Computational Frameworks enabling multi-scale multi-physics models

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Abstract

In computational models, there is an increasing need for coupling: ranging from coupling at the equation level, to tensor-level coupling and field coupling. Coupling can occur either on model boundaries, or throughout the model. Traditionally, such coupling has been done on an ad-hoc basis, and coupling of traditional computational codes can be so difficult as to require almost complete rewriting of the codes to facilitate coupling. The computational codes we have developed for ACCESS and CIG, such as Snac and Snark, were developed with coupling in mind, and as we have evolved these codes, the support for coupling has gradually improved and become both simpler and yet more powerful. This paper will present our experiences in coupling models and equations within the StGermain Framework, and the lessons we have learned from implementing such coupling.

Keywords: Model Coupling; Multi-scale; Multi-physics; Frameworks

Introduction

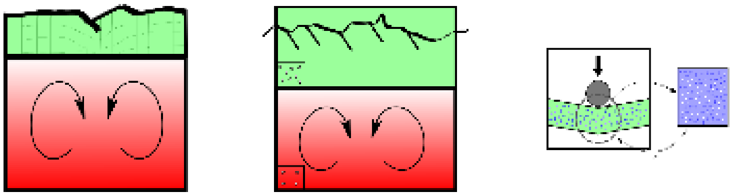
Contemporary research funding has a significant focus on facilitating e-Research. This entails enabling geoscientists to access vast amounts of data located anywhere around the world. It entails enabling geophysicists to utilise vast amounts of computational cycles, also, located anywhere around the world. An often overlooked, but equally relevant facet is that e-Research is enabling modellers to construct increasingly complicated simulations, through the guided application of software "best practices". All three facets are a producer of, and a consumer of masses of data in the Earth sciences.

Our group is primarily focussed on the latter facet of e-Research. That is, facilitating the construction of higher fidelity, more sophisticated computational models of phenomena. In terms of geodynamics, this focus includes the Snark and SPModel projects of the ACcESS MNRF, a consortium focussed on providing Australia with a common resource for geodynamics modelling. We also partake in the e-Research facilitation of CIG, a recently established equivalent organisation within the United States, and its precursor – GeoFramework, through the Snac project.

The evolution of the three software projects, Snark, SPModel and Snac is instructive. They all began with the scientifically modest goals of creating parallel, 3D versions of existing codes of well-established phenomena (mantle convection, erosion, and crustal deformation respectively). However the natural evolution of models, facilitated by effectively applied software engineering, has pushed the focus to multi-phenomena problems, entailing multi-scale, multi-physics capabilities. This includes refining the fidelity of existing phenomena models, as well as encapsulating the effects of two or more phenomena within the one model. Some examples are:

1. Lithospheric to mantle models
2. Embedding high-resolution regional models within low-resolution global models (e.g., mantle plumes within a global mantle wind model)
3. Coupled advection/diffusion models (e.g., magma melt)
4. Surface process to Lithospheric models

Naively, one might imagine that coupling two exiting codes together ("code-coupling") is a simple problem of feeding the output of one code as input into another. However, in general, coupling is far more difficult than this, and is complicated by differences in time and length scales, assumptions in the constitutive models and numerics utilised. Rather, the choice in coupling regime for a multi-phenomena problem is a function of constraints implied by each phenomenon model. Some models are sensitive to numerical error, some require accurate interface tracking, some are biased for execution speed, and so on. For example, one model may best suit, and hence be implemented by an explicit Lagrangian approach (e.g. a Lithospheric code), but its coupling counterpart may be implicit Eulerian implementation (e.g. a mantle code). In this case, neither code suits the counterpart's numerics. Hence field coupling across the two existing codes may be best. But this is not always the case.



Representative diagrams of the three styles of multi-scale, multiphysics coupling discussed.

There are Lithospheric phenomena that also suit an implicit Eulerian implementation, and in this case, the discretisation is not incompatible with the mantle convection's implementation. Consequently equation coupling can be used. That is, both phenomena are modelled in the same code on the same domain. The issue then becomes implementing the different material physics and tuned numerical methods for the both regions respectively. Another example is where one phenomenon is individually modelled at two different scales. For example, where the constitutive update of a given region of interest in the larger scale is actually resolved by modelling that same region in a separate representative domain with physics and numerics relevant to that scale (fine model in coarse model).

Software frameworks can help reduce the time, cost and effort in developing applications. StGermain is the foundation of a layered framework targeted at creating computational codes. This covers numerical, physics and computational sciences by providing people within these disciplines a common framework, and hence a medium for collaborative development. This same infrastructure provides a means to facilitate the coupling regimes described above. The result is an evolution in the ability to model real world phenomena, bringing us closer to modelling problems of real world relevance. We will discuss our experiences in enabling multi-scale, multi-physics modelling through this framework.

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