Modeling Collaboratory for Subduction RCN

Megathrust Modeling Workshop Report

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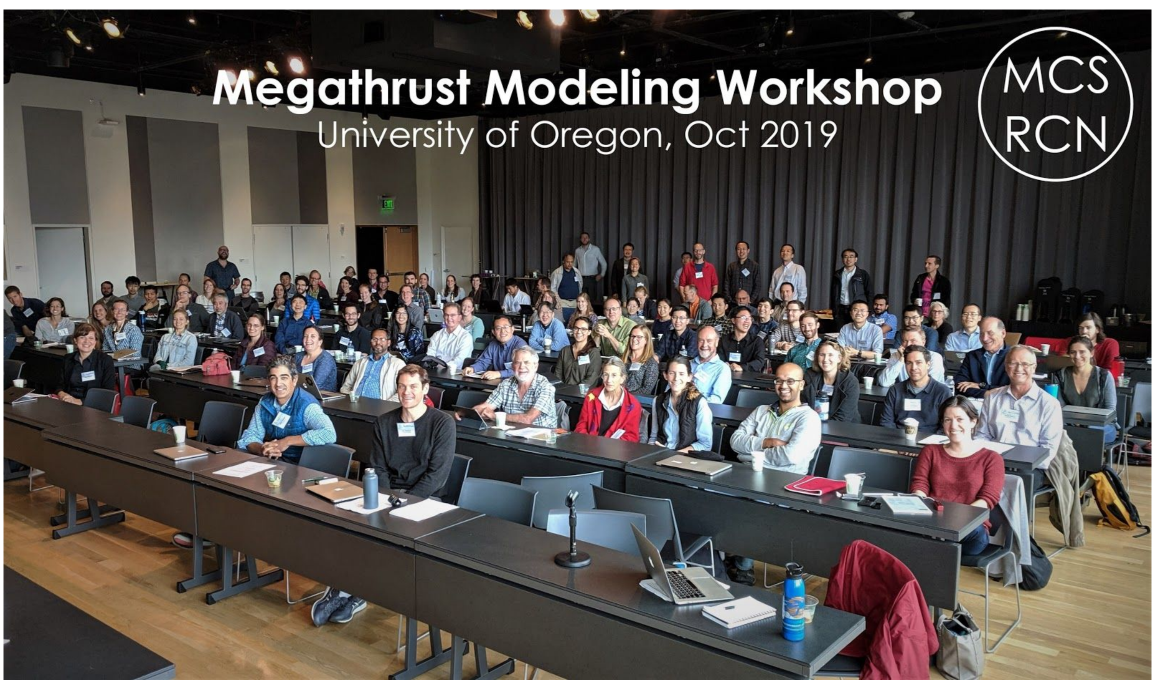

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Summary

The *Planning for a Modeling Collaboratory for Subduction Zone Science* (MCS) Research Coordination Network (RCN) is one of three RCNs funded by the National Science Foundation (NSF) following the 2016 Subduction Zone Observatory (SZO) workshop. The MCS RCN aims to facilitate the development of the integrative earthquake and volcano modeling component of SZ4D, the MCS, and explore how computational approaches and community building can best advance subduction zone systems science. This report documents the excitement and vision of the scientific community as articulated by participants of the October 2019 MCS *Megathrust Modeling Workshop*, with material from this and prior events available on the MCS RCN web site. This report reflects the efforts of the writing committee and input from the community throughout the summer of 2020.

The report begins with a brief overview of the **State of Knowledge** in three main fields comprising megathrust science: 1) dynamic rupture and tsunami, 2) sequences of earthquakes and aseismic slip, and 3) long-term geodynamics and surface processes. The report proceeds to articulate **Outstanding Science Questions** that lie at the boundary of current knowledge. These lines of inquiry will be the focus of much research in the coming years, and they have the potential to significantly advance our understanding of subduction megathrusts and the associated hazards. We are at the verge of fully integrating physics-based models into forecasting and hazard assessment for megathrusts, and working toward that goal will lead to breakthroughs in both fundamental, academic research and societally applied studies.

The report closes by outlining **Recommended Community Actions to Advance Subduction Megathrust Modeling within a Collaboratory** for immediate steps over the next few years. These actions include:

1. developing **sustained, international, distributed, and open collaborations** to facilitate comparative analysis, verification, exchange of ideas and knowledge, and joint model development;
2. organizing **focus groups dedicated to regional laboratories, and case histories of significant earthquakes**;
3. organizing **focus groups for subsets of megathrust processes,** to document the current state of knowledge, provide guidance for code and workflow development, and provide science focus;
4. **integration of modeling efforts with observations and experiments** in a manner that includes transparency of assumptions, data resolution, and joint development of falsifiable hypotheses, in conjunction with the regional laboratories;
5. thorough **code benchmarking, verification, and validation** exercises; and
6. the **immediate development of three specific models** that would benefit the community:
    a. a viscoelastic earthquake sequence model with fluid transport;
    b. a global, 3-D, thermo-mechanical mantle circulation model with two-phase flow;
    c. a flexible modeling framework for multi-physics, multi-scale modeling including rupture, earthquake cycle, and tectonic time scales.

If pursued further, these community actions will facilitate the next generation of scientific discoveries and physics-based understanding of megathrust systems. These efforts will form a major component of the MCS within the SZ4D effort, and will advance computational geoscience at large.

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Introduction

Subduction zones offer compelling and only partially answered scientific questions about earthquakes and faulting, volcanoes and magma transport, and landscape evolution. Subduction zones also host the largest earthquakes and associated tsunamis on Earth and pose a significant hazard to communities globally.

Over the last decades, fundamental advances in earthquake science have refined our understanding of this most hazardous type of plate boundary. For example, analysis of geodetic and seismic records led to the discovery of slow fault slip that had previously eluded detection. Analysis of data from the M9 2011 Tohoku-oki earthquake and tsunami has led to fascinating insights into pre-, co-, and post-seismic stages of a megathrust event. Advances in the quality and density of global geophysical monitoring networks have led to systematic analyses of large and great earthquakes to determine their overall features, and observations of spatial and temporal behavior of megathrust systems over a significant fraction of the earthquake cycle. These discoveries beget further questions into the nature of subduction megathrusts and the degree to which we can link seismic activity to our understanding of how the stresses that load faults evolve over the wide range of spatio-temporal scales of relevance, from long-term strain partitioning and orogeny to earthquake nucleation, rupture propagation, and tsunamigenesis.

Answering these scientific questions, through the development of predictive modeling tools validated and calibrated against observations, is required to inform governmental agencies and the general public about hazards from earthquakes, tsunamis, volcanic eruptions, and landslides. While subduction zones have been studied for decades, the subduction science community is currently poised for transformative and impactful research advances over the next 5-10 years.

For example, novel offshore instrumentation ranging from seafloor geodesy to cabled sensor networks will constrain fault slip and seafloor deformation before, during, and after earthquakes with unprecedented resolution. Similarly, monitoring and elucidating the causes of volcanic unrest will be facilitated by instrumentation advances in fluid and gas transport measurements, seismology, geodesy, and infrasound, together with laboratory analytical techniques. At the same time, experimental studies on exhumed or in-situ fault zone rocks yielded important insights on material behavior, and those can be incorporated into enhanced, multi-physics numerical models on improved computational platforms.

However, all of these observational and experimental constraints still need to be formally integrated into a consistent mechanical framework, and that integration must occur through data-centric, multi-scale numerical modeling, taking into account uncertainties. Megathrusts are one example where computation has to be the complement to observational and laboratory approaches to arrive at a more complete understanding of system dynamics. Such integrative modeling has long been discussed, but we are now poised to make good on this promise of computational geoscience (e.g., Lapusta et al., 2019; NASEM, 2020).

The MCS RCN *Megathrust Modeling* workshop, which convened at the University of Oregon in October of 2019, focused on assessing the critical aspects of fault system dynamics within long-term plate tectonic loading, earthquake sequences and aseismic slip, and megathrust rupture dynamics that should be included in the future integrative community modeling framework for subduction zones.

The meeting brought together a diverse group of international scientists at various career stages to identify the disconnects and knowledge gaps that should be targets for future research efforts, and to distill potential new approaches for collaborative megathrust modeling within an MCS. The meeting objectives were to

- identify the thermo-mechanical processes at different temporal and spatial scales that are critical to subduction megathrusts;
- determine the disconnects among models of different scales and/or mechanisms, and the knowledge and implementation gaps among modelers and their algorithms;
- synthesize and direct existing efforts toward building a new modeling framework for faulting, earthquake sequences and aseismic slip, and megathrust rupture dynamics modeling for subduction zones; and
- explore what theoretical developments and constraints would be needed to interpret sensor network data streams for time-dependent, physics-based hazard assessment.

The meeting laid a foundation for development of a community plan for an integrative modeling framework and community building for the above problems and, from a megathrust perspective, further solidified a vision for the MCS within SZ4D and the wider community. This report outlines that vision.

We briefly discuss the **State of Knowledge** in the three main fields comprising megathrust science: 1) dynamic rupture and tsunamis, 2) sequences of earthquakes and aseismic slip, and 3) long-term geodynamics and surface processes. We then proceed to address **Outstanding Science Questions** that are at the current frontiers of knowledge and targets for future scientific advances. Lastly, we outline a set of **Recommended Community Actions** to further advance the state of knowledge in these areas.

State of Knowledge

1. *Dynamic Rupture and Tsunamis*

Most, though not all, deformation at plate boundaries is accommodated by slip across relatively narrow shear zones known as faults. The largest faults on Earth are found in subduction zones, making them the source of Earth's largest earthquakes and significant hazard. Megathrust earthquake ruptures initiate as frictional instabilities and propagate as wave-mediated stress transfer drives progressive reduction of frictional strength and slip along the megathrust interface. Slip occurs at a fast sliding velocity, typically > 1 m/s, arising from the rapid reduction of the frictional strength, or weakening, of the fault. Strength reduction at these fast slip velocities is widely seen in laboratory friction experiments, and inferred to occur in nature, due to the velocity-dependence of the friction coefficient or other weakening processes like thermal pressurization of pore fluids (Goldsby & Tullis, 2002, 2011; Andrews, 2002; Di Toro et al., 2004, 2006, 2011; Rice, 2006; Beeler et al., 2008; Noda et al., 2009; Brantut et al., 2010; Noda & Lapusta, 2010, 2013; De Paola et al., 2011; Brown & Fialko, 2012). Wave-mediated stress transfer leads to rupture propagation at speeds approaching or exceeding the seismic shear wave speed (Andrews, 1976; Freund, 1979, 1998; Rice, 1980).

Subduction megathrusts are complicated faulting environments, particularly in the shallow region near the trench (e.g., Hyndman et al., 1997; Hubbard et al., 2015). The shallow dip of megathrusts enhances rupture and wave interaction with the free surface, producing shear and normal stress changes along the fault that can facilitate rupture growth toward the surface (Oglesby et al., 1998; Duan & Oglesby, 2005; Ma & Beroza, 2008; Duan, 2012; Huang et al., 2012; Kozdon & Dunham, 2013; Galvez et al., 2014; Gabuchian et al., 2017). This shallow region also often features splay faults that might be activated during megathrust ruptures (Park et al., 2002; Strasser et al., 2009), raising questions regarding controls on rupture path selection through branched fault geometries (DeDontney & Hubbard, 2012).

In addition, the material and frictional properties of sediments that typically comprise this shallow region are strikingly different from those of materials deeper along the megathrust. Slip often localizes within velocity-strengthening clays (Saffer & Marone, 2003; Ikari et al., 2009; Faulkner et al., 2011). Elastic moduli and wave speeds are greatly reduced (Kitajima et al., 2012; Jeppson et al., 2018), which generally enhances slip and reduces rupture velocity (Ma & Beroza, 2008; Lotto et al., 2017, 2018). It is also possible that this region experiences inelastic deformation during great earthquakes (Ma, 2012; Ma & Hirakawa, 2013; Ma & Nie, 2019); however, whether that inelastic deformation takes the form of distributed plastic strain or is instead localized as slip on splays and other structures remains unclear.

Dynamic rupture modeling permits investigation of all of these questions, but the utility and relevance of such models hinges on the assumptions and inputs to the models: structure and geometry, material properties and rheology (elastic and inelastic), stresses and pore pressure, and the friction law and other processes governing fault strength evolution (Harris et al., 2018; Erickson et al., 2020). One the one hand, large-scale structure and geometry can be constrained from seismic imaging close to the level of detail required for many aspects of dynamic rupture applications, whereas fault-zone scale structures are poorly constrained. On the other hand, stresses and pore pressure are more challenging or, at many depths, impossible to directly measure, so must be determined indirectly, including through modeling of the system over long time scales.

Modeling at the earthquake cycle time scale of hundreds to thousands of years, accounting for aseismic and slow slip as well as past earthquakes, can account for stress redistribution and connect to geodetic and related constraints on fault locking and slip history (Li & Liu, 2016; Gallovič et al., 2019; Hirahara & Nishikiori, 2019; see also next section on *Sequences of Earthquakes and Aseismic Slip*). In order to constrain pore pressure, it is necessary to model fluid production and migration over these time scales (Wada & Karlstrom, 2020; Petrini et al., 2020), and link imaging to mechanical models. In addition, constraints on the tectonic stress state and pore fluid pressure likely require models that span geological time scales (1 to 10 Myr) over which the geometry and structure of the subduction zone evolve (e.g., van Dinther et al., 2013; Menant et al., 2019; Brizzi et al., 2020; Muldashev & Sobolev, 2020). Characterizing the rheology of the off-fault material and fault friction requires a combination of laboratory experiments (on either cores from drilling or exhumed subduction faults), understanding the geological context, and theory and modeling.

Slip and deformation during megathrust earthquakes, particularly in the region near the trench, control seafloor uplift and hence tsunami generation (Tanioka & Satake, 1996; Satake, 2015; Saito, 2019). Tsunami propagation in the offshore region is well understood, as is the tsunami-generating ocean response to seafloor uplift. However, several challenges and opportunities remain for improved tsunami hazard characterization and utilization of tsunami data to constrain the earthquake source. Foremost among these is better understanding of shallow rupture processes (i.e., activation of splays, the occurrence of plastic strain, and the importance of heterogeneous elastic properties) and accounting for these processes in the workflows that couple earthquake source models to tsunami models (e.g., Saito et al., 2019; Madden et al., 2019; Ulrich et al., 2019). Most current workflows utilize approximations, such as static solutions to fault slip in a uniform elastic half-space, that were sufficient in the past when data were limited. However, the growing availability of high-quality offshore data in and around the source region motivates revamping these workflows by relaxing these approximations (Saito and Kubota, 2020).

2. *Sequences of Earthquakes and Aseismic Slip*

Faults accommodate deformation with a variety of different mechanisms that vary in space and time. Slip phenomena outside earthquake rupture, which include transient creep, slow slip, and afterslip, are characterized by slip velocities one or more orders of magnitude larger than the plate convergence rate, but still far smaller than inertially limited slip velocities ~1 m/s characteristic of seismic ruptures (Ide et al., 2007; Peng & Gomberg, 2010; Burgmann, 2018). Because transient slip phenomena occur over significantly longer timescales than typical earthquakes, they are often either partly or completely aseismic in that they either produce no detectable seismic radiation, or their seismic manifestation is depleted in high-frequency content (i.e., > 1 Hz) relative to typical earthquakes. These transient slip events occur frequently in subduction zones around the globe and documenting their spatial and temporal properties has been the focus of much study in the last two decades (Obara, 2002; Rogers & Dragert, 2003; Beroza & Ide, 2011; Obara & Kato, 2016; Burgmann, 2018, Behr & Burgmann, 2020).

Afterslip is a widely observed form of aseismic slip that occurs when the region surrounding intermediate to large magnitude earthquakes is loaded by coseismic stress changes (Smith and Wyss, 1968; Marone et al. 1991; Miyazaki et al. 2004; Hsu et al. 2006; D’agostino et al. 2012; Wallace et al. 2018; Alwahedi & Hawthorne, 2019). The region hosting afterslip experiences transiently accelerated sliding which gradually decelerates as slip relaxes stress. The observed time dependence of afterslip is generally consistent with strength change being proportional to the logarithm of slip velocity, as is commonly observed in laboratory friction experiments and described in the framework of rate-and-state friction with velocity-strengthening character (Marone et al. 1991; Kato & Hirasawa, 1997; Scholz, 1998; Liu & Rice, 2007). While regions participating in afterslip are generally thought to be spatially exclusive of coseismically slipping regions, additional studies with high spatial resolution are required to rule out the possibility that a given fault patch could participate in both coseismic slip and afterslip (Johnson et al., 2012).

Transient slow slip events on subduction megathrusts can be quasiperiodic and are commonly found below the seismogenic zone. In some locations, they also occur in the shallow region near the trench, or can even be interleaved with seismic patches. Slow slip events exhibit a great diversity of slip rates, propagation speeds, and recurrence intervals (Schwartz and Rokosky, 2007; Beroza and Ide, 2011; Burgmann, 2018). They can be modulated by relatively small stress changes such as those from solid Earth tides and are thought to occur in environments with nearly lithostatic pore fluid pressure (e.g., Shelly et al. 2007; Audet et al. 2009; Thomas et al. 2009; Kitajima & Saffer, 2012; Hawthorne & Rubin, 2013; Burgmann, 2018). Slow slip is often accompanied by seismic tremor, thought to reflect the collective seismic expression of many low frequency earthquakes (Shelly et al., 2006, 2007; Rubinstein et al., 2008), events that are slower than typical earthquakes, but still capable of producing measurable seismic radiation. The causal relationship between tremor and slow slip is still uncertain (Bartlow et al., 2011; Villafuerte & Cruz-Atienza, 2017). Transient slow slip events require some weakening mechanism to initiate and accelerate sliding, but without the fault reaching slip speeds of typical earthquakes. Several mechanisms that reproduce this general behavior have been proposed but which, if any, of these best represents the range of observable slow slip phenomena is still debated.

Models that reproduce this behavior have 1) incorporated frictional constitutive relations that are rate-weakening at low slip rates and rate-strengthening at high slip rates (e.g., Shibazaki & Iio, 2003; Hawthorne & Rubin, 2013), 2) included heterogeneity such as mixtures of rate-weakening and rate-strengthening and/or viscous materials (e.g., Skarbek et al., 2012; Tong & Lavier, 2018; Goswami & Barbot, 2018), 3) called upon dilatancy to stabilize slow rupture (e.g., Segall et al., 2010), and 4) appealed to a characteristic length scale to stabilize rupture (e.g., Liu & Rice, 2007; Rubin, 2008). Others have suggested the possibility of fluid flow and/or pore pressure transients (Skarbek & Rempel, 2016; Warren-Smith et al., 2019), sometimes coupled with fault slip (Garagash, 2012; Zhu et al., 2020). The slow slip problem has also been approached from the geologic perspective through studies that document the geologic environs of slow slip and tremor (e.g., Fagereng et al. 2014, Saffer & Wallace, 2015; Platt et al., 2018; Kotowski & Behr, 2019; Behr and Burgmann, 2020). These studies document deformation mechanisms, lithologies, and conditions that have only begun to be explored within the modeling community. Clearly, formulating falsifiable hypotheses for slow slip and testing them through the integration of modeling and observations (both geophysical and geologic) is of fundamental importance for understanding slip behavior in subduction zones.

The spatial and temporal history of fault slip undoubtedly influences the location, timing, and size of future earthquakes. As such, models that simulate the behavior of fault systems over many earthquake cycles, which include periods of slow tectonic loading and aseismic slip, earthquake nucleation, coseismic rupture, afterslip, and postseismic relaxation processes are essential to understanding the behavior of subduction megathrusts and the variety of aforementioned slip behaviors (Rice, 1993; Lapusta et al., 2000; Shibazaki & Iio, 2003; Hori et al., 2004; Liu & Rice, 2005, 2007; Lapusta & Liu, 2009; Matsuzawa et al., 2010; Noda & Lapusta, 2010, 2013; Kaneko et al., 2011; Barbot et al., 2012; Segall & Bradley, 2012; Hashimoto et al., 2014; Cubas et al., 2015; Li & Liu, 2016; Noda et al., 2017; Barbot, 2018; Shibazaki et al., 2019; Erickson et al., 2020).

There are many exciting applications of earthquake cycle models to subduction systems. For example, in most subduction settings, the time period over which high resolution geophysical measurements are available is short relative to a typical megathrust earthquake recurrence interval and we are afforded only snapshots of slip behaviors in time. Earthquake cycle models provide powerful tools to understand how the variety of slip behaviors interact in space and in time, redistribute stress along subduction megathrusts, and set initial conditions for hazard-scale earthquakes over much longer time periods. Additionally, using earthquake cycle models to determine initial conditions for dynamic rupture would obviate the artificial prescribing of prestress conditions and ad-hoc rupture initiation practices commonly employed in dynamic rupture models (Harris et al., 2018; van Zelst et al. 2019; Erickson et al. 2020; Muldashev & Sobolev, 2020).

In summary, a rich variety of slip behaviors are known to operate on global subduction megathrusts. Continued observations of these phenomena combined with earthquake sequence modeling will undoubtedly lead to new insights into the nature of faults. A modeling collaboratory could provide the framework for such integration across regional natural laboratories.

3. *Long-term Geodynamics and Surface Processes*

The large-scale structure of subduction zones evolves at time scales from tens of thousands to millions of years, affecting slab geometries and subduction speeds, and in the process forming faults, building topography, and fluxing fluids and melts. This dynamic system sets the deviatoric stress, dynamic pressure, mineralogy, and pore fluid conditions that control earthquake and fault slip. A complete understanding of the dynamics of subduction thus involves huge spatio-temporal scales. It is often challenging to confidently isolate parts of the system for study since our understanding of the physics of the interactions between processes pertaining to different scales is still incomplete. However, we have made great progress in our understanding over the last decades, and a range of coupled models (e.g., between surface mass transport and long-term subduction) and integrated inversions (e.g., mantle wedge rheology consistent with long-term flow and post-seismic relaxation) are being explored.

On the longest time scales, subduction has controlled planetary evolution through a process similar to the current style of plate-tectonics for at least 1 Gyr, and likely much longer. Arc systems are the major sites of continental crust formation within thermo-chemical mantle convection, and subducting plates make up the major plate driving force. Recycling of oceanic plates affects volatile fluxes, including the carbon cycle, and subduction dynamics affects the distribution of economically relevant mineral deposits along with the most dangerous volcanic systems.

In each subduction zone, the plate tectonic setting controls the state under which the shallow wedge, the seismogenic zone, the shear zone further downdip, and the deeper slab-mantle wedge interface operate (e.g. Arcay et al., 2007; Wada & Wang, 2009; Syracuse et al., 2010; England & Katz, 2010). Most straightforward to analyze are the instantaneous parameters of convergence rate and plate age, the product of which (the thermal parameter) governs the thermal state of a subduction interface, to first order (e.g., England & Wilkins, 2004; van Keken et al., 2011; Maunder et al., 2019). Basic differences in the type of megathrust state are a result of this thermo-kinematic setting (e.g., Wada & Wang, 2009; Abers et al., 2017; Sun et al., 2018; Brizzi et al., 2020, Muldashev & Sobolev, 2020). However, we now understand that there are a number of complexities that lead to fluctuations in fault loading and must thus be considered.

For example, the 3-D, regional setting of a subduction zone with transiently evolving, possibly irregular slab geometries will affect advective transport of heat, leading to along-strike variations of wedge temperature (e.g., Kincaid & Griffith, 2004; Wada et al., 2015; Morishige & van Keken, 2017; Ji et al., 2017; Plunder et al. 2018). Any adjacent slabs will further modify the mantle flow field in the mantle wedge, along with rheological feedbacks mediated by fluid transport (e.g., Billen & Gurnis, 2001; Arcay et al., 2005, 2007; Honda & Yoshida, 2005; DeFranco et al., 2008; Zhu et al., 2009; Wada et al., 2012; Barbot, 2018; Holt et al., 2018). As a consequence the volatile, grain-size and partial melt state of the wedge affect rheology, which in turn affects dynamic pressure, and hence stress transfer and therefore the spatial distribution of slow slip and other megathrust systematics, for example.

Thanks to geophysical imaging, we have some handle on the along-arc distribution of lithospheric density and thickness anomalies underneath the subducting and overriding plate in some regions. Those are additional sources of fault stresses that are not part of simple tectonic loading. For example, the resulting forces due to overriding and subducting plate structure and fluid distributions may lead to variations in along-strike coupling and mantle-flow-induced changes of surface topography (e.g., Wiens et al., 2008; Becker et al., 2015; Martin-Short et al., 2015; Zhou et al., 2018; Gao, 2018; Bodmer et al., 2020). Such effects need to be better understood, and then corrected for, for example in order to arrive at better models of regional, visco-elastic megathrust earthquake cycles as constrained by geodetic and geological constraints on vertical motions (e.g., Wesson et al., 2015; Hashima & Sato, 2017; Delano et al., 2017; Johnson & Tebo, 2018; Govers et al. 2018; Li et al., 2018; Jolivet et al., 2020).

Subduction trenches are often not stationary in a lower mantle fixed reference frame, but are rather advancing or retreating over Myr scales, with possible consequences for fault loading and the stress state of the plate boundary (e.g., Jarrard, 1986; Garfunkel et al., 1986; Otsuki, 1989; Conrad et al., 2004; Heuret & Lallemand, 2005; Alpert et al., 2010; Alisic et al., 2012; Heuret et al., 2012; Holt et al., 2015; Brizzi et al., 2018). Determining trench motions and slab dip evolution requires an understanding of global mantle circulation and regional slab interactions (e.g., Alisic et al., 2012; Gerault et al., 2012; Rudolph and Zhong. 2014), and geodynamic models can now resolve such interactions at regionally relevant scales (e.g., Alisic et al., 2010; Jadamec et al., 2013; Jadamec 2016; Ghosh et al., 2013, 2019; Osei Tutu et al., 2018).

On comparable geological time scales, strain accumulation at convergent margins involves the coupled problem of surface evolution and mantle dynamics. For example, erosion of topography associated with plate collision and the resulting variation in the effective near-surface normal stress will affect exhumation of the lower crust and the degree to which a given fault's orientation remains mechanically efficient (e.g., Olive et al., 2014; Ueda et al., 2015). Such effects will interact with asperity dynamics and the variations in seismicity as expected from topographic roughness and sediment supply on the incoming plate (e.g., Uyeda, 1982; Ruff & Kanamori, 1983; Cloos & Shreve, 1996; Heuret et al., 2012; Fujie et al., 2013, 2020; Wang & Bilek, 2014; Bassett & Watts, 2015; Han et al., 2017; Wallace, 2020).

Moreover, the sediments from eroded topography at a convergent margin may locally deposit on the convergent plate, where, upon subduction, they can affect the wedge stress and pressure regime, as well as the effective shear stress on the deeper shear zone. Along with the topographic load, the latter may co-determine plate speed, which in turn controls accumulation rate of sediments (e.g., Currie et al., 2007; Meade & Conrad, 2008; Behr & Becker, 2018; Sobolev & Brown, 2019). Such important feedbacks between long-term convection, tectonics, surface processes, and fault loading can now be explored with coupled geodynamic models. For example, sediment transport and wedge dynamics may lead to changes in slab dip, megathrust geometry, and hence seismic moment release (Brizzi et al., 2020; Muldashev & Sobolev, 2020).

Particularly for the time evolution of the subduction-arc system, it is thus crucial to incorporate constraints from geology and petrology. Those can make sure that any geophysically determined model of present-day margin mechanics and fault loading is consistent with the transport of mass and energy that are implied by the long-term system evolution, along with the constraints on rheology provided by rock mechanics experiments and field observations.

Outstanding Science Questions

Given the current state of knowledge and the progress in observational, laboratory, and modeling work which we can expect over the next decade, we proceed to identify a few key questions that can serve to catalyze a range of research efforts. While the Catalyzing Opportunities for Research in the Earth Sciences (CORES) report asks the most general question, *What is an earthquake?* (NASEM, 2020), we ask the following more detailed questions in the context of the megathrust component of the MCS:

1. *What are asperities and how do they relate to past and future earthquakes?*

The concept of seismic asperities describes heterogeneities of the subduction zone interface and their relationship with earthquake occurrence (Lay & Kanamori, 1981). From the seismological point of view, asperities determine the rupture extent of megathrust earthquakes; geodetically, they appear as regions with high coupling between major earthquakes. Therefore, in its simplest form, the asperity model relates the extent of past and future earthquakes to present day geodetic locking. However, recent observations have proven that the two do not always coincide. Earthquakes can sometimes rupture a fraction of previous ruptures or locked areas (e.g., Avouac et al., 2015; Schurr et al., 2014; Melgar et al., 2017) or break through regions that had been assumed to be creeping or experiencing slow slip (e.g., Simons et al., 2011; Noda & Lapusta, 2013, Lin et al. 2020). Moreover, locking patterns are not always stationary: geodetic studies in Japan (Johnson et al., 2016) and Kamchatka (Bürgmann et al., 2005) have inferred a reduction of the locked area with time. To explain these discrepancies between geodetic and seismic asperities, we need to understand how they arise from underlying heterogeneities in friction/rheology, geometry, and/or stress and pore pressure; numerical simulations play a vital role in this effort, as illustrated below.

Among the hypothesized explanations for asperities are frictional or rheological heterogeneities, such as velocity-weakening seismic patches embedded in an otherwise velocity-strengthening creeping fault (Chen & Lapusta, 2009; Dublanchet et al., 2013; Barbot, 2019; Cattania & Segall, 2019), and geometrical heterogeneities, such as subducted seamounts and other structural complexities (Cloos, 1992; Scholz & Small, 1997; Bangs et al., 2006; Watts et al., 2010; Wang & Bilek, 2011; Duan, 2012; Kopp, 2013; Wang & Bilek, 2014; Bletery et al., 2016; Hubbard et al., 2016; Kyriakopoulos & Newman, 2016; Collot et al., 2017; van Rijsingen et al., 2018). Of course, it is possible that frictional/rheological heterogeneities might be directly coupled to geometrical heterogeneities (Sagy & Brodsky, 2009; Wang & Bilek, 2011). For example subducted seafloor relief influences erosion and transport of fluid-rich sediments (Cloos, 1992; Scholz & Small, 1997; Bangs et al., 2006), and sediments and high pore pressures are often correlated with stable sliding.

In the frictional hypothesis, such asperities can, if large enough, rupture partially during earthquakes; in this case the extent of a seismic rupture is not determined by underlying frictional heterogeneity, but by prestress conditions that vary with time (e.g.,Barbot, 2019; Cattania, 2019). Rate-and-state asperities can also exhibit a reduction of the locked area between earthquakes (Chen & Lapusta, 2009; Barbot, 2019; Cattania & Segall, 2019). However, for this mechanism to explain observations on larger megathrust asperities would require nucleation lengths on the order of tens of kilometers, a possibility that is inconsistent with laboratory experiments and contradicted by the occurrence of small earthquakes in these areas. Thermal pressurization of pore fluids has been proposed as a mechanism to explain the propagation of seismic ruptures into regions that had been thought to be creeping, such as the near-trench region in the 2011 Tohoku-oki event (Noda & Lapusta, 2013; Noda et al., 2017; Shibazaki et al., 2019). This mechanism also predicts a reduction of locked areas across the seismic cycle (Jiang & Lapusta, 2016; Mavrommatis et al., 2017), without requiring unrealistically large nucleation lengths.

Alternatively, asperities may result from heterogeneities in fault structure and geometry. Many have argued for the important role of subducted seamounts and other seafloor bathymetric features in altering how sediments are transported and distributed along the plate interface (Cloos, 1992; Scholz & Small, 1997; Bangs et al., 2006). Seamounts, bends, and other geometrical features also introduce stress concentrations that might either facilitate or inhibit slip, or even cause yielding and inelastic deformation off of the main plate interface (Wang & Bilek, 2011, 2014; Bletery et al., 2016; Hubbard et al., 2016).

Numerical modeling across the full range of length and time scales, from long-term geodynamical modeling that explores the evolution of roughness and geometry to earthquake sequence and dynamic rupture modeling to determine the nature of deformation and slip, will help us better understand the nature of asperities.

2. *What is the nature of deformation, structure, and rupture behavior in the toe of the subduction zone and how do these relate to tsunamigenesis?*

Seismic reflection images of the accretionary prism in the frontal parts of subduction zones demonstrate that slip on the megathrust is transferred over geological time scales into fault-related shortening of the hanging wall. The frontal thrusts of these systems can be assumed to be active, and while many landward splay faults have been oversteepened or refolded and abandoned, others, like the Nankai megasplay, appear to continue to host seismic slip events (e.g., Park et al., 2002; Miura et al., 2005; Moore et al., 2007; Hubbard et al., 2015; Han et al., 2016). Because the frontal parts of subduction zones are far from land-based sensors, most geodetic networks are relatively insensitive to slip in these regions, and many coupling inversions have suggested that the faults there are continuously creeping (e.g., Loveless and Meade, 2010, 2011; Wang & Trehu, 2016). Recent physics-based modeling, however, has shown that this area is in the stress shadow of down-dip locking zones and therefore must slip more sporadically, either during earthquakes or in the post-seismic period (Almeida et al., 2018). This new perspective amplifies the need to understand this region and its potential to generate earthquakes and associated tsunamis. It also highlights the importance of combining geological and geophysical studies with mechanical modeling.

The soft muds of this frontal region are likely to have distinctly different material and seismic properties than the more consolidated rock further downdip (e.g., Saffer & Marone, 2003; Ikari et al., 2009; Faulkner et al., 2011; Kitajima et al., 2012; Jeppson et al., 2018). As yet, we do not fully understand whether earthquakes can initiate, how slip propagates, and how seismic radiation is emitted within this region, and examples of earthquakes where we can sufficiently resolve slip in the updip section of the megathrust (e.g., 2010 Mentawai, Hill et al., 2012) remain rare.

One hint at seismic slip in this region is the occurrence of so-called “tsunami earthquakes,” which generate larger tsunamis than can be readily explained by the earthquake magnitude as estimated from standard seismic wave analysis (Kanamori, 1972). These earthquakes are characterized by low rupture speeds and are believed to occur in the frontal sections of the megathrust (Pelayo & Weins, 1992; Bilek & Lay, 2002; Lay et al., 2007). Tsunami energy is a function of the square of the height of the wave, integrated over the area of the wave, and thus more focused uplift over a smaller area (as is expected due to slip on steeply dipping thrusts and associated off-fault deformation) should produce a more energetic wave than the broad zone of uplift above a deeper, low angle décollement. However, narrower seafloor uplift patches will also be damped by the water column (Kajiura, 1963). Tsunami generation is further complicated by the fact that typical empirical relationships between seismic slip and magnitude may not hold in the soft sediments within the accretionary prism.

Resolving these questions is complicated by the fact that it is difficult to access these regions far from shore. A large slip event within the accretionary prism would likely produce measurable kinematic deformation, seismic waves, and ocean waves, but because these events are rare it is unlikely that such signals will be captured without broad instrumentation of large areas of subduction zones. Nevertheless, recent physics-based modeling of fault coupling, off-fault deformation, and tsunami has proven promising and can provide more guidance on what types of signals might be most useful for understanding the deformation processes in this region.

3. *How do different parts of the megathrust interact across space and time?*

Subduction zones accommodate deformation through a variety of mechanisms, and numerous studies have demonstrated significant interaction between slip phenomena in space and time, including intriguing observations of precursory seismicity and deformation prior to megathrust events (e.g., Kato et al., 2012; Ito et al., 2013; Ruiz et al., 2014; Obara & Kato, 2016; Soquet et al., 2017; Pritchard et al., 2020). Observations of these interactions place constraints on the nature of heterogeneity of the megathrust system, thereby offering a means to test hypotheses regarding asperities, segmentation, and the processes that determine whether deformation is accommodated aseismically or in hazardous earthquakes.

Several recent studies have pointed to intriguing spatial and temporal relationships between coseismic slip, afterslip, and transient creep (e.g., Rolandone et al., 2016). Regions hosting slow slip and tremor often abut those known to slip coseismically (e.g., Nishikawa et al., 2019), possibly suggesting fixed rheological, frictional, and/or geometric controls on deformation style. However, there is some evidence of regions that host slow slip overlapping with regions that slip coseismically (Lin et al. 2020). Other examples of spatial interactions include model predictions and/or observations of stress transfer from repeated slow slip events onto regions capable of hosting large megathrust earthquakes (e.g., Uchida et al., 2016, Cruz-Atienza et al., 2020), slow slip events evolving into megathrust earthquakes (Segall & Bradley, 2012), and coseismic slip penetrating into regions known to host slow slip (Noda & Lapusta, 2013; Ramos & Huang, 2019; Lin et al. 2020). Slip behaviors also have temporal relationships that vary throughout the seismic cycle. Afterslip and postseismic relaxation are well-known phenomena that relieve stress imparted by coseismic slip on the adjacent regions. Slow slip transients and foreshock sequences have either been observed or inferred prior to several significant events, including the 2011 Mw 9.1 Tohoku-Oki earthquake (e.g., Kato et al., 2012; Ito et al., 2013) and 2014 Mw 8.1 Iquique, Chile, earthquake (e.g., Ruiz et al., 2014; Brodsky & Lay, 2014; Soquet et al., 2017). Apparent changes in coupling have also been observed during the interseismic period (e.g., Mavrommatis et al., 2014; Yokota & Koketsu, 2015; Socquet et al., 2017; Iinuma, 2018; Materna et al., 2019).

Understanding how seemingly disparate parts of the megathrust interact in space and time and which underlying processes are responsible for these interactions is an outstanding challenge that is best addressed using a combination of observations and modeling. Longer duration geophysical observations that sample progressively larger fractions of the megathrust earthquake cycle will soon be available and should provide insight into slip behaviours in multiple subduction zones. These records can be used to better understand the processes responsible for triggering. It is well known that static and dynamic stress transfer drive earthquake interactions, but the specific mechanisms responsible for triggering (e.g., elastic stress transfer, triggered creep, pore fluid diffusion, etc.) have not yet been thoroughly explored or validated against observations. The next decade holds much excitement with the advent of new offshore observational capabilities that will constrain and guide model development and understanding. Seafloor geodesy (Bürgmann & Chadwell, 2014), ocean bottom seismometer and pressure sensor networks (Toomey et al., 2014; Kawaguchi et al., 2015; Nishikawa et al., 2019), repeat bathymetry surveys (Fujiwara et al., 2011), scientific drilling (Tobin & Kinoshita, 2006; Wallace et al., 2019), and additional novel technologies like fiber distributed acoustic sensing (Lindsey et al., 2019; Sladen et al., 2019) will permit a new understanding of structure and deformation behavior, including slow slip transients, across the full seismogenic zone including the region near the trench. This shallow region, which in some subduction zones hosts slow slip (Saffer & Wallace, 2015), is the likely target of focused instrumentation efforts in the near future.

If sufficient progress in understanding spatial and temporal relationships among distinct parts of the megathrust can be made, it may be possible to incorporate that information into time-dependent hazard assessments. Such assessments could combine information from various sensor networks to identify slip behaviors in real time and quantify associated hazards through a physics-based modeling framework.

4. *What processes are responsible for deformation below the seismogenic zone?*

Seismologists generally treat the subduction zone interface in the seismogenic zone as a discrete slip surface; the transition into aseismic behavior at depths of 30-50 km is analyzed in terms of changes in frictional behavior, such as a change to velocity-strengthening friction during slip (e.g., Hyndman et al., 1997). The geological evidence from rocks exhumed from depths of 40 km or more on sediment-rich convergent margins suggests that rather than a discrete slip surface, the subduction zone interface may transition into a shear zone or subduction channel, within which deformation is largely ductile (e.g., Gerya et al., 2002; van Dinther et al., 2013; Behr et al., 2018; Platt et al., 2018; Behr & Burgmann, 2020). Figuring out how to incorporate such brittle-ductile interactions into mechanical frameworks of plate boundary deformation, either through approximations or direct micromechanical modeling, is a major challenge.

On sediment-rich margins the subduction channel may be several kilometers thick (perhaps up to 10 km), and may host a zone of return flow, driven either by buoyancy or by the arc-trench topographic gradient (e.g., Gerya et al., 2002). Sedimentary rocks in the subduction channel appear to deform predominantly by pressure-solution creep, at differential stresses less than 20

MPa (e.g. Wassmann & Stockhert 2013; Fagereng & den Hartog, 2017; Platt et al., 2018; French & Condit, 2019). If ductile flow is able to accommodate the relative plate motion, a discrete slip surface may not be present. In contrast, in sediment-starved margins, where basaltic oceanic crust comes in contact with the subduction zone interface, a full transition to ductile shear may not take place until ~80 km depth.

The deep transition zone from seismic slip to aseismic creep appears to be one of the main source regions for slow slip and tremor, and as such is both enigmatic and of particular interest. Several processes have been suggested to explain these phenomena, nearly all of which call on fluid pressures approaching or even in excess of lithostatic (Liu & Rice, 2005, 2007; Segall et al., 2010; Hawthorne & Rubin, 2013). This is supported by geologic observations on rocks from this region, which show abundant evidence for hydraulic fracturing in the form of dilational veins and microscale fractures filled with quartz, calcite, and other minerals. Accumulating evidence that tremor may be triggered or at least modulated by tides, teleseismic earthquakes, and possibly even changes in atmospheric pressure, suggests very low effective stress and hence very low shear stress, on the order of tens to hundreds of kPa (Shelly et al., 2007; Rubinstein et al., 2008; Thomas et al., 2009; Hawthorne & Rubin, 2010). Processes invoked to explain tremor and slow slip are reviewed in the *Sequences of Earthquakes and Aseismic Slip* section of the **State of Knowledge.**

These hypothesized processes can be tested against geophysical observations. We can, for example, assess the range of slip rates predicted by each of these models and how those slip rates depend on event size. Slow earthquakes appear to have slip rates that range from 100 nm/s to 1 mm/s, and the largest-scale trend among the events observed to date implies that smaller slow earthquakes are faster (Ide et al, 2007). We can also assess the range of material properties that allow for slow earthquakes in each of these hypotheses. Transient aseismic slip occurs on a wide range of faults and depths, suggesting that a wide range of material properties and conditions allow for slow earthquakes (Rubin, 2008; Yabe & Ide, 2017). We can assess the detailed response of slow earthquakes to tidal loading and distant seismic waves. Tremor and slow slip appear to respond differently to shear and normal stresses (Miyazawa & Brodsky, 2008; Thomas et al, 2012). Lastly, we can attempt to identify the source of slow earthquakes' spatial and temporal complexity. Some observations and models suggest that spatially varying material properties control slow earthquakes' increasing and decreasing slip rates, but some variations could arise simply from stochastically varying stress fields (Chestler & Creager, 2017; Ide & Maury, 2018).

Thus far, however, we have not identified which, if any, of the proposed models are correct, making it difficult to use slow earthquake observations to infer properties of plate interfaces at depth. All of the proposed slow earthquake mechanisms have at least a few unknown parameters, so in order to test geologically motivated models with geophysical observations we need to integrate a range of observations. This sort of approach has allowed us to eliminate some proposed models, at least in their simplest form (e.g., Liu & Rice, 2009; Hawthorne & Rubin, 2013), but to really identify the deformation processes active during aseismic transients, we must think deeply about the proposed processes and consider a large number of geological and geophysical observations. Moreover, we need to formulate and then test comprehensive mechanical models incorporating available constraints and possible constitutive laws.

5. *What is the state of stress and pore pressure in and around the megathrust?*

How is the megathrust loaded? What controls fault motion across spatio-temporal scales? Can we broadly validate and generalize the constitutive laws describing frictional, plastic, and viscous deformation, and how plate boundary systems transition in a geologically heterogeneous setting?

The state of stress and pore pressure are of central importance in controlling fault strength, slip behavior, and deformation in subduction zones (e.g., Brodsky et al., 2020). Except in shallow regions accessible by drilling, stress and pore pressure are impossible to directly measure and hence must be constrained indirectly, including seismologically (e.g., Shebalin & Narteau, 2017; Warren-Smith et al., 2019) and from exhumed paleo-subduction interfaces (e.g., Behr & Burgmann, 2020). Seismically determined focal mechanisms can be used to infer stress orientations, and changes in orientation after megathrust events have been used to place some constraints on the absolute stress level (e.g., Hasegawa et al., 2011; Hardebeck, 2012, 2015; Hardebeck & Okada, 2018). Except in these exceptional cases, absolute stress is poorly constrained from observations and must be inferred from modeling efforts. These models range from critical wedge solutions and their relatives (e.g., Dahlen, 1990; Wang & Hu, 2006) to complex geodynamic models (e.g., Mannu et al., 2016; Brizzi et al, 2020; Muldashev & Sobolev, 2020), both of which predict ambient stress levels, to earthquake sequence models (see the *Sequences of Earthquakes and Aseismic Slip* section of the **State of Knowledge**) that predict earthquake cycle loading, unloading, and stress transfer between various parts of the megathrust system.

The stress state is intimately connected to rheology, which controls viscous flow below the brittle-ductile transition and inelastic yielding above it. Furthermore, rheology often changes within fault zones due to localization, grain-size reduction, foliation, presence and flow of fluids, and other processes that alter the composition and properties of materials. An outstanding challenge from the modeling perspective is to determine a self-consistent constitutive law that explains and predicts system behavior over a wide range of time scales, from the longest geologic scales that determine the structure, geometry, and loading of the subduction zone to the shortest scales of earthquake cycles and dynamic rupture. While some new efforts are bridging these time scales (e.g., van Dinther et al., 2013; Sobolev & Muldashev, 2017; Tong & Lavier, 2018; Barbot, 2018; Herrendörfer et al., 2018), many challenges remain due to incomplete representations and numerical implementations. For example, geodynamic models often use strain-weakening (or similar) bulk plasticity formulations to create localized deformation features that are identified as faults, whereas earthquake sequence and dynamic rupture models are based on friction laws relating shear and normal tractions on pre-existing and often planar fault interfaces.

Furthermore, friction and flow processes are influenced by the presence of pore fluids, which alter deformation behavior through both mechanical and chemical processes. Pore fluid pressure enters through the effective stress principle (e.g., Hubbert & Rubey, 1959; Hirth & Beeler, 2015; Beeler et al., 2016) and is determined by fluid production rates as well as transport pathways and properties. The deformation processes that create and maintain fault zones also influence permeability and fluid transport properties (e.g., Caine et al., 1996; Evans et al., 1997; Faulkner et al., 2010). Modeling efforts that explicitly account for fluid production and migration, with coupling to mechanical deformation and fault slip, are needed to advance the field. The field is currently taking steps in this direction (e.g., Skarbek & Rempel, 2016; Cruz-Atienza et al., 2018; Zhu et al., 2020; Petrini et al., 2020).

6. *What is the role of structure, geology, geometry, and rheology in controlling slip behavior?*

What are the links between structural and seismic heterogeneity, and what sorts of geological and geophysical constraints on structure and composition and stress/temperature/pressure state, on what scale, are needed to predict the extent of future ruptures? How does the system evolve over geologic time?

The essence of a friction-based description of megathrusts is that slip will occur when the shear stress resolved on the plate interface exceeds a threshold proportional to the effective normal stress. In the widely used framework of rate-and-state friction (Dietrich, 1979; Ruina, 1983), the sliding velocity and hold-time dependence of friction can be parameterized by the experimentally-determined parameters a, b, and d_c (Marone, 1998). Their values and thus the stability of slip depends on lithology, pressure, and temperature, which provides a first-order framework for aseismic to seismic slip transition at a megathrust (e.g., Scholz, 1998; Rice et al., 2001; Saffer & Marone, 2003). Frictional dynamics also depends on the effective normal stress (e.g., Liu & Rice, 2007) and elastic properties, and the rate-state parameters may also themselves depend on slip velocity (Im et al., 2020). Of course, that dependence might be more naturally captured in alternative friction formulations, such as those based on micromechanical models (e.g., Den Hartog & Spiers, 2014; Ikari et al., 2016; Van den Ende et al., 2018).

Numerical models also show that slip behavior can be influenced by off-fault plasticity (Andrews, 2005; Templeton & Rice, 2008; Dunham et al., 2011; Gabriel et al., 2013) and coseismic damage (Thomas et al., 2016). Recent work further suggests that stress interactions within a dense fault network can make a nominally unstable fault experience slow slip (Romanet et al., 2018). The seismogenic behavior of a megathrust is therefore likely to be influenced by the structural, stress, and damage state of the overlying forearc and underlying slab. Novel modeling frameworks are needed to assess the relative effects of each of the aforementioned processes and their possible interactions. An outstanding question is whether heterogeneities primarily represent rheological variability of fault rocks or structural complexities in the near/off-fault domain.

The next generation of models should also account for the nonplanar geometry of real megathrusts (e.g., Hubbard et al., 2016; Dal Zilio et al., 2019), as fault geometry strongly modulates the shear and normal components of stress resolved on individual fault patches. High-resolution geophysical imaging will be needed to resolve these geometrical complexities and characterize the damage state of the off-fault domain.

The stress state of a subduction zone can be thought of as the sum of a visco-elastic cycle component of sometimes unsteady interseismic loading, coseismic unloading (e.g., Kanamori, 1986; Dmowska et al., 1988; Saffer & Tobin, 2011; Hardebeck & Okada, 2018; Warren-Smith et al., 2019) and transient relaxation (e.g., Wang & Hu, 2006; Wang et al., 2012; Hu et al., 2016; Loveless & Meade, 2016; Freed et al., 2017) and a background, convective and plate tectonic loading stress, which reflects a complex visco-elasto-plastic deformation history (e.g., Brizzi et al., 2020; Muldashev & Sobolev, 2020). Understanding both contributions, and how they are possibly coupled, is essential to assess the failure potential of a megathrust.

While the visco-elastic cycle component can be reasonably well characterized through modeling of geodetic observations (e.g., Wang et al., 2012), the tectonic contributions and the context for the cycle models require a broad understanding of the long-term evolution of the subduction system. These include changes in slab dip and position like slab retreat (e.g., Lallemand & Heuret, 2005; Cerpa et al., 2013; Holt et al., 2015; Yang et al., 2017; Bercovici et al., 2019; Alsaif et al., 2020; Oryan & Buck, 2020), flexure of the downgoing plate (e.g., Buffett, 2006; Babeyko and Sobolev, 2008; Kanda & Simons, 2010; Capitanio et al., 2009), transport of sediments (e.g., Cloos, 1982; van Huehne et al., 2004; Currie et al., 2007; Malatesta et al., 2013), building of topography (e.g., Gerbault et al., 2009; Tan et al., 2012; Avouac, 2015; Bassett & Watts, 2015), partitioning of deformation in the upper plate, 3-D geometry of flow in the mantle wedge (e.g., Behn et al., 2007; Kneller & van Keken, 2008; Hasenclever et al., 2011; Morishige & Honda, 2013), and potential slab tears (e.g., Yoshioka & Wortel. 2005; Andrews & Billen, 2009; Hale et al., 2010; van Hunen & Allen, 2011; Duretz et al., 2013; Menant et al. 2016). A promising path to better characterizing these phenomena is the joint use of geodynamic modeling employing laboratory and geological constraints as well as geophysical imaging from seismology and electromagnetic-magnetotelluric methods to constrain long-term mantle flow and its impact on megathrust stress.

Understanding the connection between short-term and long-term deformation at subduction zones could unlock new constraints on the seismogenic behavior of megathrusts. Subduction landscapes and seascapes, which reflect the net contribution of thousands of seismic cycles on time scales of 10–1000 kyr, are likely influenced by the geometry of repeated ruptures and geological processes not directly linked to earthquake activity (e.g., Avouac, 2015). Models that couple tectonic and surface processes are an avenue to disentangle the various contributions to the morphology of an active margin (e.g., Ueda et al., 2015; Mannu et al., 2016), and can possibly invert landscape features for key unknowns such as the persistence of heterogeneities over many cycles.

Recommended Community Actions to advance megathrust modeling within a Subduction Zone Modeling Collaboratory framework

The scientific objectives of the Modeling Collaboratory for Subduction Zone Science (MCS) should involve developing a new generation of general, cross-scale numerical modeling tools for hypothesis testing, as well as specific regional implementations that can fully incorporate geological and geophysical constraints.

An MCS could form a major, integrative component of SZ4D, and turn out to be crucial for cross-validation of diverse observations for an integrative physical theory of earthquake occurrence. Within the context of computational solid Earth geoscience, the MCS could interface well with other community initiatives such as the Computational Infrastructure for Geodynamics (CIG) or Community Surface Dynamics Modeling System (CSDMS), where CIG/CSDMS would focus more on general tools, computing access, and training, and the MCS on science-driven code development and collaborative science.

Fully understanding the subduction system in this way must involve international collaboration. Moreover, in many cases, the optimal approaches to these challenging modeling problems are yet unknown, and regional models will only have predictive power if their ingredients are well benchmarked and validated by global, comparative analysis first. The MCS would thus have a global outlook, focusing on open subduction zone earthquake science collaboration. These goals imply that large-scale, distributed, and collaborative code development and benchmarking will have to play a prominent role in any such collaboratory, alongside community science exchange and training efforts.

Besides the general, methodological approach to subduction zone science, we suggest that a two-pronged approach with dedicated working groups could provide a complementary framework for how to best realize such efforts and how to most productively collaborate between modelers, experimentalists, and observationalists: one centered around regional laboratories and case histories and a second focused on specific processes.

Some of the guiding principles for a modeling collaboratory and concrete next steps are briefly explored further below:

1. *International, distributed collaboration*

Regional, along-margin variations in the megathrust setting, such as seafloor topography and sediment load, and variations in megathrust seismic and tectonic behavior provide important clues for the processes controlling megathrust dynamics. However, no single regional realization can provide the parameter variations that are needed to robustly and comprehensively quantify the spectrum of megathrust behavior in a predictive sense, even if that one subduction zone were optimally instrumented.

Moreover, different subduction zones are in various stages of their earthquake and volcanic cycles, providing a range of important, but incomplete, windows into system behavior. The need for comparative analysis and verification alone motivates a collaborative and international approach to subduction zone science. Moreover, the diversity of scientific cultures, approaches, and viewpoints that the international community provides is another crucial contribution that can potentially accelerate our efforts toward understanding megathrust behavior. By proceeding jointly, international communities can leverage one another's efforts and complement each other's strengths.

A number of international communities have, for example, been at the forefront of imaging and instrumenting convergent margins for decades. Japan is one example, where extensive on- and offshore seismological imaging and dense onshore geodetic and seismic networks were complemented by seafloor acoustic GPS campaigns, offshore drilling, and now two permanent seafloor seismological and pressure sensor networks. These datastreams are being complemented by renewed efforts for integrative numerical modeling (including in a monitoring context), as well as efforts to utilize the biggest supercomputers for such initiatives.

New Zealand, Chile, and Costa Rica are other subduction zones where much is known geologically and geophysically, and major event sequences can teach us about intra-cycle dynamics such as stress transfer, earthquake triggering, and slow slip. These are just some examples of how existing and growing international observatories supplement whatever major investments the U.S. might commit to in the future, along with our existing and ongoing initiatives in constraining margins such as Cascadia and Alaska.

Any future subduction systems research will therefore have the highest likelihood of achieving transformative results if we can establish modeling and collaboration frameworks that can draw upon open exchange of data and best practices from subduction zone scientists internationally. A Modeling Collaboratory can, in turn, provide the tools that can bridge heterogeneous sensor data streams and probabilistic hazard assessment or early warning for operational observatories. For those observatories in their planning phases, the modeling framework can be used for optimal experimental design, such that observations can be made where and when they are likely to lead to the maximum knowledge gain and uncertainty reduction.

Perhaps more importantly, aside from joint models and exchange of data, there is a clear need to continue to expand collaborational capacity among scientists internationally. This has to involve collaboratively training the new generation of interdisciplinary scientists by means of shared educational and mentoring activities. A Modeling Collaboratory can help with all of these efforts, and form a platform for international collaboration, providing not just the framework for data-integrative, physics-based hazard assessment, but also the venue for academic, industry, and government agency discourse as to the modeling and monitoring of subduction zones. International workshops, summer schools, hackathons, and regional study groups are just some examples of how a Modeling Collaboratory could play a central role in international collaboration.

2. ***Focus groups for specific regions and case histories of past events***

Focusing model deployment on a few selected regions and bringing in case histories of event sequences can provide guidance for code and workflow development, help facilitate and accelerate international collaboration, and, of course, serve to answer key science questions.

Possible regional sites could include Japan (Nankai Trough and Japan Trench), New Zealand (Hikurangi Trench), Cascadia, Chile, and Costa Rica. When taken as a set, these margins span a range of tectonic conditions (e.g., sediment coverage and seafloor topography). They are also relatively well characterized seismologically and geologically, and have observational networks consisting of land-based seismometers and GNSS stations, as well as varying degrees of offshore instrumentation.

Comparative analysis between the most complete margin models that we might be able to build can serve to explore global processes (e.g., control of pressure and temperature on slow vs. seismic slip from consistent geodynamic background models). However, regional models should also consist of an assembly of all available constraints on structure and dynamics (e.g., locking estimates) which can be interpreted with different mechanical models and numerical tools for benchmarking efforts, and in order to better understand the role of boundary and initial conditions. Particular efforts should be dedicated to using these test cases to distill places of agreement or disagreement as to best practices and core physics ingredients.

Alongside geographically defined natural laboratory focus sites, a Modeling Collaboratory should also consider megathrust event sequences, recorded in both the instrumental and paleoseismologic records. Major events can allow us to study perturbations in the subduction system, including triggering of both seismic and slow slip events, postseismic response, and other system dynamics including potential tectonic precursors. Focus events could include the 2011 Mw 9.1 Tohoku-oki, 2016 Mw 7.8 Kaikoura, 2012 Mw 7.6 Nicoya, and 2014 Mw 8.2 Iquique earthquakes. Closely comparing results can provide the basis for consensus approaches, reference models, and evaluation of uncertainties from data and theory.

The Modeling Collaboratory could support regional and event focus groups in a number of ways, including workshops, sustained electronic collaboration, benchmarking exercises, and database repositories of a reference set of constraints for inversion exercises, as well as workflows showcasing modeling tools as applied to community test cases.

3. ***Focus groups for specific processes***

Complementing efforts focused on specific regions are efforts that focus on processes that are common to most or all subduction zones. These efforts could take the form of small workshops or, for sustained effort, focus groups that might work for several years, meeting virtually and/or in person to accomplish a specific goal. There are many processes for which understanding could be advanced in this manner, such as the first four Science Questions from the previous section. Integration and consistency across disciplines is of fundamental importance, but here the efforts would also benefit from comparing and contrasting observations and modeling studies across multiple subduction zones.

As one example, consider focused attention to Science Question 2 on understanding deformation and rupture behavior in the shallow subduction toe. A great diversity of geometries, faulting styles, and stress and pressure states exist as a consequence of variations in sediment input, convergence rate, plate age, and tectonic history. Only by studying multiple examples, some featuring slip to the trench and others not, some involving splay fault activation and others not, etc., will we identify the controls on shallow rupture behavior. Likewise, focusing on Science Question 3 on interactions might involve a concerted effort to translate hypotheses regarding the nature of asperities and interactions between regions of slow slip and seismic behavior into models that make testable predictions. These predictions can then be compared to observations, particularly those that have been and will be made in the offshore region.

Community efforts of this sort can focus attention on gaps in knowledge, critical observational constraints, and modeling needs that can drive the alignment of future research projects with funding to advance the field. There are clear ties with the regional focus groups where the process-focused products and hypotheses can be tested, but a focus on process is helpful when designing and creating the numerical tools needed to understand the physics. Focus groups could be expected to closely interact with any computational and programming efforts.

4. *Integration of modeling with observations and experiments*

Better integration of modeling efforts with both the observational and experimental communities is critical to advancing our understanding of subduction zone processes and hazards. This integration necessitates iterative communication between observationalists, experimentalists, and modelers (recognizing that many individuals practice more than one discipline).

At the interface between the modeling and observational communities, subduction zone science would benefit from modelers better highlighting which observations could be used to validate or falsify proposed mechanisms for observed phenomena. Observationally, there needs to be more emphasis on making meaningful observations, potentially ones that inform proposed mechanisms, as opposed to simply more observations of phenomena that have been otherwise well documented. Also, more transparency surrounding the limitations of observations (i.e., uncertainties, reliability, importance, etc.) is needed, and often this requires viewing the parameters constrained by observation in a dynamical modeling context.

Observational efforts in the coming decade will likely focus on the offshore region that has previously been challenging to instrument and monitor. Such efforts already underway in Japan, New Zealand, and Cascadia, for example, have uncovered a great diversity of slip and deformation behaviors, including shallow slow slip events, deformation transients, repeating earthquakes, and foreshocks that in some cases might even be precursors to megathrust events. Other studies highlight complex interactions between slow slip and earthquakes. High-resolution constraints on slip, locking, and seismicity patterns, and how those change in time due to interactions, will allow modelers to test hypotheses for the nature of asperities and the role of frictional, rheological, and geometrical controls on slip behavior across the seismogenic zone and below it. Collaborative design of instrumentation involving modelers and observationalists will benefit both communities.

Experimentally, there are only limited results on materials and at conditions thought to be important for subduction zones. These noteworthy data gaps must be filled if we are to understand certain parts of the subduction system. For example, the modeling community would benefit from having more experimental data corresponding to lithologies thought to occupy the deep (i.e., >10 km) portions of subduction megathrusts at the appropriate pressures, temperatures, and hydrothermal conditions. There have been few experiments that have measured frictional properties at pressures above 300 MPa and no experiments at the relevant pore fluid pressures. This is problematic because pressure dependence at these conditions may become nonlinear and the effective stress law may no longer be valid at conditions near the brittle-ductile transition. Additionally, intrinsically weak materials often comprise shallow subduction environments (the accretionary wedge and shallow thrust). A better understanding of friction and dynamic weakening mechanisms that operate in these environments is needed to understand shallow megathrust faulting and tsunamigenesis.

We anticipate that the workshops and focus groups described in Community Actions 2 and 3 will facilitate interaction between the relevant communities.

5. ***Benchmarking, verification, and validation***

The Modeling Collaboratory can also play a leading role in vetting research codes through code comparison (i.e., benchmarking) efforts as well as code verification and validation. Similar efforts by the Southern California Earthquake Center (SCEC)'s Dynamic Rupture Code verification group over the past decade were instrumental in building confidence in several dynamic rupture codes and their outputs (e.g., rupture and slip history, strong ground motion seismograms), understanding the problem-specific strengths and weaknesses of various numerical methods, and pushing modelers to include additional processes (e.g., plastic yielding of fault-bordering rocks, dynamic weakening) as their importance became recognized by the community.

More recent efforts at SCEC have transitioned toward validation of ground motion modeling using dynamic rupture models and verification of earthquake sequence modeling codes (through the Sequences of Earthquakes and Aseismic Slip verification group). In the long-term geodynamics community, a range of influential benchmarks have likewise been conducted for kinematic mantle wedge problems and large-scale subduction dynamics over the last decades. However, similar community-level code comparison efforts have never before been attempted for subduction megathrust problems, which potentially have to cross spatio-temporal scales as well as consider complex and coupled physics, such as fluid-solid interactions.

The unique structure of subduction zones (e.g., shallowly dipping faults adjacent to a water-covered seafloor, huge contrasts in materials properties across the plate interface, splay faulting) offers many modeling complications that challenge dynamic rupture and earthquake sequence simulation codes. It is imperative to gauge the accuracy and validity of various codes and numerical methods for subduction problems. These activities are best carried out by the small group of modelers who design and use these codes. In-person or virtual workshops to plan new benchmarks and review results from previous benchmarks will be required, along with web-hosted platforms for visualizing and comparing simulation results from multiple groups that are uploaded in a common file format.

6. Recommended model development

The Megathrust Modeling workshop illuminated several opportunities for advancing modeling capabilities by development of new models that either bridge time scales previously relegated to separate models or integrate processes in a novel manner. Several of these opportunities are highlighted below. These models are within reach over the next years and can provide guidance for more ambitious, later models in a regional observatory context:

a. *Viscoelastic earthquake sequence model with fluid transport*

One major need for subduction megathrust and fault slip modeling is an earthquake sequence model that accounts for viscoelastic flow at depth as well as fluid transport and pore pressure evolution. Current earthquake sequence models for subduction zones, with a few exceptions, employ elastic half-space boundary element solutions for stress transfer together with rate-and-state friction. These models are widely used to study and interpret slow slip behavior and to explore the relation between frictional and strength heterogeneities and the style of fault slip (i.e., the nature of asperities).

However, current models generally neglect viscoelastic deformation at depth, despite evidence of its occurrence from geodetic studies of postseismic and interseismic deformation as well as laboratory experiments. Viscoelasticity is undoubtedly important in controlling stress transfer and interaction between nearby parts of the megathrust, and is also of fundamental importance in determining the nature of shear deformation in the deep aseismic continuation of the plate boundary below the seismogenic zone.

In addition, most current models simply assume a fixed pore pressure (or effective normal stress) distribution along the plate interface and neglect poroelastic effects within the fault zone and surrounding bulk. The opportunity here is to introduce a fluid transport model, with evolving pore pressure, permeability, and storage properties, that self-consistently predicts fault slip and pore pressure. Subduction zones are well known locations of dehydration reactions and vigorous fluid transport (as compared to continental faults), making them obvious targets for the development of coupled models. Viscoelasticity and fluids are also coupled, as pores and fluid-filled cracks at depth will creep closed to equilibrate fluid pressure and mean stress. Thus a poroviscoelastic rheology will be required. This new class of models will be essential to properly explore several hypothesized explanations for slow slip events and aseismic slip.

The models can also be used to investigate interactions between frictionally and/or rheologically distinct portions of the subduction zone, as well as the role of structural and geometrical complexities. What controls segmentation? What are asperities? Are regions currently exhibiting different slip behaviors fixed in space and time or can the slip behaviors vary in response to stress changes and fluid interactions? Under what conditions are hazardous earthquakes preceded by precursory deformation transients, slow slip events, and/or foreshock sequences? These questions can best be addressed in models that account for additional processes than are captured in most current codes.

One can envision many complementary uses for such a model. First, it can be used in idealized geometries and set-ups to explore processes and the coupling between fluids, deformation, and slip. Second, it can be used in realistically complex geometries and set-ups to connect with observational constraints from specific regions. Finally, such a model could be used to explore the processes accommodating stress relaxation (e.g., afterslip) after large earthquakes. These complementary uses echo our recommendations for focus groups organized around both specific regions and processes. For regional studies, it is essential to account for complex geometries and material properties as constrained by seismic imaging and other geophysical methods, frictional and flow properties from drilling and experimental studies of exhumed analogs, and constraints on loading from crustal deformation.

b. Global, 3-D, thermo-mechanical mantle circulation model with two-phase flow

Megathrust systems respond to plate tectonic forcing as part of mantle convection, and in recent years we have seen progress in estimating the related deviatoric stresses, pressures, and temperatures that serve to load faults and set the tectonic environment in which they operate. The MCS should provide a consistent modeling framework to estimate these parameters, with the goal to dynamically and consistently match kinematic constraints (e.g., global plate motions including trench advance and retreat) and provide estimates of wedge conditions - including deviatoric stress, pressure and temperature - that are consistent with regional constraints such as heat flow.

Besides fault loading conditions, a mantle circulation model can also provide predictions of dynamic topography and uplift rates which are important for the interpretation of geodetic vertical, and long-term topographic loads. Such a unified flow model has not been constructed yet on a global scale and would pose a number of challenges, but seems within reach given improved seismological constraints on upper mantle structure, advances in our understanding of mantle rheology, and increased computational capacity.

In a second step, such a model could include two-phase flow transport and fractionation (melting) of the mantle wedge and slab, which would expand the range of predictions to the long-term transport of fluids, petrological signatures in arc volcanism, and links between dehydration reactions and seismicity within a consistent, long-term context.

c. *A flexible modeling framework for multi-physics, multi-scale modeling including rupture, earthquake cycle, and tectonic time scales*

A number of groups have recently presented numerical models which seek to bridge the time scales over which different processes operate within a subduction zone. Such models can provide many insights, e.g., linking between the viscoelastic earthquake cycle, the distribution of rheological properties on the megathrust and deeper shear zone, and the response of the fault system overall, including the formation of topography and the partitioning of deformation in the accretionary wedge. Such models also have the potential to test if any fault constitutive law or rheology of the mantle wedge is consistent with the long-term evolution of subduction zones, how seismic and geodetic asperities relate and co-evolve, etc. Integrated models can thus bridge scientific efforts with the model development in the previous two subsections a) and b), and can serve to explore two-way coupling, rather than just, say, prescribing loading stresses from b) for earthquake sequence or dynamic rupture modeling from a).

While there are promising algorithmic approaches in the works, it is still debated how to deal with some aspects of the related multi-scale problem. An MCS might therefore benefit from supporting a flexible framework of codes or a toolkit to allow for implementation of alternative physical descriptions. Existing software frameworks such as Fenics/Firedrake could be used to assemble a set of benchmarked reference implementations and allow experimenting with different solution approaches, and ways to implement the physics.

Conclusions

The earthquake science community is poised to make major advances toward understanding megathrust systems in the next 5-10 years. Utilizing experimental and observational results to their fullest potential necessitates the development of physics-based modeling tools that make predictions about system behavior and can be used to develop a more complete understanding of the physical processes that operate in subduction zones and their interaction. Here, we have described the current state of knowledge surrounding subduction zones, identified areas that lie at the boundary of that knowledge, and listed a set of community actions that will advance subduction zone science. A Modelling Collaboratory would provide the organizational and computational tools required to complete these recommended actions catalyzing future scientific discovery and increasing resilience of the communities affected by these dynamic systems.

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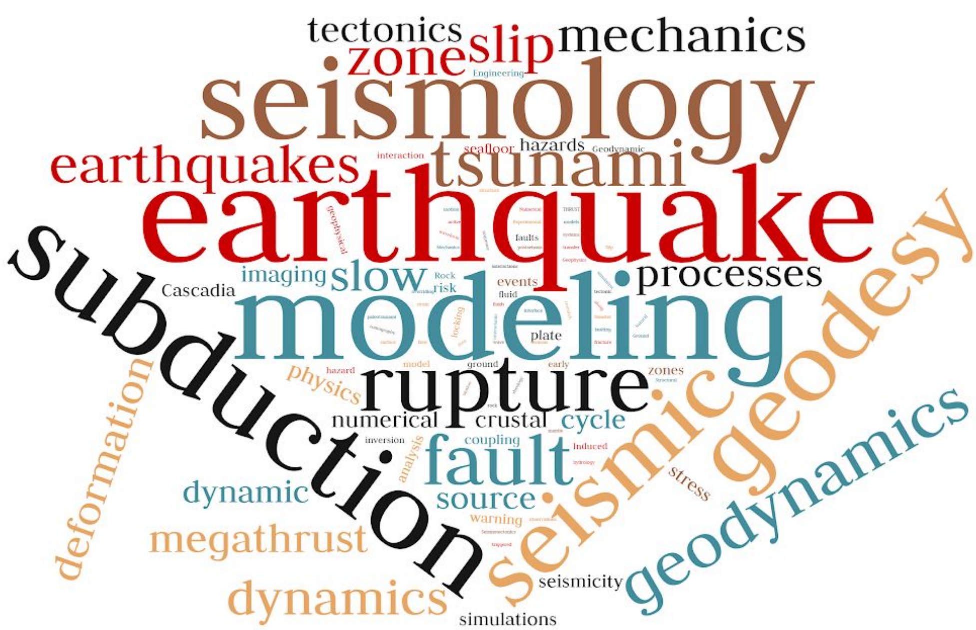
Appendix: Detailed Workshop Information

Workshop Participation

The MCS RCN Megathrust Modeling Workshop was hosted at the University of Oregon on Oct 6-9, 2019, and organized by Amanda Thomas (Univ. of Oregon) and Eric Dunham (Stanford Univ.), with support from Gabriel Lotto and Thorsten Becker (UT Austin). It was attended in person by 107 people representing 59 institutions, from across North America, South America, Europe, Asia, and New Zealand. Of all in-person attendees, 25% were students, 34% were early career scientists (non-student), 21% were mid career scientists, and 20% were senior scientists. Broken down by gender, 64% identified as male and 36% as female. Of invited speakers who were not also conference organizers, 6 of 13 were female; of breakout group leaders and scribes, 12 of 24 were female. Workshop participants were invited to submit a brief introduction and photo prior to the workshop, and those introductions were compiled into an informal directory of biosketches, viewable here. The workshop was broadcasted online via Zoom and attended remotely by an additional 123 unique viewers, representing 24 countries.

The workshop featured three main sessions - *Sequences of Earthquakes and Aseismic Slip* (SEAS), *Dynamic Ruptures and Tsunamis* (DRT), and *Geodynamics and Surface Processes* (GSP) - plus an optional introductory session geared toward early career scientists and a concluding keynote address.



Word cloud of self-described research interests from potential participants, from the initial workshop application.

Workshop Sessions and Presentations

Besides the talks below, there was also an evening poster session featuring 42 poster presenters, listed here. Presentation slides are available here, and videos from several presentations are available here.

Early Career Session (Introductory Talks)
- Roland Bürgmann (UC Berkeley): "Slow slip, asperities and deformation"
- Eric Dunham (Stanford Univ.): "Megathrust rupture dynamics and tsunamis"
- Thorsten Becker (UT Austin): "A short introduction to subduction zone geodynamics"

Session 1: Sequences of Earthquakes and Aseismic Slip (SEAS)
- Victor Cruz-Atienza (UNAM): "Short-term interactions between silent and devastating earthquakes in Mexico"
- Camilla Cattania (Stanford Univ.): "Fracture mechanics insights into the earthquake cycle of seismic asperities"
- Jessica Hawthorne (Univ. of Oxford): "Can we constrain the fault zone processes that create slow earthquakes using few-minute subevents and atmospheric modulation?"
- John Platt (USC): "Geological expression of the seismic-aseismic transition along the subduction zone interface"

Session 2: Dynamic Ruptures and Tsunamis (DRT)
- Shuoshuo Han (UT Austin): "Links between sediment properties and megathrust slip behavior - the North-Central Cascadia example"
- Shuo Ma (San Diego State Univ.): "Dynamic wedge failure and tsunamigenesis in the Japan Trench and Cascadia Subduction Zone"
- Alice Gabriel (LMU Munich): "Large-scale multi-physics earthquake and tsunami modeling"
- Tatsuhiko Saito (NIED): "Tsunami generation by megathrust earthquakes"

Session 3: Geodynamics and Surface Processes (GSP)
- Ylona van Dinther (Utrecht Univ.): "Cross-scale modeling of tectonics and earthquakes: its past, present, and future"
- Jean-Arthur Olive (ENS): "Non-recoverable deformation around partially-locked megathrusts"
- Judith Hubbard (Earth Observatory of Singapore): "The impact of megathrust geometry on earthquake ruptures and fault behavior"
- Noah Finnegan (UC Santa Cruz): "Long-term deformation of subduction margins is recorded in the morphology of the continental shelf"

Concluding Keynote
- Kelin Wang (Geological Survey of Canada): "The megathrust in 4D+"