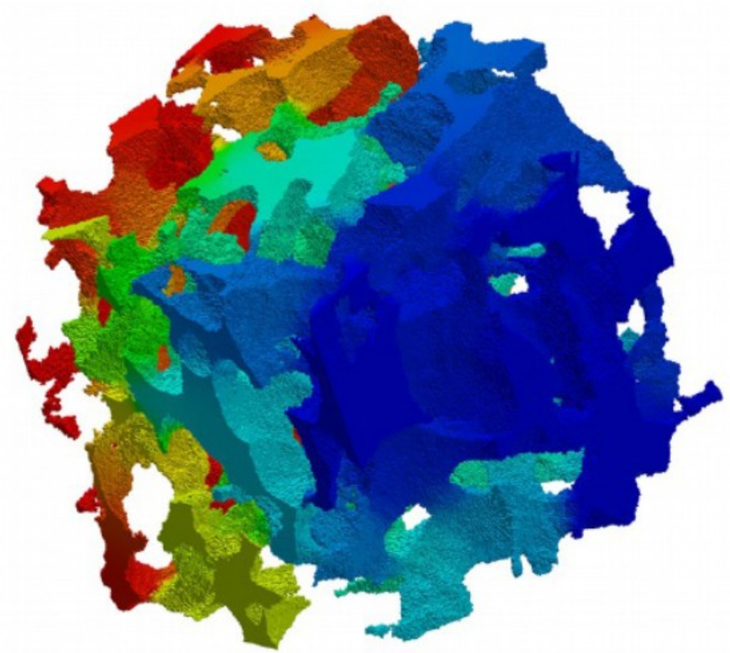
Mineral Dissolution and Wormholing from a Pore-Scale Perspective

Interpore Conference, Rotterdam

May 8-12, 2017



Cyprien Soulaine (csoulain@stanford.edu)

Sophie Roman,

Anthony Kovscek,

Hamdi A. Tchelepi

Stanford
SCHOOL OF EARTH, ENERGY & ENVIRONMENTAL SCIENCES | Energy Resources Engineering

Pore-scale processes associated with subsurface CO_2 injection and sequestration

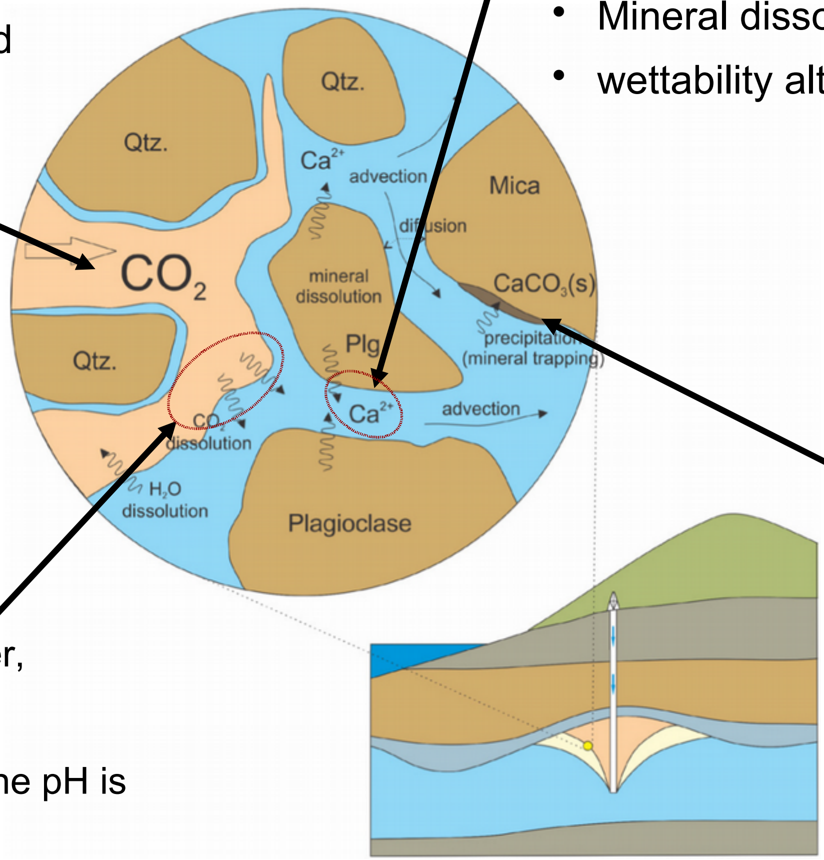
1 Drainage, imbibition and trapping mechanism

2 Interphase mass transfer, sCO2/brine dissolution,

Aqueous speciation, brine pH is lowered

3
- Transport of acid to the mineral surface,
- Mineral dissolution,
- wettability alteration

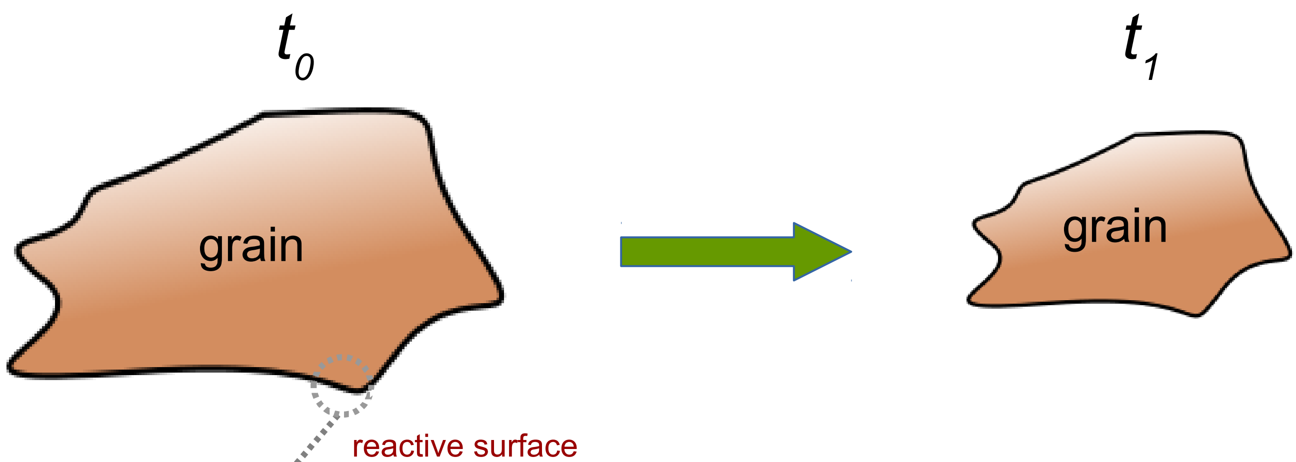
4 Precipitation

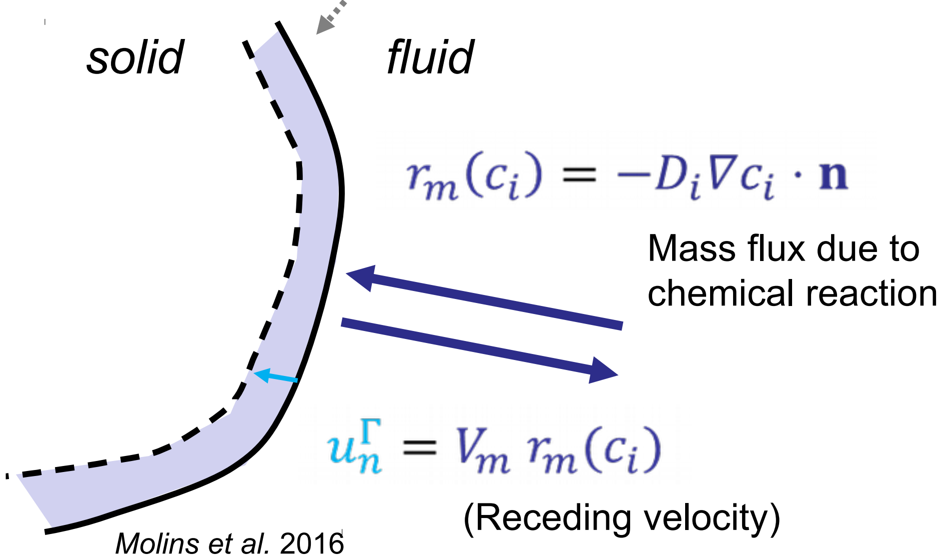


Steefel et al. 2013

Steefel et al., *Pore Scale Processes Associated with Subsurface CO2 Injection and Sequestration* Reviews in Mineralogy and Geochemistry, 2013, 77, 259-303

Solid dissolution at the grain scale

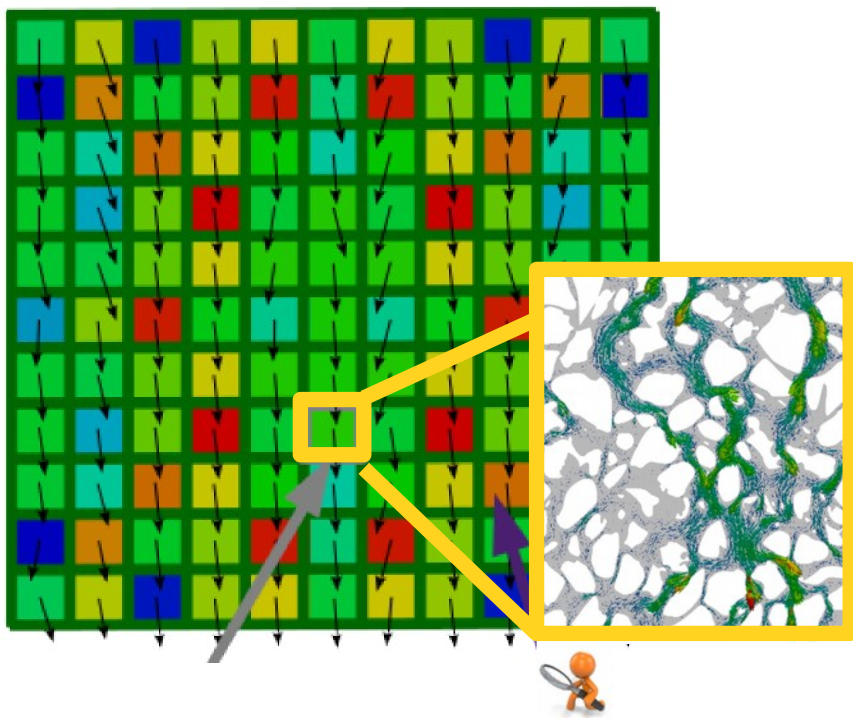




Physics of fluid:

- Navier-Stokes equations
- Advection-diffusion equation for the acid component
- Boundary conditions

Modeling dissolution at Darcy's scale



- Darcy scale = averaged equations with averaged properties (permeability, surface area...)
- How does the permeability evolves when the pore-structure changes due to the dissolution/precipitation?
- What is the surface area accessible to the acid component? Complex interplay of diffusion, convection, reaction, gravity*

$$\langle \dot{m}_A \rangle = A_e k \alpha \left(\langle C_A \rangle - C_{eq} \right)$$

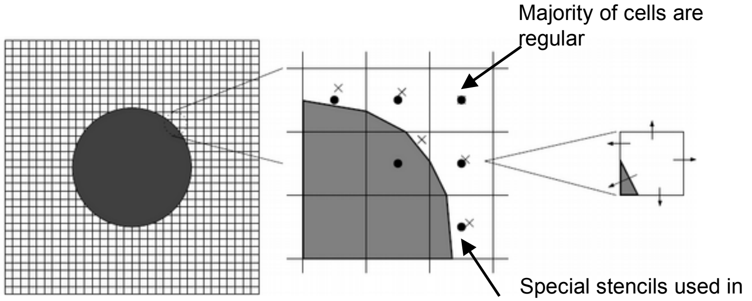
Bottom-up strategy: go back to the pore-scale to

- Improve our understanding of the phenomena,
- Derive better Darcy's scale model,
- Characterize effective properties (effective surface area, permeability, exchange coefficient, dispersion tensor….)

*Oltéan et al. *Numerical and experimental investigation of buoyancy-driven dissolution in vertical fracture* Journal of Geophysical Research: Solid Earth, Wiley Online Library, 2013, 118, 2038-2048

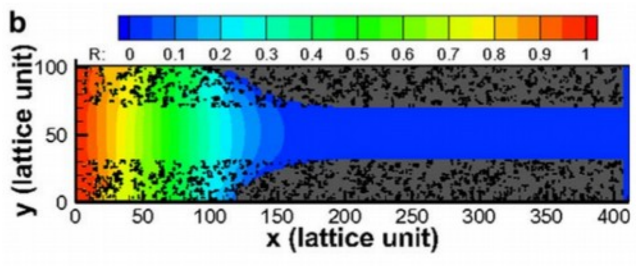
What approaches for pore-scale dissolution?

1. Embedded boundary method (*Trebotich and Graves* 2015), Level Set (*Li et al.* 2008, *Li et al.* 2010, *Xu et al.* 2012...)



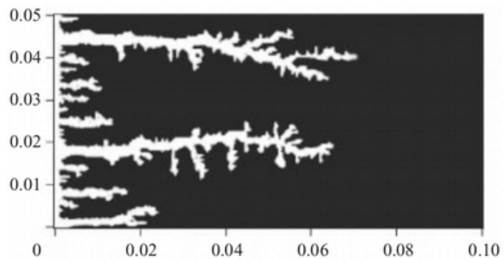
Trebotich and Graves 2015

2. Lattice Boltzmann approach (*Kang et al.* 2003, *Szymczak and Ladd* 2004, *Szymczak and Ladd* 2009, *Huber et al.* 2014, *Chen et al.* 2014...)



Chen et al. 2014

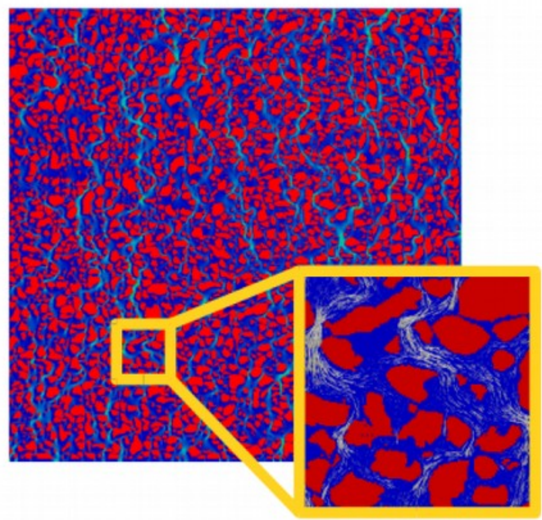
3. Micro-continuum approach (*Golfier et al.* 2002, *Luo et al.* 2012, *Luo et al.* 2014, *Guo et al.* 2015, *Guo et al.* 2016, *Soulaine and Tchelepi* 2016...)



Golfier et al. 2002

Micro-continuum: an intermediate approach

direct modeling

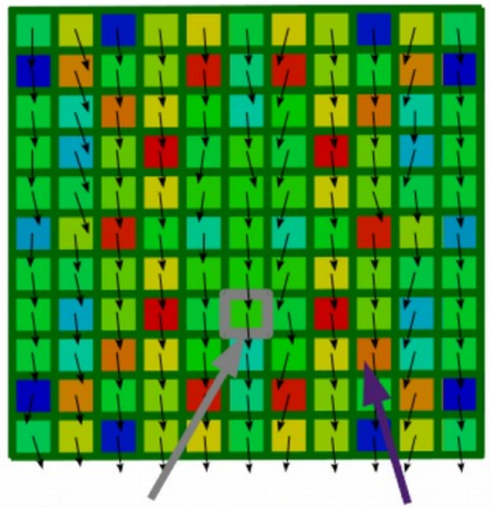


(Navier-Stokes)

Micro-continuum

- Volume averaged equations
- Flow governs by Darcy-Brinkman-Stokes equation (DBS)
- Degenerates to direct models in cells containing fluid only
- Porous media formulation in the matrix
- Immersed boundary conditions

continuum modeling

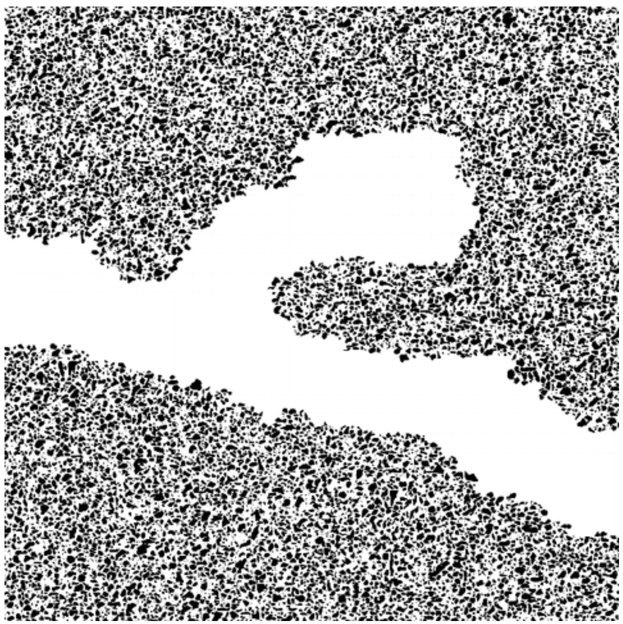


(Darcy)

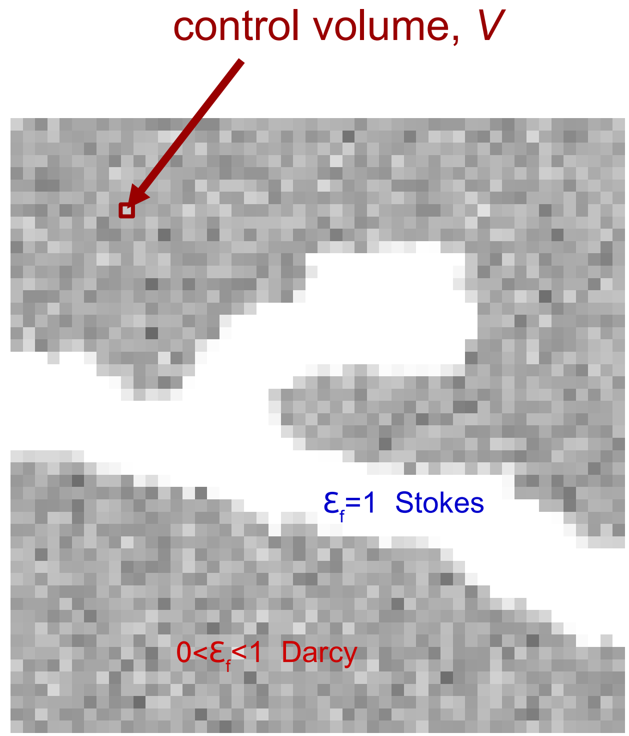
for every point of the domain

fluid **OR** solid | fluid **AND/OR** solid | fluid **AND** solid

A micro-continuum approach



Full Navier-Stokes approach



Filtering approach

Solid and fluid differentiated by the void fraction per control volume:

$$\varepsilon_f$$

Volume averaged variables:

$$\bar{\mathbf{v}}_f = \frac{1}{V}\int_{V_f} \mathbf{v}_f dV$$

$$\bar{p}_f = \frac{1}{V_f}\int_{V_f} p_f dV$$

The Darcy-Brinkman-Stokes equation allows a single domain formulation

$$0 = -\nabla \bar{p}_f + \frac{\mu_f}{\varepsilon_f}\nabla^2 \bar{\mathbf{v}}_f - \mu_f k^{-1} \bar{\mathbf{v}}_f$$

Vanishes in the void space

Dominant in the porous region

Soulaine and Tchelepi *Micro-continuum approach for pore-scale simulation of subsurface processes* Transport in Porous Media (2016)

Micro-continuum model for reactive surface[1,2]

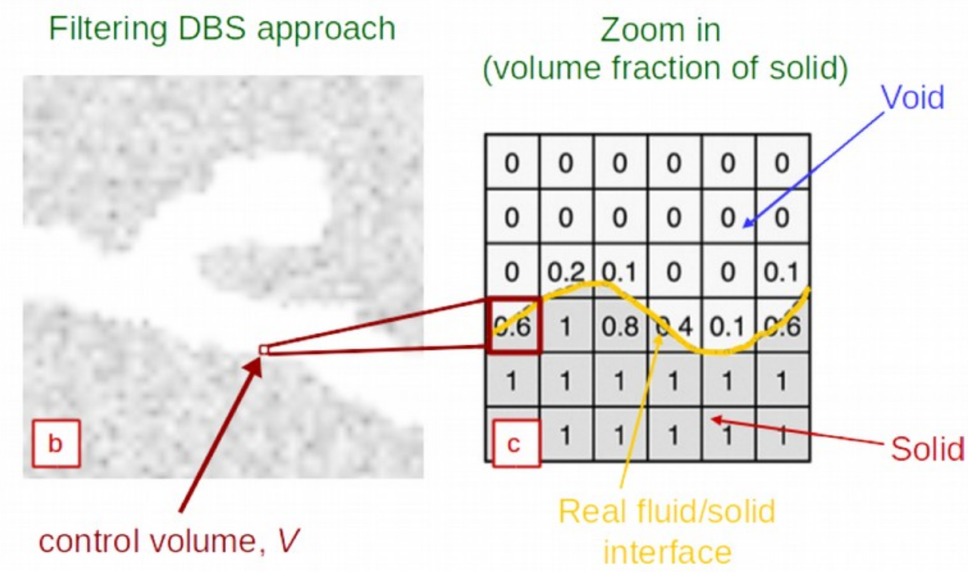
- Darcy-Brinkman model

- Mass balance for solid

$$\frac{\partial \varepsilon_s \rho_s}{\partial t} = -\dot{m}$$

- Mass balance for fluid

$$\frac{\partial \varepsilon_f \rho_f}{\partial t} + \nabla.\left(\rho_f \bar{\mathbf{v}}_f\right) = \dot{m}$$



- Mass balance equation of acid in the fluid

$$\frac{\partial \varepsilon_f \rho_f \bar{\omega}_{f,A}}{\partial t} + \nabla.\left(\rho_f \bar{\mathbf{v}}_f \bar{\omega}_{f,A}\right) = \nabla.\left(\varepsilon_f \rho_f D_A^* \nabla \bar{\omega}_{f,A}\right) - \dot{m}_{f,A}$$

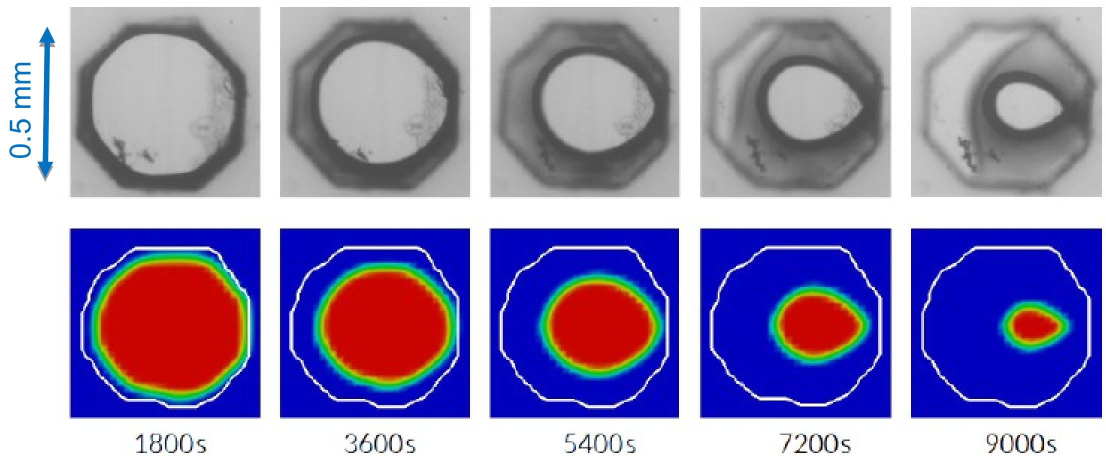
- Rate of dissolution modeled from grain scale

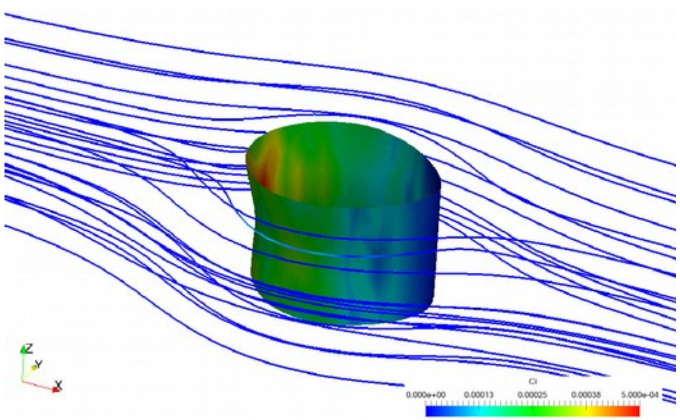
$$\dot{m} = \Gamma \dot{m}_{f,A} \qquad \dot{m}_{f,A} = \rho_f \alpha^* \left(\bar{\omega}_{f,A} - \omega_{eq}\right) \qquad \alpha^* = k a_v = k \left\|\nabla \varepsilon_s\right\|$$

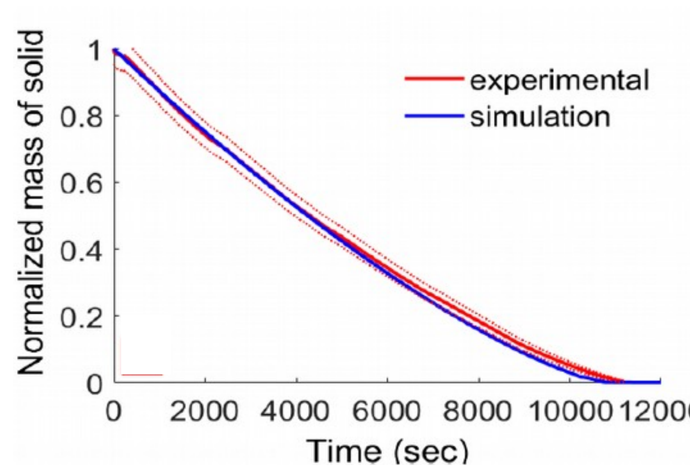
[1] Golfier et al. *On the ability of a Darcy-scale model to capture wormhole formation during the dissolution of a porous medium*. Journal of fluid Mechanics (2002)
[2] Soulaine and Tchelepi *Micro-continuum approach for pore-scale simulation of subsurface processes* Transport in Porous Media (2016)

Calcite dissolution: simulation vs experiment*

- Dissolution of a calcite crystal in a micro-channel (collaboration with Sophie Roman and Tony Kovscek, Stanford University, SUPRI-A),
- Acquisition of a high resolution dataset to compare with numerical simulations.

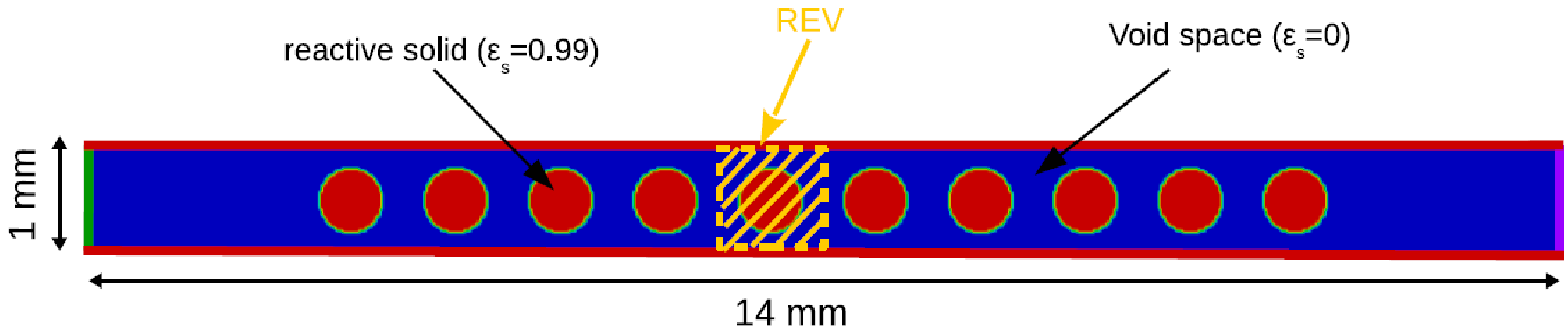






*Soulaine et al. *Mineral dissolution and wormholing from a pore-scale perspective* (under review)

Upscaling of the pore-scale dissolution



- Solve the pore-scale dissolution problem for different flow conditions,
- Upscale the results by averaging on a REV,
- Find correlation based on dimensionless numbers.

Péclet number (Pe)

$$P\acute{e} = \frac{v_0 l_c}{D} = \frac{v_0 \sqrt{k}}{D}$$

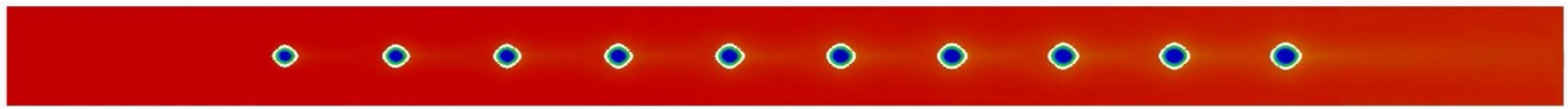
Damkhöler number (Da_{II})

$$Da_{II} = \frac{r l_c}{D} = \frac{r}{A_e D}$$

*Soulaine et al. *Mineral dissolution and wormholing from a pore-scale perspective* (under review)

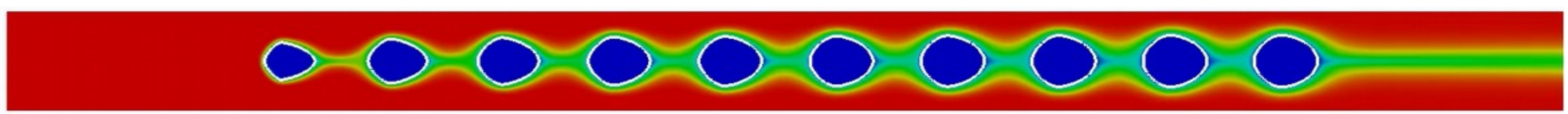
Simulation results

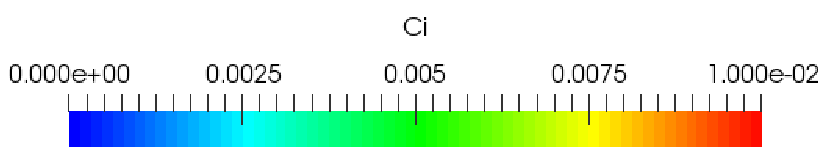
(Pé = 9 ; Da_{II} = 0.5)



(Pé = 0.9 ; Da_{II} = 50)

(Pé = 90 ; Da_{II} = 50)





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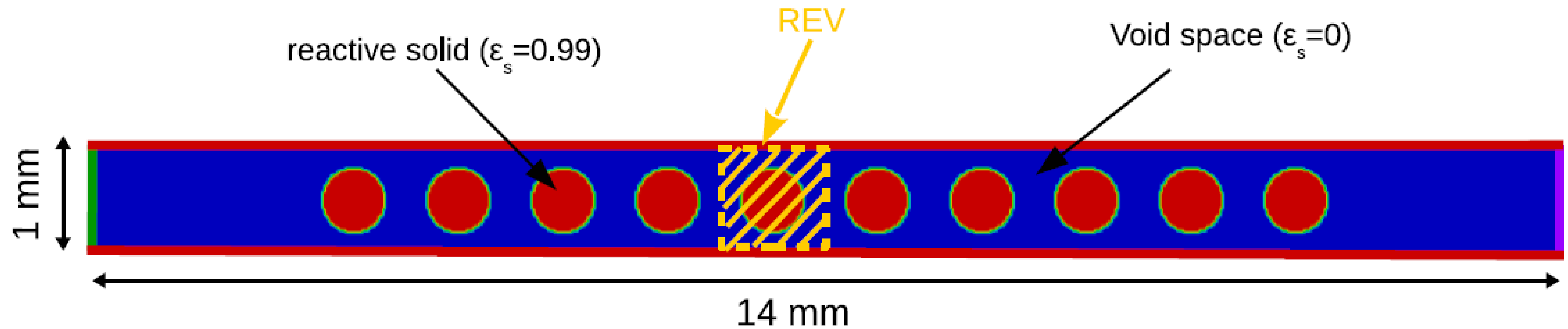
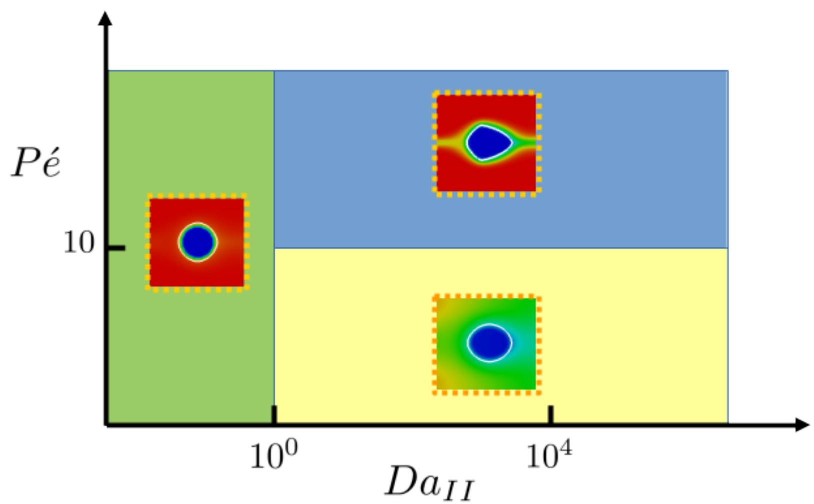
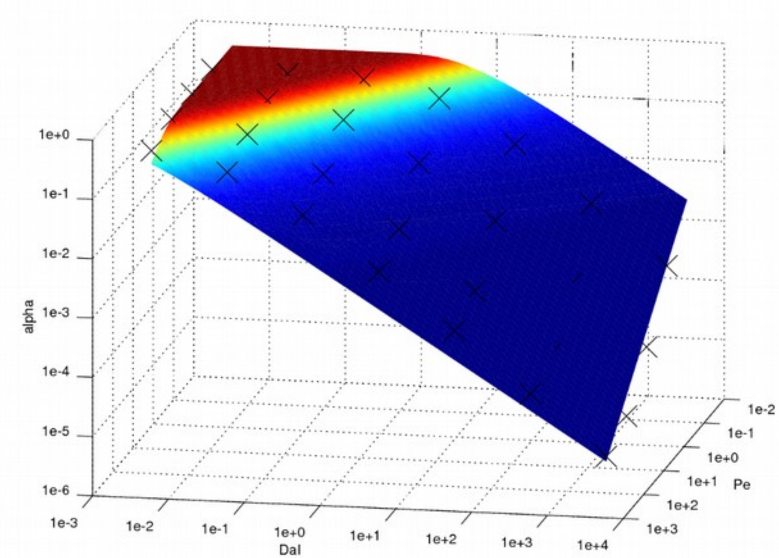
Upscaling of the pore-scale dissolution



$$\langle \dot{m}_A \rangle = A_e k \alpha \left(\langle C_A \rangle - C_{eq} \right)$$

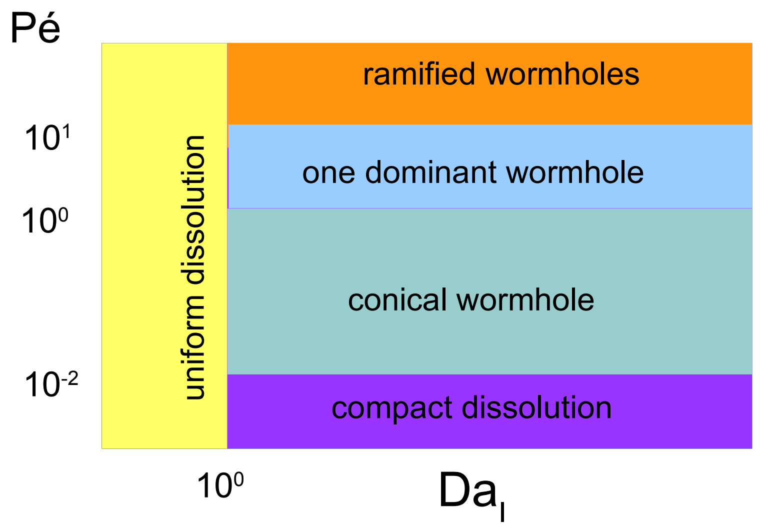


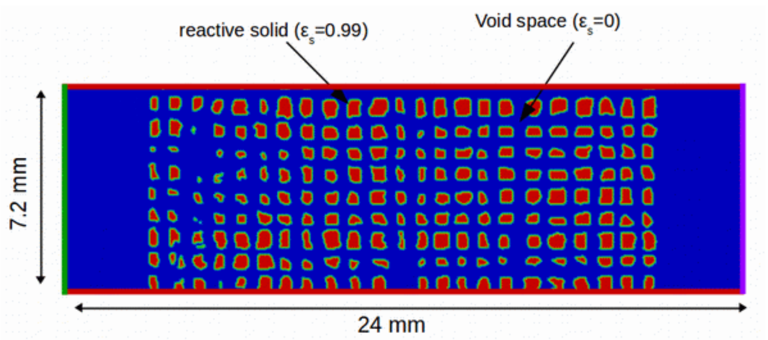


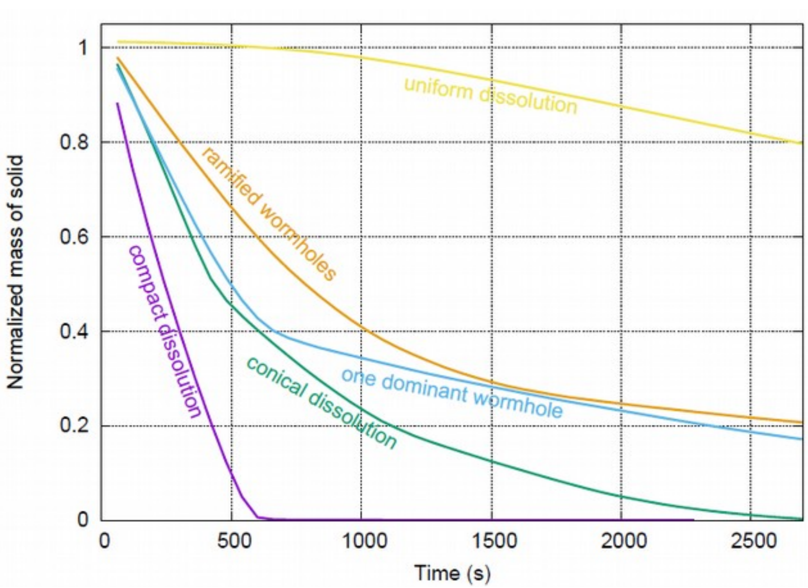
$$\alpha = 1 - \exp\left(-Pe^{-n} \left(\frac{Da_{II}}{Pe} \right)^{-m} \right)$$

*Soulaine et al. *Mineral dissolution and wormholing from a pore-scale perspective* (under review)

Differents dissolution regimes*



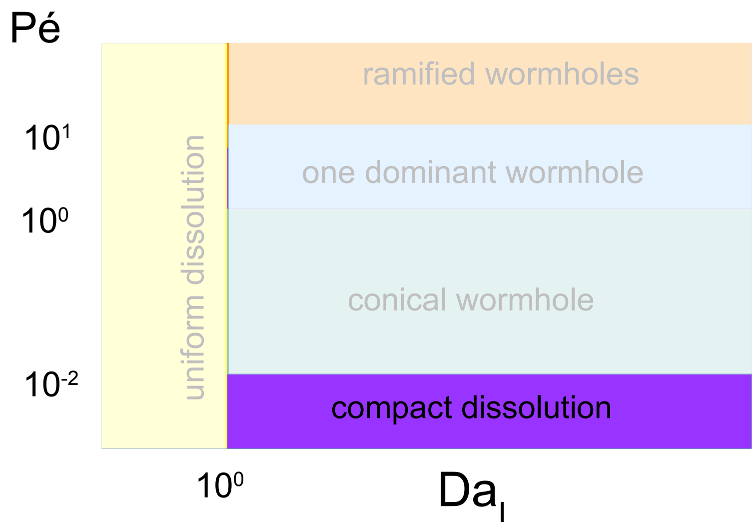


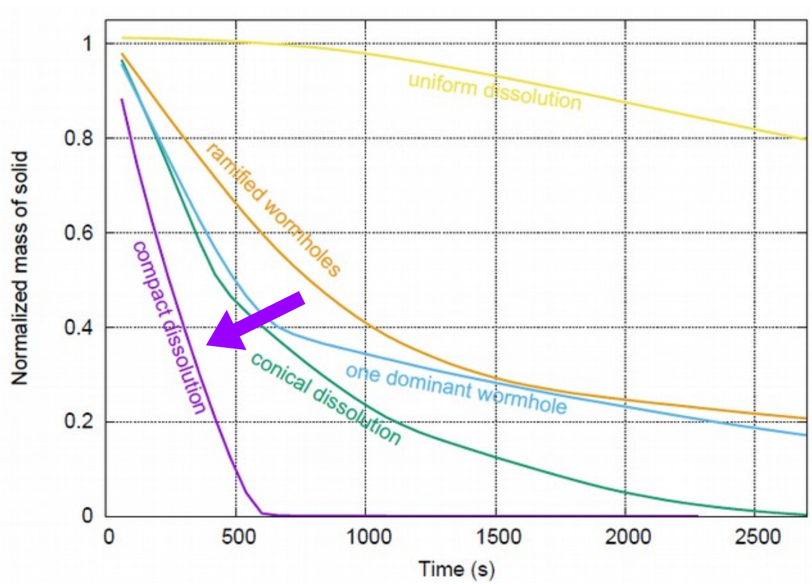


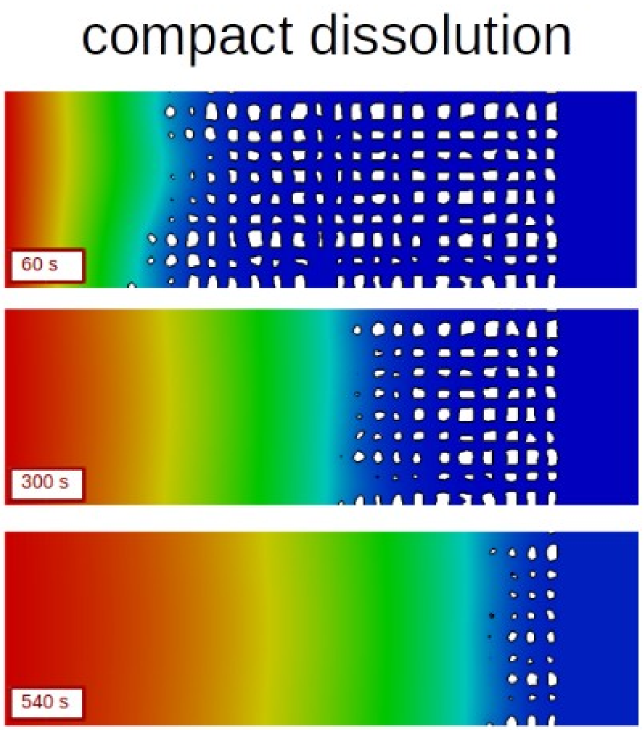
- Identification of 5 dissolution regimes according to the injection flow rate and the mineral reactivity,
- Emergence of dissolution instability due to the local heterogeneities in the velocity profile,
- Direct consequences on the mean dissolution rate and the permeability/porosity relationship.

*Soulaine et al. *Mineral dissolution and wormholing from a pore-scale perspective* (under review)

Differents dissolution regimes*

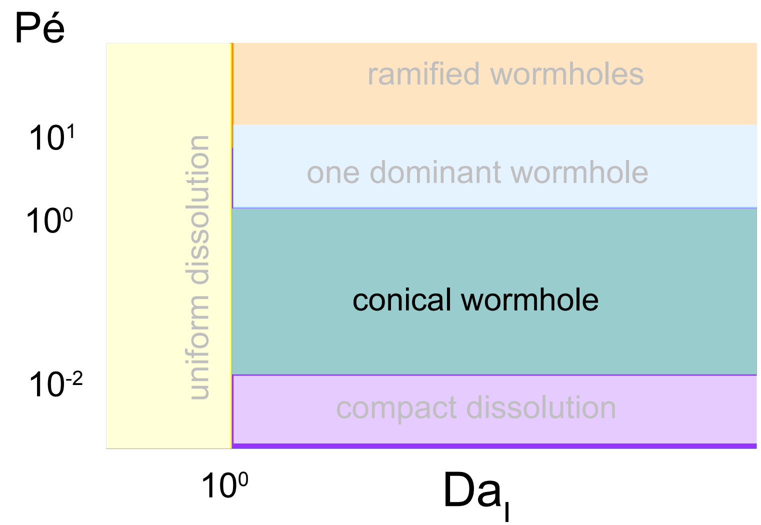


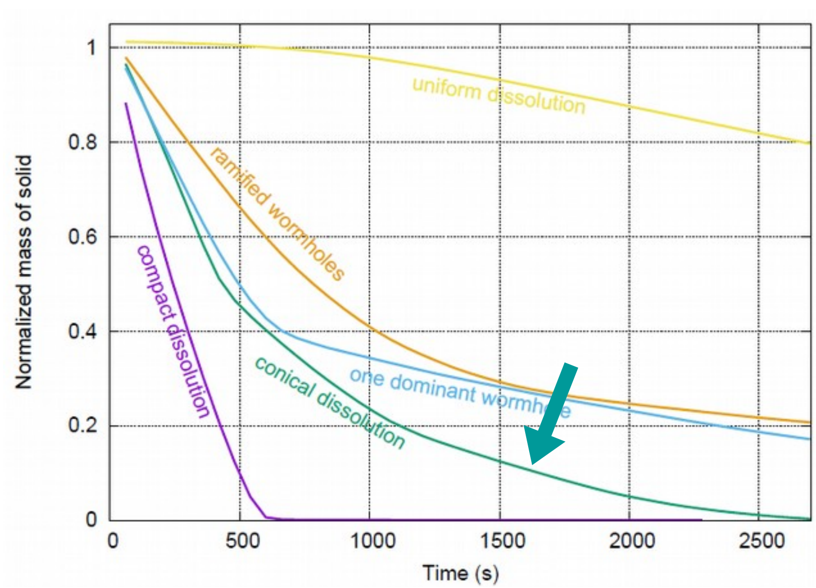




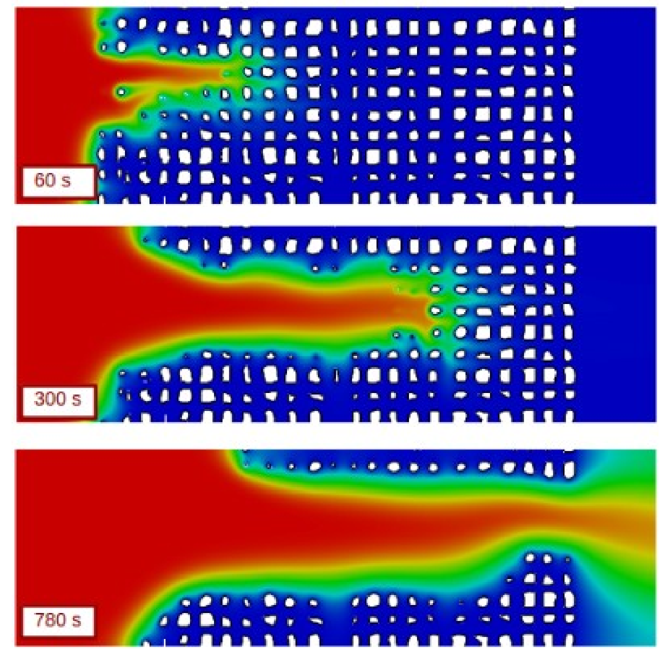
*Soulaine et al. *Mineral dissolution and wormholing from a pore-scale perspective* (under review)

Differents dissolution regimes*





conical dissolution



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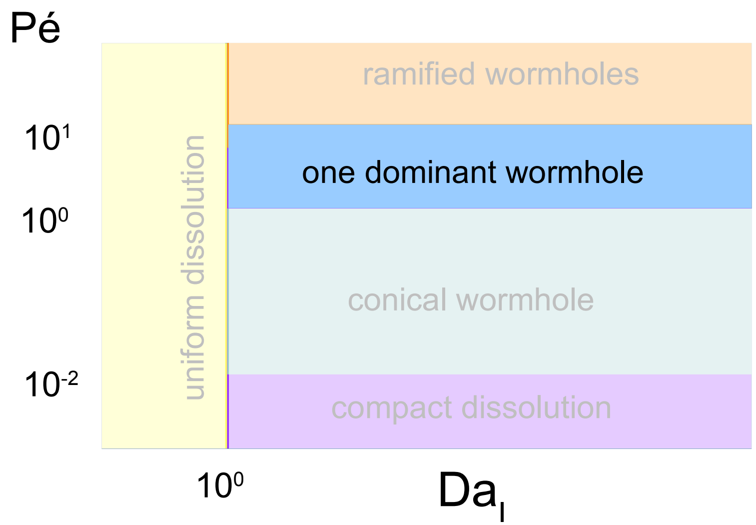
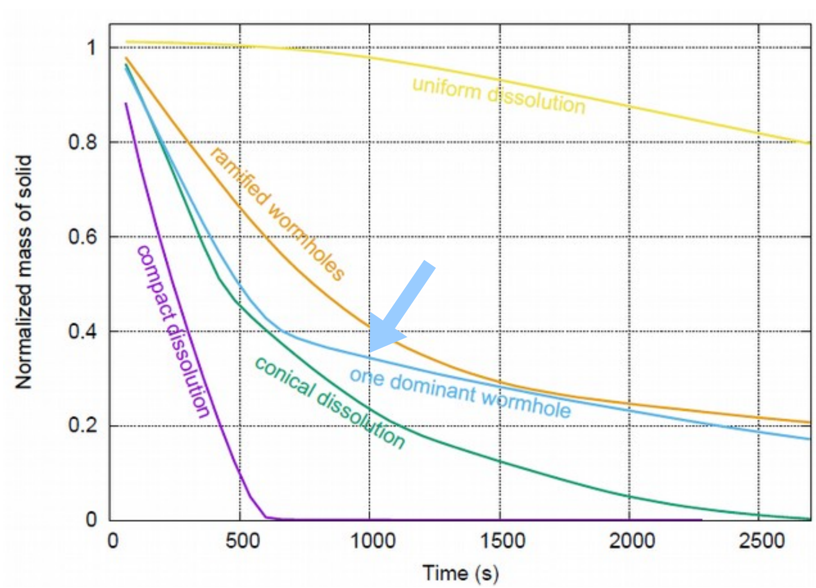
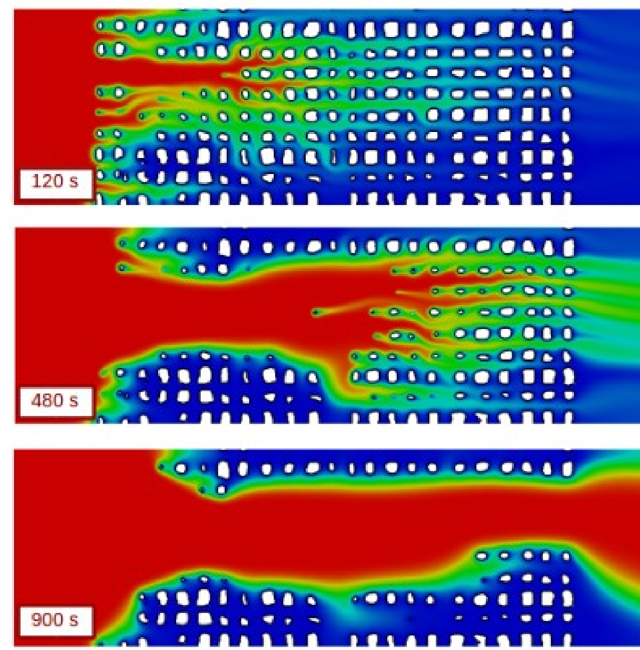




one dominant wormhole



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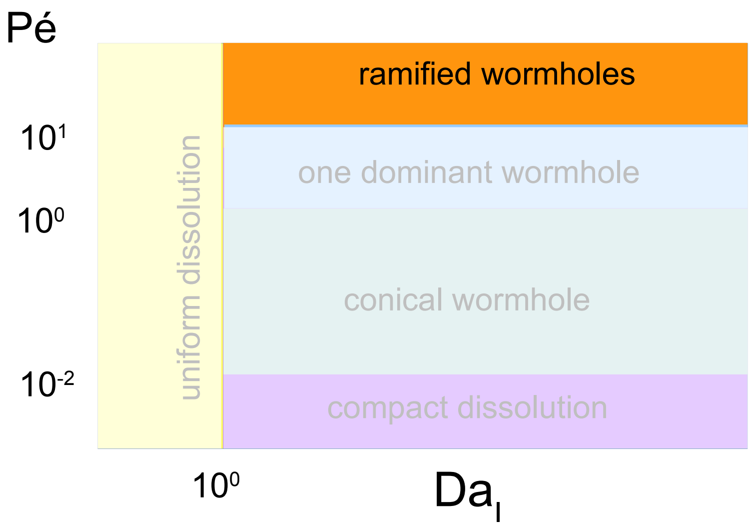
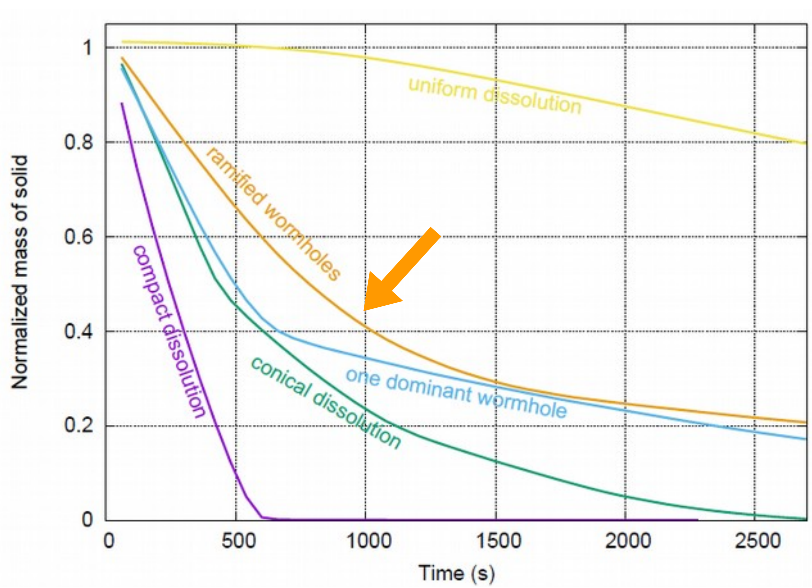
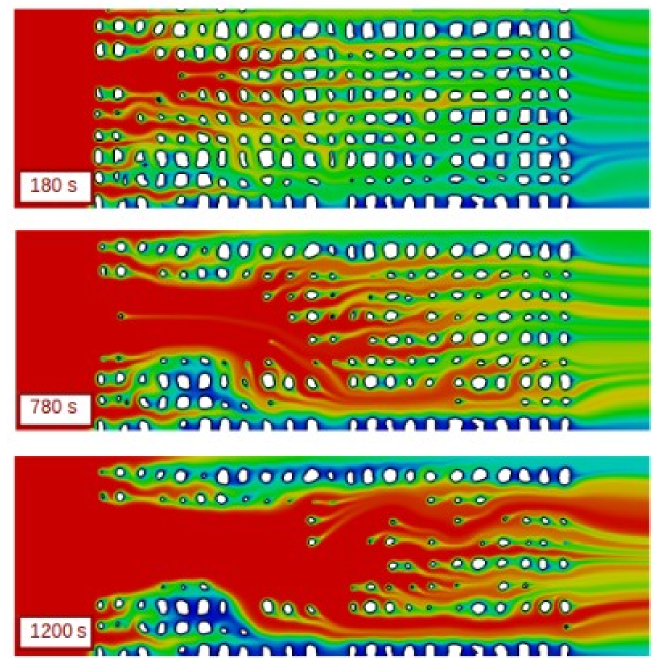




ramified wormholes



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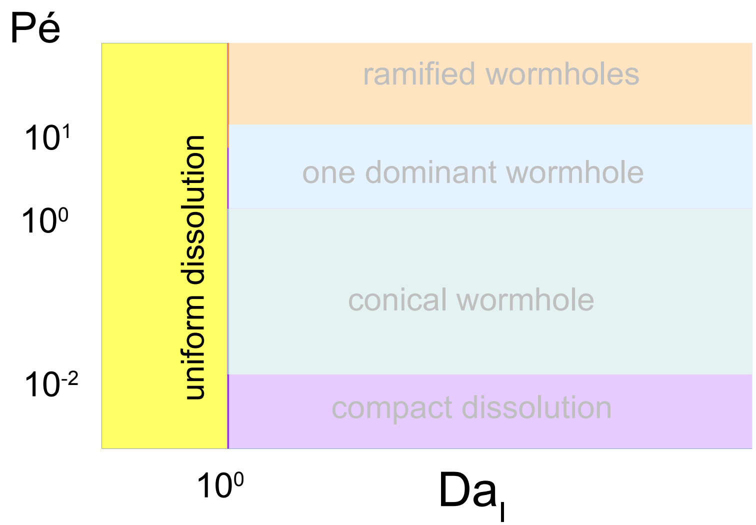

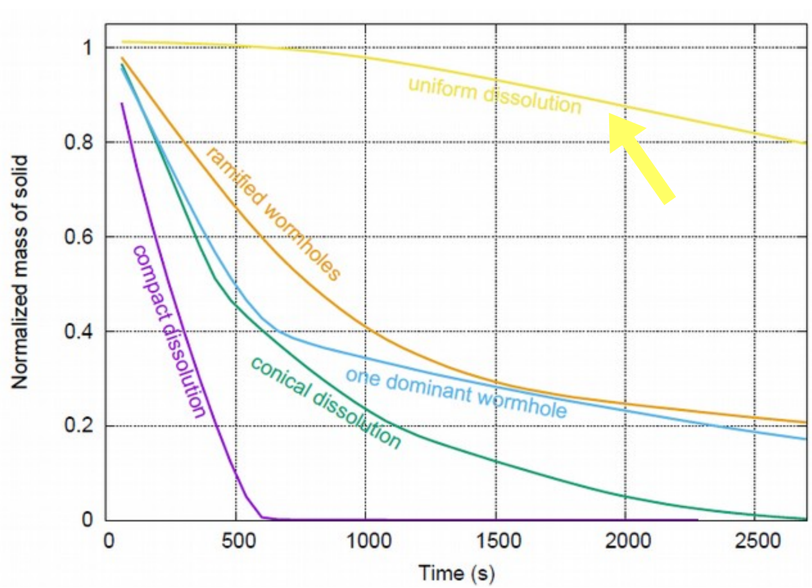

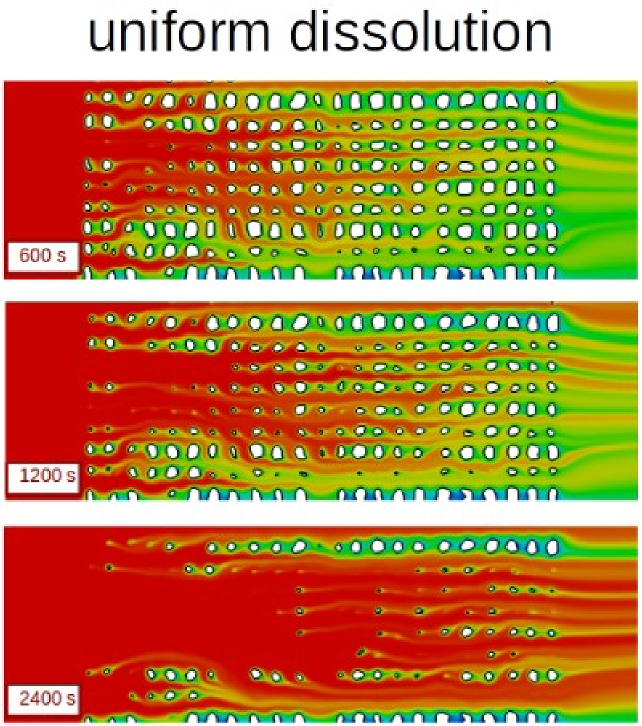

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Summary

- Micro-continuum model for pore-scale dissolution,
- Validation of the formulation thru ALE benchmark and micromodel experiments,
- Upscaling to Darcy-scale (Obtain the exchange coefficient from pore-scale simulation as a function of Da, Pé…),
- Investigation of the emergence of dissolution instabilities,
- Extension of the micro-continuum framework for multiphase systems.

Acknowledgements

- TOTAL STEMS project,
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- SUPRI-B affiliates,
- Stanford Center for Computational Earth & Environmental Sciences,
- Sophie Roman, Wen Song and Tony Kovscek from SUPRI-A, for providing experimental data for multiphase dissolution.

Thank you for your attention.

Question?

csoulain@stanford.edu

Reactive surface with a core-scale DBS model

- Core-scale model (Darcy formulation)
- Diffuse Interface Model (DIM)
- Now the porous region has porosity and permeability
- The solid contains multiple minerals with different dissolution rates

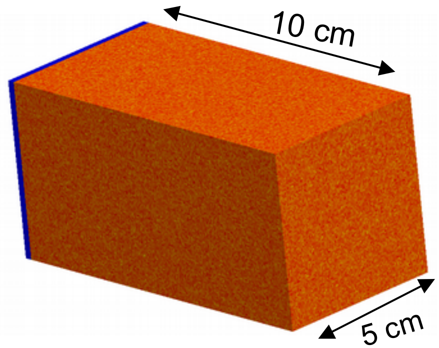
$$\dot{m}_{f,A} = -\rho_f \alpha^*_\beta \left(\bar{\omega}_{f,A} - \omega_{eq,\beta}\right) - \rho_f \alpha^*_\gamma \left(\bar{\omega}_{f,A} - \omega_{eq,\gamma}\right)$$

$$\alpha^*_i = \alpha_{i,0} \underbrace{\varepsilon_f \bar{\omega}_{s,i}} \text{ with } i = \beta, \gamma$$

Input parameter that should depends on Da, Pe, interfacial area...

The reaction only occurs in cells containing solid and fluid

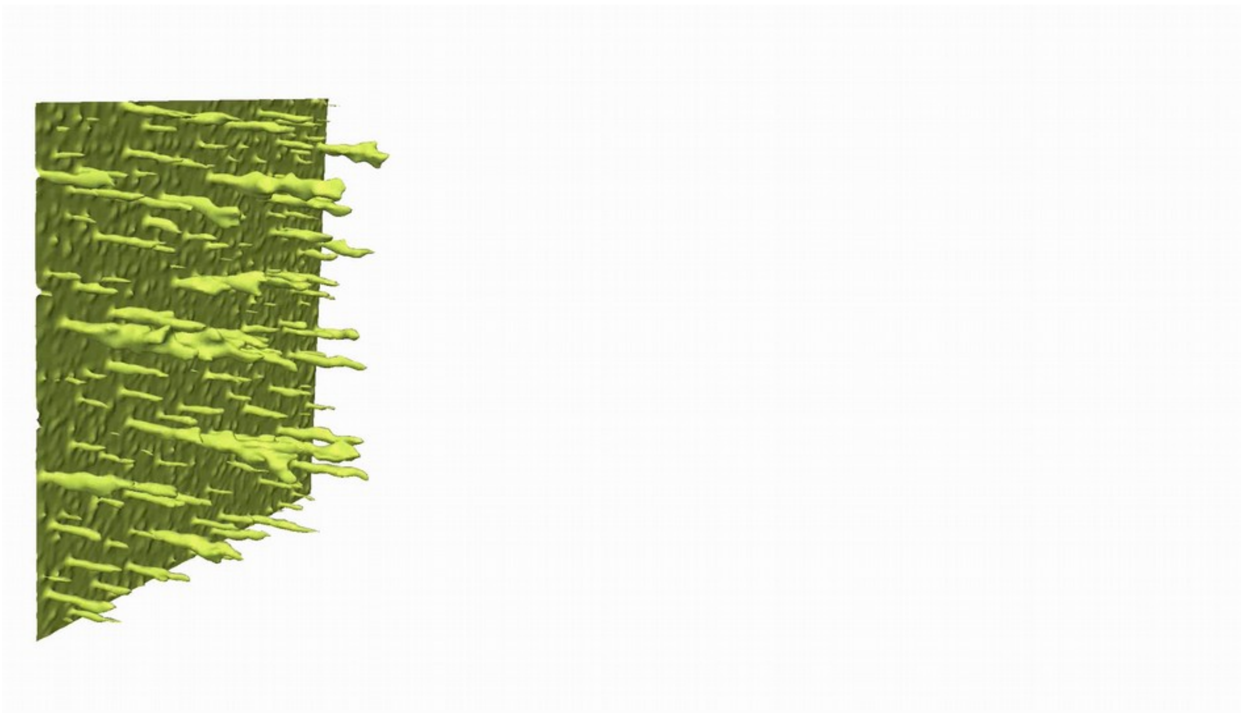
Simulation of wormholes formation

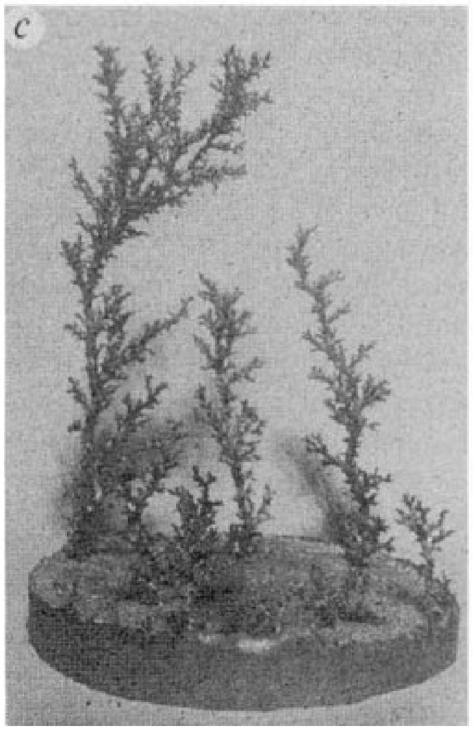


Grid with 150x150x300 hexahedrals (= 6.75×10^6 cells)**

$\varepsilon_0 = 0.1 \pm 3\%$ and $k_0 = 10^{-11}\ m^2 \pm 10\ \%$

Simulation takes less than 2 hours with 242 cores (Stanford CEES cluster)





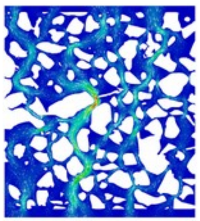
Daccord and Lenormand, 1987*

*Daccord, G. and Lenormand, R. *Fractal patterns from chemical dissolution*. Nature, 1987, 325

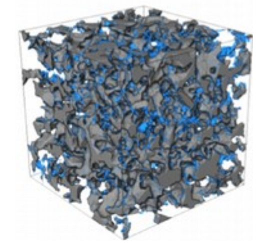
**Soulaine and Tchelepi *Micro-continuum approach for pore-scale simulation of subsurface processes* Transport in Porous Media (2016)

Conclution: application of the *micro-continuum* formulation

Single phase with immersed boundary conditions[1]

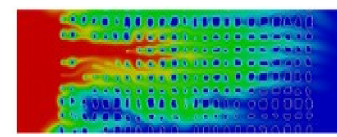


Digital Rock Physics with microporosity[2]



Micro-continuum model

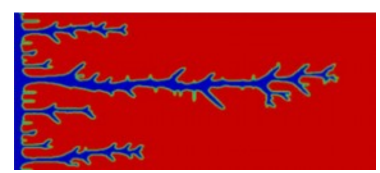
Reactive mass transfer at the pore-scale[3]



Solid mechanics

Extension to multiphase flow (CO_2 release during dissolution, oil generation and expulsion…)

Wormholing in core acidizing experiments[1]



[1]Soulaine and Tchelepi *Micro-continuum approach for pore-scale simulation of subsurface processes* Transport in Porous Media (2016)

[2]Soulaine et al. *The impact of sub-resolution porosity of X-ray microtomography images on the permeability* Transport in Porous Media (2016)

[3]Soulaine and Tchelepi *Micro-continuum formulation fpor modelling dissolution in nature porous media* ECMOR XV, Amsterdam (2016)

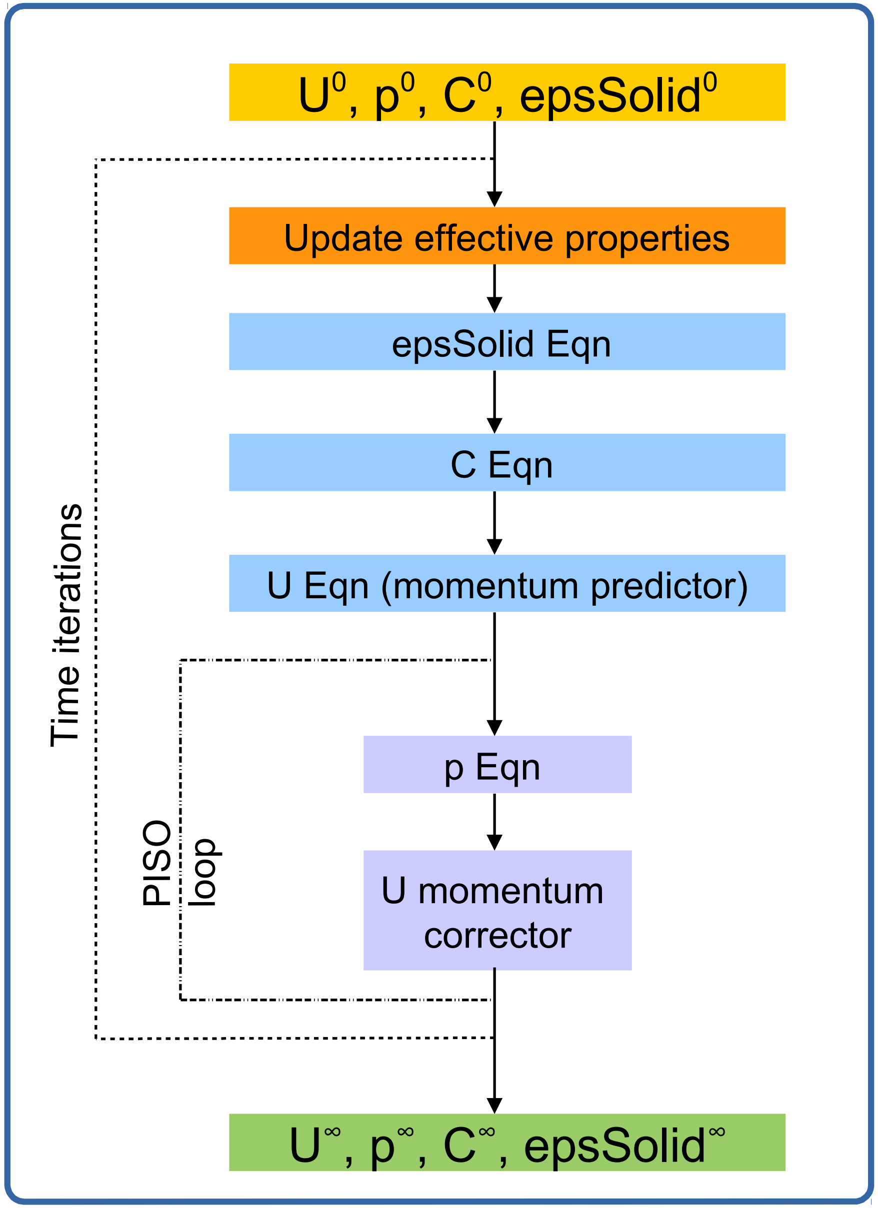
Solution algorithm with OpenFOAM®

OpenFOAM®

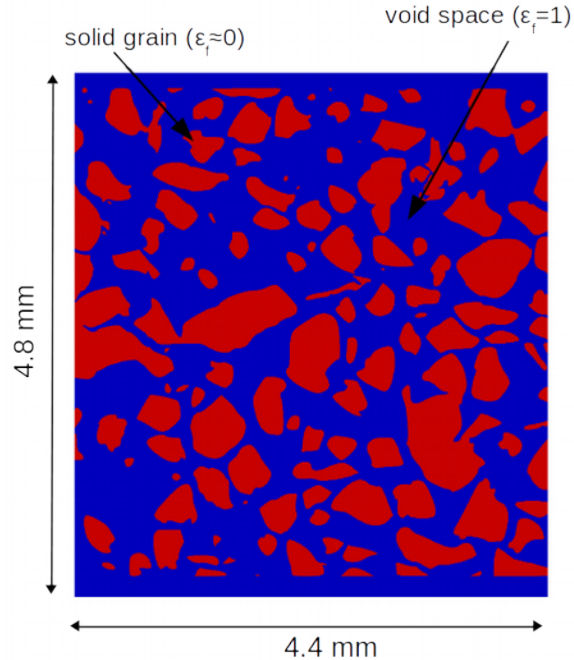
=

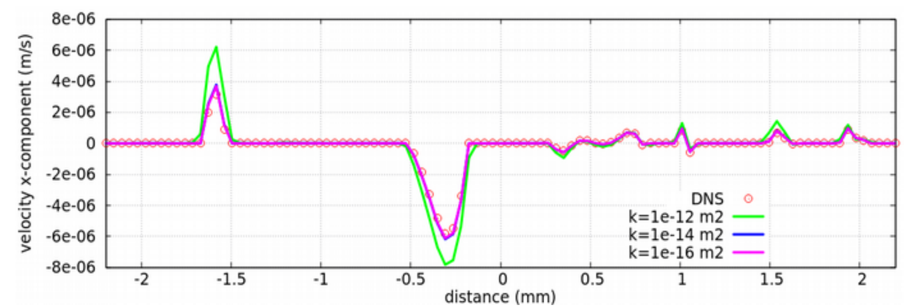
Open Field Operation And Manipulation

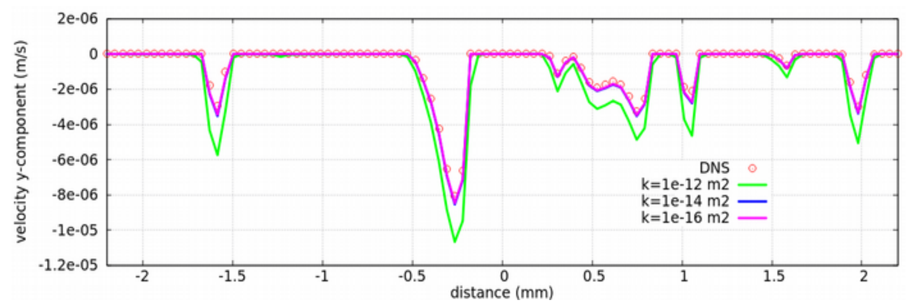
- Finite volume method
- Manage 3D grids by default
- Parallel computation
- Sequential algorithm (PISO–like)

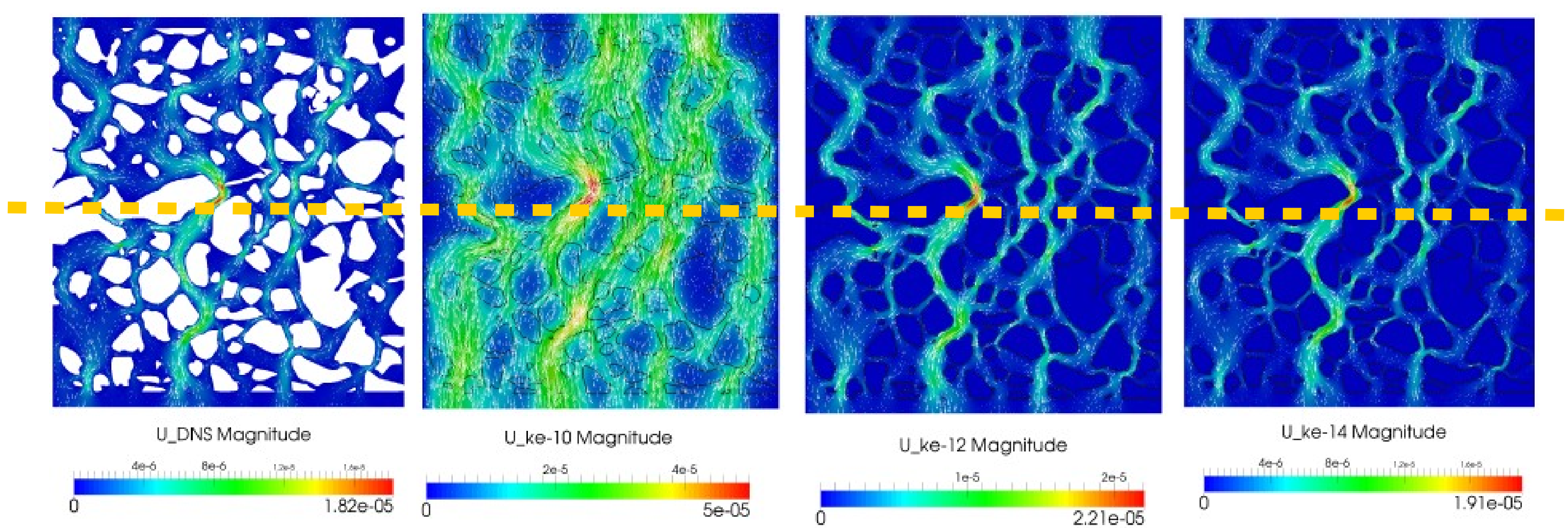


Embedded boundaries with micro-continuum approach









Soulaine and Tchelepi *Micro-continuum approach for pore-scale simulation of subsurface processes* Transport in Porous Media (2016)

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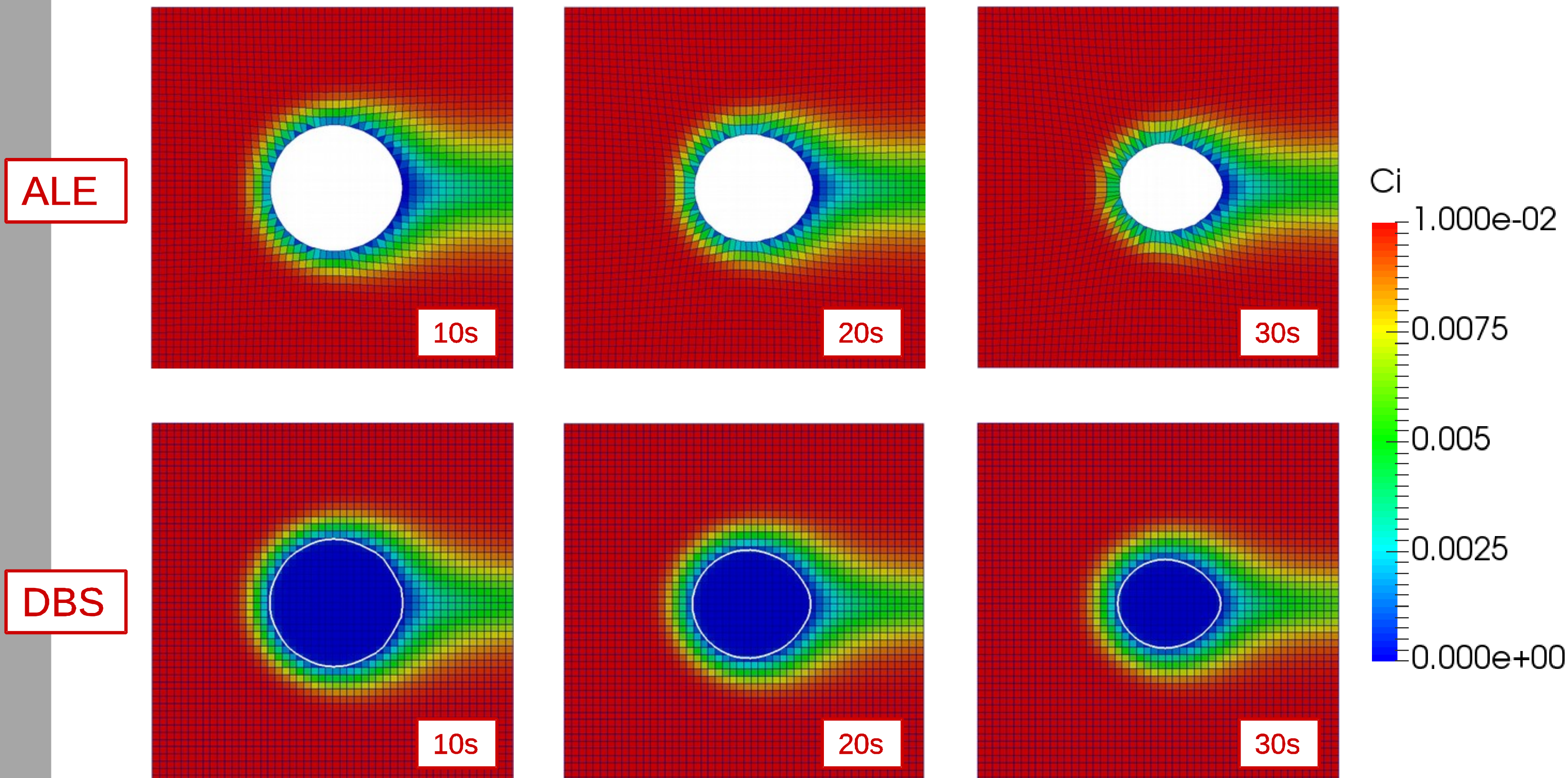
Micro-continuum vs ALE



*Soulaine et al. *Mineral dissolution and wormholing from a pore-scale perspective* (under review)