Modeling Volcano-Magmatic Systems: Crustal Magma Transport, Storage and Eruption

Workshop Report - Modeling Collaboratory for Subduction RCN

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This draft report is a community document and work in progress. Comments and input are welcome and can be provided through mid-June 2021 in two ways:

1.) By providing comments through an online form: https://docs.google.com/forms/d/e/1FAIpQLSdxx8XIZ8kXrLZyo-KKBRmI0Q5EbkuPhkuMEIdEi6Zk3wwniw/viewform
2.) By providing comments or suggestions on a Google Docs version of this report. To obtain access, please contact Helge Gonnermann (helge@rice.edu) or Kyle Anderson (kranderson@usgs.gov)

Summary

This document summarizes the outcomes of the Modeling Collaboratory for Subduction Zone Science (MCS) Volcanic Systems Workshop and presents a vision for advancing collaborative modeling of volcano-magmatic systems within a Modelling Collaboratory for Subduction (MCS).

Modeling volcanic systems is challenging due to the diversity of physical processes, limited available observations, and wide range of spatiotemporal scales involved. Models range from very simple approximations to highly sophisticated systems of coupled nonlinear differential equations, the solution of which falls at the limits of the state of the art in numerical modeling. These challenges, coupled with the small size of the volcanological community, require that models be developed and utilized as effectively and efficiently as possible.

Although models have importantly advanced the field of volcanology, progress is to some extent limited by several factors. First, there is insufficient direct support for model development as a first-order scientific outcome. Secondly, model codes are now in many cases just as important -- if not more important -- than the publications on which they are based, but better support is needed to build upon initial model development through model enhancement, integration with other models, documentation, and user training. As a consequence, the current modeling landscape is fragmented and consists of models that are generally not interoperable, are rarely used outside of small research groups, may be independently duplicated (re-invented), and are typically inadequately verified, validated, benchmarked, and documented. Overcoming these

limitations requires enhanced and dedicated support, and will result in new opportunities and collaborations for advancing volcano-magmatic systems science -- ultimately accelerating scientific progress in ways not currently possible.

A key outcome of the workshop is a recognition of the transformative potential of diverse groups of scientists, working together on common problems, to advance the science of volcanology through models that allow the integration and interpretation of observations within a framework that is rooted in the physics and chemistry of volcano-magmatic systems and processes. Such collaborative environment would be centered about community working groups -- consisting broadly of focus groups organized around workshops, summer schools, and long-term collaborative research efforts -- and will enable and support new collaboration between scientists studying different aspects of volcano-magmatic systems, between modelers and non-modelers, and between volcanologists and outside experts from fields such as mathematics and statistics. These community working groups can provide the foundation from which model development and ensuing integrative and collaborative modeling-centric science will ensue. Working groups would focus on the study of volcano-magmatic systems or subsystems and could be geologically based (e.g., magma storage, magma supply, or with a focus on a particular volcanic system), process based (e.g., reactive transport, multiphase flow), or organized around another aspect of volcano system modeling (e.g., model benchmarking, data assimilation). Working group activities, including workshops and associated model development, require coordinated funding to enable collaborative work over time periods longer than the usual 2-3 year grant cycle, providing an umbrella organization and synergistic network that will leverage and enhance, but not supplant, projects that are based on funding at the PI level.

The formation of community working groups is the next logical step for --- or on the way toward --- an MCS. Each focus group would hold a series of workshops that lead to one or multiple collaborative proposals for a funded community working group. These groups would support model development (inclusive of benchmarking, documentation, interoperability, etc.), training, and other activities, culminating generally in model implementation and use through discovery or hypothesis driven collaborative science. Thus, aside from providing an umbrella organization to facilitate collaborative community working groups, an MCS would provide support and expertise for model integration, interoperability, benchmarking, documentation, user workshops, and so forth.

Support for this vision, and ultimately an MCS, would not only encompass working groups and workshops themselves, but also provide programmatic support for model development in the form of student and postdoc funding; incentives for cross-disciplinary collaboration with computational experts that may be MCS staff and/or PIs/students/postdocs from other disciplines such as for example computer science, applied mathematics, or data science; and lastly support for the model-based collaborative science projects.

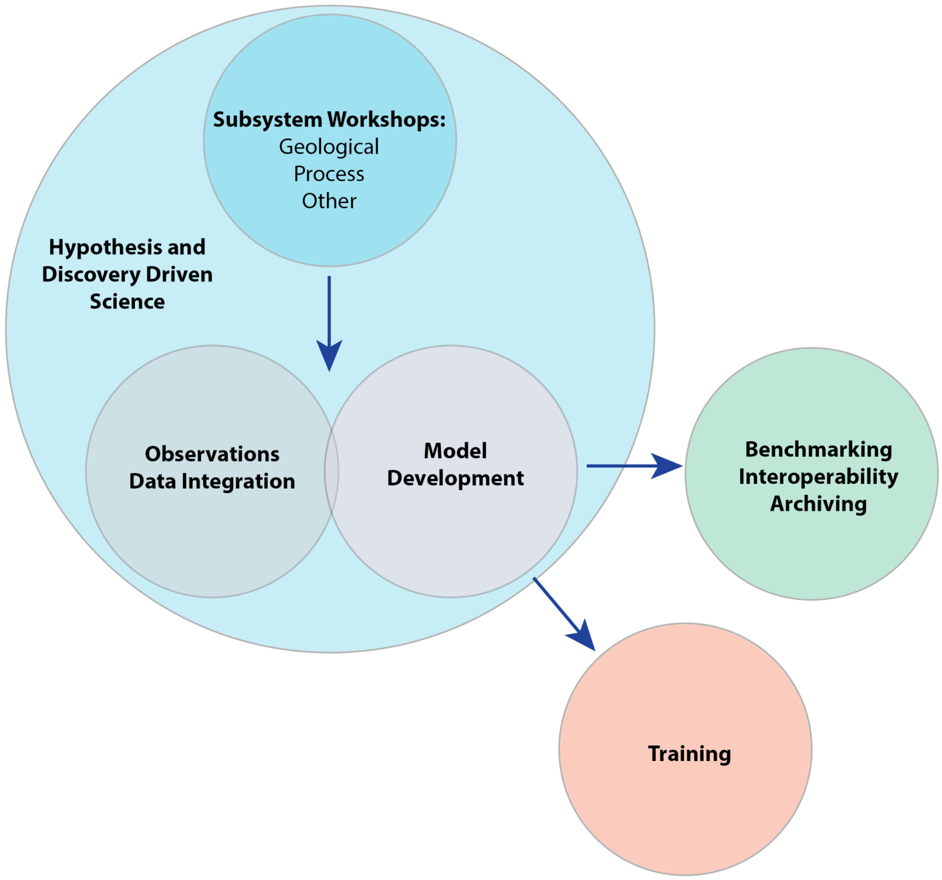

Figure 1: Subsystem focus group workshops and ensuing MCS activities. *(This figure is a placeholder until someone comes up with something better. Contact Helge for an editable version of this figure.)*

1. Introduction

1.1 Purpose

This document summarizes the outcomes of the Modeling Collaboratory for Subduction Zone Science (MCS) Volcanic Systems Workshop and presents a vision for a magmatic and volcanic systems component of a future MCS. The report encompasses two parts: (1) potential science objectives for volcanic systems science; and (2) a potential vision for how a modeling collaboratory would best advance the science objectives.

1.2 Scope and objectives of a volcano modeling collaboratory

A modeling collaboratory can facilitate the integration of community-wide science and development of science capabilities, identify and overcome barriers to interdisciplinary science, and serve the development of human resources through workshops and training, as well as outreach coordination. There is broad agreement on the need for improved organization and coordination within the volcano-magmatic systems science community, also highlighted as a major goal in the NAS ERUPT report (2017). A main motivation for the MCS Volcanic Systems Workshop has been to advance toward that goal with concrete recommendations for a future modeling collaboratory aimed at advancing our understanding of volcano-magmatic systems and ensuing hazards within subduction zones and beyond.

Crustal magmatic processes, and the initiation of eruptions at arc volcanoes, are both central and overarching parts of the SZ4D framework. Mantle-derived melts, modulated by the crustal magma system, ultimately drive volcanic activity and associated hazards. Crustal-scale magma transport and storage operate at a wide range of spatial and temporal scales through processes that ultimately drive the system toward an *eruption threshold*, which can either be crossed solely as a consequence of internal dynamics or by external forces, such as tectonic earthquakes.

This document focuses on volcano-magmatic systems within subduction zones, where the majority of active subaerial volcanism occurs. However, the volcanology community is small and volcanoes share commonalities that transcend geological settings. **Thus, while recognizing a subduction zone focus, a modeling collaboratory must also allow room for work on volcanoes in other tectonic settings.** Furthermore, a collaboratory should include both magmatic and volcanic processes, as well as linkages between them, especially insofar as they have ramification for volcanic hazards. Consideration must also be given to linkages between magmatic processes, fluid migration in subduction zones, as well as geodynamic and seismo-tectonic aspects.

1.3 Relation to other MCS activities

The supply of magma and volatiles from the mantle to the crust provides the mass and energy input to the crustal magma system. It thus constitutes the link to the deeper subduction-zone fluid transport system, which was the subject of the MCS ***Fluids Transport Workshop*** held in 2019 (Wada et al., 2109). The crustal response to these deep inputs manifests in the evolution of thermal, rheological and stress states, all of which are inherently intertwined through mechanical and dynamical feedback with magma transport and storage.

2. Workshop organization, participation and activities

The MCS Volcanic Systems Workshop was organized into four themes based on volcano-magmatic subsystems, plus a final theme focused on data integration and forecasting.

- ***Crustal-scale magma transport***

- ***Magma storage***
- ***Eruptive magma ascent***
- ***Eruption plumes***
- ***Integrative Volcano Modeling and Forecasting***

These subdivisions reflect to some extent the range in spatial and temporal scales that must be considered; however, processes under each theme itself act on a wide range of spatiotemporal scales. For example, eruptions typically have durations of days to months with recurrence times of years to centuries or millennia. The lifespan of individual volcanic edifices is of the order of 1 million years, whereas the underlying plutonic/transcrustal system may persist and evolve for 10s of millions of years.

The emerging view is that crustal scale magma transport and storage is spatially interconnected, albeit perhaps temporally episodic, across a vertically and laterally complex storage/transport system consisting of multiple magma bodies at different states of existence. Although volcanic activity is ultimately staged from shallow subvolcanic reservoirs, it may be the consequence of (upward/downward/laterally) cascading instabilities or events within the entire transcrustal system. Alternatively, it may be due to the exceedance of certain threshold conditions within the shallow subvolcanic system, or due to external triggers. Thus eruption precursors that are directly or indirectly observable at the surface may be sought within the deeper realms of the transcrustal system or within its shallow subvolcanic parts, with the latter in general observationally more accessible. These considerations were encompassed by the ***Crustal-Scale Magma Transport*** and the ***Magma Storage*** themes of this workshop.

Ultimately our interests are in large part motivated by advancing the understanding of episodes of unrest at volcanic systems and improving our abilities to assess hazards as well as the advancing toward potential forecasting of the onset of eruptive activity, style, vigor, and duration. These were the subjects of the ***Eruptive Magma Ascent***, the ***Eruption Plume***, and the ***Integrative Volcano Modeling and Forecasting*** workshop themes, including potential linkages with the ***Community Network for Volcanic Eruption Response (CONVERSE) RCN*** (https://volcanoresponse.org/).

2.1 Workshop implementation

The volcanic systems workshop was originally envisioned and planned as an in-person workshop to be held in Portland, Oregon during the summer of 2020. The COVID-19 pandemic required a transition to a virtual format consisting of a series of webinars and planning meetings, which ultimately took place from September 2020 through May 2021. Each of the five workshop themes consisted of four invited presentations spread over two webinars held on a Tuesday and Thursday of one week. The Tuesday webinars were held in conjunction with the International Volcanology Seminar Series organized through the University of Oregon and the Smithsonian Institution. Presentations spanned a range from science-focused topics to overviews of various magmatic/volcanic systems models and modeling. All webinars were recorded and made available for participants and the general public through the workshop website (https://www.sz4dmcs.org/volcano-workshop).

Crustal-scale magma transport (26, 28, 29 January, 2021)

- Thomas Sisson (US Geological Survey): An introduction to the crustal structure and dynamics of arc magmatic systems with current issues amenable for modeling.
- George Bergantz (University of Washington): Making Sense of Mush: The Geology, Physics and Chemistry of Magmatic Systems.
- Matthew Pritchard (Cornell University): *Advancing geophysical models of crustal scale magma transport: Comparing techniques, volcanoes, and inversion strategies*.
- Matthew Jackson (Imperial College of London): *Melt fraction change and magma differentiation in crustal mush reservoirs: Insights from mathematical and numerical models*.

Magma storage (23, 25, 26 February, 2021)

- Philipp Ruprecht (University of Nevada, Reno): *We ask, the crystal answers: Constraining magma storage systems from the crystal record*.
- Mark Ghiorso (OFM Research): *Modeling magma storage: A data science perspective*.
- Emilie Hooft (University of Oregon): *Magma storage from a geophysical perspective*.
- Christian Huber (Brown University): *Modeling magmatic processes… which model is appropriate for what?*

Eruptive magma ascent (23, 25, 26 March, 2021)

- Eleonora Rivalta (Geoforschungszentrum Potsdam, Germany): *Mechanical models of magma transport by diking: Coupling host rock and magma rheology*.
- Diana Roman (Carnegie Institution of Science): *A seismological perspective on magma ascent*.
- Mattia de' Michieli Vitturi (University at Buffalo): *Numerical modeling of magma ascent in volcanic conduits: equilibrium and disequilibrium*.
- Madison Myers (Montana State University): *Rates of Magma Ascent: A Petrological Perspective*.

Eruption plumes (15, 17 September, 2020)

- Josef Dufek (University of Oregon): *The fluid dynamics of volcanic plumes*
- Antonio Costa (Istituto Nazionale di Geofisica e Vulcanologia, Bologna, Italy): *Overview of various approaches of volcanic plume modeling.*
- Costanza Bonadonna (University of Geneva, Switzerland): *Determination of eruption source parameters for modeling of volcanic ash transport and deposition.*
- Larry Mastin (US Geological Survey): *Operational aspects of dispersal modeling.*

Integrative volcano modeling and forecasting (4, 6, 7 May, 2021)

- Hélène Le Mével (Carnegie Institution of Science): *Modeling volcano deformation*
- Mary Grace Bato (Jet Propulsion Laboratory, California Institute of Technology): *Towards better model-data fusion frameworks: [Sequential] Data assimilation for Volcano Applications*

- Michael Poland (US Geological Survey): *The role of a Modelling Collaboratory in forecasting volcanic eruptions and impacts*
- Paul Segall (Stanford University): *Thoughts on the power of a volcano modeling collaboratory*

2.2 Soliciting community input

A major concern was to achieve broad community participation and to provide ample opportunity for the magmatic/volcanic systems community at large to contribute to the MCS vision and this report. For this purpose we held four separate Planning Meetings, each following the Tuesday and Thursday webinars on the subsequent Friday. The planning meeting consisted of discussions and breakout sessions aimed at defining a vision for a future MCS upon which this report is based.

Furthermore, starting in February 2021, we periodically made draft versions of this report available on the workshop webpage, together with a Google Form through which anyone was able to ask questions or provide feedback. The organizers also provided direct access to the editable, online workshop draft for those interested in contributing more extensively to the report. The primary contributors of this report are listed on the title page of this report.

2.3 Workshop participation

The MCS RCN Volcanic Systems Modeling Workshop convened virtually via Zoom from Sep. 2020 – May 2021. The workshop was hosted by Helge Gonnermann (Rice Univ.) and Kyle Anderson (USGS), with support from Arianne Snyder, Gabriel Lotto, and Thorsten Becker (UT Austin). It was attended remotely by 760 people representing 44 countries, from across North America, South America, Europe, Africa, Asia, and the Pacific.

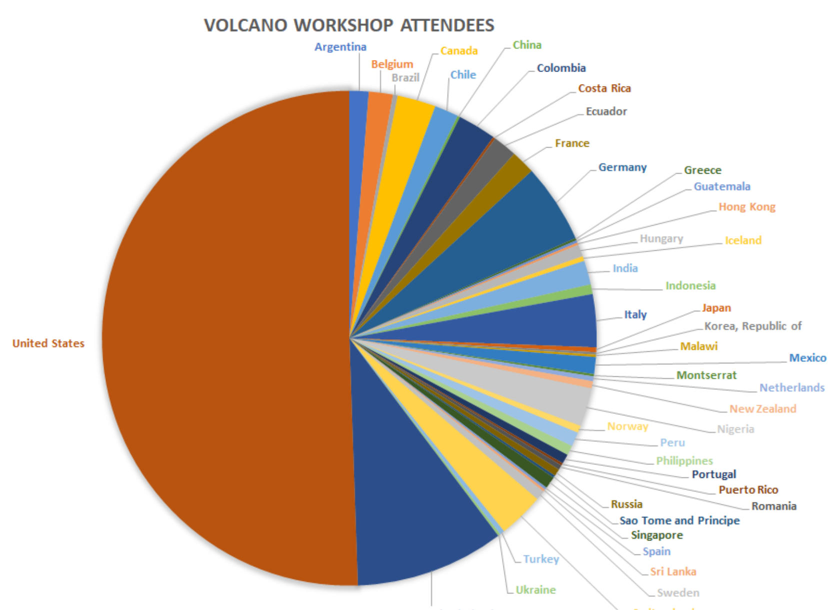

Figure 2: Participation in MCS volcano systems workshops.

3. The scientific challenges

To achieve the decadal scientific objectives outlined through ongoing SZ4D activities and in the ERUPT report (National Academies of Sciences, Engineering, and Medicine, 2017) requires ***numerical models that can provide the broader integration of observations, leading to advanced syntheses and understanding.*** Segall and Anderson (2016) have pointed out that a critical limitation of discipline-specific models is that they can only utilize a small subset of available observations. In other words, a broad range of forward and inverse modeling strategies is applied to study magmatic systems and their application depends on the science objective as well as the type of data it connects to. The main goal of an MCS will be enhancing interoperability, integration and collaboration within the volcano-magmatic modeling universe.

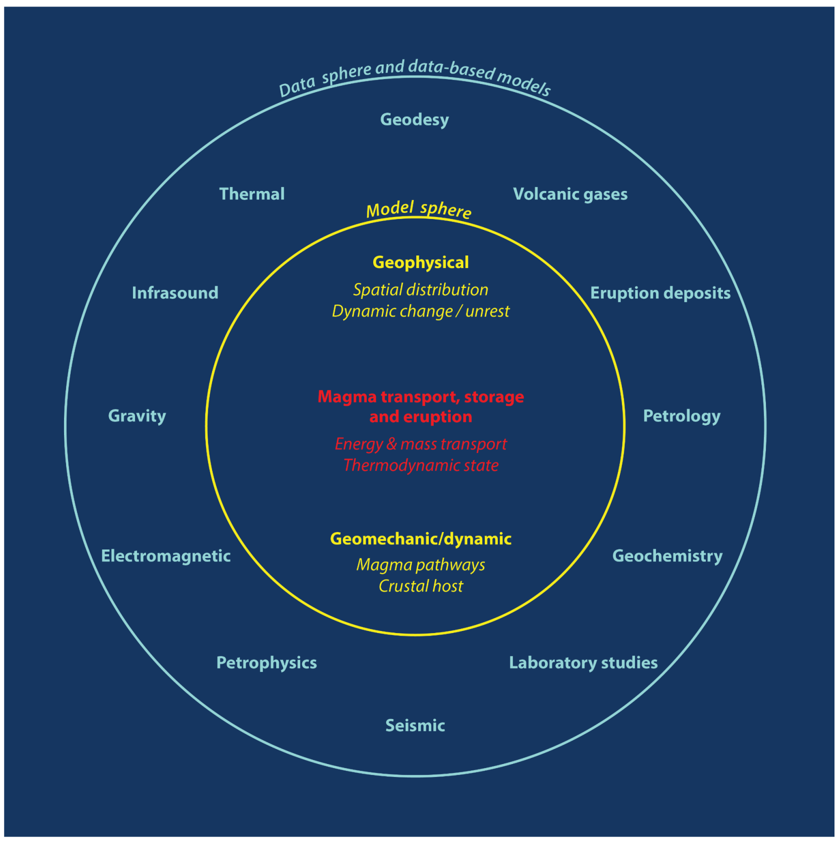

Figure 2: Observational and modeling spaces encompassed by a modeling collaboratory for volcano-magmatic systems, with a focus on magma transport, storage and eruption.

Throughout the workshop, discussions frequently centered on geological subsystems where there exists a multitude of unsolved questions and challenges. At the same time discussions invariably evolved toward issues that transcend individual subsystems, largely motivated by the recognition that an interpretation of observations requires the integration across subsystem boundaries, which can be facilitated by collaborative modeling. In the following, key geological subsystems and associated processes are considered in conjunction with the associated model requirements, including forward models of magma transport, storage and eruption. We also include in our discussion the use of models together with data for parameter estimation (inverse analysis) and forecasting. This is, however, not meant to be a comprehensive review, and the exclusion of a particular topic is not meant to preclude its inclusion in an MCS.

Volcano-magmatic models range over a tremendous range of spatial and temporal scales, encompassing an equally broad range of physical and chemical processes. They are often process-oriented and encompass reactive mass and energy transport of/within materials ranging from plastic/viscoelastic/brittle rocks and glasses, silica melt with suspended crystals and gaseous bubbles, partially solidified magmas known as crystal/magma mushes, supercritical fluids, and dusty gases. Magmas originate as partial melts in the mantle with transport dominated by reactive porous-media flow. As magma rises into crustal reservoirs it differentiate via fractional crystallization, assimilation, and mixing, and melt transport may become increasingly localized. Throughout protracted crustal magma transport and storage, magmas are thought to exist in crystal-rich mushes, likely together with a mobile exsolved volatile phase. The nature and geometry of this crustal magma transport and storage system remains in many aspects poorly understood, despite recent advances in geophysical and petrological methods (e.g. workshop presentations by E. Hooft; M. Pritchard; and T. Sisson).

A unifying theme among models of magma transport, storage and eruption is reactive transport and the multiphase nature of the natural system. When juxtaposed against the wide range of spatial and temporal scales at which observations inform the study of magmatic systems and over which scientific inquiries are focused, this inherently requires a wide variety of modeling approaches, ranging from the molecular scale (e.g., bubble/crystal nucleation, crystal growth), to the granular scale (where individual crystals or bubbles within a multiphase assemblage are resolved; e.g. workshop presentations by M. Myers, and P. Ruprecht), to the continuum scale capable of simulating processes at kilometer or greater spatial scales and over time scales of individual eruptions or longer. Upscaling, downscaling, and synergistic interconnectivity of such models is therefore of great importance.

The multi-phase nature of subsurface magma transport and storage systems constitutes one of the primary challenges for model development, particularly in terms of overall complexity, but also in terms of the range of spatial scales (e.g. workshop presentations by G. Bergantz and M. Jackson). There are tremendous challenges related to understanding and modeling spatially complex magma systems (including dikes, conduits, and reservoirs) and their interaction with the surrounding rock host rock (e.g. workshop presentations by E. Rivalta and H. Le Mével). An additional challenge is the immense range of temporal scales that come into play, from subseconds (rock fracture, or bubble nucleation), to millions of years (longevity of individual volcanic systems), to tens or hundreds of millions of years (subduction-zone and plate-tectonic evolution). There is no *'one size fits all'* solution, and these challenges require a diverse ecosystem of models that draw heavily from expertise in disciplines within engineering and physical sciences beyond geosciences, as well as applied mathematics and computer sciences.

The word "model" will have different meanings to different readers. The main categories of models discussed herein include process- or physics-based models (the primary focus of Sections 3.1, 3.2, 3.4, 3.5); inverse models in the broadest sense (the primary focus of Section 3.3); thermodynamic, kinetic and constitutive models (Section 3.7); and models of data assimilation and forecasting (Section 3.8). We apologize in advance for any potential omissions, they should not be interpreted to imply exclusion from an MCS.

3.1 Crustal magma transport processes and problems

A key question that links the volcano-magmatic system to fluid/melt production and transport in the asthenosphere is how large-scale subduction parameters control magma production and delivery within the crust. This requires consideration of the linkage between energy and mass input to subduction variables, such as slab dip, convergence angle and rate, and slab properties (slab age, hydration, sediment thickness etc.), mantle temperature, and regional mantle convection patterns. A large degree of fractional crystallization is required to take mantle-derived melts into the compositional field of bulk continental crust (half the mass has to be removed to produce common andesites and dacites) and probably requires *'delamination'*. How that happens is another outstanding problem that ties crustal scale magma transport at the geodynamic scale to the subduction zone system. Furthermore, to what extent and how mantle-supplied magmatic input rates control magma storage depths, crustal residence times, and erupted magma composition remains an open question.

Within the crustal magmatic system a major challenge is the development of models in which primitive magmas naturally stall in the deep crust and mature into observed arc sections. Most models are highly idealized in terms of the geometry of magma transport and storage. They are thus still far from addressing the question of how magma pathways form and evolve. For example, what is the aperture of the crustal magmatic feeding system and how does it evolve? To what extent is it possible to link crustal chemical evolution with crustal stress? What is its vertical continuity and what are the temperatures in the deep crust? Where does magma stall forming reservoirs and what is the overall magmatic flux? Related is the question whether deep seismic events are actually sites of magma supply. For example, quiet zones directly beneath volcanoes are thought to represent the hot and plastic magmatic system, with the seismogenic halo interpreted to represent cooler and brittle crust wherein seismic signals may be due to fluid egress. By and large there is a lack of observational constraints to go beyond simplified models and, for example, going to higher dimensions remains challenging from a modeling perspective. Field relations of exposed sections suggest deep that storage regions are dominated by vertical mass transport, whereas conceptual models commonly highlight sill-like emplacement. Can models predict evolution toward real-looking arc sections with steep-sided tabular intermediate plutions in the upper and mid-crust, and primitive cumulates deep and mostly gone?

In terms of temporal scales, magmatic systems are long-lived and relatively immobile. Volcanic growth is defined by major stages occurring at 10,000-100,000 years, whereas single edifices have average life spans of 0.5-1 my, and ancestral and successor volcanoes 1-2 my. At the same time, compositional excursions are typically brief in andesitic stratovolcanoes (~100 y), consistent with *small* active volumes. In contrast, volcanic centers that persist for 5-10 my and usually evolve toward substantial volumes of rhyodacite-rhyolite, consistent with arc intrusive suites. A key question is why such systems evolve toward felsic compositions and hence lower temperatures, and why lower temperature felsic magmas and eruptions are more voluminous. A related question is how much eruptible magma exists in a given volcanic system as a function of time, where it is located, and what variables control this. Progress on questions like these is contingent upon adequate representation of the complex multiphase rock-melt-crystal-volatile assemblage. The recognition that active magmatic systems are vertically extensive and may to a large extent consist of crystal-rich magma mushes (REFERENCE) imposes a significant challenge to the modeling community. Given such observations, what modeling approach is appropriate for melt extraction and migration at many scales, patterns, and over a wide range of rheological complexity? For example, to resolve grain scale processes recorded in the crystal record within models of magma transport and storage at relevant scales requires upscaling and coupling between different models, something that is still in its infancy and at the vanguard of volcano-magmatic modeling. Simplified box models for crustal deformation, chemical evolution, and multiphase transport may be the best initial approach for some of the problems outlined above. They can be conducive to up- and down-scaling, as well as integration of diverse data from geophysics, petrology, and geochronology. They could be viewed as fundamental system-scale models and a basis for integration of more sophisticated subsystem models developed by individual PIs, with an MCS facilitating support for model integration and interoperability.

3.2 Magma storage processes and problems

Magmas are stored in the crust feeding volcanic eruptions, supplying energy to hydrothermal systems, and evolving toward moribund plutons. The *'storage container'* remains a central and useful concept when developing the process-based models for crustal evolution and volcanic eruptions. A related but separate issue are the roles of heat flow and crustal rheology, with important implications for the evolution of magma reservoirs and for magma eruptibility. The basis for improved model development of magma storage are high fidelity records that constrain magma storage conditions (pressure, temperature, composition) within the “container” in space and time. Petrologic studies provide those constraints through phase equilibria experiments, petrography, thermodynamic-based geothermobarometry and detailed mineral-chemistry studies of the crystal cargo. These techniques reveal insight on the internal state of the magma system, whether it is mush- or melt-dominated and regardless of whether it is primarily controlled by open- or closed-system processes.

Magma storage systems operate over hundreds of thousands to millions of years, as recorded in radiometric ages from accessory phases. However, it remains a major question, if these systems experience cycles of rejuvenation with fundamental changes to their mechanical and dynamic response and on what spatial scales such changes may occur. Furthermore, the role of a fluid phase has become increasingly recognized as a major agent in not only driving associated magmatic-hydrothermal systems that produce societally relevant ore deposits, but also drive such rejuvenation through enhanced heat transport. Recognizing the fundamental role that fluids play highlights the need for better constraints on when free fluids are present or magmas reside in a state of fluid undersaturation.

Constraints on fluid saturation may not only come from petrology itself, but also through the integration of observations within geophysical datasets and dynamical models of mass and energy transport. The latter require improved constraints on the boundary conditions of the *'containers'*. For example, what is the spatial extent of magma storage and the rheologic coupling with the surrounding crust? How do these boundary conditions ultimately drive magma eruptiblity and magma evolution, in addition to the internal state of stored magma? Lastly, a major challenge in modeling magmatic storage systems is identifying meaningful simplifications that are necessary to construct models.

Crystal records often demonstrate a complex assembly from different containers with distinct storage conditions. In some cases, such assembly may encompass the entire crustal column and multiple batches of magma. Crystal records are complex and suggest that erupted magmas are often assembled from multiple components. How is this complexity best treated in a modeling framework? Key questions are temperature and pressure of storage, as well as the phases (crystal, melt, fluid) that are present and in what proportions, all of which require robust thermodynamic models. In particular the question of whether magmas are undersaturated or coexist with a free fluid phase are of critical importance. In case of the latter, its mobility and fate can be of critical importance for rejuvenation of morbibund reservoirs and for eruptions.

With the recognition that magmatic systems are vertically extensive and involve predominantly partially solidified magmas (i.e., crystal-rich magma mushes), the modeling community has increased efforts towards understanding the multiphase nature of these magmas and how it affects their transport, their emplacement, and the growth of crustal magma storage reservoirs. Because such storage regions are largely in thermal and often chemical disequilibrium with the host crust, the magmas undergo cooling, crystallization and chemical hybridization. At the same time the surrounding crust is not in static equilibrium and its stress state and rheology in turn affect magma transport as well as the evolution and growth of magma storage over time.

The petrological diversity of magmas observed on Earth is primarily caused by the physico-chemical processes that take place in these magma storage regions. Over the past decades important observations have shaped our current understanding that crustal magmatic systems are long-lived but characterized by episodes of growth that seem to occur in pulses. From a mass balance standpoint, the emplacement of large chemically evolved magmatic systems requires significantly larger inputs of primitive magmas and the loss of these mafic roots. Overall crustal magmatic systems require an incubation period before being able to generate colder and more evolved magmas, a process generally referred to as thermal maturation. While these observations put important constraints on models of magma storage, they also prompt important questions already touched upon in the previous section on crustal scale magma transport.

Recent studies have highlighted that the mechanics of phase separation, which is central to crystal fractionation, is modulated by interactions among the magma constituents (individual crystals, volatiles in bubbles, melt) at the discrete granular scale. Microscale observations of mushes and their crystal constituents are opening new possibilities that offer great opportunities for modeling. This, however, requires a modeling framework that couples the magmatic system and its host over time scales of minutes up to millions of years as well as over spatial scales of microns to tens of kilometers. Future modeling challenges will have to contend with the these broad scales and a future MCS could facilitate progress in several areas: (1) granular scale dynamical models of growing complexity (e.g. involving crystals of various size and shapes and deformable bubbles of exsolved volatiles); (2) flexible continuum scale model frameworks that are coupled with granular scale models; and (3) new upscaling paradigms where homogenization methods are tailored to faithfully serve the complexity of the granular models. An MCS would assist in the development of model interconnectivity which is key to upscaling, it would provide resources for the development of state-of-the art models at both ends of the spectrum (granular dynamics and continuum reactive transport) and finally it should facilitate collaborations between the magmatic modeling community and researchers in applied mathematics, physics and engineering who are facing similar challenges with multiphase and multiscale physical models.

3.3 Constraining crustal magma transport and storage through observations

Integration, analysis and interpretation of diverse observational data sets relies on inverse methods, which have been extensively developed in the field of geophysics. They allow models to be quantitatively compared with observations to constrain system parameters. In this way, inverse methods provide the critical link between data and models. Inverse models encompass a variety of techniques that can provide subsurface constraints on the rates, volumes, and melt distributions to provide constraints on the architecture and dynamics of real magmatic systems. Techniques vary widely, from simple optimization approaches to sophisticated Bayesian frameworks that permit utilization of independent *a priori* information and full quantification of the uncertainties associated with parameter estimates. Inverse models are not only complementary to physics- or process-based models, but in many cases they are based on such models. Because these approaches are so important for relating volcanological models with observations, they must be a key part of an MCS. Much important work remains to be done in applying such methods to volcanological problems, and an MCS must support such efforts.

Inverse models often suffer from limited resolution and inherent non-uniqueness, which can be overcome by combining different, yet complementary, geophysical approaches with petrological, laboratory, and geochemical measurements. Recent progress has been made by the development of three or four dimensional petrophysical models that infer the extent of partial melt and volatiles at several subduction zone volcanoes, including Soufriere Hills Volcano, Montserrat (SEA-CALIPSO, REFERENCE), Mount St. Helens (iMUSH, REFERENCE), Uturuncu, Bolivia (PLUTONS, REFERENCE), Laguna del Maule, Chile (REFERENCE), and Santorini, Greece (PROTEUS, REFERENCE). These projects demonstrate the value in using multiple, dense geophysical datasets combined with petrology and geochemistry in order to consistently interpret different types of data and to determine whether anomalies are caused by partial melt, brines, sulphides, or other petrophysical characteristics.

In conjunction with SZ4D, collaborative projects would benefit from a "global approach" of studying many volcanoes through synthesis of the broadest range of data. However, there is also great value in studying a small number of volcanic systems using the data from dense monitoring networks in conjunction with a comprehensive suite of other observations including field relations and geochemical and petrological observations. In addition, there is potential linkage to volcano drilling. An MCS would leverage such observations to develop the next generation of models, especially by facilitating the development of joint inversions that explain multiple (possibly all) datasets. Such models should leverage data types with complimentary sensitivity to structure or processes and include: deformation; seismicity; seismic P&S wave velocity and ambient noise tomography, interfaces (receiver functions and seismic reflection), attenuation, and anisotropy; electromagnetics; gravity (and time variable gravity); geochemistry and petrology, gas and thermal emissions. There are several approaches to joint inversion for magmatic system architecture with promising results to date, but much model development remains to be done, especially with linkages to petrophysical models using laboratory results (see for example the SIGMELTS program for electromagnetic data, REFERENCE), or linking magmatic processes with seismic data. Aside from advancing our fundamental understanding, progress in this direction would enable better assessment of hazards during periods of volcanic unrest. Data assimilation techniques can even be used not only to assess the state of a system, but to quantitatively forecast future behavior -- an extraordinarily challenging problem whose nonuniqueness can be reduced through assimilation of multiple diverse datasets together with more realistic subsurface models consistent with all available data.

3.4 Eruptive magma ascent

This section still needs to be written. Are any speakers from the "eruptive magma ascent" theme interested?

3.5 Surface processes and hazards

Surface processes such as lava flows, pyroclastic flows, and ash plumes are a direct threat to millions of people around the world, and models of such processes would be an important part of an MCS. Due to time constraints, however, the volcano workshops were only able to explicitly cover the topic of ash plumes.

The eruption plume theme of the workshop encompassed the set of physical processes starting above the eruptive vent and extending to the long-range dispersal of pyroclastic material in the atmosphere as well as final deposition. The workshop presentations and discussions focused on a range of research questions and strategies for collaboration centered about modeling of the eruption plume subsystem. They encompassed an ecosystem of models ranging from research to operational models, as well as the incorporation and archiving of observational data. Given that much of our understanding of the deeper parts of the volcanic system is seen through the filter of plume dynamics, there was an emphasis on how to connect plume dynamics to the outcome of models focused on deeper processes (i.e., reservoir and conduit models) and how to link different scales of plume models within a volcano-magmatic model ecosystem. In particular, the multiscale challenge for predicting ash dispersal over long distances received significant consideration. Because of the immediate hazard implications another focus was on the integration and development of models that can be rapidly run on widely available resources, and that would be easily accessible/usable at volcano observatories and academic researchers during volcanic crises.

Current innovation in plume models (and associated challenges) include linking reservoir/conduit models and conditions to eruptive plumes; compressibility effects and choked flow conditions; entrainment; fluid-particle interactions and turbulence modification, and incorporation of new turbulence models; heterogeneity in near-field plumes; microphysical processes including aggregation, hydrous phase change, heat transfer; and rapid incorporation of eruption source parameters. Workshop participants suggested that an MCS could help in the integration of new algorithm design and experimental/observational constraints related to physical processes in eruptive plumes. This was seen as particularly important for research codes (higher dimensionality models) although parameterization of some of these processes could eventually be incorporated in more rapid/reduced dimensionality approaches. One suggestion was to use an collaboratory as a way of using research codes to develop user friendly modules/approximations.

Also important is improving the integration between plume models and models of magma ascent and with large scale atmospheric simulations. This could be approached in a variety of ways. Component models (e.g., rheology) could be developed that could be coupled with one another to facilitate construction of larger system models. An MCS could facilitate development, testing, hosting, and sharing of these subsystem (building block) models. Some subsystem models already exist and can provide a useful starting point, such as 1D transient conduit flow models and reservoir models in the "lumped parameter" framework with flexible initial/boundary conditions, and 1D/2D/3D thermal conduction models with simple equilibrium petrologic coupling (f-T or MELTs).

Eruptive plumes are hazardous for local populations, regional air quality, air traffic and a range of infrastructure. As a result, a modeling collaboratory could support modeling activities that would aid the operational use of plume and tephra dispersal models. To make these simulations useful in a rapid response situation by a broad community of users on widely available computation resources (desktop computers), much of the development of these types of models has focused on parameterized or reduced dimensionality simulations. Workshop speakers and participants identified a number of important goals for plume models within the context of an MCS, including probabilistic tools for tephra hazard assessment; the development of computational tools (and resources) to conduct simulations during times of unrest; the incorporation of data into simulations to update forecasts for dispersion, aviation safety, and deposition; the integration of model results with satellite observations; the development of user friendly interfaces to place multiple satellite observations in a common framework and for making plume models more accessible; and the development of *(Tobias Fischer could add a linkage to the discussion of CONVERSE at this place).*

3.6 Thermodynamic, rheologic, and kinetic models

Currently this section has an emphasis on kinetic models and was led by Philipp Ruprecth. Mark Ghiorso was going to contribute something about thermodynamic models. What about volatile solubility models? Is Madison Myers interested to contribute to this section? Other contributors are welcome. Perhaps Alan Whittington would be interested to contribute as well?

A major advance in the study of magmatic systems has been the increasingly detailed record of physico-chemical changes derived from the crystals in the magma. Pressure-temperature-time paths of magma batches have become trackable at increasing spatial and temporal resolution, allowing inferences on how magmas evolve during storage, ascent, mixing, and eruption.

During long-term storage magmas can approach equilibrium and thermodynamic models constrain the abundance of phases under a set of intensive parameters as well as the distribution of elements within those phases. However, during times of magma transport and/or mixing magmas are substantially removed from equilibrium conditions and the system responds by phase changes and/or diffusive re-equilibration, producing diffusive chemical and isotopic gradients in crystals and glasses. Kinetic models can provide detailed information about the length- and timescales of the underlying processes. It is increasingly recognized, however, that crystal growth or dissolution may play an important role, requiring the joint solution of crystal growth and solid state diffusion through moving boundary problems. Other kinetic models focus specifically on phase transformations, such as crystal nucleation, growth, and dissolution in response to the varying degree of undercooling or superheating. Similar efforts exist regarding the formation and evolution of bubbles in magmas. In these models, the chemical evolution of the system can be connected to the textural observations made in erupted products or plutonic rocks. For example, rapid versus slow crystal growth related to the degree of undercooling leads to distinct crystal habits that range from skeletal, dendritic to polyhedral as well as from more acicular to more isometric crystal shapes. Models, however, are still a long way from being able to simulate these processes in adequate detail to be able to leverage observations. This within itself represents a significant challenge. Moreover, embedding such kinetic models at the sub-grid scale within meso-scale models of magma transport and storage has not yet been achieved to any significant extent and remains one of the major challenges. With future progress in these areas will come a growing need to curate and standardize models so that results can be compared and individual case studies can be synthesized into a greater understanding of magmatic processes.

3.7 Forecasting and pattern recognition / artificial intelligence

Is a forecasting section needed? If so, someone needs to take the lead, perhaps Grace Bato and/or Mike Poland and/or Diana Roman? Note overlap with section 3.3.

4. Vision for a Volcano Modeling Collaboratory

The SZ4D program is an infrastructure-intense endeavor with a strong emphasis on instrumentation for observing active subduction system processes. Its science goal is understanding the processes that underly subduction zone geohazards, which requires the synthesis of data using process-oriented models.

Model generation is a complex process. Like observational data or experiments, models are first class objects of the scientific endeavor. There is as much research and intellectual effort that goes into the generation of models, as there is in gathering measurements and observational data, or in the conception and construction of experiments. Consequently, models must be treated such that their generation, evaluation, and documentation can be viewed as just as important an activity as the generation of observational data, whether experimental, analytical, geophysical, geological, or other. In other words, there is a need for investing in model development and collaborative modeling efforts at a scale that is proportional to the investments into observing active subduction system processes.

In this section we summarize why current approaches towards volcano system modeling are inadequate, lay out goals for a modeling collaboratory, and detail how these goals could be achieved through a combination of interdisciplinary focus groups, supporting grants, and computational infrastructure.

4.1 Limitations of the Status Quo

Workshop participants identified key shortcomings to the status quo. The complexities of volcano-magmatic systems are enormous, requiring state-of-the-art models that often push the limits of numerical techniques. But model development is often treated as a by-product of other research goals, rather than as first order science. Consequently, funding opportunities for pure model development are limited and have not been conducive to model codes being adequately validated, verified, or benchmarked. Furthermore, there may be missed opportunities for collaboration with outside experts in fields such as applied mathematics, statistics/data science, or computer science, that could be overcome by programmatic support for such endeavors.

Models also lack integration, interoperability and modularity between subsystems and/or processes. Model codes can be difficult to find, are often not open source, and usually not well documented. This is in part a consequence of a lack of incentives to make models more accessible, benchmarked, documented and so forth. This is in conjunction with an academic cycle for graduate students and postdoctoral researchers that is not conducive for longer term efforts of sustaining user friendly code beyond code development. In other words, if the onus is on code developers to make models more accessible, benchmarked, documented and so forth, then what should be expected of non-modelers or users? Overall, the status quo -- no clearly defined programmatic funding opportunities for model development, yet free sharing of models is expected -- is not sustainable, limits scientific progress, and presents a range of opportunities for an MCS.

4.2 What can a Modeling Collaboratory Achieve?

4.2.1 Fostering the development of subsystem and integrative system models

The types of models that might be supported by a modeling collaboratory must be rooted in the primary science objectives defined during the workshop itself; within the ERUPT Report (National Academies of Sciences, Engineering, and Medicine, 2017); within the USGS Plan to Advance Subduction Zone Science (Gomberg et al., 2017); within the SZ4D white paper by Segall and Anderson (2016), which contributed to the recommendation for a modeling collaboratory within the SZ4D Vision Document (McGuire et al, 2017); as well as the efforts and report by the SZ4D Working Group for Magmatic Drivers of Eruption (MDE). At the same time one must consider the overarching role of models within the context of broader collaboration.

Workshop participants expressed concern about “top-down” science directives to guide research and modeling efforts; rather, there was a clear preference for a volcano MCS that supports, on some level, any models which fall under the broad umbrella of volcano-magmatic systems. It was, however, recognized that there are different classes of models, not all of which are equally amenable or at equal stages to meet criteria like interoperability and user friendliness ultimately desired. In essence the modeling ecosystem can be viewed as two or more branches with different expectations, needs, end-users, and purposes. On the one hand there are models where processes and physics are well established, understood and prescribed, and which are useful for exploring outcomes. Such models could constitute a portfolio wherein models are easily accessible to users with relatively limited knowledge of modeling, underlying theory, or numerical methods. For this branch it makes most sense to have a staff-supported 'center' with models that are archival and amenable to updating and small improvements.

The aforementioned branch of models may not be adequate for more complex questions where models are still in a flux and evolving. Such models, although being developed by individual research groups, may benefit from enhanced technical expertise. The challenge, however, is that these codes are unique and there is no one-size-fits-all in terms of methodology or expertise. Although a longer term goal would be that these model codes evolve toward a state of interoperability and accessibility that could be facilitated through a staffed center, these models would still be in a state of flux and far from archival. For such model codes developers would benefit from the various collaborative aspects that an MCS would offer (e.g., workshops, summer schools), whereas technical expertise could be supported through enhanced funding aimed at collaboration between model developers and such experts in other fields, such as for example applied mathematics or computer science.

Thus, while there may have to be variability and flexibility in how the various collaboratory objectives will be achieved, it was recognized throughout the workshop that an MCS should facilitate the development of a new generation of models that are not well-served by the existing funding and research structures. Very broadly, these include: (1) integrative system models which relate diverse physics and observations, possibly over a range of spatiotemporal scales;

and (2) subsystem “building block” models which can be directly linked to one another and used to more efficiently and effectively construct larger system models.

An ecosystem of interoperable subsystem models. In contrast to -- but complementary with -- holistic system models, an ecosystem of subsystem models can be centered on either processes or specific parts of the volcano-magmatic system. The latter would for example include melt generation and extraction, magma chambers, conduits, or eruption plumes. Process-based subsystem models could serve to link models with experiments, and could be organized around topics such as multiphase flow (in the mantle wedge, during crustal transport, in magma chambers, in conduits), thermodynamics, dike propagation. To the extent practical, these subsystem models would be interoperable using well-defined or even standardized sets of inputs and outputs (APIs), permitting their use within broader integrative models. This could take the form of something like a scrapbook of different types of highly resolved simulations (or modules), developed somewhat independently yet useful together.

Integrative system models. Throughout the workshop it was recognized that the development of models by individual research groups tends to produce models that are targeted to specific disciplinary problems. An important role for an MCS would be to encourage and facilitate the development and integration of system-scale models that cross boundaries of disciplines, problems, and scales, and that can predict diverse observations. Workshop discussions identified a fully integrated model of crustal magma transport, storage, and eruption, spanning huge spatial and temporal scales, as an aspirational but unrealistic goal. Nonetheless, there is great promise for models which incorporate diverse physics from magma storage, ascent, and even eruption. Such models can provide the "glue" to pull a range of disparate observations together (Segall and Anderson, 2016).

[This subsection is important but still needs a lot of work -- it’s currently just notes. Can borrow material from the Segall and Anderson white paper … **alternatively, the above may actually be good enough**.] Here we can discuss 1) sophisticated multiphysical models, particularly those that predict diverse data, and 2) simple 0-order “box” models that capture essential physics and can predict, for instance, both ground deformation and eruption rate.

Workshop notes:

- Unified system models. Try to build holistic volcanic system behavior models, integrating data from different volcanic research disciplines. These could be used for forecasting. Basic “zero-order” models of fundamental physics; e.g., for effusive silicic eruptions.
- Improved ability to connect models with very different spatial and temporal scales and with data of very different scales (petrologists versus reactive flow modellers versus mantle scale geodynamics); frameworks that can model volcanic processes in terms of time and space and across scales (Analogy with rock mechanics sampling experiments scaled to the fault processes).
- Example: The question of how magmatism is expressed at the surface over 1-100s kyr scales is an example grand challenge in volcanology that will require bridging disciplines:

we need to understand tectonic forcing on these scales, we need to understand preservation potential and landscape evolution (ie, role of climate both as forcing on magma system and as agent of erosion), we need to understand melt supply from the mantle and therefor mantle dynamics.

As an example, “classical” magma chamber models, describing magma storage as a fluid inclusion in an elastic halfspace, are regularly applied both to active volcanoes, ancient geologic landforms (e.g., laccoliths like the Henry Mountains, flood basalt volcanism) and volcano-adjacent analogs (e.g., mud volcanoes, planetary volcanism, cryovolcanism). There is considerable ongoing work to extend this “reservoir averaged” or “lumped parameter” or “box model” approach, including time-dependent, multiphase crustal rheology and multiphase fluid evolution including extensions that connect easily to mush concepts of magma transport.

4.2.2 Facilitating the development of public, open-source modeling codes

Models, and the computer codes from which they are built, are far less useful if they are not available to the community for use and -- ideally -- modification and reuse. While there are many modeling problems in volcanology that are in early developmental stages, there are only a very few models that have wide community buy-in and have been applied to interpret multiple different types of data over a range of scales. In this sense, the volcanological community lags behind many other sciences in which code publication is seen --- and supported --- as a standard (even required) part of the scientific process.

Public, open source codes confer numerous well-documented benefits, as already identified in other science communities. Open source codes may be more robust, more easily extensible, more widely utilized and better cited, and more easily linked with other model building blocks. These benefits are particularly important to the volcano modeling community, which is small enough that the size of research groups and complexity of software that can be produced is necessarily limited. Why has open source volcanology code not yet taken root? Firstly, models tend to be developed by graduate students, as part of hypothesis-driven science projects. There is often little funding support to develop subsystem-scale public codes, which requires far more effort than research codes. The latter may be useful despite kludges, inefficiencies, poor documentation, and idiosyncratic coding habits (volcano models are rarely developed in collaboration with professional programmers). Secondly, the publication of model codes does not yet confer the same career benefits as manuscript publication, so at present there is limited incentive for the major time investment required to document, carefully test, and publicly release code. Thirdly, researchers lack the funding needed to provide the long-term support required for public codes and there is no career incentive to do so, even if there were funding. In summary, funding mechanisms and career pressures for academic researchers are not consistent with the development and long-term support of public, open-source model codes.

These limitations may be overcome by a community-based approach. An MCS should encourage, support, and enable the development and maintenance of codes that are easy to configure, use, reuse, and extend and scale. These codes must be citable and, when possible, not be disassociated from their underlying data resources. Models should be maintainable and updatable by a community of model users. (A community of model users will also prevent geographic isolation that can be a challenge, particularly for early-career scientists.) Finally, although the problem of inadequate recognition for code development is broader than an MCS, the MCS must support DOI numbers for codes, track model access and usage, and encourage model users to include original authors in derivative works.

4.2.3 Making code robust: Facilitating code verification, validation, and benchmarking

The importance of verifying, validating, and benchmarking model codes is well established throughout the sciences. Verification may be roughly defined as an assessment of solution quality (that is, ensuring that the conceptual model is implemented correctly), which can be done by comparing against analytical results. Validation is designed to determine if the model agrees with physical reality, and is "a continuous process, in which the credibility of a model with respect to its intended use(s) is progressively improved by comparisons with...experiments" (Ongaro et al., 2020). Benchmarking, finally, involves comparing different models of the same physical process to one another.

Verification, validation, and benchmarking ensure that codes are modeling the correct system, and that the codes do what they are supposed to do. They make outputs from different models more directly comparable, permit users to better understand model uncertainties and limitations, may guide the observational community to address key data limitations, and improve understanding of how parameterization and initial conditions affect results. Importantly, only properly tested codes can become trusted and widely-used community resources.

Despite these clear benefits, very few volcanological codes are carefully verified, validated, and benchmarked. This work is time-intensive and offers few direct rewards, and codes may not even be available for intercomparison work. As a result, only a few community intercomparison efforts have occurred in volcanology, including: lava flows (Dietterich et al. 2017), ash plumes (Suzuki et al. 2016), conduit models (Sahagian 2005), and pyroclastic density currents (Valentine 2019). Currently the lack of rigorous uncertainty quantification in these models (especially with respect to the nonlinear dynamics of eruption cycles) limits progress.

An MCS would support these activities by providing programmatic funding and other support for modelers to collaborate with each other and with experimentalists/observationalists on validation projects, by hosting open-source codes amenable to this work, by treating models as first-class objects (thus making model verification more rewarding), and by providing structures and facilities that make doing this work as easy and appealing to scientists as possible.

4.2.4 Facilitating code discovery and sharing

Code is far less useful if the community of potential users is unaware of its existence or if it cannot readily be accessed. Absent this, codes must be reinvented over and over in individual research groups. Unfortunately, awareness of existing codes is a major problem in volcanology since no well-established centralized code repository -- or index of external codes -- exists. In the field of volcano geodesy, for instance, dozens of independent implementations of analytical source models are in existence. A previous community effort (VHUB) failed to gain broad acceptance, in part because it was built on older technologies (Expand?), and although “local” repositories can be useful (e.g., http://www.cas.usf.edu/~cconnor/codes.html) these are not community-based and can still be challenging to locate. A primary limitation to existing "repository" efforts is that they are viewed and construed as static archives. An MCS that is focused on making codes verified, validated, benchmarked, interoperable, and open source would lead to a dynamic repository amenable to code discovery and sharing.

An MCS should also facilitate the sharing of model results, such as the IRIS repository for geophysical and inverse models (ds.iris.edu/ds/products/emc-earthmodels). An MCS that facilitates sharing of model results will enable not only interdisciplinary studies but also comparative volcanology of a greater diversity of magmatic systems, which is critical to overcome our current biased sampling of a small fraction of the world’s volcanoes, as outlined in the ERUPT report. It should be expected that an MCS would synthesize available data and develop new hypotheses that could be tested with, and will inform the design of, focused multi-disciplinary field or laboratory experiments. The best way forward on this path would be the formation of focus groups that tackle problems at the subsystem scale, starting with workshops aimed at further refining questions and approaches, leading to proposals for model development and projects that integrate observations through collaborative modeling science.

4.2.5 Enhanced interdisciplinary collaboration

Making models and model codes more accessible to a broader user community is aspirational, but needs to account for the fact that models are first order science objects, are highly sophisticated, and require substantial expertise in using. The assumption that sharable and open-source models will automatically lead to wider use is simply naive. Instead, broader use of models is best achieved within the framework of collaboration that involves a significant component of cross-disciplinary training and education. The role of an MCS would be to facilitate and enhance collaboration through workshops that are focused on volcano-magmatic sub-systems and include a significant component of training and education aimed at enhancing collaborative synergy.

Volcanology is an inherently interdisciplinary field and model development requires interdisciplinary expertise, not only within the geosciences, but also with mathematics, engineering and computer science. Therefore, enhanced collaboration with other fields will have to be an important goal of an MCS in order to improve model efficiency, increase confidence in results, and enable more difficult problems to be tackled. Examples of opportunities for this sort of cross-disciplinary collaboration include improving code structure, optimization, parallelization, and utilization of computational resources through collaboration with computer scientists. Collaboration with statisticians who can improve data and model uncertainty quantification through the utilization of more sophisticated statistical techniques. With adequate investment in modeling, it may even be possible that volcano science could become a producer of quantitative techniques with broad interdisciplinary appeal. For example, the development of strongly multiscale, time dependent, inhomogeneous and anisotropic deformation models is a frontier area in a range of disciplines.

4.2.6 Enhancing modeling-based collaborative volcano-magmatic system science through education and training

To advance hypothesis-driven science objectives through integrative modeling of magmatic-volcanic systems requires a critical mass of geoscientists that are skilled both in model development and in the subsequent application of models through collaborative model simulation. In other words, advancing science objectives through modeling requires a pipeline of scientists with diverse skill sets, rooted in the geosciences, trained to understand complex geological systems, adept at advanced numerical methods, and who can integrate diverse geological datasets into simulations. The breadth of skills required is striking, and separates volcano science from many other fields. Augmenting and sustaining this pool of geoscientist modelers is a necessary requirement and a fundamental challenge for nurturing a thriving and competitive geoscience program for the 21st century.

Achieving this goal requires enhanced investment in student and postdoctoral researchers who are focused on the development of the prerequisite numerical models, beyond a paradigm whereby a majority of support for geoscience modeling is solely tied to hypothesis-driven projects and contingent upon the prior existence of modeling capabilities. Ultimately, models are rooted in the scientific questions they seek to address; however, the path to model simulation invariably goes through model development, which is thus an integral part of the broader science objectives. For example, converting satellite radar data into maps of volcano deformation requires the development of sophisticated algorithms. The latter constitutes model development, which requires funding. Similarly, the derivation of physics-based models and their implementation is science that needs to be supported. The same, of course, holds true for the ultimate collaborative use of process-based models in hypothesis-driven simulations aimed at deeper insight into observations. Thus, a competitive science program for volcano-magmatic systems, whether within the broader SZ4D objectives or beyond, requires enhanced and sustained support of students and postdocs engaged in model development. An MCS could serve as a programmatic conduit in this regard. Moreover, it could simultaneously assure, through workshops and networking, that a growing pool of nascent "modelers" will be optimally positioned for collaboration with experimental and observational scientists through hypothesis-driven model simulation.

4.3 Proposed Volcano Modeling Collaboratory

Based on community feedback during the workshop, this section defines a proposal for how an MCS would best advance volcano-magmatic systems science. The proposal elements are designed to facilitate model accessibility and training, science collaboration, and interconnectivity between models and between models and observations. **At its heart this represents a new vision for community-driven collaborative science of volcano-magmatic systems, with modeling as the nexus between observations and understanding.** The proposal is composed of three primary elements:

1. ***Community Working Groups***
2. ***Grants***
3. ***A Modeling Collaboratory Network and/or Center***

4.3.1 Community Working Groups

Perhaps add some kind of diagram to illustrate the interaction between PIs, summer schools, topical workshops, software, development of new synergistic ideas that couldn't exist with just PI-driven science, etc.

Volcanology is a small, geographically-dispersed community working with limited data to understand highly complex nonlinear systems. A successful collaboratory will need to allow and encourage individual PI's and their teams to devise new computational techniques, or employ traditional methods in new ways, as their vision, scientific impulses, and insights direct them. The idea of "shared master codes" maintained in a repository by technicians was viewed by some participants as an outdated solution that would lead to code obsolescence. A collaboratory might rather be most successful by providing support for researchers (including postdocs and graduate students) and workshops for various communities, in which creativity and forward-looking is encouraged, leading to the creation of a hierarchy of modeling tools that reflect the needs of a diverse community.

Thus, perhaps the single most important activity a modeling collaboratory can undertake to improve volcano modeling efforts -- and thus advance the field of volcanology -- is to bring groups of diverse scientists together for extended periods of time to work on common problems, and with results that are openly shared with the broader volcano-magmatic systems community. To enable long-term collaborative work, these community working groups (CWGs) must be funded at the group level. In this section we discuss the implementation of CWGs, and in section 4.3.2 we discuss funding mechanisms.

We define a CWG as a diverse group of scientists seeking, through long-term cooperative work, to advance a particular aspect of volcano model research, and whose model codes will ultimately become part of an MCS ecosystem of (ideally) interoperable models accessible to the broader community. A defining feature of CWGs is that they would be designed to include (as appropriate) an interdisciplinary range of modelers, observationalists, and experimentalists; early career and more advanced scientists; and geoscientists and outside experts such as applied mathematicians and computer scientists, in order to focus on problems that are otherwise difficult to tackle. CWGs would work collaboratively to produce proposals and subsequently pursue collaborative projects. Any given CWG could produce multiple collaborative projects, including workshops and summer schools.

Currently no similar framework exists in the field of volcanology. Focused workshops and meetings already occur, of course, often arranged around conferences, and often with training as a primary goal -- but these are brief and rarely interdisciplinary. IAVCEI commissions are not designed for long-term collaborative modeling efforts. Perhaps most similar, although with a broader focus, is the Cooperative Institute for Dynamic Earth Research (CIDER) summer school series. Only a single CIDER has been focused on volcanology, but that meeting was heavily oversubscribed and highly successful. It was attended by several report authors and workshop participants and inspired in part the CWG model proposed here.

CWGs could take a number of forms depending on the focus. These might include intensive summer schools or hackathons, or intermittent workshops held regularly over a period of years. Significant cost savings are possible by mixing less-frequent in-person meetings with more frequent remote collaboration. In one model, a community group would get initial seed funding to hold a workshop (an interdisciplinary proposal incubator), with the objective of producing collaborative proposals to carry out the work. This could occur in an intense period of weeks, or over years. Rather than serving as the equivalent of science committees that direct or sanction science objectives or projects, the CWGs are meant to act as incubators and nexi for collaborative projects at the individual PI level and which include a significant component of modeling or model development.

Some CWGs could be arranged around a specific science topic, such as magma ascent in dome forming eruptions, eruption cycles in distributed volcanic fields, or the kinetics of crystallization. Others could be arranged around a specific geography, such as a recently-active magmatic system, or a volcanic region (or even an entire arc), or an exhumed plutonic system. Still other CWGs could focus on a particular type of process or model. CWGs would directly address many of the modeling collaboratory goals identified above, including 1) training and education, 2) interdisciplinary collaboration, and 3) fostering the development and testing (verifying, validating, and benchmarking) of public, open-source model codes. Critically, CWGs would enable science advances by leveraging the current mechanism of individual PI-level research grants.

CWGs would include a mix of early career and more advanced researchers, thereby serving as important networking and training venues. They would maximize diverse community engagement and enhance collaboration between geoscientist modelers and expert communities outside the geosciences (e.g., applied mathematics, physics, statistics/data science, and engineering), and across magma/volcano science disciplines. CWGs would put modelers, observationalists, and experimentalists together to educate all and design studies, at the same time providing a venue for model users and developers to interact in order to encourage collaboration rather than competition. This would serve to break down barriers of institution, discipline, and geography (volcanology is very fragmented in the US across states and institutions, and models reflect this), forging and strengthening community bonds at both the personal and institutional level (for instance, between volcano observatories and the academic community). Furthermore CWGs, assuming they are supported beyond the usual 2-3 year grant cycle, would be well suited to assure long term broader utility, use and integration of models, as well as facilitate model verification, validation, and benchmarking, all of which were repeatedly highlighted during workshop discussions.

Some illustrative examples around which CWGs could coalesce could be: (1) Building a system model of a recent volcanic eruption, where a mix of academic and observatory scientists gather to explore multiparameter eruption monitoring data, develop conceptual subsystem-scale models, implement them numerically and interoperably so that they can be linked to form a system-scale model, and finally compare model simulations to data with the assistance of statisticians. (2) Joint inversions of eruption data sets using various approaches/models by *a* group of volcanologists who work with statisticians. (3) Forecasting, similar to the above, but focused on forecasting the evolution of an eruption (or hindcasting a past one). (4) Task forces that develop best-practice recommendations in order to improve their multi-use in models as well as the generation of interoperable experimental and observational data sets that are more useful for modeling endeavors. (5) CWGs focused on temporal-based subsystems, such as eruptive time scales (days to years), volcano life spans (thousands to hundreds of thousands of years), and life cycles of magmatic centers (millions of years). Activities such as these could be initiated through CIDER-like summer schools. At the same time such summer schools could produce collaborative proposals, while also enabling sustained collaborations on, and synergies between, existing projects. *[More could be added here if so desired.]*

4.3.2 Programmatic funding (grants)

Grants would provide support for students and postdocs in order to establish and sustain a pipeline for geoscience modelers. The need for such grants is based on the recognition that the majority of model development, model innovation, and model simulations are pursued by graduate students and postdocs. However, under the status quo there is no viable pathway to go from a research grade model, which is the basis of many hypothesis-driven publications, to the desired benchmarking, model documentation, archiving and publication, as well as accessibility and collaborative training. None of these activities translate into citiable publication or otherwise lead to tangible career advancement. Moreover, the resources spent on the development of models are not further multiplied because the models often end up as single-use efforts. At the same time, there is a dearth of postdoctoral funding opportunities for graduating students. Ideally, any solution would simultaneously overcome the aforementioned limitations while at the same time enhancing student and postdoctoral funding.

The objective of these proposed grants program would be to: (1) attract talented students with interests in physics-based numerical modeling into the geosciences; (2) train students in all facets of numerical modeling, from model development to science collaboration and simulation; (3) provide a pathway for graduates whose PhD involved numerical modeling into science careers through post-graduate grants that support professional development, collaboration involving the integration of observations into model simulations; (4) support and enhance the development of numerical models within volcanic-magmatic systems science, inclusive of funding for collaboration with applied mathematicians and computer scientists; (5) move research efforts of model development into a path of long-term synergistic use; and (6) to make models more viable for collaboration: benchmarking, documentation, publication and archiving, accessibility and training. In summary, within this vision the grants would support the development of an ecosystem of numerical models. They could augment hypothesis driven science grants, but would predominantly be full grants in their own right. Because models are in a dynamic flux of development and improvement, within this ecosystem there could be multiple sets of potentially overlapping models. However, the MCS framework would facilitate integration and interoperability between individual models by supporting grants which build upon those supporting the initial model development and application.

4.3.3 Network / Center

A Modeling Collaboratory might consist of two primary elements: 1) administrative and technical staff to assist with implementation of MCS activities, and 2) computational infrastructure. Whether such a facility should be distributed (a Network), centralized (a Center), or some combination of the two. Although there was no conclusive workshop discussion on this question, a suggestion was for a significant part (perhaps even 100%) of an MCS to be distributed and decentralized, with permanent technical staff embedded within the scientific community.

Staff
Opinions diverged on whether a modeling collaboratory should include staff with expertise in computer sciences and applied mathematics. On the one hand it seems difficult to consider how the envisaged objectives, such as model interoperability, documentation, accessibility, and so forth, can be achieved without a center and expert staff. On the other hand, caution was expressed to avoid that such a "center" with expert staff could quickly become obsolete and perhaps even become an impediment to enhanced collaboration. There was, however, unanimous support for summer schools, workshops and training activities that, if facilitated by an MCS, would require coordinating staff.

Any technical staff would primarily be dedicated to assist in model development, benchmarking, documentation, best practices, and even developing graphical user interfaces (GUIs) and other methods to make codes easier to use. Administrative staff would provide logistical support for CWG activities, which could otherwise take large amounts of time and deter participation and leadership. Both technical and administrative staff would manage computational infrastructure (below), handling protocols and streamlining processes. This approach is analogous to lab work, in which technicians are often hired to help run the experiments. We emphasize that support staff would serve to support community-based science efforts, not establish top-down research priorities.

In one model, the MCN staff would be hosted by different institutions under a rotational system that assures continuity and overall employment considerations. For example, a postdoctoral program could stipulate that some of the postdocs' time beyond code development and research activities is devoted to some of the broader collaboratory objectives. This would provide a much needed boost to postgraduate professional development opportunities, if it translates into more postdoctoral opportunities overall, while at the same time furthering many of the objectives outlined in this report. For example, postdocs could be supported for staggered three-year durations in order to assure continuity and in accordance with evolving project needs, somewhat akin to Southern California Earthquake Center (SCEC), while at the same time providing sufficient time to advance research portfolios.

Computational infrastructure

[To do in this section: detail how this will differ from VHUB, which was useful but also unsuccessful in a number of ways. Can somebody relatively familiar with VHUB tackle this?]

Many goals listed above require that model codes be robustly tested, documented, and (usually) maintained in an open-source community archive. In an MCS this would be enabled through a cyberinfrastructure component that includes at least some of the following:

- A git-based (version controlled) model repository with associated documentation, which could include non-traditional "publications" such as Jupyter Notebooks. Documentation would carefully detail inputs and outputs to enable model interoperability. Similar efforts to host code (not all git-based) exist in other organizations, such as the Southern California Earthquake Center.
- A centralized index of external modeling codes and repositories will help to achieve broad community buy-in and overcome regulations that some government organizations (e.g., USGS) face in distributing code.
- Training materials (recordings of training workshops, etc.).
- Information on best practices and information about strengths/limitations of various modeling approaches.
- A communication infrastructure.
- Ability to assign DOI numbers for model codes, encouraging model publication
- A mechanism for matching expertise with problems, and for publicizing interesting problems to solicit involvement by outside experts.
- Links between models and associated permanent data archives.

This broad outline does not cover the details of implementation, which were not discussed in the workshop. Open questions include: whether the cyberinfrastructure would require local hardware or utilize cloud services; procedures for code submission and, possibly, review; relation to other SZ4D proposal activities; and how a cyberinfrastructure component of an MCS could leverage or cooperate with existing efforts such as CSDMS, CIG, or EarthCube. Regardless, within the context of SZ4D, a cyberinfrastructure component can serve as the nexus between data acquisition, processing and dissemination, and data integration within models.

4.4 Relation with Other Organizations and Initiatives

In this section we highlight several key efforts and organizations with which an MCS should establish a strong coordination and working relation. The list is not meant to be exhaustive.

4.4.1 Community Network for Volcanic Eruption Response (CONVERSE)

[This section requires more work. Ideally, Tobias Fischer could take a stab at it.] CONVERSE is primarily concerned with eruption response to maximize scientific value of rare data collected during volcanic activity. MCS is dedicated to development of community codes to better understand subduction at a variety of scales, from arc to volcano scales. MCS can be quite

valuable to CONVERSE and vice-versa in developing synthetic eruptions at specific high threat volcanoes, like Mauna Loa. A simulated eruption, using MCS tools, can inform how existing instrument networks respond and on what time scales, and how sensor networks can be improved. Such an exercise will also reveal gaps in modeling that the MCS community can address.

- Use models to determine what data need to be collected during an eruption, and design sensor networks
- CONVERSE is focused on data collection. Models might be involved in how you collect data – how one might prioritize data collection. Innovative data sets will drive model development. Conversely, model application will drive where and how instruments are deployed.
- Facilitating the use of research software in eruption response scenarios (may require modification to code and training)
- Need an infrastructure/process by which models can easily ingest data on a timeframe that is useful to an eruption response
- Can look at the 2008 Etna eruption scenario that used modeling to forecast the evolution of the eruption as an example of what could be done. This exercise required preparation of a variety of data that is usable for the modelers
- Eruption response exercises, for instance coordinated with CONVERSE, could be strong motivators for researchers to release and/or open-source their codes for use therein.
- Idea of a virtual volcano observatory
- To what level should academic groups be involved in forecasting? To what level should *they want to be* involved?
- Ultimately, forecasts are made by humans. The models inform forecasts but are not the forecast themselves.
- We don’t want it so that people doing independent modeling can just make statements to the public.
- Interested in the **Match.com idea** discussed during the breakout. Examples of a similar scenario that has worked in the past are Geo Hack-A-Thon Weeks where they poll everyone about their level of knowledge and expertise and mix people up.
    - Or if you wanted to search for someone who had expertise in a certain area, you could look that up through this Match.com service. For instance, if a researcher needed someone with more subsurface geophysics knowledge, they could find an expert. This would be a more transparent, accessible way for people to network than bumping into some random expert at a conference.

4.4.2 U.S. Geological Survey (USGS)

[This section requires more work.]

- Note that PI-driven funding mechanisms exclude USGS scientists
- What value is MCS adding for USGS?
- Gomberg et al. (2017)

- This is a blueprint for “prioritizing USGS science activities and for delineating USGS interests and potential participation in subduction zone science supported by its partners.”
- Science theme 1: “Advancing observations and models of subduction zone processes”. This includes “Understanding cycles of volcanic eruptions”, that lists as frontier research “studies that systematically sample volcanic rocks, lavas, and gasses and apply state-of-the art age-dating methods improve knowledge of eruption chronologies and reveal the causes and characteristics of eruption clustering. Improving eruption chronologies, in turn, improves the confidence and accuracy of volcano hazard assessments at high-threat volcanoes.”
- Science theme 3: “Forecasting and situational awareness” includes “Providing reliable, high-fidelity volcano warnings” and “Projecting Ash Cloud Trajectories More Accurately”
- Developing Tools for Cascading Hazards: Importance of building models “that include the interaction of multiple, linked phenomena” -- cascading hazards.
- Stakeholder need: “coupled geologic and atmospheric models validated by real-time observations (ground-based and remotely sensed); interagency collaborations to clearly communicate hazards, ensure safe transportation, and minimize costly disruptions”
- Shared Scientific Infrastructure: “Our understanding of subduction zones would benefit from shared scientific data centers, laboratories, field instruments, and computational facilities, which would extend observations at minimal cost, maximize efficiencies, and facilitate the exchange of data and knowledge.”

4.4.3 NASA

[This section needs to be written or deleted.]

5. Synthesis / Conclusion / Next Steps

Needs to be written up. Notes below in part based on Paul Segall's presentation and input.

A potential next step toward a modeling collaboratory could be the formation of focus groups and workshops, organized around the concept of subsystems. Subsystems could be geologically based (e.g., source, reservoir, conduit), process based (e.g., multiphase flow), or scale based (e.g., arc scale, eruption scale, VEI<=5 vs. VEI>=6). Most natural is probably the definition of subsystems based on the overall geological volcano-magmatic system itself. This would be conducive to bring together people with different backgrounds and it would inherently intersect with the various process- and scale-based subsystems. The objective would be to identify key problems that are both significant and ripe for progress, and to set the stage for models and collaborations aimed at these problems.

Identify potential subsystems here?

Big-picture things to think about

- What can we achieve with volcano MCS that we cannot achieve with the current funding mechanisms?
- How can we get broad volcano community buy-in for a Modeling Collaboratory for *Subduction*, which by definition excludes some of Earth's most active volcanoes and much of the volcano community?
- How do we link volcanoes into their broader subduction zone (or other) contexts?

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