructions by Sun and Iacovino
17:10 – 17:30	Discussion with all participants	Representative from each group of 8 presents key points discussed. Remaining time opened to the room for discussion.

Day 1 (Thursday, May 30)

7:40	*Breakfast*	
8:20 8:35 8:50 8:55 9:55	**MCS RCN overview** Workshop overview and Day 1 schedule **Theme 1** overview Presentation 1a Presentation 1b Presentation 1c Discussion	Lotto Wada and Karlstrom Simon and Trehu *Taras Gerya* *Rachel Lauer* *Johannes Vrijmoed*
10:20	*Morning Break*	
10:50 10:55	**Theme 2** overview Presentation 2a Presentation 2b	Caricchi and Haney *Richard Katz* *Janine Kavanagh*

 11:55	Presentation 2c Discussion	*Tobias Keller*
12:20	*Lunch*	
13:20 13:30	Breakout #1 Instructions **Breakout #1**	Simon, Trehu, Caricchi and Haney Breakout #1 leaders
15:00	*Afternoon break*	
15:30 16:00 16:10 16:25 16:40	Other RCN overviews Discussion ECS group discussion summary Discussion Lightning talks	SZ4D RCN and CONVERSE 1-minute talks by poster presenters
17:00	**Poster reception**	
19:00	*Break for dinner*	

Day 2 (Friday, May 31)

7:40	*Breakfast*	
8:20 8:30 9:00 9:15 9:20 10:00	Summary of Day 1 and Day 2 schedule Breakout 1 Summaries Discussion **Theme 3** overview Presentation 3a Presentation 3b Discussion	Wada and Karlstrom Breakout #1 leaders (10 min/group) Fulton and Warren *Pengcheng Fu* *Viktoriya Yarushina*
10:25	*Morning Break*	
11:00 11:10	Breakout #2 Instructions **Breakout #2**	Fulton and Warren Breakout #2 leaders
12:30	*Lunch*	
13:35 13:40	**Theme 4** overview Presentation 4a Presentation 4b Presentation 4c	Lithgow-Bertelloni and Montesi *Eric Sonnenthal* *Diane Arcay* *Cian Wilson*

14:40	Discussion	
15:05	*Afternoon break*	
15:35 15:40	Breakout #3 Instructions **Breakout #3**	Lithgow-Bertelloni and Montesi Breakout #3 leaders
17:00	*Break for dinner*	

Day 3 (Saturday, June 1)

7:40	*Breakfast*	
8:20 8:30 9:00 9:15 9:45	Summary of Day 2 and Day 3 schedule Breakout #2 Summaries Discussion Breakout #3 Summaries Discussion	Wada and Karlstrom Breakout #2 leaders (10 min/group) Breakout #3 leaders (10 min/group)
10:00	*Morning Break*	
10:30 11:30 **12:00**	**Synthesis Discussion** Concluding remarks and unfinished business ***End of workshop***	Wada and Karlstrom *** Regular participants start leaving
13:00 - 16:00	*Planning of workshop report writing*	*Writing committee only*