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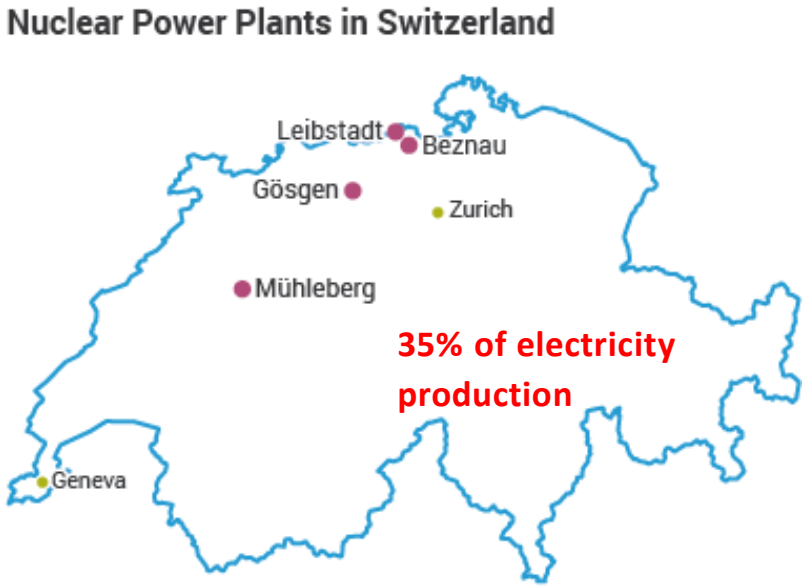
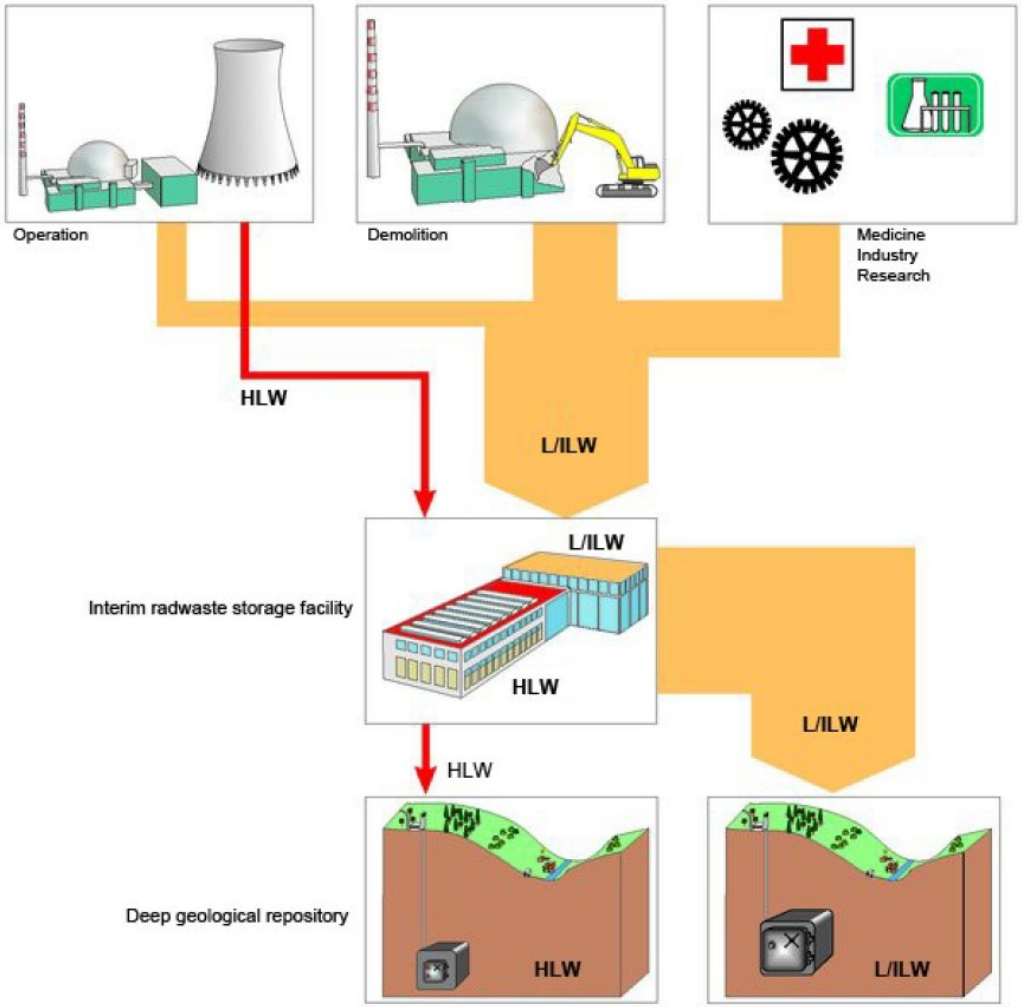
N. Prasianakis: Head of transport mechanisms group: Laboratory for Waste management
In collaboration with R. Haller, L.H. Damiani, M. Mahrous, S. Churakov

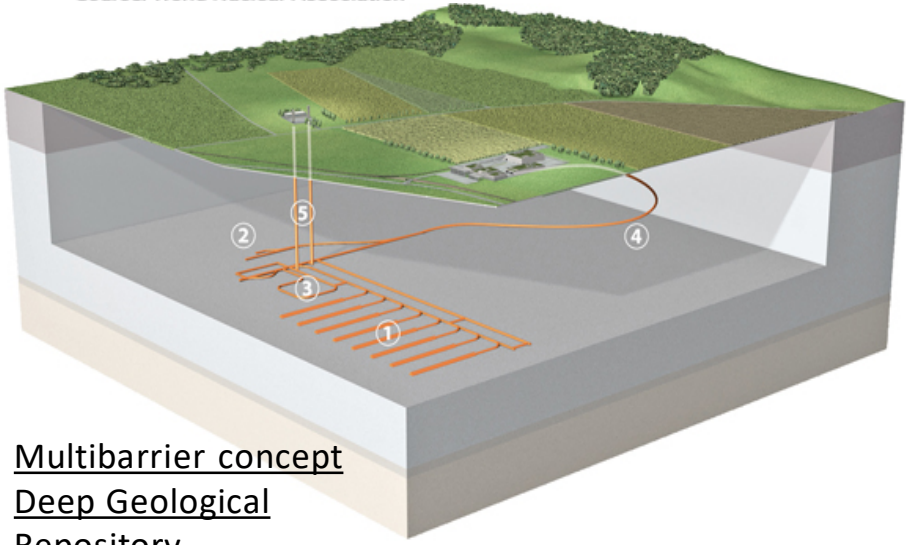
ML workshop meeting 15.06.2021

Machine Learning for Digital Twins and multiphysics simulations

Nuclear Waste Management concept

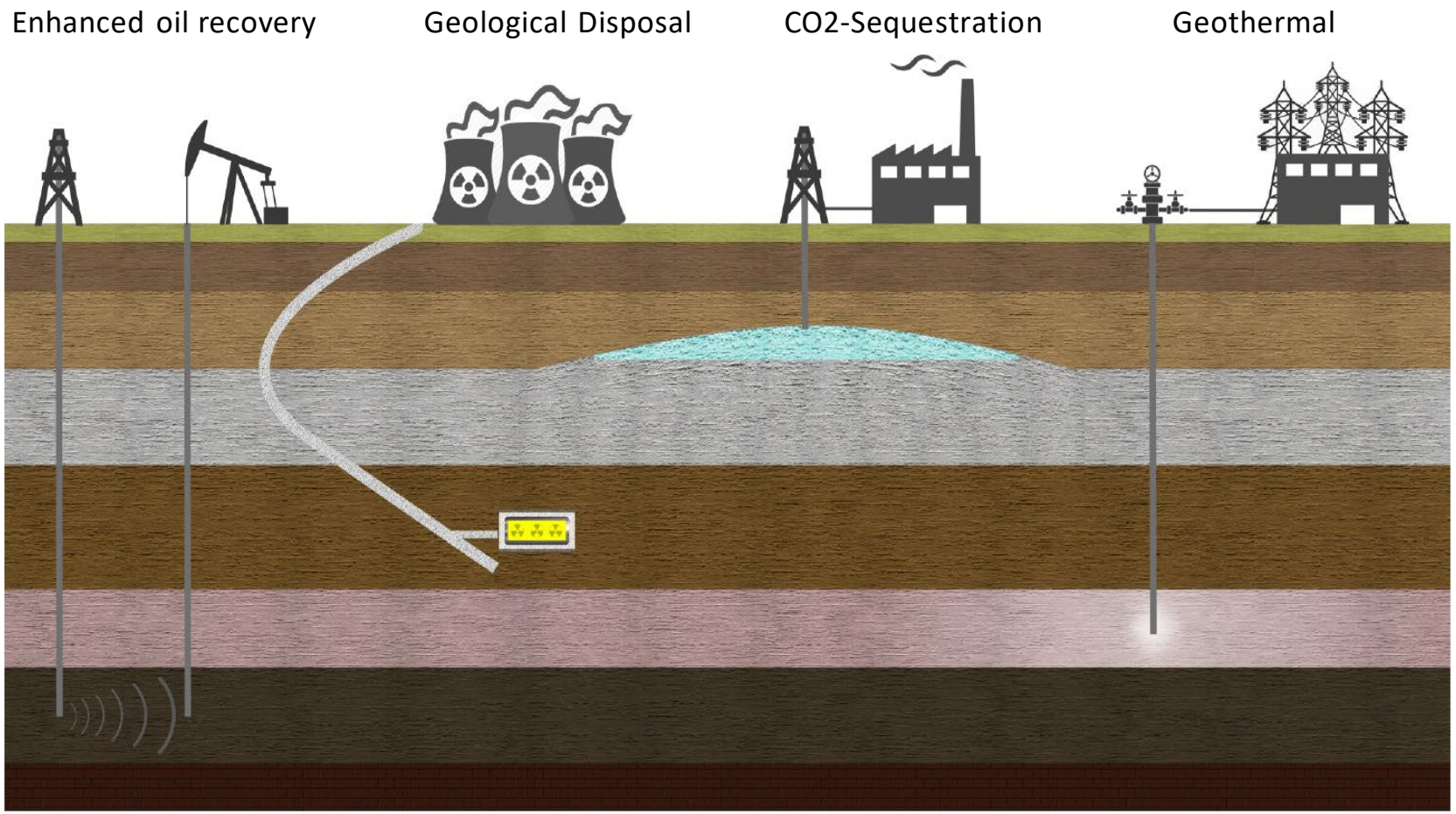






Multibarrier concept
Deep Geological Repository

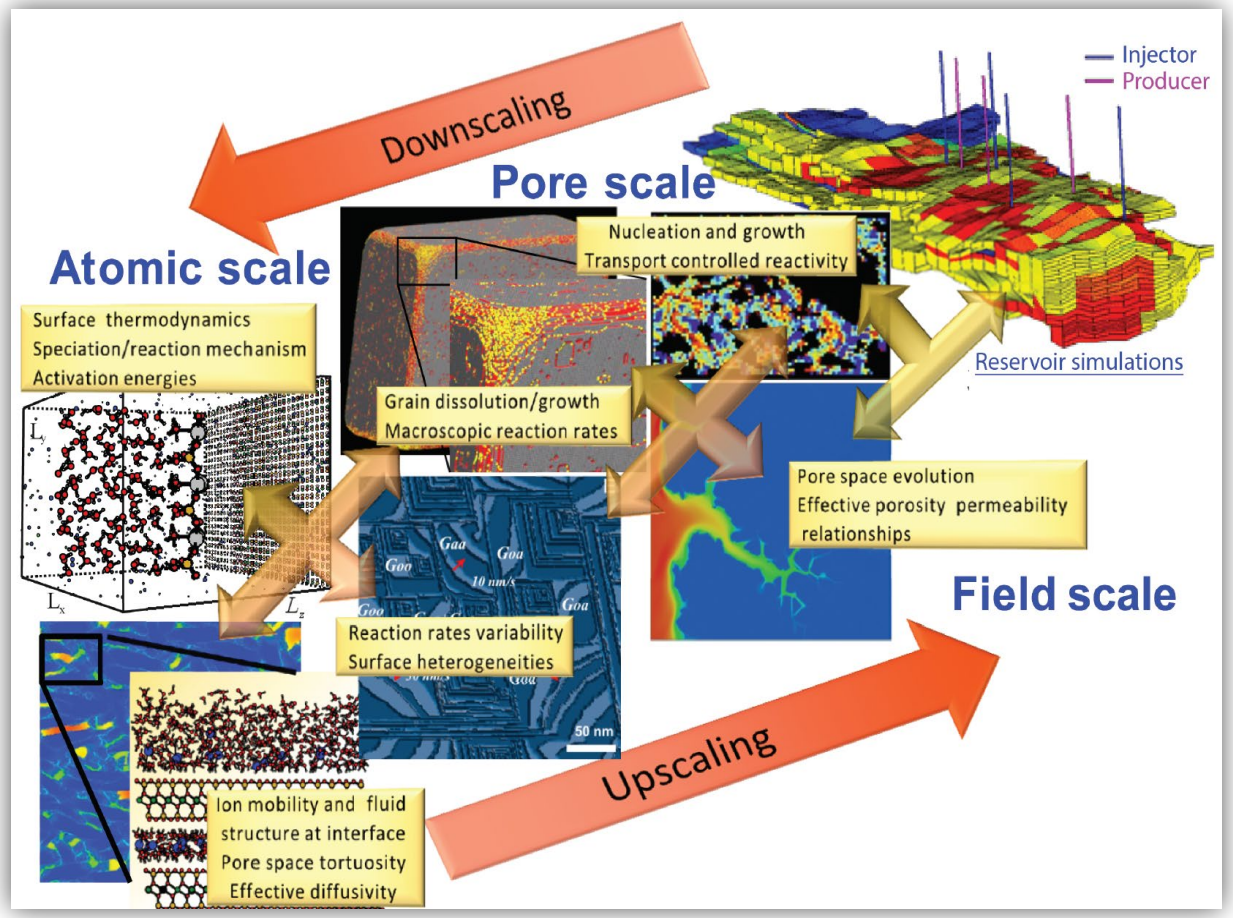
Subsurface processes are governed by dissolution precipitation processes



Multiscale description is necessary

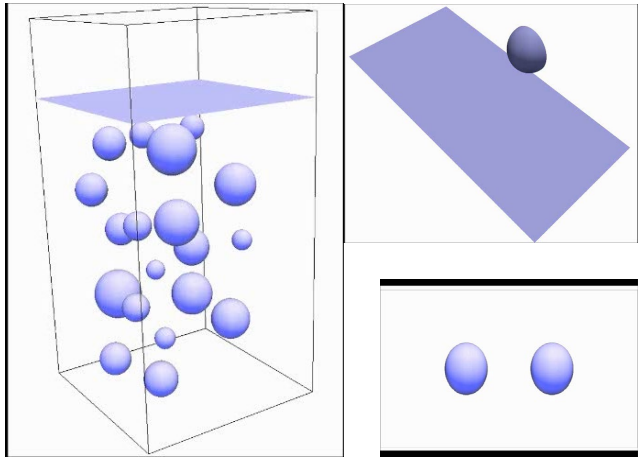
Geochemical evolution of repository is governed by mass transport and phase changes: all scales matter

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.

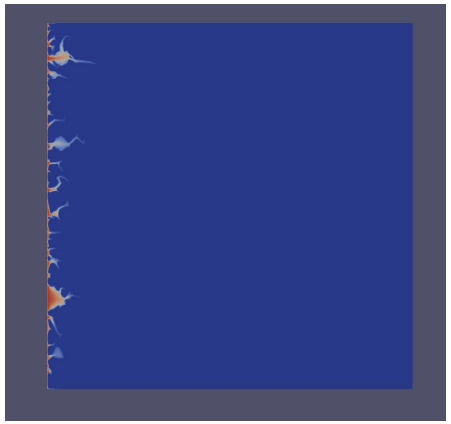


Churakov & Prasianakis, *Holistic process-based description of mass transport and mineral reactivity in porous media.* **Am. J. Science, 318 (9)** 921-948 (2018)

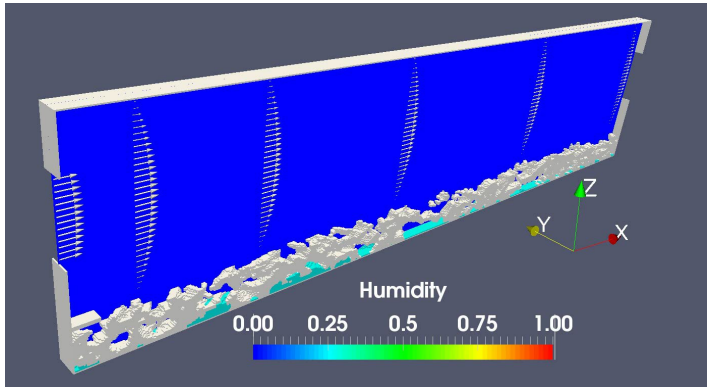
Lattice Boltzmann activities at PSI



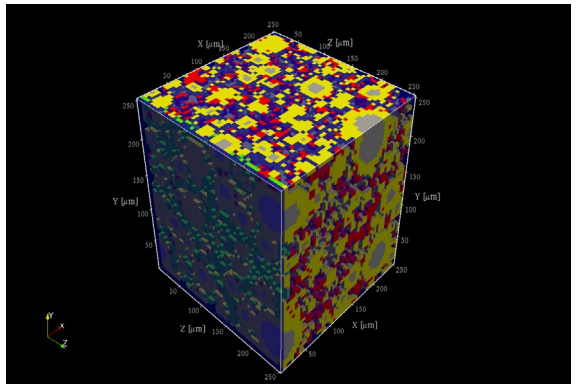
Multiphase Models
(Nuclear reactors, fuel cells)



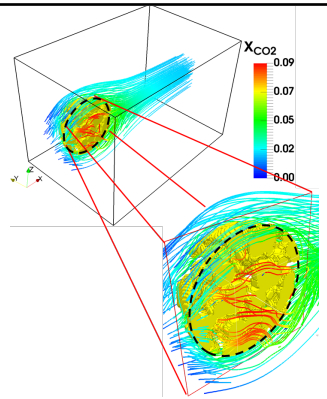
Geochemical reactions
(wormholes during acidification)



Evaporation in porous media (fuel cells)



Cement Evolution

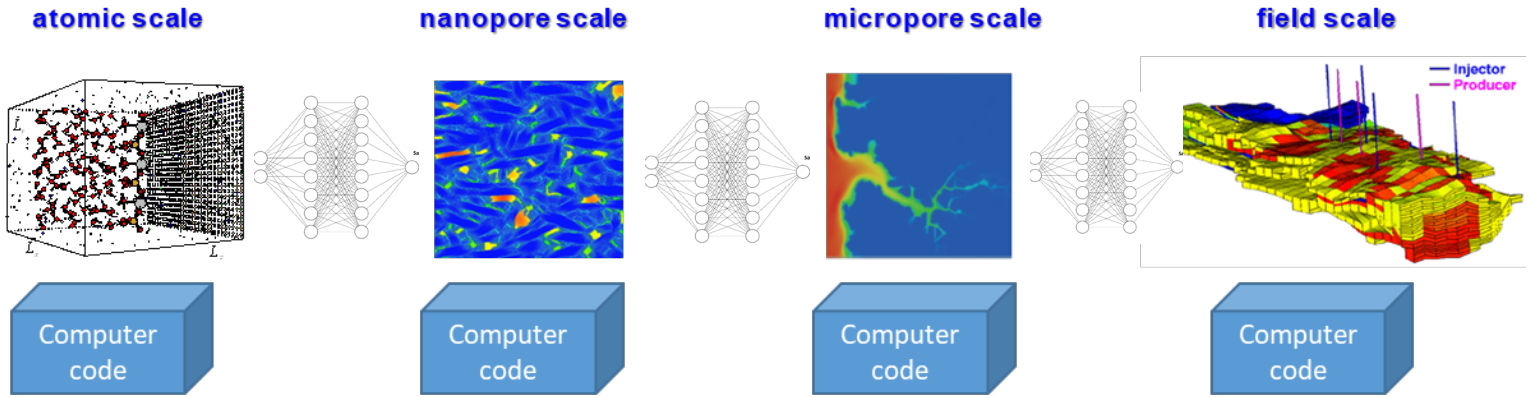


Catalytic particulate flow

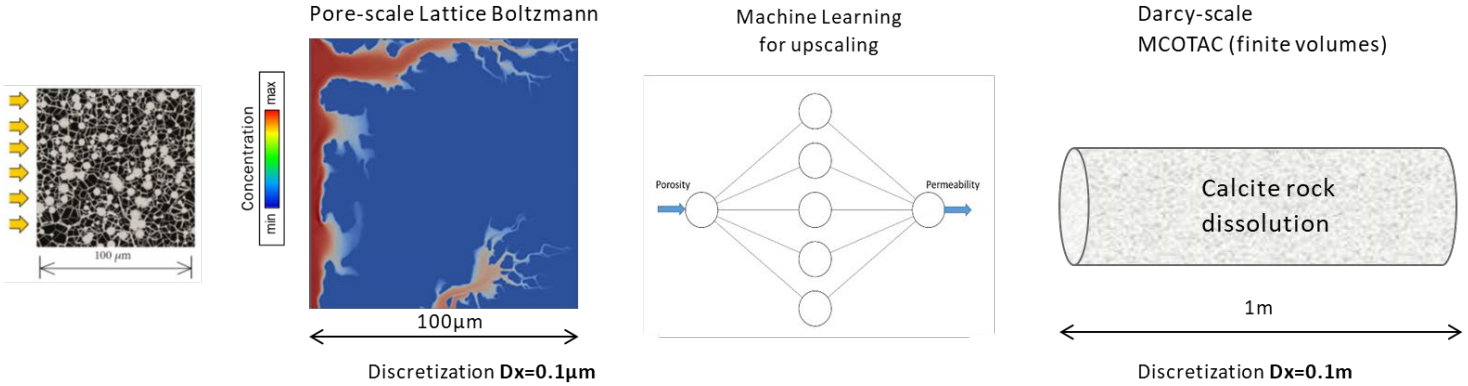
Lead: N.I. Prasianakis (LES/NES/PSI).
Development Team: A. Safi, J. Kang, M. Khatoonabadi, R. Patel (developer of yantra), M. Mahrous, S.V. Churakov, J. Mantzaras

Neural network based multiscale modelling for reactive transport simulations

Multiscale modelling is limited by the communication between heterogeneous codes which operate at different scales and physical descriptions. Data driven deep-learning (neural network) framework is proposed and demonstrated



Demonstration: Pore-scale Lattice Boltzmann simulations provide the porosity permeability correlations in reactive environment (micrometer level). e.g. calcite rock dissolution due to acidification. Simulation output was encoded in a neural network and integrated in a finite element solver (meter level).



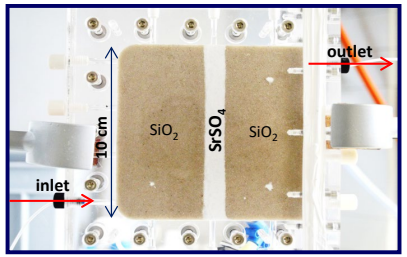
Prasianakis, N.I., Haller, R., Mahrous, M., Poonoosamy, J., Pfingsten, W. and Churakov, S.V., (**2020**). Neural network based process coupling and parameter upscaling in reactive transport simulations. ***Geochimica et Cosmochimica Acta***, ***291***, pp.126-143.

Lab on a chip Digital Twin

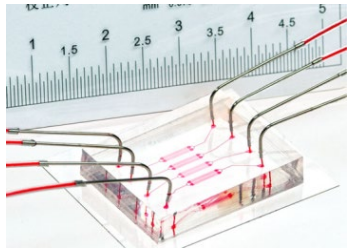
Advantages: miniaturized environment, shorter time-scales, small quantities of reactants, continuous monitoring, parallel

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

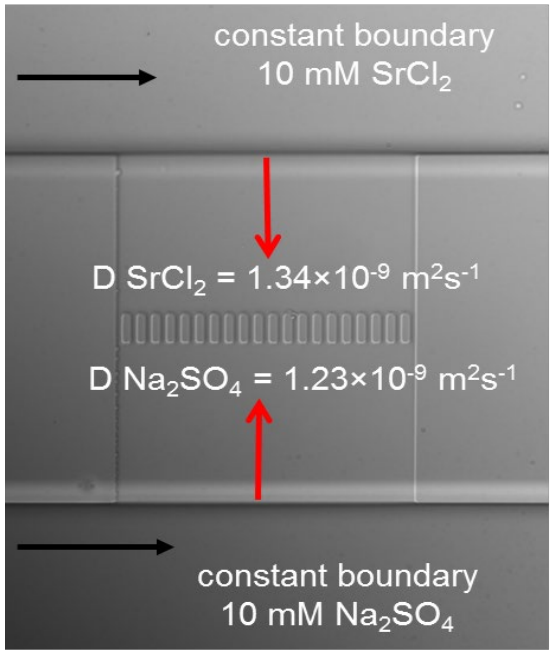
Typical lab experiment
(**cm** scale)

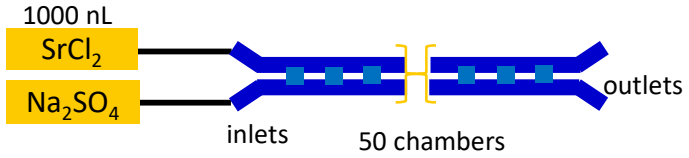


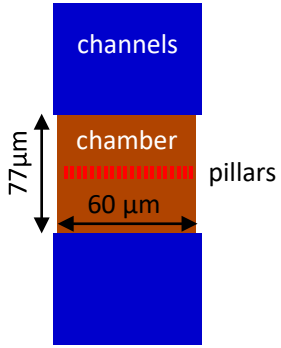
Microfluidic reactor
(**µm** scale)



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

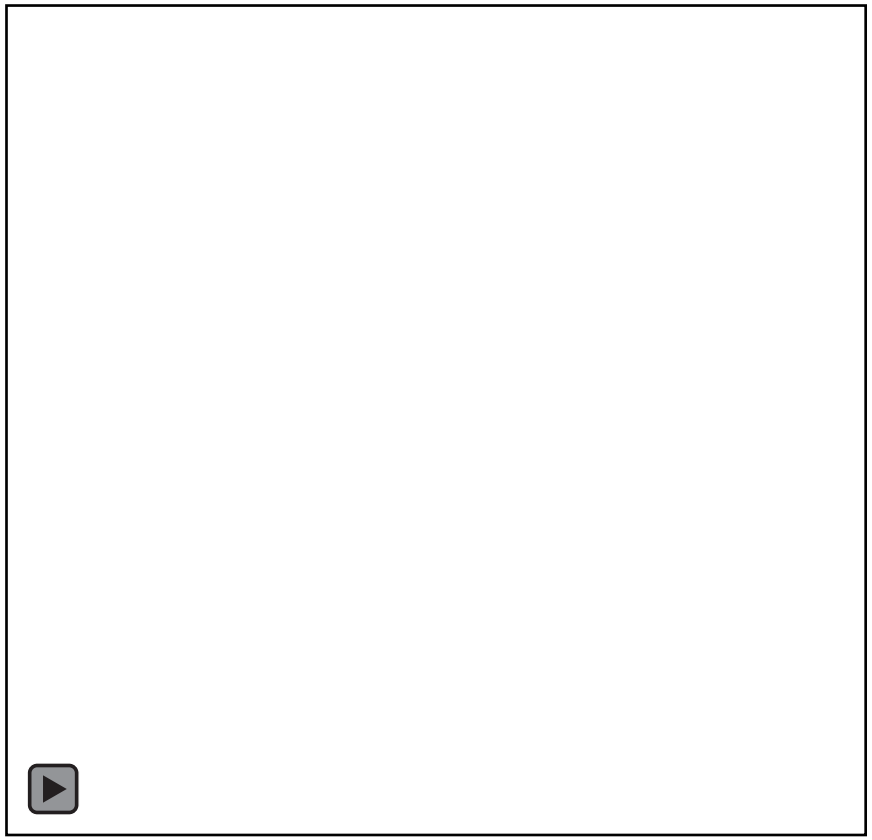
Evolution of experiment (camera)

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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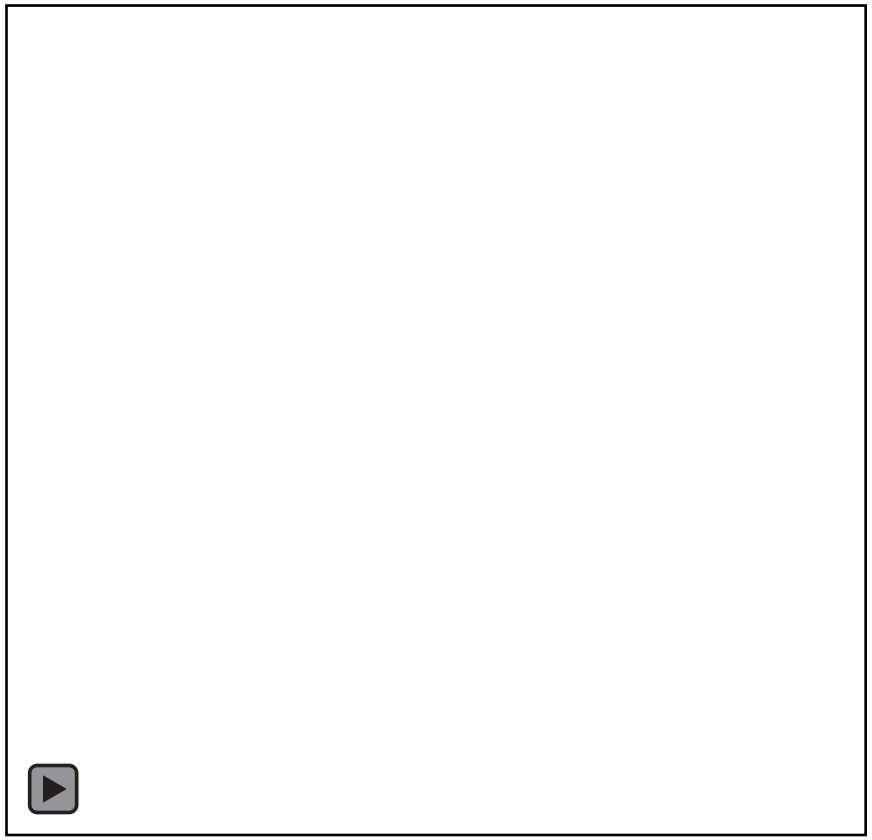

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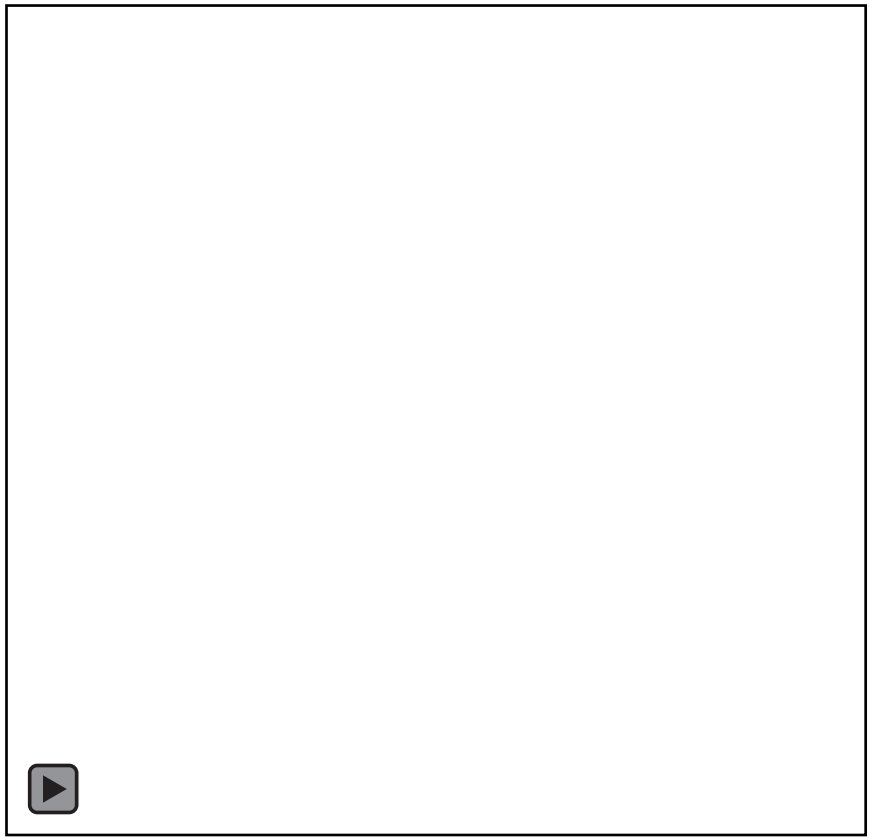

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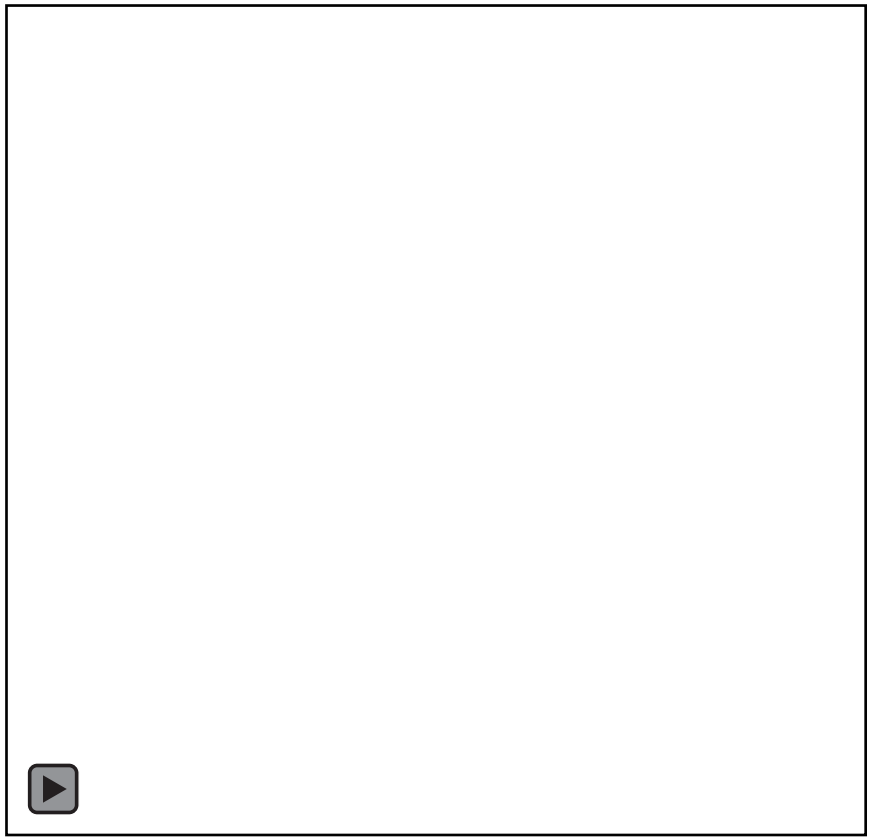

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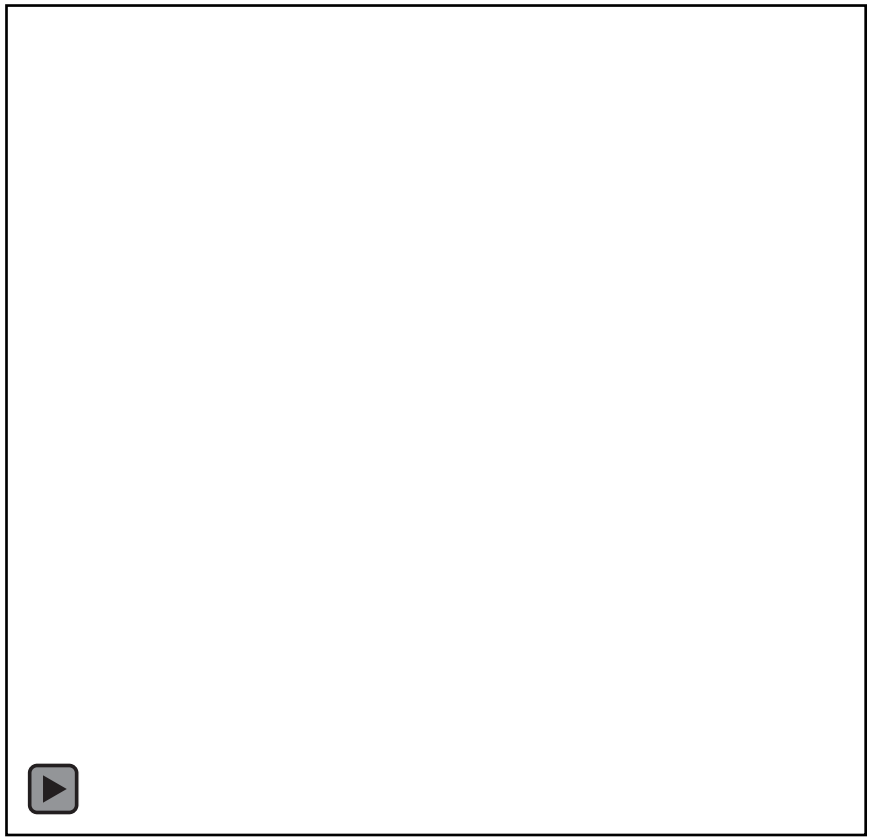

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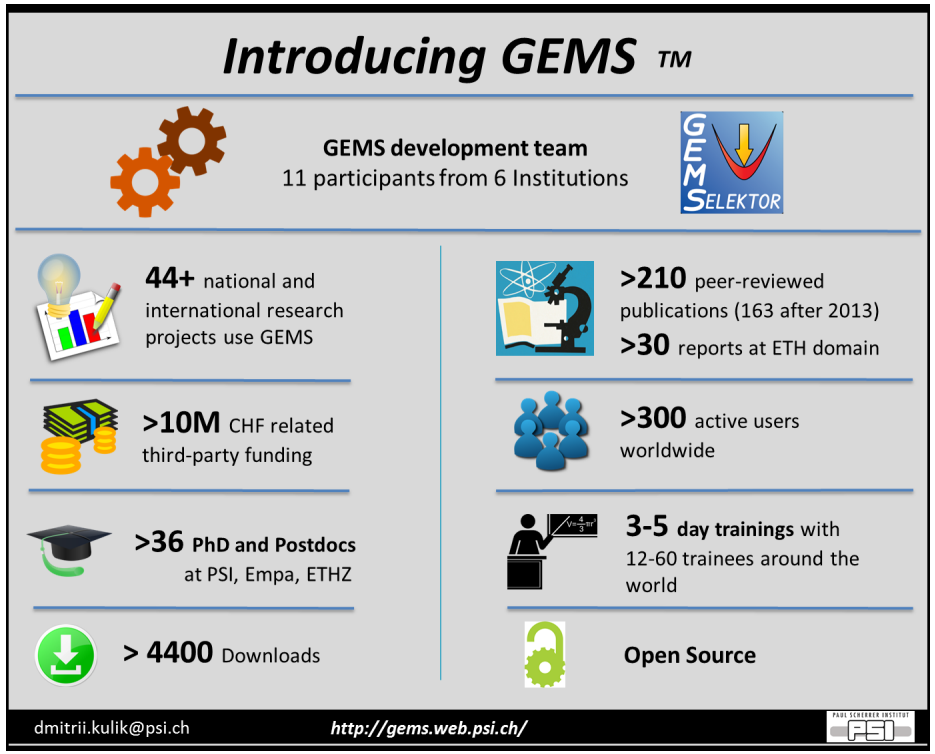
Equilibrium Speciation and geochemical calculations GEMS

1



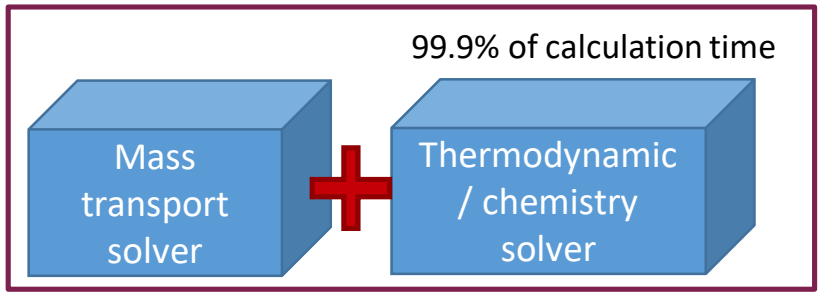
Example: **GEM-Selektor** full speciation for **sea water** at 1 bar and 80°C. Concentrations are in molar (mol/L) scale, and only species with concentrations > 10^{-10} M are shown.

a_aq_gen	54.66756		K(SO4)-	0.000229486		Na(CO3)-	1.09E-05		NO3-	1.00E-09
Cl-	0.54518692		Na(HCO3)@	0.000187894		HSiO3-	7.12E-06		Li+	9.87E-10
Na+	0.45936644		Mg(HCO3)+	0.000176174		NaOH@	2.70E-06		HPO4-2	9.41E-10
Mg+2	0.047302479		SiO2@	0.000142668		CaOH+	2.10E-06		Sr+2	8.97E-10
SO4-2	0.014423941		MgOH+	0.000100842		Mg(HSiO3)+	1.74E-06		B(OH)3@	8.86E-10
K+	0.009948141		Mg(CO3)@	5.18E-05		MgSiO3@	1.16E-06		Ba+2	7.94E-10
Ca+2	0.009408134		Ca(HCO3)+	3.63E-05		Ca(HSiO3)+	2.31E-07		F-	5.50E-10
Na(SO4)-	0.007373634		CO3-2	2.96E-05		KOH@	4.79E-08		MgF+	3.55E-10
MgSO4@	0.005341611		Ca(CO3)@	2.92E-05		HSO4-	2.77E-08		Ba(SO4)@	2.01E-10
HCO3-	0.001318276		CO2@	2.91E-05		H+	2.61E-08		BO2-	1.14E-10
Ca(SO4)@	0.000778619		N2@	2.74E-05		CaSiO3@	1.83E-08		Sr(SO4)@	9.74E-11
O2@	0.000244295		OH-	1.97E-05		SiO3-2	2.95E-09			

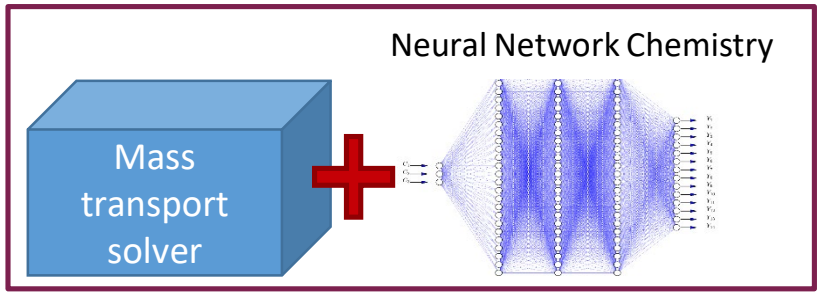
Neural network based process coupling and code acceleration in reactive transport simulations

In reactive transport simulation a transport and a chemical solver are usually coupled. The thermodynamic/chemical calculations consume > 99.9% of the total simulation time. Data-driven acceleration of the geochemistry at practically zero loss in accuracy was demonstrated

Typical reactive transport solver

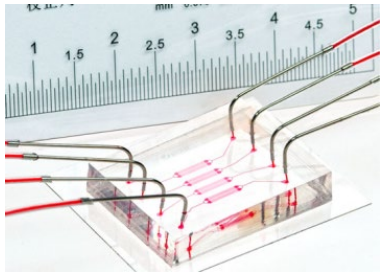


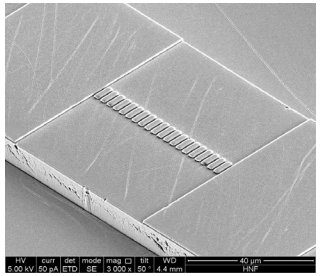
Machine learning assisted reactive transport solver

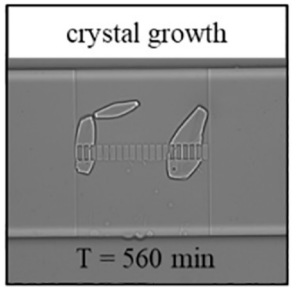


First tests show a **10'000x** acceleration of the chemical solver, without loss in accuracy and an overall speed up > **1000x**

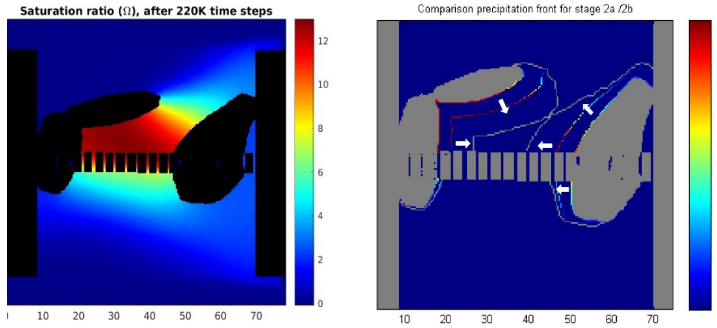
Demonstration: This acceleration was an enabling step for the realization of the digital twin and modelling diagnostics including crystal growth prediction of microfluidic experiments (FZ-Julich)







Microfluidic Experiement



Digital Twin and modelling diagnostics

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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

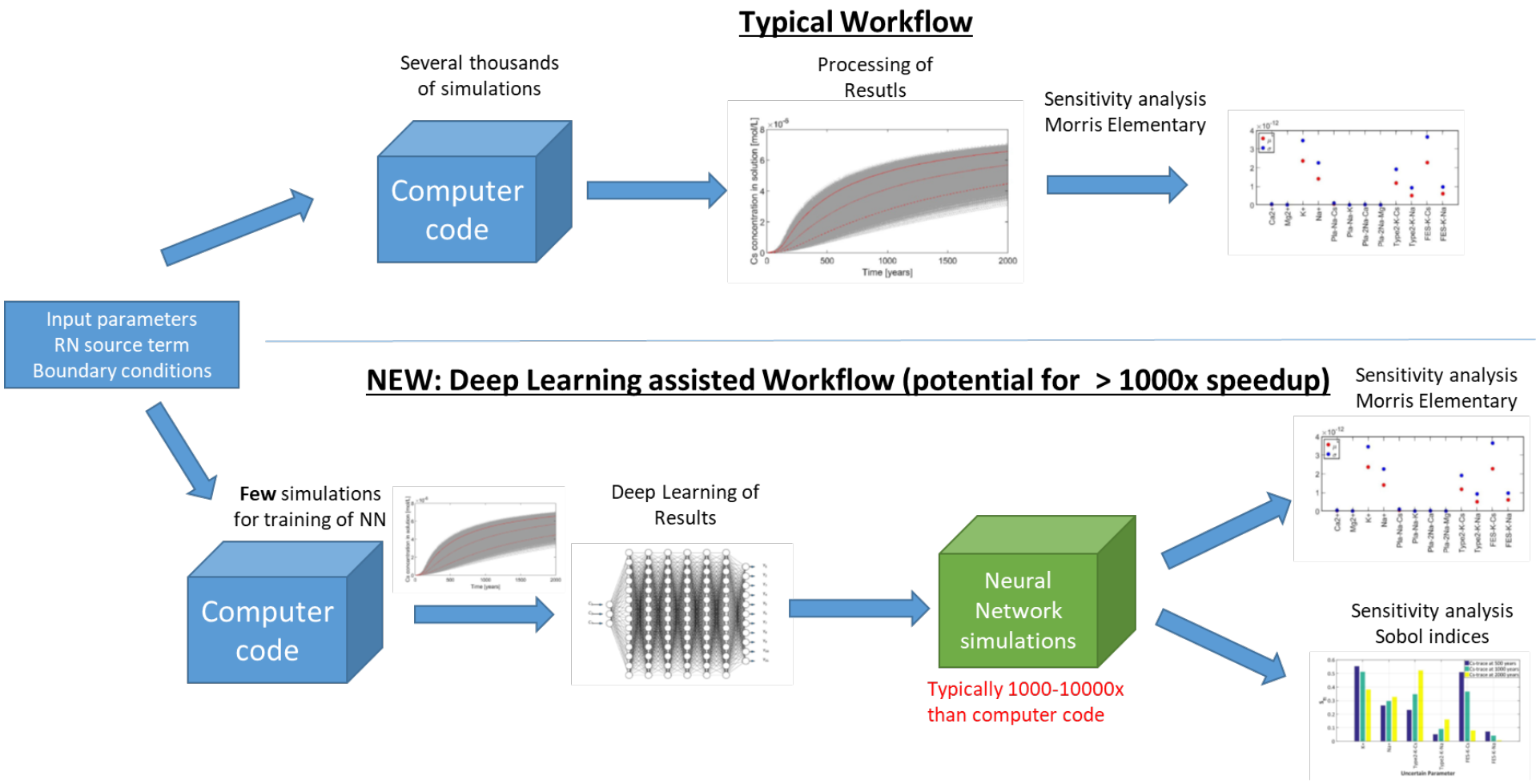
Chemistry GEMS / PHREEQC	Transport (flow) Lattice Boltzmann	Chemistry Neural Network
1 CPU-core ~ 1'000/s	1 CPU-core, 4 species ~ 1'000'000/s	1 CPU-core (depending on system) ->more than 1'000'000/s
1 GPU -> **Impossible** **Code not available**	1 GPU, 4 species -> 100'000'000/s	1 GPU -> Expected speedup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

Challenge: Train surrogate models for input dimension >4 e.g. 10 and maintain accuracy

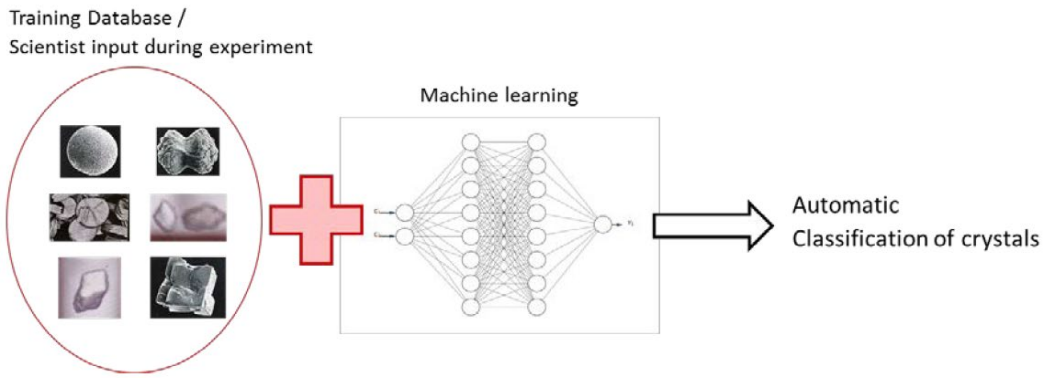
Training Metamodels for sensitivity analysis in radionuclide transport

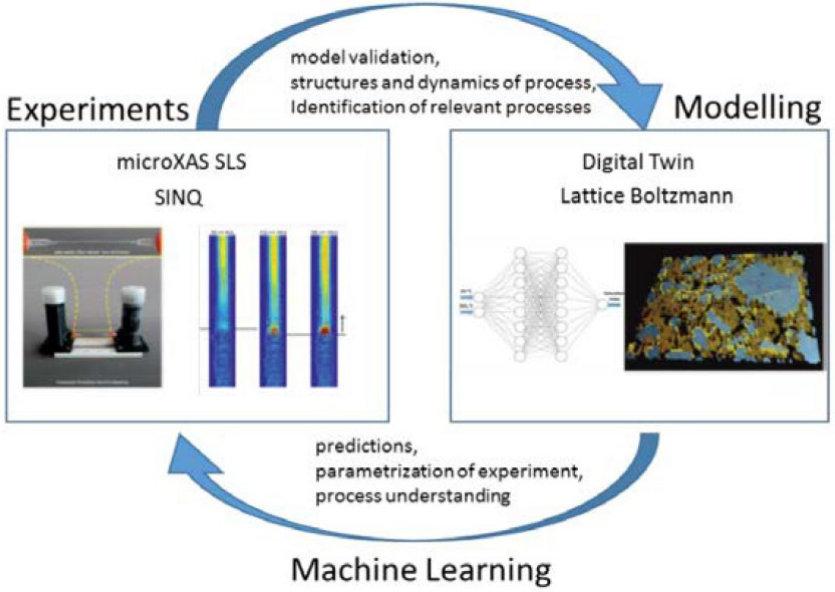
2

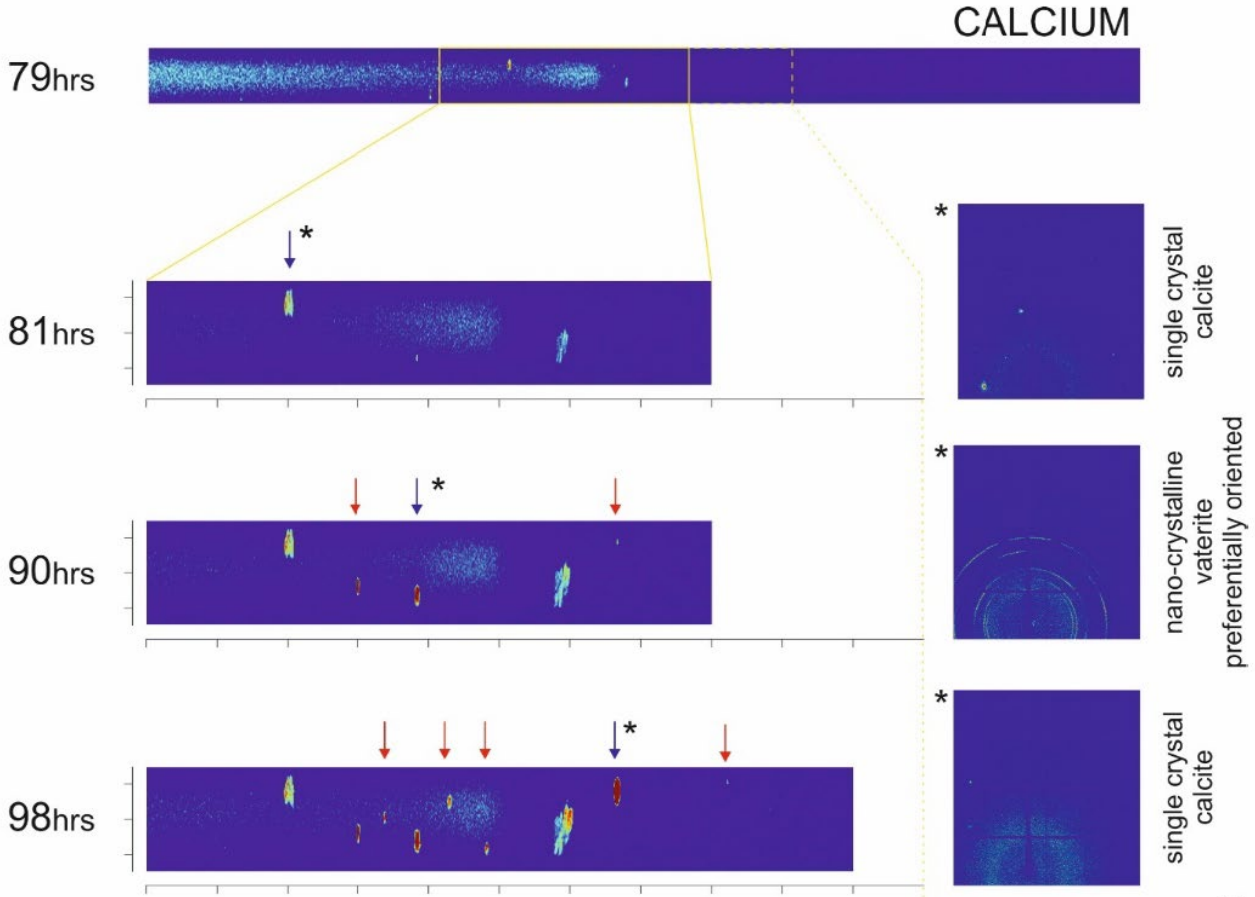


Challenge: Train surrogate models for input dimension >4 e.g. 10 and maintain accuracy, training dataset might be scarce ?

3 Deep Learning for characterization of X-ray tomography output (beamlines PSI, CROSS project)







Multidimensional Data, Chemical Imaging

Summary

1) Surrogate modelling, data driven interfaces between heterogeneous codes → Accelerate Geochemistry, cross platform (2019-2023, EURAD, Nagra)

Challenge: Train surrogate models for input dimension >4 e.g. 10 and maintain accuracy. Optimum training dataset to represent multidimensional spaces

2) Metamodelling for sensitivity analysis (2021- …)

Challenge: Can a metamodel be trained in a smaller number of costly numerical simulations and achieve similar accuracy at sensitivity analysis studies? Can be used for intensified design of experiment?

3) Image recognition, classification of X-ray multidimensional chemical data (e.g. microXAS beamline at PSI) for characterization, digital Twin (CROSS project at PSI, 2021-2025, PhD search is ongoing)

Challnege: Classification of multidimensional data, use small sample of input images, couple with reactive transport solvers for real-time predicitons

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Thank you