Contribution ID: **1088**   Type: **Poster Presentation**

Alquimia: A generic interface to biogeochemical codes

Wednesday, 24 May 2023 16:10 (1h 30m)

Multicomponent reactive transport codes couple biogeochemical models with solvers for flow and transport and other relevant processes. Many of these codes are the legacy of years of development and research, over which model complexity has increased incrementally. Often the complexity of implementing a comprehensive and flexible treatment of biogeochemistry is a significant obstacle to the development of new biogeochemical capabilities. As a result, this step is often circumvented by coupling flow and transport codes to existing biogeochemical codes. However, this is typically done as a one-off to a specific code. In this poster presentation, Alquimia, an open-source software library is introduced that provides a generic interface to existing biogeochemical capabilities. This software is intended to facilitate interoperable code development by exposing tried-and-true biogeochemical capabilities in existing software. To exemplify its use, the geochemical capabilities in the open-source reactive transport codes PFLOTRAN and CrunchFlow are made available via Alquimia's generic interface. This interface is then used to add geochemical capabilities to Amanzi and ParFlow. We show that because Alquimia allows for different geochemical codes to share flow and transport solver, and therefore the same spatial discretization, time stepping control, and coupling schemes, it may be a useful tool for benchmarking. We also present examples of how Alquimia has enabled incorporation of geochemical capabilities to codes for a range of applications.

Participation

In-Person

References

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Session Classification: Poster

Track Classification: (MS08) Mixing, dispersion and reaction processes across scales in heterogeneous and fractured media