EGU2020-1631
https://doi.org/10.5194/egusphere-egu2020-1631
EGU General Assembly 2020

Chemical speciation in GPU for the parallel resolution of reactive transport problems.

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Reactive Transport modelling (RTM) involves the resolution of the partial differential equation that governs the transport of multiple chemical components, and several algebraic equations that account for chemical interactions. Since RTM can be very computational demanding, especially when considering long term and/or large scale scenarios, several effort have been made on the last decade in order to parallelize it. Most works have focused on implementing domain decomposition technics for distributed memory architectures, and also some effort have been made for shared memory architectures. Despite the recent advances on GPU only few works explore this architecture for RTM, and they mainly focused on the implementation of parallel sparse matrix solvers for the component transport. Solving the component transport consumes an important amount of time during simulation, but another time consuming part of RTM is the chemical speciation, a process that has to be performed multiple times during the resolution of each time step over all nodes (or discrete elements of the mesh). Since speciation involves local calculations, it is a priory a very attractive process to parallelize. But, to the author's knowledge, no work on literature explores chemical speciation parallelization on GPU. One of the reasons behind this might be the fact that the unknowns and the number of chemical equations that act over each node might be different and can dynamically change in time. This can be a drawback for the single instruction multiple data paradigm since it might lead to the resolution of several systems with potentially different sizes all over the domain. In this work we use a general formulation that allows to solve efficiently chemical specialization on GPU. This formulation allows to consider different primary species for each node of the mesh and allows the precipitation of new mineral species and their complete dissolution keeping constant the number of components.