Whitepaper Reporting Outcomes from NSF-Sponsored Workshop:

## **CTSP:** Coupling of Tectonic and Surface Processes

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#### 1. Executive Summary

Feedbacks between geomorphic and tectonic processes play a key role in the Earth's Wilson cycle—modulating mountain building, continental rifting, and the interactions between landscapes and climate. These feedbacks occur over both geologic and human time-scales. They have direct societal relevance through their influence on natural hazards—for example in the triggering of landslides by large earthquakes—and on Earth's habitability, through the role of erosion and basin evolution on the global carbon cycle. Further, understanding these feedbacks is important in evaluating surface responses to changing sea level and dynamic lake levels. While many of the basic feedbacks between tectonic and surface processes are well established, the details of these interactions remain poorly constrained—which in turn hinders our ability to predict the evolution and future state of these systems. Indeed, one of the Grand Challenges identified in the recent NSF-sponsored report on *Challenges and Opportunities for Research in Tectonics* is "Understanding the dynamic interactions among Earth-surface processes and tectonics" (Huntington and Klepeis, 2017). To do so, we must investigate the linkages between deformation and rheology in the Earth's lithosphere with erosion and erodibility in the near surface, across a range of spatio-temporal scales.

One approach to study these interactions is through numerical models that couple surface and tectonic processes in order to quantify the effects of a range of geologic and geomorphic parameters. This approach allows for hypotheses derived from field observations to be quantitatively tested, and for new hypotheses to be developed, which can later be validated through field and laboratory experiments. Great progress has been made over the last several decades on modeling lithospheric deformation and landscape evolution (e.g., Koons 1990; Willgoose et al., 1991; Beaumont et al. 1992; Willett et al. 1993; Howard, 1994; Tucker et al., 2001; Zeitler et al. 2001; Whipple 2009; Koons et al., 2010; 2012: 2013). However, while both the tectonics and surface processes communities have developed their own families of models through individual and/or community efforts (e.g., the Computational Infrastructure for Geodynamics (CIG) and the Community Surface Dynamics Modeling System (CSDMS)), interactions between these communities have been limited and few fully coupled codes are openly available to the academic community.

To address these needs, the National Science Foundation sponsored the Coupling of Tectonic and Surface Processes (CTSP) workshop, held in Boulder, Colorado in April 2018. The stated goals were:

- **Goal 1:** Work toward developing the next generation of coupled long-term tectonic and surface processes models in order to explore key questions linking tectonics, climate, and landscape evolution.
- **Goal 2:** Strengthen the US long-term tectonics modeling community and build new links/collaborations between the long-term tectonics community at CIG and the surface processes community at CSDMS.

With almost 100 on-site attendees (and an additional ~50 remote participants), the CTSP workshop was highly successful in achieving both of these objectives. Workshop participants spent two full days identifying the numerical techniques used by the different communities, and elucidating the challenges in coupling numerical models across different temporal and spatial scales. The workshop was arranged around a series of keynote lectures, posters presentations, and break-out group discussions. Both communities were well represented, and care was taken to

ensure that the speakers and participants represented gender and career diversity. Discussions focused on numerical techniques and reproducibility in model development, the degree to which mass transport properties are constrained, and new scientific directions (e.g., the role of climate in modulating tectonic processes, and linkages between landscape evolution and biodiversity).

Several major themes came out of the CTSP discussions. First, several computational bottlenecks were identified for establishing efficient numerical algorithms to couple landscape evolution and tectonic deformation across multiple spatial and temporal scales. These include the need for improved grid resolution (particularly in 3-D tectonic models), the lack of parallelized surface processes codes, and the need to develop methodologies for parameterizing and upscaling sub-grid-scale features. Second, it is unclear what level of coupling is necessary to include in numerical models. For example, are there scales at which surface processes impact tectonics more than others, and vice-versa? If so, the level of coupling must be tuned to the problem of interest. This is an avenue in which modeling can play an important role by testing the sensitivity of model outputs to scenarios in which different levels and scales of coupling are incorporated.

Another important theme discussed throughout the CTSP workshop was the need to integrate model results with geologic and geophysical datasets. New observations often motivate and inspire new modeling. Similarly, modeling results can identify key data gaps needed to answer key scientific questions. Deliberate efforts are necessary to ensure that modeling and data scientists work together. One exciting topic discussed at the workshop was new inverse modeling approaches that can be used to infer specific geomorphic and geologic parameters. However, in all cases, in order for data to be useful they must be accessible and understandable. Standards for metadata and data formatting are required, along with common data storage areas and open data access. This is an excellent opportunity for the CIG and CSDMS communities to expand their efforts to interface with ongoing EarthCube data archiving and workflow efforts.

Lastly, it was clear that bringing the tectonics and surface processes communities together facilitated more than just technical discussions of code development. It enabled new scientific perspectives to existing questions and ideas. The workshop stimulated new collaborations and proposal ideas that would not have been possible if the CIG and CSDMS communities had met in isolation. Many participants advocated for future meetings/workshops to follow-up on the CTSP discussions, and possible funding sources/venues were discussed, including for workforce development and training (e.g., Penrose, Chapman, and CIDER). However, it was also clear that new funding streams will be necessary in order to achieve all the scientific goals highlighted at the workshop.

In the document below, we provide details on the workshop activities (Section 2), discuss what specifically was learned by bringing the communities together (Section 3), and lastly provide recommendations for efforts that could be undertaken to facilitate future research directions (Section 4).

## 2. The CTSP Workshop

The CTSP workshop took place from April 25–27 in the SEEC (Sustainability, Energy, and Environment Complex) building at the University of Colorado Boulder. At total of 95 participants, including the organizing committee attended on site. On-site participants included 28 graduate students, 26 postdoctoral scholars, 19 early-career scientists, and 22 mid-career to



*Figure 1.* Group photo of workshop participants outside the SEEC building at the University of Colorado Boulder.

senior scientists (Appendix 1). Of the onsite participants, 40% were female. The keynote speakers were also balanced by gender and career stage. An online venue was provided for remote participation using Zoom as a provider for video conferencing (https://www.zoom.us/). Up to 54 remote participants attended concurrently during the main sessions of the workshop, and 10–20 participated in online breakout sessions, which were tasked with addressing the same questions as the onsite attendees. Remote participation allowed the workshop to expand its reach to those unable to attend in person due to monetary constraints and limited space at the venue. The total CTSP participation of ~149 scientists (**Figure 1**) was significantly larger than anticipated and reflects the community's keen interest in the scientific challenges and opportunities addressed at the workshop.

The workshop was structured around two days of talks, breakout sessions, and posters, followed by a half day dedicated to developing the outline for this white paper (see Appendix 2 for complete workshop agenda). Below we briefly summarize the main points made in each of the keynote presentations. Abstracts of the talks and posters and videos of the talks and presentation slides are available at: <u>https://csdms.colorado.edu/wiki/Form:Meetingconfirmation#</u><u>Meeting\_presentations</u>.

Breakout sessions focused on the key questions, opportunities, and challenges, for both the individual tectonics and surface processes communities, as well as across communities. The discussions covered a range of topics, including: How can strain predictions from a tectonic model be translated to erodibility in a landscape evolution model? Do tectonic models need 2D topographic information, or is collapsing topography into 1D sufficient? At what time scales should models be coupled? The overarching themes identified in the breakout sessions are presented in Section 3; a detailed record of the breakout group discussions is provided in Appendix 3.

#### 2.1 Summary of oral sessions

The invited presentations provided critical information and knowledge relevant to the questions posed in the breakout sessions. Day 1 included two oral sessions. The first was focused on a subset of big picture questions that are, and could be, addressed by modeling the

interactions between seismo-tectonic and surface processes. Alison Duvall (University of Washington, Seattle) provided an overview of a community effort to link short-term tectonic and surface processes through collaborative sharing of models, data, labs. Alison pointed to the importance of cross-disciplinary training. As an example of such collaboration she presented the case of a potential Cascadia M9 megathrust earthquake (Figure 2). In the second talk, Katy Barnhart (University of Colorado, Boulder) focused on problems associated with the inversion of Landscape Evolution Models (LEMs) to infer both geomorphic and tectonic processes. Katy outlined many challenges associated with the calibration and validation of LEMs, the coupling of geodynamics and climate processes, and the ultimate comparison of models and data. Her inversions of geomorphic processes showed that lithology, erosion threshold, and non-linear hillslopes were all required for the models to reproduce the observations in her particular field site. The relationship between these parameters is non-linear and the results of the inversions are related to the objective function used to extract parameters when matching observations. Katy showed that synthetic experiments could be used as guides for inversion and the addition of constraints such as thermochronologic data could improve parameter estimations and landscape evolution. Her talk also highlighted the value of the community cyberinfrastructure resources that are enabled by the CSDMS and CIG facilities.

The second oral session on Day 1 focused on models that couple surface and tectonic processes. Jean-Arthur Olive (Ecole Normale Supérieure. Paris, France) presented an exploration of the coupling of brittle deformation and surface extensional processes in settings. He argued that halfgrabens bounded by normal faults (such as the Wassuk Range in Nevada) are natural laboratories to study the effect of erosional processes on the localization of deformation in fault zones. Combining numerical and analytical approaches he showed that increased erosion promotes localization on a single normal fault. He further explored extensional settings by calibrating stream power incision parameters to equilibrium river profiles from the East African Rift and the Basin & Range Province, and illustrated how surface



**Figure 2.** Schematic illustration (top) of the overall goals of the M9 project which also illustrates the importance of understanding the coupling between tectonics and surface processes (provided by Nasser Marafi, University of Washington). Physical processes along a subduction zone pose many hazards for people and the built environment and scientists must work with communities so that they can better prepare for these hazards. Figure from Alison Duvall's presentation.

processes control how quickly these half-grabens reach steady state. Phaedra Upton's (GNS Science, New Zealand) presentation focused on efforts to link rock cohesion and landscape erodibility using a coupled scheme in which the CSDMS-hosted landscape evolution model CHILD (Tucker et al., 2001) was coupled to the geodynamics code FLAC3D<sup>™</sup>. This coupled model provides a method to directly relate erodibility to rock rheology using cohesion, fracture spacing and grain size (Roy et al., 2016). Phaedra then presented the Failure Earth Response Model (FERM) (Figure 3) and showed how erodibility can be directly related to strain, a product of the state of stress at the surface, through the rheological properties of the rocks. FERM has the potential to relate surface and tectonic processes through the ratio of total stress to rock strength within the lithosphere and at a free surface (topography). Simultaneously solving for the evolution of both surface and tectonic processes using the momentum balance would eliminate the need for parameterization of surface processes using stream power and diffusion laws. Challenges such as the effects of stresses associated with stream hydrodynamics can be accounted for with other numerical methods. In the final talk of Day 1, Jean Braun (GFZ German Center for Geosciences, Potsdam, Germany) presented an approach to modeling surface processes during the orogenic cycle by parameterizing a non-linear power law for fluvial and glacial erosion, and showing that analytical and numerical solutions of erosion laws provide accurate estimates of the steady state response time for mountain building as well as the landscape response time to periodic climate variations. Jean also showed that climate variability (weather) can affect the way surface processes respond to climate change.

# Failure Earth Response Model (FERM)

FERM uses a Mohr-Coulomb approach to failure of Earth materials wherein failure occurs if the local differential stress  $(\tau)$  exceeds the local strength (C) of the Earth material.



**Figure 3.** Schematic illustration of the Failure Earth Response Model (FERM). Estimation of the total stress at the Earth's surface incorporates geodynamic (tectonic, seismic) and geomorphic (topographic, fluvial, glacial) stresses into a single reference frame to determine if failure will occur at a given point. Failure occurs when the local stresses overcome the local strength of the material. Figure from Phaedra Upton's presentation.

Day 2 also included two oral sessions. The first was focused on the challenges associated with implementing the coupling of surface and tectonic processes in numerical models. Brian Yanites (Indiana University, Bloomington) gave an account of successes and failures when trying to reconcile LEMs with data from natural systems. He showed that complexities in natural systems limit our ability to use simplified models and that the available physical formulations may not describe all river systems. The variation in rock types renders the translation of lithology into erodibility difficult and diminishes the applicability of the present formulations. One possible solution would be to calibrate erodibility using river incision profiles. Brian also discussed the challenges of incorporating climate into LEMs, including the role of mean climate state, as well as climatic timescales and weather variability. Finally, Brian noted that channel width must be accounted for in a more realistic way to properly explore how slope adjusts to external forcing. In the following talk, Louis Moresi (Melbourne University, Australia) showed that to couple LEMs and tectonic models efficiently, LEMs must be parallelized such that they do not act as a computational bottleneck to the standard parallel long-term tectonic codes. To do so, Louis proposed a mathematical method loosely based on graph theory that allows a fluvial channel network to be formulated in a matrix form. This formulation allows for the direct use of parallelized linear algebra tools such as the Portable Extensible Toolkit for Scientific Computing (PETSc), which are already widely used in tectonic codes, to simulate landscape evolution. When implemented in LEMs this method allows for the seamless two-way coupling of dynamic models of lithospheric evolution and LEMs. The corresponding tool Quagmire, developed by Louis, was provided in a Python framework. The use of Python tools (as already used at CSDMS) should provide flexibility when choosing what formulation to use in LEMs for different environments.

Finally, during the afternoon of Day 2, representatives from CSDMS and CIG provided overviews of the tools and methods currently available to model landscape and lithospheric evolution, respectively. Mark Piper (CSDMS) described the CSDMS philosophy that grew from the needs of the surface-dynamics community. Specifically, Mark discussed the use of frameworks such as the Basic Modeling Interface (BMI), Python Modeling Tool (PyMT), and Babel to develop high level wrappers around LTT and LEM software to simplify communication between tectonic and surface processes models (Figure 4). One of the main advantages of such an approach is that it allows for flexibility in the choice of models to couple. These needs arise from the wide diversity of models used by the CSDMS community: models that treat different types of environment (for example, polar, fluvial, coastal, and marine), on spatial scales ranging from grains to global, and at temporal scales from storms to geologic epochs. Mark highlighted that a strength of the CSDMS "plug and play" approach is the ability to address coupled problems by combining models in a single framework, and to test hypotheses by swapping in alternative process components. John Naliboff (University of California Davis, CIG) showed that similar considerations apply to long-term tectonic models. The diversity of length and time scales simulated by the lithospheric deformation community (i.e., mountain building to earthquakes) forces the long-term tectonic community to choose a great variety of approaches when modeling lithospheric deformation. This includes the choice of reference frame (Eulerian versus Lagrangian), rheology (e.g., elastoplastic, viscoplastic, thin sheet approximation, etc.), boundary conditions, and solvers. John also pointed out the need for each code to follow a process of verification and validation to develop open-source methods that allow for reproducibility. Lastly, he pointed out the need to equip open-source software with a framework for inversion (e.g., Bayesian) both for validation, as well as to address scientific questions. Akin



**Figure 4.** Illustration of how the CSDMS Basic Model Interface (BMI) and Babel allow two different models 'A' and 'B', which are written in different languages, to be coupled together. At left, by adding BMI, this in essence ensures that both models have some standard functions so that they can talk to each other. At center, Babel allows models written in different languages can talk to each other. BMI and Babel allow models 'A' and 'B' to be coupled in the CSDMS plug and play architecture. Figure from Mark Piper's presentation.

to the need to use inversion techniques to constrain parameters for stream power laws and erodibility (as discussed by Katy on Day 1), parameters for the effective rheology of the lithosphere must be constrained through inversion using geophysical observations such as deformation rates. John gave some pointers for accessibility to computational resources that are available for running parallelized dynamic models with coupled surface and tectonic processes. Collectively, the presentations by Mark Piper and John Naliboff highlighted the critical role of the CSDMS and CIG facilities in supporting computational science within the scientific communities that they serve.

#### 3. What we learned by bringing the communities together

#### 3.1 The value of learning from one another

A consistent theme to emerge from the workshop was the need for, and benefits of, further communication and mutual education between the tectonics and surface-processes communities. The workshop provided an opportunity to share information about motivating scientific questions, key datasets and their uncertainties, and computational and numerical methods. Meeting participants expressed enthusiasm for holding additional workshops to continue and intensify the conversation.

#### 3.2 Computational issues: similarities and differences

Regarding numerical methods, advances in both communities are limited by computational bottlenecks. Model resolution emerged as a common limitation. In the tectonics community, models of upper crustal deformation do not generally resolve faults explicitly, but instead depict shear zones, the minimum width of which is limited by grid resolution. Similarly, models of fluvial erosion, sediment transport, and deposition often treat river channels as sub-grid-scale features and can experience grid-resolution sensitivity as a result. In the tectonics community, numerical models of three-dimensional deformation typically require parallel computing on distributed memory systems to achieve practical run times; however, most surface process codes

run on a single processor. Development of parallel techniques in the surface-processes community is therefore a key future direction in creating the next generation of coupled models.

Both communities use models of varying complexity to address different types of science questions. For example, some crustal deformation models are 2D (vertical slices; e.g., SiStER), where others are 3D (e.g., ASPECT, PyLith). Tectonic models also vary in their representation of rheology (e.g., visco-elasto-plastic vs. visco-plastic). Similarly, some models of erosion and sedimentation at Earth's surface represent topography as a 1D "slice" (in which elevation is a function of distance along a transect), whereas other models treat elevation as a function of two independent spatial dimensions, and may include information about subsurface material properties such as stratigraphy and rock strength (making them quasi-3D). Moreover, landscape evolution models also vary in nature and sophistication in their representation of processes. Coupling such diverse codes can be a challenge. The earth-surface dynamics community, through CSDMS, has developed standards, protocols, and a framework for coupling numerical models, including coupling of models written in different languages. These developments provide a starting point for coupling tectonics and surface processes. However, in order to be computationally efficient for 3D tectonics models, the current framework and protocols needs to be adapted to handle tight, fully parallel coupling. Such tight coupling could be achieved through an enhanced version of CSDMS' Basic Model Interface (BMI) standard (Peckham et al., 2013). The Python programming language is popular in both communities, and has the advantage that codes written in compiled languages such as C can in principle be "wrapped" in Python, thus taking advantage of its high-level features and libraries.

The solid-earth geodynamics community, through CIG, has developed best practices for developing and disseminating scientific software that is correct, useable, discoverable, and attributable (**Figure 5**). CIG has also established methods for attribution of software authorship, which includes the usage of DOIs. Further, CIG has invested in and recommends the use of standard scientific computing libraries when possible, and provides a model for how to contribute methodologies back to these libraries. Similarly, CSDMS promotes a "best practice" approach that incorporates unit testing and continuous integration. The CSDMS model repository allows model authors to tag their software with a Digital Object Identifier, and can track citation of models through a bibliometric index that is linked to a particular model program rather than to a particular author. These types of best-practice innovation should be adopted in the development of coupled tectonic/surface processes codes.

Finally, both communities described benchmark testing of models as an ongoing research need. Potential case studies for benchmark tests range from simple analytical solutions to laboratory experiments to real geological cases. Benchmarks will be needed for coupled models as well as for individual (uncoupled) ones.

#### 3.3 Data needs in the tectonics and surface-dynamics communities

The use of data to validate numerical simulations is key to both communities, but it became apparent during the meeting that several aspects of data collection and reporting need to be refined to enable their use across the disciplines. In particular, concerns were raised regarding what data will be needed to constrain future models, how those data would be stored and collected, and what would be the availability of those data in established or future databases. Additionally, data uncertainty and links between effective behavior and state and compositional variables predicting them was a major concern. Methodologies for quantifying uncertainty in data collection methods, analytical methods, and the numerical models used to interpret these data were all raised as points where communication is paramount. Addressing the above questions was viewed as essential to developing robust collaborations between the communities.

Members of both communities presented examples of the types of data used to test models. For instance, metrics extracted from digital topography data are commonly used to test the predictions of landscape evolution models. Models of crustal deformation might be compared with estimates of total fault slip, spacing between faults, strain partitioning, and/or seismicity. An open question lies in determining what kinds of data are needed to test coupled models, and what constitutive laws might describe key material behavior such as erodibility. Here, there is an opportunity to take advantage of data sets produced in both communities, including topography, seismic imagery, and stratigraphy.

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## Software Development Best Practices

Best practices for developers of CIG hosted codes are specified at three different levels:

- Minimum Best Practices. Minimum expectation for all codes hosted by or distributed by CIG.
- Standard Best Practices. All codes should be following this level of best practices. If not, codes should have a plan of active development to achieve this level.
- Target Best Practices. Codes under active development should have a long-term plan to implement these practices.

#### Summary Table

## **Minimum Best Practices**

Practices that codes must follow in order to be accepted by CIG.

- 1. Licensing
  - a. Open source license. GPL preferred. See licensing.
- 2. Version control
  - a. Use of version control (e.g., subversion, git) to manage code changes
- 3. Portability, configuration, and building
  - a. Code builds on Unix-like machines (Linux, Darwin) with free tools (compilers)
  - b. Well designed, portable build system (e.g. cmake, make, configure-unix only, setup.py, etc.)
- 4. Testing

*Figure 5.* Illustration of some of the recommendations made on the CIG best practices for software development webpage: <u>https://geodynamics.org/cig/dev/best-practices/</u>.

#### 3.4 When coupling matters (not just in models, but in observations)

Significant discussion at the CTSP workshop revolved around determining when coupling of surface processes and tectonics models actually matters. The consensus was that it depends on the question being asked, in particular as to which spatio-temporal scales are concerned (see below). At the scale of individual faults, coupled models such as SiStER have demonstrated that the effect of surface processes on fault evolution is to further enhance the fault lifespan in thinner/weaker faulted layers for a given erosion and slip rate (Olive et al., 2014; Figure 6). In collisional settings, the weakening of rocks along zones of highly concentrated strain/shear zones can dictate the fate of the landscape by virtue of their reduced cohesive strength and hence enhanced erodibility (e.g., Roy et al., 2015; 2016). During CTSP examples were shown in which coupled models demonstrated that the cohesion of a material dictates its erodibility and, therefore, the ultimate grain size distribution in channels (Roy et al., 2015). One question that emerged was: to what extent are the rock properties that dictate rheologic response to stress in the Earth's interior the same as those that set the material's response to various weathering and erosional processes, which can generate near-surface stresses? Brian Yanites presented data from channels in the Salmon River Watershed, Idaho, USA, which illustrate that channel evolution varies depending on rock type (Figure 7). Findings such as these are necessary to tackle this question. By bringing the communities together, we learned that the coupling of tectonic and surface processes models at the scale of individual structures can enrich our understanding of how surface processes are fundamentally linked to the underlying tectonic processes. We also saw examples of topography and relief directing affecting tectonic processes. In regions of high relief, topography (which can include ice loading) rather than tectonic driving forces dominate the stress tensor and can influence the style of faulting, the permeability structure and hence transfer of fluids and heat (Upton and Sutherland 2014; Sutherland et al. 2017; Upton et al., 2018).

At the scale of entire orogens, modeling must start addressing mass balances at the crustal scale. Large-scale river and landscape morphology can inform the style and timing of mountain building (Zeitler et al., 2001; Koons et al., 2013). Currently a challenge of coupling models at this scale is the understanding of the degree of complexity that is necessary and the contrasts in resolutions (both with respect to the model components as well as the available data; here again, a model-coupling framework would add value because it allows for experimentation on different levels of complexity, and handles re-mapping between grids of different resolution and/or geometry). One common thread that emerged when discussing methodologies to constrain large-scale models was the need to incorporate stratigraphy and basin evolution.

Further, in coupling tectonic and surface process models, different timescales are relevant for different questions. The presentations and discussions at the CTSP highlighted that both communities struggle with the problem of timescales. Moreover, we learned that linking short-scale processes such as earthquake cycles, which can greatly influence surface processes such as landslides (e.g. Dadson et al., 2004; Li et al., 2014; Meunier et al., 2007), to long-term tectonics, such as the evolution of an active continental margin, is a challenge. Indeed, despite the groundbreaking conceptual model of a two-sided wedge by Koons (1990) and subsequent numerical modeling by Willett (1999), the communities have still not fully quantified the underlying feedbacks between surface processes and tectonics that take place in convergent settings. Modeling the long-term evolution of convergent zones will require understanding what goes on in the short timescale and what cause-effect relationships exist there. On the other hand,



**Figure 6.** Example of numerical model SiStER (Simple Stokes for Exotic Rheologies) coupling of surface processes and fault evolution. (a) Model setup with an elasto-plastic layer of thickness H. A weak fault initially seeded at an angle  $\theta = 60^{\circ}$  undergoes extension at a half-rate V. The cohesion and friction coefficient of intact rocks are C and  $\mu$ , respectively, and cohesion is decreased to  $C_o$  in the fault zone. Surface processes cause footwall erosion and partial filling of flexural basins. (b-d) Snapshots of numerical simulations after 22 km of extension in a 15-km thick layer extending at a half-rate of 1 mm/yr. Surface topography is subjected to erosion rates of (b) 0.015, (c) 1.0, and (d) 15 mm/yr. Yellow dashed lines indicate faults that have been abandoned in a sequence indicated by the numbers. Blue faults are actively growing at the time of the snapshot. Colored areas indicate the material that deposited while the fault of corresponding color was active. In the case of panel (b), where faults are short-lived and closely spaced, the blue material integrates deposits associated with the successive growth of fault #2 and fault #3. Figure from Olive et al. (2014).



**Figure 7.** Channel profiles from two channels incising into different rock types in the Salmon River watershed, Idaho, USA. The form of the knickpoint in the channel at left differs from that in the channel at right, suggesting that incision processes may differ between channels with different rock types. Figures were shown in Brian Yanites' presentation and were provided by graduate student Nathan Mitchell, Indiana University Bloomington.

the long-term contribution of surface processes to the evolution of a convergent zone might help understand how short-term tectonics-surface processes links change through time. It is important to advance our understanding in these topics, especially because the coupled studies may provide valuable information for hazard assessment.

#### 3.5 Weather and climate

Climate has long been considered a driver of landscape evolution (**Figure 8**), though clear geologic evidence for such a link has been difficult to establish (Whipple, 2009). For decades, our communities have focused on finding mechanistic examples of mountain ranges where climate influenced tectonics through surface processes (e.g., Brozovic et al., 1997; Finnegan et al., 2008; Gabet et al., 2008; Enkelmann et al., 2009). However, how climate drives surface processes depends on the climate. In cold locations where glaciers dominate, some studies argue that glaciers are very efficient eroders, even acting as a "buzzsaw" (e.g., Mitchell et al., 2006; Egholm et al., 2009). By contrast, other studies have shown that cold-based glaciers erode at relatively slower rates (e.g., Thomson et al., 2010; Koppes et al., 2015). In unglaciated landscapes, there are similar disparities in data relating climate (rainfall, temperature) and processes such as weathering and hillslope and fluvial erosion (e.g., von Blanckenburg, 2005; Perron, 2017). Whether global climate cooling has led to increased erosion has been actively debated for the last three decades and drives much of the research linking climate and surface processes (e.g., Molnar & England, 1990; Willenbring & Jerolmack, 2016; Herman & Champagnac, 2016; Schildgen et al., 2018).

A common theme discussed throughout the CTSP workshop and highlighted in Jean Braun's talk was how weather events, as opposed to climate, and tectonics interact. Weather, via rainfall events and floods, provides a better window to explore mechanistic links between surface processes and tectonics. In the past, studies have investigated the frequency distribution of flood events and explored how they play a role in moving sediment of a relevant grain size to incise



**Figure 8.** Scenarios in which a landscape might respond to a change in climate, here modeled as a change in erodibility, K, in the stream power model; doubling K simulates a wetter, more erosive climate, and halving K simulates a drier, less erosive climate. The 'fixed' model assumes that width of a mountain range is fixed and cannot respond to climate, whereas in the 'wedge' model the mountain range width can vary with climate. Plots show temporal response of (a) normalized mountain half width, (b) normalized relief, (c) normalized erosional efflux, or spatially integrated erosion rate, and (d) normalized rock uplift rate to a change in climate. Figure from Whipple (2009).

into bedrock (e.g., Tucker and Bras, 2000; Molnar, 2001; Tucker, 2004; Lague et al., 2005; DiBiase & Whipple, 2011; Rossi et al., 2016; Deal et al., 2018). Trade-offs between mountain building and atmospheric circulation provide an avenue to explore the feedback mechanisms between relief enhancement and the recurrence intervals of large rainfall and discharge events (e.g., Ehlers and Poulsen, 2009). The community is only now starting to explore how the minimum discharge necessary to move grains large enough to incise into bedrock varies in time due to tectonic and long-term climatic change (**Figure 9**). These are avenues for future research and could even involve additional couplings with atmospheric models.

#### 3.6 Life and landscape

How surface processes and tectonics interact can dictate the topology of drainage basins, which in many cases define boundaries for biota (e.g., Stokes et al., 2018). Defining the pace and mechanistic links between surface processes and tectonics can provide new information on the coevolution of landscape and life and vice versa (e.g., Burridge et al., 2006; Waters et al., 2007; Wallis et al., 2016; Craw et al., 2016; 2017).

In the case of short-term surface processes, drainage capture is an important process that is capable of drastically changing the sizes of the drainage basins involved, causing expansion of one basin at the expense of another (e.g., Bishop, 1995; Prince et al., 2011; Yanites et al., 2013). These processes may merge species that were previously separated all the while increasing the drainage area, which is termed "reach expansion" in the biologic community. This process is a



**Figure 9.** (left) Schematic of the coupled WRF/WRF-Hydro/Landlab modeling environment. WRF produces rainfall that is routed across the landscape using WRF-Hydro, modeled discharge is then used to predict erosion rates in Landlab. (right) Example of discharge exceedance probabilities in three rivers on the west side and east side of the Andes at 20°S using this modeling environment. The red line illustrates the discharge necessary to entrain ~4 cm for the slopes and widths of the channels analyzed here. Figures presented by Brian Yanites and provided by Brigid Lynch, Indiana University Bloomington.

recipe for increased biodiversity. On the other hand, the basin losing drainage area can experience extinction if the basin size is reduced to a critical drainage area below which life for some species is unsustainable. Investigating if and when tectonics can trigger drainage capture events can provide direct links to understanding the distribution and richness of species that are sensitive to the shape, size, and evolution of drainage basins.

In the case of long-term tectonics and surface process interactions, we learned that plateaus are capable of governing the shapes of drainage basins by sustaining flexurally-elevated plateau edges, which can also dictate species distributions (**Figure 10**). In addition, orographic relief above mantle upwellings can alter global climate, and moderate the generation of typhoons and hurricanes. Thus, investigating the evolution of plateaus in regions that were once tectonically active can shed new light on the coevolution of landscape and life. In the case of mountain building, the connectivity of drainage basins is drastically changed. There are multiple examples in the literature of how the evolution of tectonically active mountain ranges is imprinted on the species that reside in those regions (i.e., Andes, New Zealand). In some cases, genetic signatures extracted from biota in today's basins can provide a rough timing of appearance of a new species and sometimes this age falls within a well-defined tectonic event. Conversely, lacustrine speciation and migration patterns may be controlled by erosion and tectonic events (e.g., E. Africa). We have learned that the legacy of tectonic processes on the landscape may dictate the evolution of some species. What we do not know is if there is a mechanistic link between the pace of tectonics and surface processes and the appearance or disappearance of species.



**Figure 10.** (left) Map of showing the centers of endemism across Madagascar from Wilme et al. (2006). Distribution of these centers is linked to evolution of river catchments, which are in turn related to uplift patterns. In the case of Madagascar, uplift is controlled by the flexural response of the lithosphere to rifting (shown schematically in the right panel)—leading to potentially exciting feedbacks between life and the deep Earth. Figure from Jean Braun's presentation.

#### 3.7 Science and model development need to proceed together

Lastly, there was consensus that development of relevant science questions and coupled numerical simulations should proceed together. The emergent behavior expected from tightly coupled surface processes and lithosphere dynamics models is likely to yield transformative science, but it is difficult to determine the behaviors likely to emerge prior to development of such coupled models. As these coupled models are developed, there will be a need for explorational modeling that does not focus on calibration or particular field areas. Results from theoretical modeling will raise new scientific questions and drive future data collection and exploration.

Although the community is highly motivated to develop coupled models, there are several challenges remaining before model coupling can be achieved. One of these challenges is the lack of a framework for communication between the surface processes and lithosphere dynamics communities, which is manifest in code development efforts. The CSDMS community has put significant effort into creating a multi-layered framework for code communication, but this framework does not currently operate in a fully parallel mode. Because most lithosphere dynamics codes are highly parallelized, this presents a major challenge to model coupling. One

possible solution raised at the meeting (which itself was a first step toward improving communication between communities) was to build on the current CSDMS model-coupling framework to add parallel capability. In the following section, we provide some specific recommendations for developing the next generation of coupled tectonic/surface processes models.

## 4. The Road Ahead

## 4.1 Continued community building

As outlined above, the CTSP workshop was highly successful in bringing together a wide range of researchers from both the surface dynamics and the long-term tectonics modeling communities. We see this as the beginning of an ongoing process of community building and workforce development. We identified the need to continue building links between these two communities via a variety of methods. We also identified other communities to engage with, both other modelers and the wider community of geoscientists who can help to constrain our models and will have their own scientific questions that modeling can help answer.

#### 4.1.1 Workshops and Tutorials

The CTSP identified needs for (1) knowledge transfer between the communities, (2) transfer of skills within and between the communities, and (3) continued promotion of communication. Workshops and tutorials or clinics, as well as conferences, are efficient ways to achieve these goals.

*Tutorials:* Both the surface dynamics and the long-term tectonics modeling communities already have established avenues for training and knowledge transfer in their fields, taking the form of online and offline resources provided by CSDMS and CIG. Nevertheless, the workshop made clear that more effort is necessary to spread this information across communities, for example in the form of combined tutorials discussing the coupling and interaction of surface and tectonic processes.

#### **Recommendations:**

- Develop a simplified community tutorial. A first step could be to take existing resources and by the smallest possible modification build a module that covers a simplified coupling between example software packages (~90 min content). Existing codes could be used to start with first order couplings between 1-D or 2-D landscape evolution models and 2-D tectonic models. This information can be created with reasonable effort and presented online—e.g. in form of a recorded tutorial such as the CIG webinar series, or in the form of a documented web tutorial like the CSDMS labs. This would not only transfer necessary skills, but would also further help in identifying obstacles for the more challenging full coupling case. After establishing a first resource, it would be straightforward to use the existing tutorial opportunities (like clinics at the annual CSDMS workshop, GeoPrisms mini-workshops at the AGU Fall Meeting) to extend the developed module from an online to an in-person tutorial, and to educate about prospects and challenges when coupling tectonic and surface evolution models.
- *Extend simplified tutorial into a suite of tutorials in accordance with technical progress.* As technical challenges are resolved, additional modules of increasing complexity could be

developed to document different levels of coupling that involve 2-D landscape evolution models and 3-D tectonic models.

• Collect a suite of created tutorials and create an inter-community course. A long-term project could allow for the establishment of a collaborative training and research program for coupling tectonics and surface modeling analog to the CIDER program (<u>http://www.deep-earth.org/</u>) for deep Earth research. This would require a significant investment for a single research group, but might be feasible if it is organized as a community effort, and would strongly support the transfer of critical skills and the creation of a combined community.

*Workshops:* The current workshop received an overwhelming response from the community, and there was a lot of support to pursue more similar opportunities. In general, such workshops can either concentrate on transferring knowledge between communities or be focused around developing a common project/proposal or tackling a specific problem.

## **Recommendations:**

*Submit special topics or sessions*. A moderate first step is to include coupling of software as a special topic into existing workshop programs by CIG and CSDMS, or to submit a special session proposal to conferences such as the AGU Fall Meeting and GSA Annual Meeting. Both allow for scientific exchange and would continue the community building that has been started.

- *Opportunities for new specialized workshops.* Another conference exclusively dedicated to coupling of processes (either in the format of this workshop, or as a dedicated conference within a conference series such as Penrose, Chapman, GRC) would provide a venue to make focused progress in defining coupling interfaces and actively work on the challenges that were identified during the CTSP workshop.
- *Include practical components.* We recommend including practical components (e.g., hackathons, hands-on tutorials, and break-out sessions focused on specified tasks) into upcoming workshop proposals. Each of these practical components would have defined products that they would deliver, for example: (1) an idealized workflow for coupling models, (2) a set of benchmark definitions, (3) a practically implemented interface for a particular software, and so on.

A dedicated workshop would also enable other communities to attend who can provide crucial input for the coupling of surface and tectonic processes as described in the next section.

## 4.1.2 Other communities

This workshop focused on bringing together the long-term tectonics and surface processes modeling communities. In doing so, we identified other communities that are vital to coupling tectonics and surface processes, but were underrepresented at the CTSP.

#### **Recommendations:**

• Include short-term tectonics and biological communities. The first of these is the short-term tectonics modeling community, which is also a component of CIG. This includes researchers who model earthquake, volcanic eruptions, and other processes that occur on a short timeframe. In many ways these processes are the link between long-term tectonics and the surface and it is essential that this community is part of our conversation. Further, new insights into the linkages between life and landscape evolution were discussed at the workshop, but a lack of expertise from the biological community precluded us from gaining

substantial insight in this area. Future workshops should strive to broaden their scope into these emerging fields.

- Seek more connections to data and constraints. Looking more widely than modeling brings us to researchers who provide both the data with which we build and constrain our models. These include but are not limited to: seismologists, geodesists, structural geologists, petrologists, sedimentologists, and basin analysis researchers. Seismologists and geodesists provide constraints on present-day rates and stress states, while structural geologists can inform us about past and present stress states. Sedimentologists and the sediments and basins they study hold the key to a library of information about tectonics, erosion and deposition through time. Not only do these researchers maintain this observational data, but they also have research questions that modeling may be able to answer. Finally, seismologists and petrologists have data sets that place bounds on the elusive lower crustal composition, fluid content, and rheology to which the numerical models are sensitive. Thus, it is vital that our modeling communities interact with field-based scientists. This can be challenging as it is often easiest to remain within one's field of expertise, but there are ways to facilitate these conversations:
  - Inviting field-based researchers to modeling workshops.
  - Specifically developing workshops with a field component.
  - Ensuring that our communities present results at structural seismology, geodesy, geology, and geomorphology meetings in a way that is accessible to non-modelers.
  - Special sessions at conferences such as GSA and AGU that are aimed at bringing the communities together.
- *Include international community*. International links are and will continue to be important. The CSDMS and CIG communities already have strong links with a number of overseas researchers, several of whom contributed to the workshop in April (both in person, as well as, through the online platform); however, it is critical to continue to cultivate these relationships.

## 4.2 Code Development Efforts

While the challenges and goals identified by individual participants in the breakout sessions were diverse, common themes emerged that should guide future code development. The first major challenge is the coupling frameworks and underlying computational infrastructure needed to support coupling of models of Earth's surface and its interior. The CSDMS Basic Model Interface (BMI) standard and PyMT model coupling framework were identified as good first steps towards such an interface. A second major challenge pertains to developing appropriate and feasible methods for careful model-data comparison and estimation of uncertainty. Below we describe the challenges and opportunities associated with each of these two themes for code development and make recommendations for tackling outstanding problems.

## 4.2.1 Tools to support model coupling

A set of standards for model inter-communication are required in order to couple two models, be they two models of the Earth's surface or a model of Earth's surface and of its interior. The creation of a model interface standard, such as the CSDMS BMI provides a template for a coupling framework. In addition, CSDMS provides PyMT, a model coupling tool that implements the BMI standard. Wrappers can be created to make existing models compatible with a coupling framework, and new models can be designed to fit such a framework.

Discussion identified that the BMI and PyMT provide an excellent starting point, but must be extended to meet the needs of both communities. Specifically, the BMI framework and PyMT were not designed to support the coupling of MPI parallel models *and* were not designed to support the tight coupling of models, in which coupling occurs at the level of the numerical solver. Instead, the BMI makes it possible for models to be coupled "loosely" at the level of passing state variables between models and running each model forward in time independently, which may be insufficient for highly nonlinear problems, though this question remains untested.

A major theme of discussion was the "right" level of necessary complexity to couple models. Does a geodynamic model of whole-mantle convection need to be coupled tightly to a surface processes model that resolves reorganization of drainage basins and tracks sediment fluxes to create stratigraphy? Ultimately this is an empirical question that is not possible to answer unless alternative couplings are created and compared. For comparison of model output with observations such as sediment fluxes through time inferred from the stratigraphic records in a terrestrial or oceanic basin, models must include state variables that are related to comparison data. However, it may be computationally intractable to couple such an Earth surface model with a geodynamic model. A path forward could be nested model coupling—in the example above a full-complexity geodynamic model could run with tight coupling to a simple surface process model, and then used as a forcing boundary condition (one way coupling) with a high complexity stratigraphy-producing model.

To address the described challenges the following are needed:

- 1. Development of a model coupling standard that supports coupling of MPI-parallel models and tight (solver-level) coupling.
- 2. Discussion between and within both communities related to the creation of such a standard.
- 3. Lobby the community to incorporate computational training into undergraduate geosciences education.
- 4. Training sessions (including week to multi-week hack-a-thons) in which established researchers and students learn the model coupling standard and frameworks so that the models they develop can fit within existing and future tools.
- 5. Continued development of Earth surface and interior models and modeling packages designed for a variety of time and space scales that permit modeling at varying levels of complexity.
- 6. Develop test models that can be run to isolate the influence of different levels of coupling.
- 7. Resources for PI-lead code development efforts, as CIG and CSDMS do not currently have the personnel and/or financial resources to do this alone.

## **Recommendations:**

• Leverage existing widely-used open-source frameworks. PETSc & Python are the currently best-supported common open-source standards that are widely used with the geodynamics

community, and Python is emerging as a standard within the Earth surface process modeling community. Through the use of Jupyter-Notebooks, or Jupyter-Lab, these tools are readily useable and can be combined with a wide variety of plotting routines. This will also help using the tools for teaching. We recommend that development of models and coupling frameworks use these tools or other similar tools, and when possible that effort is put into reengineering existing codes to better facilitate them. We recommend that the model coupling standard first prioritize MPI-parallel communication and then prioritize tight coupling. This can be achieved by first developing an MPI-parallel compatible Python interface for loose coupling, and then incrementally changing existing codes to provide required state variables for joint numerical solutions using PETSc.

- *Build off of existing coupling standards and frameworks*. The CSDMS PyMT and BMI are an important first step in creating a generic and usable coupling framework, albeit it for "loose" coupling at the upper level. Future work should build from them and support teaching members of both communities at all career levels about their existence and protocols.
- *Need for MPI-parallel Surface Processes codes.* Few surface processes models are designed to work in MPI-parallel computing environments, yet nearly all 3D geodynamics codes require such an environment. Having an MPI-parallel framework that does surface processes is a key requirement to couple models from these two communities.
- Facilitate creation of different codes & have them talk to each other. Progress in computational geodynamics over the last decade has shown that creating a single code for the community is not a good way forward, as it is often not clear which numerical technique is best for solving the governing tectonic processes. This finding is echoed by the experience of the surface processes modeling community. Instead, more progress is being made by creating generic computational tools that make it simpler to deal with problems that are common to the different codes. (An example is particle advection methods, widely used by different tectonic codes, which are now natively supported by PETSc and work for structured and unstructured meshes). Additionally, models designed for one time or space scale, or that include all possible physical processes, may not be appropriate in another context. The construction of modular model frameworks such as the Landlab Earth surface dynamics package (e.g., Hobley et al., 2017) provide reusable model components that can be mixed and matched to meet the needs of individual researchers. We recommend support for the continued development of both that are scalable on large number of processors, and are welldocumented. We recommend that future work support both generic computational tools and modular modeling frameworks.
- Dynamic re-gridding and adaptive mesh refinement. Geodynamic processes warp the surface of the Earth through processes such as rifting and mountain building. Modeling surface processes in these contexts thus requires a computational mesh that can be re-gridded and refined without loss of continuity of mass. Surface process models typically do not use adaptive mesh methods. Work in support of this capability is necessary and we recommend that it is done using the standards employed by the geodynamic modeling community.

4.2.2 Comparisons with observational data and estimation of uncertainty

The second theme related to code development was the development and accessibility of appropriate and feasible methods for careful model-data comparison and estimation of

uncertainty. Broad motivation exists for these tools: from model-parameter calibration based on observed geophysical data to uncertainty quantification of hazard prediction. Many challenges still remain at even the most preliminary steps. For example, it is not clearly established which statistics of the topographic surface are most appropriate to use for model data comparison. One key avenue for future progress is to better leverage data discoverability through EarthCUBE.

Inverse modeling approaches: One way with which to compare models to observations is to assess through inversion the model parameters that minimized the misfit between modeled quantities and observed quantities. Whereas in many fields, inversion has become routine, this is not yet the case within computational lithosphere dynamics and is not extensively used within Earth surface processes. Partly this is caused by the significant computational requirement of the forward models, which in the case of lithospheric dynamics necessitates that each individual forward model be run on parallel machines. There is thus a need to develop new methods to couple data with models, and compute uncertainty bounds. Using a full Bayesian approach may be one way forward in that it can deal with multiple minima in the parameter space. Indeed, Bayesian approaches are already implemented in the surface processes modeling community, as much effort has been put into developing highly efficient algorithms (e.g., Braun & Willett, 2013). However, given the computational requirements in fully coupled models, it may not be feasible for simulations with many input parameters. Alternative (gradient-based) approaches, utilizing adjoint gradients may be more practical, though they have the disadvantage that they may converge to a local minimum in the parameter space. Other (maybe hybrid) inversion approaches under development in related scientific disciplines (numerical mathematics, computer science) should be explored. For this to be practical, both the inverse and forward modeling tools should be accessible from the same computational framework. Part of this is already achieved within the geodynamics modeling community in TAO (Toolkit of Advanced Optimization), which is part of the PETSc framework. By contrast, CSDMS has worked extensively to integrate the DAKOTA framework (e.g., Adams et al., 2015) into its modeling tools. There are, additionally, many other packages for uncertainty quantification (e.g., MUQhIPPYlib). We advocate for careful investigation of existing and under-development uncertainty quantification and model analysis framework to identify which meet the needs of the community.

*The Challenge of Disparate Data:* Inversion approaches to model-data comparison require a formal objective function that defines the model-data misfit. Within each of geodynamics and Earth surface processes models, the definition of such an objective function is non-trivial. Take as an example the calibration of surface processes model parameters based on topographic information. A straight difference of observed and modeled topography is not appropriate as we often do not expect modeled and observed ridges and channels to be in exactly the same location. There is no accepted misfit statistic for comparison and often multiple statistics are appropriate. This means that either appropriate weights for each statistic must be determined or multiobjective inverse methods must be used. This example with comparison based on topography is much simpler than many real examples, in which topography, basin stratigraphy, and geochronologic data all provide constraint on model fit.

*Model sensitivities and underlying model physics:* Many input parameters to computational geodynamics and Earth surface processes models are uncertain. An important question is how uncertainties in the data affect the model results, and which of the input data is of key importance. For simple geodynamic models, insights from analytical solutions (such as the key non-dimensional parameters that control the rising of low density spheres in the mantle) give

some clear ideas on what the governing physics and the key model parameters are. For more complicated models, with nonlinear viscosities and brittle rheologies, this is typically much less clear. A focused effort is therefore required to combine the insights from analytical models with the results of numerical simulations. In addition, the use of automatic methods to obtain the key model parameters, for example by utilizing adjoint gradients, should be increasingly explored. Doing this on a routine basis requires adjoint gradients to be computed from the main geodynamic and surface processes models, which could probably be made available through a common model interface.

## **Recommendations:**

- *Compilation and synthesis of inversion and uncertainty quantification frameworks*. Based on the experience that committing to a single model code is not the best for the advancement of the science and the community, we do not advocate for identifying a single inversion and/or uncertainty quantification framework. Rather we recommend that the communities identify a place to compile and compare existing uncertainty quantification frameworks. This will increase the discoverability of existing tools and improve the ability of users to select the framework best suited to their needs.
- Create teaching resources related to inversion and uncertainty quantification methods. Associated with the prior recommendation is the creation of teaching tools related to inversion and uncertainty quantification. Many members of both communities are not experts in inversion and uncertainty quantification methods. To support scientists at all career levels we recommend that teaching/self-study resources related to these topics be created. When possible coordinate with IRIS and UNAVCO in sharing training materials. These resources would provide an introduction to the use of these methods, the terminology used, and information regarding the appropriateness of different methods to different problems. These resources would not replace finding collaborators who are experts in inversion and uncertainty quantification, but would provide the background a student or established scientist would need to start such a collaboration.
- *Creation of guidelines and tools for developing loss functions.* Ultimately the comparison of models and data requires the construction of a loss function that describes numerically the degree of misfit between models and data. We recommend the development of formal loss function guidelines. These guidelines would include information regarding options for constructing loss functions with good mathematical properties and information about how to incorporate observational uncertainty and model uncertainty in weighting model data differences. Also important are guidelines about best practices for creating non-direct comparisons (e.g., when a pointwise comparison between model and data is not appropriate). Finally, these guidelines would provide recommendations for assessing if the defined loss functions are appropriate for use in inversion.

## 4.3 Resources needed

Some of the recommendations given above can be done with very few resources—e.g., organization of AGU and GSA special sessions, GeoPRISMS mini-workshops, and coordination with other communities (e.g., IRIS, UNAVCO). Moreover, ongoing efforts at CIG and the recent recommendation of funding for CSDMS 3.0 provide the critical infrastructure required for community-building efforts. However, more expensive activities including dedicated workshops and training programs (e.g., a summer school) will require a significant investment of time to

write proposals and plan and hold meetings and workshops. Finally, other recommendations will require dedicating considerable time and resources toward smaller groups of investigators, such as for creating tutorials, and for dedicated coding efforts that cannot be supported through the existing CIG and CSDMS budgets. We look forward to working with NSF and the community to pursue novel funding opportunities to help promote these efforts in the future.

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#### Appendix 2. Workshop Agenda

#### April 25 – Day 1 (Wednesday)

- 7:30 Shuttle Leaves Millennium Hotel
- 7:45–8:30 Registration / Breakfast (provided on site)
- 8:30–8:45 Intro/ Welcome (Mark Behn)

#### 8:45–10:15 Oral Session 1: *Big questions* (convener: Greg Tucker)

- Alison Duvall: From Earthquakes to Landscapes in the Cascadia Subduction Zone
- Katy Barnhart: *Testing landscape evolution models with natural and synthetic experiments*
- 10:15-10:30 Break
- 10:30–11:45 Breakout Session 1: Questions:
  - 1. What are the outstanding questions / grand challenges in understanding the linkages between surface process and long-term tectonics?
  - 2. What are the data needs required to address these questions?
  - 3. What are the modeling needs required to address these questions?
- 11:45–1:00 Lunch (box lunches provided)
- 1:00–1:30 Summary of Breakout Session 1
- 1:30–3:00 Oral Session 2a: *Time & Length Scales* (convener: Luc Lavier)
  - Jean-Arthur Olive: Feedbacks between brittle deformation and surface processes: Insights from extensional settings
  - Phaedra Upton: Coupling geodynamics and surface processes
- 3:00–3:30 Break
- 3:30–4:15 Oral Session 2b: *Time & Length Scales* (convener: Luc Lavier)
  - Jean Braun: Parameterizing Surface Processes and their Response to Tectonic and Climatic Forcing
- 4:15–6:00 Posters (snacks / beverages provided)
- 6:00 Shuttle leaves for Millennium Hotel
- 7:00 Shuttle leaves Millennium Hotel for conference dinner
- 7:30–9:30 Conference Dinner (St. Julien Hotel, Xanadu Ballroom, 900 Walnut St, Boulder)
- 9:30 Shuttle returns to Millennium Hotel

#### April 26 – Day 2 (Thursday)

- 7:45 Shuttle Leaves Millennium Hotel
- 8:00–8:30 Breakfast (provided on site)
- 8:30–10:00 Oral Session 3: *Implementation challenges* (convener: Thorsten Becker)
  - Brain Yanites: *Reconciling landscape models with reality: a spectrum of success*
  - Louis Moresi: *Quagmire Algorithms and a Toolbox for Parallel Surface Process Codes*
- 10:00-10:30 Break
- 10:30–11:45 Breakout Session 2:
  - 1. What are the challenges facing long-term tectonic models?
  - 2. What are the challenges facing surface process models?
  - 3. What are the key challenges in coupling long-term tectonic and surface process models?
- 11:45–1:00 Lunch (box lunches provided)
- 1:00–1:30 Summary of Breakout Session 2
- 1:30–3:00 Oral Session 4: *Numerical Techniques / Computational Challenges* (convener: Boris Kaus)
  - Mark Piper (CSDMS): Community cyberinfrastructure for modeling Earth-Surface processes
  - John Naliboff (CIG): *Methods, challenges and uncertainty in modeling tectonic processes*
- 3:00–3:30 Break
- 3:30–4:45 Round Table Discussion (convener: Louise Kellogg)
- 4:45–5:00 Concluding remarks
- 5:30 Shuttle to Millennium Hotel

Dinner on your own

#### April 27 – Day 3 (Friday)

9:00–12:00 Writing group convenes

#### Appendix 3. Summary of Breakout Sessions: Identifying the Scientific and Technical Opportunities

On each day of the conference, breakout groups discussed key questions, opportunities, and challenges, both for individual communities and across communities. In the first breakout session we posed the questions "What are the outstanding questions / grand challenges in understanding the linkages between surface process and long term tectonics? What are the data needs required to address these questions? What are the modeling needs required to address these questions?"

In the second breakout session we posed the questions "What are the challenges facing longterm tectonic models? What are the challenges facing surface process models? What are general challenges that both communities face? What are the key challenges in coupling long-term tectonic and surface process models?"

Below we provide a detailed summary of the breakout discussions beginning with challenges that face the individual communities and then moving into the broader challenges that span both communities.

#### Challenges facing the long-term tectonics modeling community

Validation & Verification: This includes comparing model results generated using different codes and different numerical methods, and comparing these results to observations and identifying meaningful metrics for these comparisons. This is especially important for better constraining the rheology used in long-term tectonics models, including the governing equations, the choice of model parameters, the numerical behavior, and metrics for model comparison. It is not always clear how this should be done and what observational data are required, and well constrained datasets are needed.

<u>Uncertainty</u>: Another challenge reported is the large uncertainty in both the material properties – in particular the rheology – and the initial conditions that are used as input parameters for long-term tectonic models. Inverse modeling can address how much these types of uncertainties influence the model predictions. However, inverse modeling requires heavy computational resources and more data.

<u>Mesh dependence of brittle deformation processes</u>: In models that incorporate brittle deformation processes, quantitative results such as the width and spacing of faults are related to the mesh resolution. Hence, either new descriptions of the physical mechanism of brittle failure or better numerical methods are required for robust model predictions. The community has started to address this problem, but many open questions remain.

<u>Modeling needs</u>: Both technical advancement and better documentation and support will improve current models. Better parallel scaling for models with higher resolution, particularly close to the surface, and stable multi-grid solvers for high viscosity contrasts are needed. Further, new software capabilities such as petrologic modeling, fluid/rock interactions and more physics-based models of hydrothermal processes are necessary.

## Challenges facing the surface process modeling community

<u>Validation & Verification</u>: Verifying and validating surface process models is challenging because there is no consensus on protocol and model results are compared with noisy field data. Further, there is no consensus on the appropriate physical processes to include in numerical

models, and often different processes can lead to the same solution. It is unknown whether a model validated for one region would or should work well for another similar region even if the two regions are quantifiably similar. Participants pondered potential solutions. Employing adjoint gradient or homogenization methods would help better quantify model sensitivity to parameters. Calibration of a model against only one constraint, such as topography, should be avoided. Other data, such as stratigraphic records, can provide information on temporal variation in surface processes and environmental conditions that influence them.

<u>Uncertainty</u>: The surface process community needs to formulate best practices for incorporating uncertainties in material properties and parameters in sediment transport and incision equations. Equifinality, a state in which different models produce the same results, also needs to be addressed. Although useful in many cases, empirical tuning of a parameter, into which multiple complex processes are lumped, makes uncertainty handling difficult. Great uncertainty is also involved in constraining initial conditions and past forcings (e.g., paleoelevation and paleoclimate).

<u>Improving model physics</u>: Improved physics of surface processes as well as their interactions with climate and ocean is desired. A better mechanistic understanding of river incision at the grain scale would allow for quantification of parameters in incision equations. Improved physics should be distilled in the form of better-defined governing equations that can be implemented in models. Incorporating climate or weather variability is desirable but if models become too complicated with non-essential components they will not be practical. Similar to the practice in climate modeling, ensemble models may be useful for surface processes. Coupling with ocean models might be fruitful because three quarters of the Earth's surface is underwater and we should learn how submarine surfaces get shaped.

## General challenges faced by both modeling communities

<u>Degree of complexity:</u> Both communities find choosing model complexity to be a major challenge that depends on the modeling problem. Recurring questions were:

- How much detail and complexity should be incorporated in models, and can we quantify what we learn from added complexity?
- What degree of complexity is required to produce predictions?
- How much averaging between different scales is appropriate? How does it affect results?
- Which part of the parameter space should be explored, and how do we determine the relevant parameters?

<u>Modeling across scales</u>: Models in both communities span a wide range of time and length scales, and processes are linked across different scales. Modelers must determine what temporal and spatial scales are important for which physical processes, reconcile processes and rates that may vary between scales, and upscale/downscale certain forcings. For the long-term tectonics community, one example is the link between long-term lithospheric deformation and earthquakes, which is not well understood. Modeling this kind of coupling also necessitates transient formulations opposed to the stationary formulations of the Stokes equations that is used in many model. The landscape evolution community faces similar problems. For example, how can we scale up nearly instantaneous processes like landslides over thousands to millions of years.

<u>Reconciling spatial and temporal scales</u>: Linking surface and tectonic models requires a better understanding of how the coupling is achieved over different spatial and temporal scales. In particular, it is not clear how to reconcile the different time and length scales over which seismic (seconds–minutes), tectonic (kyr–Myr) and surface processes (seconds–Myr) act. For this, it is necessary to think in terms of processes, data and models. Participants agreed that it is crucial to identify which processes are going to have the greatest effect at various scales. Identifying the primary and secondary drivers in a given system is a first step in this direction. This will help to constrain which small scale processes influence large scale processes, and vice versa. At this point, participants identified a number of outstanding questions to be addressed such as: Is plate tectonics impacted by surface processes and the other way around? Are there scales at which surface processes impact tectonics more so than others? (e.g. Is the signal/influence of surface processes more apparent when consider local fault evolution than when considering large scale wedge dynamics?) How do sediment fluxes influence subduction dynamics and topographic uplift? How do earthquake cycles interact with surface processes? Is tectonics sensitive to climate? (i.e. coupling climate, tectonics and surface processes).

Knowledge transfer of processes occurs across scales. This translates into extrapolating understanding of the physics of specific surface processes to large scale long-term tectonic and surface processes, and vice versa. A better understanding of this scaling would inform the necessary complexity level of models, the relevant resolutions, and how to parameterize processes. How processes interact across scales impacts boundary conditions, initial conditions, and coupling. For example, when looking at the interaction of surface processes and tectonic uplift, should we model uplifted topography as initial conditions, or is it better to couple evolution of uplift with surface processes? What are the costs in each approach? This discussion, also included the distinction between transient and steady-state scenarios. It is unclear to what extent an event-based/stochastic approach is necessary (e.g. storms and discrete earthquakes) and when more continuous processes be assumed. Data and models must be integrated across scales. Both observations and models are important in deciphering the underlying physics, but deciding the necessary resolutions is challenging. There is often a discrepancy between the resolution of available data and that needed for modeling.

<u>Community building: software accessibility, training and infrastructure</u>: Information exchange is a challenge. This encompasses the training of students and new members of the community, access to state-of-the art modeling software and support, and good documentation of existing software packages and methods. Sharing of software requires access to the code and also training. This is made more difficult because there are many geodynamic and surface evolution software packages, each covering different processes or environments and with their own steep learning curve. Universities often do not have the personnel to offer geodynamic or surface evolution modeling courses. This makes entry into the community difficult.

Ideally, users should learn both the methods and application of the software. This includes how numerical methods and algorithms work and how to develop them. Users must also know how to set up a model and use the code for applications. To facilitate the use of software packages, there is a need to make them more accessible and user-friendly by designing clear interfaces, providing extensive documentation and step-by-step guides for building and using a model. Part of this challenge could be addressed by cross-disciplinary workshops with classes and projects where model development and use are taught. Community organizations like CIG, CSDMS, and CIDER (Cooperative Institute for Dynamic Earth Research, <u>http://www.deep-</u>

<u>earth.org/</u>) already do some training, but there is need beyond what these organizations are currently funded to do.

Another community need is the infrastructure to run large-scale 3D computations, and to store their output so that it can be shared with the community (for example in form of a model repository). As big computing facilities become more and more common, simpler ways to discover and access them should be created.

#### What are the key challenges in coupling long-term tectonic and surface process models?

<u>Degree of complexity</u>: Many of the challenges that the individual communities face are amplified in the context of coupling tectonic and surface evolution models, such as desired degree of complexity. For coupled models this means establishing the appropriate process coupling for each application and scientific question. Questions to address include what are the temporal and spatial scales of meaningful interactions, and what up/downscaling of different processes are required?

<u>Numerical challenges</u>: Evaluating the robustness, stability and accuracy of a coupled model is more challenging than for an individual model. Different numerical methods are used in different parts of the model, each with its own dependency on resolution. This is particularly important to consider because a coupled model might use more than one grid and interpolate between different resolutions. Moreover, it demands the design of new benchmark problems that can be used to verify the correctness of the implemented coupling.

Model setup must be consistent between the tectonic and landscape evolution models, such as consistent initial and boundary conditions. Choosing material properties consistently seems particularly challenging, and requires linking the parameters used in the surface evolution model (e.g., erodibility) to those in the tectonic model. Moreover, validating coupled models is more difficult, as there are more processes and more input parameters affecting the outcome.

Another key point is the performance of coupled models. Both surface evolution models and tectonic models have to cover a large spatial domain using a reasonably high resolution. Hence, both models need to be parallelized and run on a distributed system. While this is common practice for state-of-the-art geodynamic codes, the surface evolution community has only begun to address this problem.

<u>Technical challenge of the model interface</u>: In addition to that, the community identified other challenges related to the coupling itself and the interface that should be used to communicate between tectonic and surface evolution codes. Key design challenges for the interface include:

- What physical properties should be exchanged between models, and how are they defined in the different communities?
- How can different material properties and heterogeneities be related for the exchange of data (for example, how can strain and rock damage be translated to erodibility at the surface)?
- How does communication between the models work?
- How does the interface deal with different meshes and data structures?
- How should the time step be chosen?

<u>Social challenges</u>: The workshop participants also identified the need to improve the communication between the different communities, particularly regarding the needs, knowns and unknowns of each community. This includes exchanging information about numerical methods, model results and limitations, and the need to find scientific questions that motivate both communities. These questions can then be used to assess which models to couple and how. Better communication of algorithms, negative models results, general lessons learned from modeling studies, and model limitations and uncertainties is needed to facilitate the understanding and reuse of these models across disciplines.

## What are the data needs required by the two communities?

<u>Coupling data with models</u>: New observations and techniques often motivate and inspire new modeling. Similarly, modeling results can identify key data gaps needed to answer big questions. Deliberate efforts to ensure that modeling and data scientists work together will advance scientific progress on all fronts. There was general enthusiasm for focusing on data collection in field areas that are of interest to both communities. These field areas would represent controlled experiments, or locations where the impacts of different forcings or material properties could be isolated. No specific site was identified, although the idea that it should involve source-to-sink was appealing. Outstanding data/model coupling questions include:

- How can we use observations to decipher underlying physics?
- Is non-unique interpretation of data inevitable? If so, how much does it matter?
- What data should be collected and at what scale?
- How do rock rheology and material properties regulate couplings?

Generally, there was a desire for data on paleotopography, paleoclimate, paleotectonics, and paleo-erosion rates. Specific desired datasets include:

- High resolution 3D maps of lithology, including rock properties beyond lithology, such as fracture spacing, grain-scale properties, and rock strength.
- Increased LiDAR coverage in tectonically active areas.
- Sediment cores from depositional areas.
- More data on fault populations and stress states in the upper crust.
- Material properties and rock rheology are important for both tectonic and surface processes, and represent a potential bridge between these two fields.
- Experimental data from physical models.

Just as the science questions cross spatial and temporal scales, so too do the data needed to support modeling efforts. One example is data crossing time scales, such as erosion rates averaged over different time scales. These data are critical for modeling efforts from both directions, yet there are gaps in the times scales that different chronometers can measure, such as exhumation rates measured by thermochronology and erosion rates measured from cosmogenic radionuclides. Even when data exist across different scales, there are challenges for incorporating them into a single study. For example, data measured over longer time scales are lower resolution and data measured over shorter durations are often higher resolution.

<u>Community and technical challenges</u>: Data need to be accessible and understandable. Standards for metadata and data formatting are desired, along with common data storage areas and open data. Making raw data available is essential because data processing methods will change over. Ideally disparate datasets would be combined in a common GIS/3d framework for visualization. Handling big data will also be a challenge and machine learning algorithms that help generate large synthesis datasets could be helpful.