Modeling Volcano-Magmatic Systems

Workshop Report for the Modeling Collaboratory for Subduction Research Coordination Network

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Disclaimer: *This workshop report has not been through a full peer review process.*

Summary

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

The U.S. Geological Survey (USGS) has identified 161 potentially active volcanoes in the United States and its territories, of which 57 are considered to be high or very high threats (Ewert et al., 2018). All western states, including Alaska and Hawaii, have potentially active volcanoes. Eruptions range from the quiet effusion of sluggish lava flows over hours to decades to immense explosive ejections of tephra which produce massive calderas.

Understanding these volcanoes and assessing their threat to society requires the development of quantitative models, rooted in physics and chemistry, which can be used to interpret diverse observations including real-time monitoring data. Existing models have tremendously advanced our understanding of volcanic systems and have improved our ability to assess hazards and forecast future activity, contributing directly to reductions in the number of lives lost to volcanic eruptions and helping mitigate their costs to society. Magmatic system models also provide a quantitative framework for understanding processes that occur at depth beneath volcanoes, linking volcanic systems with a broad range of deeper processes associated with the production, transport, and storage of magma and associated fluids above subducting slabs.

Despite this exciting progress much remains to be accomplished and workshop participants identified several important opportunities. First and foremost is the recognition that enhanced support for the development and dissemination of volcano-magmatic system models and associated methodologies will enable advances in ways not currently possible. A key outcome of the workshops is a recognition of the transformative potential of diverse groups of scientists working together on common problems. Support for collaborative working groups will enable communication across disciplines and between modelers and non-modelers, leveraging expertise from scientists studying different aspects of volcano-magmatic systems, and between geoscientists and outside experts from fields such as mathematics, statistics, and material sciences. Better support will also enable modelers to more fully verify, validate, benchmark, and document their codes, and also provide new training opportunities. Enhanced model sharing and interoperability will reduce the need for different groups to independently duplicate (re-invent) code and increase confidence in published results.

This report lays out a proposal for a collaborative modeling environment that is centered in large part around community working groups manifested as workshops, summer schools, and sustained long-term research collaborations involving diverse groups of scientists working on common problems. Programmatic support is envisioned in the form of enhanced student and postdoc funding for model development, incentives and support for cross-disciplinary collaborative research projects, and related support for these activities. This support will fundamentally improve our ability to integrate and interpret observations using volcanic and magmatic system models.

Table of Contents

1. Introduction

1.1 Purpose

The Volcanic Systems Workshop was organized under the aegis of the Planning for a Modeling Collaboratory for Subduction Zone Science (MCS) Research Coordination Network (RCN), which aims to facilitate the development of integrative earthquake and volcano modeling. This report documents the vision of the scientific community as articulated by participants in the Volcanic Systems Workshop, which took place online from September 2020 to May 2021. The report encompasses two parts: (1) challenges and opportunities for modeling and collaboration; and (2) a potential vision for how a modeling collaboratory would best advance the science objectives.

1.2 Relation to other activities

In 2019 the MCS supported two other workshops focused on different aspects of the subduction zone system: the MCS Fluids Transport Workshop (Wada and Karlstrom, 2019), and the MCS Megathrust Modeling Workshop (Dunham et al., 2020). These workshops also necessarily touched on important aspects of volcano-magmatic systems science. The Fluids Transport workshop covered the supply of magma and volatiles from the mantle to the crust, which provides the mass and energy input to most crustal magma systems, as well as aspects of lithospheric magma transport and hydrothermal fluids. 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 Megathrust Modeling workshop covered recycling of oceanic plates, which affects volatile fluxes, and subduction dynamics, which affects the distribution of volcanic systems. The report (Dunham et al., 2020) also recommended the development of a global, 3D, thermo-mechanical mantle circulation model, with implications for fluid transport and the petrological signature of arc volcanism.

A number of important science objectives, and to some extent modeling approaches, have also been defined recently within the ERUPT Report (National Academies of Sciences, Engineering, and Medicine, 2017); within the USGS Plan to Advance Subduction Zone Science (Gomberg et al., 2017); the NASA decadal survey (National Academies of Sciences, Engineering, and Medicine, 2018); 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); and within the report of the SZ4D Working Group for Magmatic Drivers of Eruption (MDE).

The outcomes of the Volcanic Systems Workshop echo to some extent the conclusions of the National Academies ERUPT report. In particular the two principal motivations for volcano-magmatic systems science are relevant: (1) to advance our knowledge and understanding of how volcanic systems work; and (2) to advance our ability to forecast eruptions. Furthermore, the key aspects through which a future MCS can support and facilitate these goals broadly overlap and complement the ERUPT report's recommendations for strengthening volcano science: (1) enhancing interdisciplinary collaboration; (2) training of future scientists; (3) supporting access to data, data products, models, and modeling; (4) maximizing the value of collaborations between observation- and modeling-focused scientists; and (5) building an effective volcano-magmatic systems science community.

1.3 Volcano-magmatic system models

The word “model” will have different meanings to different readers and is viewed herein as broadly encompassing, ranging from forward models of magma transport, storage and eruption through models for parameter estimation and forecasting. The main categories of models discussed herein are those covered within the volcanic systems workshops and planning meetings, including process- or physics-based models; thermodynamic, kinetic and constitutive models; and inverse models in the broadest sense as well as data assimilation for eruption forecasting. Omissions are due to space and time limitations and should not be interpreted to imply exclusion from an MCS.

Model generation is a complex process. Like observational data or experiments, models are first class objects of the scientific endeavor, requiring considerable research and intellectual effort. Observations and experimental outcomes are far less useful if not interpreted in the context of models. Furthermore, field and laboratory observations motivate models, and those models in turn motivate more focused field tests that feed back into improved models. There is thus a need for investing in collaborative model development at a scale that is comparable to investments in observing active subduction system processes.

Models of volcano-magmatic systems provide a quantitative framework, rooted in physics and chemistry, and in which to interpret diverse observations, including real-time monitoring data (Figure 1). Combining such models and data, often through sophisticated statistical inverse or data assimilation techniques, in turn improves our ability to understand underlying processes, assess hazards, and sometimes forecast future activity. Models also bring together the diverse disciplines involved in studying magmatic, volcanic, and associated hydrothermal systems. This diversity is an important aspect of volcano-magmatic research, making the field fundamentally interdisciplinary and offering stimulating and fertile challenges brought about by the myriad of physical and chemical processes involved, our inability to directly observe processes deep in the crust or even within eruptions at the surface, and because the spatiotemporal scales of critical phenomena range from smaller than individual crystals to many kilometers and from seconds to millions of years.

Volcano-magmatic system models range from very simple approximations of the governing physics to highly sophisticated systems of coupled nonlinear differential equations, the solution of which falls at the limits of the state of the art in numerical modeling. Examples include the emergence of multiphase (melt, crystals, gas) models for magma transport from the source region to crustal storage reservoirs, within the storage reservoirs, and during ascent to the surface; the propagation of hydraulic fractures (dikes) and associated earthquakes; models of lava flows, eruption plumes, and pyroclastic density currents; predictive models for the atmospheric dispersal of volcanic ash; and the embedding of physics-based models within statistical and data assimilation frameworks. These models have greatly enhanced our ability to understand processes, assess the state of volcanic systems, and infer future activity. Practical implications encompass natural hazards and their societal/economic impacts, the production of geothermal energy, and the formation and exploration of mineral resources.

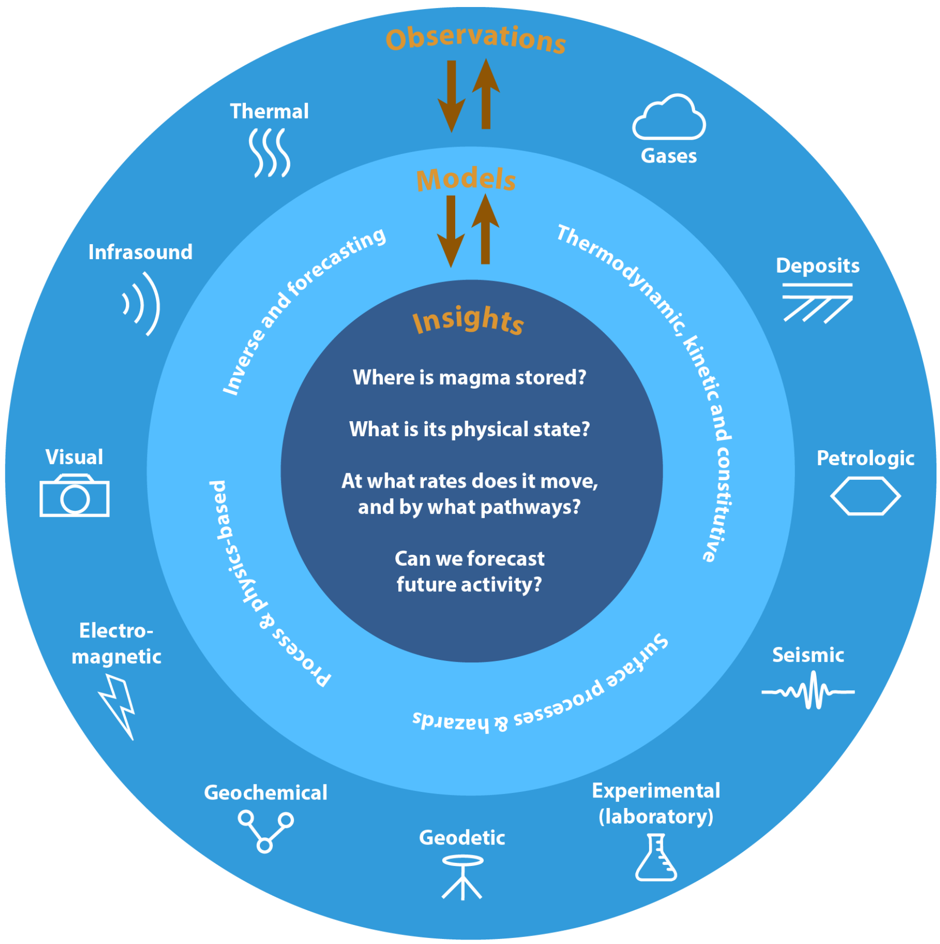

Figure 1: Models are the link between observations and improved understanding. *Observational and modeling spaces encompassed by a modeling collaboratory for volcano-magmatic systems, with expected insights shown in the dark blue central circle. Arrows indicate that observations inform models and that models allow the integration and interpretation of observations, and can also help inform the collection of observations. Likewise, models yield insights into volcano-magmatic systems which, in turn, help improve models.*

1.4 Scope and objectives of a volcano modeling collaboratory

A modeling collaboratory can promote the development of community-wide science frameworks and capabilities, identify and overcome barriers to interdisciplinary science, and develop human resources. There is broad agreement on the need for improved organization and coordination within the volcano-magmatic systems science community, also highlighted as a major goal in the NAS ERUPT report (National Academies of Sciences, Engineering, and Medicine, 2017). A main motivation for the MCS Volcanic Systems Workshop has been to make progress toward that goal through the development of concrete recommendations for a future modeling collaboratory aimed at advancing our understanding of volcano-magmatic systems and related hazards within subduction zones and beyond.

The evolving SZ4D (Subduction Zone 4D) initiative has a strong emphasis on instrumentation for observing active subduction system processes. Its science goal is understanding the processes that underlie subduction zone geohazards, which requires the synthesis of data using process-oriented models. Crustal magmatic processes, and the initiation of eruptions at arc volcanoes, are central and overarching parts of the SZ4D framework. Mantle-derived melts are the consequence of plate subduction and deep subduction zone processes. This melt supply, while modulated by the crustal magma system, ultimately drives volcanic activity and associated hazards, hydrothermal systems, and the formation of mineral deposits. Magma transport and storage occur at a wide range of spatial and temporal scales through processes that ultimately drive the system toward an eruption threshold, which can either be crossed solely as a consequence of internal dynamics or by external forces, such as tectonic earthquakes or surface processes.

This document focuses on volcano-magmatic systems within subduction zones, where the majority of active subaerial volcanism occurs. However, the volcanology community is small and volcanoes share commonalities that transcend geological settings. ***Thus, a modeling collaboratory must also allow room for work on volcano-magmatic systems in other tectonic settings.*** In conjunction with SZ4D, collaborative projects would on the one hand benefit from a “global approach” of studying many volcanoes through synthesis of the broadest range of observations and measurements. However, there is also great value in studying a small number of volcanic systems using the results from dense monitoring networks in conjunction with a comprehensive suite of other observations including field relations and geochemical and petrological observations. Furthermore, an MCS should include both surface and subsurface processes, as well as connections between them, especially insofar as they have ramification for volcanic hazards. The extent to which an MCS should support efforts associated with operational hazard models remains somewhat of an open question and relevant considerations and potential solutions fall at the intersection of an MCS and the Community Network for Volcanic Eruption Response (CONVERSE). Lastly, it was recognized that consideration must also be given to coupling between magmatic processes and fluid migration in subduction zones, as well as geodynamic and seismo-tectonic aspects, which are the subjects of separate MCS workshop reports.

2. Workshop organization, participation, and activities

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

- ***Crustal-scale magma transport***
- ***Magma storage***
- ***Eruptive magma ascent***
- ***Eruption plumes***
- ***Integrative volcano modeling and forecasting***

These subdivisions reflect to some extent the range in spatial and temporal scales that must be considered, although processes under each theme also 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 tens of millions of years.

The emerging view is that crustal scale magma transport and storage are spatially interconnected, albeit perhaps temporally episodic, across a vertically and laterally complex - intrusive system consisting of multiple magma and rock bodies in different physical states with respect to temperature, melt fraction, volatile content etc. 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, eruptions may be due to the exceedance of certain threshold conditions within the shallow subvolcanic system, or due to external triggers. Thus, eruption precursors that are directly or indirectly observable at the surface may be sought within the deeper realms of the transcrustal system or within its shallow subvolcanic parts, with the latter in general observationally more accessible. These considerations were encompassed by the ***Crustal-Scale Magma Transport*** and the ***Magma Storage*** themes of the workshop.

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

2.1 Workshop implementation

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

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

- Thomas Sisson (U.S. 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, University of Bologna, Italy): *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 (U.S. Geological Survey): *Operational aspects of ash dispersal modeling.*

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

- Hélène Le Mével (Carnegie Institution of Science): *Modeling volcano deformation*

- Mary Grace Bato (Jet Propulsion Laboratory, California Institute of Technology): *Towards better model-data fusion frameworks: [Sequential] Data assimilation for volcano applications.*
- Michael Poland (U.S. Geological Survey): *The role of a modeling collaboratory in forecasting volcanic eruptions and impacts.*
- Paul Segall (Stanford University): *Thoughts on the power of a volcano modeling collaboratory.*

2.2 Soliciting community input

A major goal of the workshops 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 on the Friday following the Tuesday and Thursday webinars. The planning meetings consisted of discussions and breakout sessions aimed at defining a vision for the volcano component of a future MCS, and together with the webinars largely form the basis of this report.

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

2.3 Workshop participation

The MCS RCN Volcanic Systems Modeling Workshop convened virtually via Zoom from Sep. 2020 – May 2021. The workshop was hosted by Helge Gonnermann (Rice Univ.) and Kyle Anderson (USGS), with support from Arianne Snyder, Gabriel Lotto, and Thorsten Becker (UT Austin). It was attended remotely by a total of 760 people from 44 countries across North America, South America, Europe, Africa, Asia, and the Pacific (Figure 2). Each webinar was attended by between 200 and 400 people.

3. Challenges and opportunities for modeling and collaboration

3.1 Overview

To achieve the decadal scientific objectives outlined through ongoing SZ4D activities and in the ERUPT report (National Academies of Sciences, Engineering, and Medicine, 2017) requires ***numerical models that can provide broader integration of observations, leading to advanced syntheses and understanding.*** (Participants also pointed out that model predictions can be used to guide data collection, which in turn will improve the models.) A broad range of discipline-specific forward and inverse modeling strategies are applied to study volcano-magmatic systems. Their application depends on the science objective as well as the type of data that they connect to. Segall and Anderson (2016) pointed out that a limitation of discipline-specific models is their utilization of only a subset of the available observations. The main goal of an MCS would be to enhance interoperability, integration and collaboration within the volcano-magmatic modeling universe.

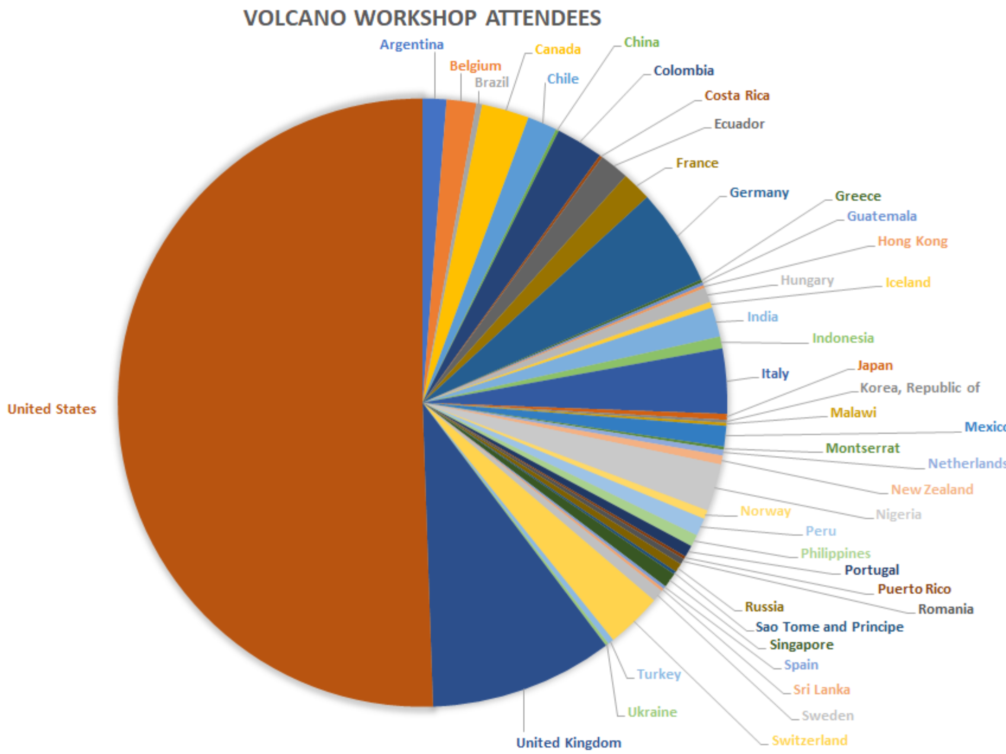

Figure 2: Participation in MCS volcano systems workshops.

Throughout the workshop, discussions frequently centered on geological subsystems and encompassed a multitude of unsolved questions and challenges. At the same time, discussions invariably evolved toward issues that transcend individual geological subsystems, due to the recognition that a robust interpretation of observations often requires integration across subsystem boundaries, facilitated by collaborative modeling. In the following, key geological- and process-based subsystems are considered, together with the associated model requirements.

Volcano-magmatic models span a tremendous range of spatial and temporal scales, encompassing an equally broad spectrum of physical and chemical processes (e.g., workshop presentation by P. Segall) (Figure 3). A major challenge is identifying meaningful simplifications that are necessary to construct tractable models. Forward models are typically process-oriented and encompass reactive mass and energy transport of and within a wide range of materials, for example: plastic/viscoelastic/brittle rocks and glasses; igneous melt with suspended crystals and gaseous bubbles; extensively solidified magmas known as crystal/magma mushes; supercritical fluids; and dusty gases. Inverse methods couple models with observations in order to resolve system parameters, increasingly using probabilistic (often Bayesian) approaches in order to quantify uncertainties. Near real-time data can also be coupled with models using data assimilation algorithms, making it possible to track the changing state of the system and, in principle, to forecast its future behavior (e.g., workshop presentations by D. Roman, M. Poland, and G. Bato). Similarly, there have been advances in the simulation of eruption plumes, which can now in some cases be operationally forecast (e.g., workshop presentations by J. Dufek; A. Costa; C. Bonadonna; and L. Mastin).

The great majority of magmas originate as partial melts in the mantle, with transport dominated by reactive porous-media flow. As magma rises into crustal reservoirs it differentiates via fractional crystallization, assimilation, and mixing, and melt transport may become increasingly localized. Simulation capabilities for the thermodynamic evolution of magma during transport and storage has seen significant advances, including a transition to cloud-based simulation tools (workshop presentation by M. Ghiorso). Throughout protracted crustal magma transport and storage, magmas are thought to exist in crystal-rich mushes (e.g., workshop presentation by G. Bergantz), likely together with a mobile exsolved volatile phase. The nature and geometry of this crustal magma transport and storage system remains in many aspects poorly understood, despite recent advances in geophysical and petrological methods (e.g., workshop presentations by E. Hooft; M. Pritchard; and T. Sisson).

A unifying theme among models of subsurface magma transport, storage, and eruption is reactive transport (e.g., workshop presentation by M. Jackson) and the multiphase nature of the natural system (e.g., workshop presentations by G. Bergantz and M. de' Michieli Vitturi). The wide range of spatial and temporal scales of observations and processes requires an equally wide variety of modeling approaches, ranging from the molecular scale (e.g., bubble/crystal nucleation, crystal growth), to the granular scale where individual crystals or bubbles within a multiphase assemblage are resolved (e.g., workshop presentations by M. Myers, and P. Ruprecht), to the continuum scale capable of modeling processes at kilometer or greater spatial scales and over time scales of individual eruptions or longer. Upscaling, downscaling, and interconnectivity between these various subscale models is of great importance and remains a major challenge (e.g., workshop presentation by C. Huber).

The multiphase nature of subsurface magma transport and storage systems constitutes one of the primary challenges for developing computational models, particularly in terms of overall complexity, but also in terms of the range of spatial scales (e.g., workshop presentations by G. Bergantz and M. Jackson). There are tremendous challenges related to understanding and modeling spatially complex magma systems (including dikes, conduits, and reservoirs) and their interaction with the surrounding rock host rock (e.g., workshop presentations by E. Rivalta and H. Le Mével). Here too a major challenge is the immense range of temporal scales that come into play, from subseconds (rock fracture or bubble nucleation), to millions of years (longevity of individual volcanic systems), to tens or hundreds of millions of years (subduction-zone and plate-tectonic evolution). There is no “one size fits all” model; rather, a diverse ecosystem of models is required that draws heavily on expertise in other disciplines (e.g., engineering, physical sciences, applied mathematics, and computer sciences).

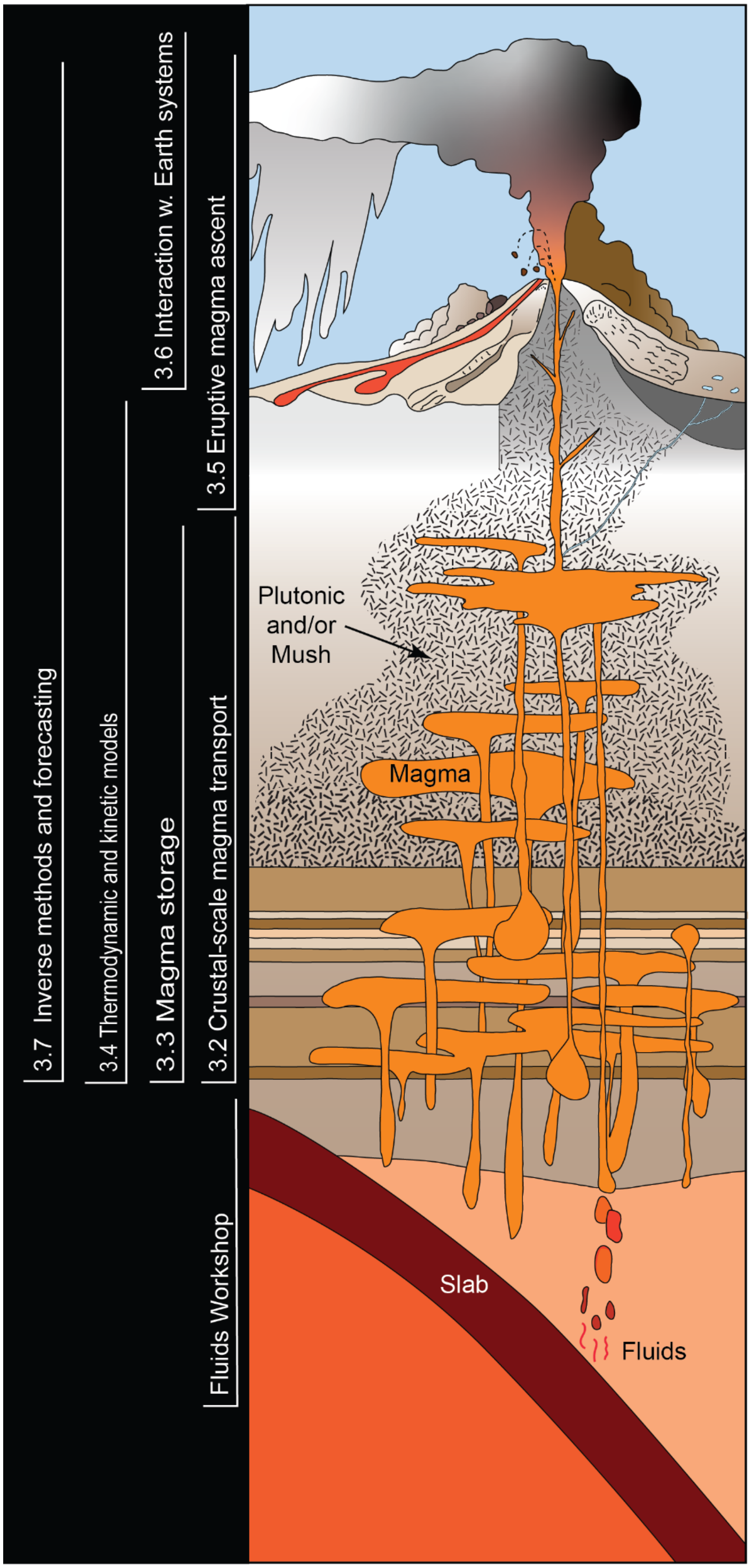

***Figure 3**: Conceptual cross section of a subduction zone magmatic-volcanic system, extending from the subducting slab through the crust to eruption of volcanic products at the surface. Labels on the left side of the figure denote sections of this report in which these parts of the system are discussed. Figure by Marcy Davis (University of Texas, Institute of Geophysics), modified from figures in the ERUPT report (National Academies of Sciences, Engineering, and Medicine, 2017).*

3.2 Crustal-scale magma transport

A key question that links the volcanic system to fluid/melt production and transport in the asthenosphere is how large-scale subduction parameters control magma production and delivery within the crust. This requires consideration of the coupling between energy and mass input to subduction variables, such as slab dip, convergence angle and rate, and slab properties (slab age, hydration, sediment thickness, etc.), mantle temperature, regional mantle convection patterns, two-phase mantle wedge dynamics and reactive transport, and time-evolving lithospheric thickness. These factors determine melt supply for crustal-scale magma transport which, in turn, provides the basis for magma storage and ultimately leads to volcanic eruptions. A fundamental question is the mode of magma transport and the formation of magma reservoirs which are preserved as plutons, but modeling advances are beginning to improve our understanding of these processes (for example, the important role of thermoviscoelastic effects on transport via dikes by Karlstrom et al. (2017)). Furthermore, a large degree of differentiation is required to take mantle-derived broadly basaltic melts into the compositional field of bulk continental crust, while at the same time about half the mass of the original basalt or basaltic andesite has to be removed to produce common andesite and dacite liquids. One-dimensional models of reactive two-phase magma transport, advancing on similar considerations in the mantle wedge (McKenzie, 1984) and accounting for melt percolating upwards through and reacting with crystals to produce chemically differentiated (silicic) magmas (Jackson et al., 2018), are first steps toward addressing these questions. Models such as the ones highlighted here are very promising, but still depend on a tremendous set of simplifying assumptions and parameters, particularly with respect to the thermomechanical-chemical coupling between fluid and solid phases. They illustrate the degree to which modeling of crustal-scale magma transport remains in its infancy, with tremendous potential for groundbreaking work to come.

Future models will have to tackle questions including the fate of the (ultra)mafic residue produced during the differentiation and formation of andesite and dacite magmas. It probably requires “delamination” (e.g., Dufek and Bergantz, 2005a), but how that happens remains an outstanding problem that ties crustal scale magma transport at the geodynamic scale to the subduction zone system. Within this context another open question is how and to what extent mantle-supplied magmatic input rates control magma storage depths, crustal residence times, and erupted magma composition (Hughes and Mahood, 2011). Another major challenge is the development of computational models in which primitive magmas naturally stall in the deep crust and mature into observed arc sections (e.g., Keller and Suckale, 2019). Most models of active magma transport and storage utilize highly simplified geometries such as spheroids or planes and consider elastic mechanics of host rocks, reflecting not only a preference for simpler models but also a lack of observational constraints for more complexity. Thus, on the one hand there is a dire need for more observations to improve our understanding of how magma pathways form and evolve; and on the other hand, there is equal need for models that can capture these processes. Here again a challenge lies in the wide range of timescales involved, because the timescale at which magma transport causes deformation can range from much shorter to much longer than the viscous relaxation time of the crust. Consequently, magma transport may be accommodated through a range of mechanisms from brittle fracture to viscous flow and assimilation of the rock host. Important questions include: What is the aperture of the crustal magmatic feeding system, and how does it evolve? To what extent is it possible to link crustal chemical evolution with crustal stress? What is the vertical continuity of crustal-scale magmatic systems and what are the temperatures in the deep crust? Where do magmas stall forming reservoirs and what is the overall magmatic flux?

A related question is how geophysical signals relate to deeper magmatic processes. For example, are deep seismic events actually sites of magma supply? By the same token, do seismically quiet zones directly beneath volcanoes represent the hot and plastic magmatic system, with the seismogenic halo representing fracture of cooler and brittle crust (Aso and Tsai, 2014)? To what extent are such seismic signals due to fluid egress, rather than magma transport? Geodetic and seismic tomographic images of the same volcano often do not agree on the location and extent of magma reservoirs (Lerner et al., 2020), suggesting frequency dependence (or poor resolution) that has not been well studied. Electromagnetic methods clearly image localized fluid structures in 3D (Bedrosian et al., 2018), but these have yet to be integrated with other methods.

Moreover, there is uncertainty as to whether crustal reservoirs are fed by episodic dikes or persistent conduits, which may depend on the magmatic setting and will have different implications for monitoring. By and large, geologic observations of crustal intrusions currently lack the temporal resolution to go beyond simplified models. Consequently, magma ascent models (crustal-scale or conduit models) often have insufficient constraints to go beyond 1D or idealized 2D geometries and quasistatic elasticity. This highlights a clear need for more observational data to overcome these limitations and, in conjunction, for models capable of more realistic geometries and dynamic fidelity. The challenges increase with depth within the magmatic system. Field relations of exposed sections suggest that storage regions exhibit mass transport on a range of scales that likely reflect different modes of crustal deformation. Plutonic bodies have characteristic scales that vary between elastic fracture (dikes) and larger flow structures that require ductile deformation and may reflect transport on a variety of timescales (e.g., Cruden et al., 2017). The relations between such magmatic system architecture and tectonic stresses, magma supply rate, lithospheric thermal history, and surface eruptions are still unclear. What physical pathways reproduce magmatic evolution toward real-looking arc sections with steep-sided tabular intermediate plutons in the upper and mid-crust, transitioning to sheet-like mid-crustal structures, and primitive cumulates at depth (which may not necessarily be preserved)? How much eruptible magma exists in a given crustal system? Here too the need for more observational data and for collaboration, to integrate data into models of greater complexity and sophistication, clearly exists and highlights the opportunities and challenges for subduction zone science in general and an MCS in particular.

In terms of temporal evolution, magmatic systems are long-lived. At the arc scale, zircon populations from plutonic systems reveal that magmatism is likely pulsed on ~10 Myr scales (Paterson and Ducea, 2015). At the surface, volcanic growth is defined by major stages occurring at 10,000–100,000 years, whereas single composite edifices have average life spans of <0.5–1 million years that may inherit and pass on structure over 1–2 million years (Calvert, 2019). Compositional excursions are typically brief in andesitic stratovolcanoes (~100 years), consistent with small active volumes. In contrast, volcanic centers that persist for 5–10 million years usually evolve toward substantial volumes of rhyodacite-rhyolite, consistent with arc intrusive suites (Jagoutz and Kelemen, 2015). A key question is why such systems evolve toward felsic, lower temperature, and higher viscosity compositions, and why lower temperature felsic magmas and eruptions are more voluminous. Progress on questions like these is contingent upon adequate representation of the complex multiphase rock-melt-crystal-volatile assemblage, and reactive transport dynamics in a heterogeneous medium with frequency dependent rheology.

The recognition that active magmatic systems are vertically extensive and may to a large extent consist of crystal-rich magma mushes (Cashman et al., 2017) is a manifestation of this significant modeling challenge. What modeling approach is appropriate for melt extraction and migration at the full range of temporal and spatial scales, and over a wide range of rheological complexity? For example, resolving grain-scale processes recorded in the crystal record at appropriate scales requires upscaling and coupling between different models of magma transport and storage. Such techniques are in their infancy and at the vanguard of volcano-magmatic modeling. Reduced-order models (sometimes called “lumped element” models), which parameterize the description of spatially distributed physical systems and reduce the state space to a set of ordinary differential equations with a finite number of parameters, are a possible approach for some of these problems. Reduced-order models can be scaled up to integrate tectonic histories and down to incorporate crystal and bubble dynamics but are generally nonlinear so require careful numerical development and parameter exploration.

3.3 Magma storage

Ultimately, magmas that are stored in the crust may feed volcanic eruptions or evolve into moribund plutons. Magma storage zones supply energy to hydrothermal systems and also contribute to the formation of societally important ore deposits. Historically, the concept of magma storage was commonly taken to be synonymous with a melt-filled reservoir from which magma is supplied to volcanic eruptions. The emerging concept of magma storage, in contrast, encompasses spatially distributed storage zones, linked by variable degrees of interconnectivity, which contain magmas which range from crystal-rich mushes to crystal-poor melts (Hildreth, 1981; Hildreth and Moorbath, 1988; Bachmann and Bergantz, 2008; Bachmann and Huber, 2016; Cashman et al., 2017; Sparks et al., 2019). The plumbing of crustal magma storage zones remains for the most part poorly understood, although recent projects have made important progress. Mechanically, magma storage regions host heterogeneous and complex mixtures of melt, crystals, fluids, and wall rock that display an extremely wide range of physical properties. Magma storage regions are also out of thermal, mechanical, and often chemical equilibrium with the surrounding crust; these environments are therefore evolving dynamically in response to internal and external processes. One such process is magma transport between individual storage reservoirs, at different levels within the entire crustal column and within the uppermost mantle, often referred to as magma “supply” and “withdrawal.” Another occurs within individual storage reservoirs, mostly in conjunction with convective heat transfer.

Although often a simplification, the magma reservoir concept remains central and useful when developing process-based models for magma evolution and volcanic eruptions. Early numerical models related to magma reservoirs (e.g., Knapp and Norton, 1981; Spera, 1984; Spera et al, 1986; Brandeis and Jaupart, 1986; Oldenburg et al., 1989; Bergantz, 1992; Bergantz and Ni, 1999) were followed recently by a re-emergence in numerical modeling of magma storage. Some highlights include advances in the simulation of magma thermodynamics (http://enki-portal.org; Bohrson et al., 2014; Gualda et al., 2012); crystal scale dynamics including two-phase (melt+crystal) flow simulations (Bergantz et al., 2015); three-phase simulations with exsolved volatiles within a crystal-rich magma mush (Parmigiani et al., 2011); coupling of parameterized convective heat transfer and thermodynamics (Huber et al., 2009; Huber and Parmigiani, 2018); as well as crustal scale heat transfer simulations (Annen et al., 2006; Annen, 2009; Gelman et al., 2013) and reactive transport simulations aimed at the formation and evolution of magma storage regions (e.g., Dufek and Bergantz, 2005; Karakas and Dufek, 2015; Karakas et al., 2017; Jackson et al., 2018; Solano et al., 2012). These examples not only illustrate that modeling of magma storage is a growing field, but also that a broad range of modeling strategies (from discrete to continuum approaches) and numerical methods are required to address the spatial and temporal scales of magma storage systems. Much of this work is at the forefront of research related to the theoretical and numerical challenges posed by such rheologically complex multiphase systems.

At the crustal scale, the petrological diversity of magmas observed on Earth requires large inputs of primitive magmas and the loss of mafic roots produced by fractional crystallization. The mechanics of phase separation, which is central to crystal fractionation, is likely modulated by interactions among crystals, volatile bubbles and melt at the discrete granular scale. Thus, micro- and macro-scales are intimately intertwined and modeling of magma storage will have to contend with a wide spectrum of scales. Interim goals could focus on (further) developing a range of modeling approaches for specific length scales or processes, and identifying methods to upscale across these, in order to incrementally move towards an integrated modeling framework that encompasses increasingly wider ranges of spatial and temporal scales.

On the temporal side, future models will have to contend with the fact that magma storage systems operate as generally open systems over hundreds of thousands to millions of years, as recorded by radiometric ages from accessory phases and in crystal zoning profiles of slow-diffusing elements (e.g., Reid et al., 1997; Reid, 2003; 2008; Claiborne et al., 2010; Cooper, 2015). Storage regions are also subjected to the dynamic evolution of the surrounding crust, as its mechanical state affects magma transport and, especially, the inception, evolution, and growth of magma storage over time. Given the complexity of the storage-host system, progress in modeling requires consideration of a wide range of observational and experimental constraints, for which broad collaboration is a necessary requirement.

For example, a potential basis for improved modeling is the existence of high-fidelity temporal records of magma storage conditions (pressure, temperature, composition). Petrologic studies provide such constraints through phase-equilibria experiments, thermodynamic-based geothermobarometry and detailed mineral-chemistry studies of the crystal cargo (e.g., Wallace et al., 1999; Putirka, 2008; Cooper and Kent, 2014; Barboni et al., 2016; Neave and Putirka, 2017; Shamloo and Till, 2019; First et al., 2021; Rout et al., 2021). These techniques reveal insight into the internal state of the magma storage system, whether it is mush- or melt-dominated and regardless of whether it is primarily controlled by open- or closed-system processes. Crystal records often imply a complex assembly from different magma sources with distinct storage conditions, in some cases perhaps encompassing the entire crustal column and multiple batches of magma (e.g., Davidson et al., 2007, Ruprecht and Plank, 2013, Kahl et al., 2015, Cashman et al., 2017).

As progress is made towards constraining the state of magma reservoirs from melt-crystal equilibrium, consideration of the presence of a fluid phase is warranted. Recent studies have clearly illustrated the fundamental role that a fluid phase plays on the thermo-mechanical evolution of the reservoir (Bachmann et al., 2002; Bachmann and Bergantz, 2003; Blundy et al., 2010; Huber et al., 2010; Buret et al., 2016; Parmigiani et al., 2016; Townsend et al., 2019) and the generation of ore deposits (e.g., Hedenquist and Lowenstern, 1994; Weis et al., 2012; Wilkinson, 2013; Blundy et al., 2015; Mungall et al., 2015; Chelle-Michou et al., 2017). Thus, there is a need to better constrain when free fluids are present or when magmas are fluid undersaturated. Constraints on fluid saturation may not only come from petrology, but also through the integration of observations within geophysical datasets.

3.4 Thermodynamic and kinetic models

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. It is now possible to track the pressure-temperature-time paths of magma batches at increasing spatial and temporal resolution, allowing inferences on how magmas evolve during storage, ascent, mixing, and eruption.

During long-term storage, magmas can approach equilibrium, at least between mineral surfaces and melt. Under the assumption of equilibrium, thermodynamic models are then able to constrain the abundance and composition of phases under a set of intensive parameters (Ghiorso and Sack, 1995). Calculation of equilibrium phase assemblages has advanced greatly as more experimental datasets have been completed, creating a growing thermodynamic database. With this database has come the creation and promulgation of thermodynamic models, of which the ENKI simulation platform (http://enki-portal.org) is the most recent development and a useful example for collaborative, web-based modeling implementation. Despite such recent advances there remain unsolved issues, such as prediction of the stability and composition of complex, volatile-based phases like igneous calcic amphiboles and biotite. This gap leaves the community with the inability to model, interpret and understand the origins of intermediate and evolved arc and other magmas, and limits our ability to predict accurate volatile solubilities at middle and lower crustal pressures.

There also remain ample opportunities for improvement when it comes to the treatment of volatiles in thermodynamic models. For example, the need for the incorporation of sulfur and sulfide–sulfate equilibria into models is highlighted by the fact that our current ability to analyze volcanic gas emissions far exceeds our ability to relate their compositions and fluxes to eruptive and shallow subvolcanic processes. In addition, an improved assessment of the depths from which magmas ascend and are stored during transport through the crust is of critical importance for our understanding of volcanic systems, but the tools for inferring depths remain limited. For example, pressure estimates may be based on measurements of volatiles in melt (glass) inclusions, which typically require careful reconstruction due to post-entrapment modification, and are generally thought to be minimum estimates (Wallace et al., 2021). Mineral geothermobarometry relies upon understanding the temperature and pressure of the formation of minerals within igneous rocks and is based on laboratory studies in which minerals are grown at known temperatures and pressures. Geothermobarometers rely on several assumptions, in particular chemical equilibrium. During times of magma transport and/or mixing, however, magmas are substantially removed from equilibrium conditions and the system responds through phase changes and/or diffusive re-equilibration, resulting in crystal growth and dissolution. This produces diffusive chemical and isotopic gradients in crystals and glasses. Their interpretation and improved understanding of the underlying processes requires numerical modeling at spatial and temporal scales relevant for crystal growth, as well as upscaling and integration into models at spatiotemporal scales that are relevant for magma chambers.

Related models focus specifically on phase transformations, such as crystal nucleation, growth, and dissolution in response to the degree of undercooling or superheating. Similar efforts exist regarding the formation and evolution of bubbles in magmas. In these models, the chemical evolution of the system can be connected to the textural observations of erupted products or plutonic rocks. For example, rapid versus slow crystal growth related to the degree of undercooling leads to distinct crystal habits that range from skeletal, dendritic, to polyhedral, as well as from more acicular to more isometric crystal shapes. Moreover, crystals and bubbles in magmas display substantial polydispersity in size and shape. Although substantial advances continue to be made through integrated analytical and modeling endeavors, numerical models are still a long way from being able to capture these processes in adequate detail to leverage the observations. This in itself represents a significant challenge. Moreover, embedding such models at the sub-grid scale within meso-scale models of magma transport and storage has not yet been achieved to any significant extent and remains a major challenge. With future progress in these areas will come a growing need to curate and standardize models so that results can be compared and individual case studies can be synthesized into a greater understanding of magmatic processes.

3.5 Eruptive magma ascent

Volcanic eruptions span a wide range of styles and magnitudes, thereby presenting different societal and environmental risks. Our capacity to mitigate volcanic risks is in part contingent upon forecasting of eruptions, including vent location, occurrence time, intensity, duration, and style, as well as the movement of lava flows, pyroclastic density currents, and volcanic ash clouds during explosive eruptions. Understanding of magma ascent to the surface together with the related observables (seismicity and its characteristics, surface deformations, gravity changes, gas emissions, etc.) is important in itself and it also is a key element for forecasting volcanic activity and hazards (Sparks, 2003). The interdependent processes that modulate magma ascent include crystallization, nucleation and growth of bubbles, the migration and loss of magmatic gases, as well as their effect on magma rheology, and the response of the host rock to magma-induced stress changes. Because these processes are not amenable to direct observation during eruptions, numerical modeling is of paramount importance. Such modeling has to rely on a diversity of experimental and observational research, making multidisciplinary collaboration essential for progress in eruption modeling (e.g., Polacci et al., 2017) and provides a clear incentive for a future MCS.

Numerical simulation of eruptive magma ascent has been a productive area of research with seminal early work by Wilson and coworkers (Wilson et al., 1980; Wilson and Head, 1981). Subsequently, a vibrant eruption modeling community has produced advances on multiple fronts. Examples, which are by no means comprehensive, include: the conduit model of Dobran and Papale (Dobran and Papale, 1992; Papale and Dobran, 1993), which marked the beginnings of a succession of subsequent generations of conduit models; exploration of the role of conduit wall erosion and collapse (Macedonio et al., 1994; Aravena et al., 2017, 2018); the loss of magmatic volatiles through conduit walls (Woods and Koyaguchi, 1994; Jaupart, 1998); the incorporation of bubble nucleation (Massol and Koyaguchi, 2005); the inclusion of disequilibrium bubble growth during eruptive magma ascent (Proussevitch and Sahagian, 2005); the coupling of magma chamber and conduit (Bower and Woods, 1998; Huppert and Woods, 2002; Macedonio et al., 2005, Anderson and Segall, 2011), including crystallization and the formation of plugs and domes (Schneider et al., 2012; Kozono and Koyaguchi, 2012, Wong et al., 2017); coupling of dykes and cylindrical geometries together with elastic wall-rock deformation (Costa et al., 2007a); time-dependent eruption models constrained using observations in a Bayesian framework (Anderson and Segall, 2013; Wong and Segall 2020); forays into transient two-phase (gas-melt) flow in one-dimension (Melnik et al., 2005; La Spina et al., 2017); magma flow in dikes (Woods et al., 2006); and dike propagation (Weertman 1971; Rubin, 1995; Mériaux and Jaupart, 1998; Dahm, 2000; Segall et al., 2001). Especially notable in this context are the publicly available user-friendly CONFLOW model of Mastin and Ghiorso (2000) and the conduit model intercomparison workshop discussed in Sahagian (2005).

Most of the aforementioned models are one-dimensional, but when juxtaposed against the rheological and multiphase complexities of magma flow, this approximation likely bears severe limitations and unexplored feedback. Even if the volcanic conduit is geometrically simple, magma viscosity will be strongly strain-rate dependent. Thus, a single and/or constant value of viscosity at a given depth within the volcanic conduit is generally insufficient. At high crystallinity and/or vesicularity, shear banding and deformation partitioning are commonly observed in experiments, leading to further nonlinear rheological behavior that cannot be encapsulated in a single viscosity value. The resulting conditions likely require at least two-dimensional models. For example, Dufek and Bergantz (2005b) modeled the transient two-dimensional dynamics in the upper conduit of a rhyolitic eruption to elucidate the role of particle collisions in redistributing momentum after fragmentation; Costa et al. (2007b) studied the thermo-rheological feedbacks due to viscous dissipation; and Massol and Jaupart (2009) used a finite-element model to study magma extrusion in dome eruptions. In terms of code development, higher-dimensional models are challenging because of the multiphase and multi-scale (temporal and spatial) nature of magma ascent processes. Obtaining and utilizing observations to provide constraints on higher-dimensional models will be challenging and will require careful assessment to what extent going to higher dimensions is justifiable based on observations (Trafton and Giachetti, 2021). Such endeavors would undoubtedly benefit from the collaborative synergies envisaged for a modeling collaboratory.

All of the aforementioned models require extensive integration of magma properties and coupling with the host rock, which are based on a vast and critical body of experimental and theoretical work, and which in turn highlight the importance of collaborative modeling. Furthermore, although simulations of eruptive magma ascent provide insights within themselves, ultimately models may be more useful if they can be used to predict observations or, equivalently, be constrained by observations. In this respect, although there has been undeniable progress in developing models aimed at both simulating the physics of the specific processes and the expected geophysical and geochemical observables, only a small subset of models have achieved robust estimation of eruption source parameters through inversion of observations from eruptions (e.g. Anderson and Segall, 2013; Heimisson et al., 2015; Massaro et al., 2018, Wong and Segall, 2020). Such parameter estimations rely on building blocks to simulate seismicity, deformation, gravity changes, dispersion of eruptive material, and so forth. Filling the remaining gaps and constructing more comprehensive models, which can retrieve eruptive source parameters from both the geophysical and geochemical domain, and which are able to provide reliable predictions for a wide range of observations, represents one of the key roles that a future collaboratory should embrace.

An important challenge for magma ascent modeling is a better understanding and anticipation of the path that magma will take on its way to the Earth’s surface. In detail this remains poorly understood and challenging to forecast. Magma may intrude a pre-existing pathway, make use of structural features amenable to intrusion, or force a new path by hydraulic fracturing. Surprisingly, geodetic and seismological observations indicate that magma may take tortuous pathways through “intact” rock to erupt, even in the presence of well-established conduits. Thus there exists a pre-existing conduit vs. hydraulic fracturing ambivalence that has led to the development of separate “conduit flow” and “diking” models. In reality, eruptions may involve both, with diking first creating a pathway, followed by wallrock erosion and the development of a pathway or conduit with a more mature and persistent geometry, or even with magma flowing through a pre-existing conduit and at the same time opening a new pathway as a dike. Advancing predictive capabilities involving the formation of eruptive magma ascent pathways also requires consideration of and constraints on the presence and role of fluids other than the magma itself, on magma properties, on the mechanical properties of the host rock, on the geometry of existing pathways, on the presence of hydrothermal systems, and on the surrounding crustal stress field that controls the creation of new pathways. Recently we have seen the emergence of the first models able to address some of these factors (Heimisson et al., 2015; Pinel et al., 2017; Rivalta et al., 2019). Models such as these rely on information from multiple disciplines, such as geomechanics, thermodynamics, and geophysics. Simulating and perhaps forecasting eruption initiation thus requires complex and integrated transient models that are still in early stages of development, and which could benefit from the collaborative aspects envisioned for a future MCS.

Transient behavior over different time scales is also important. On the one hand, during the initial phases of an explosive eruption, a fragmentation wave propagates within the conduit at very high speeds, and transient models capable of properly simulating the propagation of shock and rarefaction waves are required (La Spina et al., 2017). On the other hand, once an eruption has begun and a volcanic conduit has been established, changes in the eruption conditions may occur over time-scales much longer than the travel time of magma in the conduit, allowing the use of steady-state models (e.g., Macedonio et al., 2005). Many eruptions go through a temporal progression that may involve distinct episodes of eruptive activity and even hiatuses in eruptive activity (e.g. Hildreth and Fierstein, 2012). Such transient activity may in part be a consequence of conduit wall-rock erosion or conduit collapse (e.g., Aravena et al., 2018), but likely also involves complexities within the magma chamber, such as zoning in magma composition, geometric complexities, or complex feedback mechanisms during ascent (Kozono and Koyaguchi, 2012). Thus it is necessary to couple magma ascent and magma reservoir models in order to advance understanding of unsteady eruptive behavior. Transients on even short time scales are presumably associated with complex feedbacks during magma flow within the volcanic conduit. They are responsible for the generation of seismic and acoustic signals, which can be utilized as observational constraints on eruptive behavior (e.g., Niu and Song, 2021). Most eruption models, however, still assume steady behavior and the models required to address the multitude of transient behavior during volcanic eruptions remain at the vanguard of model development and application (e.g., La Spina et al., 2017). Early efforts at coupled reservoir-conduit models have also generally neglected much or all of the complex spatiotemporal variability within the reservoir itself (e.g., Bower and Woods, 1998; Huppert and Woods, 2002; Macedonio et al., 2005, Anderson and Segall, 2011).

Recent insights from petrological and geochemical studies point to an emerging need for better integration of disequilibrium reactive transport processes into eruptive magma ascent models. To date most models are based on simplified descriptions of such processes. For example, crystallization and degassing are often treated as equilibrium processes (Melnik and Sparks, 2002), in part due to the complexities of upscaling from crystal- or bubble-scale models, especially if they encompass more realistic polydisperse crystal or bubble populations. Equilibrium or disequilibrium should, however, be model outcomes rather than model assumptions. In this context, Kozono and Koyaguchi (2012) modeled the effects of gas escape and crystallization to understand the complexity of conduit flow dynamics during lava dome eruptions by introducing a finite crystallization rate; La Spina et al. (2016) used a similar formulation for the simultaneous exsolution of volatiles and crystallization.

The importance of the multiphase nature of magma is paramount in this regard and highlights the need for eruption models that can adequately represent and resolve the multiphase flow of magma across relevant spatial and temporal scales, something that remains a challenge theoretically and numerically (see workshop presentation by M. de Michieli Vitturi). In fact, most existing magma ascent models are based on mesoscale descriptions of the multiphase nature of magma, with the crystal and gas phases represented by their volume fractions. This approach does not allow a direct comparison with the crystal and bubble size distributions from eruptive products. A proper treatment and modeling of these size distributions (nucleation and growth) on one side would allow for better comparisons with observations and samples, and on the other it would allow reconstruction of eruption dynamics by a model inversion of the observations. A promising approach in this direction is represented by the use of the method of moments, well established in the field of chemical engineering, which makes it possible to rigorously simulate the space-time evolution of a distribution of sizes.

An important mechanism during explosive eruptions is magma fragmentation, with direct impact on eruptive behavior. Fragmentation is usually based on the assumption of a sharp transition from a bubbly flow regime to a gaseous flow with suspended pyroclasts, with the transition based on some parameter threshold (e.g., Papale, 1999). Although this makes incorporation of magma fragmentation in eruption models tractable, it is likely an oversimplification and there remains much room for further developments (e.g., Giachetti et al., 2021), including consideration of the interaction of magma with external water (e.g., Wohletz et al., 2013), which has thus far received little attention in eruption models.

3.6 Interaction with Earth systems

The overarching question of this section is how landscapes, the hydrosphere, and the atmosphere interact in the long and short term with the volcano-magmatic system (and vica versa). Due to time constraints, in terms of Earth systems interactions the workshop only covered volcanic plumes and associated deposits — that is, physical processes starting above the eruptive vent and extending to the long-range dispersal and deposition of pyroclastic material (tephra). In addition to a discussion thereof we do provide, however, a brief summary of landscapes, hydrosphere, and atmosphere interactions. For a complementary discussion of other volcanic and subduction zone surface processes we also refer to recent efforts encompassed by the CONVERSE Research Coordination Network (https://volcanoresponse.org/) and the recent NSF-sponsored Coupling of Tectonic and Surface Processes Workshop whitepaper (Barnhart et al., 2018).

Surface processes associated with magmatic activity include volcanic landform evolution, lava flows, pyroclastic density currents (PDCs), tephra plumes, lahars, volcanic flank failure, and caldera collapse. Volcanic landscape evolution records many generations of such processes over long time scales, along with surface uplift by intrusive magmatism (O'Hara et al., 2021) or collapse due to magma withdrawal, competing with erosion to define topography. Erosion may be driven by climate or magmatism and can provide external forcing on the volcanic system, for example through landslides or long-term erosion. Surface processes can also provide external forcing on the volcanic system, including glacial loading and groundwater. How magmatism is expressed at the surface over 1-100s kyr timescales is also of critical importance to regulation of long-term climate through silicate weathering — for example, chemical weathering rates in arcs correlate with extent of basalts (Börker et al., 2019).

Often overlooked is the importance of pervasive and deeply circulating arc hydrothermal systems. Interactions between magmatic and groundwater systems produce geophysical and geochemical signals that can be difficult to interpret. For example, time-dependent volcanic ground deformation may reflect poroelastic physics associated with hydrothermal circulation rather than magma (Nespoli et al., 2021). To date there has, however, been relatively little work aimed at the integration of magmatic system and hydrothermal system models (e.g., Fu et al., 2010). The cooling, depth, and lateral aperture of magma reservoirs, the opening of eruptive pathways, and volcano stability ultimately are all impacted by hydrothermal processes.

Magma-hydrothermal systems are also critical for human resources. Hydrothermal ore deposits are of critical importance for emerging low carbon technologies (Sillitoe, 2010), and extensive aquifers representing significant water resources are often hosted in volcanic deposits (Farley et al., 2011). Finally, there are significant hazards associated with hydrothermal unrest (Currenti et al., 2017; Fournier and Chardot, 2012), and stratovolcano flank collapse is promoted by hydrothermal alteration (Finn et al., 2007). Thus, the inclusion of hydrothermal systems and processes are an important facet for an Earth systems component of the SZ4D/MCS endeavor.

Presentations and discussions during the Volcanic Plumes workshop theme focused on strategies for both research and operational modeling. One of the main questions that emerged from the discussions was how to connect plume dynamics with deeper reservoir and conduit processes, as well as large scale atmospheric dispersal simulations. It was recognized that component models, such as rheological models, could be developed and coupled with one another to facilitate construction of larger system models. Such subsystem models already exist to some extent and could provide useful starting points. Current examples include one-dimensional conduit flow and reduced order reservoir models with flexible initial and boundary conditions, as well as thermal conduction models with simple equilibrium petrologic coupling using thermodynamic subsystem models such as the magma chamber simulator (Bohrson et al., 2014) or rhyolite-MELTs (Gualda et al., 2012) for example. Ongoing challenges include the modeling of multiscale ash dispersal over long distances, compressibility effects and choked-flow conditions; higher-dimensional models (2D/3D); entrainment of ambient air; fluid-particle interactions and turbulence; heterogeneity in near-field plumes; and microphysical processes including aggregation, hydrous phase change, and heat transfer. Related to this is the rapid assessment of eruption source parameters, which is ultimately a monitoring and data assimilation challenge.

Forecasting ash clouds is important for aviation safety and the societal impacts of ashfall. Workshop participants thus suggested that establishing a modeling collaboratory could spur the improvement of plume modeling and have a global impact on aviation safety. Consequently, there was discussion about the integration and development of models that can be rapidly run by observatories during volcanic crises using widely available computation resources — for example through parameterized or reduced-dimensionality simulations. Further modeling goals include the development of probabilistic tools for tephra hazards assessment; the incorporation of research codes into more user-friendly modules; eruption response activities in collaboration with CONVERSE; and the incorporation of multiple types of observations (satellite, ground-based radar, infrasound, thermal cameras, and visible cameras) into simulations to ‘automatically’ update forecasts (e.g. data assimilation) for dispersion, aviation safety, and deposition. Some of this work will be motivated by a new requirement from the International Civil Aviation Organization that large ash-cloud forecasts include model-based contours of ash concentration (ICAO Met. Panel, 2019), extending a European requirement established in 2010

(Beckett et al., 2020). Efforts to develop this practice are still in the early stages (e.g. Pelley et al., 2015).

3.7 Inverse methods and forecasting

Inverse methods allow models of magmatic systems to be compared quantitatively with observations to enable us to constrain otherwise inaccessible properties and processes of magmatic systems, thereby providing the critical link between data and models. Through computational parameter estimation, inverse methods have been widely and successfully applied to a diverse range of problems in volcanology; for instance, magnetotelluric observations have been used to constrain subsurface resistivity; gravity data used to map density anomalies; ground deformation and seismicity used to reveal faulting, pressure, or volume changes; and seismic imaging used to resolve variations in seismic shear and compressional velocity, anisotropy, and attenuation. Importantly, data-model assimilation algorithms can also be used to forecast the future state of a volcanic system given constraints on its current state. Model-based forecasting techniques remain in their infancy in volcanology but show great promise (Poland and Anderson, 2020).

3.7.1 Inverse methods for constraining crustal magma transport and storage

Inverse methods encompass a variety of techniques that can provide insight on a range of volcanic system models, thereby informing our understanding of the architecture and dynamics of real magmatic systems. Techniques vary widely, from simple optimization approaches to sophisticated Bayesian inference frameworks that permit the utilization of independent *a priori* information and full quantification of the uncertainties associated with parameter estimates. Because inverse approaches are so important for relating volcanological models with observations, they must be a part of an MCS.

Because magma systems are complex, nonlinear, and observed only indirectly, the future success of magma system modeling hinges on the integration of diverse data types such as geodetic observations with eruption rate and gas emissions data (e.g., Anderson and Segall, 2013; Wong and Segall, 2020). There remains great promise in the combination of new types of observations. For instance, petrology and geochemistry measurements may be combined with geodetic and geophysical datasets — the former providing crucial information about the thermodynamic state of the magma integrated up to a point in the past, and the latter providing a contemporaneous view of the host-reservoir system. Particularly powerful is the development of inverse methods that combine different, yet complementary, geophysical approaches with petrological, laboratory, and geochemical measurements, as well as with the results of independent past studies. In contrast, inverse models of single data types can suffer from limited resolution and inherent non-uniqueness. A major issue has been the interpretation of seismic tomography and related studies with regards to melt fraction. Recent progress has been made by the development of three or four-dimensional petrophysical models that infer the extent of partial melt and volatiles at several subduction zone volcanoes, including Soufriére Hills Volcano, Montserrat (SEA-CALIPSO; Voight et al., 2014; Paulatto et al., 2019), Mount St. Helens (iMUSH; e.g., Kiser et al., 2016; 2019), Uturuncu, Bolivia (PLUTONS; Pritchard et al., 2018), Laguna del Maule, Chile (e.g., Singer et al., 2014), and Santorini, Greece (PROTEUS;

Hooft et al., 2019). These projects demonstrate the value of using multiple, dense geophysical datasets combined with petrology and geochemistry to consistently interpret different types of data and to determine the structure of subsurface magma storage and whether anomalies are caused by, for instance, partial melt, brines, or sulphides.

An MCS would leverage abundant and diverse observations to develop the next generation of models, especially by facilitating the development of joint inversions that explain multiple datasets. Such models should leverage data types with complimentary sensitivity to structure and processes and include: deformation; seismicity; seismic P&S wave velocity (body wave and ambient noise tomography) interfaces (receiver functions and seismic reflection), attenuation, and anisotropy; electromagnetics; gravity (and time variable gravity); geochemistry and petrology; and gas and thermal emissions. There are several approaches to joint inversion for magmatic system architecture with promising results to date, but much model development remains to be done, especially coupling petrophysical models with laboratory results (see for example the SIGMELTS program for electromagnetic data, Pommier and LeTrong, 2011), or linking magmatic processes with seismic data. Aside from advancing our fundamental understanding of magma system architecture, progress in this direction would also enable better assessment of hazards during periods of volcanic unrest.

3.7.2 Forecasting

To be able to accurately forecast a volcanic eruption and the hazards associated with it is one of the grand challenges of volcanology (National Academies of Sciences, Engineering, and Medicine, 2017). Eruption forecasting involves a variety of questions that should be addressed on a societally relevant timeframe such as: If, when, and where will the eruption occur? What will be the magnitude of the eruption? How will it evolve? What are the transient events that could take place? Also important, but less often asked: When will the eruption end? To address these questions it is important to know what physical parameters and processes will improve forecasts. Future advances in eruption forecasting will require improved linking between monitoring and process. Of particular importance is the move toward more physics-based forecasting models (National Academies of Sciences, Engineering, and Medicine, 2017), which involves the tight integration of data and thermo-mechanical models of magma systems. The MCS can play an important role in fostering the development of such models.

At present, some volcanoes still erupt with no detected precursors and lives and livelihoods are placed in peril (Poland and Anderson, 2020). Yet, recent advances in volcano observing systems allow us to obtain data with improved spatial and temporal resolutions, opening the door to a new generation of eruption forecasts. Anomaly detection and pattern recognition have been revolutionized with machine learning techniques and benefited greatly from the overwhelming quantity of data that is now freely available. However, caution has to be exercised when interpreting these data-driven outputs as they can be misleading and they provide no physical understanding of the volcanic system. Thus, advances in forecasting will benefit from the implementation of multidisciplinary monitoring of the full range of phenomena during repose, unrest, and eruption at many more volcanoes, as well as the development of flexible, open-access databases of diverse observations for immediate use, as well as their long-term maintenance (National Academies of Sciences, Engineering, and Medicine, 2017). This is also something a MCS can play a valuable role in.

Eruption forecasts that are based on dynamical models of the underlying physical processes are now, at least for certain volcanoes and eruptions, within grasp. These models can be combined with observations using Bayesian-based Markov chain Monte Carlo or data assimilation techniques of the kind that are now widely used in numerical weather prediction centers. Such techniques can be used not only to track and assess the current state of a system, but also to quantitatively forecast future behavior (e.g., Segall 2013, Gregg and Pettijohn, 2016, Bato et al., 2017, Zhan et al., 2017, Albright et al., 2019). Forecasts will always remain uncertain due to our lack of direct subsurface observation, but non-uniqueness can be reduced through the assimilation of multiple diverse datasets using more realistic subsurface models. The incorporation of volcano models into probabilistic, unified forecasting frameworks — which integrate insights from various techniques including expert elicitation and machine learning — may also prove useful (Poland and Anderson, 2020), and it is worth remembering that model-based eruption forecasts will provide guidance to decision-makers, whose expertise will be necessary to interpret these results appropriately. Ultimately, eruption forecasting requires sophisticated modeling techniques in conjunction with deep collaborative work to understand the observations and complexities that distinguish each individual volcanic system — efforts that could be directly benefited by an MCS.

4. Vision for a Volcano Modeling Collaboratory

Volcano-magmatic system models are challenging and time-consuming to develop. They enable understanding of natural and experimental observations, and therefore require comparable levels of support. **In this section we summarize how current approaches towards volcano-magmatic system modeling can be improved in order to enable new scientific advances, lay out goals for a modeling collaboratory, and detail how these goals could be achieved.** We emphasize that this is a vision for how an MCS can benefit modeling-based collaborative science, not a list of topics modelers should focus on, nor a formula for how they should go about doing so.

4.1 Limitations of the Status Quo

Workshop participants identified key shortcomings to the status quo. The complexities of volcano-magmatic systems are enormous, requiring state-of-the-art models that often push the limits of numerical techniques. Yet, model development is often treated as a by-product of other research goals, resulting in a lack of incentives and resources, and many codes are developed by graduate students and postdoctoral researchers in relatively isolated research groups on short-term academic cycles. As a result:

- Opportunities for collaboration are missed — between research groups, between observationalists and modelers, and between volcano modelers and outside experts in fields such as applied mathematics, statistics, data science, and computer science.

- Models of different — but physically related — subsystems and/or processes typically lack integration, interoperability and modularity, even when such interoperability is not technically challenging.
- Many (if not most) codes are not adequately validated, verified, benchmarked, and documented.
- Model codes are often not freely shared, can be difficult to access, and are often not open source.
- Training opportunities are limited.

Clearly defined programmatic funding opportunities for model development and an integrated approach to collaborative volcano science, in which modeling is included as a full partner, lies at the heart of the vision for a volcano modeling collaboratory.

4.2 What can a Modeling Collaboratory Achieve?

4.2.1 Fostering flexible development of subsystem and integrative system models

While the types of models that might be supported by a modeling collaboratory must be rooted on some level in the primary science objectives discussed above, workshop participants expressed concern about prescribing *top-down* science directives aimed at guiding future research and modeling efforts. Instead ***there was a clear preference for a volcano collaboratory that would support, on some level, any models falling under the broad umbrella of volcano-magmatic systems.*** Therefore, the types of models supported by an MCS are envisaged to emerge organically during the MCS process itself, rather than following a preordained list of research goals.

It was also recognized that not all models will be fully amenable to certain MCS goals, such as interoperability with other models. Rather, ***the modeling ecosystem consists of different branches with different expectations, needs, end-users, and purposes***. For some models, observational constraints as well as underlying processes and physics are relatively well established, understood and prescribed, with model solution techniques that may be relatively straightforward. These models can be useful for exploring outcomes (with necessary caution) even by users with limited knowledge of underlying theory or numerical methods, and such models can benefit from MCS tools and resources for open-source sharing or interoperability.

Other models are evolving more rapidly, or are more complex or rudimentary, and may not be ready in the short term for broad distribution or interoperability with other models. Although a longer-term goal could be that these model codes evolve toward a state of interoperability and accessibility that could be facilitated through an MCS, this outcome could take many years, or on some levels even never be practical. Developers of such model codes would benefit from the various collaborative aspects that an MCS would offer (e.g., workshops and summer schools), as well as technical expertise through enhanced funding aimed at collaboration between model developers and experts in other fields, such as applied math and data science. Thus, there will have to be flexibility in how the various collaboratory objectives will be achieved.

Regardless of the mechanism, it was recognized throughout the workshop that an MCS can facilitate the development of a new generation of models that are not well-served by the existing funding and research structures. For convenience we here divide models into two classes: (1) integrative system models which relate diverse physics and observations, possibly over a range of spatiotemporal scales, and (2) subsystem "building block" models which can ideally be directly linked to one another and used to more efficiently and effectively construct larger system models. Below we detail how an MCS can benefit both classes of model.

Integrative system models. Throughout the workshop it was recognized that the development of models by individual research groups tends to target specific disciplinary problems. An important role for an MCS would be to encourage and facilitate the development and integration of system-scale models that cross boundaries of disciplines, problems, and scales, and that can predict diverse observations. Workshop discussions identified a fully integrated model of crustal magma transport, storage, and eruption, spanning huge spatial and temporal scales, as an aspirational but probably unrealistic goal. Nonetheless, there is great promise for models which incorporate diverse physics from magma storage, ascent, and even eruption. Such models can provide the *"glue"* to pull a range of disparate observations together (Anderson and Segall, 2013; Segall and Anderson, 2016). To begin with, this work can be facilitated by the use of reduced-order "box" or "lumped parameter" models which average physical properties across spatial domains, such as a magma reservoir, but which nevertheless capture the essential physics and which can be conducive to up- and down-scaling, as well as integration of diverse observational and experimental data. These models are highly simplified yet can be viewed as fundamental system-scale models that form the basis for integration of more sophisticated subsystem models, which constitutes one of the principal goals for an MCS.

An ecosystem of interoperable subsystem models. In contrast to — but complementary with — holistic system models, an ecosystem of subsystem models can be centered on either processes or specific parts of the volcano-magmatic system. The latter would, for example, include melt generation and extraction, crustal magma transport, magma storage reservoirs, conduits, or eruption plumes. Process-based subsystem models could serve to link models with experiments and could be organized around topics such as multiphase flow (in the mantle wedge, during crustal transport, in magma chambers, in conduits), thermodynamics, or dike propagation. Subsystem models are a necessary requirement for advancing sophisticated simulation capabilities, due to the immensely complex nature of any given natural system. To the extent practical, subsystem models would be interoperable using well-defined or even standardized sets of inputs and outputs (application programming interfaces [APIs]), permitting their use within broader integrative models. This could take the form of something like a scrapbook of different types of highly resolved simulations (or modules), developed somewhat independently yet useful together. For instance, the Community Surface Dynamics Modeling System (CSDMS; Tucker et al., 2021), which supports the development of integrated software modules that predict fluxes of fluid and sediments at Earth's surface, has demonstrated that in many cases coupling can be performed after-the-fact between existing codes (even those written in different languages), and can lead to important advances. An interoperability objective is, however, not always appropriate. Efficiently modeling complex multiscale coupling may sometimes require close algorithmic coupling, and furthermore, many research codes are simply not well-suited for coupling with others. Thus, an MCS must remain flexible enough to accommodate different needs in terms of model integration and interoperability.

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

Models, and the computer codes from which they are built, are not mere "tools" — they are first-order science objects. They are designed to simulate aspects of natural systems under specific science objectives but are not, of course, digital copies by which a user can exactly reproduce nature. Models therefore require understanding of the natural system they are meant to simulate, and they require mathematical representations and simplifications that are suitable to address specific science objectives. It is important to emphasize that model development and scientific insight are intimately intertwined. In other words, more scientific insight may be gained during model development than during subsequent model application. Thus, public open-source modeling codes are not generally the implementation of an easily accessible tool, but rather they are based on first order scientific projects in the form of model development and as such they are entirely contingent upon such efforts.

Open-source, community-supported codes confer numerous well-documented benefits, as already identified in other science disciplines. There are only a very few models in volcanology that have wide community acceptance and have been applied to interpret multiple types of data over a range of scales. In this sense, the volcanological community lags behind many other sciences in which code publication is seen — and supported — as a standard (even required) part of code development and the scientific process. A key point here is that such code publication, which requires time and effort, is only feasible if supported through funding and if there are tangible career benefits associated with doing so (i.e., publications and citations).

Open-source codes tend to be more robust, more easily extensible, more widely utilized and better cited, and more easily linked with other model building blocks. These benefits are particularly important to the volcano modeling community, which is small enough that the size of research groups and complexity of software that can be produced is necessarily limited. Why has open-source volcanology code not yet taken root? Firstly, models tend to be developed by graduate students, as part of hypothesis-driven science projects. There is often little funding support for the development of public codes, which requires far more effort than the development of research codes. The former may be useful despite kludges, inefficiencies, poor documentation, and idiosyncratic coding habits (volcano models are rarely developed in collaboration with professional programmers). Secondly, the publication of model codes does not yet confer the same career benefits as manuscript publication, so at present there is limited incentive for the major time investment required to document, carefully test, and publicly release code. This is something that other communities have dealt with. For instance, lessons learned from the Computational Infrastructure for Geodynamics (CIG) program and its best practices (https://github.com/geodynamics/best_practices) can be applied to a future MCS. In summary, funding mechanisms and career pressures for academic researchers are not consistent with the development and long-term support of public, open-source model codes.

These limitations may be overcome by a community-based approach. An MCS should encourage, support, and enable the development and maintenance of codes that are easy to configure, use, reuse, and extend and scale. In many ways the envisaged access to models is complementary to the ERUPT report's recommendation for supporting access to data and data products (National Academies of Sciences, Engineering, and Medicine, 2017). Shared codes must be citable and, when possible, not be disassociated from their underlying data resources. Models should be maintainable and updatable by a community of model users. A community of model users will also prevent the geographic isolation that can be a challenge, particularly for early-career scientists. Finally, although the problem of inadequate recognition for code development is broader than an MCS, the MCS must support DOI numbers for codes, track model access and usage, and encourage model users to include original authors in derivative works.

4.2.3 Facilitating code verification, validation, and benchmarking

Code verification, validation and benchmarking goes in hand with the development of public, open-source codes. The importance of verifying, validating, and benchmarking model codes is well established throughout the sciences. Verification may be roughly defined as an assessment of solution quality (that is, ensuring that the conceptual model is implemented correctly), which can be done by comparing against analytical results. Validation is designed to determine if the model agrees with physical reality, and is “a continuous process, in which the credibility of a model with respect to its intended use(s) is progressively improved by comparisons with… experiments” (Ongaro et al., 2020). Benchmarking, finally, involves comparing different models of the same physical process to one another. (We acknowledge that these terms are used in different ways, and that models can never be confirmed to completely represent natural processes; Oreskes et al., 1994).

Verification, validation, and benchmarking ensure that codes are modeling the correct system, and that the codes do what they are supposed to do. They make outputs from different models more directly comparable, permit users to better understand model uncertainties and limitations, may guide the observational community to address key data limitations, and improve understanding of how parameterization and initial conditions affect results. Importantly, only properly tested codes can become trusted and widely-used community resources. The required efforts are time-intensive and offer few direct rewards. As a result, despite the clear benefits, only a few community intercomparison efforts have occurred in volcanology, and very few volcano-magmatic codes are carefully verified, validated, and benchmarked (a point also echoed during other workshops; e.g., https://sites.google.com/view/civworkshop/home). Early progress has been made only in a few instances, including lava flows (Dietterich et al. 2017), tephra plumes (Bonadonna et al. 2012, Suzuki et al. 2016), conduit models (Sahagian 2005), and pyroclastic density currents (Valentine 2019).

An MCS should facilitate more verification, validation and benchmarking activities, for instance through the development and dissemination of model intercomparison parameters and guidelines, and by providing a venue for documenting model verification results. An MCS could support such activities by, for instance, providing support for modelers to collaborate with each other and with experimentalists and observationalists on validation projects.

4.2.4 Facilitating code discovery and sharing

Code is far less useful if the community of potential users is unaware of its existence or if it cannot readily be accessed. Absent this, codes must be reinvented over and over in individual research groups (we make a clear distinction between intentionally reinventing code for training purposes and unnecessarily reinventing code because existing code is not available). Unfortunately, awareness of existing codes is a problem in volcanology since no well-established centralized code repository — or index of external codes — exists. In the field of volcano geodesy, for instance, dozens of independent implementations of analytical source models are in existence. Additionally, it is also important that model outputs (results), not just models, be made available, such as in the IRIS repository (http://ds.iris.edu/ds/products/emc-earthmodels).

Improved access to codes will enable not only interdisciplinary studies but also comparative volcanology of a greater diversity of magmatic systems, which is critical for overcoming our current biased sampling of a small fraction of the world's volcanoes, as outlined in the ERUPT report (National Academies of Sciences, Engineering, and Medicine, 2017). It should be expected that an MCS would synthesize available data and develop new hypotheses that could be tested with, and will inform the design of, focused multi-disciplinary field or laboratory experiments.

A previous community effort (VHUB) hosted codes and related information and was widely used in its early stages — particularly for teaching students and by observatories worldwide in regions with less access to research information. However, VHUB used an older and somewhat inflexible technology, and use declined as funding for training and outreach ran out (https://vhub.org/about/usage). VHUB thus demonstrates a strong need for a modern modeling hub that facilitates code development, discovery, and sharing. Recent efforts such as online modeling portals and shared public repositories can be useful (e.g.,https://gscommunitycodes.usf.edu/geoscicommunitycodes/index.php, https://laharflow.bristol.ac.uk, and various git repositories hosted by individuals or research groups), but are not community-based and can still be challenging to locate. A primary limitation to existing "repository" efforts is that they are viewed and construed as static archives. An MCS that is focused on open-source codes with verification, validation, benchmarking, and interoperability would lead to a dynamic repository amenable to code discovery and sharing.

4.2.5 Enhanced interdisciplinary collaboration

Making models, model codes, and model outputs more accessible to a broader user community is aspirational but needs to account for the fact that some models require substantial expertise to use. The broader use of such models is best achieved within the framework of collaboration that involves a significant component of cross-disciplinary training and education. An MCS should facilitate and enhance collaboration (through workshops, for instance) that include a significant component of training and education aimed at enhancing collaborative synergy.

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

4.2.6 Enhancing modeling efforts within the CONVERSE initiative

CONVERSE is primarily concerned with eruption response to maximize scientific return through the collection of key data before and during eruptions. Within CONVERSE the academic scientific community coordinates with scientists from federal agencies (primarily the USGS) to respond to volcanic unrest and eruptions in a timely manner. Because MCS is dedicated to collaborative modeling, model benchmarking, interoperability and documentation, there is the potential for significant synergy between these two initiatives. As emphasized in the ERUPT report, the collection of multidisciplinary data at volcanoes is critical to inform physical-chemical volcano models that in turn enable a better understanding and quantification of volcanic processes (National Academies of Sciences, Engineering, and Medicine, 2017). While CONVERSE is focused on US volcanoes and not exclusively on convergent margins, the broad overlap between physics and processes across all volcano-magmatic systems, inherently leads to significant potential synergies between MCS and CONVERSE. In an ideal case, the data collected through CONVERSE will feed into models in near real-time to inform eruption forecasts and hazard assessment. As MCS develops interconnected multi-disciplinary volcano models from magma to the surface, data collected by CONVERSE scientists can inform various parts of these models. For example, gas and deformation measurements during eruption run-up can inform the models of magma-chambers while drone-based measurements on lava and pyroclastic flows can inform conduit models.

Facilitated through the Volcanic Systems MCS workshop, there are preliminary synergistic activities between CONVERSE and MCS being explored. Specifically, a synthetic magmatic event, such as a dike injection at a US high threat volcano, could be simulated such that models generate synthetic deformation signals. The CONVERSE deformation community would then evaluate whether such deformation events are detectable with the current sensor network on the selected volcano and propose network modifications based on the data obtained. This scenario exercise would result in testing and benchmarking of various volcano deformation models as well as an outcome that enables network testing and modification to better detect such events and maximize scientific return. The scenario exercise would also reveal gaps in modeling capabilities that the MCS community can address.

In summary, CONVERSE and MCS share a number of commonalities that provide opportunities for synergy. They include improvements of sensor network designs on volcanoes, the potential to inform models with real-time multi-disciplinary data collected during run-up and eruptions, training of scientists to use models to forecast volcanic activity and providing a forum for modeling scientists and data collection scientists to exchange ideas and advance our understanding of how models can be most effectively informed by data.

4.2.7 Enhancing science community and preparing future scientists

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

Preparing future volcano scientists has already been identified as a major goal for strengthening and building an effective volcano science community (National Academies of Sciences, Engineering, and Medicine, 2017). Achieving this goal requires enhanced investment in student and postdoctoral researchers who are focused on the development of the requisite numerical models. It must go beyond a paradigm whereby a majority of support for geoscience modeling is solely tied to hypothesis-driven projects and contingent upon the prior existence of modeling capabilities. A competitive science program for volcano-magmatic systems, whether within the broader SZ4D objectives or beyond, requires enhanced and sustained support of students and postdocs engaged in model development. An MCS could serve as a programmatic conduit in this regard, assuring through workshops and networking that a growing pool of nascent "modelers" will be optimally positioned for collaboration with experimental and observational scientists through model development and hypothesis-driven model simulation.

4.3 Proposed Volcano Modeling Collaboratory

Based on community feedback during the workshop, this section defines a proposal for how a modeling collaboratory would best advance volcano-magmatic systems science. **At its heart this represents a new vision for community-driven collaborative volcano-magmatic system science, with modeling as the nexus between observations, analysis, synthesis, and understanding (Figure 4).** The proposal elements are designed to facilitate the goals identified in section 4.2 above. The collaboratory vision is composed of two primary elements:

1. Community working groups

2. Programmatic funding (grants)

These are discussed in the next sections, along with the support necessary for making an MCS work.

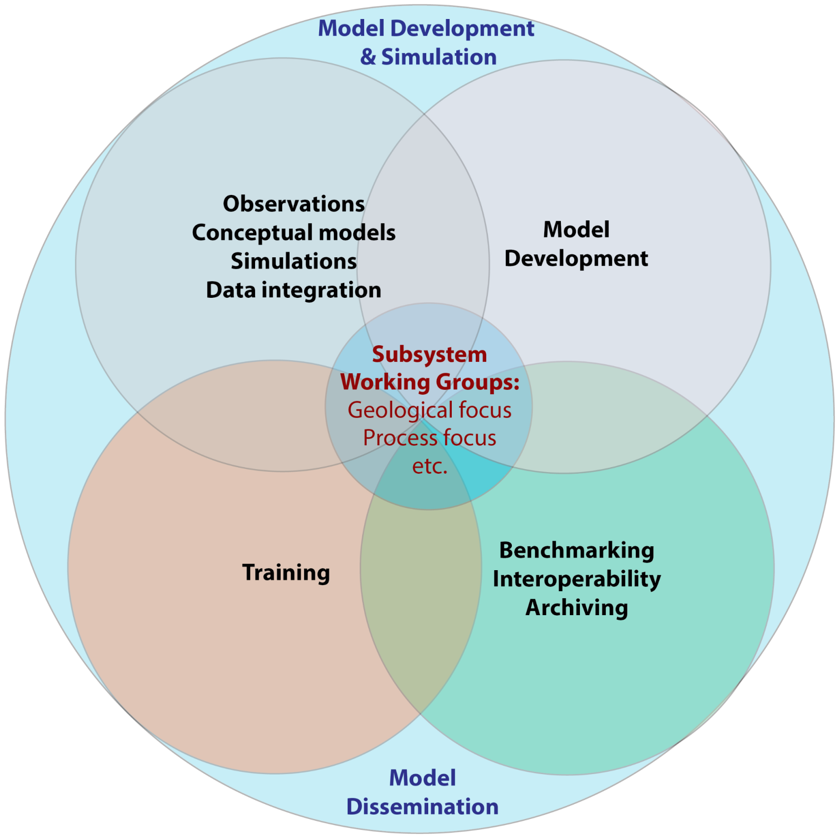

Figure 4: *Potential MCS structure with model development and simulation activities originating through working groups that may be geologically, process, or otherwise focused. Essential activities are model development, often at the PI level, and integration of observations through the development of conceptual models and simulations. Model dissemination integrally follows model development and includes activities such as benchmarking, making models interoperable, model archiving, and training.*

4.3.1 Community Working Groups

Volcanology is a small, geographically-dispersed community working with rich but fragmentary information to understand highly complex systems. This offers great opportunities but also unique challenges. A successful collaboratory will need to allow and encourage individual research groups to devise new computational techniques, or employ traditional methods in new ways, as their vision, scientific impulses, and insights direct them. Furthermore, the idea of "shared master codes", maintained in a repository by technicians, was viewed by some workshop participants as an outdated solution that would lead to code obsolescence. On the other hand, the development and maintenance of open modeling codes by an interdisciplinary community of users — when appropriate — could prevent obsolescence and lead to scientific sharing in ways not currently possible. To be successful a collaboratory must therefore provide support for model development by researchers (including postdocs and graduate students), community-based working groups, and platforms and tools necessary for efficient and open sharing of codes and ideas. Creativity and forward-looking approaches should be encouraged, with the goals of collaborative analysis, synthesis, and ultimately a universe of different models and modeling approaches.

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

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

The CWG vision was inspired by workshop discussions, as well as by the activities of the USGS John Wesley Powell Center for Analysis and Synthesis (https://www.usgs.gov/centers/powell-ctr) and the Cooperative Institute for Dynamic Earth Research (CIDER) summer school. Inspiration was also found in other fields, such as in weather forecasting, where collaboration between observationalists, theorists, and modelers has led to remarkable improvements in forecast accuracy.

In the MCS model, individual CWGs would work to promote understanding through modeling-centric analysis and synthesis of existing data. Some CWGs could be arranged around a specific science topic. Others could be arranged around a geographically focused problem, such as a recently-active magmatic system, a volcanic region or arc, or an exhumed plutonic system. Still other CWGs could focus on a particular type of process, model, or even methodology. CWGs would directly address many of the modeling collaboratory goals identified above, including 1) training and education, 2) interdisciplinary collaboration, and 3) fostering the development and testing (verifying, validating, and benchmarking) of public, open-source model codes. Critically, CWGs would enable science advances by augmenting the current mechanism of individual PI-level research grants.

CWG activities could take on different forms depending on the focus. These might include intensive summer schools or hackathons, or intermittent workshops held regularly over a period of years. In one model, a community group would obtain initial seed funding to hold a workshop (an interdisciplinary proposal incubator), with the objective of producing several individual or collaborative proposals to carry out the work. This could occur in an intense period of weeks, or over years. Rather than directing or sanctioning science objectives or projects, the CWGs would act as incubators and nexuses for collaborative projects that include a significant component of modeling or model development.

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

4.3.2 Programmatic funding (grants)

Grants would provide support for students and postdocs in order to establish and sustain a pipeline for geoscience modelers. The need for such grants is based on the recognition that the majority of model development, model innovation, and model simulations are pursued by graduate students and postdocs. However, under the status quo there is no viable pathway to go from a research-grade model, which is the basis of many hypothesis-driven publications, to completion of the desired benchmarking, model documentation, archiving, publication, and/or training steps. Few of these activities translate into citable publications 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, even though postdocs often are the "glue" that holds together a large research team.

The objective of the 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 graduate students with expertise in numerical modeling to move into science careers by funding professional development and collaborative modeling activities; (4)

support and enhance the development of numerical models within volcanic-magmatic systems science, inclusive of funding for collaboration with applied mathematicians and computer scientists; (5) move research efforts of model development into a path of long-term synergistic use; and (6) make models more viable for collaboration through benchmarking, documentation, publication and archiving, accessibility, and training. In summary, within this vision the grants would support the development of an ecosystem of numerical models. They could augment hypothesis driven science grants, but would predominantly be full grants in their own right, and may or may not be awarded in conjunction with a CWG.

4.3.3 Supporting an MCS

Activities outlined above will require at least some administrative support (for instance, to assist with coordinating the CWGs). However, workshop discussions reached no conclusion regarding the need for a permanent technical or administrative staff, nor if the collaboratory should be based at a centralized facility. We therefore set aside these decisions for the broader MCS.

Workshop participants were generally in agreement, however, that some form of basic web infrastructure support would be required, although there were different visions regarding the implementation. Specifically, many goals listed above require that model codes be robustly tested, documented, and (usually) maintained in an open-source community archive. These activities could be enabled through a cyberinfrastructure component that includes at least some of the following:

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

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

5. Synthesis

Model development is an integral part of scientific discovery and a critical step leading to the advancement of knowledge and understanding. Models have provided tremendous insights into magmatic and volcanic systems, with a remarkable diversity of models now available for magma transport and storage, from crystal-scale processes to the evolution of entire magma systems over thousands of years. Now, enabled in part by new technologies for collaborative communication and code development, there are exciting opportunities for improving the ways in which models are developed and shared. Chief among these is the great potential for bringing diverse groups of scientists together for collaborative research efforts which utilize models to tackle some of the great outstanding questions in volcanology.

The vision of a collaboratory in which modeling serves as the nexus for integration of magma system observations across subdisciplines is the result of community input solicited in the MCS volcano workshops. It is also inspired in part by the success of collaborative efforts such as the Cooperative Institute for Dynamic Earth Research (CIDER), the USGS Powell Center for Analysis and Synthesis, and the Southern California Earthquake Center. Through diverse, interdisciplinary working groups and targeted grants, the collaboratory will foster the development (including distribution, testing, and archiving) of a new generation of community volcanic system and subsystem models. Working groups could be organized around particular subsystem models (e.g., source, reservoir, conduit), process models (e.g., multiphase flow), or scales (e.g., arc scale, eruption type). A key objective for initial activities would be to identify key modeling challenges (some are outlined in this report) that are ripe for progress, thereby setting the stage for proposals aimed at model development and model-centric collaborative science integration. Such a modeling collaboratory will bring together scientists with different backgrounds and at different career stages for sustained, interdisciplinary, collaborative research and modeling efforts. The results should be remarkable new insights into the magmatic and volcanic systems on planet Earth, with important societal implications for economic activity and hazards mitigation.

Disclaimer

This workshop report has not been through a full peer review process. Any use of trade, firm, or product names is for descriptive purposes only and does not imply endorsement by the U.S. Government.

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