Automating forward and adjoint coupling in finite element geoscience simulations

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This project will extend the capabilities of the Firedrake and dolfin-adjoint model generation system from single domain modelling to coupled models. This will deliver into the hands of working geoscientists the practical capability to create models of coupled processes which would hitherto have been too mathematically complex, too slow to execute, or too expensive to code using existing technology.

The need to conduct simulations of continuous systems described by partial differential equations (PDEs) pervades geoscience. Whether the domain is ocean, atmosphere, cryosphere, lithosphere, ground water, or flooding; the core physical processes of geoscience are continuous mechanical systems modelled by PDEs. However, none of these systems operate in isolation. It is the interaction of processes which characterises the natural world and our interaction with it. Ocean and atmosphere exchange momentum, temperature and salinity; ocean and ice move each other and exchange water and heat; rivers move sediment which in turn alters their course. Even the shape of the Geoid is the consequence of a tight coupling between ice sheets, solid earth deformation and sea level. Coupled modelling is therefore a core geoscience requirement.

The current hand-tooled approach to simulation software development depressingly often results in PhD students and post-docs spending much or most of their time coding and debugging known methods, at the expense of time to conduct new science. For the simulation of coupled systems, the combined complexity of multiple models and their combination often makes development infeasible for most researchers. As is the case across the economy, the key to increasing productivity is to automate laborious, technical, and error prone tasks. In this project, the creation of coupled modelling software from the equations describing the physical system will be automated.

Automated model generation enables scientists to write high-level code which is very close to the mathematical description of a model system that they would write on paper. The high-performance parallel implementation of this is then generated automatically by a specialist simulation-aware compiler. This enables the scientist to write maths, and get simulation. Changing the equations, numerics, or solvers requires a few lines of code, so the scientist can experiment to achieve the best results. This revolutionary new approach to model development is available for single process geoscientific models through the Firedrake project, which has already been taken up at over 30 institutions around the world. This project is a response to demand from geoscientific modellers for an equally high productivity way of creating high performance models of coupled systems.

Many of the critical questions in the geosciences are so-called inverse problems. Here instead of asking a "what happens if" question, the scientist asks a "what causes this" question. Examples of inverse problems include inferring the cause of phenomena, and matching model systems to real data. A key tool in inverse modelling is a so-called adjoint model. This runs backwards in time to discover what inputs influence the model outputs. Creating a backward running version of a complex computer code is exceptionally difficult and typically runs slowly. However the automated code generation approach also extends to this scenario via the dolfin-adjoint system. By ensuring the new technology created here is dolfin-adjoint compatible, we will create a completely unique automatic way to solve inverse coupled problems. This will enable geoscientists to solve this class of problems in circumstances where this is currently infeasible or too computationally expensive.