A community plan towards reproducible simulations of complex lithospheric dynamics

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Over the past decade, the computational lithospheric dynamics community has made significant technical progress in its ability to simulate a wide range of long-term tectonic processes, including rifting, subduction, and intra-continental tectonics. In particular, multiple open source lithospheric dynamics codes can now efficiently utilize high-performance computing resources and run high-resolution 3D simulations across 10^3-10^4 processors. Furthermore, recent advances in simulating two-phase fluid transport, coupling to landscape evolution algorithms, and integration with inverse and adjoint methods have provided new pathways to investigate complex geologic processes, thus obtaining insights into nonlinear feedbacks between processes acting across different scales.

However, significant challenges still remain in simulating complex lithospheric dynamics in a scalable and reproducible manner. Simulations incorporating plasticity suffer from mesh-dependent localization behavior and in many cases exhibit extremely poor nonlinear convergence behavior. In the ductile domain, different formulations for grain size evolution may lead to significantly varying deformation patterns within shear zones and may also pose difficulties for nonlinear solvers. Two-phase flow fluid transport also poses significant challenges for non-linear solvers, and when used in combination with plasticity (i.e., hydrofracturing), produces even further challenges that require multiple stabilization methods. From a thermodynamics point of view, compressible formulations are necessary to properly capture phase transitions within the lithosphere, but to date few such algorithms have been tested for realistic applications. Similarly, the proper simulation of the interaction between fluids (melt, volatiles) and rocks requires either defining simple analytical expressions for these reactions or coupling in an efficient fashion to an external thermodynamics code. Compounding these technical challenges is the question of what geologic and geophysical observations should be used for validating complex and highly nonlinear models.

While daunting, we believe many of these challenges can be overcome through a targeted series of activities in CIG IV focussing on (1) new community numerical benchmarking efforts, and (2) close collaboration with the observational and experimental lithospheric dynamics communities towards a series of investigations that center on specific geologic and geophysical data sets and locations. The benchmarking efforts will be critical to learn where codes perform differently and ensure that all codes using such features as nonlinear plasticity, coupled two-phase flow, rate-state friction, and compressible deformation are able to approximately reach the same results for a given problem. While highly technical, we note that in the last 2-3 years new methods have been proposed for implementing these features that remove any mesh dependency and achieve stable convergence behavior. In parallel, the outcomes of the 2020 CIG Tectonics Workshop will be used to define one or more targeted field sites and associated data sets, such as the New Zealand Alpine Fault or the Insubric Line in the European Alps, and to initiate cross-disciplinary modeling and physics validation efforts across distinct lithospheric domains. The validation efforts will utilize a range of forward and inversion approaches, including recently developed methods for performing geodynamic inversions. Combined, these two parallel approaches will provide the lithospheric dynamics community with a new suite of robust and reproducible methods for simulating nonlinear multiphysics processes, which have been explicitly tested against specific geologic and geophysical data sets.

To accomplish these goals and maximize the impact across the lithospheric dynamics communities, we propose a series of alternating virtual and hybrid workshops for benchmarking and targeted collaborations with the observational and experimental lithospheric dynamics communities. These workshops will serve as platforms for both review of yearly efforts, planning of new activities, and disseminating the working groups findings across the broader community. To ensure progress, resources should be allocated to coordinate between different research groups, design benchmarks, and test new algorithms that can be implemented by other codes.