Reactive flows at pore scale with hybrid computing

Jean-Matthieu Etancelin
Laboratoire de Mathématiques et leurs Applications de Pau
UMR CNRS 5142, IPRA
Université de Pau et des Pays de l'Adour

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Context

Simulations of reactive flows at pore scale

Motivations

- Flows through porous media (geological structures or artificial material)
- Studies at large dimensions (reservoir) with macroscopic models w.r.t physic phenomenons
- Need of microscopic simulations in order to further calibrate macroscopic models.
- Intrusive physical measurements of rocks samples replaced by simulation from X-ray imagery
- Applications to reservoirs safety and long term CO_2 mineral storage

Challenges of simulations of reactive flows at pore scale

Application

- 3 time scales
  - hydrodynamic scale : $\sim 100\,ms$
  - chemical equilibrium : $\sim 10\,s$
  - dissolution : $\sim 1\,h$
- Complex chemical phenomenons: dissolution, precipitation, crystallization
- In a geological context : need years of simulation

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Computing

- Long term simulations w.r.t time-steps
- Large data from X-ray high resolution sample scans

High order remeshed particle method on GPU

Vortex method

Solving conservation equations:

$$\frac{\partial u}{\partial t} + \mathrm{div}(a : u) + Au = F$$

where $u(x, t)$ is a conservated quantity (unknown) and $a(x, t)$ is the velocity

Vortex method

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Operator splitting

- Solve $\frac{\partial u}{\partial t} + \mathrm{div}(a : u) = 0$ with remeshed particle method
- Solve $\frac{\partial u}{\partial t} + Au = F$ with best suited method

Vortex method

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Discretisation using particles (x_p, v_p, u_p)

- Approximation: $u_h(x, t) = \sum_p u_p(t)\delta(x - x_p(t))$
- Particles trajectories: $\frac{\mathrm{d}x_p}{\mathrm{d}t} = a(x_p, t)$
- Transported quantities: $u_p(t) = u(x_p, t)v_p$
- Particles volume: $\frac{\mathrm{d}v_p}{\mathrm{d}t} = \text{div}(a(x_p, t))v_p$

Remeshed particle methods

Remeshing step

- Velocity distortions may lead to unoverlapping particle distribution
- Redistributing particles (particle-grid interpolation) every few timesteps enforce a sufficient regularity of the particle distribution
- remeshing at every timestep[1]: remeshed particle methods = forward and conservative semi-Lagrangian method

[1] Koumoutsakos and Leonard, JFM, 1995

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Particle-grid interpolation

$$u_i^{n+1} = \sum_p u_p^n \Gamma\left(\frac{x_p^{n+1} - x_i}{\Delta x}\right)$$

with x_i a point of a regular grid of size Δx and $(\cdot)^n$ the quantity at time t^n. Γ is a remeshing formula.

[1] Koumoutsakos and Leonard, JFM, 1995

Numerical analysis of remeshed particle method

- Multidimensional cases reduces to 1D analysis with dimensional splitting

[2] GH Cottet, **JME**, F Perignon and C Picard, ESAIM: M2AN, 2014

Numerical analysis of remeshed particle method

- Multidimensional cases reduces to 1D analysis with dimensional splitting

Consistency with transport equation[2]: $\frac{\partial u}{\partial t} + (a \cdot \nabla)u = 0$

Under the Lagrangian CFL condition $\Delta t < ||a'||_\infty^{-1}$, the remeshed particle method is consistent with a transport equation and the consistency error is bounded by $\mathcal{O}(\Delta t^\alpha + \Delta x^{min(p,r)})$ provided that :

- α-order in time for advection
- Remeshing formula Γ satisfies the conditions:
  - $\sum_k \Gamma(x-k) = 1$ and $\sum_k (x-k)^j \Gamma(x-k) = 1$, $1 \leqslant j \leqslant p$
  - $\Gamma \in C^r(\mathbb{R})$, $r \geqslant 1$
  - $\Gamma(i-j) = \delta_{ij}$, $i,j \in \mathbb{Z}$
  - Γ support is $[-p/2-1; p/2+1]$
  - Γ is even, piecewise polynomial of degree $2r+1$ over integer intervals

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Stability of the scheme[2]

Same hypothesis as above

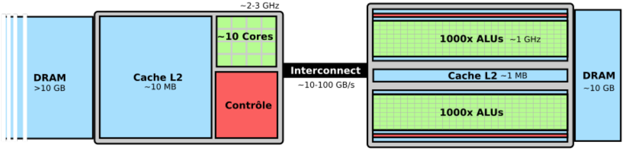
[2] GH Cottet, **JME**, F Perignon and C Picard, ESAIM: M2AN, 2014

Remarks towards implementation

- High order remeshing $\Rightarrow$ large support and high polynomial degree $\Rightarrow$ large number of computations per particle
- Dimensional splitting $\Rightarrow \mathcal{O}(d(p+2))$ complexity (instead of $\mathcal{O}((p+2)^d)$ with tensorial formulas)
- Usage of regular cartesian grid $\Rightarrow$ regular data structure and stencils scheme for homogeneous transport equation
- Usage of regular cartesian grid $\Rightarrow$ use grid-based method for other terms of the conservation equation.
- Method well suited to GPU architecture (regular data structure, high arithmetic intensity) and parallel implementation

Hybrid high performance computing – GPU

CPU-GPU comparison



CPU:

- Large memory
- Small core nb. at high freq.
- Several cache levels
- Important instruction controller
- Multitask (OS, devices, ...)

GPU:

- Small dedicated memory
- Very large cores nb. at low freq.
- Programmable cache
- Massively parallel (SIMD)
- ~ 6 *TFLOPS* (DP)

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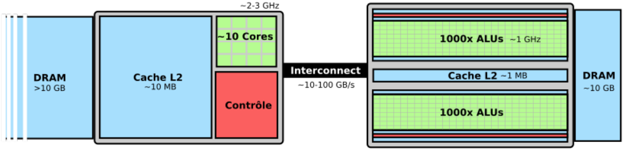

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Major difficulties of hybrid programming

- Important vectorization needed
- Data transfers
- Regular patterns for data access

Need to think about this architecture when designing the methods

High performance computing

HySoP (Hybid Simulation with Particles)

- Open Source python package (not released yet)
- Low level computations in compiled languages (Fortran, C, OpenCL)
- Generated and autotuned low level (OpenCL) code
- Distributed and parallel computations (MPI + GPU)
- High level of abstraction (user interface $\sim$ eDSL)
- Coarse grained task parallelism
- Dimensional splitted operators implemented in best transposition state for data (similar to fftw)

Reactive flows

Remeshed particle method with penalization

Handle obstacles in fluid : Brinkman penalization method

- extend flow velocity inside solid bodies
- add an external force on the flow following a Darcy law[3]
- penalization term depending on a specific permeability parameter
- handle rigid body motion
- no need to specify a boundary condition at fluid-solid interface

[3] Kevlahan and Ghidaglia, Eur. J. Mech. B - Fluids, 2001

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Penalization term for vorticity equation

$$\nabla \times (\lambda\chi(u_b - u))$$

- λ : permeability parameter (0: fluid, ∞ : solid)
- χ : solid body indicator function
- u_b : solid body velocity

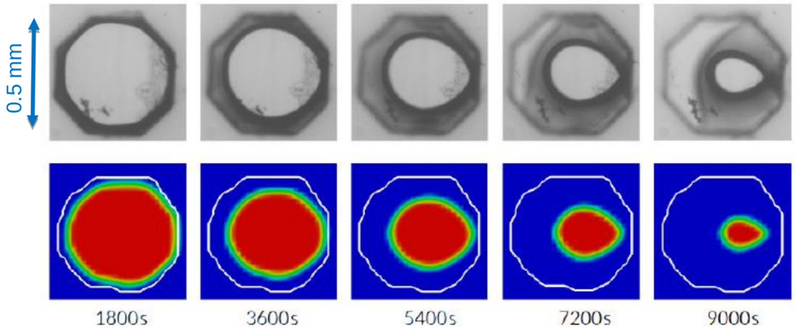
One more step in operator splitting, solved implicitly

[3] Kevlahan and Ghidaglia, Eur. J. Mech. B - Fluids, 2001

Validation benchmark

Calcite crystal dissolution in a micro-channel

- high resolution dataset from experiment (S. Roman, Stanford University)
- Validation against experiment in 2D[4]



[4] P Poncet, **JME** and L Hume, InterPore conference 2018

3D calcite dissolution with remeshed particle method

Full model

$$CaCO_3 + 2\,H^+ \rightleftharpoons {Ca_2}^+ + {HCO_3}^- + H^+ \rightleftharpoons {Ca_2}^+ + H_2O + CO_2$$

- dissolution and precipitation
- solid in suspension
- gas emissions

3D calcite dissolution with remeshed particle method

Simplified model (solid-fluid)

$$CaCO_3 + 2\,H^+ \rightleftharpoons {Ca_2}^+ + {HCO_3}^- + H^+$$

$$\begin{cases} \varepsilon^{-1}\dfrac{\partial \rho u}{\partial t} - \mathrm{div}(\varepsilon^{-1}\mu(\varepsilon)\nabla u + \varepsilon^{-2}\rho u : u) + \mu(\varepsilon)\underbrace{K_0^{-1}\dfrac{(1-\varepsilon)^2}{\varepsilon^3}u}_{\text{Kozeny-Carman law}} = -\nabla p \\ \mathrm{div}\, u = 0 \\ \dot{\varepsilon} = K_d(1-\varepsilon)C_H - K_p C_{Ca} C_{HCO_3} \upsilon \\ \dfrac{\partial C_{H,Ca}}{\partial t} + (u\cdot\nabla)C_{H,Ca} - \mathrm{div}(\underbrace{\sigma(\varepsilon)}_{\text{Archie law}}\nabla C_{H,Ca}) = \pm\dot{\varepsilon}/\upsilon \\ + \text{ adequate initial and boundary conditions} \end{cases}$$

- ε : porosity ($[CaCO_3] = (1-\varepsilon)/\upsilon$)
- $C_{H,Ca}$: concentration in either H^+ or Ca^{2+} and ${HCO_3}^-$
- K_d : dissolution reaction constant
- Kozeny-Carman law : Poiseuille law in porous media, K_0 : permeability
- Archie law : molecular diffusion in porous media ($\sigma(\varepsilon) = \varepsilon D_M$)

3D calcite dissolution with remeshed particle method

Simplified model (solid-fluid, dissolution only and constant viscosity)

Stokes flow

$$CaCO_3 + 2\,H^+ \longrightarrow {Ca_2}^+ + {HCO_3}^- + H^+$$

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Simplified model (solid-fluid, dissolution only and constant viscosity)

Stokes flow, as a fixed point

$$CaCO_3 + 2\,H^+ \longrightarrow {Ca_2}^+ + {HCO_3}^- + H^+$$

$$\begin{cases} \dfrac{\partial u_e}{\partial s} - \nu \Delta u_e + \nu K_0^{-1} \dfrac{(1-\varepsilon)^2}{\varepsilon^2} u_e = -\nabla p \qquad \text{(fixed point iterations)} \\ \text{div}\, u = 0 \\ \dot{\varepsilon} = K_d (1-\varepsilon) C_H - K_p C_{Ca} C_{HCO_3} \upsilon \\ \dfrac{\partial C_{H,Ca}}{\partial t} + (u \cdot \nabla) C_{H,Ca} - \text{div}(\sigma(\varepsilon) \nabla C_{H,Ca}) = \pm \dot{\varepsilon}/\upsilon \\ + \text{ adequate initial and boundary conditions} \end{cases}$$

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- $u(x,t) = \lim_{s \to \infty} u_e(x,t,s)$ et $u_e(x,t,0) = u(x, t - \Delta t)$

3D calcite dissolution with remeshed particle method

Simplified model (solid-fluid, dissolution only and constant viscosity)

Stokes flow, as a fixed point, in u-ω formulation

$$CaCO_3 + 2\,H^+ \longrightarrow Ca_2{}^+ + HCO_3{}^- + H^+$$

$$\begin{cases} \dfrac{\partial \omega}{\partial s} - \nu \Delta \omega + \nu K_0^{-1} \nabla \times \left(\dfrac{(1-\varepsilon)^2}{\varepsilon^2} u_e \right) = 0 & (u\text{-}\omega \text{ formulation}) \\ \Delta u_e = -\nabla \times \omega & (\omega = \nabla \times u_e) \\ \operatorname{div} u = 0 & \\ \dot{\varepsilon} = K_d (1-\varepsilon) C_H - K_p C_{Ca} C_{HCO_3} \upsilon & \\ \dfrac{\partial C_{H,Ca}}{\partial t} + (u \cdot \nabla) C_{H,Ca} - \operatorname{div}(\sigma(\varepsilon) \nabla C_{H,Ca}) = \pm \dot{\varepsilon}/\upsilon & \\ + \text{ adequate initial and boundary conditions} & \end{cases}$$

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3D calcite dissolution with remeshed particle method

Spatial and temporal multi-scale problem

3 time scales:

- hydrodynamic: time of domain traversal (<1s)
- Chemical reaction characteristic time: quasi-stationary state for rate of reaction ($\simeq$ 10s)
- dissolution time: solid evolution ($\simeq$ 10 min at $pH = 1$)

2 space scales, high Schmidt number ($Sc = \frac{\nu}{\sigma(\varepsilon)} = \sqrt{\frac{\eta_\nu}{\eta_\sigma}} >> 1$):

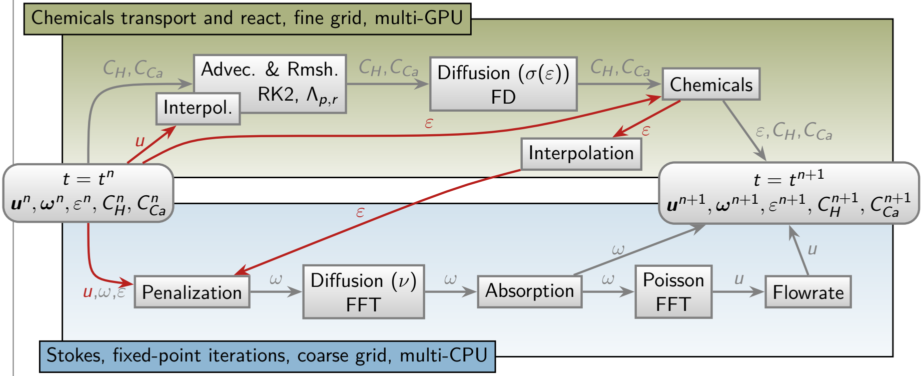
- Flow scale (coarse)
- Chemical species concentration (fine)

Simulation features

- One spatial grid size for each scale
- Transport-diffusion-reaction solved on the fine grid on GPU
- Implicit penalization (solid influence on flow)
- Time scale separation (using a fixed point to reach flow stationary state)

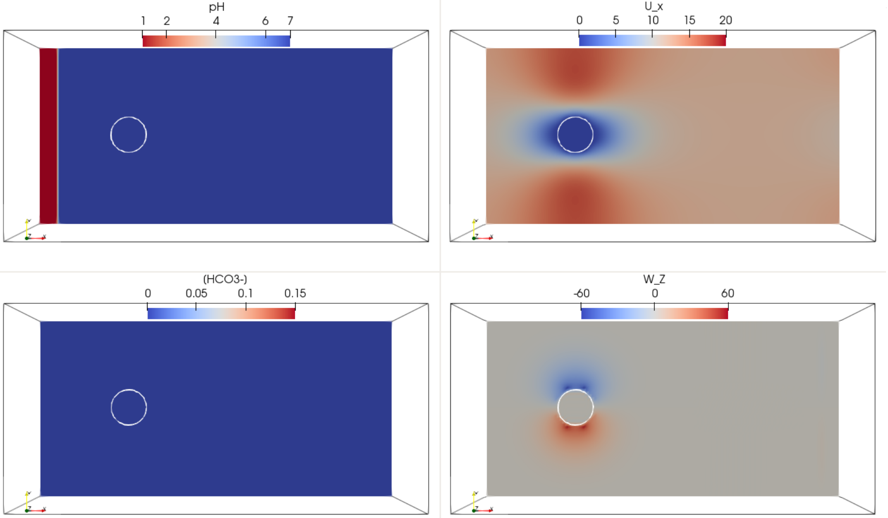
3D calcite dissolution with remeshed particle method

Sketch of the algorithm for Stokes reactive flow



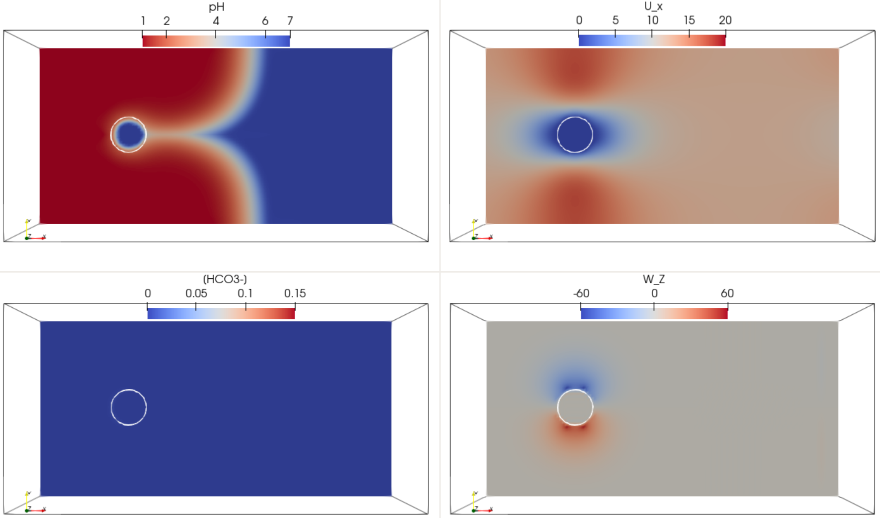
3D calcite dissolution with remeshed particle method

Numerical illustration : $Re = 0.12,\ t = 0$



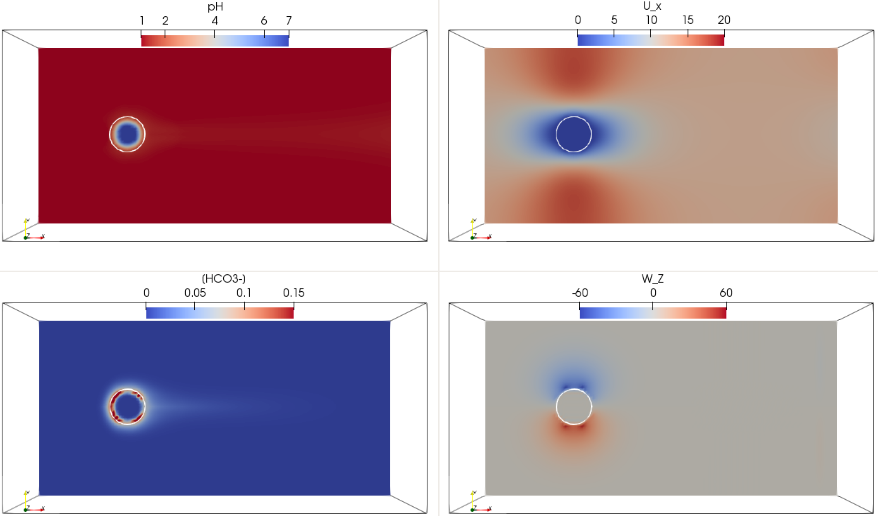
3D calcite dissolution with remeshed particle method

Numerical illustration : $Re = 0.12,\ t = 0.30176$



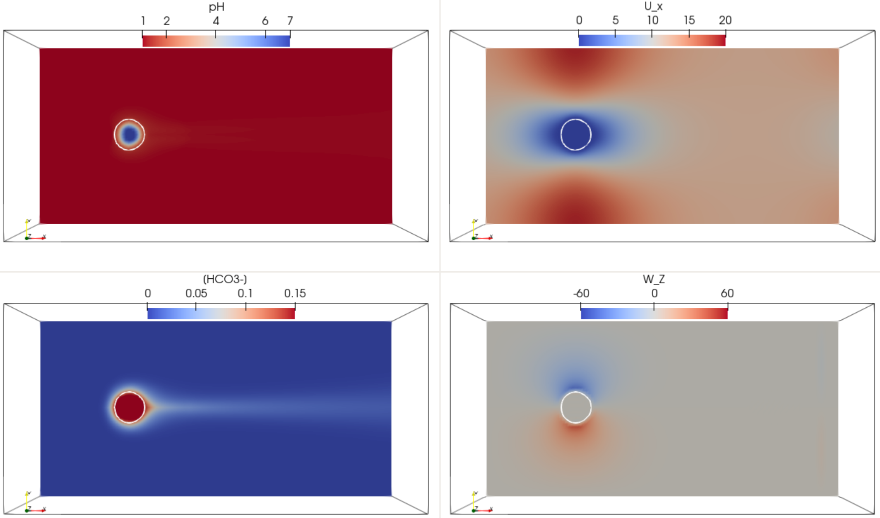
3D calcite dissolution with remeshed particle method

Numerical illustration : $Re = 0.12$, $t = 1.01725$



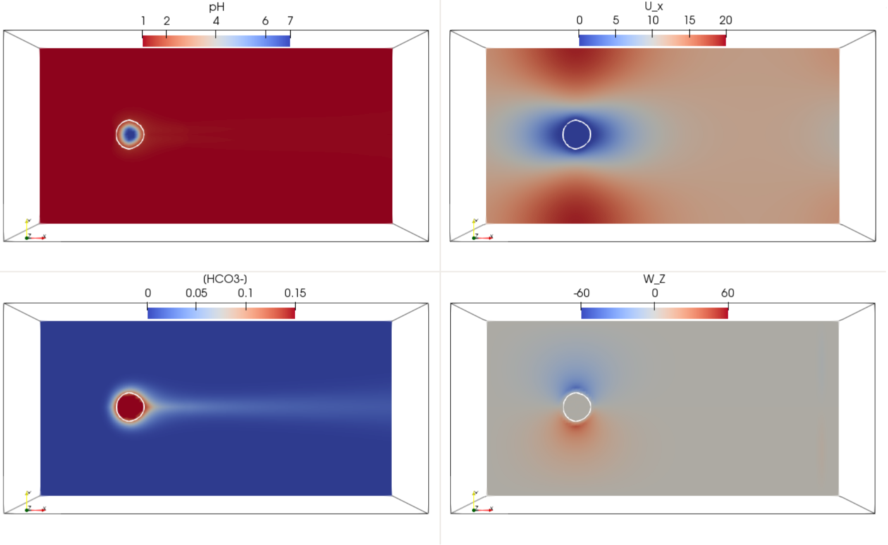
3D calcite dissolution with remeshed particle method

Numerical illustration : $Re = 0.12$, $t = 40.69$



3D calcite dissolution with remeshed particle method

Numerical illustration : $Re = 0.12,\ t = 61.0352$



3D calcite dissolution with remeshed particle method

Reduced model (solid-fluid, dissolution only and constant viscosity)

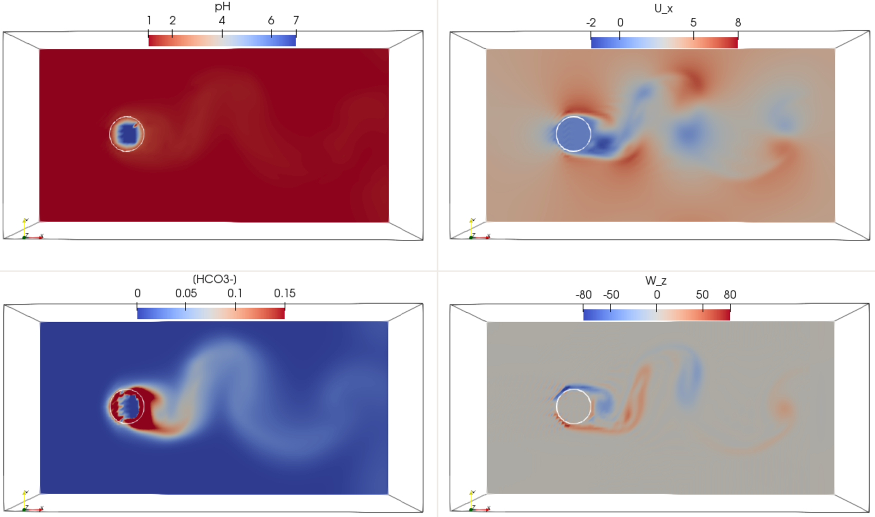
Turbulent flow

$$CaCO_3 + 2\,H^+ \longrightarrow Ca^{2+} + HCO_3^{\,-} + H^+$$

$$\begin{cases} \dfrac{\partial \omega}{\partial t} + (u\cdot\nabla)\omega + (\omega\cdot\nabla)u - \nu\Delta\omega + \nu K_0^{-1}\nabla\times\left(\dfrac{(1-\varepsilon)^2}{\varepsilon^2}u_e\right) = \nabla\times f \\ \Delta u_e = -\nabla\times\omega \qquad (\omega = \nabla\times u) \\ \operatorname{div} u = 0 \\ \dot{\varepsilon} = K_d(1-\varepsilon)C_H \\ \dfrac{\partial C_{H,Ca}}{\partial t} + (u\cdot\nabla)C_{H,Ca} - \operatorname{div}(\sigma(\varepsilon)\nabla C_{H,Ca}) = \pm\dot{\varepsilon}/\upsilon \\ + \text{ adequate initial and boundary conditions} \end{cases}$$

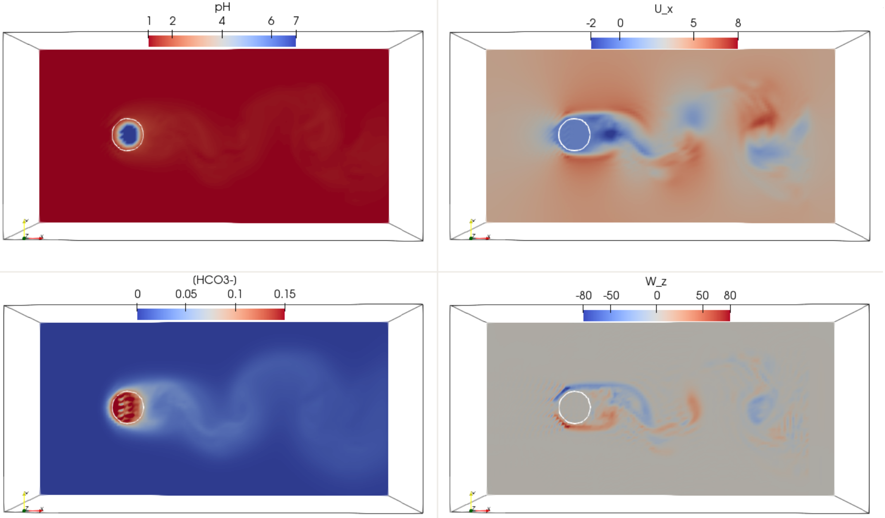
3D calcite dissolution with remeshed particle method

Numerical illustration : $Re = 960,\ t = 4.026$



3D calcite dissolution with remeshed particle method

Numerical illustration : $Re = 960$, $t = 29.234$



Conclusions and future works

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Conclusions

- Exploiting several levels of parallelism
- Multi-scale resolution (spatial and temporal)
- Multi-physics simulation (flow + chemical)
- Robust method and implementation : from microfluid ($Re = 0.12$) to turbulent reactive flows ($Re = 960$)

Conclusions and future works

Future works

- Overall optimization of the code (MPI-GPU interactions on modern architectures)
- Handle precipitation, solid in suspension in flow
- Use of real complex geometries from X-ray tomography (flow is ok, need chemistry)