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Combining machine learning and equation based models in reactive transport: POET

MARCO DE LUCIA[1], MICHAEL KÜHN[1,2], MAX LÜBKE[1] AND BETTINA SCHNOR[2]

[1]GFZ German Research Centre for Geosciences
[2]University of Potsdam
Presenting Author: delucia@gfz-potsdam.de

The reduction of the computational cost of reactive transport simulations is paramount to ensure wide adoption of this class of models without recurring to supercomputing facilities, which may be difficult to access for geoscientists. Such a goal can be achieved by means of approximated computing, including the use of surrogate models based on machine learning and artificial intelligence (ML/AI), but also by adapting the simulators to heterogeneous computing environments and especially to hardware accelerators such as GPUs (Graphical Processing Units) and FPGAs (Field Programmable Gate Array). In this contribution we describe the recent and ongoing developments of POET [1], which originates from the cooperation between geoscientists and computer scientists and which combines classical numerics, AI methods and state of the art algorithmic improvements such as lookup from fast Distributed Hash Tables. It is therefore an ideal environment to test novel approximated methods. Achieved improvements and the future roadmap are demonstrated in application of subsurface nuclear waste disposal.

[1] De Lucia, Kühn, Lindemann, Lübke & Schnor (2021), *Geoscientific Model Development*, 14, 7391--7409.