Simulation of dissolution, precipitation and crystallization at the pore scale of porous media using particle methods

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This talk presents advances in numerical methods for the simulation of single-phase flow, reactive transport and solid geometry evolution at the pore scale, involving dissolution, precipitation and crystallization.

Firstly, we will present the semi-Lagrangian approach of the problem and the related models [1], involving particle treatment of the transport phenomena, and underlying grids for the diffusion, reactions and flow computation.

We will then describe the validation of the method by a dissolution process of 2D and 3D calcite cores (including experimental validation) with a benchmark approach [2]. The codes used in this benchmark cover a good portion of the wide range of approaches typically employed for solving pore-scale problems in the literature, including discretization methods, characterization of the fluid-solid interfaces, and methods to move these interfaces as a result of fluid-solid reactions. Results show remarkable agreement both quantitatively and qualitatively, providing cross-validation of our method.

We will also focus on the simulations of precipitation and crystallization in 3D porous media. This last aspect includes nucleation of the dissolved chemical species and then crystal growth due to their interactions with the solid material.

The numerical method, developed and running on the cluster Pyrene, is currently extended to GPU-CPU computing using the HySoP HPC platform developed at UPPA-LJK-CNAM.

References:

[1] J-M. Etancelin, P. Moonen, P. Poncet. *Improvement of remeshed Lagrangian methods for the simulation of dissolution processes at pore-scale*. Advances in Water Resources 146, Elsevier, 2020, p.103780. DOI: 10.1016/j.advwatres.2020.10378

[2] S. Molins, C. Soulaine, N. I. Prasianakis, A. Abbasi, P. Poncet, A. J. C. Ladd, V. Starchenko, S. Roman, D. Trebotich, H. A. Tchelepi, and C. I. Steefel, *Simulation of mineral dissolution at the pore scale with evolving fluid-solid interfaces: Review of approaches and benchmark problem set*, Computational Geoscience, 2020. DOI: 10.1007/s10596-019-09903-x