

Alquimia: an application programming interface for geochemical codes- Development and application

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The fate of reactive solutes in the subsurface is the result of the coupling between physical processes and complex reaction networks. Capabilities available in geochemical codes reflect this complexity, typically including a wide range of homogeneous and heterogeneous reactions, under kinetic and equilibrium assumptions. For convenience, implementation of new geochemical capabilities into flow and transport codes is often circumvented by coupling them to existing reaction codes. While these couplings have been successfully accomplished on a case by case basis, a systematic way to carry them out may improve efficiency and facilitate code maintenance. Further, interoperability can make it possible to access a range of capabilities not available in legacy codes.

In this contribution, we will introduce Alquimia, a biogeochemistry API and wrapper library that provides a unified interface to the biogeochemistry routines from geochemical codes. Alquimia has two parts: (1) an engine-independent application programming interface (API) consisting of function call signatures and data structures and (2) an optional utility library. The API works by enforcing a signature for geochemical subroutines using a single cell model. Required parts of the API include function call signatures, data structures and constants. Development of Alquimia adheres to a set of practices that ensure software quality and enable interoperability between components [1]. Among others, this implies that Alquimia uses a CMake-based build system, provides a comprehensive test suite, provides a documented, reliable way to contact the development team, and has an accessible repository.

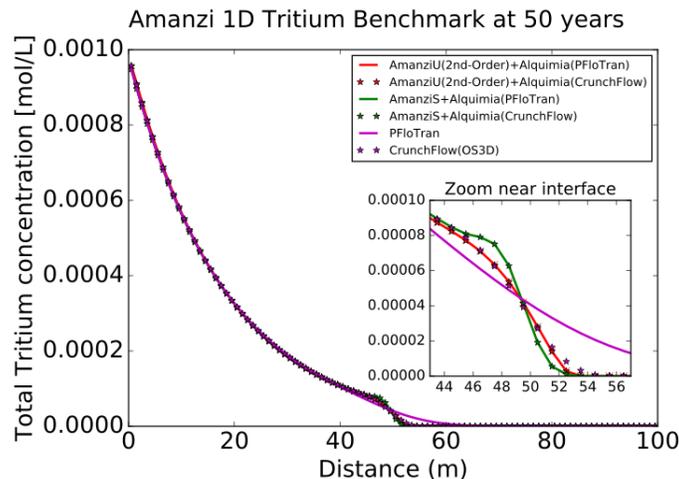


Figure 1: Comparison of results for a simple 1D, first-order decay reactive transport benchmark

We demonstrate the development by describing the implementation of interfaces to the geochemical capabilities of two widely used reactive transport codes, PFLOTRAN [2] and CrunchFlow [3]. Next, we demonstrate its use in the addition of geochemical capabilities to a newly developed flow and transport simulator, Amanzi [4]. Amanzi is a multi-process high performance computing (HPC) simulator that provides a flexible and extensible simulation capability, in which unstructured and structured mesh approaches are available in a single code base. While the ability to select between unstructured and structured meshes is powerful and the use of external packages facilitates development, this approach poses some challenges to code structure and design. The single-cell coupling implemented in Alquimia provided a suitable software solution.

Once implemented in the code base, Alquimia allows for the selection of geochemical engine at runtime via the input file. Because in Amanzi different discretization methods are also available from the input file, several simulations can be carried out for different combinations of discretizations and geochemical engines (*Figure 1*). Comparison of results between the different runs shows that interoperable approaches such as the one made possible by Alquimia may also be a useful tool for benchmarking.

References

- [1] Bartlett, R., Demeshko, I., Gamblin, T., Hammond, G., Heroux, M. A., Johnson, J., ... Yang, U. M. (2017). xSDK Foundations: Toward an Extreme-scale Scientific Software Development Kit. *Supercomputing Frontiers and Innovations*, 4(1), 69–82. <https://doi.org/10.14529/jsfi170104>
- [2] Lichtner, P. C., Hammond, G. E., Lu, C., Karra, S., Bisht, G., Andre, B., ... Frederick, J. M. (2017). *PFLOTRAN Web page*.
- [3] Steefel, C. I., Appelo, C. a. J., Arora, B., Jacques, D., Kalbacher, T., Kolditz, O., ... Yeh, G. T. (2014). Reactive transport codes for subsurface environmental simulation. *Computational Geosciences*, 19(3), 445–478. <https://doi.org/10.1007/s10596-014-9443-x>
- [4] *Amanzi: Amanzi primary repository*. (2017). C++, Amanzi. <https://github.com/amanzi/amanzi>