GEOS: A performance portable multi-physics simulation framework for subsurface applications

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Summary

GEOS is a simulation framework focused on solving tightly coupled multi-physics problems with an initial emphasis on subsurface reservoir applications. Currently, GEOS supports capabilities for studying carbon sequestration, geothermal energy, hydrogen storage, and related subsurface applications. The unique aspect of GEOS that differentiates it from existing reservoir simulators is the ability to simulate tightly coupled compositional flow, poromechanics, fault slip, fracture propagation, and thermal effects, etc. Extensive documentation is available on the GEOS documentation pages (*GEOS Documentation*, 2024). Note that GEOS, as presented here, is a complete rewrite of the previous incarnation of the GEOS referred to in (Settgast et al., 2017).

Statement of need

The threat of climate change has resulted in an increased focus on mitigating carbon emissions into the atmosphere. Carbon Capture and Storage (CCS) of CO_2 in subsurface reservoirs and saline aquifers is an important component in the strategy to meet global climate goals. Given the 2050 net-zero emissions goals, CO_2 storage capacities required to offset emissions is orders of magnitude greater than current levels (Intergovernmental Panel on Climate Change IPCC, 2023). Evaluation of reservoir performance and containment risks associated with the injection of liquefied CO_2 in the subsurface in a reproducible and transparent manner is an important consideration when evaluating new storage sites. As an example of typical complexities in carbon storage reservoirs, the 11th Society of Petroleum Engineers Comparative Solution

Project (SPE11) ([Nordbotten et al., 2024](#)) provides a benchmark example for evaluating the the predictions of carbon storage simulators. The goal of GEOS is to provide the global community with an exascale capable open-source tool that is capable of simulating the complex coupled physics that occurs when liquefied CO_2 is injected into a subsurface reservoir. To this end, GEOS is freely available and focused on the simulation of reservoir integrity through various failure mechanisms such as caprock failure, fault leakage, and wellbore failure. Open source projects such as OPM ([Rasmussen et al., 2021](#)), OpenGeoSys ([Naumov et al., 2024](#)), DuMux ([Koch et al., 2020](#)) and Darts ([Voskov et al., 2024](#)) are example efforts that share similar objectives. However, GEOS stands out in two key areas: the explicit fault modeling coupled with flow and mechanical deformation, and the focus on performance portability on platforms ranging from workstations to exascale supercomputers.

GEOS Components

The core C++17 infrastructure provides common computer science capabilities typically required for solving differential equations using a spatially discrete method. The components of the infrastructure provided by GEOS include a data hierarchy, a discrete mesh data structure, a mesh-based MPI communications interface, degree-of-freedom management, IO services, and a physics package interface.

By design, GEOS is intended to be a generic multi-physics simulation platform. The physics package interface in GEOS is intended to encapsulate the development of numerical methods applied to the solution of governing equations relevant to a problem. When implementing a physics package for a set of coupled physics equations, each individual physics package is first developed as a stand-alone capability. The single physics capabilities are then applied together in a coupled physics package and solved through a flexible strategy ranging from solving the fully monolithic system to a split operator approach.

To solve the linear systems that arise from the boundary value problem, GEOS maintains a generic linear algebra interface (LAI) capable of wrapping various linear algebra packages such as hypre ([Falgout & Yang, 2002](#)), PETSc ([Balay et al., 2024](#)), and Trilinos ([Heroux et al., 2005](#)). Currently, in GEOS only the hypre interface is actively maintained. For every multi-physics problem involving the solution of a coupled linear system, GEOS currently relies on a multigrid reduction preconditioning strategy available in hypre ([Bui et al., 2020](#), [2021](#)).

The performance portability strategy utilized by GEOS applies LLNL's suite of portability tools RAJA ([David A. Beckingsale et al., 2019](#)), CHAI ([CHAI, 2023](#)), and Umpire ([D. A. Beckingsale et al., 2020](#)). The RAJA performance portability layer provides [performance portable](#) kernel launching and wrappers for reductions, atomics, and local/shared memory to achieve performance on both CPU and GPU hardware. The combination of CHAI/Umpire provides memory motion management for platforms with heterogeneous memory spaces (i.e., host and device memory). Through this strategy, GEOS has been successfully run on platforms ranging from GPU-based Exa-scale systems to CPU-based laptops with near-optimal of performance.

In addition to its C++ core, the GEOS project provides a Python3 interface that allows for the integration of the simulation capabilities into complex Python workflows involving components unrelated to GEOS.

Applications

To date GEOS has been used to simulate problems relevant to CO_2 storage, enhanced geothermal systems, hydrogen storage, and both conventional and unconventional oil and gas extraction. Often these simulations involve coupling between compositional multiphase flow and transport, poroelasticity, thermal transport, and interactions with faults and fractures.

As an example of a field case where GEOS has been applied, we present a coupled compositional flow/mechanics simulation of CO_2 injection and storage at a large real-world storage site. Figure 1a illustrates the computational mesh and Figure 1b shows results after 25 years of injection. Simulations such as this will play a critical role in predicting the viability of potential CO_2 storage sites.
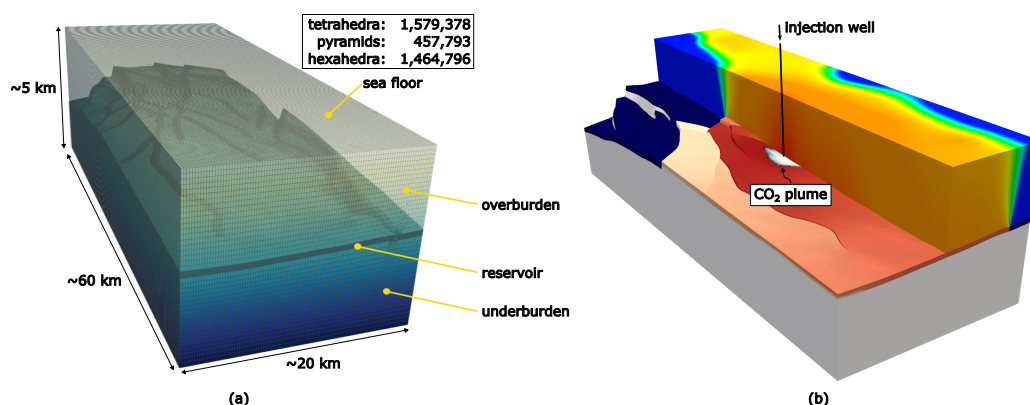

tetrahedra:	1,579,378
pyramids:	457,793
hexahedra:	1,464,796

Figure 1: Real world CO_2 storage site: (a) discrete mesh, transparency is used for the overburden region to reveal the complex faulted structure of the storage reservoir; (b) results of a compositional flow simulation after 25 years of CO_2 injection. The CO_2 plume is shown in white near the bottom of the well. Colors in the reservoir layer indicate changes in fluid pressure, and the colors in the overburden indicate vertical displacement resulting from the injection. Note that color scales have been removed intentionally.

As an example of the weak scalability of GEOS on an exascale class system, we present two weak scaling studies on a simple wellbore geometry run on the Frontier supercomputer at Oak Ridge National Laboratory. Frontier is comprised of 9,472 Cray EX235a nodes that each contain a single AMD EPYC 7A53 CPU and four AMD MI250X GPUs (Atchley et al., 2023). Note that each MI250X is comprised of two Graphics Compute Dies (GCD), with each GCD appearing as a GPU to the operating system. A more detailed discussion and instructions to reproduce the results are available in the Performance Benchmarks of the GEOS documentation.

The weak scaling results for mechanics are presented in (Figure 2a) and shows nearly flat scaling of the GEOS processes (assembly/field synchronization) up to 32,768 GPUs (81.3×10^9 degrees-of-freedom). There is a moderate decrease in efficiency with the application of the hypre preconditioner setup and solve, but given the complexity of those algorithms, this level of scaling efficiency is excellent. The weak scaling results of compositional flow are presented in Figure 2b shows excellent scaling up to 2,048 GPUs.
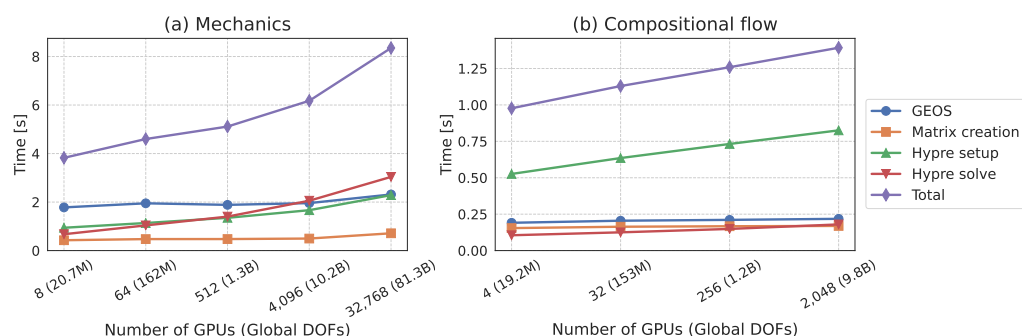

Figure 2: Weak scaling results on ORNL/Frontier: average execution time per newton iteration vs number of GPUs for a mechanics (a) and a compositional flow (b) simulation, respectively.

Acknowledgements

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