J. David Moulton

Multiphysics Frameworks and Scalable Solvers for Environmental Applications

Applied Mathematics and Plasma Physics
Los Alamos National Laboratory
Los Alamos
NM 87545
moulton@lanl.gov
Ethan Coon
Gianmarco Manzini
Markus Berndt
Rao Garimella
Konstantin Lipnikov
Scott Painter

Modeling and simulation are playing an increasingly critical role in understanding and predicting climate impacts and feedbacks in terrestrial systems. Managing the complexity of these process-rich integrated hydrologic and biogeochemical models requires flexible software designs that enable exploration of model features and model coupling. In addition, flexibility in meshing and robust discretization techniques are required to capture topographic features, such as hill slopes and rivers, and suburface stratigraphy. This combination of process-rich applications with advanced discretizations creates significant challenges for efficient solvers, and efficient time-evolution.

In this talk we highlight a flexible and extensible approach to multiphysics frameworks for these applications that specifies interfaces for coupled processes, automates weak coupling and supports strong coupling strategies to manage this complexity. We use a prototype implementation this multiphysics framework, dubbed Arcos, to support both model and algorithm development for environmental applications in the open-source codes Amanzi and the Arctic Terrestrial Simulator (ATS). Amanzi provides infrastructure for general unstructured polyhedral meshing with a flexible operator-based implementation of the Mimetic Finite Difference method as well as two-point flux Finite Volume method. Amanzi is used for subsurface flow and reactive transport, while ATS includes capabilities for coupled non-isothermal surface/subsurface flow.

Here we examine the increasingly important problem of coupled surface/subsurface flow where we use a diffusive wave approximation for surface flow, and a Richards equation for subsurface flow as a testbed for discretizations and solvers. In both equations, the coefficients of the div/grad operator are strongly nonlinear, and the surface and subsurface flows are strongly coupled. The challenges of designing a preconditioner for Krylov-based nonlinear solvers with first-order backward Euler time discretization are discussed. For example, upwinding of the nonlinear coefficient is required to evolve the system efficiently, but breaks the symmetry of the operator on general meshes. Furthermore, as the ponded height of the surface water goes to zero (e.g., water runs off or infiltrates into the subsurface) the nonlinear coefficient goes to zero, making standard formulations that involve its inverse invalid. Finally, the system is strongly coupled through continuity of both pressure and flux at the surface/subsurface interface, and adaptive time-stepping is required to evolve the system efficiently. We discuss the performance of the nonlinear and multilevel linear solvers (e.g., Hypre BOOMERAMG), on this fully coupled system at various times in the simulation, and the hueristics used to control the dynamic time-step. We show results for several benchmark problems, as well as physically relevant, large-scale simulation of rainfall on arctic tundra based upon LIDAR data from Barrow, Alaska.