

# New trends in Vortex Methods for reactive flows

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# Summary

New trends in  
Vortex Methods for  
reactive flows

Philippe Poncet

Vortex methods

Complex 3D flows  
Complex geometries  
Rheology

Reactive flows  
Reactive model  
Calcite dissolution

Conclusion and  
perspectives

## Vortex methods

### Complex 3D flows

Complex geometries  
Rheology

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## Conclusion and perspectives



# What is a Vortex Method ?

Particle method involving vorticity and underlying grids

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- Navier-Stokes equations:

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

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

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

Vortex methods  
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*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*  
 *$\text{Grid} \Leftrightarrow \text{Particles}$*

- 
- M. El Ossmani and P. Poncet, *Efficiency of multiscale hybrid grid-particle vortex methods*, SIAM Multiscale Modeling & Simulation 8(5), 1671–1690 (2010).  
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- A particle is defined by a triplet Vortex-Location-Volume  $(\omega_p, \mathbf{x}_p, \mathbf{v}_p), p = 1..N$ :

$$d\omega_p/dt = [\omega \cdot \nabla \mathbf{u} + \mu \rho^{-1} \Delta \omega]_{\mathbf{x}_p(t)}, \quad d\mathbf{x}_p/dt = \mathbf{u}(\mathbf{x}_p(t)), \quad d\mathbf{v}_p(t)/dt = \mathbf{v}_p \text{div}(\mathbf{u}(\mathbf{x}_p)) = 0$$



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

$$\frac{\partial \mathbf{C}}{\partial t} + \text{div}(\mathbf{u} \mathbf{C}) - \text{div}(\sigma \nabla \mathbf{C}) = \mathbf{F}(\mathbf{C}) \implies d\mathbf{C}_p/dt = \mathbf{F}(\mathbf{C}_p) + [\text{div}(\sigma \nabla \mathbf{C})]_{x_p(t)}$$



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# High resolution Newtonian flow in sandstones

Simulations at  $1024^3$

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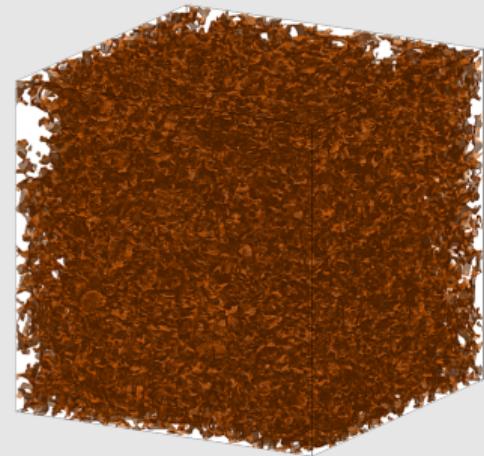
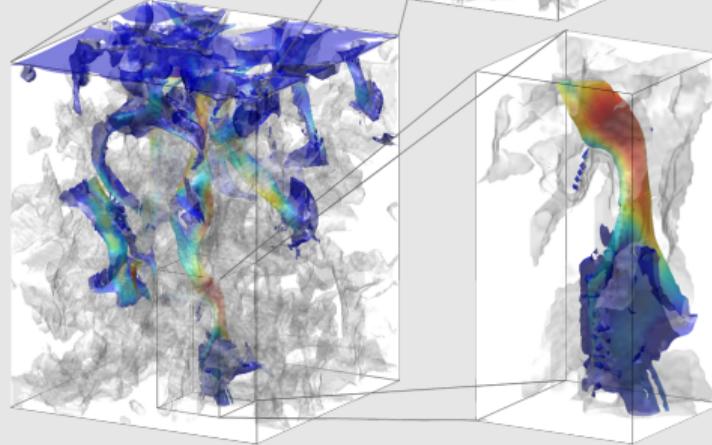
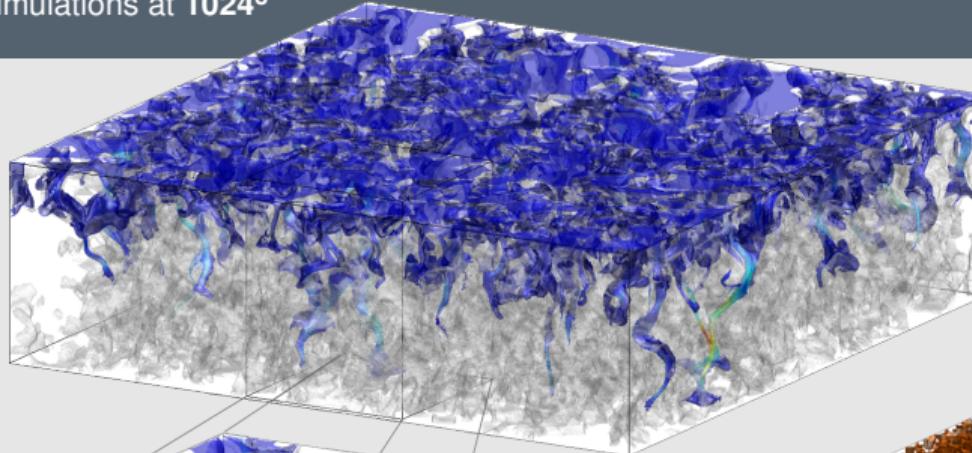
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# Newtonian flow around bead stacks

## Permeability estimation of real rock sample

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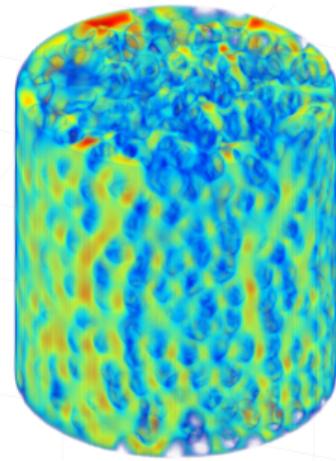
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$$-\operatorname{div}(2\mu D) + \chi_{B(t)} K^{-1} u = f - \nabla p$$

where  $D = (\nabla u + \nabla u^T)/2$  and  $\operatorname{div} u = 0$

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).



# Rheology and shear-thinning flows

## Miscible heterogeneous Xanthan transport

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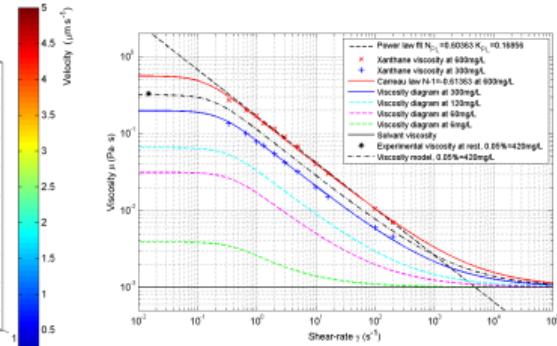
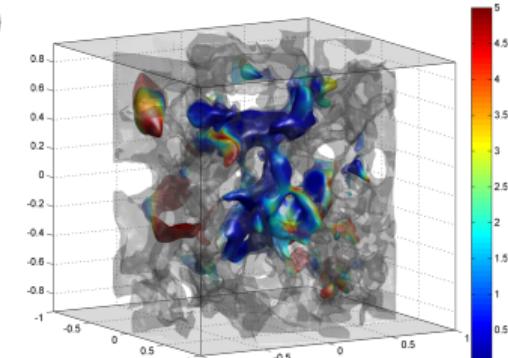
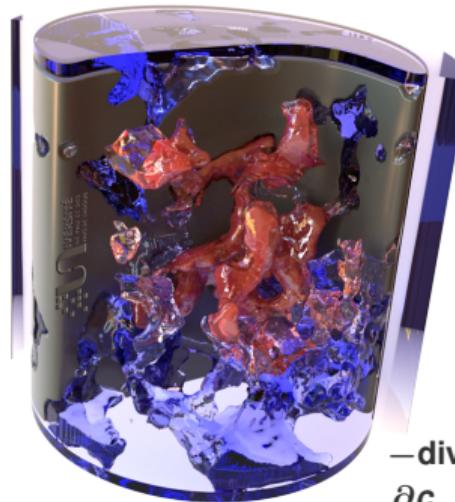
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$$\begin{aligned}
 & -\operatorname{div}(2\mu(c, D) D) + \chi_{B(t)} K^{-1} u = f - \nabla p \\
 & \frac{\partial c}{\partial t} + \operatorname{div}(uc) - \sigma \Delta c = 0, \quad \text{where } D = (\nabla u + \nabla u^T)/2 \text{ and} \\
 & \mu(c, D) = \mu_\infty + (\mu_0(c) - \mu_\infty) (1 + 2\beta(c)^2 |D|^2)^{\frac{q(c)-2}{2}}
 \end{aligned}$$

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*, Submitted.

R. Chatelin, D. Sanchez and P. Poncet, Analysis of penalized variable viscosity 3D Stokes equations coupled with transport and diffusion, *ESAIM: Math. Model. Numer.* 50:2, 565-591 (2016).



# Reactive flow using superficial velocity

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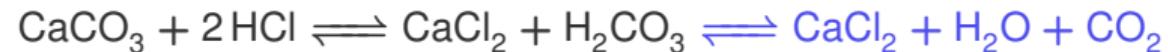
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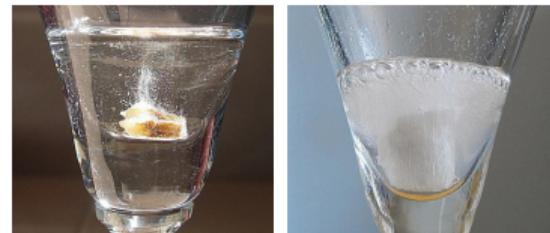
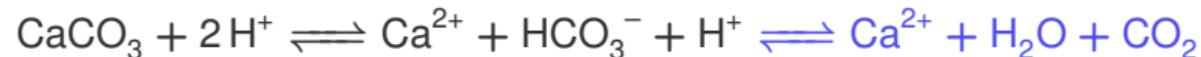
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or



Calcite in Hydrochloric Acid



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

$$\varepsilon^{-1} \frac{\partial \rho \mathbf{u}}{\partial t} + \varepsilon^{-1} \operatorname{div}(\varepsilon^{-1} \rho \mathbf{u} \otimes \mathbf{u}) + \nabla p - \varepsilon^{-1} \mu \Delta \mathbf{u} + \mu \underbrace{\frac{(1-\varepsilon)^2}{\varepsilon^3} K_0^{-1} \mathbf{u}}_{\text{Kozeny-Carman law}} = \mathbf{f}$$
$$\operatorname{div} \mathbf{u} = 0$$
$$\frac{\partial \varepsilon}{\partial t} = K_d(1-\varepsilon)\mathbf{C} - K_p v \mathbf{C}_2 \mathbf{C}_3$$
$$\frac{\partial \mathbf{C}}{\partial t} + \operatorname{div}(\varepsilon^{-1} \mathbf{u} \mathbf{C}) - \underbrace{\operatorname{div}(\sigma(\varepsilon) \nabla \mathbf{C})}_{\text{Archie law}} = -\dot{\varepsilon}/v$$

+ adequate initial and boundary conditions

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



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$$\left\{ \begin{array}{l} u(x, t) = \lim_{s \rightarrow +\infty} u_e(x, t, s) \text{ with } u_e(x, t, 0) = u(x, t - \delta t) \text{ and} \\ \frac{\partial u_e}{\partial s} - \mu \Delta u_e + \mu \frac{(1 - \varepsilon)^2}{\varepsilon^2} K_0^{-1} u_e = \varepsilon(f - \nabla p) \\ \operatorname{div} u = 0 \\ \frac{\partial \varepsilon}{\partial t} = K_d(1 - \varepsilon)C \\ \frac{\partial C}{\partial t} + \operatorname{div}(\varepsilon^{-1} u C) - \operatorname{div}(\sigma(\varepsilon) \nabla C) = -\dot{\varepsilon}/v \\ + \text{adequate initial and boundary conditions} \end{array} \right.$$

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# Vortical formulation

Time-splitting method

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$$\frac{\partial \omega}{\partial s} - \mu \Delta \omega + \mu K_0^{-1} \operatorname{curl} \left( \frac{(1-\varepsilon)^2}{\varepsilon^2} u \right) = 0 \iff \frac{\partial u}{\partial s} - \mu \Delta u + \mu K_0^{-1} \frac{(1-\varepsilon)^2}{\varepsilon^2} u = -\nabla(\dots)$$

where  $u = \operatorname{curl} \Psi - \nabla \phi$  and  $-\Delta \Psi = \omega$

↓

$\frac{\partial u}{\partial s} + \mu K_0^{-1} \frac{(1-\varepsilon)^2}{\varepsilon^2} u = 0$	: Exact solution
$\omega(t) = \operatorname{curl} u(t)$	: Straightforward FD scheme
$\frac{\partial \omega}{\partial s} - \mu \Delta \omega = 0$	: FD or Fast solver based of pure FFT
$u = \operatorname{curl} \Delta^{-1} \omega - \nabla \phi$	: FFT + FD
$\frac{\partial C}{\partial t} + \operatorname{div}(\varepsilon^{-1} u C) - \operatorname{div}(\sigma(\varepsilon) \nabla C) = -\dot{\varepsilon}/\nu$	: Lagrangian + Interpolation

Computational time still scales as  $\mathcal{O}(N \log N)$

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# Calcite dissolution – Snapshots

Different time scales, Re=0.24, pH=2, at resolution **512 × 256**

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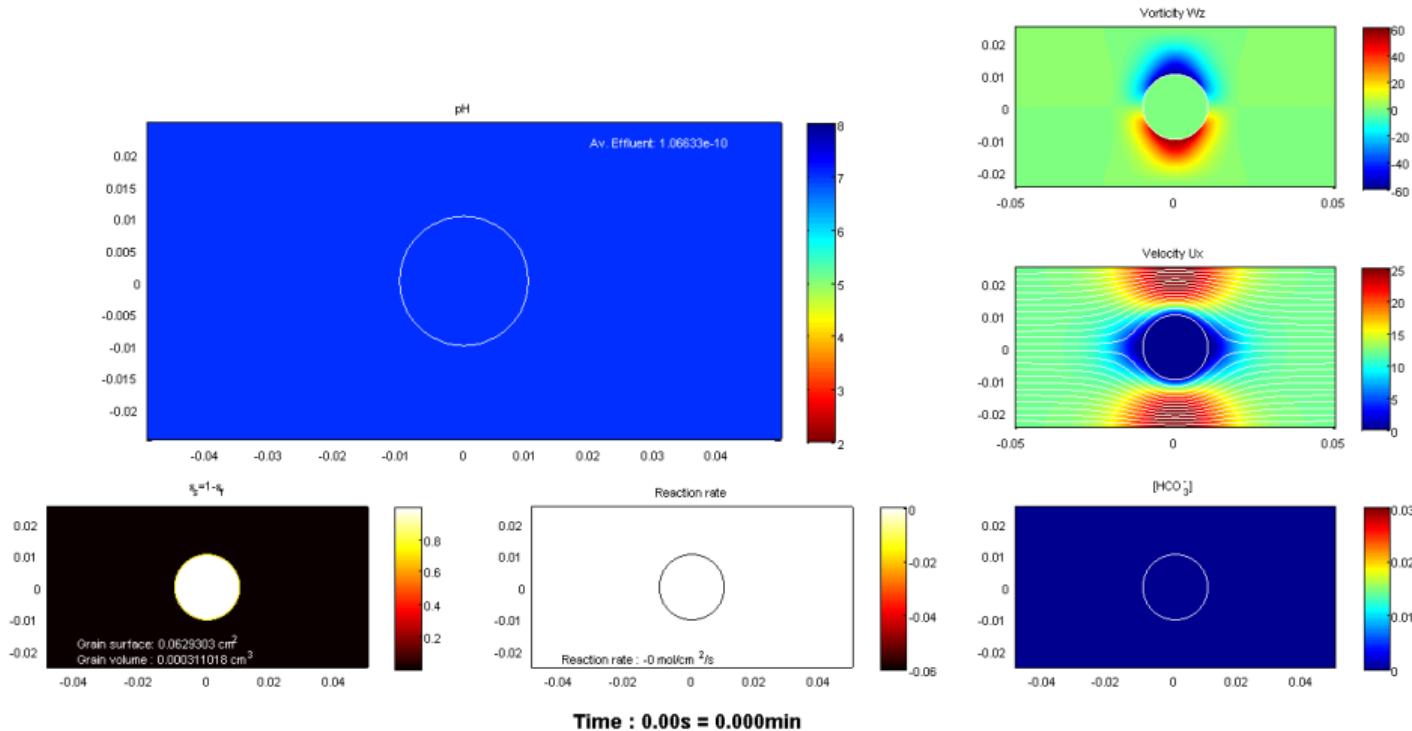
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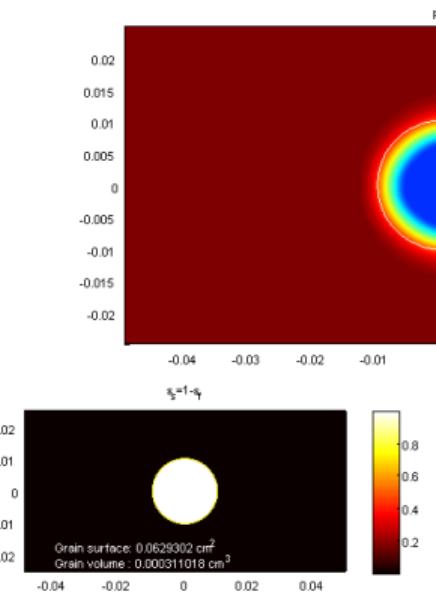
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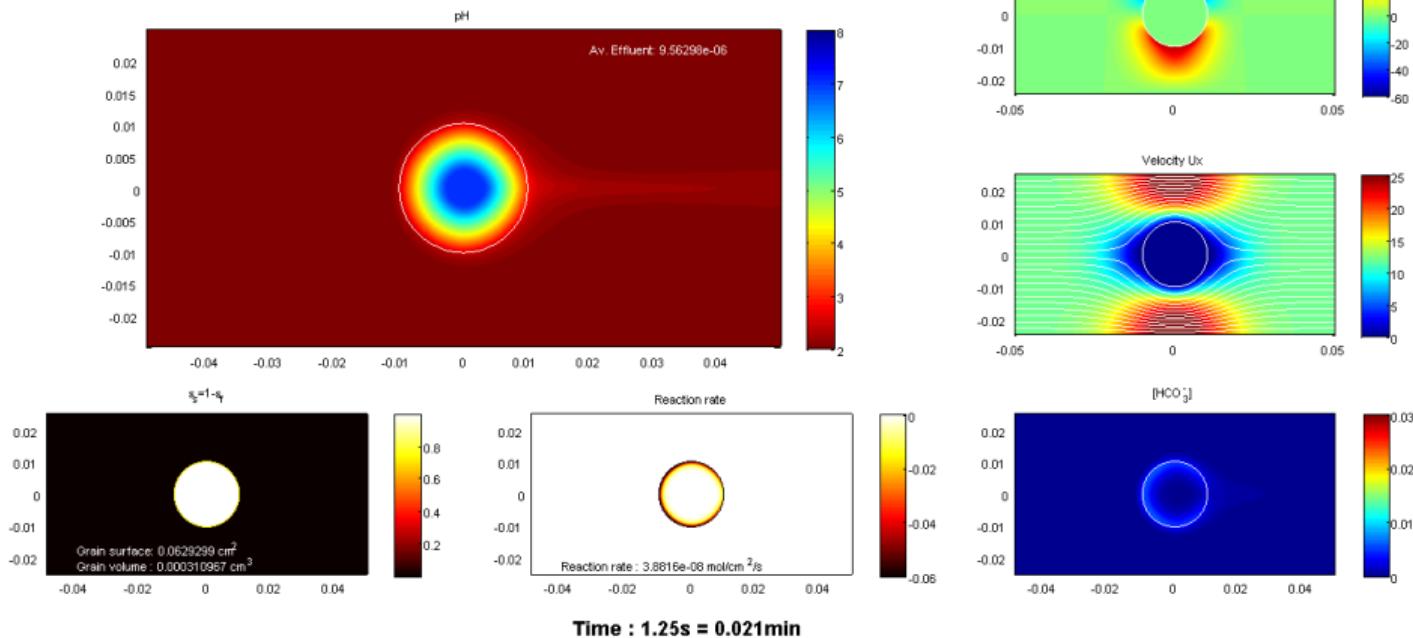
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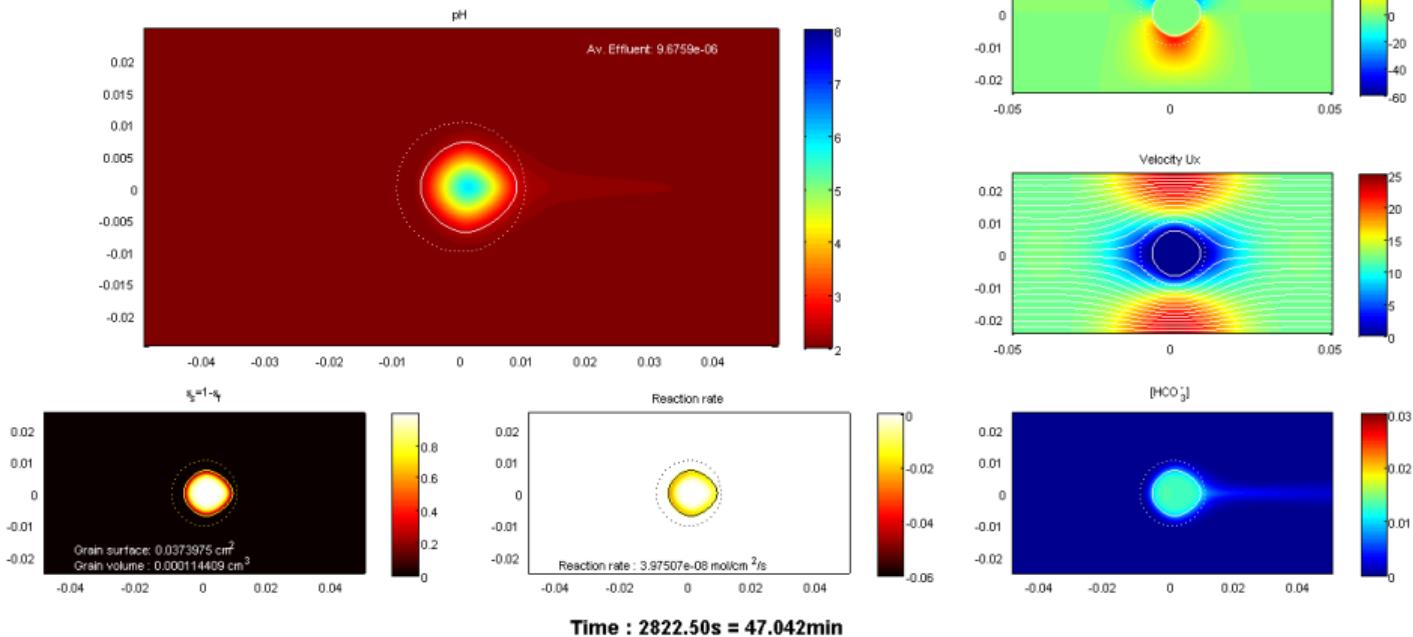
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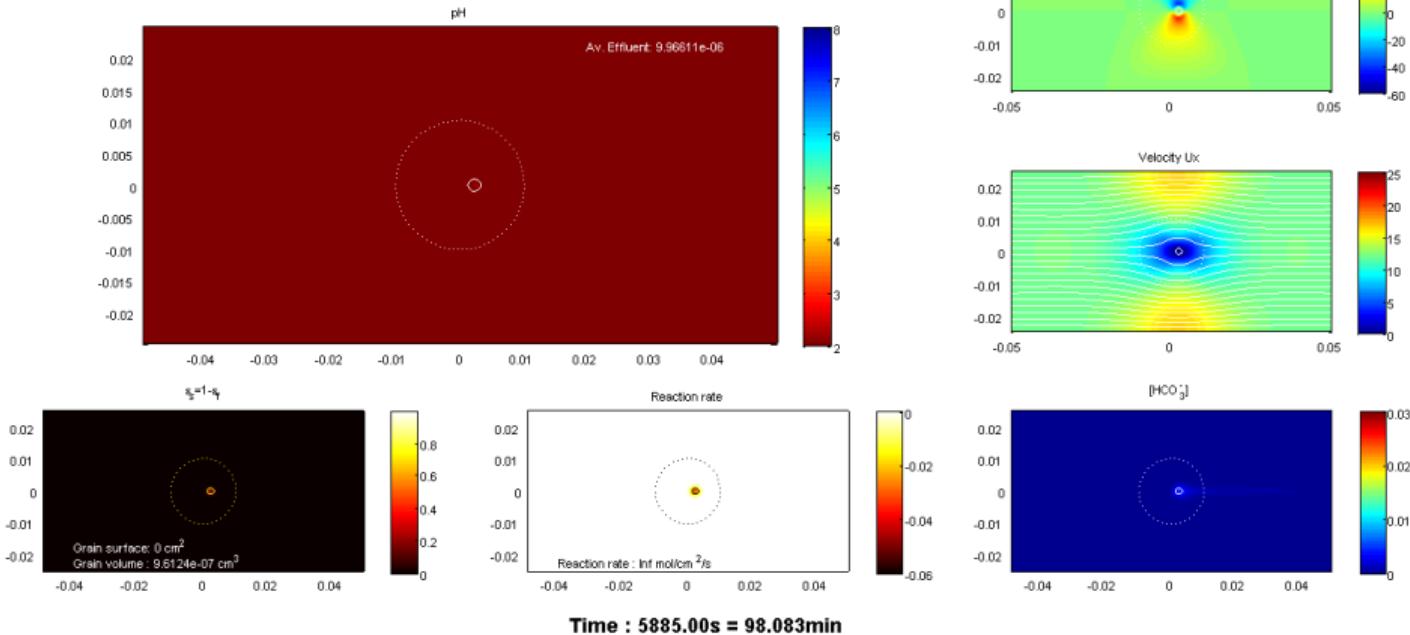
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# Calcite dissolution – Comparison at $t = 45\text{min}$

Joint work with S. Molins, C. Soulaine, N. Prasianakis and A. Abbasi.

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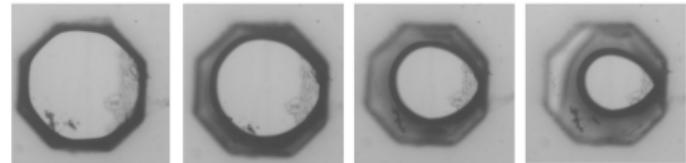
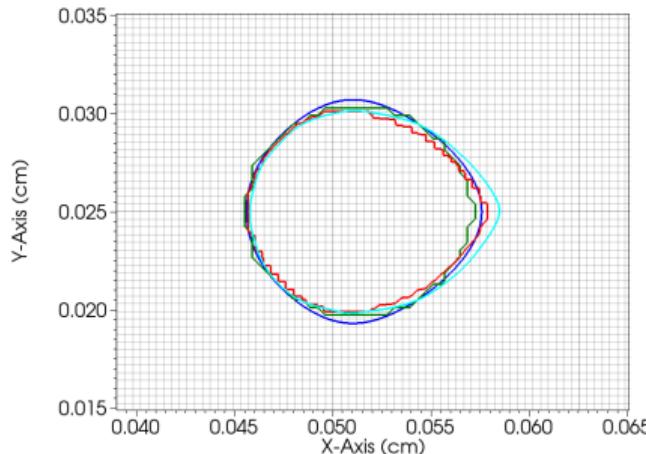
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- ▶ Cyan line is by S. Molins (Berkeley) using Chombo-Crunch,
- ▶ Red line is by C. Soulaine (JFM 827, 2017) using OpenFOAM,
- ▶ Green line is by N. Prasianakis and A. Abbasi (PSI, Zürich) using Lattice Boltzman,
- ▶ Dark blue line is the present method (Vortex Method),
- ▶ Experimental work is from S. Roman.



# Flexibility and robustness of 3D Vortex Methods

Dissolution at  $\text{Re}=24$ ,  $\text{pH}=1$

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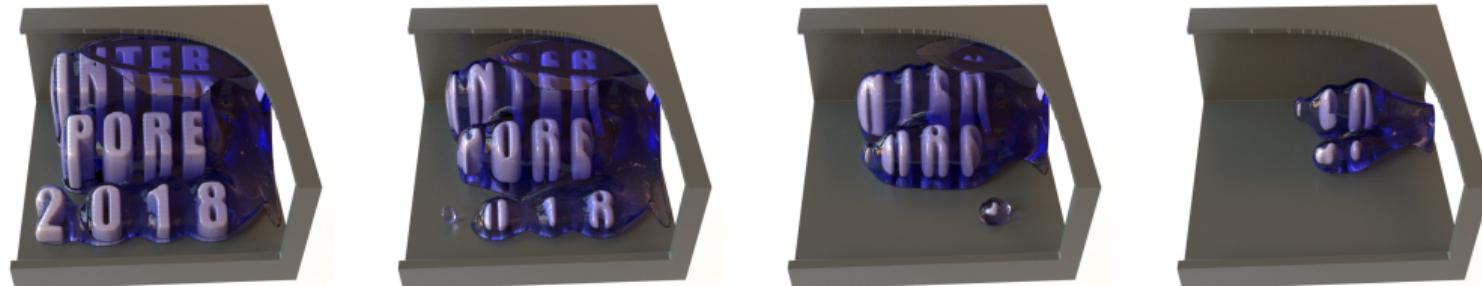
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# Flexibility and robustness of 3D Vortex Methods

Animation at Re=24, pH=1

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# Conclusion

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- ▶ Currently extended to GPU-CPU computing (library HySoP),
- ▶ Still "young" methods in geo-science, but they show a good potential,
- ▶ Intensive use of the method high efficiency for sensitivity analysis and uncertainty management,
- ▶ Acknowledgment of the following fundings:



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# Thank you for your attention



## Supplementary material :





# Vortical formulation

## Stokes-Brinkman and its vorticity

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Complex 3D flows

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Calcite dissolution

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One gets the Stokes-Brinkman equation:

$$\frac{\partial \mathbf{u}}{\partial \mathbf{s}} - \mu \Delta \mathbf{u} + \mu \frac{(1-\varepsilon)^2}{\varepsilon^2} K_0^{-1} \mathbf{u} = \varepsilon (\mathbf{f} - \nabla p)$$

||  
↓  $\omega = \operatorname{curl} \mathbf{u}$

$$\frac{\partial \omega}{\partial \mathbf{s}} - \mu \Delta \omega + \mu K_0^{-1} \operatorname{curl} \left( \frac{(1-\varepsilon)^2}{\varepsilon^2} \mathbf{u} \right) = \nabla p \wedge \nabla \varepsilon \simeq 0$$

where  $\mathbf{u} = \operatorname{curl} \Psi - \nabla \phi$  and  $-\Delta \Psi = \omega$

or  $-\Delta \mathbf{u} = \operatorname{curl} \omega + \mathbf{B.C.}$

---

If needed,  $-\operatorname{div}(\varepsilon \nabla p) = \mu \mathbf{u} \cdot \nabla K^{-1}(\varepsilon)$



# Vortical formulation

General philosophy of time-splitting –or fractional step– methods

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$$\begin{cases} y'(t) = (A + B)y(t) \\ y(0) = y_0 \end{cases} \quad \text{implies} \quad y(t) = e^{(A+B)t}y_0$$



$$\begin{cases} y'_1(t) = Ay(t) \\ y_1(0) = y_0 \end{cases} \quad \text{and} \quad \begin{cases} y'_2(t) = By(t) \\ y_2(0) = y_1(\delta t) \end{cases}$$

$$\text{imply } y_2(\delta t) = e^{Bt}y_2(0) = e^{Bt}y_1(\delta t) = e^{At}e^{Bt}y_0$$



$$\begin{cases} y(\delta t) = \left( I + \delta t(A + B) + \frac{\delta t^2}{2}(A^2 + AB + BA + B^2) + \dots \right) y_0 \\ y_2(\delta t) = \left( I + \delta t(A + B) + \frac{\delta t^2}{2}(A^2 + 2AB + B^2) + \dots \right) y_0 \end{cases}$$

$$\text{finally leads to } y_2(\delta t) = y(\delta t) + [AB - BA]\delta t^2/2 + \mathcal{O}(\delta t^3)$$



# Diffusion into quasi-impermeable media

## Archie law and related models

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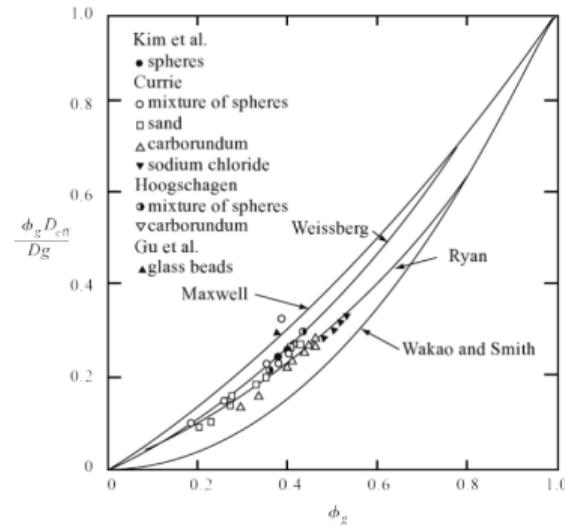
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$$\text{Diffusion } \sigma(\epsilon) = \epsilon D_M$$



Crystal porosity  $\epsilon = 10^{-3} - 2 \cdot 10^{-2}$



# Calcite dissolution – Benchmark setup

Joint work with S. Molins, C. Soulaine, N. Prasianakis and A. Abbasi.

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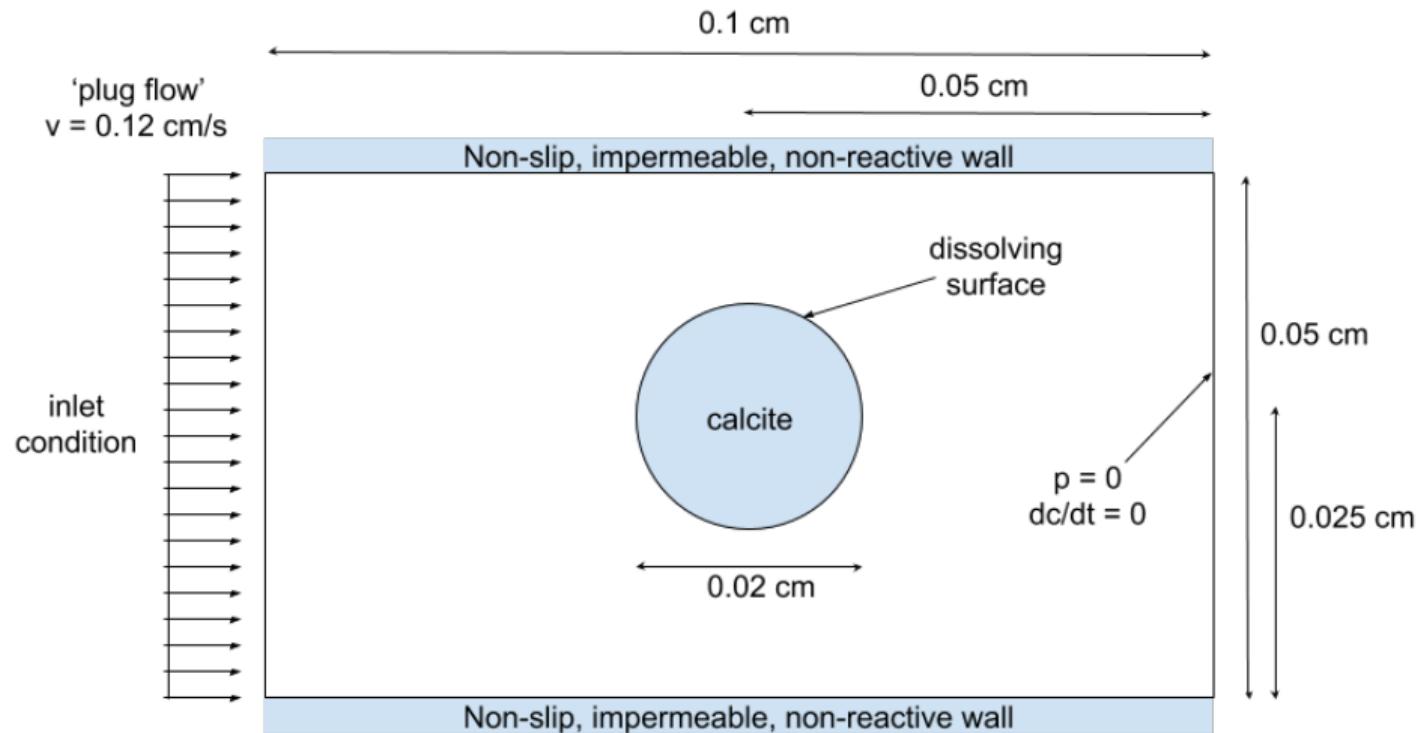
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