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Towards digital twins: machine learning based process coupling and multiscale modelling of reactive transport phenomena

Goldschmidt 2020

25.06.2020

Outline of presentation

- Motivation, multiscale, digital twins and machine learning
- Bridging heterogeneous codes at different scales (slide 9)
- Numerical diagnostics and digital twin of a microfluidic experiment. (slide 12)
- Accelerating reactive transport calcualtions (slide 19)
- Significance implications and challenges (slide 22)
- Summary (slide 24)

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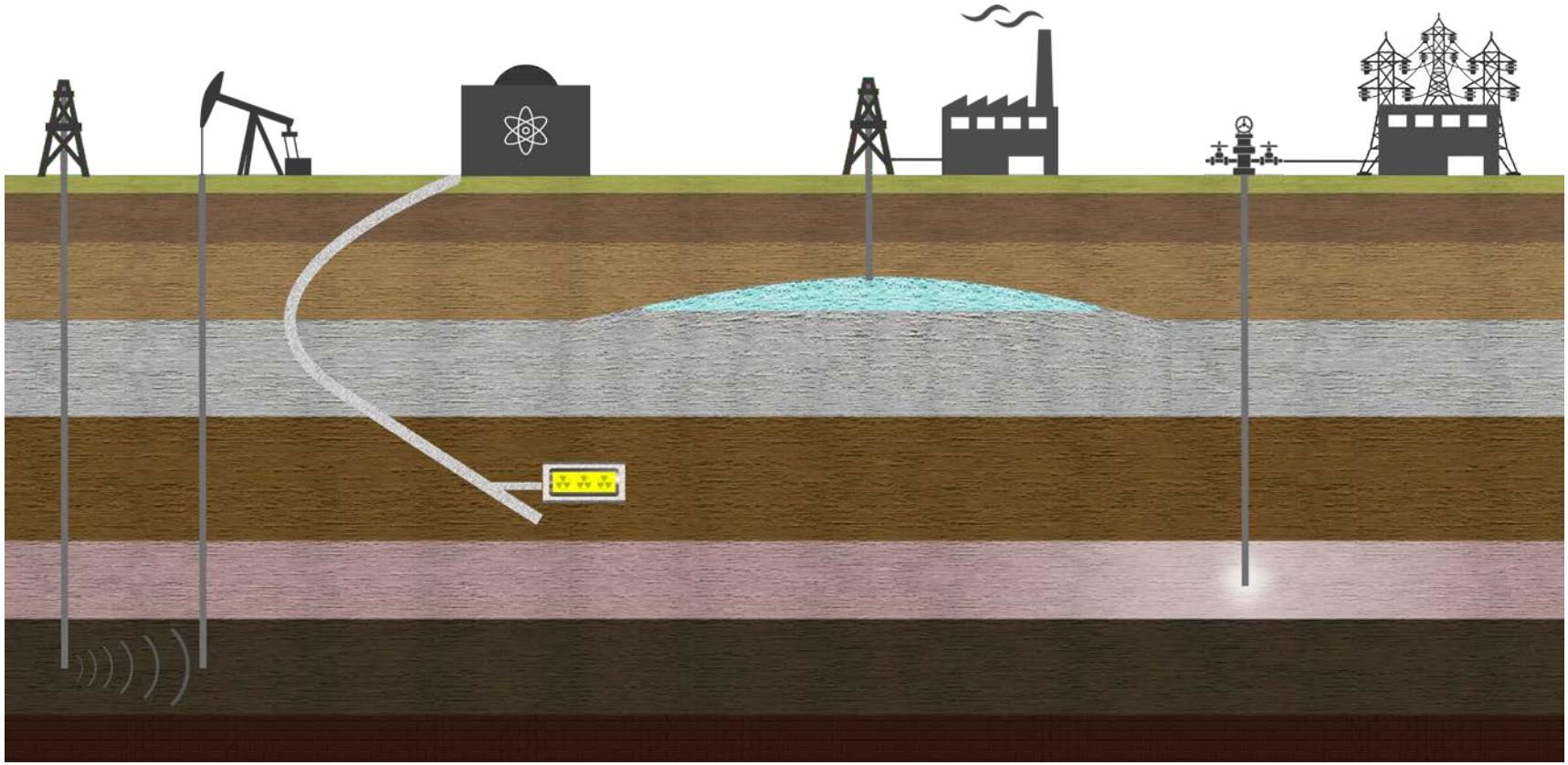
Motivation: Realistic multi-scale multi-physics modelling

- *Subsurface processes are governed by mass transport and phase change processes that act at several scales.*
- *Well established numerical tools and process understanding exists at each spatial scale (atomistic-, pore-, field- scale).*
- *Digital twins of the real physical systems require enhanced code-, physics- and scale- couplings.*

Subsurface processes are governed by mass transport and phase change processes

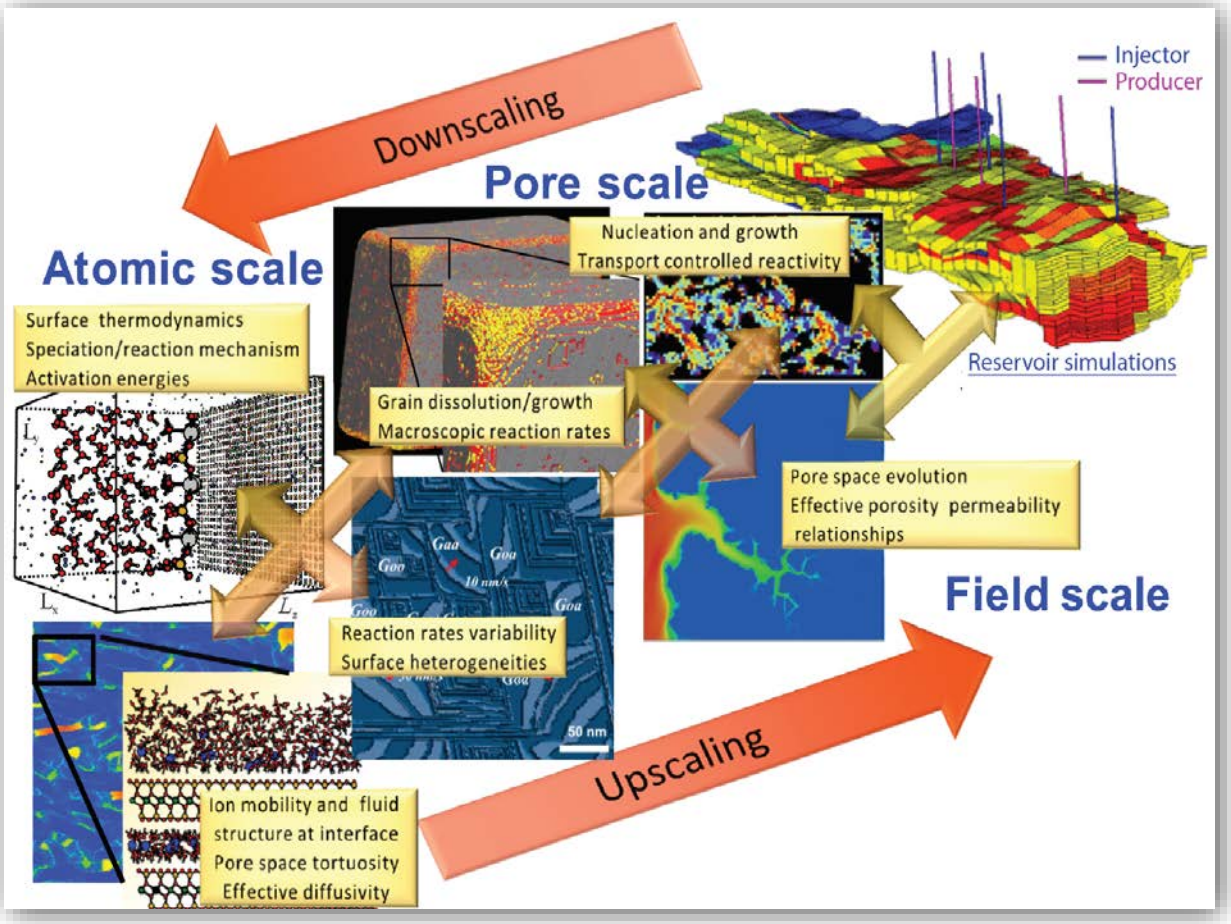
Enhanced oil recovery | Geological Disposal | CO2-Sequestration | Geothermal



⇒ Realistic representation of the processes requires multiscale multiphysics description

All scales matter: breakdown of relevant scales

Processes occurring at the atomic- and pore- scale control the evolution of the geochemical systems. Currently, there exist several mature numerical tools, and good process understanding, at each scale.



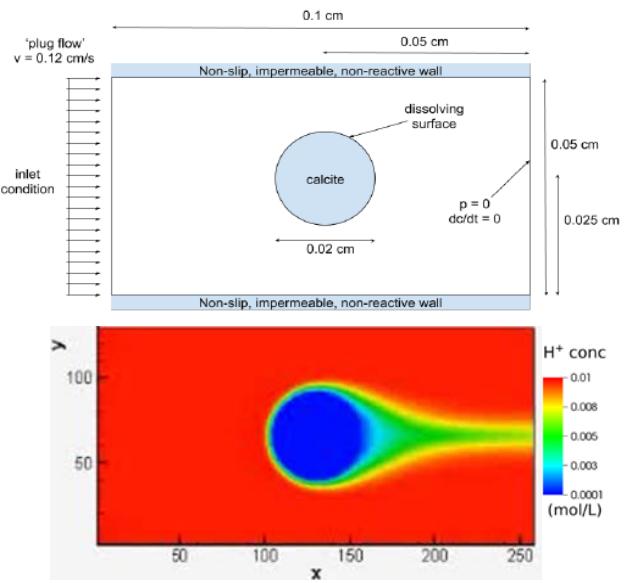
Churakov & Prasianakis, *Holistic process-based description of mass transport and mineral reactivity in porous media.* **Am. J. Science, 318 (9)** 921-948 (2018)

Well established tools and process understanding exists at each scale: pore-scale benchmark example.

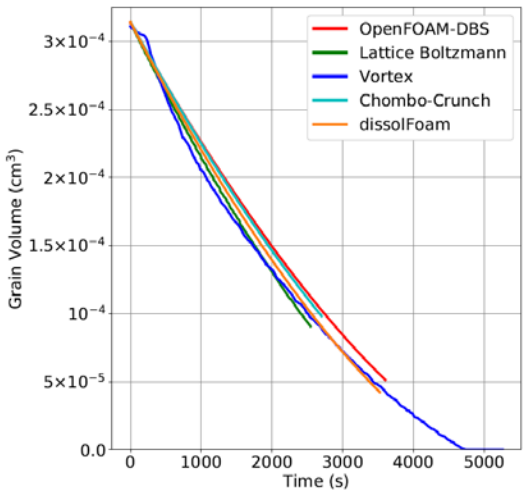
Such an example is the pore-scale dissolution benchmark with evolving fluid-solid interfaces.
A calcite rock is dissolved due to the convective flow of acid solution.
Six different codes participated and gave similar results.

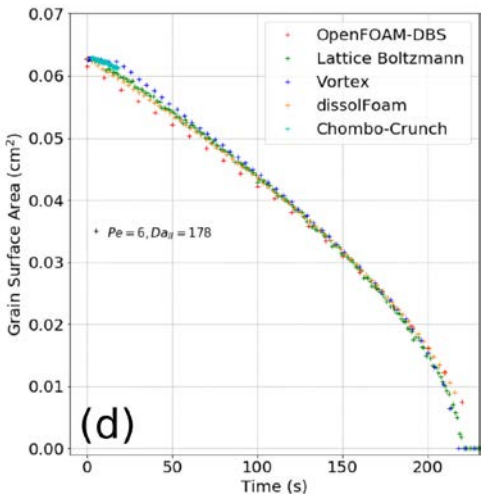
***Remaining Challenge:* Transfer information and connect the scales / codes**

Institute:	OAK RIDGE National Laboratory	PAUL SCHERRER INSTITUT PSI	BERKELEY LAB Lawrence Berkeley National Laboratory	UNIVERSITÉ DE PAU ET DES PAYS DE L'ADOUR	UNIVERSITY OF FLORIDA	Stanford University / brgm
Participant code:	**dissolFoam**	**Lattice Boltzmann**	**Chombo Crunch**	**Vortex method**	**dissolFoam**	**OpenFoam-DBS**



H+ Concentration contours pH=2



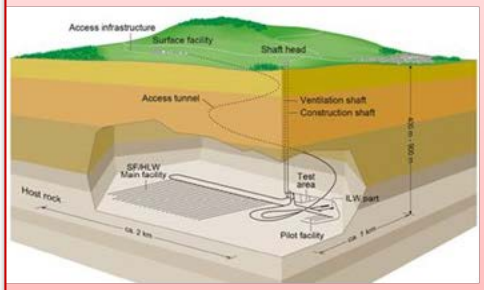


Molins et al, *Simulation of mineral dissolution at the pore scale with evolving fluid-solid interfaces: Review of approaches and benchmark problem set*, **Computational Geosciences, 1-34** (2020), https://doi.org/10.1007/s10596-019-09903-x

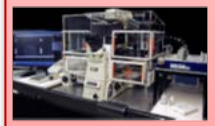
Geochemical digital twins

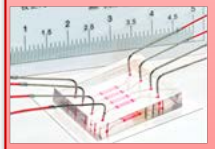
Digital Twin is a modelling based tool of increased realism. For geochemical applications, it should cover several spatial and temporal scales, as well as all major underlying mechanisms.

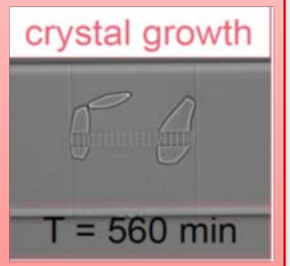
Real physical process



Field scale, nuclear waste repository







Laboratory experiment, microfluidics

Design optimization

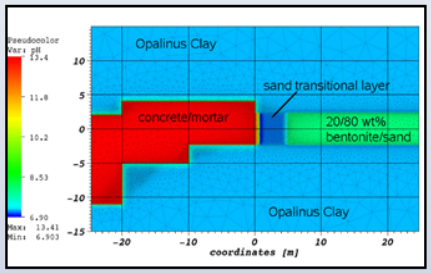
Predictive capability

Process Understanding

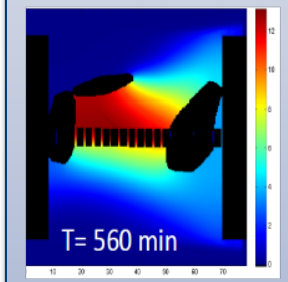
Numerical Diagnostics

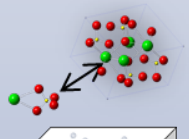
Digital Twin

Physics based models

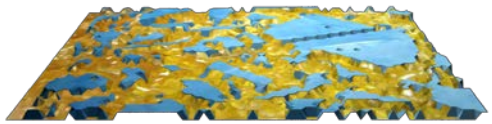


Field scale, numerical simulation

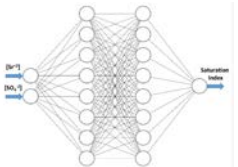




Cross-scale microfluidic precipitation simulation



- High fidelity simulations
- Multiscale description
- Multiphysics description
- Ultrafast computations
  Sensitivity analysis
- Machine learning
- Augmented reality of experiment
- Real-time experiment companion



Machine learning, integral part of a digital twin

Machine learning is a set of numerical algorithms and models that allows a system to automatically learn and improve without being explicitly programmed.

- Novel algorithms and increased computational power drive the new machine learning wave

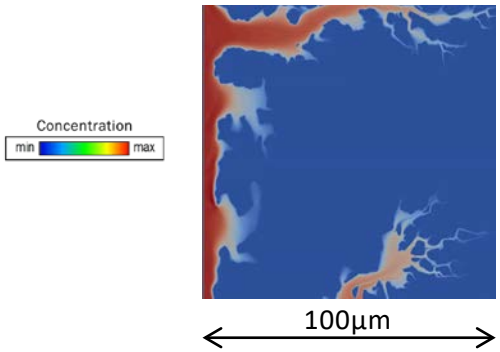
- Artifical Neural Networks (ANN) are machine learning tools

- ANNs are used here in two examples:
  a) for coupling heterogeneous codes at different scales,
  in an effort to automate communication between scales and codes
  b) for accelerating geochemical calculations coupled to a lattice Boltzmann solver

Bridging heterogeneous codes at different scales

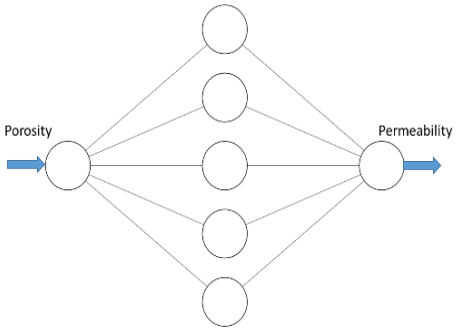
Communication and interfacing of heterogeneous codes at different spatial scales can be based on neural networks.
The scale specific mechanisms and their dependence on several parameters can be used as the training input.

Pore-scale
Lattice Boltzmann

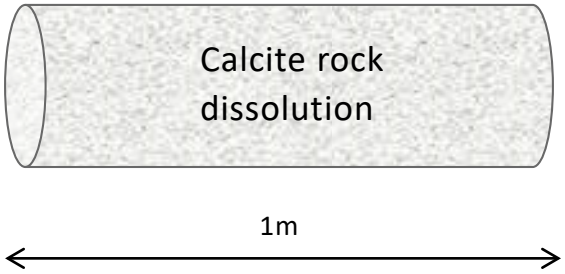


Discretization **Dx=0.1µm**

Machine Learning
for upscaling



Darcy-scale
MCOTAC (finite volumes)



Discretization **Dx=0.1m**

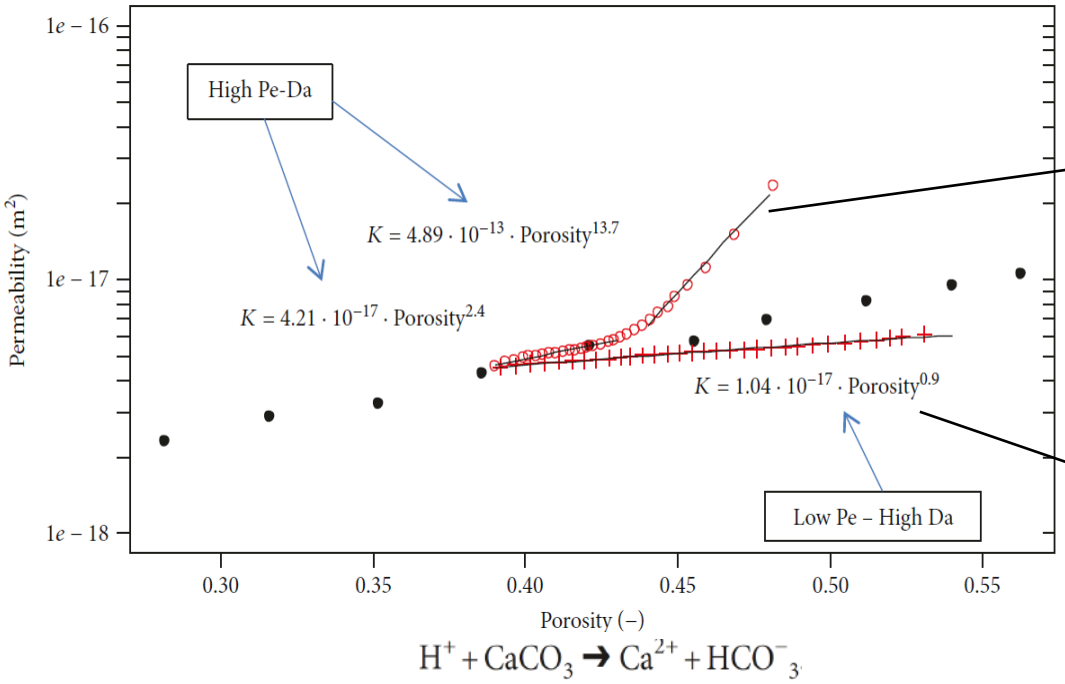
⇒ Trained neural networks are light and robust functions that can be easily integrated in any code, written in any of the major programming languages.

Prasianakis, N.I., Haller, R., Mahrous, M., Poonoosamy, J., Pfingsten, W., Churakov S.V.,
Neural network based process coupling and parameter upscaling in reactive transport simulations (In revision 2019)

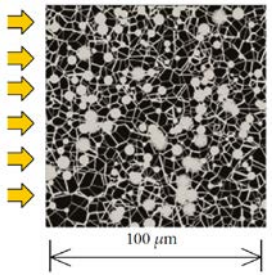
Upscaling strategy: case specific correlations, extracted from detailed pore-level simulations.

During dissolution, the permeability-porosity correlations **deviate** from typical Kozeny-Carman, and depend highly on the chemical and flow gradients. The **Peclet** (Pe) and **Damkohler** (Da) numbers can be used for classification of the expected **evolution paths** (e.g. wormhole formation / face dissolution). It is common to fit such correlations in power laws.

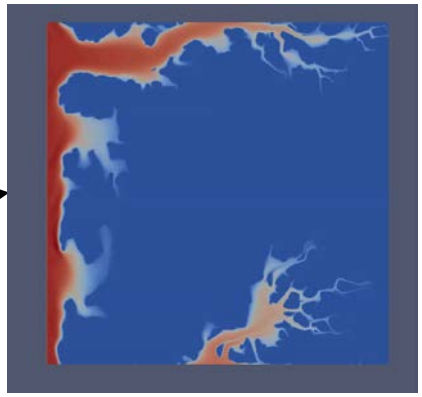
Permeability (K) – porosity correlation: $K = a \cdot porosity^{b}$



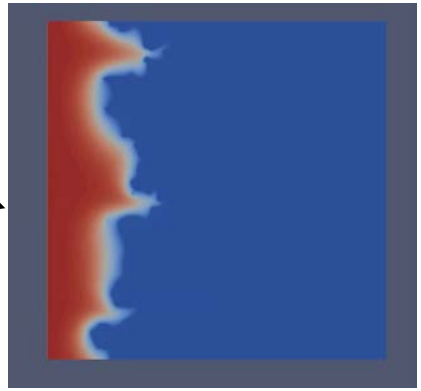
$H^{+} + CaCO_3 \rightarrow Ca^{2+} + HCO^{-}_3$



Wormhole formation



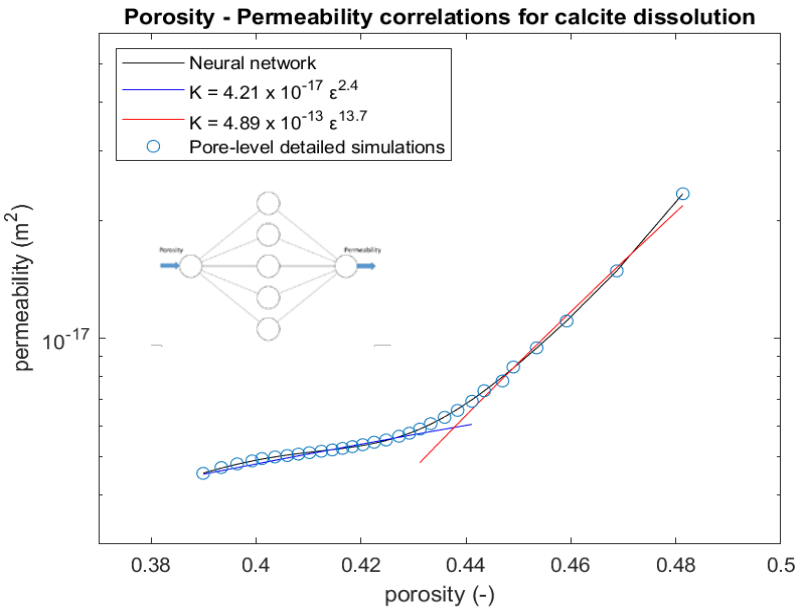
Face dissolution



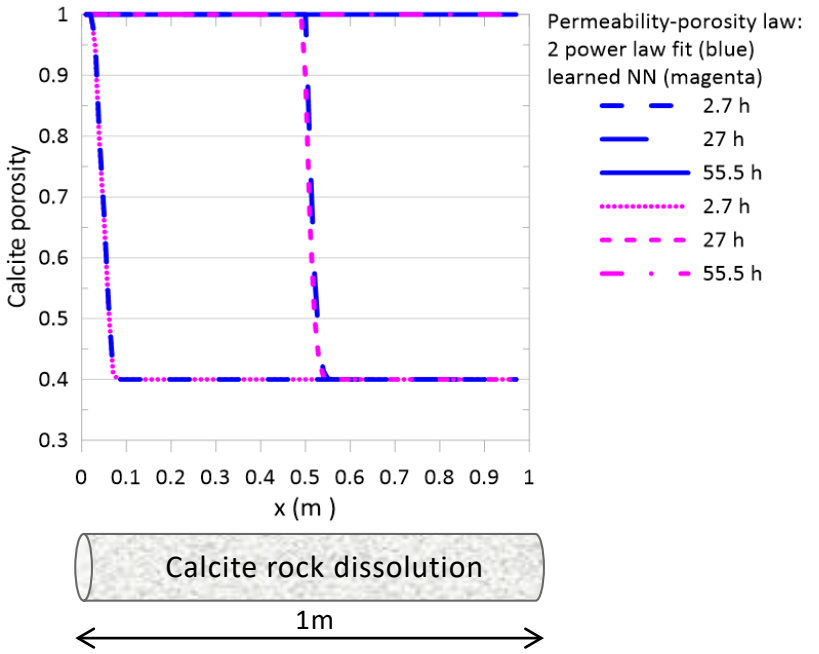
Prasianakis, N.I., Gatschet, M., Abbasi, A., & Churakov, S. V. Upscaling Strategies of Porosity-Permeability Correlations in Reacting Environments from Pore-Scale Simulations. ***Geofluids*** 9260603 (2018).

Upscaling porosity-permeability correlations into a macroscopic Darcy-scale code

The Permeability-porosity correlation in the case of wormhole formation is not possible to be fitted by a single power law, and usually requires human-machine interaction for segmenting the correlation to two or more domains (**blue**-**red**).
A shallow neural network can be used instead (**black**). Training is completed in few seconds. **Process can be automated**.



Calcite porosity distribution during acidification along the macroscopic domain for two different approaches



The ANN was trained on the microscopic LB simulations, and was subsequently embedded in the Darcy scale code MCOTAC.
If data exist, the neural network can represent higher dimension parameter spaces:
e.g. porosity permeability correlations as functions of K=*f*(*Pe*, *Da*, *initial porosity*, *heterogeneity,…)*.

Numerical diagnostics and digital twins

Lab on a chip experiment (Celestine precipitation)

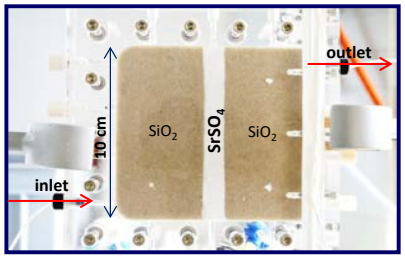
Augmented reality via modeling diagnostics

Lab on a chip: design and concept

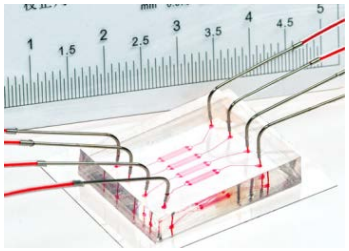
Advantages: miniaturized environment, shorter time-scales, small quantities of reactants, continuous monitoring, parallel

Challenges : in-situ conditions of flow and chemistry unknown, control of experiment, manufacturing, design of experiment

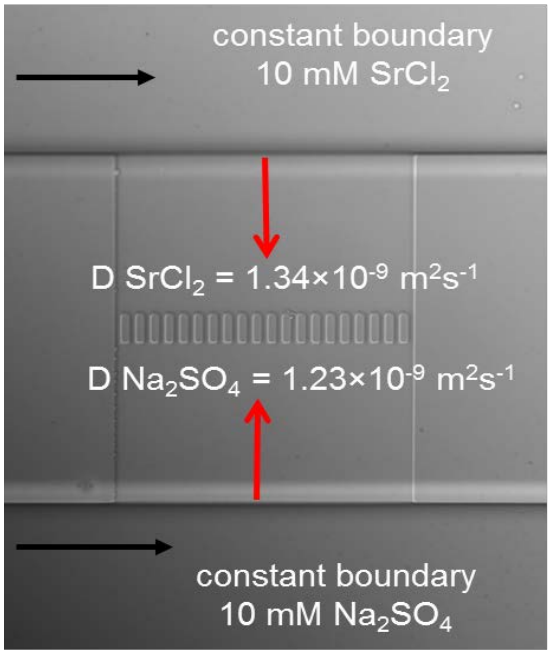
Typical lab experiment
(**cm** scale)

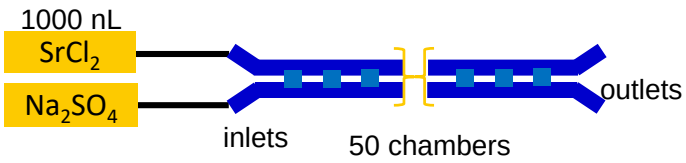


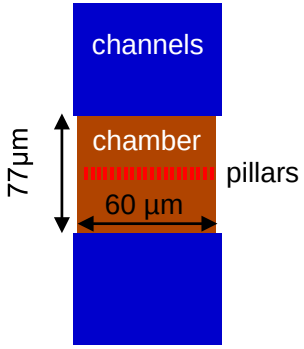
Microfluidic reactor
(**µm** scale)



laminar flow







$SrCl_{2(aq)} + Na_2SO_{4(aq)} \rightarrow SrSO_{4(s)} + 2NaCl_{(aq)}$

Collaboration with J. Poonoosamy, FZ-Jülich, Germany

Digital Twin and Numerical diagnostics

Augmented reality by combining cross scale lattice Boltzmann modelling diagnostics. Numerical model includes: a classical nucleation theory (CNT) implementation (nanoscale processes), multicomponent transport, kinetic reactions.

Injection of 10 mM $SrCl_2$ and 10 mM Na_2SO_4 → celestine precipitation, crystal growth

Layers of diagnostics

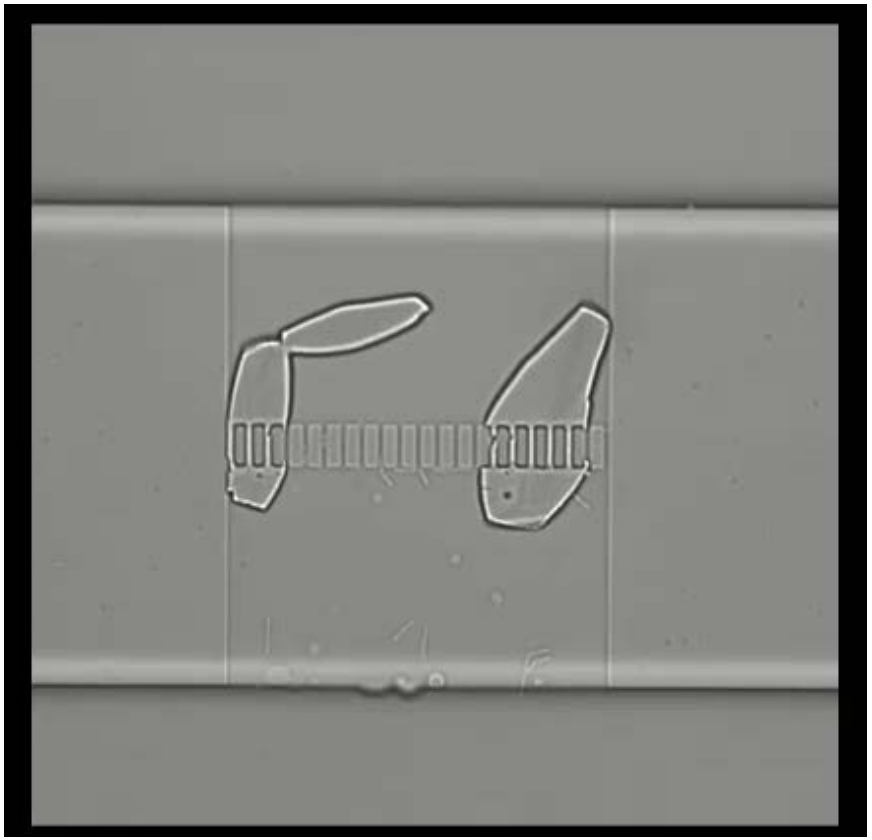
Evolution of experiment (camera)

Local flow-field and streamlines visualization (numerically calculated, experimentally verified).

Spatial resolution of velocity field at different stages of the experiment (numerically calculated)

Local species concentrations, saturation ratio (numerically calculated, interplay of advection/diffusion)

Local precipitation rates at fluid-solid interface, prediction of directional differential growth (numerically calculated, color: precipitation rate)



Poonoosamy, J., Westerwalbesloh, C., Deissmann, G., Mahrous, M., Curti, E., Churakov, S.V., Klinkenberg, M., Kohlheyer, D., Von Lieres, E., Bosbach, D., Prasianakis, N.I., A microfluidic experiment and pore scale modelling diagnostics for assessing mineral precipitation and dissolution in confined spaces, ***Chemical Geology, 528, 5, 119264 (2019)***

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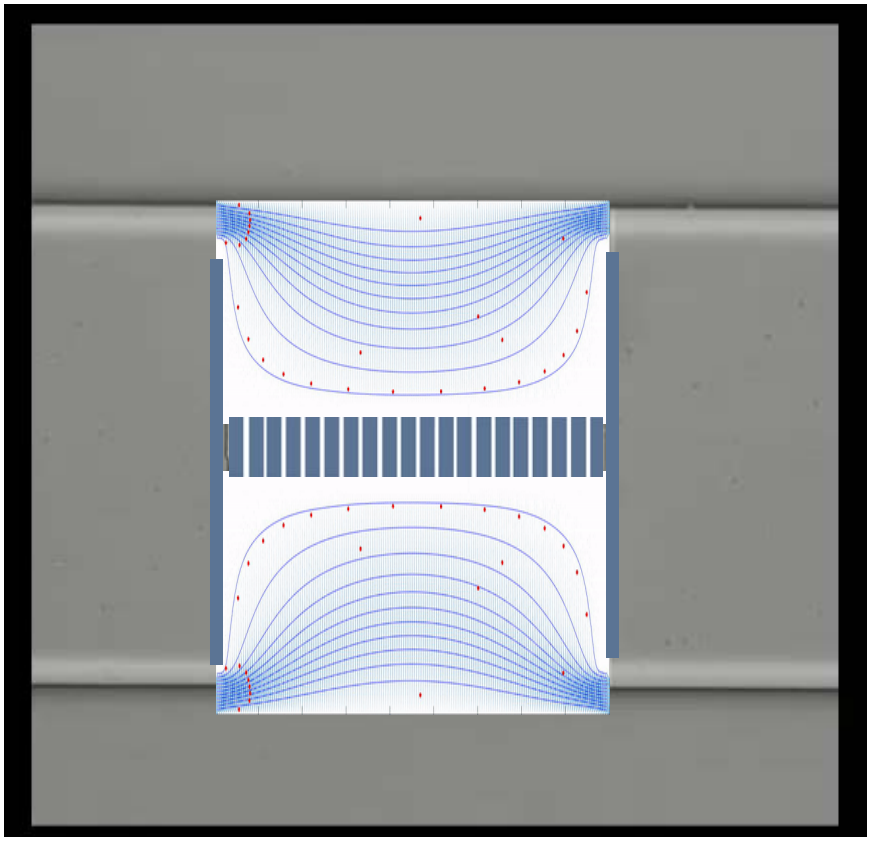

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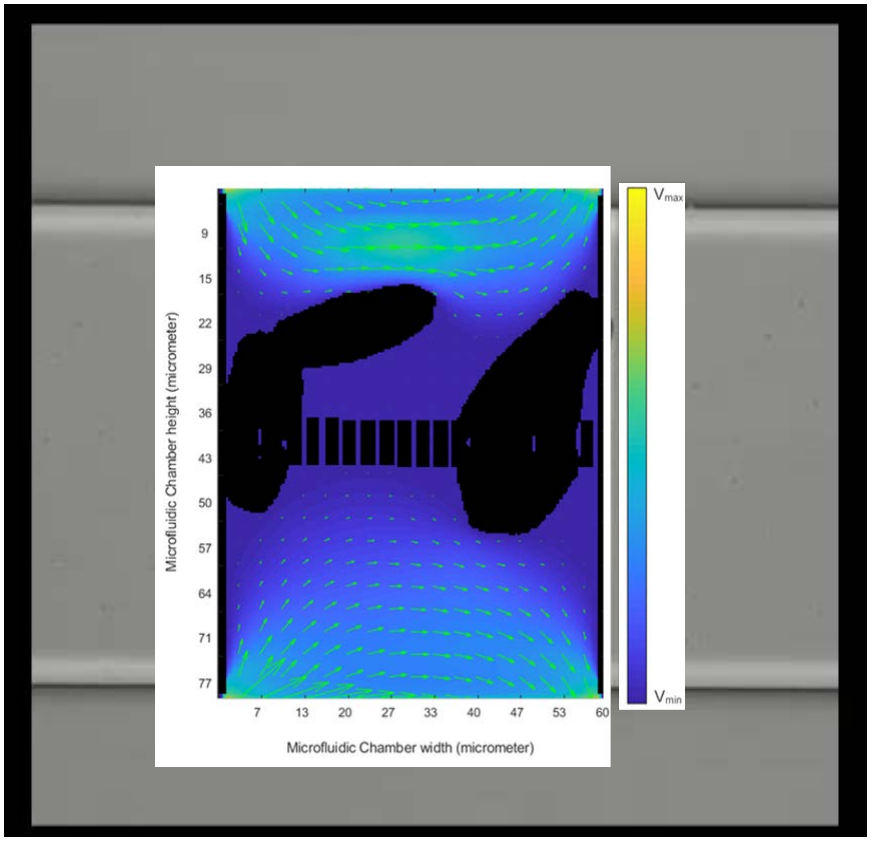

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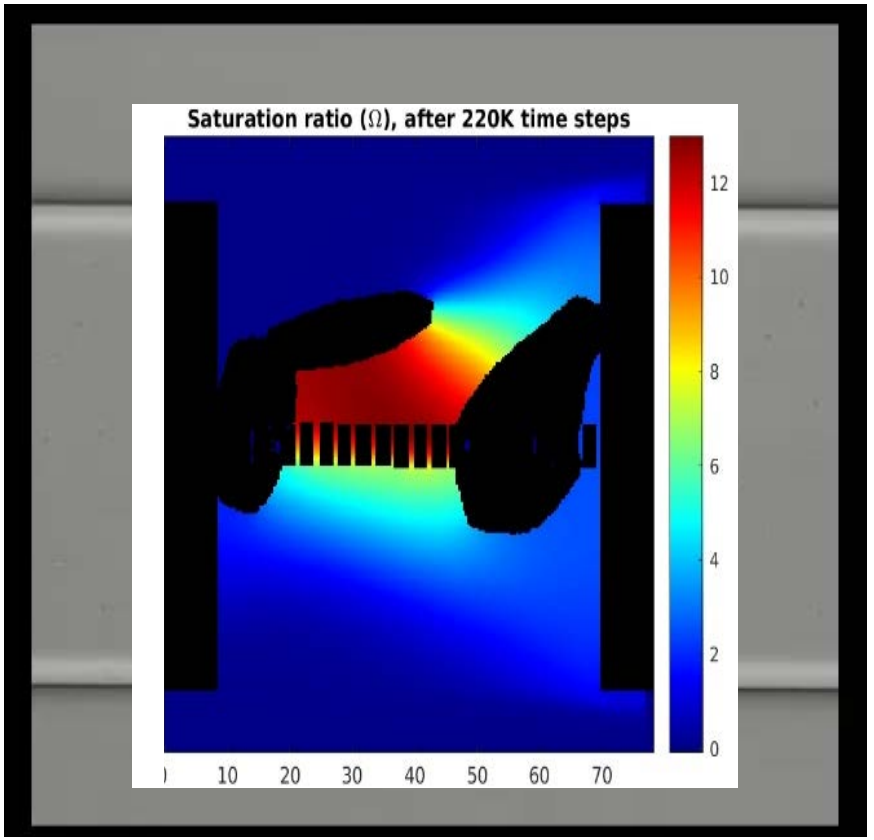

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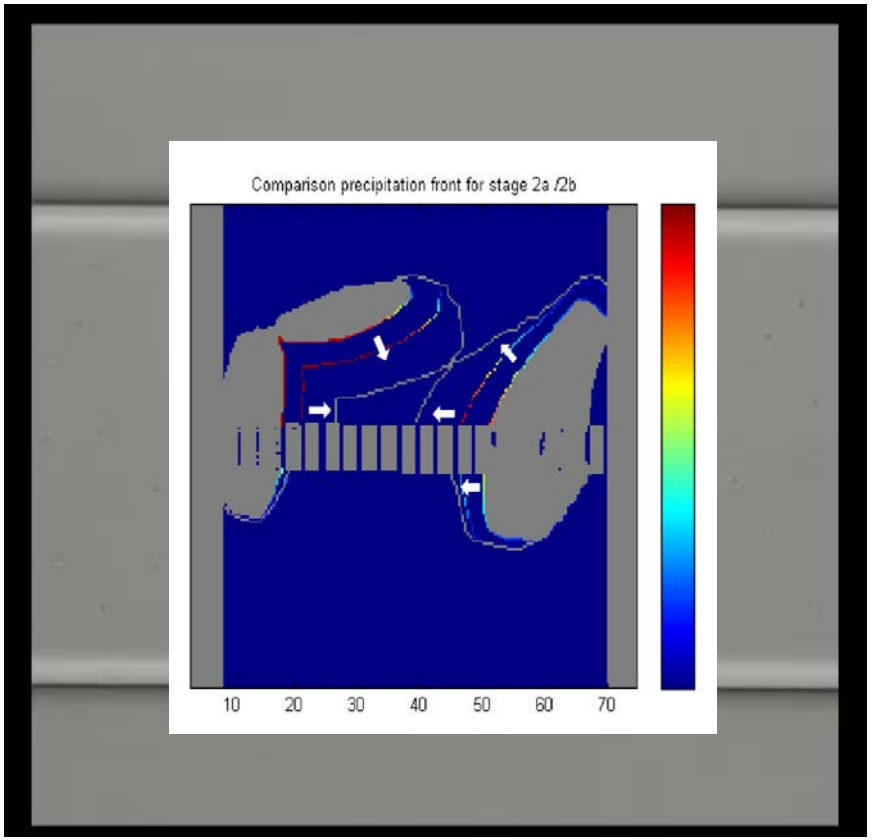

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Accelerating reactive transport calculations: Chemical calculations is the bottleneck

Machine learning has been used in several fields of computational physics that involve reactive transport in the past. Lately there are several efforts also in the field of geochemical reactive flows. Advanced algorithms and available computing power are the **drivers of innovation**.

Accelerating chemistry in the filed of combustion, reactive flows

Christo, F. C., A. R. Masri, and E. M. Nebot."Artificial neural network implementation of chemistry with PDF simulation of H2/CO2 flames." Combustion and Flame 106, no. 4 (1996): 406-427.

Accelerating geochemistry and geochemical reactive transport calculations

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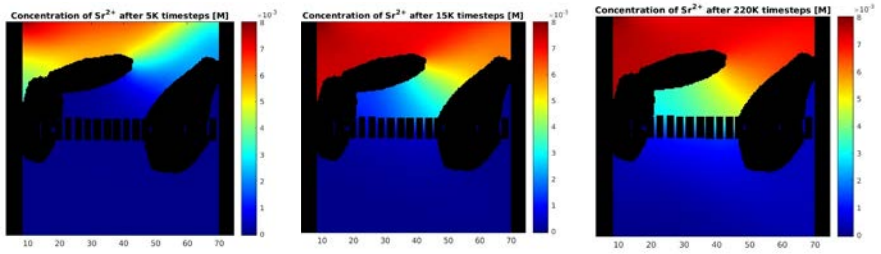
Prasianakis, N.I., Haller, R., Mahrous, M., Poonoosamy, J., Pfingsten, W., Churakov S.V.,
Neural network based process coupling and parameter upscaling in reactive transport simulations (In revision 2019)

Simple speciation, complex reactive transport and phase change setup: celestine precipitation

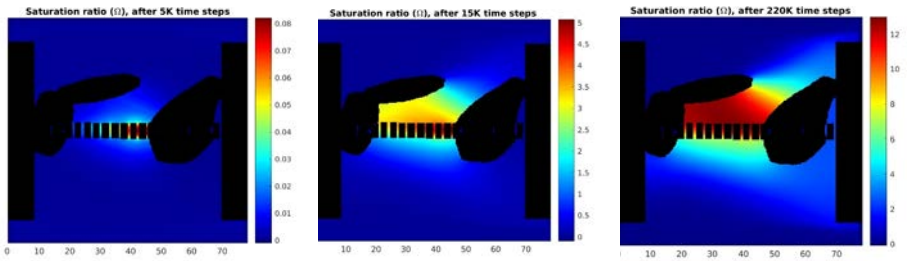
For the digital twin of the microfluidic experiment it is necessary to calculate at each time step, and at each node the chemical speciation and the saturation index (SI). Local SI drives the precipitation kinetics.

Injection of fresh 10 mM $SrCl_2$ and 10 mM Na_2SO_4 mixture
→ celestine precipitation, crystal growth

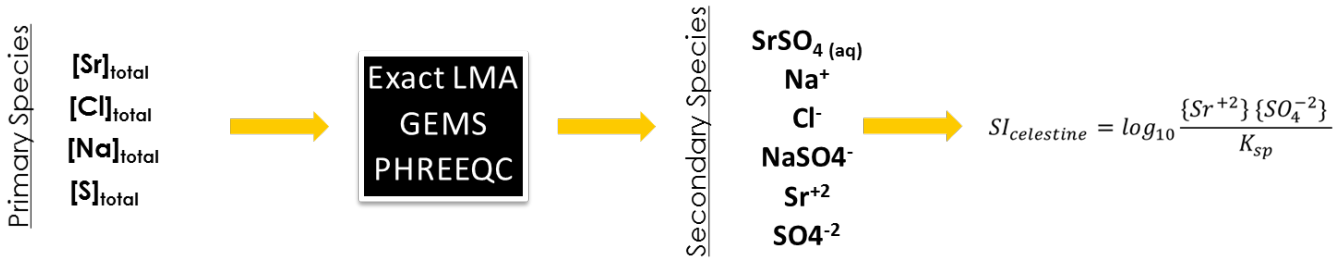
Evolution of Concentration of Sr^{+2}



Evolution of Saturation ratio



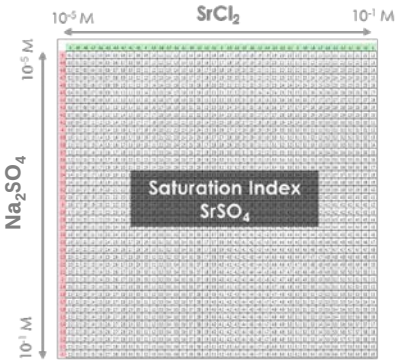
Typical workflow for calculation of SI: Knowing the concentrations of primary species, an external LMA solver, e.g. GEMS / PHREEQC is invoked for the calculation of the chemical speciation



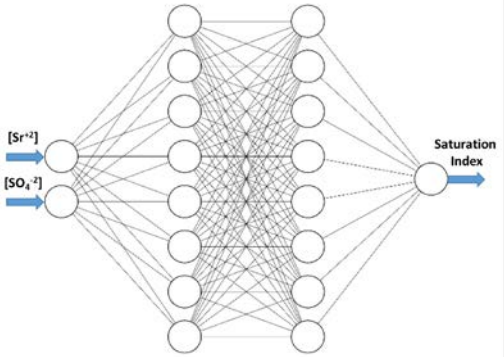
Accelerating geochemistry, and accuracy considerations
Comparison of Exact LMA, Lookup table, Neural Network

Exact LMA
GEMS
PHREEQC

Vs



Vs

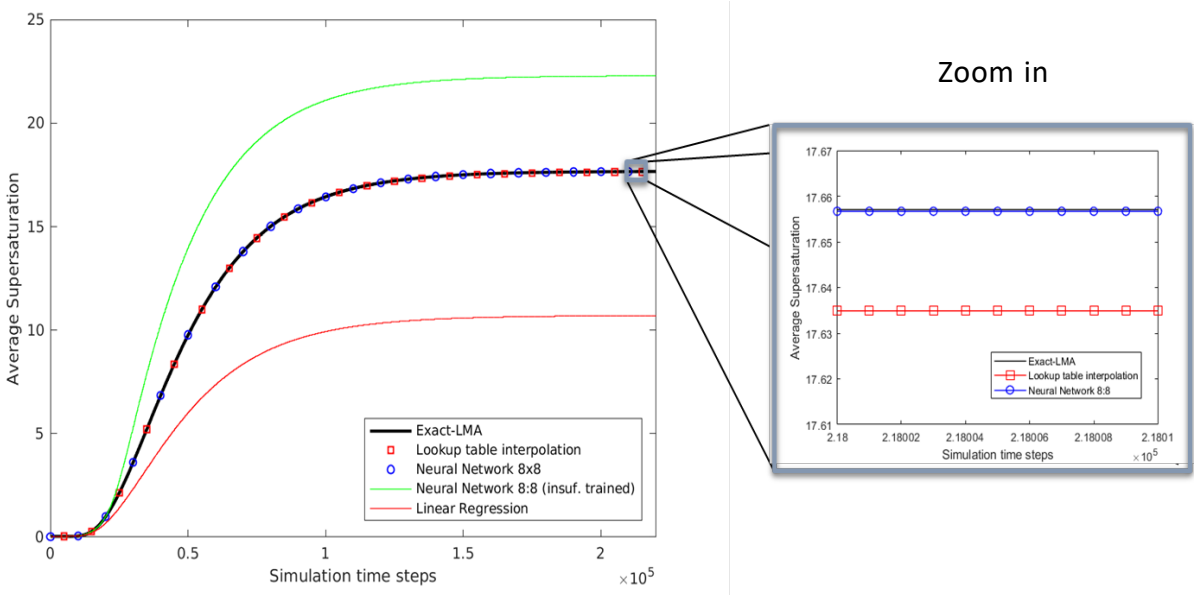


Exact LMA coupled to lattice Boltzmann (LB)

40x40 lookup table generated from exact LMA, coupled to LB

Neural network trained on 70% of the lookup table entries, RMSE=6.64 * 10^{-5} , coupled to LB

Evolution of the domain average supersaturation for the different methods: exact LMA, lookup table (linear interpolation), neural network with 2 hidden layers.



In this setup, ANN proves to be orders of magnitude faster compared to LMA and extremely accurate also compared to lookup table.

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Significance, implications and challenges

- A typical ***Lattice Boltzmann code*** for 4 master species can perform ~ **1'000'000** grid (lattice) point updates per second (1 MLUPS), on a single CPU core. Geochemical calculations occur at every timestep / every lattice point

- Typical ***geochemical speciation code*** (GEMS/PHREEQC) delivers ~ **1'000** cold start geochemical calculations per second on a single CPU core (e.g. Xeon E5-2650v4 2.2 GHz). In this case, chemistry consumes 99.9% of the computational time (*1000 times slower than the flow solver*)

- The ***neural network*** shown here, with 2 hidden layers and 8 neurons per layer, has a sustained throughput performance of ~ **13'000'000** calculations of SI per second, on the same cpu core (c code function). This is a speed-up of geochemical calculation ~ *four orders of magnitude, chemistry is not anymore the bottleneck* ***!***

- Similar speed-up is observed also from the ***lookup table*** implementation, and for simple problems it can be more straightforward to implement. However, linear interpolation can be less accurate, and for more complex problems the lookup table grows exponentially. E.g., precision of 100 points per dimension (input variable), for 6 dimension (input), results in a 1 Trillion points (10^12) and occupies in memory 31 Exabyte (100 times more than the storage capacity of the largest supercomputer)

- *Training* a ***neural network*** for higher dimensions, to achieve the desired accuracy is still very challenging, and the difficulty increases with the complexity of the geochemical problem. ***High quality of training data*** is also required. However, the network performance does not decrease with the number of dimension rather than with the number of neurons per layer. Pre-training or training on-the-fly are both very promising options.

- See next slide for high performance computing.

Supercomputing: Transport is fast, chemistry is slow, hybrid computer architecture

Current supercomputers allow to simulate geometries with > 10 billion voxels (grid points). Most advanced systems have hybrid CPU/GPU computational nodes. Transport and chemical calculations take place at every voxel, at every timestep

Swiss Supercomputing Center (CSCS)

Piz Daint Nvidia Tesla P100 GP-GPUs

X-ray tomogram
(1 Billion Voxels)

Comparision of Calculations per second

Chemistry **GEMS / PHREEQC**	**Transport (flow)** **Lattice Boltzmann**	**Chemistry** **Neural Network**
1 CPU-core ~ 1'000/s	1 CPU-core, 4 species ~ 1'000'000/s	1 CPU-core (depending on system) ->more than 1'000'000/s
1 GPU -> **Impossible** **Code not available**	1 GPU, 4 species -> 100'000'000/s	1 GPU -> Expected speedup 10-100 times the CPU

For high performance computing, where problem can be solved entirely in parallel GPU setup (Lattice Boltzmann), **surrogate modelling is an enabling step**.

Summary

- Ever increasing realism of multiphysics simulations **is an enabling technology** for **digital twins** e.g. lab on a chip digital twin, nuclear waste repository
- Real-time **digital twins** can assist in the interpretation and the steering of laboratory experiments. The potential is yet to be explored.
- **Machine learning** can assist in **bridging** the scales and physics in multiscale multiphenomena simulations
- Artificial **neural networks** (ANN's) can replace the geochemical solver or any underlying physical process during runtime. Acceleration of several **orders of magnitude** is expected. This is especially important for conducting sensitivity and uncertainty analysis
- **Neural networks** must be trained carefully to achieve the desired accuracy. More research is needed to identify better the fields of application.
- **Lookup table** techniques work best for low dimension problems. Their exponential growth with the number of inputs is prohibitive for higher dimensional problems.

Wir schaffen Wissen – heute für morgen

Acknowledgements: Nagra, SNF, BFE, EU project EURAD WP4-DONUT funding from the European Union's Horizon 2020 research and innovation programme under grant agreement n° 847593