1. Introduction

1.1 Purpose

This draft report is a community document and work in progress. Comments and input are welcome and can be provided in three ways:

1.) By participating in one of the Volcanic System Workshop Planning Meetings: https://us02web.zoom.us/meeting/register/tZwpfuyrrj4qGtA_jMIyVSmAnHEfxignm7sv
2.) By providing comments through an online form: https://docs.google.com/forms/d/e/1FAIpQLSdxx8XIZ8kXrLZyo-KKBRmI0Q5EbkuPhkuMEldEi6Zk3wwniw/viewform
3.) 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)

The report will evolve through your input, as well as ongoing and subsequent planning meetings and webinars.

The purpose of this report is to summarize the outcomes of the Modeling Collaboratory for Subduction Zone Science (MCS) Volcanic Systems Workshop. The report encompasses two parts: (1) potential science objectives for volcanic systems science in subduction zones; and (2) a potential vision for how a modeling collaboratory would best advance the science objectives.

1.2 Scope and objectives of a modeling collaboratory

Science questions and objectives will be focused on magmatic and volcanic systems in subduction zones. A primary focus will be on subsurface magmatic processes, volcanic processes, and the linkages between them, especially insofar as they have ramification for volcanic hazards. Furthermore, consideration will be given to linkages between magmatic processes, fluid migration in subduction zones, and seismo-tectonic aspects of subduction zones.

The ultimate goal of this report is to present a vision for a magmatic and volcanic systems component of a future MCS. There will be a focus on magmatic/volcanic systems within subduction zones, where after all the majority of active subaerial volcanism occurs; however, not to the exclusion of other geological settings that have significant bearing on our understanding of magmatic and volcanic processes.

A modeling collaboratory can serve to facilitate the integration of community-wide science, 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 both broad agreement on the need for improved organization and coordination within the volcanic systems science community. This was highlighted as a major goal in the NAS ERUPT report (2017). A main motivation for the MCS Volcanic Systems Workshop is to advance toward that goal with concrete recommendations for a future modeling collaboratory aimed at advance our understanding of magmatic-volcanic systems and ensuing hazards within subduction zones and beyond.

1.4 Workshop themes

Unless indicated explicitly, material within this document was contributed by participants and presenters of the Volcanic Systems MCS Workshop, the *Modeling Collaboratory for Subduction Research Coordination Network Steering Committee*, and the *Magmatic Drivers for Eruption SZ4D Working Group*.

Crustal magmatic processes and the initiation of eruptions at arc volcanoes are central/overarching components of the SZ4D framework. The crustal magma system, modulated by mantle input, ultimately constitutes the driver for volcanic activity and associated hazards. Crustal-scale magma transport sets the stage and drives the system toward an *eruption threshold* that can be crossed solely as a consequence of internal dynamics. Alternatively, the system may be forced across this threshold by external forces, such as tectonic earthquakes for example.

For the purpose of the MCS Volcanic Systems Workshop we have subdivided the volcanic systems objectives into four process-focused themes that correspond to vertical subregions of the overall system:

- ***Crustal-scale magma transport***
- ***Magma storage***
- ***Eruptive magma ascent***
- ***Eruption plumes***

This subdivision itself reflects 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 supply of magma and volatiles from the mantle to the crust provides the mass and energy input to the transcrustal system. It thus constitutes the link to the deeper subduction-zone fluid transport system, which was the subject of the MCS ***Fluids Transport Workshop*** (https://www.sz4dmcs.org/fluids-workshop). 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.

The emerging view is that 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 are encompassed by the ***Crustal-Scale Magma Transport*** and the ***Magma Storage*** themes of this workshop.

Ultimately our interests lie in advancing the understanding of episodes of unrest at volcanic systems, as they either lead to eruption or wane towards a new "stable" state. Understanding these cycles then improves the assessment of associated hazards, and the potential for forecasting of the onset of eruptive activity, style, vigor, and duration. These are the subjects of the ***Eruptive Magma Ascent***, the ***Eruption Plume***, and the ***Integrative Volcano Modeling and Forecasting*** workshop themes. Furthermore, there are potential linkages with the ***Community Network for Volcanic Eruption Response (CONVERSE) RCN*** (https://volcanoresponse.org/).

2. Workshop organization, participation and activities

2.1 Workshop organization

All planning for the original Portland workshop, scheduled for summer of 2020 had been completed when COVID-19 forced us to cancel it. Instead a virtual workshop comprised of a series of webinars and planning meetings spread over several months, starting in the Fall of 2020 and extending through Spring 2021. Each theme consisted of four invited presentations spread over two webinars that were 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. Webinar presentations spanned a range from more science-focused topics to overviews of various magmatic/volcanic systems models and modeling. A summary of the five workshop themes and presentations is as follows.

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.*

Eruptive magma ascent (4, 6, 7 May, 2021)

- Paul Segall (Stanford University)
- Michael Poland (US Geological Survey)
- Hélène Le Mével (Carnegie Institution of Science)
- Mary Grace Bato (Jet Propulsion Laboratory, California Institute of Technology)

2.2 Workshop activities

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 made periodically updated *'work in progress'* versions of this report available to anyone as a downloadable PDF file on the workshop webpage, together with a Google Form through which anyone was able to ask questions, provide feedback, or contribute in writing to the workshop report. Moreover, participants interested to contribute more extensively to this report were able to contact the organizers for access to the working document of this report as a shared Google Document. The resultant main contributors of this report are listed on page XXX of this report.

2.3 Workshop participation

This section will be written after completion of the webinars and planning meetings. It will contain statistics of workshop participation: number of participants, breakdown in terms of career stage, international, etc.

3. Scientific drivers to advance the state of the art

3.1 Overview of modeling of magma transport, storage and eruption

Workshop discussions that were centered about the question of what an MCS should encompass, identified a fully integrated model of crustal magma transport, storage, and eruption as an aspirational but unrealistic goal. One suggestion, viewed as a more realistic goal, encompassed ***an ecosystem of models, broadly centered about magma transport, storage and eruption, which are in a dynamic flux of development and improvement through grants at the individual PI level***. Within this ecosystem there would be multiple sets of potentially overlapping models. A step beyond this would be a framework whereby individual models from such an ecosystem could be integrated and which would facilitate up- and down-scaling of models. This would not replace development of new modeling approaches, which is considered to be essential at a PI level.

The role of an MCS would be to foster and support:

- Model interconnectivity, integration, and extendability
- Publication of models
- Archiving of model results
- Cultivating the next generation of modelers
- Verification, validation, and benchmarking
- Workshops, summer schools, and other cooperative research gatherings aimed at fostering integration between models and observations with models as a nexus between observations and underlying physical processes, as well as hypothesis testing and forecasting, and training

This vision for an MCS therefore calls upon funding agencies to provide enhanced support at the individual PI-level for projects that are solely aimed at model development and for hypothesis driven projects that include model development as part of the project

scope. **This support would be complemented by some level of support for MCS staff who would collaborate with PIs, postdocs and graduate students in order to realize efficient and state of the art code development.**

Ideally a modeling collaboratory for magmatic-volcanic systems, as part of an overarching MCS, would be comprised of physics-based models for magma transport, ranging from crustal scale to individual eruptions, as well as magma storage. In essence these models are process-oriented and encompass mass and energy transport, crustal mechanics and dynamics, as well as thermodynamics. The models are informed and constrained by observations, in turn based on geophysical and geochemical/petrological models, as well as studies of eruption deposits themselves. They rely on a wide range of experimental data (e.g., petrophysics, rheology, solubilities, diffusivities, equations of state, phase relations). Synthesis of observations and integration within magma transport, storage and eruption models requires methods that can be broadly categorized as parameter estimation, inverse and data assimilation. Thus a model collaboratory must strive to facilitate integration between the physics-based models and data-based modeling methods. The nature of magmatic/volcanic systems makes magma transport, storage and eruption models complex in a variety of ways that require models to draw heavily from expertise in disciplines within engineering and physical sciences beyond geosciences, as well as applied mathematics and computer sciences.

The multi-phase and dynamical nature of subsurface magma transport and storage systems constitutes one of the primary challenges for the ensuing models, particularly in terms of overall complexity, but also in terms of the range of spatial scales. An additional challenge is the immense range of temporal scales that come into play, from subseconds for example associated with rock fracture, seismic energy release, or bubble nucleation, to millions of years in terms longevity of individual volcanic systems, to tens or hundreds of millions of years in terms of subduction-zone and plate-tectonic time scales. There is no *'one size fits all'* solution. Instead these challenges necessitate enhanced funding opportunities aimed at facilitating enhanced: (1) development of a diversity of models; (2) collaboration among model developers and users; (3) model interconnectivity; (4) model benchmarking, documentation, publication and accessibility; (5) scientific collaboration among modelers (developers and users) and non-modelers aimed at *'data synthesis'* and prediction.

A unifying theme among the magma transport, storage and eruption models are reactive transport and the multiphase nature of the natural system. When juxtaposed against the wide range in 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 in one extreme (e.g., bubble/crystal nucleation, crystal growth), to the granular scale where individual crystals or bubbles within a multiphase assemblage are resolved, to the continuum scale capable of simulating processes at kilometer or greater spatial scales and over time scales of individual eruptions or longer. A key role for a modeling collaboratory would be to facilitate upscaling, downscaling, and synergistic interconnectivity of such models.

3.2 Crustal magma transport and storage

3.2.1 Crustal magma transport

In its current state this section represents a collection of ideas and comments provided during the workshop and asynchronously. It is still seeking a champion interested in turning it into a coherent narrative.

- For arc trans-crustal magmatic systems, can we develop models in which primitive magmas naturally stall in the deep crust and that mature into observed arc sections? How long does this take? To make progress on this question requires knowledge of the aperture of the magmatic feeding system. Also, what is the temperature in the deep crust? What is the vertical continuity of the magmatic system? Where do the intrusions store or stall? What is the overall magmatic flux?
- How do the large-scale subduction parameters control magma production and delivery to the crust? Linkage of energy and mass input to subduction variables, such as slab dip, convergence angle and rate, and slab properties (slab age, hydration, sediment thickness etc.) with mantle temperature and regional mantle convection patterns.
- Do mantle-supplied magmatic input rates control magma storage depths, crustal residence times, and erupted magma composition? If so, how? Relationship between the rate of mantle-supplied magmatic input and magma storage depths, crustal residence times, and erupted magma composition.
- Crustal magma pathways become seismically active/observable prior to, during and after eruptions. There is often also ground deformation measured. What does the seismicity and ground deformation represent in these episodes?
- It takes a lot of fractional crystallization (half the mass has to be removed) to take mantle-derived melts into the compositional field of bulk continental crust (common andesites and dacites). It probably takes "delamination", but how that happens is an outstanding problem.
- Assimilation (entrainment of evolved components) is probably important to produce metaluminous andesites.
- Arc magmatic systems are long-lived and relatively immobile. Late magmas are transiting antecedent intrusions of the same magmatic system.

- Why is volcanic growth pulsed (major stages 10,000-100,000 y; single edifices 0.5-1 my, ancestral and successor volcanoes 1-2 my)?
- Systems that persist for 5-10 m.y. usually evolve into systems with substantial rhyodacite/rhyolite. This is consistent with arc intrusive suites. System evolves toward felsic and lower temperatures. Why are lower temperature / felsic magmas more voluminous?
- Ubiquitous magma mixing and mingling produce decimeter-size enclaves. What determines this characteristic size?
- Mafic sheeted sill complexes at the interface between more crystal-rich and crystal-poor magma, not at bottom of intrusion.
- Field relations of exposed sections suggest deep storage regions are dominated by vertical mass transport (up and down?), while conceptual models commonly highlight sill-like emplacement.
- Would like to have models that evolve to real-looking arc sections with steep-sided tabular intermediate plutions in the upper and mid-crust, and primitive cumulates deep and mostly gone.
- Thermal, compaction and reaction processes.
- Resolution of grain scale processes recorded in the crystal record within models of magma transport and storage at relevant scales. This requires upscaling and coupling between different types of models.
- Geometry of magma transport and storage. Most models are highly idealized, we often lack observational constraints to go beyond one-dimensional models or simplified two/three-dimensional models. At the same time going to higher dimensions remains challenging from a modeling perspective.
- Developing joint forward and inverse petrophysical models of the composition, volatiles, and partial melt within the entire transcrustal magmatic system that are consistent with all available datasets (petrology, magnetotelluric, seismology, gravity, ground deformation, etc.).
- Advances in physics of granular materials with implications for magmatic mushes. What is a modeling approach that is appropriate for field observations, with melt extraction and migration at many scales and patterns, and a wide range of rheological complexity? What controls the behavior of mush.
- Compositional excursions are typically brief in andesitic stratovolcanoes (~100 y), consistent with "small" active volumes.
- Volatiles: Parent magmas of arc systems are water rich. Gives melt to low temperatures. Aqueous fluids promote melting of wallrock and remelting of antecedent intrusions. Volatiles at the surface are composites/mixtures of fluids across depth. Make arc intrusions compressible, making it difficult to interpret deformation. - Volatiles are the primary agent to move and sequester societally relevant metals, and arc magmatic systems are among the most important settings for such ore deposit formation
- Linking chemical evolution and its relation to stress evolution in the crust.
- Should there be a link to economic geology and societal relevance for fluids in the crust causing enrichment of rare/precious minerals?

- Deep seismicity: Are deep events actually sites of magma supply? Hypothesis that quiet zones directly beneath volcanoes is the hot magmatic system (plastic), whereas seismogenic halo is cooler (brittle) and signal of fluid egress. Similarly why do we sometimes, but not always observe the seismicity and ground deformation from these deep sources together? What are the causes of the deformation (or lack thereof) and how does it relate to the seismicity?
- Goals:
    - Plutons are larger than the portions active at any given time, can they be distinguished?
    - Why are the systems pulsed?
    - Detect magma sooner, interpret signals more accurately!
- What is the role in magma transport and storage of a possibly transient shallow chamber relative to a deeper hot zone?
- How much eruptible magma is there in a given volcanic system as a function of time, where is it located, and what variables control this?
- Large volume fluxes of basalt required to create and sustain a large (trans-crustal) reservoir and produce eruptible magma. Do we see evidence for this everywhere and does the mass balance work out? What about other heat sources?

3.2.2 Magma storage

The subsequent narrative can be expanded upon, if anyone is interested in doing so.

Magmas are stored in the crust feeding volcanic eruptions, magmatic-hydrothermal systems, and moribund plutons. The “storage container“ remains a central and useful concept when developing the process-based models for crustal evolution and volcanic eruptions. 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 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. Can we develop models in which primitive magmas naturally stall in the deep crust and that mature into observed arc sections? How long does this take? What is the vertical continuity of magma storage systems? How is that complexity best treated in a modeling framework?

The following is a collection of ideas and comments provided during the workshop and asynchronously, which still need to be integrated into a narrative.

- What is T and P of storage?
- What phases are present and much of each phase?
- Volatile content of magma - undersaturated or free fluid phase?
- Role of heat flow and crustal rheology on evolution and eruptibility.
- Open or closed system?
- Reaction kinetics and phase compositions.
- Crystal records are complex and suggest that erupted magmas are often assembled from multiple components. What is a useful approach to this complexity without oversimplification?
- Thermodynamics
    - Geothermometry.
    - Geobarometry.
    - Phase equilibria.
    - Equilibrium reference state
- Magma mush
    - Microscale observations of mushes are opening new possibilities that offer great opportunities for modeling.
    - What does a "living" mush look like? Hypothesis: granular dominated system. Concept of critical melt fraction obstacle to progress.
    - Long-lived reservoirs are active mushes in a time-averaged sense, with inactive solid regions at some times.
    - Cold storage norm rather than exception?

3.3 Eruptive magma ascent

This section will be addressed in future webinars. Are any webinar speakers interested to take a lead in writing this section?

3.4 Eruption plumes

Work in progress coordinated by Joe Dufek with contributions from "eruption plume" webinar speakers.

The eruption plume workshop encompassed the set of physical processes from the eruptive vent exit to long-range dispersal of pyroclasts in the atmosphere and final deposition. The workshop presentations and discussions focused on a range of research questions and strategies for collaboration, particularly those related to modeling these systems, ecosystems of models from research to operational models, and the incorporation and archiving of useful data. As much of our understanding of the deeper systems and their products are seen through the filter of plume dynamics much of the discussion focused on how to connect plume dynamics to the outcome of models focused on deeper processes (reservoir and conduit models) and how to link different scales of plume models in a model ecosystem. In particular, the multiscale challenge was discussed for predicting ash dispersal over long distances. Due to the immediate hazard implications of these dynamics there was a focus on integration and development of models that can be rapidly run on widely available resources such as volcano observatories. The discussion particular emphasized the flexibility of the collaborative to aid a range of code development projects.

The discussion identified a number of challenges to progress that a modeling collaboratory could provide the foundation to address. In particular, much discussion focused on the training of users/students on both the physical processes and mathematical/computational tools. One suggestion to address this was to conduct regular summer schools with an online component to reach broader audiences with maintained websites to link students to resources. Another proposal focused on the development of a postdoc program where postdocs would be embedded in research groups but would have some of their time devoted to developing computational tools appropriate to the application (developing GUIs, databases, organizing community workshops/classes, archiving data etc). It was suggested that a three year postdoc would be ideal for such a program to acknowledge the time constraints of community work and give the postdocs time to develop these tools and also build their research portfolios. One further challenge was seen as the limited availability of high-quality data to validate models, and one proposal for the collaboratory was to develop a repository for this data and to provide support for benchmarking activities. Another proposed collaboratory activity included placing satellite resources (and other data) in a common and user friendly framework and to organize modeling efforts to make simulations more directly comparable to available observations.

Ecosystem of Models

The discussion emphasized the utility of a range of model types and stressed the importance of the collaboratory in supporting development of both high resolution/multiprocess research codes along with reduced dimensionality codes that can be run rapidly or with more limited computational infrastructure. One suggestions for the collaboratory is that it could be used as a repository for benchmarking conditions and results and could also provide information on best practices and information about strengths/limitations of various modeling approaches. This discussion focused on a collaboratory that could potentially provide support/funding for a number of code development projects as well as infrastructure.

Eruptive plumes are hazardous for local populations, regional air quality, air traffic and a range of infrastructure. As a result, a modeling collaboratory could also support modeling activities that would aid the operational use of plume and tephra dispersal models. To make these simulations capable of rapid response and to be run by a broad community on widely available computation resources (desktop computers) much of the development of these types of models have focused on parameterized or reduced dimensionality simulations. Some of the ideal features that the group discussed include:

- Probabilisitic tools for tephra hazard assessment
- Development of computational tools (and resources) to conduct simulations during times of unrest.
- Incorporation of developing conditions/data into simulations to update forecasts for dispersion, aviation safety, and deposition
- Integrate model results with satellite observations and develop user friendly tools for placing multiple satellite observations in a common framework
- Development of user friendly interfaces (GUI, etc) to make these types of codes more accessible.
- Development of best practices procedures to improve the accuracy and communication of results.

It was also suggested that one role of the modeling collaboratory could be to 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 paramaterizations of some of these processes could eventually be incorporated in more rapid/reduced dimensionality approaches. One suggestion was in fact to use the collaboratory as a way of using research codes to develop user friendly modules/approximations. Some of the more challenging conditions/topics of current innovation include:

- Time-dependent inflow conditions based on conditions at depth (linking reservoir/conduit conditions to eruptive plumes).
- Compressiblity effects and choked flow conditions
- Entrainment in these multiphase systems
- Fluid-particle interaction and turbulence modification, and incorporation of new turbulence models
- Heterogeneity in near-field plumes

- A range of microphysical processes included aggregation, hydrous phase change, heat transfer.
- Rapid incorporation of eruption source parameters
- Communication between plume models with models constraining processes in the crust and in large scale atmospheric simulations.

4. Potentially relevant models

4.1 Overview

The study of volcanic systems is broad and involves complex multiphase flow governed by coupled thermodynamic and mechanical processes. Magmas originate as partial melts in the mantle with transport dominated by reactive porous-media flow. As they rise into crustal reservoirs magmas differentiate via fractional crystallization, assimilation, and mixing, and melt transport may become increasingly localized. Throughout this protracted crustal magma transport and storage, magmas exist as crystal-rich mushes and contain 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).

As magma rises, pressure decreases and volatile phases (H_2O, CO_2, SO_2, etc.) exsolve to form bubbles. This exsolved volatile phase tends to be mobile relative to the melt and also modify the bulk properties of the mixture (e.g., workshop presentation by C. Huber). Furthermore, crystals nucleate and grow in the magma due to decompression, cooling, and H_2O exsolution, further changing magma properties. For example, the viscosity of the bulk magma is a strongly non-linear function of melt composition, temperature, dissolved water content, and crystal volume fraction. Together these strongly affect eruption rate and style. Moreover, the crystals are the primary record of the assembly of cooling plutons and erupted magmas and reconstruct specific processes at depth.

The question of what range of models to be considered for a modeling collaboratory must be rooted in the primary science objectives defined during the workshop itself; 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); the ERUPT Report (National Academies of Sciences, Engineering, and Medicine, 2017); the USGS Plan to Advance Subduction Zone Science (Gomberg 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.

Much progress in understanding volcanic systems has been made by interpreting data using models developed for specific subdisciplines. For instance, geodetic data is typically inverted using kinematic models to provide constraints on the locations of magma reservoirs. Seismic tomography in conjunction with rock-physics models can constrain the fraction of melt within the crust associated with volcanic systems. Geochemical and petrological observations give clues about pressures, temperature, rates, and the compositional history of a magma. Furthermore, gas emissions yield information about magma flow rates and compositions. Segall and Anderson (2016) pointed out that a critical limitation of discipline-specific models is that they can only utilize a small subset of available observations. ***Yet, only models can provide the broader integration of observations that can lead to advanced syntheses and understanding of magmatic/volcanic systems***. More specifically, models that are based fundamentally on the physics of magma processes, in other words, transport, storage and eruption, can integrate diverse observations into a coherent synthesis. The latter may range in approaches from forward modeling to joint inverse modeling, with the additional challenge of needing to be able to cross a wide range of spatial scales.

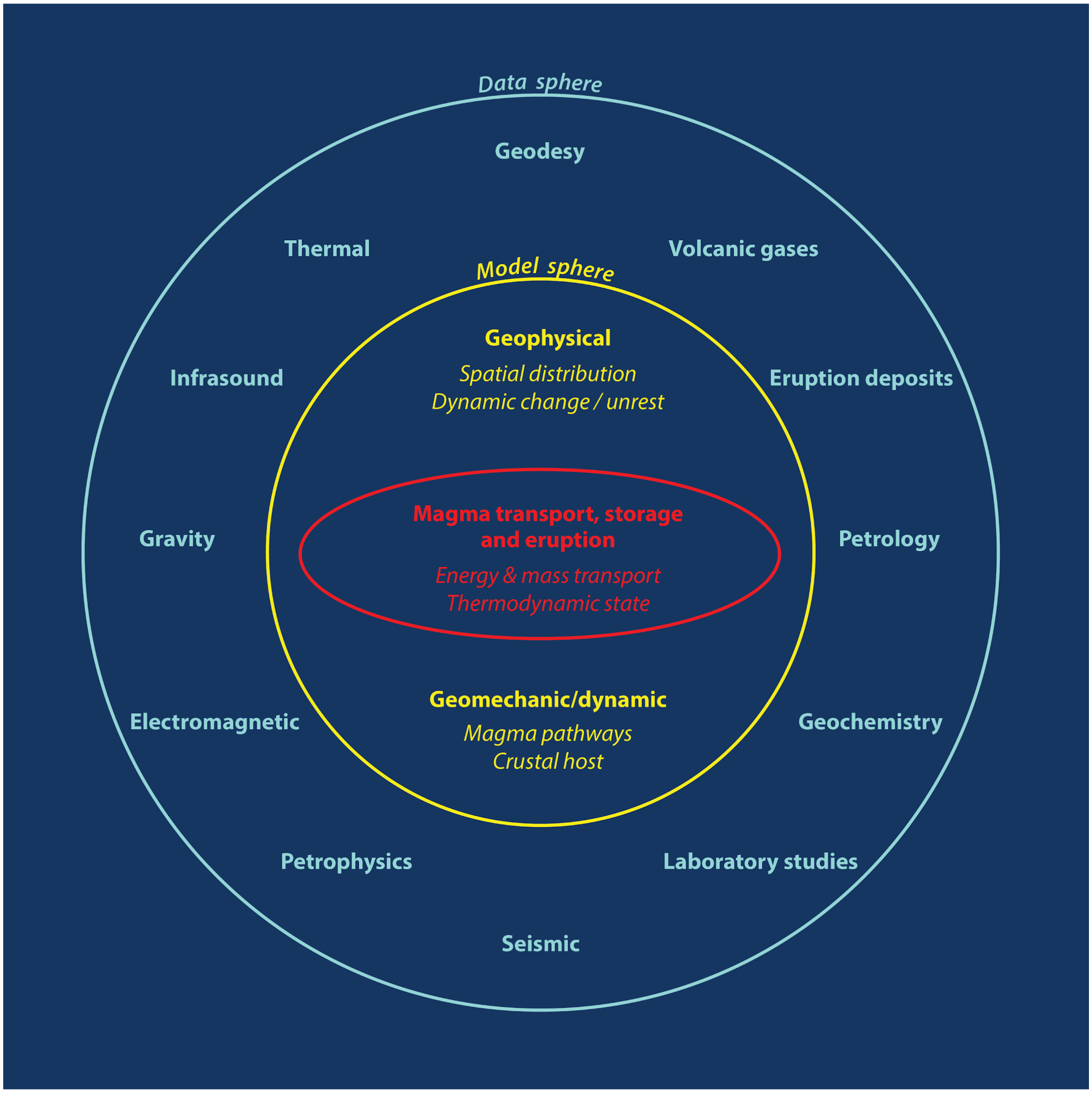

Figure 1: Magma transport, storage and eruption centric view of magmatic-volcanic systems modeling.

Thus, for magmatic/volcanic systems science, at the heart of a modeling collaboratory could be: (1) physics-based forward models of reactive magma transport, storage and eruption, which includes thermodynamics and reaction kinetics; (2) geophysical models based on inverse/parameter estimation methodologies and which constrain the presence and geometry of magma transport pathways and storage regions, as well as dynamical changes and unrest; and (3) geomechanical/geodynamical models of magma pathways and surrounding crustal host rock.

One key outcome of this workshop is ***the need to provide enhanced support for the development of a broad ecosystem of models,*** for only a critical mass of creative ventures at the individual PI level can ensure sustained innovation. Building blocks are common between domains. Examples include thermodynamics, rheology, multiphase flow. The central role for a modeling collaboratory would be to facilitate model accessibility and training, science collaboration, and interconnectivity between models and between models and observations. Integrated modeling, across a wide range of spatiotemporal scales, can provide the "glue" to pull the range of disparate observations together (Segall and Anderson, 2016). This requires ***sustained support for model development, model integration and collaboration, where integration requires sustained input from the observational community***.

4.2 Forward models of magma storage and transport dynamics

Work in progress C. Huber is working on it …

Magmatic systems are inherently multiphase, they consist of melt, crystals and sometimes exsolved volatiles. The complex thermal, mechanical and chemical interaction between these different phases control the evolution of magma storage regions. Moreover, multiphase magmas cannot be studied in isolation from their containers; various feedbacks between the reservoir and its host exert a significant control over the formation and growth of storage regions, the onset and modes of magma transport through the crust and the rate of cooling of the magma. The multiphase nature of magmas and the recognition that active magmatic systems are vertically extensive imposes a formidable challenge to the modeling community: ***models need to account for the formidable range of spatial and temporal scales involved in the evolution of crustal magmatic systems, from the discrete scale of the physical constituents (crystal, bubble) to that of the crust hosting them.***

4.2.1 Constitutive models

This section needs a champion.

- Rheology and challenges to go beyond effective medium approaches, mechanical and thermal properties of multiphase systems
- Parameterization for phase separation
- Thermodynamics (see 4.3.1)

4.2.2 Magma storage and transport models

George Bergantz, Matt Jackson, Chris Huber said they would contribute. The state-of-the-art, challenges, opportunities, future needs, opportunities, and how a modeling collaboratory could further progress on these models. Other contributors are welcome.

With the recognition that magmatic systems are vertically extensive and involve predominantly crystal-rich magmas, the modeling community has increased efforts towards understanding the multiphase nature of these magmas and how it affects the transport of magmas, their emplacement and the growth of crustal magma storage regions. These magmas are in thermal and often chemical disequilibrium with the host crust, which drives magma cooling, crystallization and chemical hybridization. Mechanically the crust is not passive, its stress state and rheology do not only influence magma transport, they also affect the evolution and growth of magma storage regions over time.
The petrological diversity of magmas observed on Earth is primarily caused by the physico-chemical processes that take place in magma storage regions. Over the past decades important observations have shaped our current understanding of crustal magmatic systems. Magmatic systems are long-lived, but episodes of growth seem to occur by pulses. From a mass balance standpoint, the emplacement of large chemical evolved magmatic systems requires significantly larger inputs of primitive magmas and the loss of these mafic roots (delamination). Overall crustal magmatic systems require an incubation period before being able to generate colder and more evolved magmas, a process generally referred to thermal maturation. While these observations put important constraints on models of magma transport and storage, they also prompt important questions:

- For arc trans-crustal magmatic systems, can we develop models in which primitive magmas naturally stall in the deep crust and that mature into observed arc sections? How long does this take? To make progress on this question requires knowledge of the aperture of the magmatic feeding system. Also, what is the temperature in the deep crust? What is the vertical continuity of the magmatic system? Where do the intrusions store or stall? What is the overall magmatic flux?
- Do mantle-supplied magmatic input rates control magma storage depths, crustal residence times, and erupted magma composition? If so, how? Relationship between the rate of mantle-supplied magmatic input and magma storage depths, crustal residence times, and erupted magma composition.
- How much eruptible magma is there in a given volcanic system as a function of time, where is it located, and what variables control this?

These questions are challenging, in part because they involve the complex interplay between multiphase magmas and their crustal host and because they span a wide range of temporal and spatial scales. In fact, recent studies have highlighted that the mechanics of phase separation, central to crystal fractionation for example, is modulated by interactions among the magma constituents (individual crystals, exsolved bubbles, melt) at the discrete/granular scale. Yet the questions listed above (as well as many others not discussed here) require a modeling framework that would couple the magmatic system and its host over time scales of millions of years and over scales of tens of kilometers.

Future modeling studies will have to contend with the challenge of scales and that effort involves three aspect of modeling that will have to be further developed: (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 will evolve with the understanding of the physics at the granular scale and (3) new upscaling paradigms where homogenization methods are tailored to faithfully serve the complexity of the granular models. A Modeling Collaboratory would be placed ideally to help our community address these three needs. It 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.

Crustal magma storage and transport models require supply of melt from the mantle, but this is poorly constrained observationally except perhaps on very long (arc-building) timescales. Its also not clear what controls the spatial evolution of transport pathways, which likely influence (but may or may not be a primary control on) surface vent or shallow storage locations. An MCS could provide support for an interdisciplinary look at this deeper component of magma transport, including the lithospheric mantle, which naturally connects to deeper fluid transport and the issues raised in the MCS fluids workshop report.

4.2.3 Eruption models

Are some of the webinar speakers interested to help writing this section? For example, *Mattia de' Michieli Vitturi, Joe Dufek, Larry Mastin, Eleonora Rivalta, Other? This would encompass: conduit, dike, eruption plumes. Includes a thorough discussion of multiphase flow.*

4.2.4 Multiscale dynamical models

Here discuss multiscale issues for both "crustal" magma dynamics and eruption dynamics. This section is seeking potential writers.

4.3 Inverse and data-driven models

As our community seeks to develop models that capture/predict the evolution of magmatic systems, the development of data-driven models, which draw information from field, petrological, geochemical and geophysical analyses is a crucial step to provide constraints about the state of a magmatic system at discrete points in time. The datasets that feed these models include the chemical composition of samples, outputs from petrology experiments, elemental profiles in crystals, geodetic and geophysical signals. The following sections provide a brief and non-exhaustive sample of models that utilize these datasets to infer/invert for the prevailing thermodynamic conditions, timing of potential perturbations perturbations and the topology of magma storage regions.

4.3.1 Thermodynamic models

Mark Ghiorso will contribute to this section. What about volatile solubility models, ask if Madison Myers is interested to contribute to this? Other contributors are welcome.

4.3.2 Kinetic models

Here discuss diffusion and crystal growth models. Philipp Ruprecht will take the lead. Other contributors are welcome

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 increasingly fine spatial and temporal scales to infer how magmas change 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 (see Section 4.3.1). However, during times of magma transport and mixing magmas are substantially removed from equilibrium conditions and the system responds by phase change and/or diffusive equilibration where kinetic models provide detailed information about the length- and timescales of specific magmatic processes. Different classes of kinetic models have been developed. A large community has documented diffusive elemental gradients in crystals and melts that emerge when crystals and melts are subjected to changing pressure, temperature, and/or composition. Here a large family of models has been developed that solve variations of the diffusion equation. However, it has been increasingly recognized that crystal growth or dissolution can in some instances be superimposed on emerging diffusive gradients, thus having led to the additional development of moving boundary problems. Such combined effects can be revealed using elements of different diffusivities as well as the differential diffusion of lighter and heavier isotopes (e.g., Mg-24 vs. Mg-26 or Fe-54 vs. Fe-56). Other kinetic models focus specifically on phase transformations. This includes the kinetics of 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 is connected to the textural observations we can make in erupted products or exposed, plutonic rocks. E.g. rapid versus slow crystal growth related to the degree of undercooling leads distinct crystal habits that range from skeletal, dendritic to polyhedral as well as from more acicular to more isometric crystal shapes. As these models become increasingly sophisticated they can be tied back to the thermodynamic drivers that not only includes partitioning, but also aspects the controls such surface tension and energies, defect structures within crystals, and the development of boundary layers at sites of phase transformation.

There is increasing need to integrate these kinetics model with the system-wide drivers such as cooling or ascent rates that are independently determined by other types of model or direct and indirect observations. Thus, the petrology community now has a broad tool box derived from experiments and natural examples that can be directly compared against geophysical, gas emission, and deformation datasets to understand in much more detail the processes that happen near the surface in the storage regions as well as in the conduit. They provide unique constraints then for fluid dynamics models that explore the non-linear behavior associated with changes in viscosity, density. Increasingly these models start to resolve processes that incorporate 2D and 3D effects such as boundary layers near the conduit walls or within the magma storage system. As a result we can study the non-linear feedbacks between degassing, changes in crystallinity and chaotic fluid flow.

On top of these first order observations, kinetic models are increasingly tested with statistical tools e.g., Bayesian and Markov Chain-Monte Carlo methods. All these represent an increasing number of interrelated and integrated models that need to be curated, advanced and to some extend standardized so that results can be compared and individual case studies are synthesized into a greater understanding of magmatic processes.

4.3.3 Geophysical models

This section is work in progress by Matt Pritchard and Emilie Hooft. Other contributors are sought and welcome.

Geophysical observations provide subsurface constraints on the rates, volumes, and melt distributions in magmatic systems, but they suffer from limited resolution and inherent non-uniqueness. To overcome these limitations, different, yet complementary, geophysical approaches must be combined with petrological, laboratory, and geochemical measurements in forward and inverse models to bound the architecture and dynamics of real magmatic systems. Recent progress has been made by development of three or four dimensional petrophysical models showing the inferred extent of partial melt and volatiles at several subduction zone volcanoes including Soufriere Hills Volcano, Montserrat (SEA-CALIPSO), Mount St. Helens (iMUSH), Uturuncu, Bolivia (PLUTONS), Laguna del Maule, Chile, and Santorini, Greece (PROTEUS). In particular these projects demonstrate the value in using multiple, dense geophysical datasets combined with petrology and geochemistry to consistently interpret different types of data and to determine whether anomalies are caused by partial melt, brines, sulphides, or other petrophysical characteristics.

A modeling collaboratory should leverage work from these and similar projects to develop the next generation of models, especially by developing joint inversions that explain multiple (possibly all) datasets to help answer the scientific questions posed in section X. The diversity of geophysical data 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); gas and thermal emissions. There are several approaches to joint inversion for magmatic system architecture with promising results to date, but there is still much model development to be done, especially with linkages to petrophysical models using laboratory results (see for example the SIGMELTS program for electromagnetic data). During periods of unrest, explaining the temporal evolution of multiple datasets simultaneously in a rheologically heterogeneous subsurface model consistent with all available data is discussed in section Y. A collaboratory should also facilitate the sharing of model results, such as the IRIS repository of geophysical models: ds.iris.edu/ds/products/emc-earthmodels. An MCS that facilitates sharing of models and 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. We expect that the 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.

In its current state the remainder of this section represents a collection of ideas and comments provided during the workshop and asynchronously. It requires further work and writers are welcome.

- Discuss Activity/Unrest
- Dikes.
- Rock deformation.
- High-resolution imaging of transcrustal magmatic systems
- Geophysical signals of fluids vs. magma.
- Not a single "tool" we should be using to study volcanic systems. Use multiple geophysical techniques and petrology.
- There is value in comparing different volcanoes.
- Studies of a small number of volcanic systems that are densely instrumented and comprehensively studied for their magmatic history.
- "Modeling" means a petrophysical model that explains one or more datasets: deformation; seismicity; seismic P&S wave velocity, attenuation, anisotropy; electromagnetics; gravity; gas and thermal emissions.
- Value in "global approach" --- studying many volcanoes (deformation) and synthesis with all geophysics data
- Joint inversion is an important goal (SHV example). Develop new algorithms.
- Need for modern dense geophysical datasets at volcanoes. Need targeted additions to what we have.
- Closer linkage between volcano drilling and geophysics, including new drilling.
- Sharing geophysical images (ds.iris.edu/ds/products/emc-earthmodels)
- Petrophysics --- models to convert geophysical inversions to rock properties.

4.4 Model integration

This section remains to be fleshed out, perhaps following the 4th theme webinars and planning meeting. Who would be potential contributors? Volunteers needed.

A means for integrating (combining) the models from the four process-focused themes above. For example, a coupled reservoir-conduit model would fall into this category. This would be important for understanding unrest (certainly that is the point of the forecasting part) but the integrative part would be more than that, it would also be a framework in which different volcanic system "submodels" would be combined -- a long-term aspirational goal both here and in the ERUPT report.

4.5 Data assimilation and operational models

This section remains to be written, perhaps following the 4th theme webinars and planning meeting. Potential contributors: Grace Bato, Kyle Anderson, Patricia Gregg, others are welcome.

- "Data assimilation is also a powerful tool for hindcasting and investigating the evolution of a system through time. I would say that forecasting is a very minimal portion of data assimilation. Rather than thinking of it as a forecasting method, I would frame it as a way to combine models and data in a statistically robust way to investigate the state of a system." [Patricia Gregg]

4.X Box models (from Leif Karlstrom)

I believe that there is broad agreement (and by that I mean agreement with data and continued use/development) of simplified box models for crustal deformation, chemical evolution, and multiphase transport associated with the magma transport system. Such models continue to be the best that the data can resolve (e.g., shallow Kilauea magma reservoir - the best instrumented on Earth - is indistinguishable from an elipsoid in an elastic halfspace), and can be straightforwardly upscales (through boundary/initial conditions) and downscaled (by providing time-evolving thermodynamic state). An MCS could support the development of community model(s), with benchmarks and an integration framework up-and-down scales (perhaps involving hired software engineers to implement ever-more-complex rheology and physics). This will not replace development of new modeling approaches, which must be at a PI level in my opinion. But box models have not been put their paces yet (huge range of parameter exploration and sensitivity yet to be explored) and these stand to be the best place to integrate diverse data from geophysics, petrology, and geochronology. I'll comment below as well in the text, but want to emphasize that this is not the approach outlined here - and I think it should be considered...

[Do we need a section here spelling out limitations in the way models are currently built/used in volcanology?]

5. Organizational vision for a Modeling Collaboratory

Comments and suggestions to this section are welcome.

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 underlying subduction zone geohazards, which requires the synthesis of data using process-oriented models.

The process of model generation is complex. Models are first class objects in that there is as much research and intellectual effort that goes into the generation of models, as there is in gathering measurements and observational data. Consequently, models have to 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.

Within the subduction zone setting, and beyond, magmatic-volcanic systems encompass a remarkably broad and complex range of physical and chemical processes. 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 represent the state of the art in terms of theory and numerical methodologies, albeit adapted to the needs of simulating magmatic and volcanic systems. A broad range of modeling strategies is applied to study magmatic systems, their application depends on the science objective as well as the type of data it connects to. For instance, the study of magma transport processes requires sophisticated multiphase models as detailed in previous sections. These models, which are by and large still in an early stage of evolution and are in a constant flux of active development, form the basis for numerical simulations. Other models are designed to specifically integrate various streams of observations to advance understanding of the underlying physical processes that give rise to the observed phenomena. Complementary to these process-oriented models, sophisticated numerical methodologies are required to transform observations into models of spatial and material properties of magmatic systems and surrounding host rocks, or to identify signals of unrest.

All of these different types of models are not only the basis for simulations aimed at yielding a deeper understanding of natural processes, but the models themselves are scientific outcomes in their own right. Consequently, to advance hypothesis-driven science objectives surrounding magmatic-volcanic systems requires a critical mass of geoscientists that are equally skilled in model development and in the subsequent application through **collaborative model simulation**. In other words, to advance science objectives, there needs to be a sufficiently large and deep pool/pipeline of scientists that are rooted in the geosciences, who are trained to be equally adept at understanding complex geological systems, at advanced numerical methods and their implementation through simulation, as well as the integration of diverse geo-datasets into simulations. Augmenting and sustaining this pool of geoscientist modelers is a necessary requirement and a fundamental challenge for nurturing a striving and competitive geoscience program for the 21st century. Volcano science has benefited from model and numerical advances in other fields, for example engineering of high speed compressible flows. Many currently used models are derivative products of other fields, slightly tweaked for volcanic settings. However, with more investment in modeling, volcano science could reverse roles and 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 and volcanology occupies a broad range of parameter space shared with other fields.

Achieving this goal requires enhanced investment in projects involving model simulation, as well as students and postdoctoral researchers who are focused on the development of the prerequisite numerical models. This vision is distinctly different from the paradigm where a majority of support for geoscience modeling is tied to hypothesis-driven projects and contingent upon the prior existence of modeling capabilities, and where progress toward the overarching science objectives will be hobbled. 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, that is observations of volcano deformation, requires the development of sophisticated algorithms. The latter constitutes model development, which is science that 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. In summary, a competitive science program for magmatic and volcanic systems, whether within the broader SZ4D objectives or beyond, requires sustained support of students and postdocs engaged in model development as well as collaboration with experimental and observational scientists through hypothesis-driven model simulation.

5.1 Grants for model development and collaborative modeling

Comments and suggestions to this section are welcome.

A vision for a Modeling Collaboratory encompasses ***Modeling Collaboratory Grants (MCG)***. Such grants would provide support for students and postdocs in order to establish and sustain a pipeline for geoscience modelers. The need of such a grants program 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 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 magmatic/volcanic 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) are to some extent tied to the aforementioned requirements that make models viable for collaboration: benchmarking, documentation, publication and archiving, accessibility and training.

In summary, within this vision the Modeling Collaboratory Grants would support the development of multiple sets of numerical models through graduate student and postdoc projects. The grants could augment hypothesis driven science grants, but would predominantly be full grants in their own right.

5.2 Modeling Collaboratory Network

Comments and suggestions to this section are welcome.

The aforementioned grants program would be complemented by a ***Modeling Collaboratory Network (MCN)***, which would be tied to the Modeling Collaboratory Grants in terms of scope. In other words, the size and budget of this network should be proportional to the grant program itself, in order to assure optimal resource allocation to students and postdocs. A Modelling Collaboratory Network would consist of staff with expertise in computer science, applied mathematics, as well as a collaboration coordinator for workshops and training activities. All staff would primarily be dedicated to working with the grant recipients. Their role would be to assist in model benchmarking, documentation and interconnectivity, as well as facilitating training, workshops, and summer schools. Although a number of these activities would be hosted online, there is value in in-person workshops at various locations and which would be facilitated/organized through the Modeling Collaboratory Network. The MCN staff would be hosted by different institutions, with some sort of rotation that is realistic in terms of assuring continuity and overall employment considerations. For example, postdocs and/or programmers could be hired according to special projects proposed to MCS, somewhat akin to SCEC, with duration of at least 3 years (for continuity).

A potential alternative or complement to a Modeling Collaboratory Network could be a Modeling Collaboratory Center, but at this stage there hasn't been sufficient workshop discussion to resolve the question of how much centralization (Center) versus decentralization (Network) a Modeling Collaboratory should entail.

In addition the Modeling Collaboratory Network could also serve as a data hub for collaborative data integration within model simulations. To what extent this would require an investment in hardware infrastructure versus being cloud-based remains an open question. Furthermore, there are already ongoing SZ4D proposal activities related to database/data dissemination cyberinfrastructure. Regardless, within the context of SZ4D a Modeling Collaboratory Network would serve as ***the nexus between data acquisition, processing and dissemination, and data integration within models***.

Collaborative modeling should encompass several key facets, as highlighted during the MCS RCN Volcanic Systems Workshop. Many of these would benefit from the activities that could be facilitated through a modeling collaboratory center:

- Model verification, validation, and benchmarking.
- Model documentation.
- Connectivity across models.
- Open source model code.
- Workshops and summer schools aimed at
  - Facilitating model development and interconnectivity
  - Training modelers
  - Educating non-modelers; fostering collaboration between modelers and non-modelers to enhance the integration of observations through modeling, perhaps leading to an interdisciplinary proposal incubator.
  - Enhancing collaboration between geoscientist modelers and expert communities outside the geosciences, such as applied mathematics, physics, statistics/data science, and engineering.

5.3 Activities facilitated by a Modeling Collaboratory

5.3.1 Workshops, working groups, summer schools, cooperative research gatherings

This section remains to be written. Potential contributors/leaders are sought. Potentially 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.

- Why have these [what to do call them in general? Collaborative gatherings??
  - They are a way to get outsiders interested in our science questions.
  - Forge and strengthen collaborations
    - With Volcano Observatories around the world to overcome barriers to collaboration.
    - Opportunity to network and meet people who are doing similar work promotes new collaborations (in avenues like this workshop).
    - Across disciplines

        - Help researchers to stay connected and working together over longer time periods
        - Focus on collaboration rather than competition
    - Ideally, PIs could come together and develop new projects that would advance the state of the art beyond what is possible in a single (even collaborative) project.
    - We all agree workshops are useful, but are smaller workshops (ex: two 8-hour days) actually useful in changing the way researchers approach their models? Or are shorter workshops mostly useful for exposure? Answer: Workshops should have a longer-term group for reinforcing the goals of the workshop, such as by helping a researcher adapt the workshop's lessons to their own work.
    - Maximize the engagement of the community (in terms of numbers and/or subdisciplines)
    - Reach both the students that are the next generation of experts, but also the students that need to be at the interface of experts and observations
    - Develop the community so that long-term curation and advancement is done by the community and not individuals (e.g. how do the atmospheric sciences advance their community models that complexities across scales and different components such as thermodynamics versus fluid dynamics)
    - Volcanology is very fragmented in the US across states, institutions. We risk becoming very siloed, and models reflect this.
- What is the current model for this?
    - Small focused meetings, often arranged around conferences, often with training as a primary goal
    - CIDER
- Why isn't that good enough?
    - CIDER is not focused on volcanology (except one very successful meeting) [say something if we can about how popular/oversubscribed it was]
    - Arranging takes a lot of effort; need support to make them more common
    - Rarely interdisciplinary
- What form would they take and who would they be for?
    - For who?
        - Both modelers and non-modelers
        - Mix of early career and more advanced scientists
        - Not only volcanologists, but also applied mathematicians, computer scientists, etc. (see next subsection)
        - Couple modelers with petrologists, geophysicists, etc. ("observational " and "experimental" scientists)
    - Common mechanisms could be workshops/Hackathons (CIG model), summer school that could be either centralized or operate similar to e.g. CIDER (rotating group of community and focus)
    - Detailed mapping/analysis of past eruption products
    - Studies of exhumed plutonic systems

    - Test the feasibility of joint inversions of observations on subsets of observations to increase understanding as we work toward integrative models (i.e., joining limited numbers of different datasets first. Get more consistent interpretations as one incorporates other types of data).
    - Allow feedback from users of the models in order to validate the results (for instance, using field data) and to request improvements / adjustments in the models.
    - Need to acknowledge the Zoom era. These could be a mix of remote and in-person
    - Short courses in how to write code for high performance computing. There is too much time spent relearning code or best practices
    - Communicate what can be done by experiments to modellers (and vice versa; or field geologists and geochemists). Design studies together from the beginning.
    - Task forces that develop best-practice recommendations for data gathering and reporting in order to improve their multi-use in models and beyond (what are the barriers to model reuse and extension?) - In this regard, can there be training for the community to generate such interoperable data sets? I think especially the petrology/chemistry community needs a little bit of help to make our data more useful to the modelers and geophysicists
    - Integration of observations from ***Notional SZ4D Experiments and Instrumental Deployments*** through process-centered conceptual and numerical models, perhaps facilitated by workshops.
    - Putting modelers and data people together; just knowing how to format data so others can use it is important (can also consider connecting with cyberinfrastructure aka EarthCube
    - CIDER-style summer school seems like a valid format to bring the community together with an emphasis on interdisciplinary exposure
        - Brings in multiple perspectives together, at least for developing a jumping-off point for the different working groups
        - This style really benefits modelers because it is more convenient for getting to an end product (data mining)
        - For modelers, provides exposure to other models and ways people have gone about answering different questions.
            - Do we present data and use that to think of ways to further develop models (concern about data sharing, credit)
                - Could we use this to setup much LARGER collaborations (longer author lists)
        - Difficult to play a primary role in these style meetings when you are an igneous petrologist/geochemist/etc.
        - If this is the birthplace for ideas, what way can we further support and push these collaborations through to fruition
- Workshops - how do students and researchers get more out of this?

  - Shorter workshops are great for exposure and a crash course in the model/code, but it is not always an easy task to then utilize it in their own work
  - Can we develop some kind of community resource/communication as a resource afterward for when you are trying to adapt these codes or models to your own work?
    - Again credit, larger collaboration possibility, networking, developing longer author lists
- Coordinate small, focused, collaborative workshops:
  - *Specific science topic*. Address a science question, such as magma ascent in a dome-forming eruption. Could be bi-disciplinary (e.g., modelers and petrologists) or multi-disciplinary. Inclusion of non-modelers is important.
    - Idea (LK): multi-year workshop sequence (perhaps 2 years with in-person or virtual meeting every 6 months?) focused on topics that are outside current modeling capability. Several examples
      - Conduit shape evolution and en echelon fissure system dynamics
      - What controls magma transport in the mid/lower crust
      - What controls the temporal and spatial variability of magma transport into the crust from the mantle
      - Eruption cycles in distributed volcanic fields
  - *Geographic focus*. Focus on a particular magmatic system or volcanic region (there is value in systematically investigating a whole arc or an arc segment.) Participants bring datasets and observations, and during the workshop combine the data into a single context. Even just putting all relevant data into the same format and plotting it together is very useful and is not done frequently. The workshop would meet once to present and discuss data, adjourn, and then come back a number of days later with a specific product that combines data sets in some way. This could lead to putting several sets of data into one integrated geomechanical model and making predictions to test hypotheses. [Collaborative work on a certain geographic setting will get people from different disciplines working together in order to attract multiple tools and perspectives. We need to identify locations, this will also allow the projects to get funded. We need to pick a few locations that will attract sufficient funding for sustained and coordinated efforts. Pick locations where phenomena occur that are of interest for different disciplines. For example if in a location two systems are adjacent and portray differences, then this is going to generate transformative science questions.]
  - *Model focus*. For instance, focus on geodynamic models and see how to fit observations using seismic imaging help constrain the starting model. This could include training of non-expert users (developing toolboxes,

basic models, training data sets, being more educated in manipulating existing models)
        - Idea (LK): Develop a community hierarchical crystal/bubble growth model, with benchmarks for different scenarios to explore uniqueness and resolving power (e.g., purely 1D sphere in hexagonal lattice, poly disperse distribution with continuum description, fully phase resolved)
        - Idea (LK): Develop a new set of conduit flow model benchmarks, aimed at non-equilibrium and transient effects.

5.3.2 Interdisciplinary collaboration

This section remains to be written. One of the 26 March breakouts could be dedicated to fleshing this section out. Potential contributors/leaders are sought.

- Collaborating with 'outside' experts (mathematicians, statisticians, computer scientists, engineers) can increase model efficiency, increase confidence in results, and enable an ability to tackle more difficult problems. Other communities have already solved some of our problems, or are well-positioned to help us do so. Some examples:
    - Computer scientists and IT professionals can help with code structure, optimization, parallelization, utilization of computational resources (memory, CPU cores, storage capacity)
    - Statisticians can assist with understanding the significance of results (e.g. how representative a crystal population is), Bayesian statistics, and a general move away from basic Gaussian approaches.
    - Machine learning while ground truthing results for a volcanic system (e.g. considering observations) (?)
    - Need to connect with earth surface processes community, who have a substantial modeling framework and community in place (CSDMS) and many similar science questions. For example, the question of eruption record completeness is perhaps better posed a geomorphic than volcanbologic question (what is preserved, how do we interpret stratigraphic columns of spatially discontinuous deposits, how does chemical weathering impact interpretations, etc).
- More interdisciplinary exchange would further the goal of code development. Would be useful to see people do modeling in a different way, but also to see people who have data and want to turn it into a model but don't know how, or who have two convergent datasets they want to bring together.
- How to get there?
    - MCS is a central link between our science and the outside community
    - Develop relations with outside academic departments
    - Widely publicize interesting problems to solicit involvement by outside experts. *This is a mechanism for matching expertise with problems*, and could work within the volcano community as well (not just outside experts)

5.3.3 Development of open-source, well-documented, interoperable model codes

This section remains to be written. One of the 26 March breakouts could be dedicated to fleshing this section out. Potential contributors/leaders are sought.

While there are many modeling problems in volcanology that are in early/developmental stages, there are a few models that have wide community buy-in and have been applied to interpret multiple different types of data over a range of scales.

For example, “classical” magma chamber models, describing magma storage as a fluid inclusion in an elastic halfspace, are regularly applied both to active volcanism (e.g., Kilauea, MSH), 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. There is no common set of benchmarks for these problems, and no common open source framework for exploring the models that is accessible or comparable between groups. This would be a fairly easy and high-reward MCS target: these models will undoubtedly see much more use, as they can be easily adapted to upscale or downscale to match petrologic, geophysical, or geochrolonic data. Currently the lack of rigorous uncertainty quantification in these models (especially with respect to the nonlinear dynamics of eruption cycles) inhibits progress.

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.

- Model generation and documentation is as important an activity as the generation of observational data. Code must be easy to configure, use, reuse, and extend and scale. It should be accessible and citable. Models should be interconnectable using standardized APIs and other inputs/outputs. Models should not be disassociated from their underlying data resources. Models should be maintainable and updatable by a community of model users.
- At present there is limited incentive for "research" models to be documented, benchmarked, open-sourced, etc. "Releasing" a model in an openly accessible and documented manner requires time and effort that is currently not rewarded. This is the major obstacle that must be overcome. Firstly, through funding to model developers. Secondly by developing a system that makes "released" models publications in their own right, assigns citable DOIs to models, tracks model access and usage, and gives model developers an optional stake in projects that use their models. The status quo where model development is inadequately funded, yet free sharing of models is expected, is neither tractable nor sustainable. In other fields, such as applied mathematics, incremental advancements in methodologies constitute bonafide publications, why not in geoscience?
- Important to advance goal of code development too. Now, code development is often done on the side and there is not enough motivation for researchers to develop new

code. Researchers need more support and acknowledgement/reward for code development.

- Open source codes permit anyone to examine and test, making them more robust
- 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.
- These goals require that code be validated, well-documented, and (usually) maintained in open-source community version-controlled archives (git-based)
- Relation to other community efforts?
- How to get community buy-in?
- Documenting inputs and outputs will reveal how codes link together like lego blocks.
- Agreement that there needs to be a community go-to group, because modelers often feel geographically isolated (ex: they are the only grad student at their school working on a certain field) and open communication channels within the community would encourage networking and collaboration. COVID has helped bridge the gap somewhat, since people no longer have to travel to attend workshops, so collaboration has become easier but still more to do. It has encouraged more international collaboration, which we want to encourage.
- When we do laboratory experiments, we often hire a technician to help run the experiments. But we don't do this with our code. We need to hire someone from IT that can help us make our code be best-practice, better, "in the right way form the beginning"
- Codes as Python (etc.) packages -- broader use (e.g., DensityX)
- Small size of our community realistically limits the size of research groups, complexity of software. Need to use existing codes as much as possible. For instance, use OpenFoam as a foundation. But -- if you want to add your own code on top, it can be very challenging unless it is very simple. Having a CS person alongside can help develop understanding. The CS person can act as a translator (this part of the code does this, this does that). This can save a lot of time.
- Importance of crossing fluid-solid boundary. Coupled conduit and plume modeling. Seismic excitation is one place where there has been coupling of fluid and solid
- Real need for IT support from the beginning. Funding needed for scientific programming.
- "There is an implicit assumption that there will be some massive simulator that you can drop a scientist into. To help the community, maybe we need an atlas of highly resolved small models that capture small constitutive processes. Don't try to do everything at all scales at the same time. Make the scrap-book of different types of highly resolved simulations - or modules. It is fine that these different models are done in isolation. Trying to make the combined super model is probably not the way to go.
- Barriers
  - It takes a lot of effort to make the code nice and clear. Time is the biggest barrier to open source
  - Where does funding for this come from? Trade-offs between model development and other activities in terms of funding
  - Time scales of academic success are not consistent with long term code development. This favors a community approach to these codes.
  - Don't want people to use it yet?

    - Embarrassing cludges?
    - Code development at PhD or postdoc level, and then they have the expectation to publish good science paper to get a job. They are not incentivized to document the code and make it more accessible and/or open source. How can we as a community provide incentives and rewards for the extra steps of making code accessible? Or are we better off hiring some computer scientists that we can say "here, make my code open source". So -- incentivization.
    - Where is the reward for doing this? Is a DOI number enough?
    - Unwilling to do user and tech support
    - Everyone has their own coding habits, variable names, etc.
    - Most of us not experts in programming
    - Afraid to share programs that are not fully finished
    - Protecting own research? Maybe not a big concern.
    - Every code has a lifetime. The moment you hit compile, the code is already beginning to expire. How much time / effort/ money do we invest in keeping code alive? In documenting it?
- Other examples
    - European CHEESE initiative. Numerical codes to exascale with partners experts in mass computing. Primarily good for developing parallelisation and HPC for the codes
    - Caltech - CLIMA - new set of climate models. Brings together computer scientists, mathematicians, etc. Facilitating group discussion
    - Weather forecasting models, science tool + forecasting tool
    - Eurovolc project, possible to give virtual access to some software codes, Pisa - several codes including source and executables, surprised by number of people who downloaded and used the codes, that computational models in demand, 3 codes offered, several hundred downloads
    - Volcanology example: MELTS. "Collaborations within the community, MELTS took a long time for others to use, MELTS - physics is pretty settled in the community, whereas mixture theory, constitutive relations not totally settled yet, issue with validation datasets, end product that goes to public (i.e. other modelers) needs to be a very reduced order model, who is the audience of this collaboration?"
    - US national labs. They are charged with having academic partnerships of some sort, and often have world-class codes.

- A related issue: Sharing of model results (e.g., 3D seismic inversion results)
- How do we get there?
    - Establish standards/best practices
    - Promote the publication of models, which should have a DOI and be citable. This also requires long-term archiving.
    - Jupyter Notebooks, for example, would work well for this. Traditional papers are static, data resources are seldom completely referenced, software resources are seldom adequately documented. Package analysis, data and software into

replicable and extensible documents (e.g., dynamic notebooks). Open questions: How to "protect" intellectual effort? What would be the incentive/award for doing so?

  - Need to define interoperability; inputs/outputs documented (e.g., sometimes can treat codes as black boxes -- still useful).
  - Encourage participation and engagement, cultivate user base (how?)
  - Facilitate model extensibility and maintainability (how?).
  - More centralised approach?
    - Someone to help developing, documenting?
    - Someone to teach best practices?
    - Some sort of training about how to share codes online, experience with codes outside geophysics, afraid to share programs that are not fully finished, but other IT communities are doing this well -- what can we learn?
  - Can be promoted/incentivized using model validation/verification/benchmarking meetings

5.3.4 Development of reusable model building blocks

- Lego-block approach: Develop sub-system (component) models (e.g., rheology) that can be coupled with one another to facilitate construction of larger system models.
- MCS would facilitate identification of suitable building blocks, hosting the models and their documentation (also validation etc.). A central facility would make the community aware that these building blocks exist, encouraging their use.
- Building blocks for a "lego volcano" that currently exist and could provide a useful starting point for MCS: 1D transient conduit flow models. Magma reservoir models in the "lumped parameter" framework with flexible ICs/BCs and crustal rheology, 1D/2D/3D thermal conduction model with simple equilibrium petrologic coupling (f-T or MELTs)
- What about subsystem models?

5.3.5 Development of models that cross boundaries of disciplines, problems, and scales

This section remains to be written. One of the 26 March breakouts could be dedicated to fleshing this section out. Potential contributors/leaders are sought.

- 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.

5.3.6 Code verification, validation, and benchmarking

This section remains to be written. Potential contributors/leaders are sought. Note that a lot of this is much more general than the volcanology community. Should this text focus on volcanology? ***[some overlap here with earlier section on documented, open-source codes]***

- Verification, validation, and benchmarking are critical for model success. Benchmarking can be done against analytical models, other numerical models, and field data. Many advantages:
    - Code is more trustworthy
    - Outputs from different models more directly comparable
    - Users can better understand model uncertainties and limitations
    - May guide the observational community to address key data limitations
    - Improved understanding of how parameterization and initial conditions affect results for different models
    - Community codes can be validated just once and then used (trusted) by the community (see next section); much less work than each group developing and validating their own models
- These are rarely done carefully though
    - They require a great deal of effort and there are few direct rewards
    - Non-trivial amount of work to make such comparisons
    - Can’t always get other codes for intercomparisons
    - Community level effort needed
    - May be relatively little reward for all the work required to validate, document, maintain code.
- What do other communities do?
    - ideas with creating DOIs that make code citable
    - Community supported facility
    - Review for inclusion in community archives/repositories (e.g., The Comprehensive R Archive Network).
    - Community comparison process/facility
        - Southern california earthquake center - software that can be used directly once agree on problem and conditions
        - Computer vision community
- Some community benchmarking efforts have occurred in volcanology as well
    - lava flows, ash plumes, conduit models (need to cite these), PDCs, but relatively few compared with the volume of models out there
- What is needed?
    - Reward system (recognizing code)
        - If build tool that widely used, the paper gets cited

        - Pays off better for data analysis tool widely applicable rather than forward models
        - Also not all codes have clearly associated papers
    - Develop structures that make doing this work appealing to scientists or else bring in the outside community to do the work for us (paid, if necessary)
    - Framework for validation
        - Common goals
        - Workshops
    - If a collab was partly a center, could it give small grants that fund workshops on a given focal point and create a framework, with the hope that once started the community as a whole would join in
        - Jumps in citing after workshops
        - Often papers resulting
        - Greater confidence in code usage
    - Explore more deeply what incentives have worked in other communities that develop community codes
    - Modelling collaboratory could provide
        - Center that provided training and support for working with the logistics of benchmarking and validation

5.3.7 Code discovery and archiving

Code may be open-source, documented, and validated, but is not ultimately useful if the community is unaware of its existence or if it is not readily available. Absent this, we are reinventing the wheel over and over. We need to move away from "please contact the author". Awareness of existing codes is a major problem in volcanology as no well-established centralized code repository -- or index of external codes -- exists. VHUB failed to gain broad acceptance and is now twilighted (?). "Local" repositories are useful (e.g., http://www.cas.usf.edu/~cconnor/codes.html) but are not community-based and can still be challenging to locate.

This problem is not unique to volcanology, and other fields have had success with centralized community-driven repositories/indexes. For instance, the Community Surface Dynamics Modeling System (CSDMS) code repository for surface processes/landscape evolution/tectonics is more than a decade old and as of the time of writing contained nearly 400 open source models and tools. There is also EarthCube [somebody fill in details; a comment that there are "issues with duplication, indexing, what's actually linked"].

MCS proposal [please edit/comment]: Combination repository (git-based) and index of external codes. Managed by MCS with professional support staff to handle protocols, streamlining process. Procedure for submission and, possibly, review. By linking to external repositories we can help to achieve broad community buy-in, and overcome regulations that some government organizations (e.g., USGS) face in distributing code. Support staff will also help to achieve community buy-in, making the process of submitting to MCS easier than going it alone. Approved codes will be assigned citable DOI numbers. Git repositories are easily cloned and migrated, ensuring that codes are not lost after the end of SZ4D (maybe some sunset provisions should be spelled out?). MCS will publicize models to the community, further incentivizing submission. Consider teaming up with community organizations like IAVCEI? Use workshops to develop models and codes for community use.

Challenges:

- How to get community buy-in?
- Who will manage/moderate a repository, and how will we ensure that it remains relevant on timescales longer than SZ4D
- Volcanoes are not only in subduction zones. How can an MCS repository serve the entire volcanology community?
- Note: most of the discussion in this section focuses on individual codes, not necessarily coupled to one another, and also not considering ‘unified’ models.
- From Leif Karlstrom: Needs to be detailed how this will differ from VHUB (which was a failed experiment and not useful anymore) and code repositories like CSDMS and CIG. Maybe the point is to generate something like IRIS but for diverse volcanologic data/models?

5.4 Computational infrastructure

This section still needs to be written. The question of "computational infrastructure" was not discussed during the workshop thus far, other than a case being made for cloud computing. To what extent there is a need for new/additional computational infrastructure for the study of magmatic and volcanic systems is unclear and would benefit from further discussion. Also potential overlap with the Network/Center section.

- What do we mean by computational infrastructure here? CPU cycles?
- Many efforts listed above will involve a cyberinfrastructure component. How would this be implemented? What form would it take? Who would develop and maintain it?

5.5 Governing/administrative structure

This section remains to be written. One of the 26 March and/or 7 May breakouts could be dedicated to fleshing this section out. Potential contributors/leaders are sought.

Administrative structure:

- Steering committee
- Other

- A key aspect would be that any "centralized" MCS staff should scale in proportion to the aforementioned grant program. The objective would be to get more funding for model development and modeling, and to avoid administrative bloat at the expense of supporting research at the PhD and postdoc level. In this model there would be multiple sets of codes, developed at the grassroots (PI/PhD) level, with MCS facilitating the next step of model connectivity, publication, accessibility, workshops etc.. To get broad buy-in the funding pipeline has to go to student/postdoc grants that augment/complement the standard hypothesis driven science grants. The should include funding to attend MCS workshops and work with dedicated MCS staff.

5.6 Relation with other organizations and groups

- Integration with SZ4D
- Integration with CONVERSE:
    - 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
- Role of USGS
    - Note that PI-driven funding mechanisms exclude USGS scientists
- Relation with international organizations

Conclusions

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?

##

This represents material that has not yet been integrated in the report above.

Programming languages

Not sure if we need to get this far into the "weeds". Maybe pull out some of this and integrate, but leave out details of languages.

A collaboratory must support models developed in a diverse range of programming languages. Commercial programming languages (e.g., MATLAB) offer certain advantages and are widely used in volcano science. However, it is important to particularly support the development of models written in open programming languages such as Python, C, or Julia, which do not require commercial licenses to fully utilize -- a major impediment, particularly in developing countries. (It may be beneficial to devote funding to porting particularly important codes from obsolete or commercial languages into modern open-source languages.) It will also be important to facilitate documentation and API development for codes that will allow them to be interoperable across programming languages to the extent possible (for instance, a MATLAB conduit flow model could call a solubility model developed in C). Finally, the collaboratory should support not only the implementation of mathematical models in computer programming code, but also input files for stand-alone software packages -- for instance, an input file that defines the geometries, physics, and boundary conditions for a finite element model.

- Open source and cloud based. Minimize the need for software installation.
- Software environment in which a model lives should not be transient or at least the model should be adaptable to the evolution of that environment.

##

Homeless text (mostly notes from meeting breakouts):

- Laboratory experiments are an essential tool in furthering our understanding of magmatic processes in arcs, and there are several urgent ways in which they can be used to begin to work on problems addressed by our hypotheses and can inform and support the design and deployment of the future main SZ4D experiments. Experiments will support the urther development of petrologic models for P-T-X-H_2O-CO_2 magma storage conditions is needed and requires the integration of laboratory experiments.
- Volcanic gas emissions (CO_2/S) or changes signaling magma rise within the deeper system and potentially precursory to eruptions. Need further development of models for pressure-composition controls on volcanic CO_2/S gas signatures measured on active

volcanoes and integration with magmatic processes at depth, as well as geophysical and other monitoring data.

- Analog modeling.
- There is value in better examining intrusive-extrusive relationships in magmatic systems.
- Data collection <--> organization / data information <--> knowledge (make predictions). How can we marry these steps?
- Understanding how melt and residual solid separate in mush reservoirs and the consequences for magmatic differentiation remains a key challenge for modelers.
- Thermal, compaction and reaction processes are all important, but models will never capture all processes at all scales. Develop and apply models to address specific hypotheses at particular scales.
- Attempt hierarchical modeling using smaller scale models to derive effective properties for use in larger scale models (upscaling).
- Volatiles make the modeling much more challenging.
- Model development is most successful and flexible at the PI-level. There need to be more funding opportunities at the PI-level for model/code development, and also for model benchmarking and reproducibility.
- There are challenges and a need for a community to work on lithospheric scale magmatic systems especially away from mid-ocean ridges. Integrating volcanism into thermomechanical models of magmatic processes
- Don’t wait to model! Modeling should occur at the same time or prior to data collection
- Petrophysics is needed to interpret geophysical observations and inform geodynamic models
- Need to move towards open science and sharing codes we have, so other people can take a look at what other people are doing, and spot errors and improvements. Learn from other subdisciplines (IRIS, seismology) to share and recognize existing work and intellectual property
- Equations and models for multiphase flow
- Poroelastic, poroviscous
- Consititutive models
- Resolution of grain scale processes recorded in the crystal record within models of magma transport and storage at relevant scales. This requires upscaling and coupling between different types of models.
- Geometry of magma transport and storage. Most models are highly idealized, we either lack observational constraints or their complexity
- In its current state this section represents a collection of ideas and comments provided during the workshop and asynchronously. It is still seeking a champion interested in turning it into a coherent narrative.
- For arc trans-crustal magmatic systems, can we develop models in which primitive magmas naturally stall in the deep crust and that mature into observed arc sections? How long does this take? To make progress on this question requires knowledge of the aperture of the magmatic feeding system. Also, what is the temperature in the deep crust? What is the vertical continuity of the magmatic system? Where do the intrusions store or stall? What is the overall magmatic flux?

- Would like to have models that evolve to real-looking arc sections with steep-sided tabular intermediate plutions in the upper and mid-crust, and primitive cumulates deep and mostly gone.
- Thermal, compaction and reaction processes.
- Resolution of grain scale processes recorded in the crystal record within models of magma transport and storage at relevant scales. This requires upscaling and coupling between different types of models.
- Geometry of magma transport and storage. Most models are highly idealized, we often lack observational constraints to go beyond one-dimensional models or simplified two/three-dimensional models. At the same time going to higher dimensions remains challenging from a modeling perspective.
- Developing joint forward and inverse petrophysical models of the composition, volatiles, and partial melt within the entire transcrustal magmatic system that are consistent with all available datasets (petrology, magnetotelluric, seismology, gravity, ground deformation, etc.).
- Advances in physics of granular materials with implications for magmatic mushes. What is a modeling approach that is appropriate for field observations, with melt extraction and migration at many scales and patterns, and a wide range of rheological complexity? What controls the behavior of mush.
- Talking with some of the volcanic systems modelers, there is interest in a grant program (student and postdoc support) that will expand the PhD modeler pipeline and also allow recent modeling PhDs to build upon their PhD through "collaborative science MCS grants". This should also include workshops, training and making code more accessible. All this would be to some extent facilitated through an MCS "program", which will include the grants with students, postdocs and PIs dispersed throughout the US, as well as some centralized computer science / applied math / organizational staff dedicated to working with the grant recipients.
- The funding stream has to go to support students and postdocs, augmenting/complementing standard hypothesis driven science grants. Any centralized MCS would have the role of providing specialized technical expertise and organizational facilitation. If the onus is on modelers to make models more accessible, benchmarked, documented and so forth, then what should be expected of non-modelers? Perhaps MCS could also serve as a data hub and integrator for enhanced collaboration. In other words, if there will be lots of money spent on instrumentation and data acquisition, there could be somewhat proportional funding for integration and collaboration with MCS, and hence modeling, as the nexus.systems, old dead plutons)
- From the volcanic systems side, we are a small community in terms of modeling. In my opinion we are underserved in terms of outright funding, which presents a growth opportunity. That needs to be conveyed to NSF.
- Informing numerical models with data from experiments (e.g., use rates from petrology to inform the rates in reactive flow modeling; or fluid dynamics experiments to inform subgrid scales of flow models)
- Always have the obstacle of resistance to sharing data and people not being open to collaboration. One way of getting around sharing data would be to use old data, but

ultimately we want to foster collaboration and more openness to sharing data. That may mean something as simple as giving credit to people who shared their data by including them in the author list. Right now, people may feel slighted if they share data but do not feel like they are a part of the process of what science their data contributes to.

- Great idea: DOIs assigned for talks. After the talk, attendees give feedback which the speaker has to address, and then once the work is properly peer-reviewed, they get a DOI. Right now, talks are often focused on one person's point of view, so this process would ensure that there is more acceptance among the community (i.e. peer review) for high-level informative talks.
- "something we have been discussing is "do we see this as a central infrastructure, or distributed infrastructure? This matters as many of us in the room are code developers. Is it best to have a central resource, or one that is distributed. I will say that… is this a zero-sum game? If there is a central infrastructure, then does that prevent resources from going to other places. You could have a place with a prof code development team that helps make code open source and useable. Or you could have longer-term postdocs that are funded to do this type of work."
- **Two models of MCS development:**
    - **1. Centralized facility and programmers are hired to write code**
    - **2. Another end-member is PI-driven and NSF – centered**
    - **What are the pluses and minuses associated with these approaches to model development.**
    - **One advantage of the centralized facility is that it a modeling framework can be developed that is robust and easily interfaced with other efforts such as geodynamics.**

Summary of other efforts

1. 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 <u>and models</u> 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.”

References

Gomberg, J.S., Ludwig, K.A., Bekins, B.A., Brocher, T.M., Brock, J.C., Brothers, Daniel, Chaytor, J.D., Frankel, A.D., Geist, E.L., Haney, M., Hickman, S.H., Leith, W.S., Roeloffs, E.A., Schulz, W.H., Sisson, T.W., Wallace, K., Watt, J.T., Wein, A. (2017), Reducing risk where tectonic plates collide—U.S. Geological Survey subduction zone science plan: U.S. Geological Survey Circular 1428, 45 p., https://doi.org/10.3133/cir1428

McGuire, J.J., T. Plank, et al. 2017. The SZ4D Initiative: Understanding the Processes that Underlie Subduction Zone Hazards in 4D. Vision Document Submitted to the National Science Foundation. The IRIS Consortium, 63 pp.

National Academies of Sciences, Engineering, and Medicine (2017), *Volcanic Eruptions and Their Repose, Unrest, Precursors, and Timing*. Washington, DC: The National Academies Press. https://doi.org/10.17226/24650.

Segall, P. and Anderson, K. (2016), *Subduction Zone Observatory multidisciplinary system scale models of volcanic systems*, White Paper 47, The Subduction Zone Observatory Workshop, Boise, Idaho, September 2016.