A benchmark for the numerical simulation of pore-scale mineral dissolution with fluid-solid interface evolution

SITRAM Conference, 2/12/2019

P. Poncet, S. Molins, C. Soulaine, N. Prasianakis, A. Abbasi, A. J. C. Ladd, V. Starchenko, S. Roman, D. Trebotich, H. A. Tchelepi, and C. I. Steefel

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Summary

Usual models

Example of pore-scale simulations

Reactive flows and benchmark

Conclusion

Brinkman-Stokes :

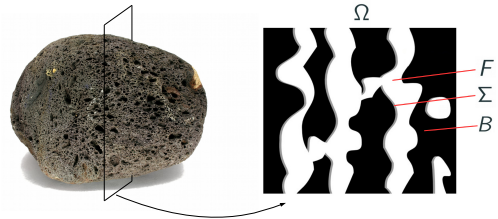
$$-\mu\boldsymbol{\Delta u} + \mu^* \boldsymbol{K}^{-1}\boldsymbol{u} = \boldsymbol{f} - \boldsymbol{\nabla p}$$

Stokes and penalization :

$$-\mu\boldsymbol{\Delta u} + \frac{\mathbf{1}_B}{\varepsilon}\boldsymbol{u} = \boldsymbol{f} - \boldsymbol{\nabla p}$$

Kozeny-Carman law :

$$\boldsymbol{K}^{-1} = \boldsymbol{K_0}^{-1}\frac{(1-\phi)^2}{\phi^3}$$



Darcy-Brinkman-(Navier)-Stokes (DBS) :

$$\phi^{-1}\frac{\partial(\rho\boldsymbol{u})}{\partial t} + \phi^{-1}\mathbf{div}\left(\phi^{-1}\rho\boldsymbol{u}\otimes\boldsymbol{u}\right) - \phi^{-1}\mathbf{div}\left(\mu\frac{\boldsymbol{\nabla u} + \boldsymbol{\nabla u}^T}{2}\right) + \mu^*\boldsymbol{K_0}^{-1}\frac{(1-\phi)^2}{\phi^3}\boldsymbol{u} = \boldsymbol{f} - \boldsymbol{\nabla p}$$

$$\Longrightarrow \qquad -\mathbf{div}(\mu(\phi)\boldsymbol{D}) + \mu^*\boldsymbol{K_0}^{-1}\frac{(1-\phi)^2}{\phi^2}\boldsymbol{u} = \phi(\boldsymbol{f} - \boldsymbol{\nabla p})$$

What is a Particle/Vortex Method ?

Particle method involving vorticity, possibly with underlying grids

- Navier-Stokes equations:

$$\frac{\partial \rho \boldsymbol{u}}{\partial t} + \mathbf{div}(\rho \boldsymbol{u} \otimes \boldsymbol{u}) - \mathbf{div}(\mu \boldsymbol{D}) + \frac{1_B}{\varepsilon} \boldsymbol{u} = \boldsymbol{f} - \nabla p, \ \boldsymbol{D} = (\nabla \boldsymbol{u} + \nabla \boldsymbol{u})^T/2, \ \mathbf{div}\boldsymbol{u} = 0,$$

$$\overset{\omega = \mathbf{curl}\boldsymbol{u}}{\Longrightarrow} \frac{\partial \omega}{\partial t} + \boldsymbol{u} \cdot \nabla \omega + \mathbf{curl}\left(\frac{1_B}{\rho \varepsilon} \boldsymbol{u}\right) = \omega \cdot \nabla \boldsymbol{u} + \mu \rho^{-1} \Delta \omega,$$

where $\boldsymbol{u} = \mathbf{curl}\Psi$ and $-\Delta \Psi = \omega$

Robust
Flexible
Fast, scales as $\mathcal{O}(N \log N)$

Lot of code to do
Several meanings of consistency

Semi-Lagrangian
High order interpolation for
Grid $\Leftrightarrow$ *Particles*

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- A particle is defined by a triplet Vortex-Location-Volume (ω_p, x_p, v_p), $p = 1..N$:

$$d\omega_p/dt = \left[\omega \cdot \nabla \boldsymbol{u} + \mu \rho^{-1} \Delta \omega\right]_{x_p(t)},\ dx_p/dt = u(x_p(t)),\ dv_p(t)/dt = v_p \mathbf{div}(u(x_p)) = 0$$

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- This method is able to transport any passive/active tracer defined by a field $\boldsymbol{C}$:

$$\frac{\partial \boldsymbol{C}}{\partial t} + \mathbf{div}(u\boldsymbol{C}) - \mathbf{div}(\sigma \nabla \boldsymbol{C}) = \boldsymbol{F}(\boldsymbol{C}) \quad \Longrightarrow \quad d\boldsymbol{C}_p/dt = \boldsymbol{F}(\boldsymbol{C}_p) + \left[\mathbf{div}(\sigma \nabla \boldsymbol{C})\right]_{x_p(t)}$$

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- This method is able to transport any passive/active tracer defined by a field $\boldsymbol{C}$:

$$\frac{\partial C}{\partial t} + \mathbf{div}(uC) - \mathbf{div}(\sigma \nabla C) = F(C) \quad \Longrightarrow \quad dC_p/dt = F(C_p) + \left[\mathbf{div}(\sigma \nabla C)\right]_{x_p(t)}$$

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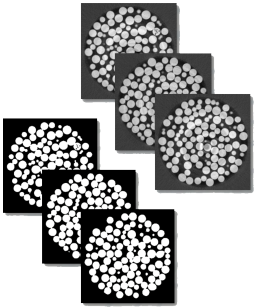
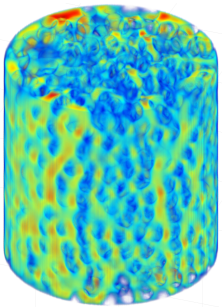
Newtonian flow through a bead stack

Permeability estimation of millimeter-scale real samples





$$\frac{\partial(\rho u)}{\partial t} - \mathbf{div}\left(2\mu \boldsymbol{D}\right) + \mathbf{1}_{B(t)}\varepsilon^{-1}\boldsymbol{u} = \boldsymbol{f} - \nabla p$$

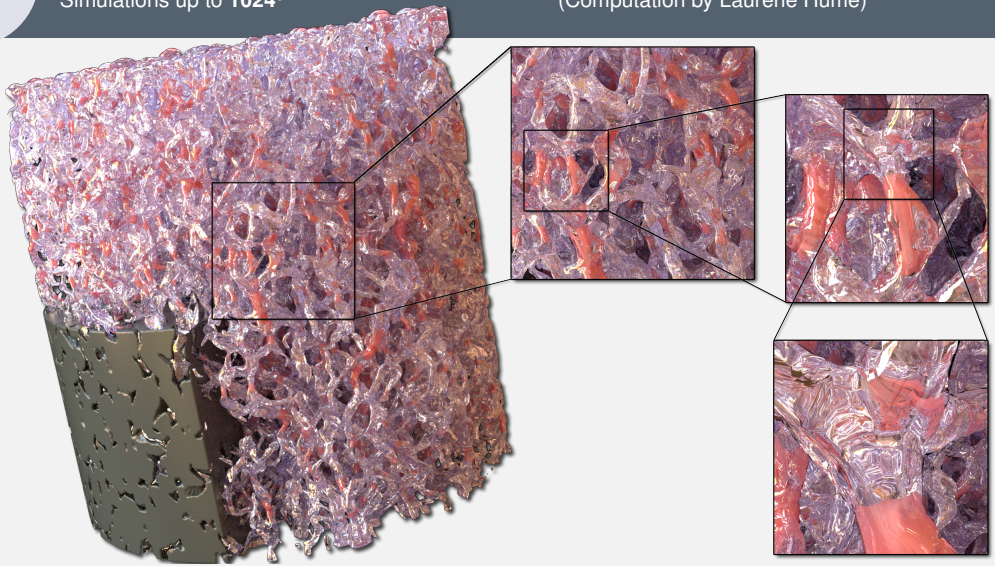
where $\boldsymbol{D} = \left(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^{T}\right)/2$ and $\mathbf{div}\,\boldsymbol{u} = 0$

MicroCT scan provided by DMEX Team at UPPA.

L. Hume, F. Guerton, P. Moonen and P. Poncet, *Experimental and numerical cross-validation of flow in real porous media*, ICTMS, Lund, Sweden (2017).

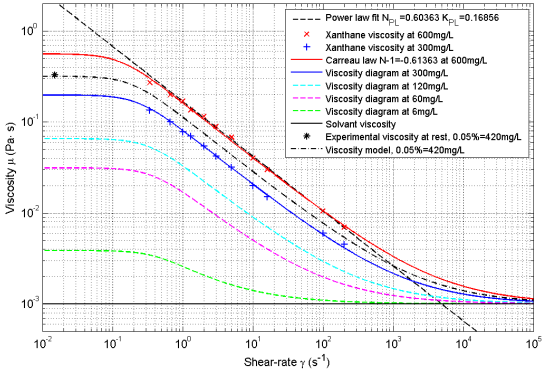
High resolution Newtonian flow in sandstones

Simulations up to 1024^3 (Computation by Laurène Hume)



Rheology and shear-thinning flows

Miscible heterogeneous Xanthan viscosity

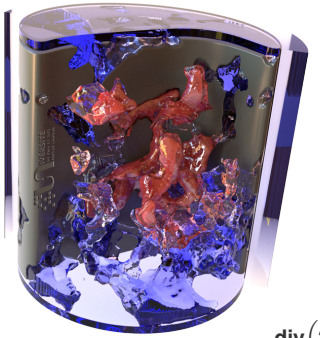


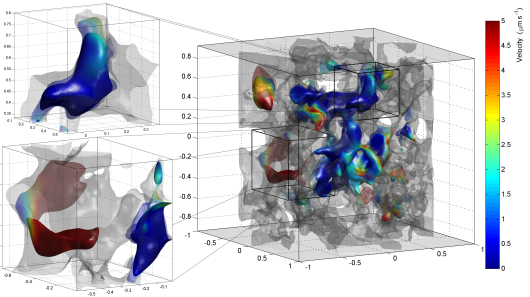
$$\mu(\boldsymbol{c}, \boldsymbol{D}) = \mu_\infty + (\mu_0(\boldsymbol{c}) - \mu_\infty)\left(1 + 2\beta(\boldsymbol{c})^2|\boldsymbol{D}|^2\right)^{\frac{q(\boldsymbol{c})-2}{2}}$$

D. Sanchez, L. Hume, R. Chatelin and P. Poncet, *Three-dimensional non-linear Stokes problem coupled to transport-diffusion for shear-thinning heterogeneous microscale flows: Applications to digital rock physics and mucociliary clearance*, in press for M2AN.

Rheology and shear-thinning flows

Miscible heterogeneous Xanthan tranport





$$-\mathbf{div}\left(2\mu(\boldsymbol{c},\boldsymbol{D})\,\boldsymbol{D}\right)+\mathbf{1}_{\boldsymbol{B}}\,\varepsilon^{-1}\boldsymbol{u}=\boldsymbol{f}-\boldsymbol{\nabla p}$$

$$\frac{\partial \boldsymbol{c}}{\partial \boldsymbol{t}}+\mathbf{div}(\boldsymbol{uc})-\sigma\boldsymbol{\Delta c}=\mathbf{0},\quad \text{where } \boldsymbol{D}=\left(\boldsymbol{\nabla u}+\boldsymbol{\nabla u}^{\boldsymbol{T}}\right)/\mathbf{2} \text{ and}$$

$$\mu(\boldsymbol{c},\boldsymbol{D})=\mu_{\infty}+(\mu_{\mathbf{0}}(\boldsymbol{c})-\mu_{\infty})\left(\mathbf{1}+\mathbf{2}\beta(\boldsymbol{c})^{\mathbf{2}}|\boldsymbol{D}|^{\mathbf{2}}\right)^{\frac{\boldsymbol{q(c)}-\mathbf{2}}{\mathbf{2}}}$$

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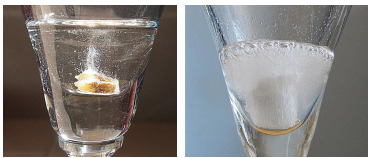
Reactive flow using superficial velocity

$$CaCO_3 + 2\,HCl \rightleftharpoons CaCl_2 + H_2CO_3 \rightleftharpoons CaCl_2 + H_2O + CO_2$$

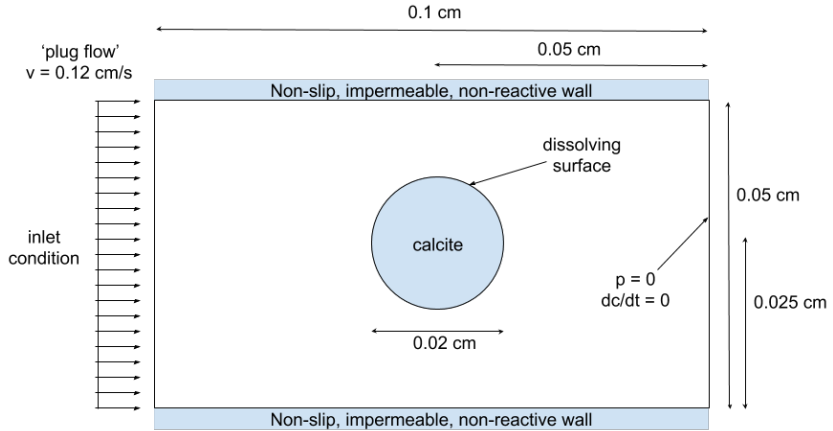
or

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



Calcite in Hydrochloric Acid

Calcite dissolution – Benchmark setup



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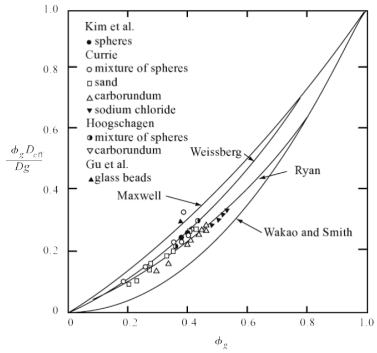


Diffusion $\sigma(\varepsilon) = \varepsilon \boldsymbol{D_M}$

Crystal porosity $\varepsilon = \mathbf{10^{-3} - 2\,10^{-2}}$

Reactive flow using superficial velocity

From *Quintard & Whitaker (1993), ..., Soulaine et al. (2017)* :

$$\varepsilon^{-1}\frac{\partial \rho \boldsymbol{u}}{\partial t} + \varepsilon^{-1}\mathbf{div}(\varepsilon^{-1}\rho \boldsymbol{u} \otimes \boldsymbol{u}) + \nabla p - \varepsilon^{-1}\mu \Delta \boldsymbol{u} + \mu \underbrace{\frac{(1-\varepsilon)^2}{\varepsilon^3} K_0^{-1}\boldsymbol{u}}_{\text{Kozeny-Carman law}} = \boldsymbol{f}$$

$$\mathbf{div}\,\boldsymbol{u} = 0$$

$$\frac{\partial \varepsilon}{\partial t} = K_d(1-\varepsilon)C - K_p v C_2 C_3$$

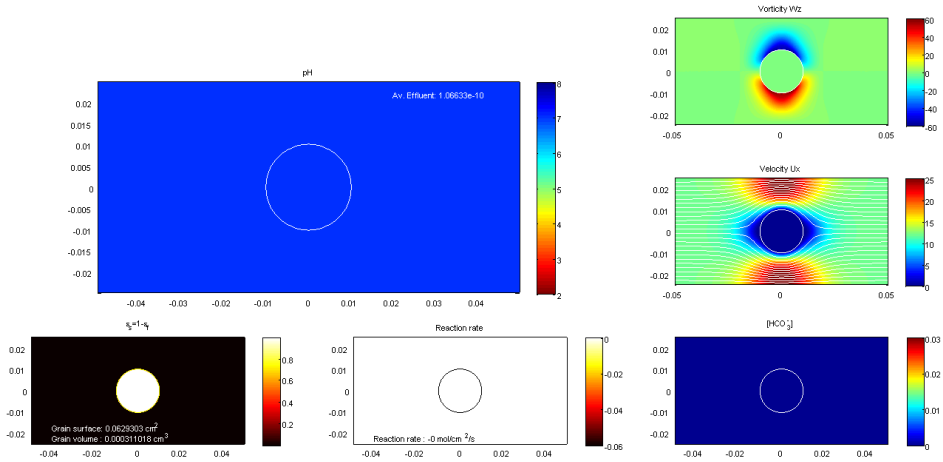
$$\frac{\partial C}{\partial t} + \mathbf{div}(\varepsilon^{-1}\boldsymbol{u}\, C) - \underbrace{\mathbf{div}(\sigma(\varepsilon)\nabla C)}_{\text{Archie law}} = -\dot{\varepsilon}/v$$

+ adequate initial and boundary conditions

- ε is porosity, v molar volume of calcite,
- $\boldsymbol{u}$ is superficial velocity, p is pressure, $\boldsymbol{D} = (\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T)/2$
- ρ and μ are liquid density and viscosity,
- K_d is dissolution rate, K_p is the precipitation rate,
- C is acid concentration, $\sigma(\varepsilon) = \varepsilon D_M$ (Wakao & Smith 1962) is acid diffusion.

Calcite dissolution – Snapshots

Different time scales, Re=0.24, pH=2, at resolution $\mathbf{512 \times 256}$



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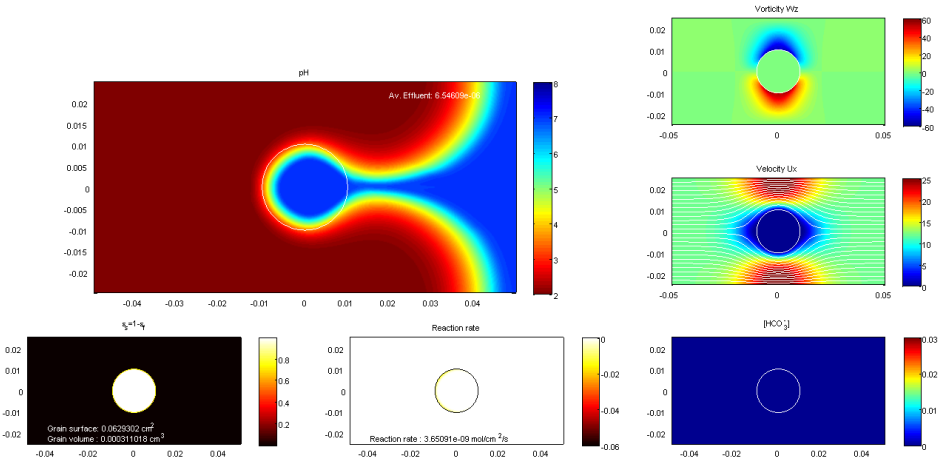

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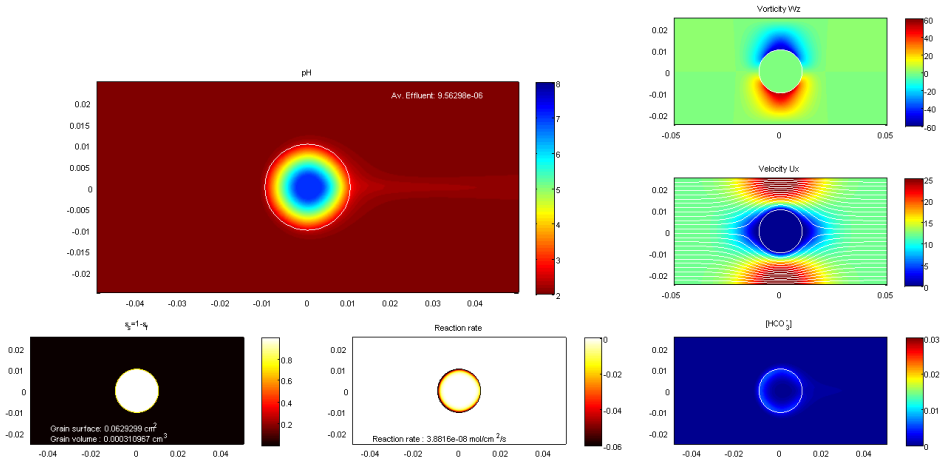

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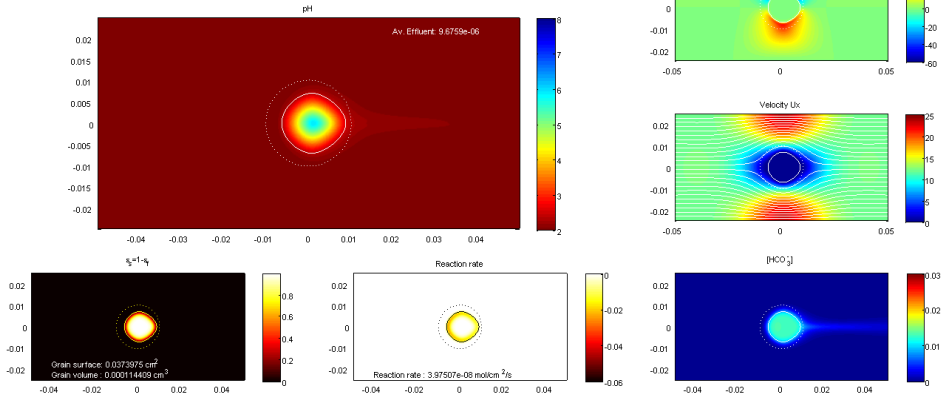

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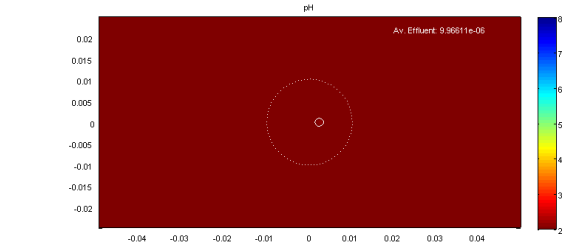
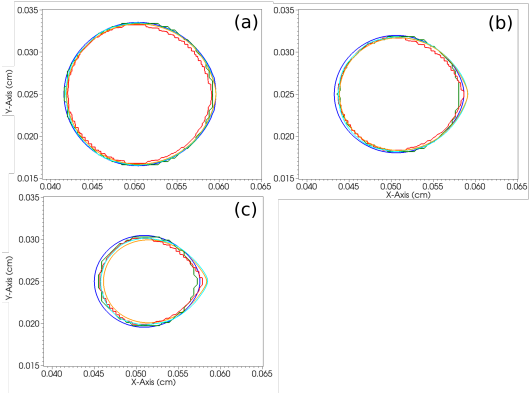
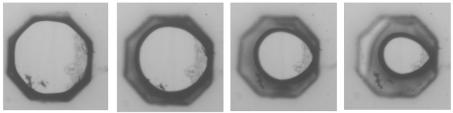


Calcite dissolution

Comparison of 2D dissolution at $t = 15, 30$ and 45min





- Cyan line is by S. Molins (Berkeley) using Chombo-Crunch,
- Red line is by C. Soulaine (Standford University) using OpenFOAM-DBS,
- Green line is by N. Prasianakis and A. Abbasi (PSI, Zürich) using Lattice Boltzman,
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- Dark blue line is the present method,
- Experimental work is from S. Roman.

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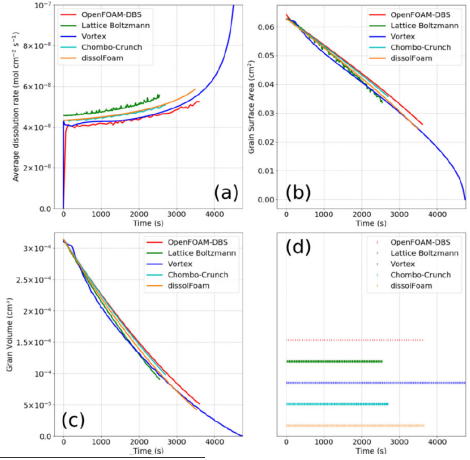

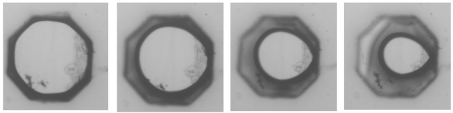

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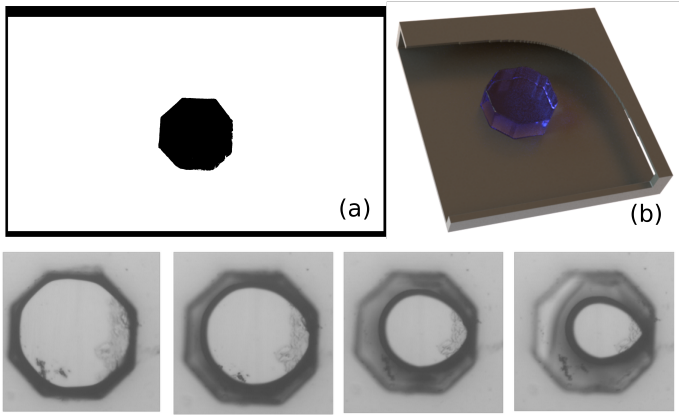

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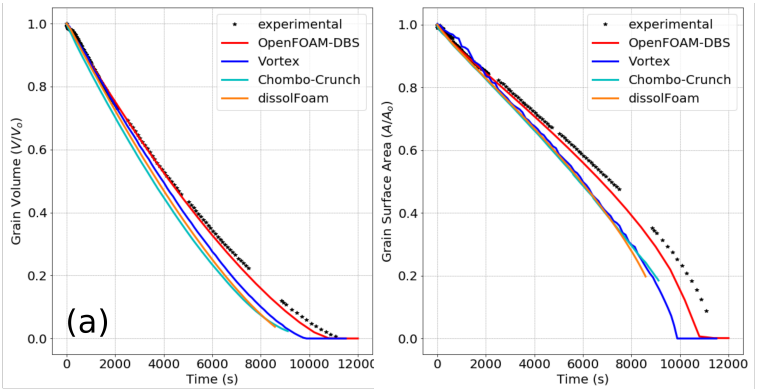

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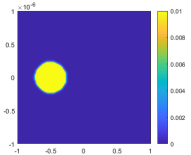
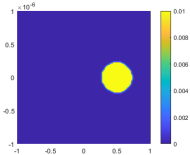
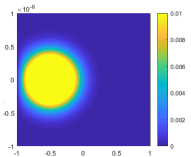
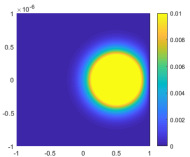
Pore-scale nucleation process (S. Perez)

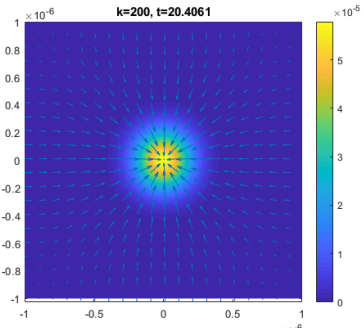
Non-divergence free velocity induced by reactive incompressible flows











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Concluding remarks

- Currently extended to GPU-CPU computing in library HySoP with J-M. Etancelin,
- Intensive use of the method's high efficiency for sensitivity analysis, uncertainty management and inverse problems,
- Particle-based methods are a good alternative for cross-validation,
- The benchmark can be extended to solid/fluid/gas (cf. C. Soulaine JFM 2018).
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