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Reactive flows at pore scale with hybrid computing

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SUMMARY

In this work, we aim at producing a generic simulation code that operates at large scale on hybrid (CPU-GPU) clusters for solving reactive micro-flows at pore scale.

The purpose of this talk is to describe how we exploit a semi-Lagrangian method based on a Remeshed Vortex Method [1]. The key feature of this method is to introduce meshless particles as the domain discretisation. These particles evolve along flow characteristics and carry the vorticity of the flow. The vorticity transport-diffusion equation is combined with a Poisson problem to recover a velocity field from the vorticity. In addition, we use a viscous splitting in order to solve convective terms in a Lagrangian framework and the other terms (stretching, diffusion, Poisson, or chemical reactions) in Eulerian framework on an underlying cartesian grid.

The proof of concept and the usability of these methods has been investigated since several years [1], especially using GPU [2] and more recently using a directional splitting and high order remeshing (particle-grid interpolation) schemes [3] on large hybrid computing resources [4].

In the application context of hydrogen, methane or carbon dioxide injection in specific geological layers for storage purposes, a fine models validation is mandatory. Gases are replacing pore fluids in rocks and are interacting with the medium. These physical and chemical phenomena that can alter the operation of the storage by modifying the chemical composition of fluids and the structures of the rocks. Numerical illustrations of this application will be presented together with the computational performances.

References

[1] G.-H. Cottet et P. Koumoutsakos, *Vortex methods: theory and practice*, Cambridge university press, 2000.

[2] D. Rossinelli, M. Bergdorf, G.-H. Cottet et P. Koumoutsakos, *GPU accelerated simulations of bluff body flows using vortex particle methods*, Journal of Computational Physics 229, 2010.

[3] G.-H. Cottet, J.-M. Etancelin, F. Pérignon et C. Picard, *High order Semi-Lagrangian particle methods for transport equations: numerical analysis and implementation issues*, ESAIM: Mathematical Modelling and Numerical Analysis 48, 2014.

[4] J.-M. Etancelin, G.-H. Cottet, F. Pérignon et C. Picard, *Multi-CPU and multi-GPU hybrid computations of multi-scale scalar transport*, Proceedings of the 26th International Conference on Parallel Computational Fluid Dynamics, 2014.

[5] P. Poncet, L. Hume et J.-M. Etancelin, *New trends in Vortex Methods for reactive flows*, InterPore 10th Annual Meeting, 2018.

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