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Reactive flows at the pore-scale of porous materials

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SUMMARY

This talk will focus on the numerical aspects of reactive flows and pore-scale modeling, and how involving vortex-like methods can substantially improve computational efficiency, that is to say optimize the use of computing resources (computational time and memory storage). After briefly describing the numerical approach (whose hybrid aspect are introduced in [4, 3]), a few numerical simulations of calcite dissolution will be presented.

The numerical method is built specifically with a time-splitting algorithm such that velocity computing and interpolations are performed meaningfully in order to avoid useless computations (in the spirit of [5]). In practice we will show that a good strategy is to compute chemistry, diffusion of species and transport on particles, while penalization, velocity computation and viscous diffusion are performed on grids. This strategy decreases the number of interpolations thus improving the computational time. In this spirit, chemistry and hydrodynamics can be considered at different resolutions, and require only a down-scaling of solid concentration, which fits very well to GPU or hybrid CPU-GPU computing, which is currently one of our main developments [2].

Concerning reactive flows, three time scales are involved: a hydrodynamic time scale (under the second) in which the flow is able to cross the domain at the pore-scale; a time scale allowing to reach a quasi-stationary reactive state of reaction rate; a dissolution time scale for which the solid body evolves. We will consider the case of a calcite core dissolution at pH=2, in the context of a [1]. For this configuration, these three time scales are about 1s, 10s and 1h, respectively.

References

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