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2D simulations of Uranium diffusion in clay: geochemical surrogate models and accelerated coupled reactive transport simulations with POET

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The computational burden associated with coupled reactive transport simulations limits their application coarse models and thus to oversimplified geological and geochemical features, with obvious repercussions on uncertainty and safety assessment of nuclear waste disposal facilities. Techniques from approximated computing can however be leveraged to accelerate simulations of large-scale, heterogeneous domains. These include both surrogate models based on machine learning and artificial intelligence (ML/AI) to replace more costly numerical geochemical simulators, and algorithmic improvements such as interpolation from previously computed geochemical simulations stored and indexed in efficient data structures such as Distributed Hash Tables during coupled simulations. In this contribution we demonstrate recent advancements in physics-based geochemical surrogates achieved within the ML-Benchmark initiative from the DONUT/EURAD project for Uranium diffusion in clay subject to exchange and sorption. Furthermore, the algorithm implemented in the reactive transport simulator POET [1] based on automatic clustering of multivariate data and subsequent interpolation enables the simulation of large-scale, heterogeneous reactive transport scenarios on uniform grids of magnitude of million grid elements at reduced computational costs.

[1] Marco De Lucia, Michael Kühn, Alexander Lindemann, Max Lübke, and Bettina Schnor, 2021: POET (v0.1): speedup of many-core parallel
reactive transport simulations with fast DHT lookups, Geoscientific Model Development, 14, 7391--7409. https://doi.org/10.5194/gmd-14-7391-2021