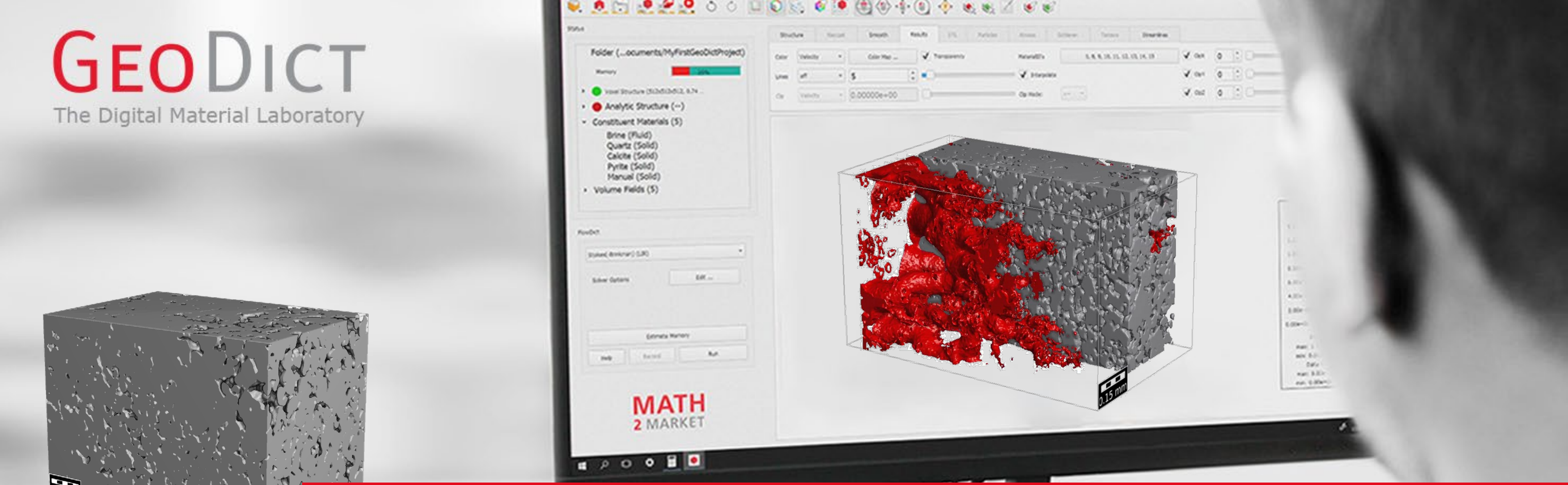

Efficient Simulation of Reactive Flow in Reservoirs Rocks at the Pore Scale

InterPore German Chapter Meeting 2021

Online conference, February 1st – 2nd

Christian Hinz, Jens-Oliver Schwarz, Andreas Weber, Andreas Wiegmann

Math2Market GmbH, Kaiserslautern

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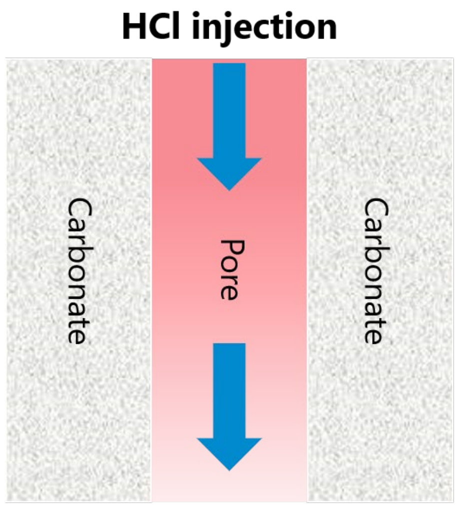
Overview

Motivation

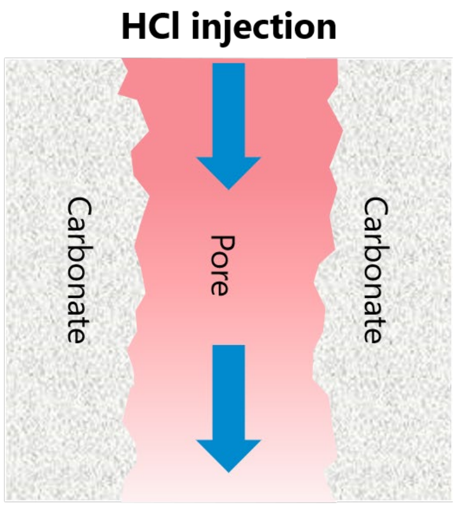
Reactive Flow in Carbonates

Acidizing treatments in carbonate reservoirs

- HCl injection into carbonate
- Effect: Dissolution, enlargement of pore space
- Establish a higher permeability
- Keep mechanical stability



Initial stage



Dissolved stage

Numerical parameter studies

- Efficient optimization of process parameters

  e.g., acid concentration, injection velocity, and pore-scale structure

➡ **Such parameter studies require efficient solvers**

Our Motivation: Efficient model capable of performing digital reactive flow experiments in large pore-scale geometries.

Reactive Flow in DRP

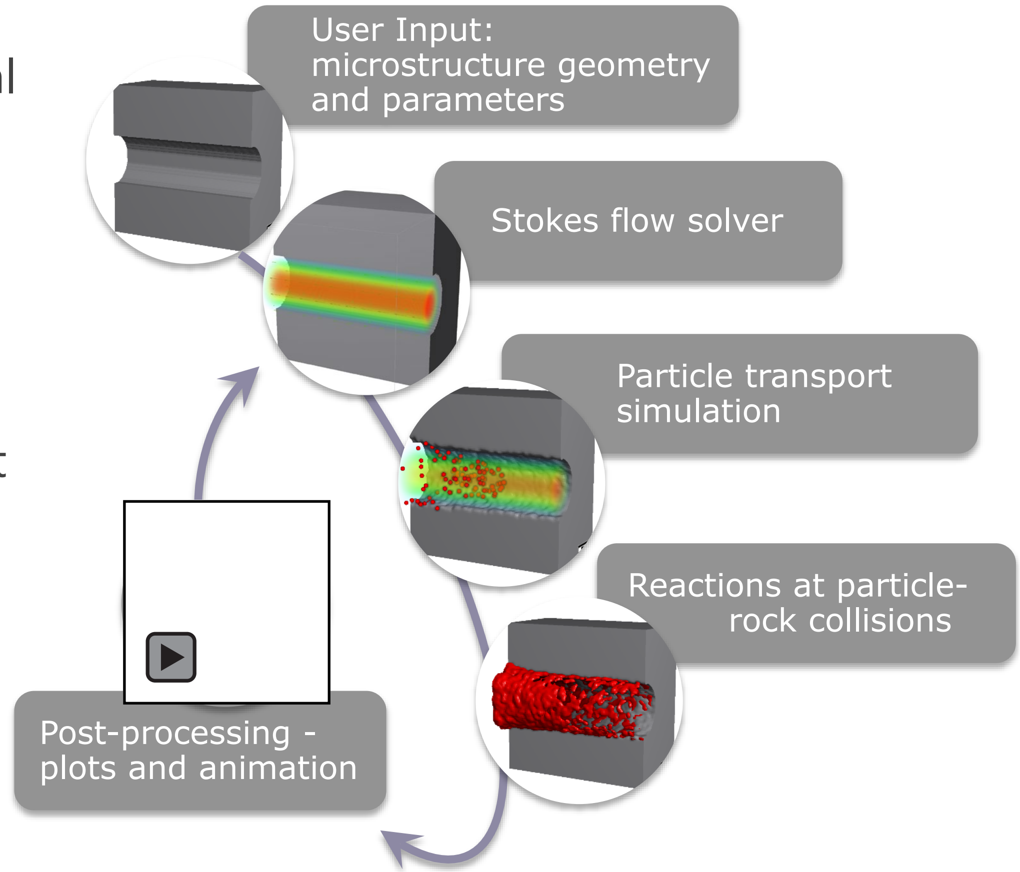
Workflow

Our **Reactive Flow** feature computes dissolution and precipitation of mineral phases during continuous inflow of reactants (e.g., acid) and predicts:

- 4D rock alteration
- Dissolution regime
- Porosity-permeability development

Reactive Flow applications in DRP:

- Permeability enhancement
  e.g., in carbonate reservoirs
- Permeability reduction
  e.g., by salt precipitation



FLOW COMPUTATION

Advective motion is optional

- Flow field is computed in the current batch's structure

  LIR Stokes solver of Linden et al. (2014)

- Flow is solved for a given fluid velocity

  Every X time steps

- Boundary Conditions (BCs) may be set individually

  Periodic or symmetric BCs,
  Convergence, Inlet/Outlet regions

PARTICLE SIMULATION

GEODICT

- Compute particle movement
  - Advective motion (Streamlines)
  - Diffusive motion (Brownian motion)
  - Motion according to molecules

Reaction Rate & pH-based geochemical Models:
We keep track of the collision points with the rock interface, where particles will react.
Particles' motion stops when they are geochemically exhausted (user-defined).

REACTION – MODELS

GEODICT

Model I: pH-based model

At particle-rock collisions, a partial acid volume dissolves the reactive solid surface partially

- Each particle represents an acid volume indicated via pH value

Model II: Reaction Rate Model

At particle-rock collisions, the solid surface reacts partially.

- Reaction is based on reaction rates, which are:
  (1) *user-defined,*
  (2) *mineral-specific, and*
  (3) *global reaction rates*

We keep track of the consumed acid volume of particles and of the solid fractions of reactive minerals.

is highlighted in red color.

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Data processing

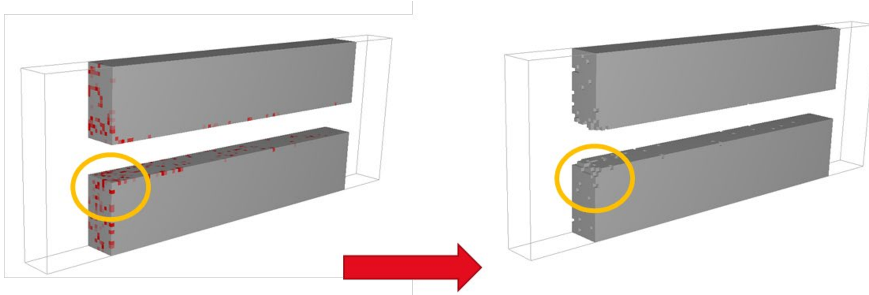
- Rock structure is automatically updated

  Remove dissolved voxels, precipitate voxels

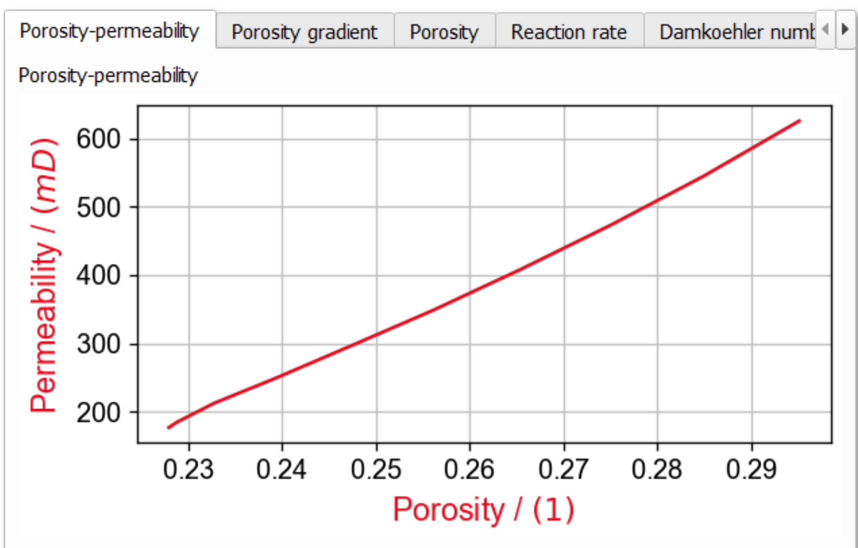
- All data may be stored

  and used for further analysis:

  Mechanical stability (Bulk Modulus), Conductivity, and more



Remove voxels of reactive material once they are completely dissolved



- Automated post-processing

  Porosity-Permeability relationship,

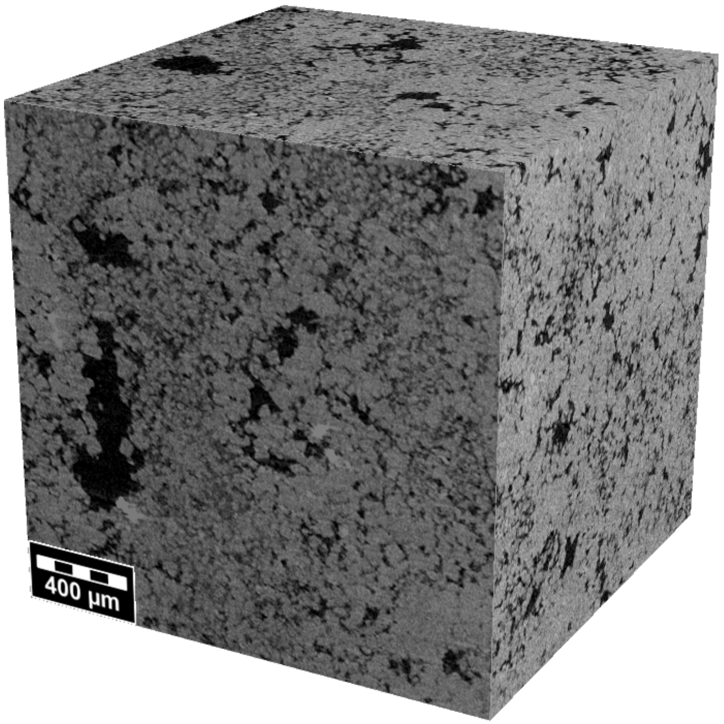
  Reaction rate, Damköhler number,

  3D Animations, amongst others

Grosmont Carbonate sample

Grosmont Formation, Alberta, Canada

- Dimensions: 1024x1024x1024 voxel
- Resolution: 2.02 µm
- Porosity: 21 %
- Permeability range: 150 mD – 470 mD
  → heterogenous pore space
- Data set is published in DRP benchmark paper (Andrä et al., 2013)

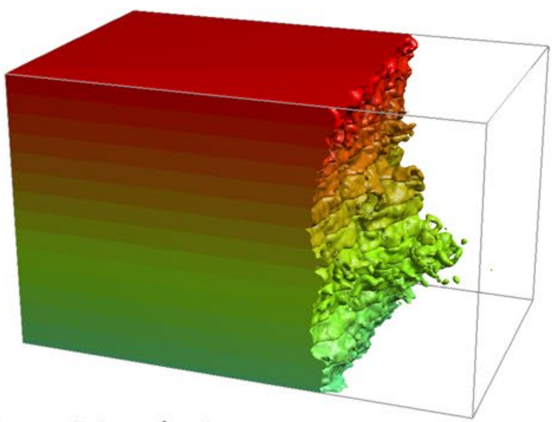


Reactive Flow – Model Evaluation

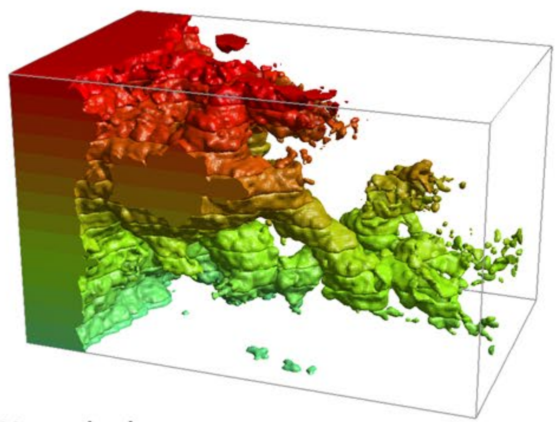
Dissolution regimes

Goal: Replicate characteristic dissolution patterns

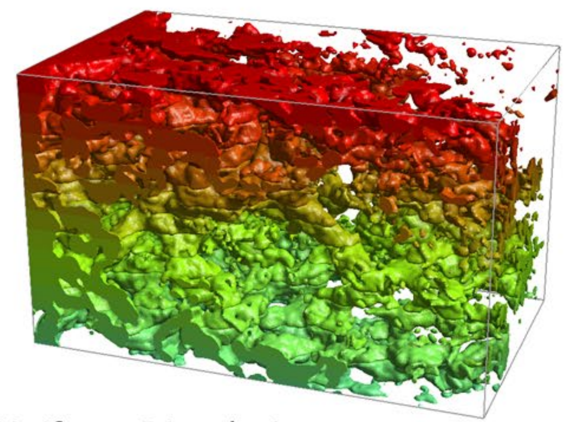
- **Face Dissolution:** Slow flow in relation to reaction rate
- **Wormhole:** Comparable transport rate and reaction rate
- **Uniform Dissolution:** Fast flow in relation to reaction rate



Face Dissolution



Wormhole



Uniform Dissolution

GROSMONT CARBONATE SAMPLE

pH-BASED MODEL

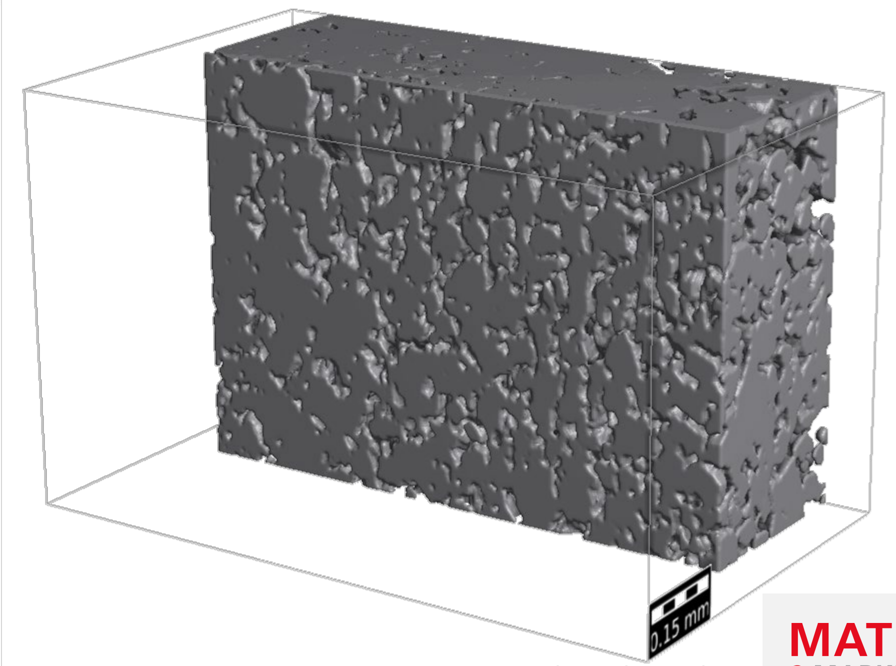
Goal: Replicate characteristic dissolution patterns

pH-based models		$v\ [\frac{m}{s}]$	$t_{sim}\ [s]$	pH	$\Delta\Phi$ [%]	$t_{runtime}\ [h]$	$\Delta permeability\ [mD]$
Face Dissolution		0.00001	500,000	3.0	11.5	30.6	160
Wormhole	256x256x362	0.0005	6,000	3.0	9.0	2.4	3,165
Uniform Dissolution		0.05	200	3.0	7.4	3.0	1,354

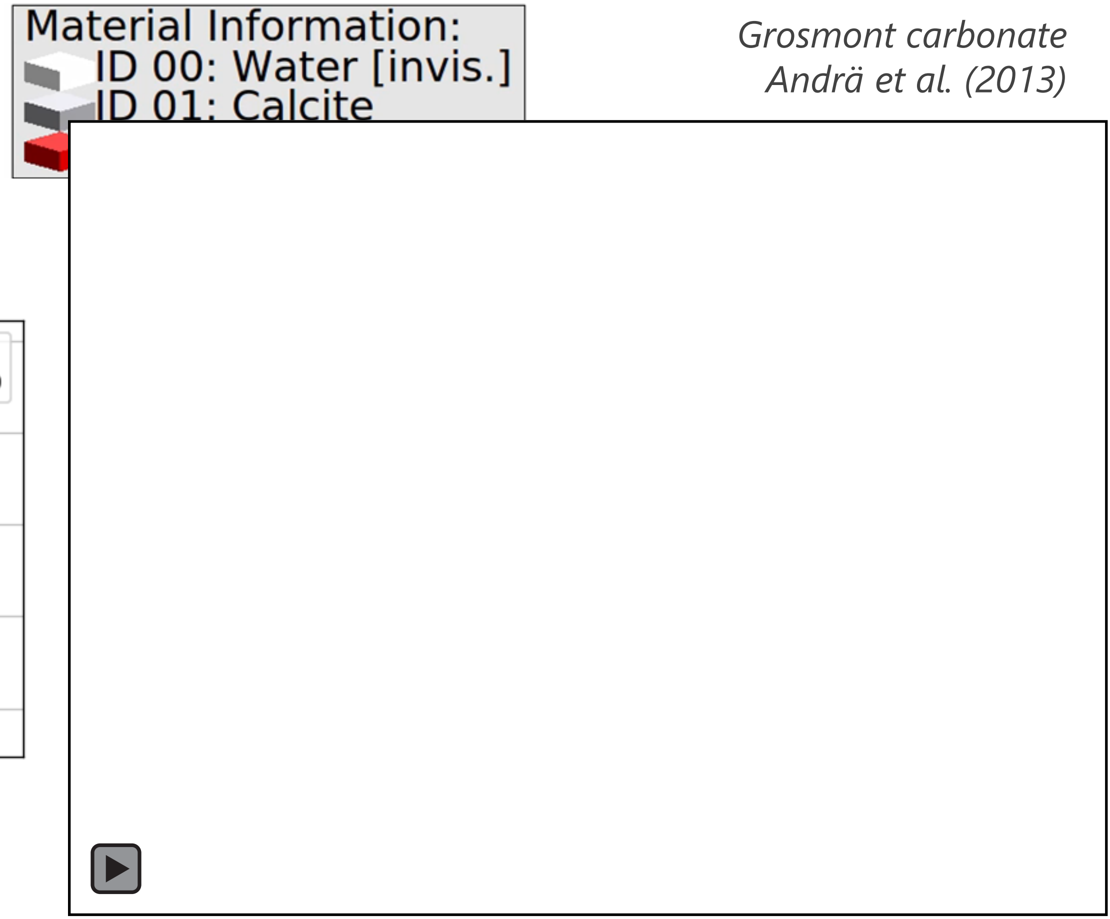
Grosmont carbonate

Andrä et al. (2013)

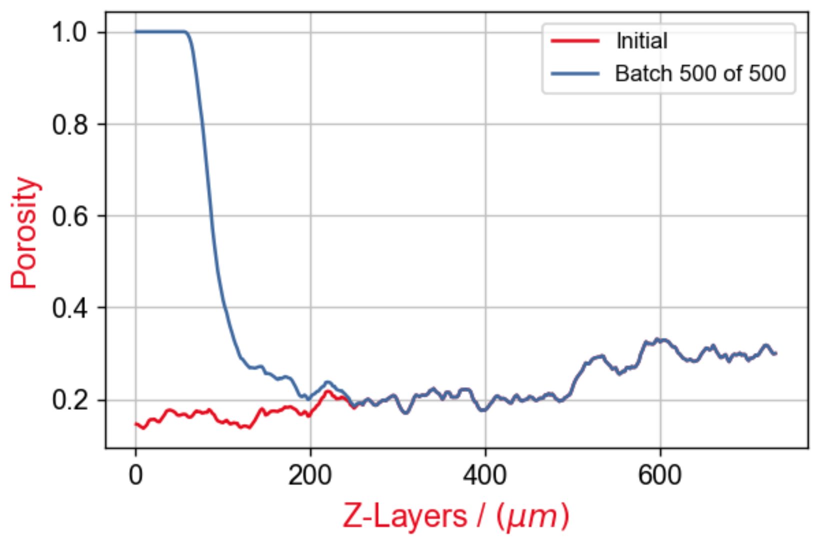
- Porosity $\Phi = 21.95\ \%$
- Voxel length: $2.02\ \mu m$
- Domain: $256 \times 256 \times 362$ voxel



FACE DISSOLUTION
GROSMONT CARBONATE SAMPLE

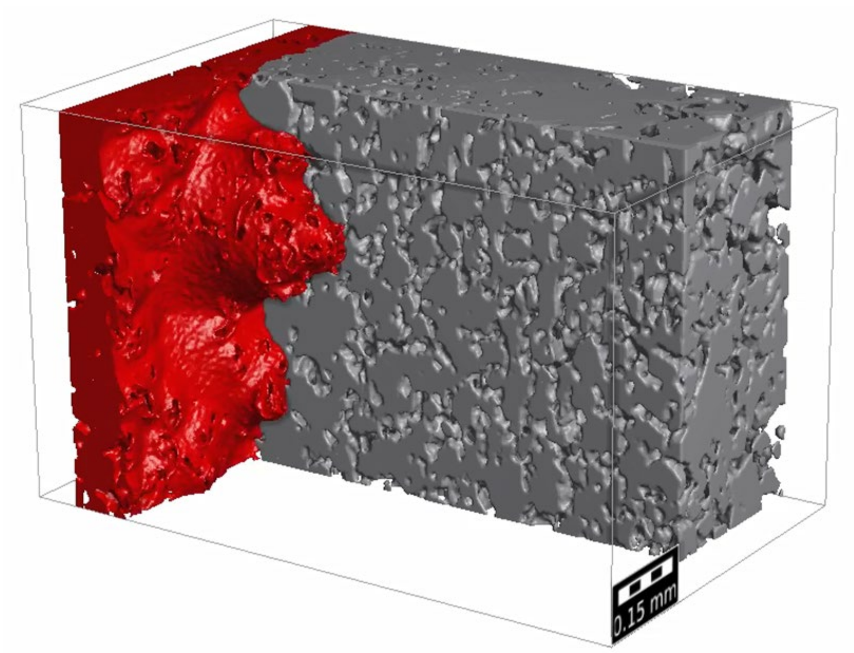


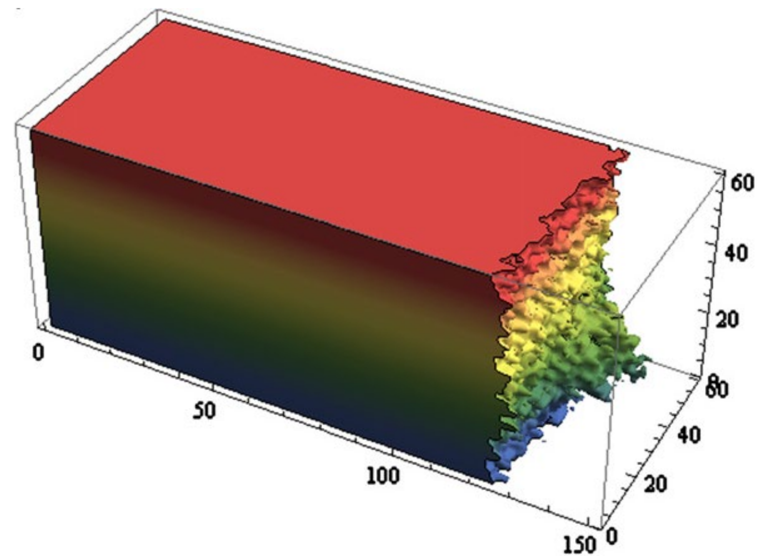
Grosmont carbonate
Andrä et al. (2013)



Comparison face dissolution pattern

Grosmont Carbonate sample





GeoDict Simulation

Pore scale modeling

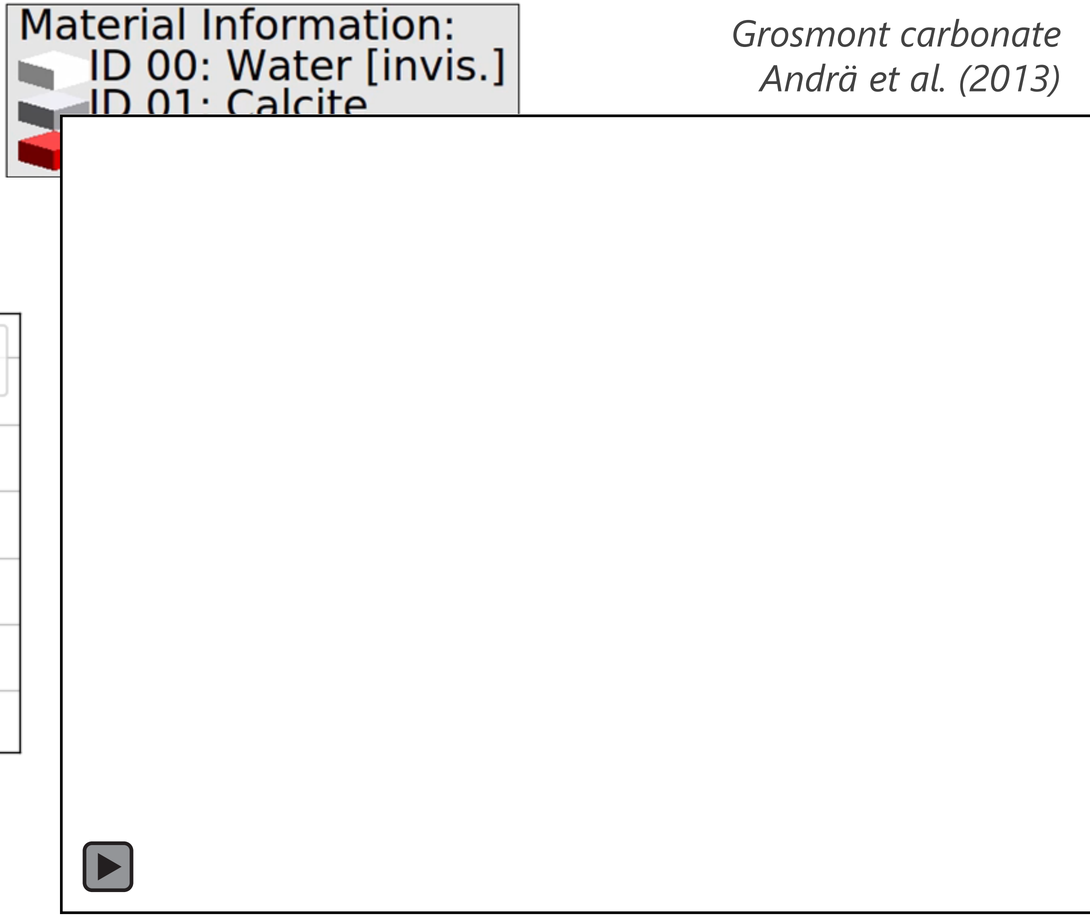
Maheshwari et al. 2013

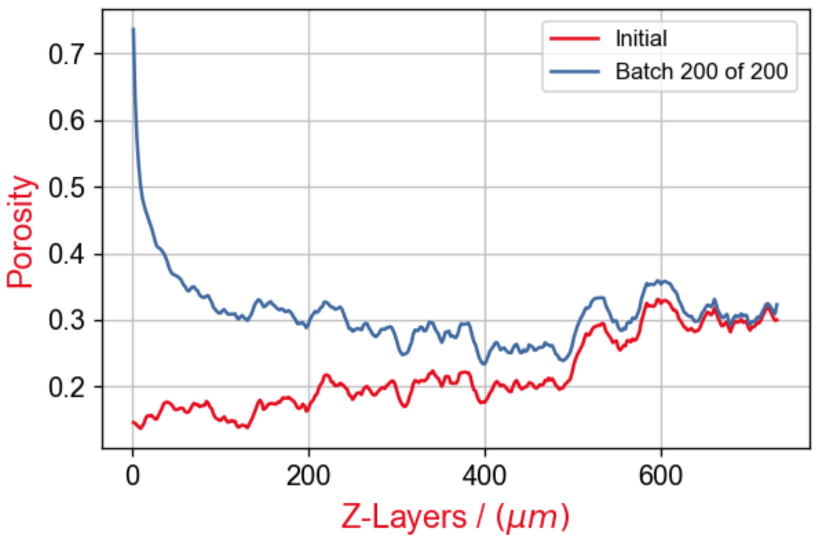
Continuum scale modeling

Wormholing

Grosmont Carbonate sample

Grosmont carbonate
Andrä et al. (2013)

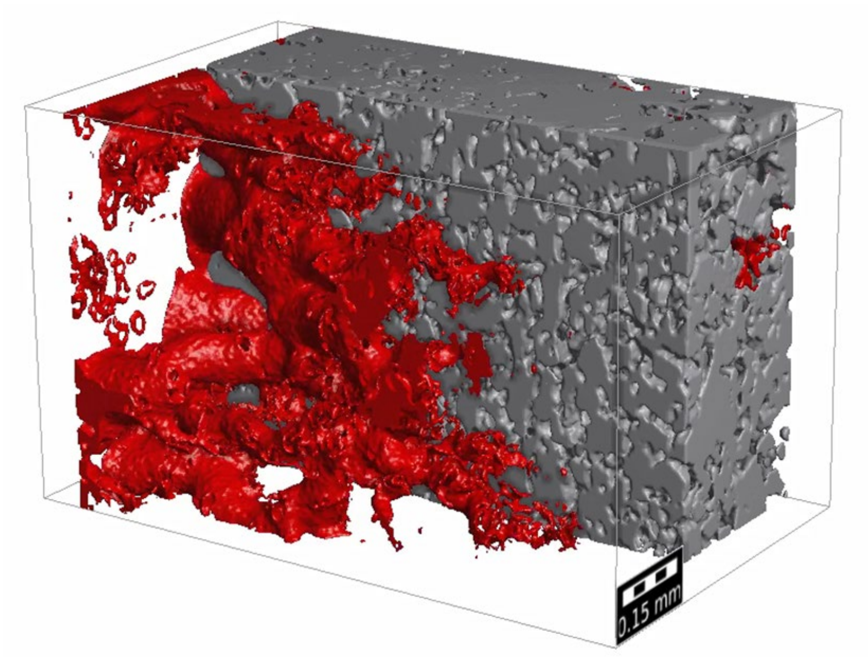


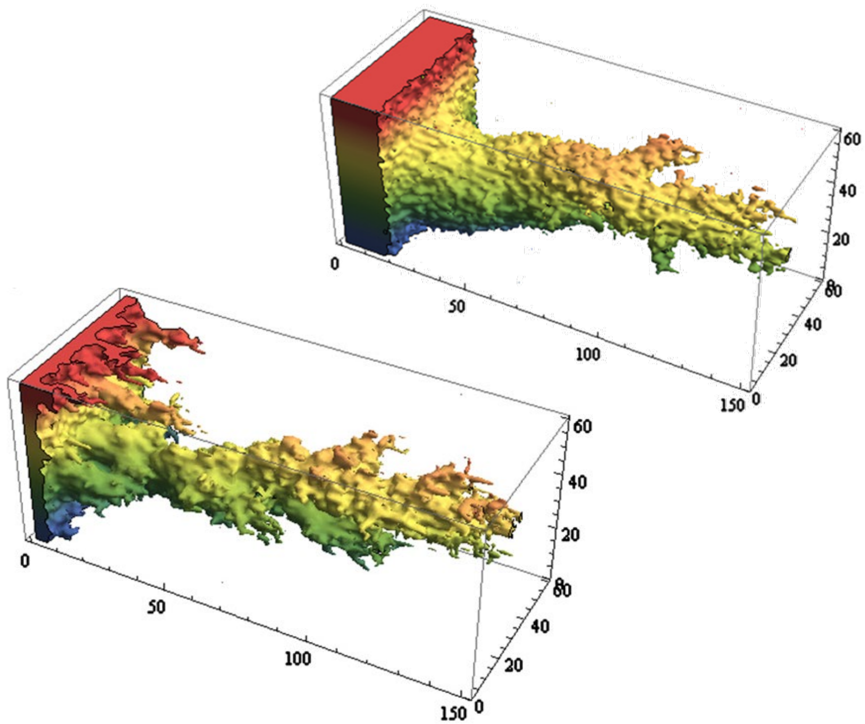


Comparison Wormhole pattern

Grosmont Carbonate sample

GeoDict





GeoDict Simulation	Maheshwari et al. 2013
Pore scale modeling	*Continuum scale modeling*

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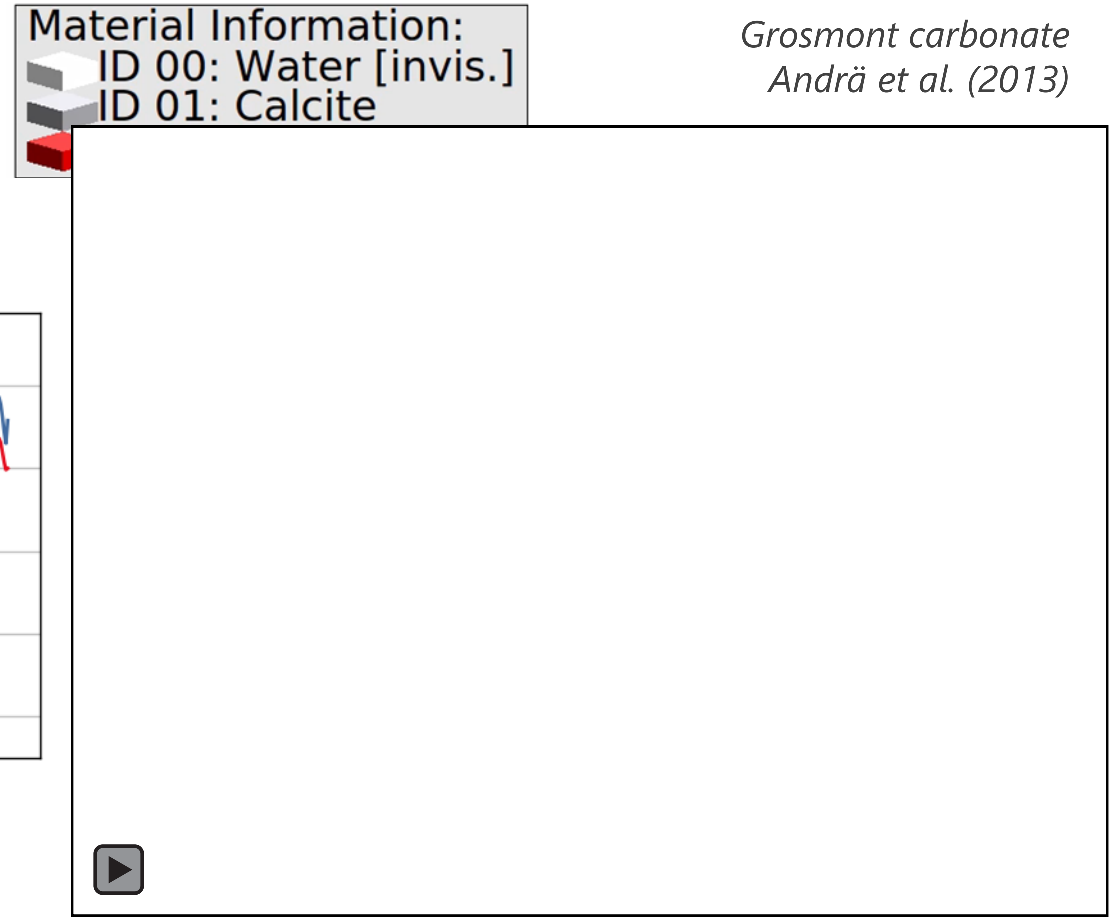
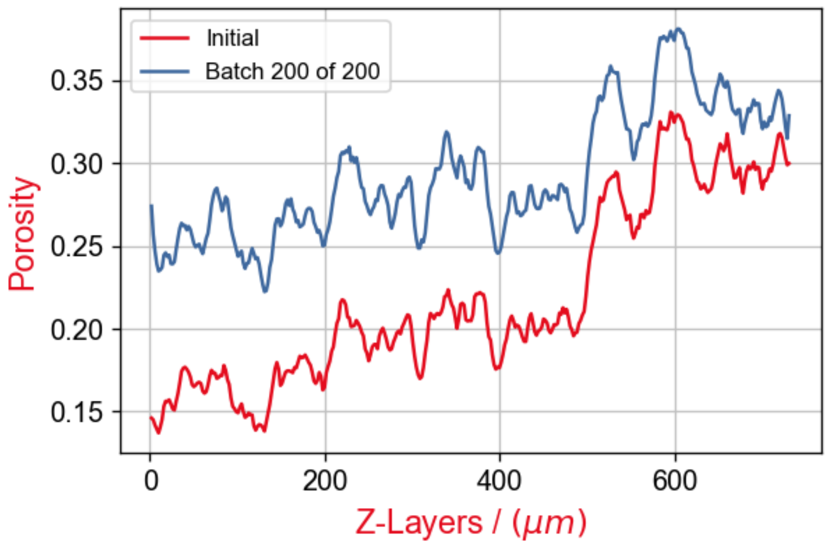
Uniform Dissolution

Grosmont Carbonate sample

Grosmont carbonate
Andrä et al. (2013)

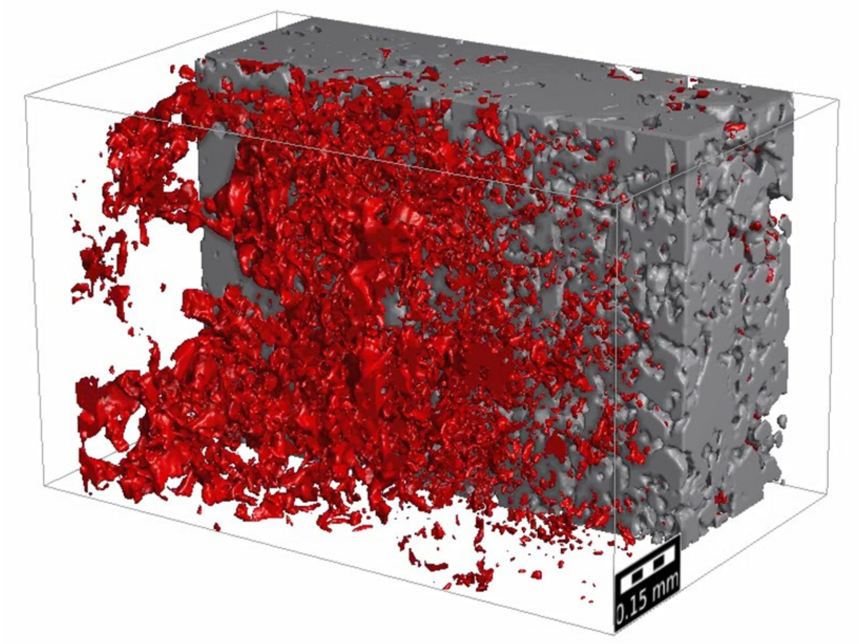


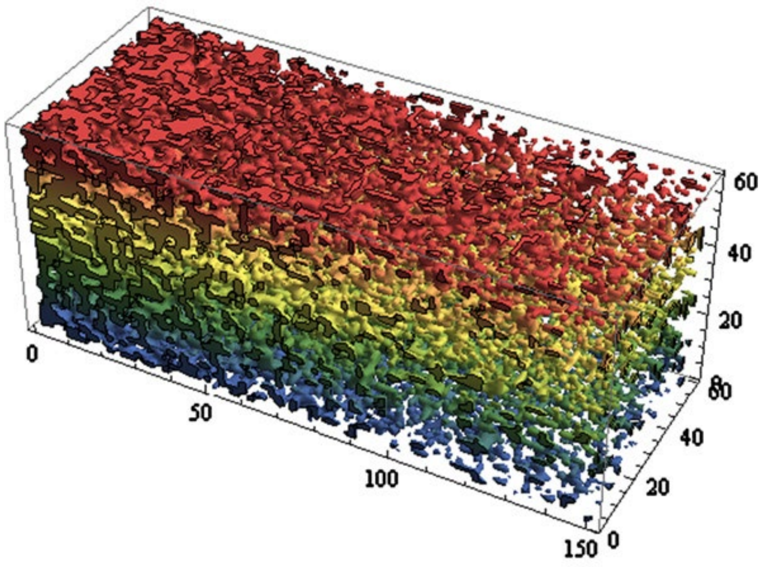


COMPARISON UNIFORM DISSOLUTION PATTERN

GEODICT

GROSMONT CARBONATE SAMPLE





GeoDict Simulation	Maheshwari et al. 2013
Pore scale modeling	*Continuum scale modeling*

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OVERVIEW

Grosmont Carbonate sample

Reaction Rate Model

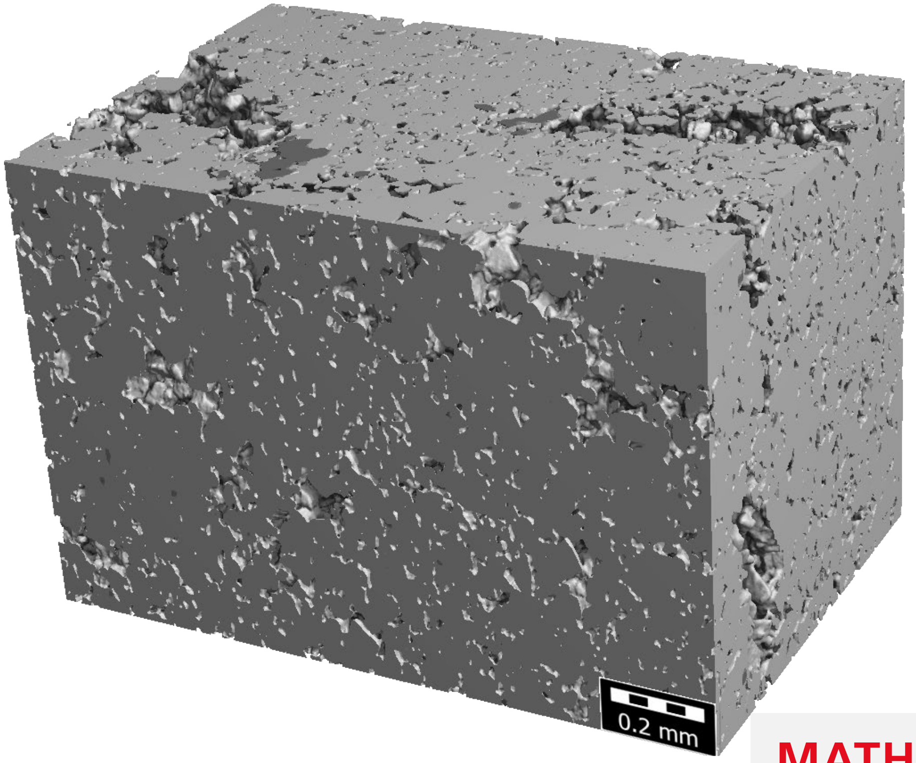
Goal: Perform kinetically-controlled carbonate dissolution

Reaction rate model		$v\ [\frac{m}{s}]$	$t_{sim}\ [a]$	$rate_{Calcite}\ [\frac{mol}{m^2 s}]$	$\Delta\Phi$ [%]	$t_{runtime}\ [h]$
Carbonate Dissolution	512x512x768	0.00005	20	0.0001	10.98	28.8

Grosmont carbonate

Andrä et al. (2013)

- Porosity $\Phi = 23.53\ \%$
- Voxel length: $2.02\ \mu m$
- Domain: $512 \times 512 \times 768$ voxel



Grosmont Carbonate sample

Reaction Rate Model

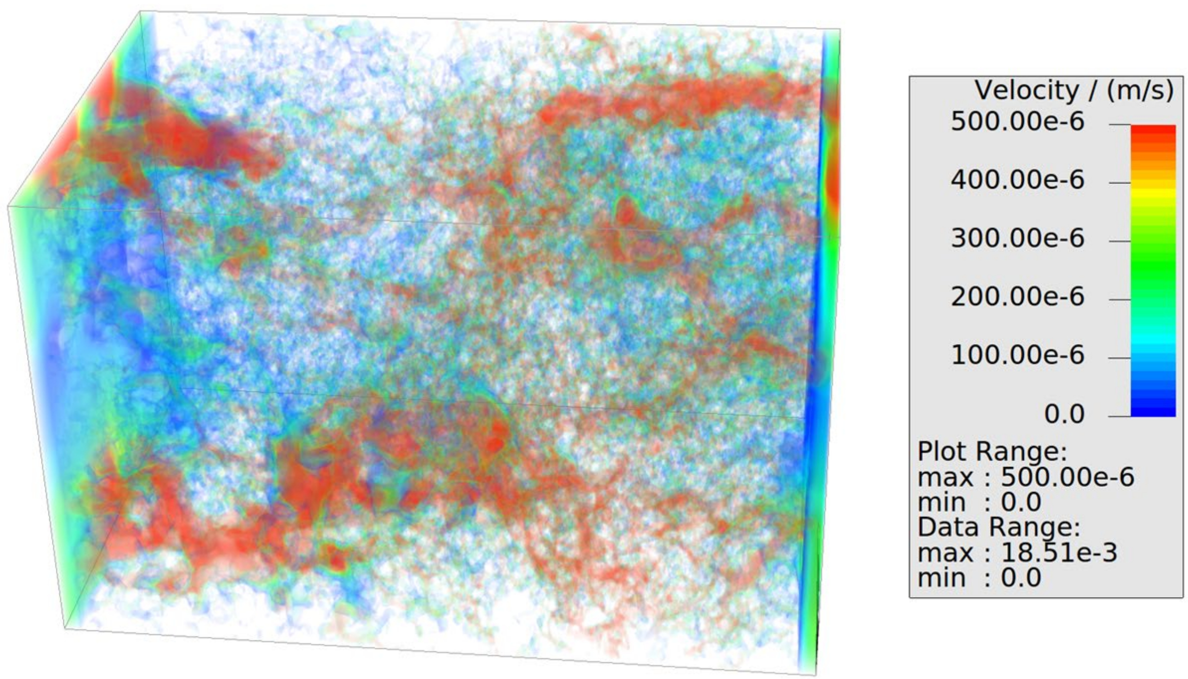
Goal: Perform kinetically-controlled carbonate dissolution

Reaction rate model		$v\ [\frac{m}{s}]$	$t_{sim}\ [a]$	$rate_{Calcite}\ [\frac{mol}{m^2 s}]$	$\Delta\Phi\ [\%]$	$t_{runtime}\ [h]$
Carbonate Dissolution	512x512x768	0.00005	20	0.0001	10.98	28.8

Grosmont carbonate

Andrä et al. (2013)

- Initial flow field
  - Heterogeneous
  - Preferred flow path

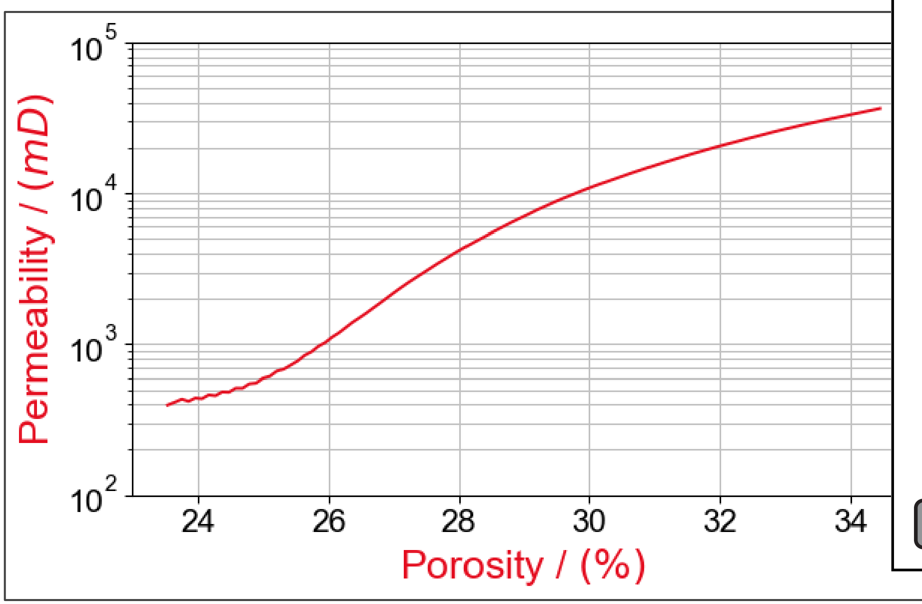


Grosmont Carbonate Sample

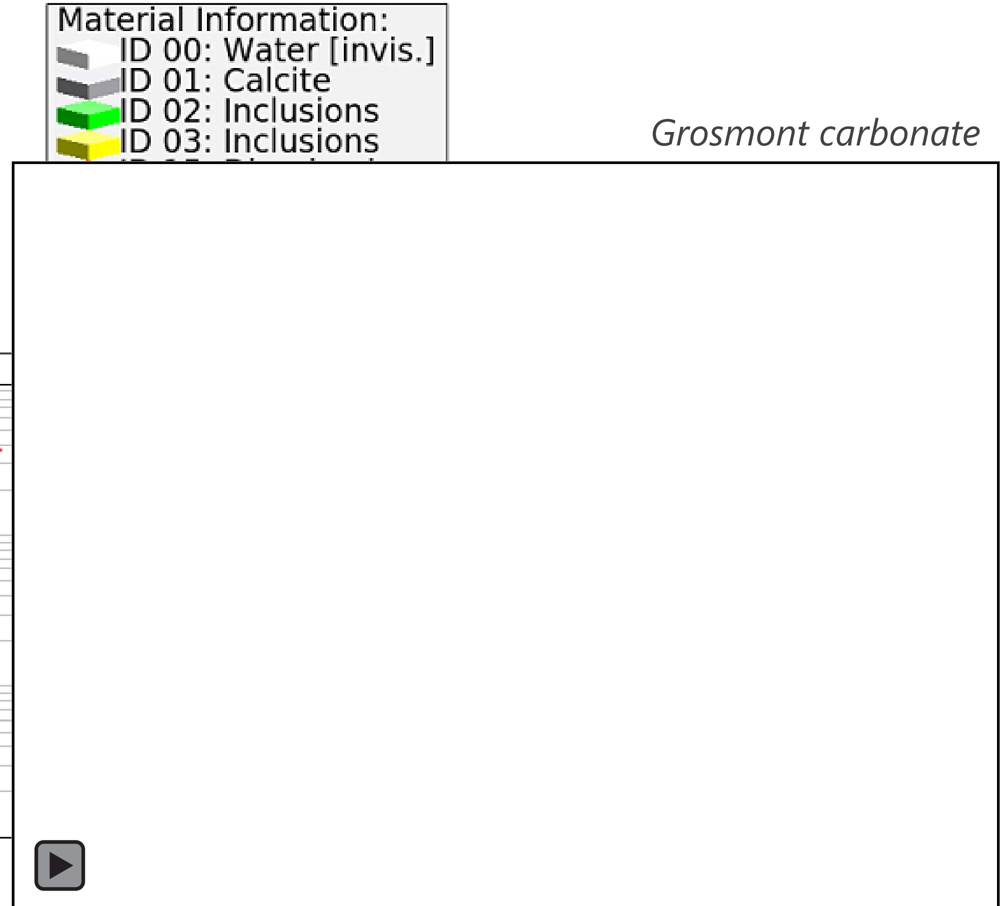
Kinetic Carbonate Dissolution

GeoDict

Parameter	Value
$t_{simulated}$	20 a
$t_{runtime}$	28.8 h



Grosmont carbonate



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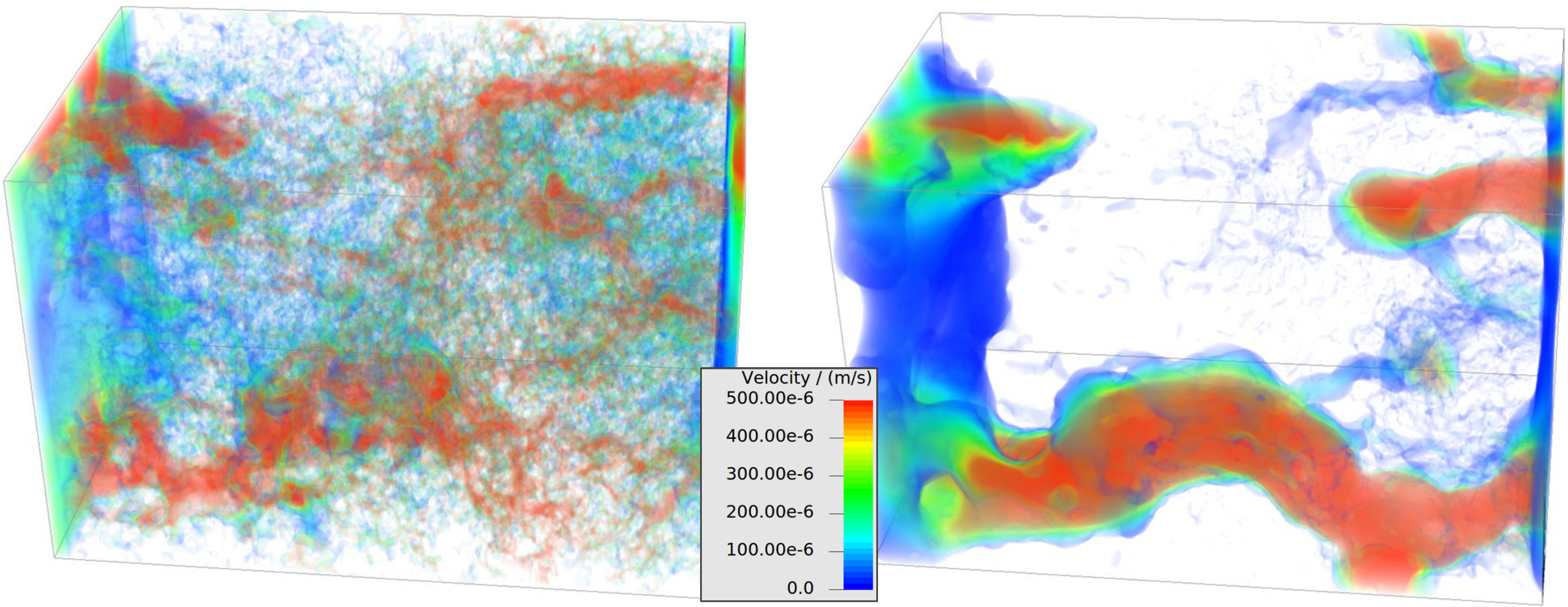
Grosmont Carbonate Sample
Kinetic Carbonate Dissolution



Initial flow field	Final flow field
Grosmont carbonate *Andrä et al. (2013)*	***Channeling*** *Dissolution Pattern*

Berea Sandstone Sample

Selective Dissolution – 2 Phases

GeoDict

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on
olved

a sandstone
et al. (2013)

Structure (v
720x720x

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CONCLUSION

GEODICT

- We presented a numerical model to simulate reactive flow
  - Different geochemical approaches
- We evaluated the model by reproducing characteristic dissolution patterns
- Computations can be run on a state-of-the-art desktop workstation
- Computational domains of > 1000^3 voxels
- On going advances in performing Digital Reactive Flow Experiments

Andrae, H., Combaret, N., Dvorkin, J., Glatt, E., Junehee, H., Kabel, M., Keehm, Y., Krzikalla, F., Lee, M., Madonna, C., Marsh, M., Mukerji, T., Saenger, E., Sain, R., Saxena, N., Ricker, S., Wiegmann, A., Zhan, A., "Digital rock physics benchmarks Part I: Imaging and segmentation", Computers & Geosciences, 43, 25-32, 2013.

Fischer, C., Arvidson, R.S., Lüttge, A., How predictable are dissolution rates of crystalline material? Geochim. Cosmochim. Acta 98, 177-185, 2012.

Maheshwari, P., Ratnakar, R.R., Kalia, N. and Balakotaiah, V., 3-D simulation and analysis of reactive dissolution and wormhole formation in carbonate rocks. Chemical Engineering Science, 90, 258-274, 2013.

Menke, H., Andrew, M.G., Blunt, M.J., Bijeljic, B., Reservoir condition imaging of reactive transport in heterogeneous carbonates using fast synchrotron tomography – Effect of initial pore structure and flow conditions. Chemical Geology 428, 15–26, 2016.

Steefel, C.I., Appelo, C.A.J., Arora, B., Jacques, D., Kalbacher, T., Kolditz, O., Lagneau, V., Lichtner, P.C., Mayer, K.U., Meeussen, J.C.L., Molins, S., Moulton, D., Shao, H., Šimůnek, J., Spycher, N., Yabusaki, S.B., Yeh, G.T., Reactive transport codes for subsurface environmental simulation. Computational Geosciences 19 (3), 445-478, 2015.

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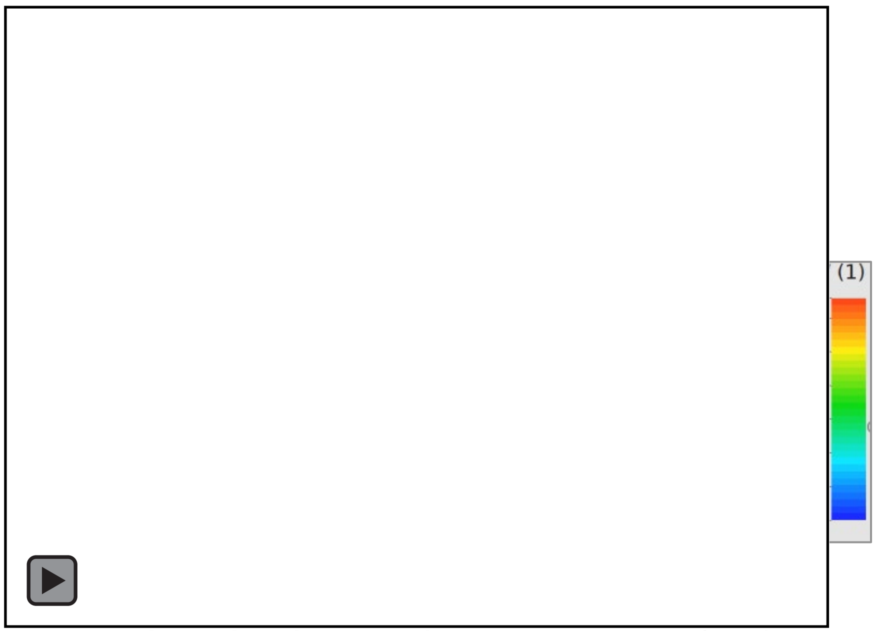
REACTIVE FLOW ADVANCEMENTS

GEODICT

- Simulate Mineral Dissolution & Crystallization upon consideration of the complete aqueous geochemistry
- Flow and transport solvers coupled to IPhreeqC (USGS)

Example: Reactive Flow setup for Carbonate dissolution using geochemical calcite reaction kinetics



pH value distribution *changes continuously due to ongoing dissolution reactions in a Grosmont carbonate sample of Andrä et al. (2013).*

Ca^{2+} concentration *increases in the pore space due to continuous dissolution reactions in a Grosmont carbonate sample of Andrä et al. (2013).*

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Thank You for your Attention

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