Data-Driven and Physics Based Modeling for Corrosion-induced Cracks

Akash Kumar, Nishant Prajapati, Martin Reder, Arnd Koeppe, Daniel Schneider, Michael Selzer, Britta Nestler

Akash Kumar, 16-17 June 2025

Motivation

Major reason for material damage in industries **---- Corrosion**

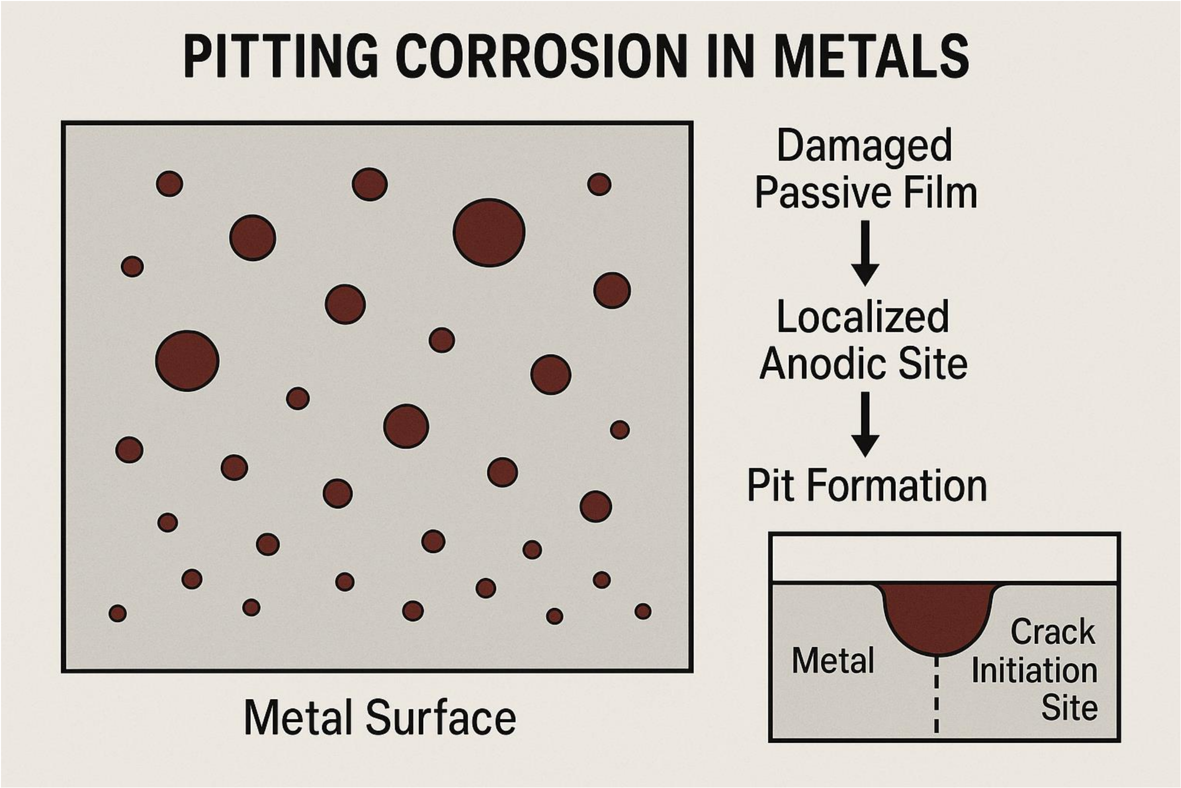
Annual economic damage: **2.5 trillion euros** (Fontes and Nistad, 2020)

Data-driven simulation enables prediction and protective measures

Background

Pitting Corrosion in Metals

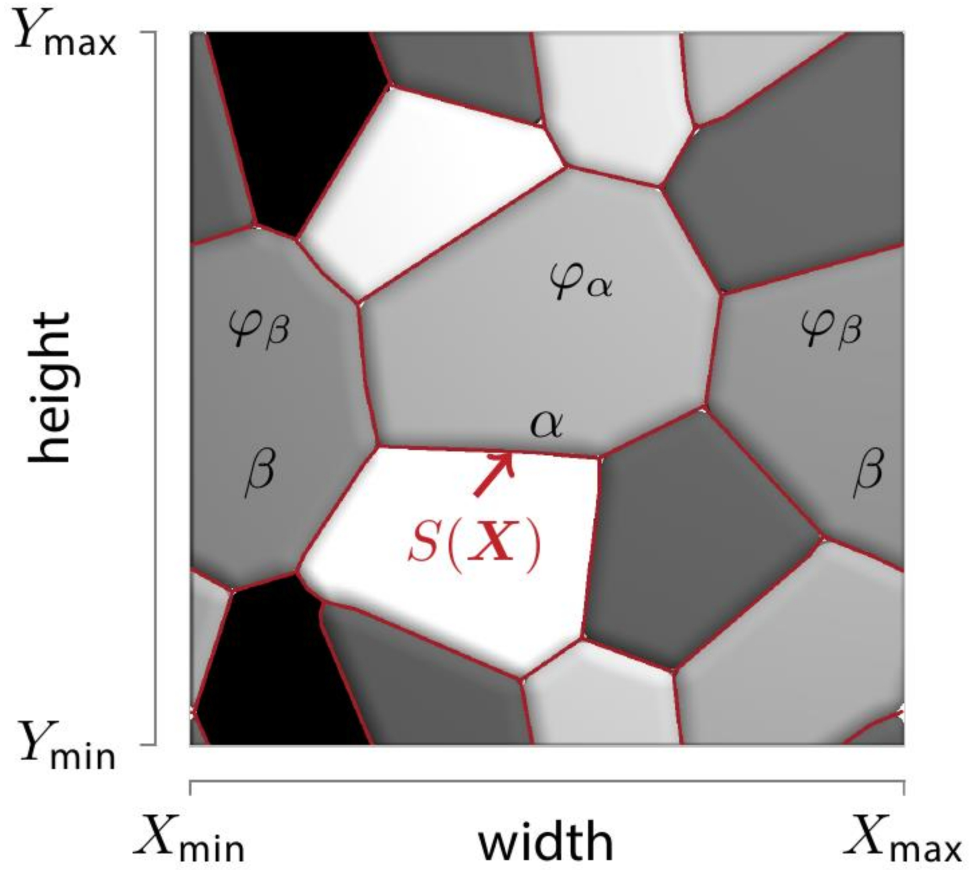
- Localized, aggressive form of corrosion causing small, deep pits
- Initiated by breakdown of protective oxide layers (e.g., by chlorides)
- Common in stainless steel, aluminum, and copper alloys
- Difficult to detect; pits can lead to crack initiation and rapid failure of the material



Schematic showing the pit formation and further crack growth zone

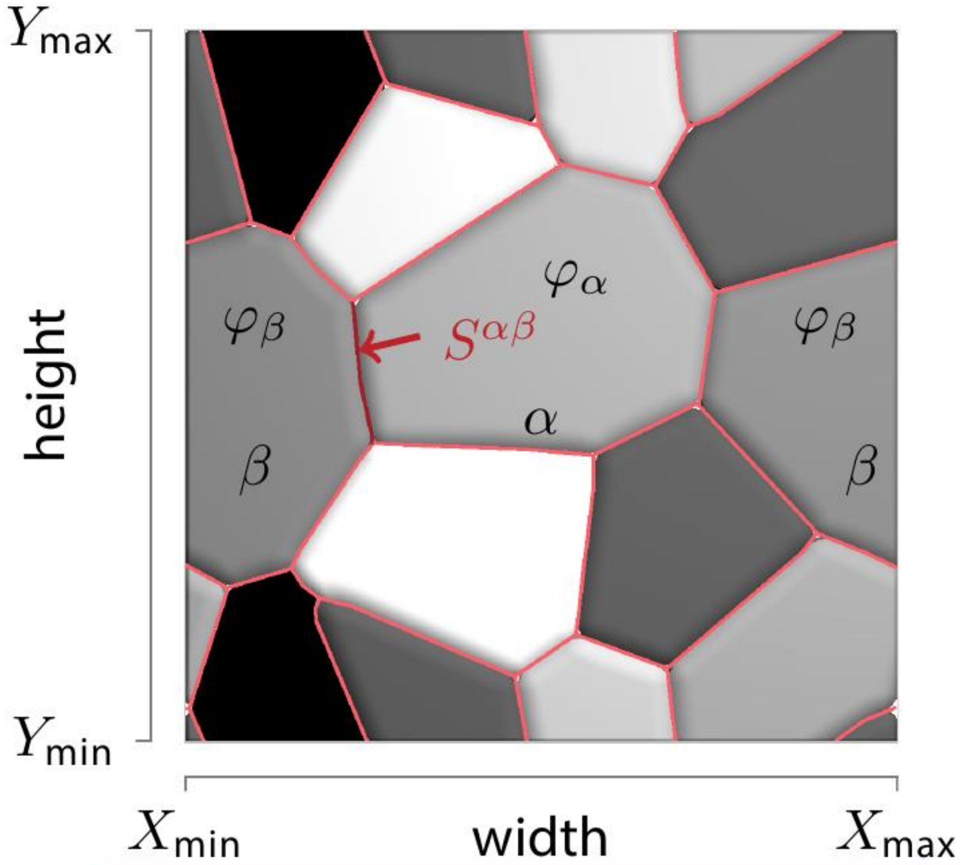
Numerical Modeling Methodology

Phase-field Method - Concept



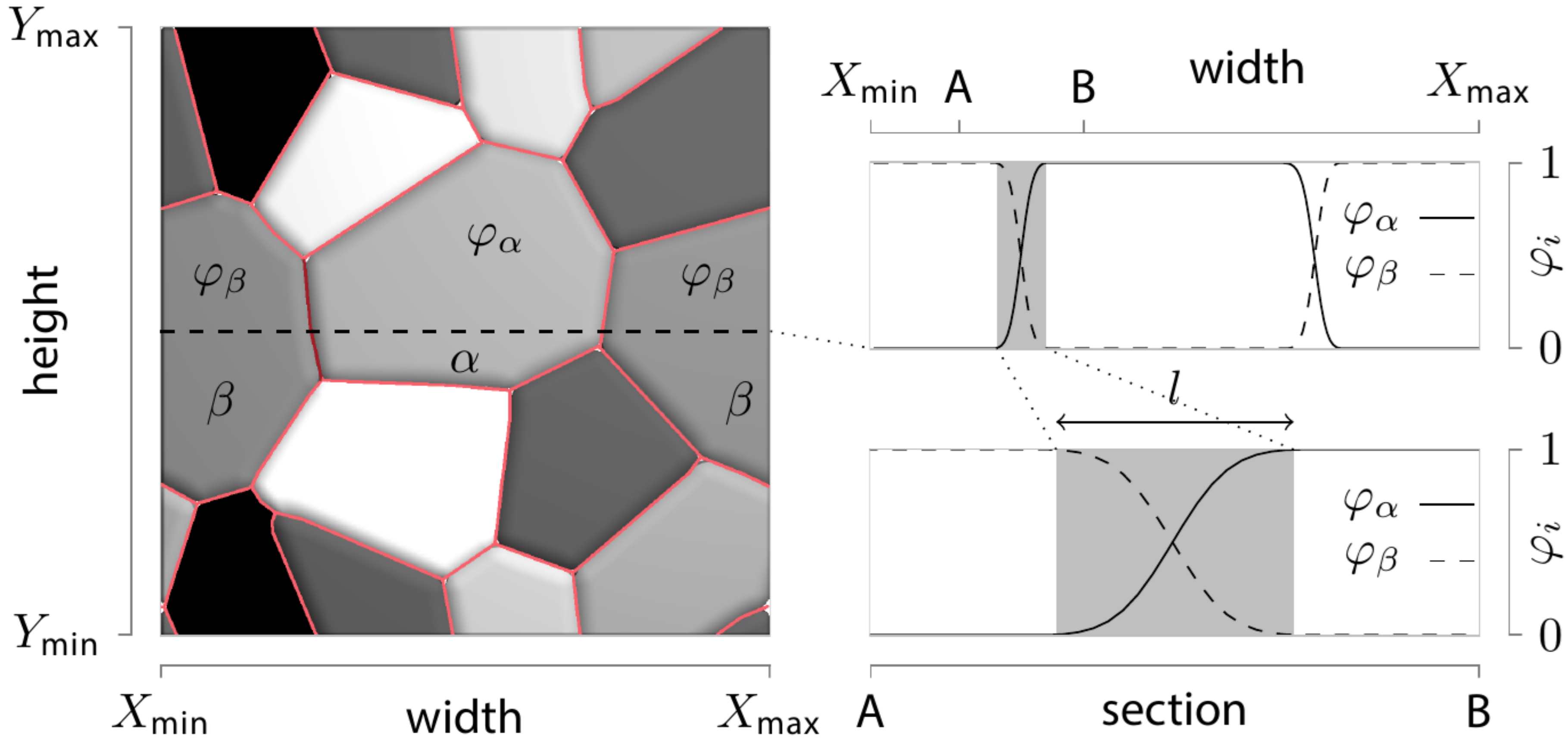
$$\mathcal{F}(\dots) = \int_{S_r} f_{se}(\boldsymbol{X}, \dots)\mathrm{d}A_r + \int_{V_r} f_{bulk}(\boldsymbol{X}, \dots)\mathrm{d}V_r$$

Phase-field Method - Concept



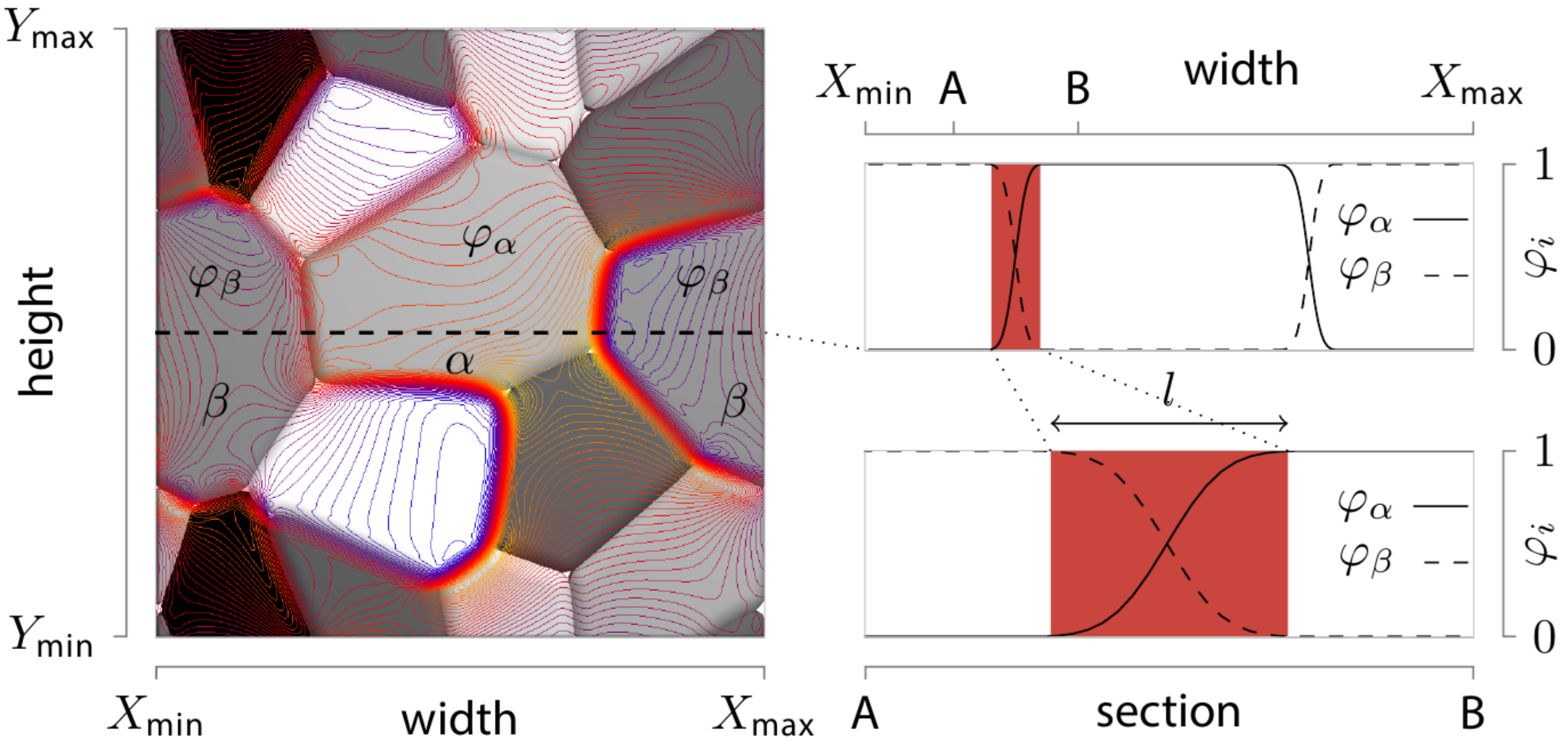
$$\mathcal{F}(\boldsymbol{\varphi}, \ldots) = \sum_{\alpha<\beta} \int_{S^{\alpha\beta}} f_{\text{se}}^{\alpha\beta}(\varphi_\alpha, \varphi_\beta, \ldots)\,\mathrm{d}A_r + \sum_{\alpha} \int_{V_r^\alpha} f_{\text{bulk}}^{\alpha}(\varphi_\alpha, \ldots)\,\mathrm{d}V_r$$

Phase-field Method - Concept



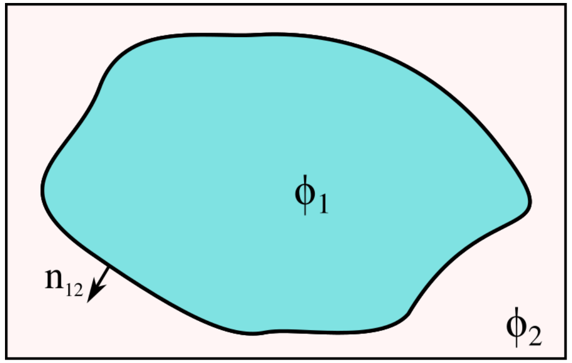
$$\mathcal{F}(\boldsymbol{\varphi}, \nabla_X \boldsymbol{\varphi}, \ldots) = \int_{V_r} \epsilon a(\boldsymbol{\varphi}, \nabla_X \boldsymbol{\varphi}) + \frac{1}{\epsilon}\omega_{ob}(\boldsymbol{\varphi}) \mathrm{d}V_r + \int_{V_r} f_{bulk}(\boldsymbol{\varphi}, \ldots) \mathrm{d}V_r$$

Phase-field Method - Concept

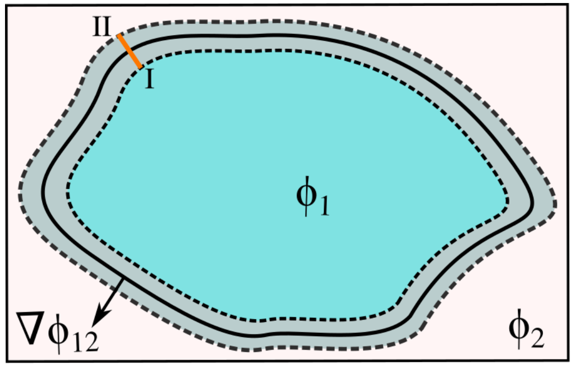


$$\mathcal{F}(\boldsymbol{\varphi}, \nabla_X \boldsymbol{\varphi}, \dots) = \underbrace{\int_{V_r} \epsilon a(\boldsymbol{\varphi}, \nabla_X \boldsymbol{\varphi}) + \frac{1}{\epsilon}\omega_{ob}(\boldsymbol{\varphi}) \mathrm{d}V_r}_{\stackrel{!}{=} \sum_{\alpha<\beta} \int_{S_{\alpha\beta}} f_{se}^{\alpha\beta}(\varphi_\alpha, \varphi_\beta, \dots) \mathrm{d}A_r} + \int_{V_r} f_{bulk}(\boldsymbol{\varphi}, \dots) \mathrm{d}V_r$$

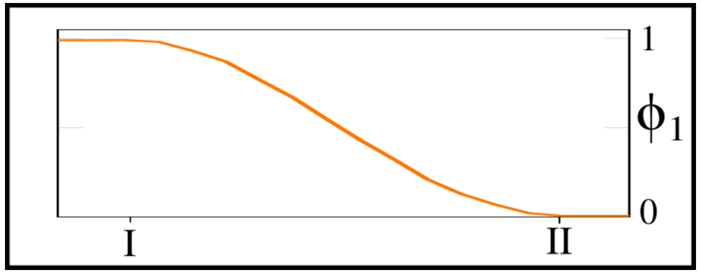
Phase-field Method - Overview



Sharp Interface



Diffuse Interface



Diffuse interface profile

- Diffuse interface approach
- Tracking evolution of a phase within a system is much easier
- Avoids remeshing during evolution
- Evolution is governed by differential equation based on minimization of free energy

Grand-chem approach for Modeling Corrosion

- Grand potential functional of the system,

$$\Psi(\boldsymbol{\phi}, \nabla\boldsymbol{\phi}, \boldsymbol{\mu}) = \psi_{\text{int}} + \psi_{\text{bulk}} = \int_V \left[\frac{1}{\epsilon}\omega(\boldsymbol{\phi}) + \epsilon a(\boldsymbol{\phi}, \nabla\boldsymbol{\phi}) + \psi(\boldsymbol{\phi}, \boldsymbol{\mu})\right] \mathrm{d}V$$

- Evolution of order-parameter of the system is governed using,

$$\frac{\partial \phi_\alpha}{\partial t} = -\frac{M_{\alpha\beta}}{2\epsilon}\left(\frac{\delta\psi_{\text{int}}}{\delta\phi_\alpha} - \frac{\delta\psi_{\text{int}}}{\delta\phi_\beta} + \frac{8\sqrt{\phi_\alpha(1-\phi_\alpha)}}{\pi}\Delta^{\alpha\beta}_{\text{bulk}}\right)$$

- Evolution of concentration of the system is governed using,

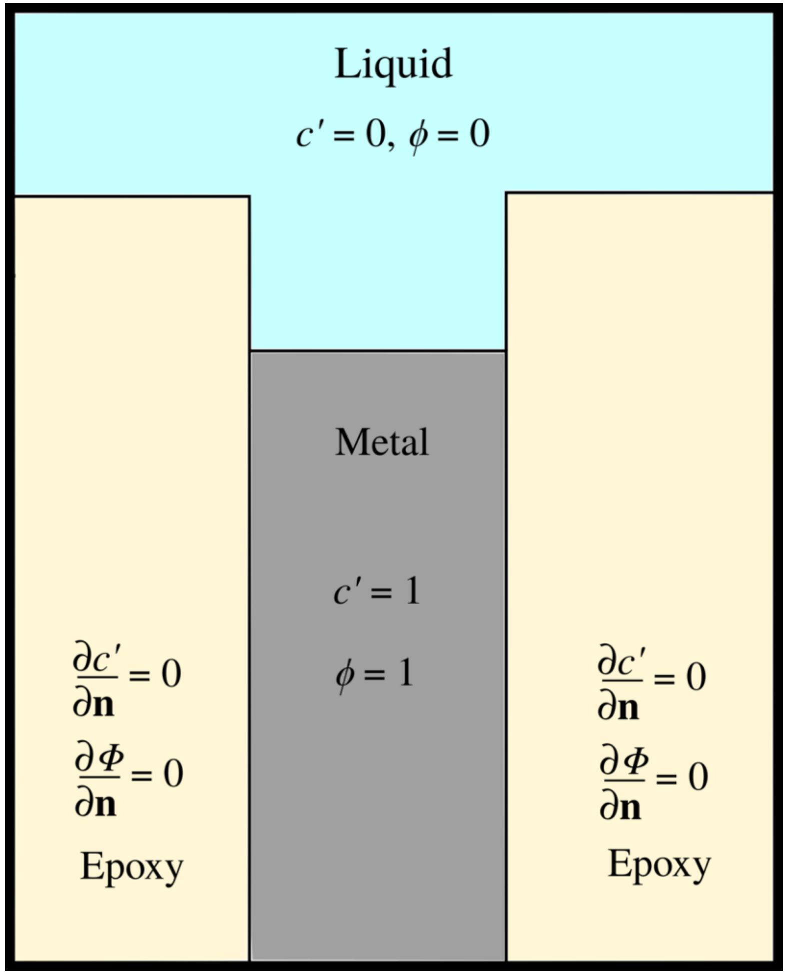
$$\frac{\partial \bar{c}}{\partial t} = \nabla \cdot \left(\bar{M}(\phi_\alpha)\nabla\mu\right), \quad \bar{M}(\phi_\alpha) = \phi_\alpha M^\alpha + (1-\phi_\alpha)M^\beta, \quad M^\alpha = D^\alpha \frac{\partial c^\alpha(\mu)}{\partial \mu}$$

- Evolution of chemical potentional of the system is governed using,

$$\frac{\partial \mu}{\partial t} = \left[\phi_\alpha \frac{\partial c^\alpha(\mu)}{\partial \mu} + (1-\phi_\alpha)\frac{\partial c^\beta(\mu)}{\partial \mu}\right]^{-1}\left(\nabla \cdot \bar{M}(\phi_\alpha)\nabla\mu - (c^\alpha(\mu) - c^\beta(\mu))\frac{\partial \phi_\alpha}{\partial t}\right)$$

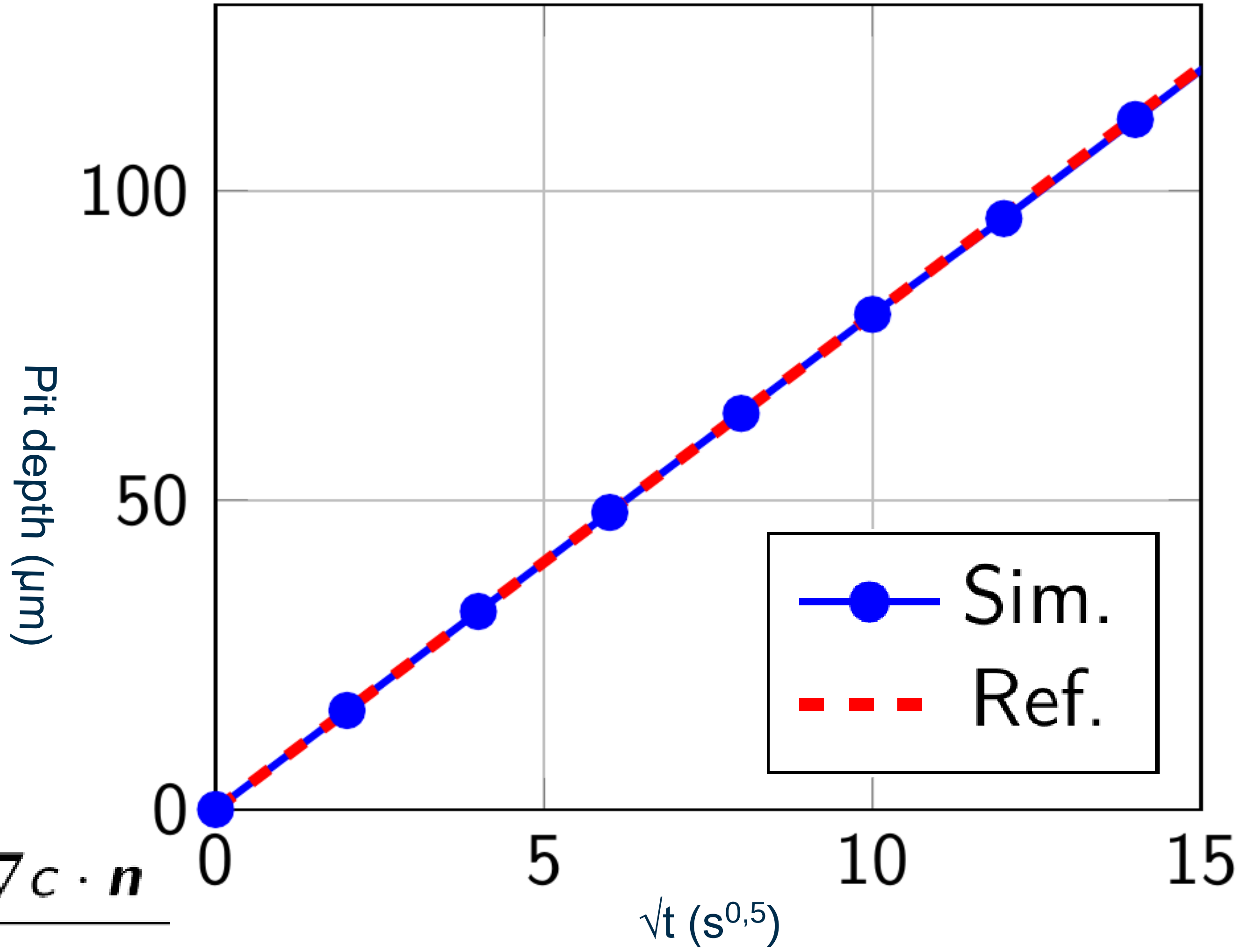
Simulation Analysis using PACE3D

Validation – Pseudo-1D Simulation



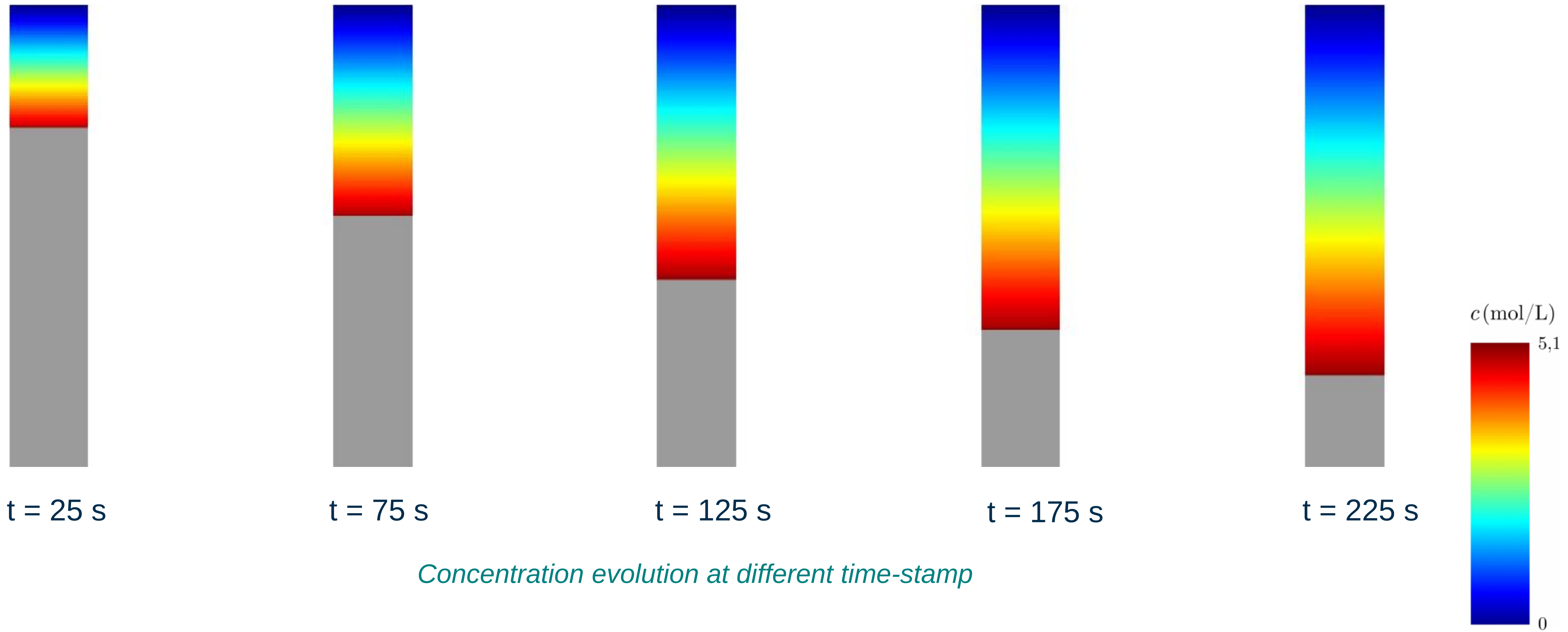
Schematic illustration 1D simulation-setup

$$v_n = \frac{D\nabla c \cdot \boldsymbol{n}}{c_{solid} - c_{sat}}$$



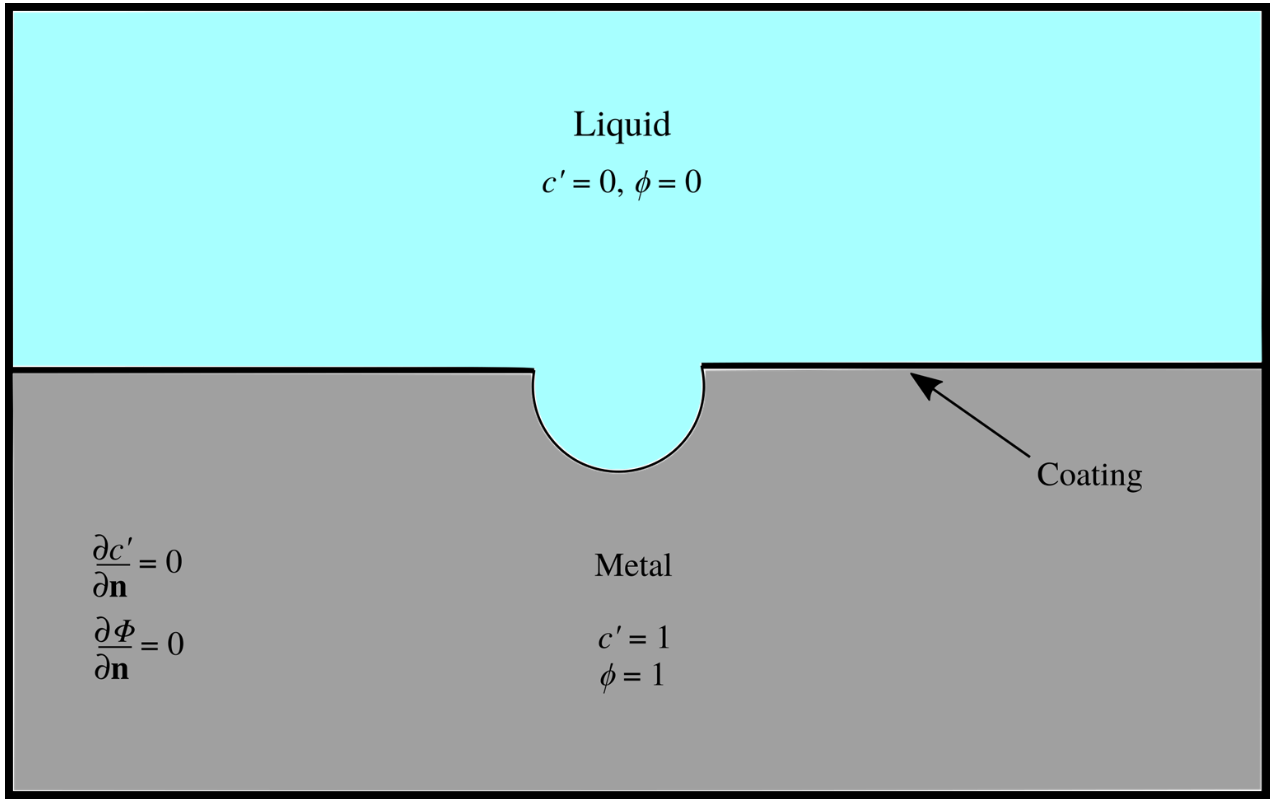
Validation of 1D-simulation

Validation – Pseudo-1D Simulation

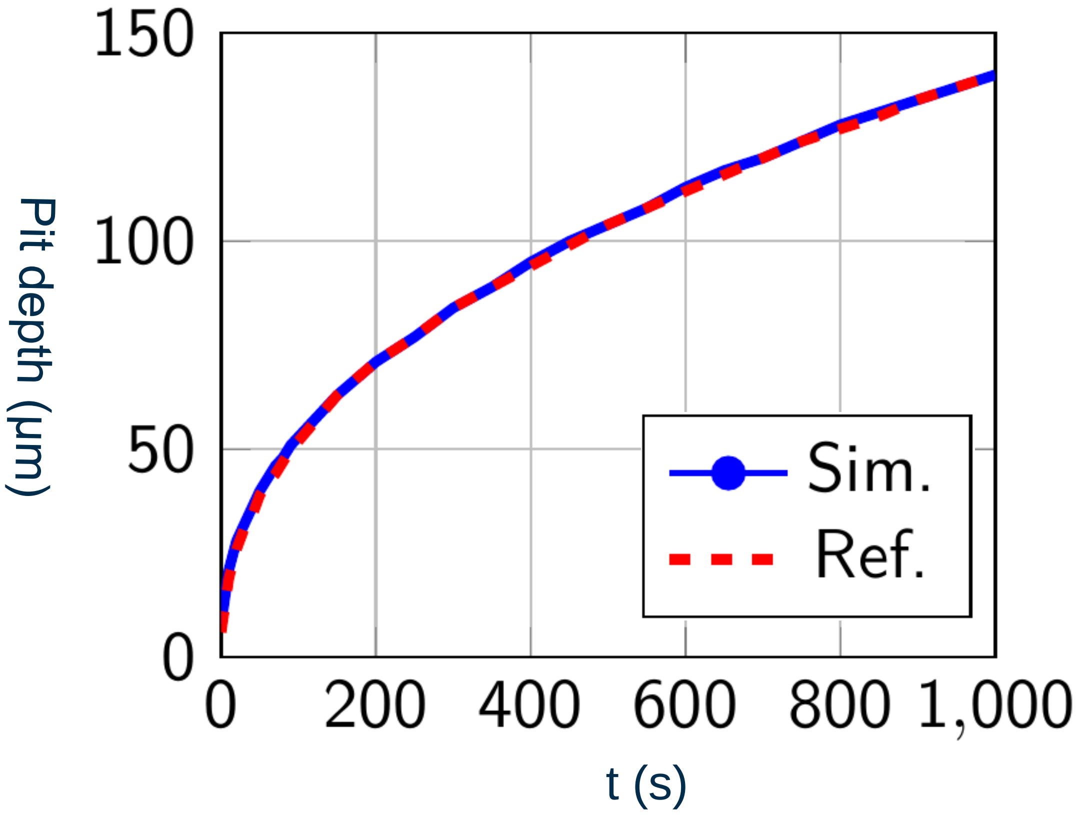


Concentration evolution at different time-stamp

Validation – 2D Simulation

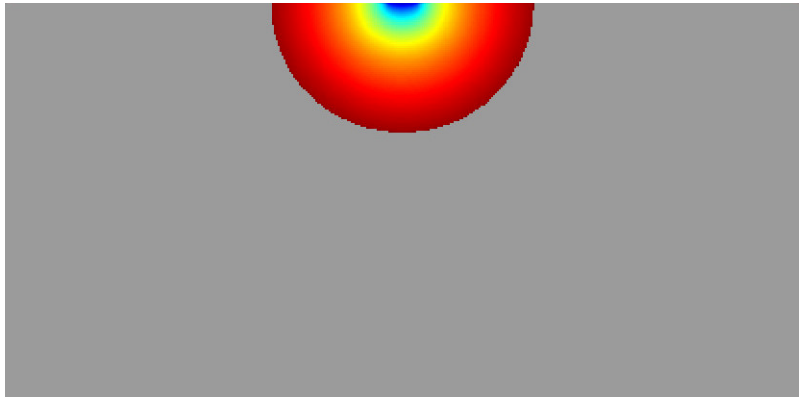


Schematic illustration 2D simulation

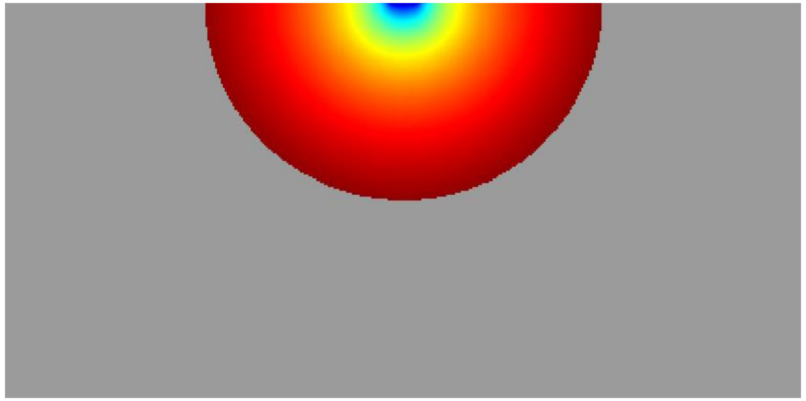


Validation of 2D-simulation

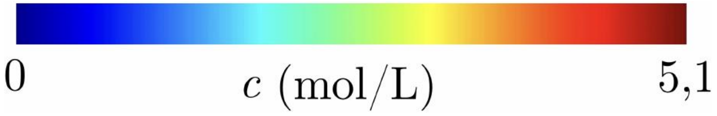
Validation – 2D Simulation

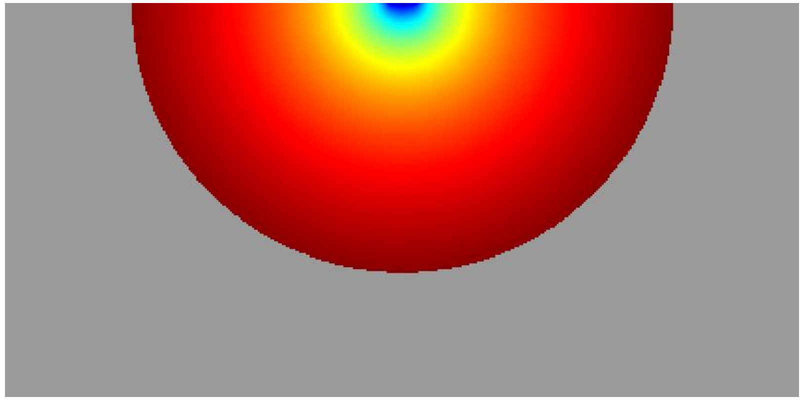


t = 200 s



t = 500 s

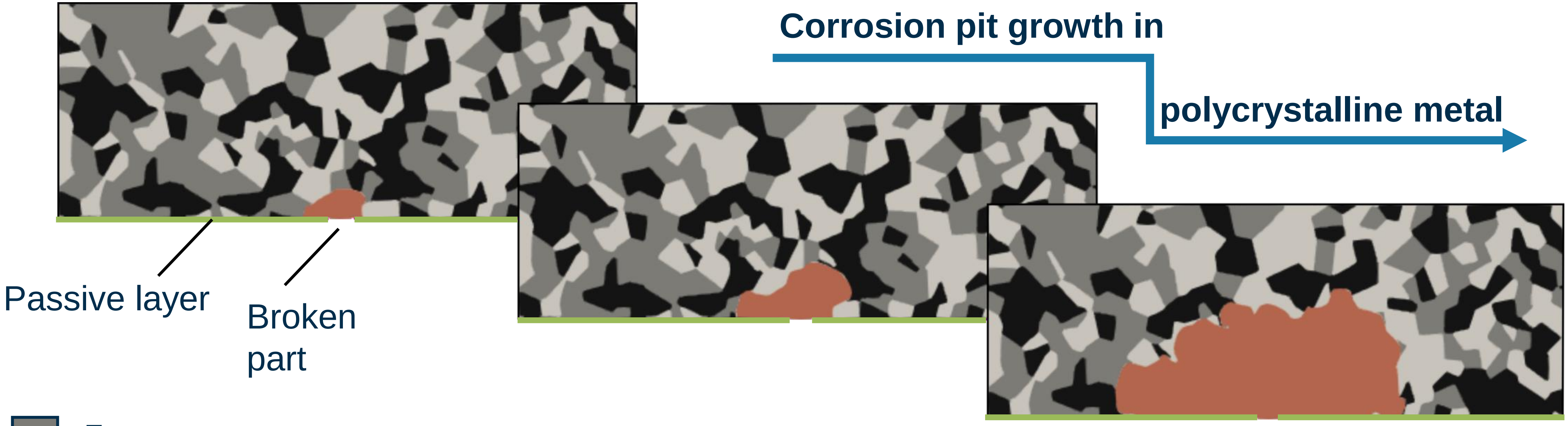




t = 1000 s

Concentration evolution at different time-stamp

Results – Pitting corrosion in Polycrystalline materials (Fe-Mn-Al alloys)

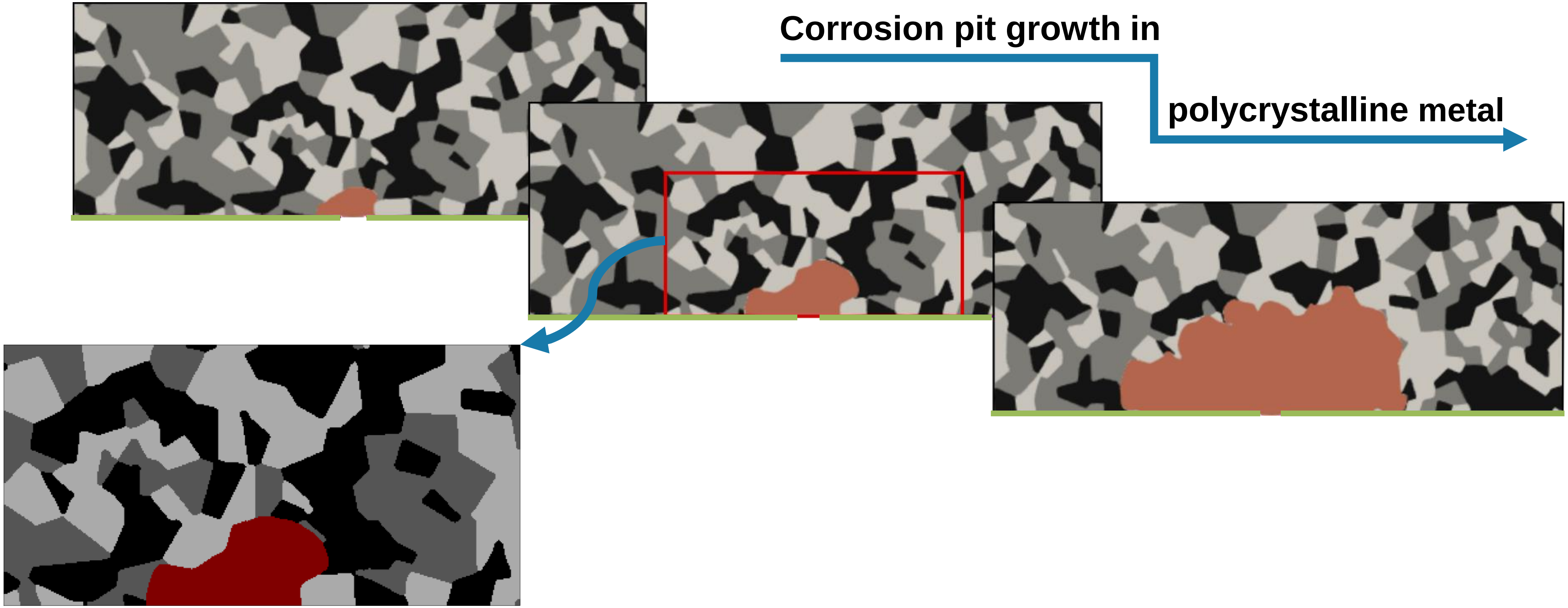


- Corrosion occurs preferentially in the ferrite phase of Fe-Mn-Al alloys.

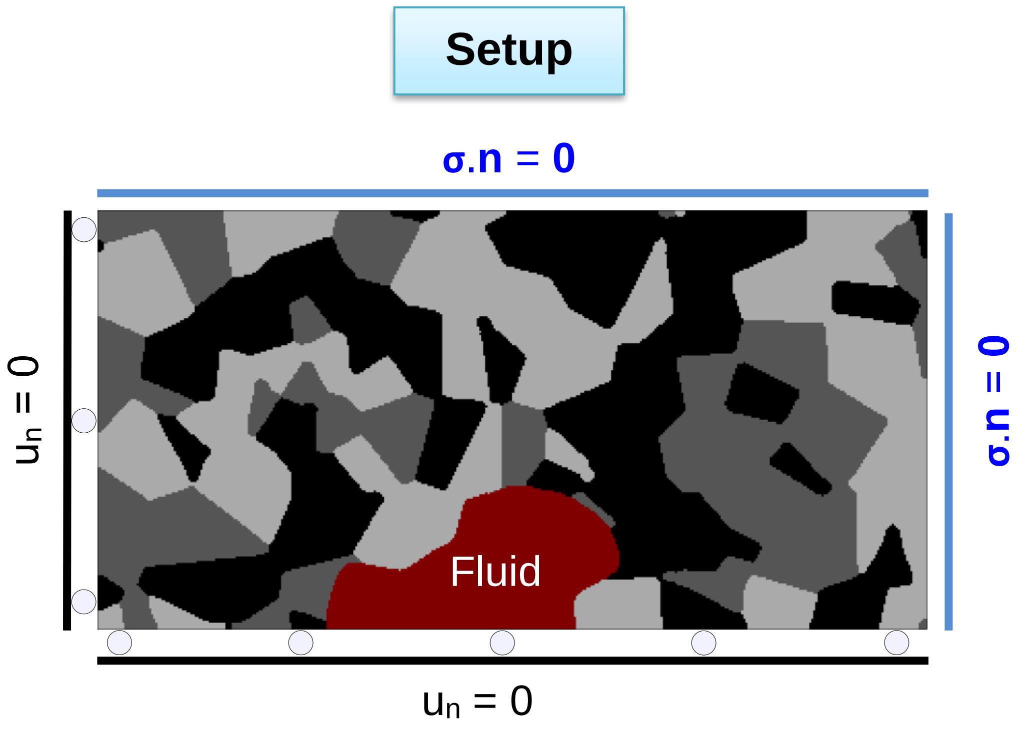
Here, $\frac{m1}{m2} = 3$

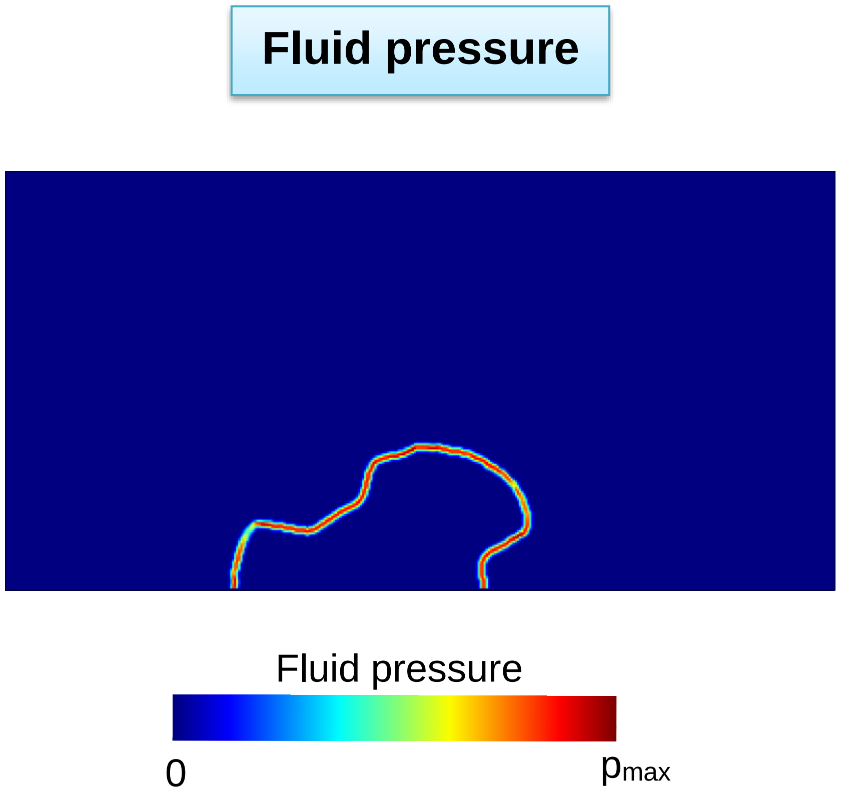
- $m1$ – Kinetic parameter of Fe
- $m2$ – Kinetic parameter of Mn and Al

Pressure-induced cracks in corrosion pits



Pressure-induced cracks in corrosion pits





Pressure-induced cracks in corrosion pits

Diffuse stress boundary condition

Momentum balance

$$\nabla \cdot \left(h(\phi_c) \sum_{\alpha}^{N_s} \phi^{\alpha} \boldsymbol{\sigma}^{\alpha} \right) = p \delta_d \boldsymbol{n}$$

Pressure

Surface normal vector

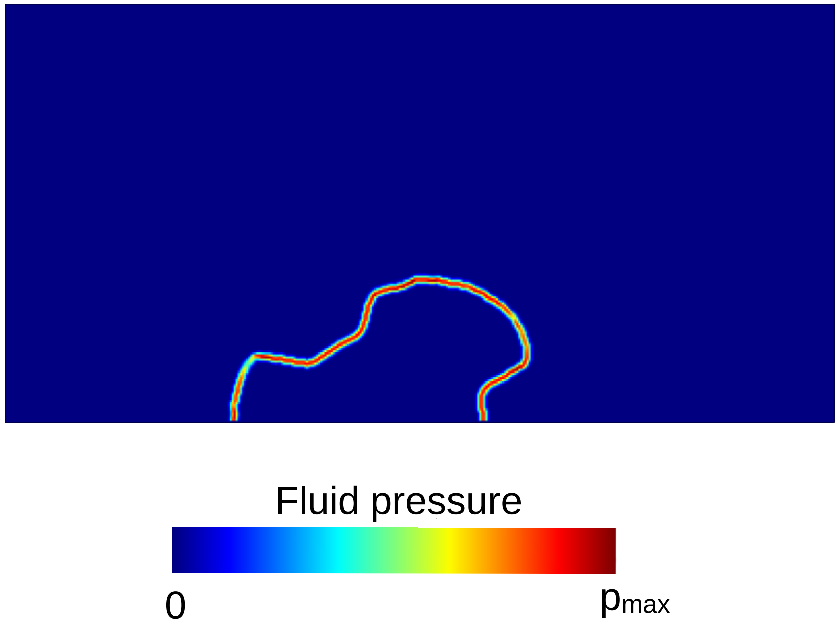
Surface Dirac Distribution approximation

$$\delta_d = 6\phi_s(1-\phi_s)||\boldsymbol{\nabla}\phi_s||$$

Solid phase-field

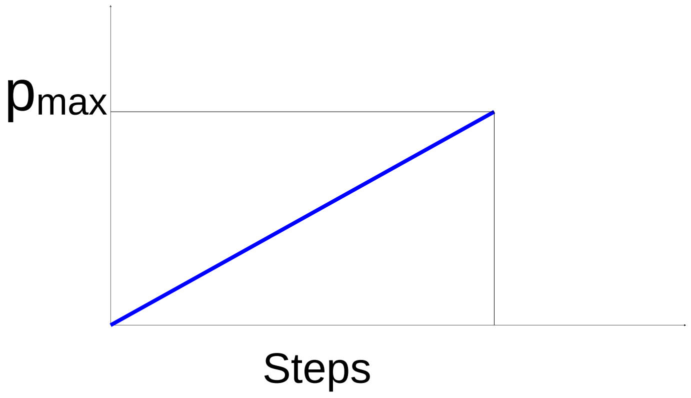
$$\phi_s = \sum_{\alpha}^{N_s} \phi_{\alpha}$$

Fluid pressure

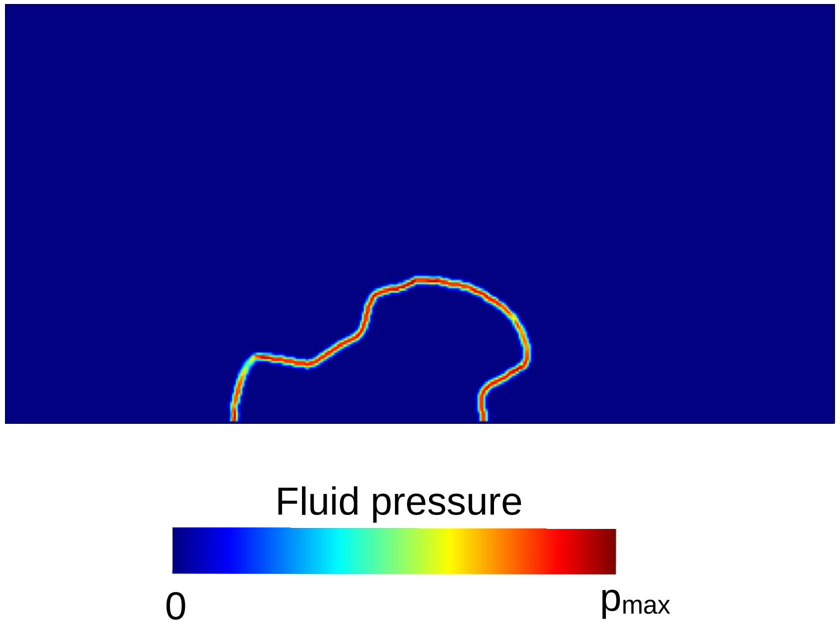


Pressure-induced cracks in corrosion pits

Pressure ramping

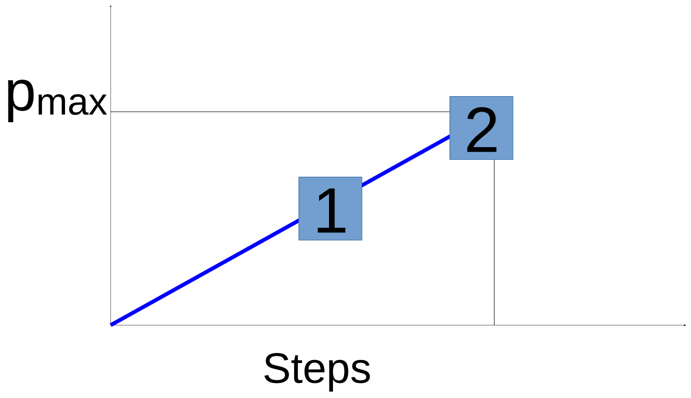


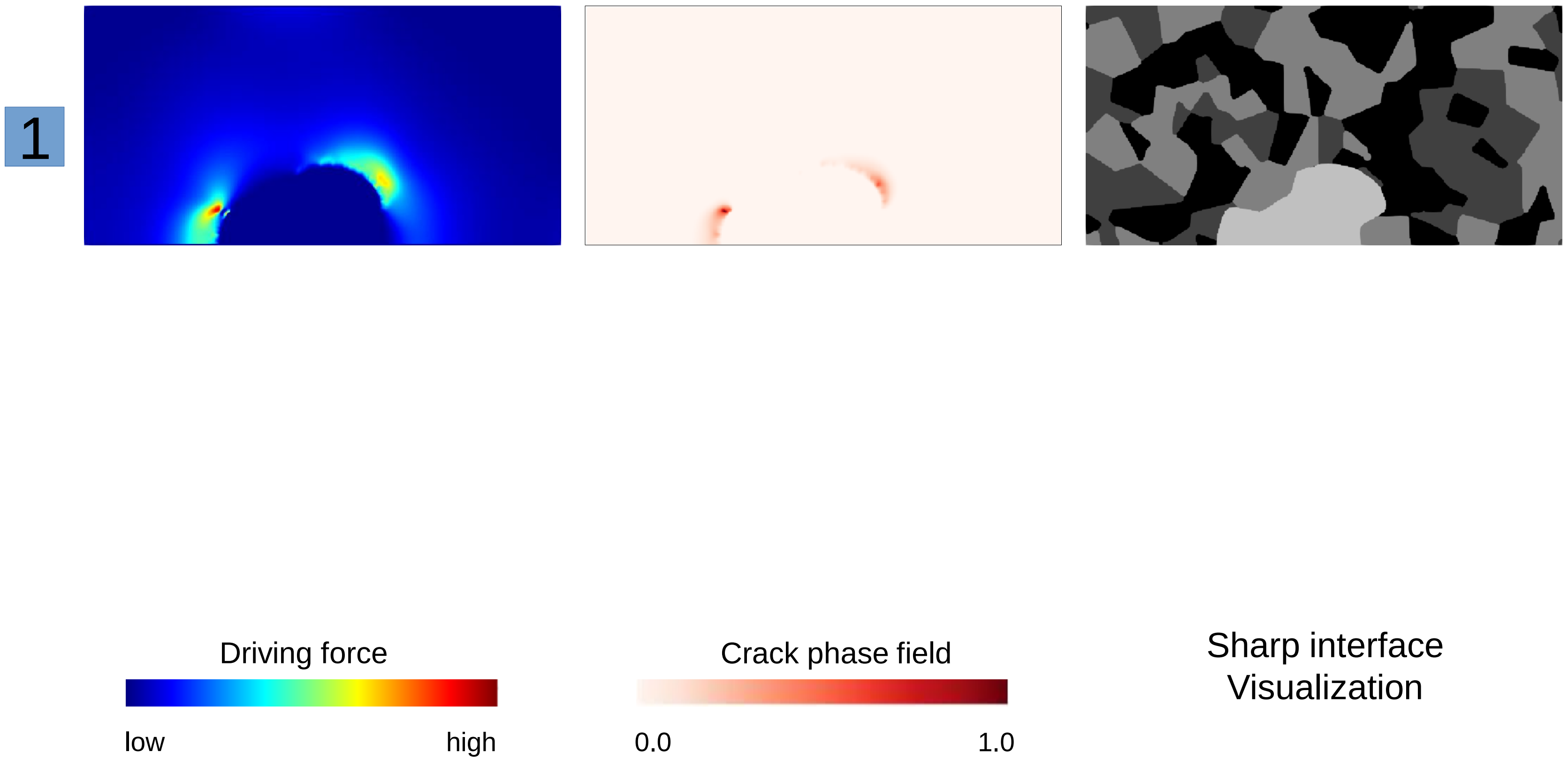
Fluid pressure



Pressure-induced cracks in corrosion pits

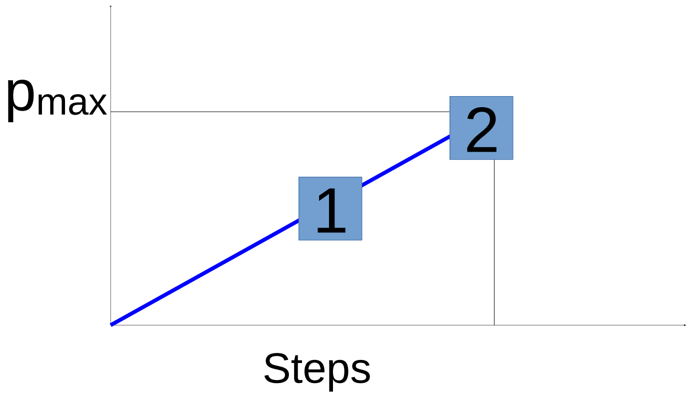
Pressure ramping

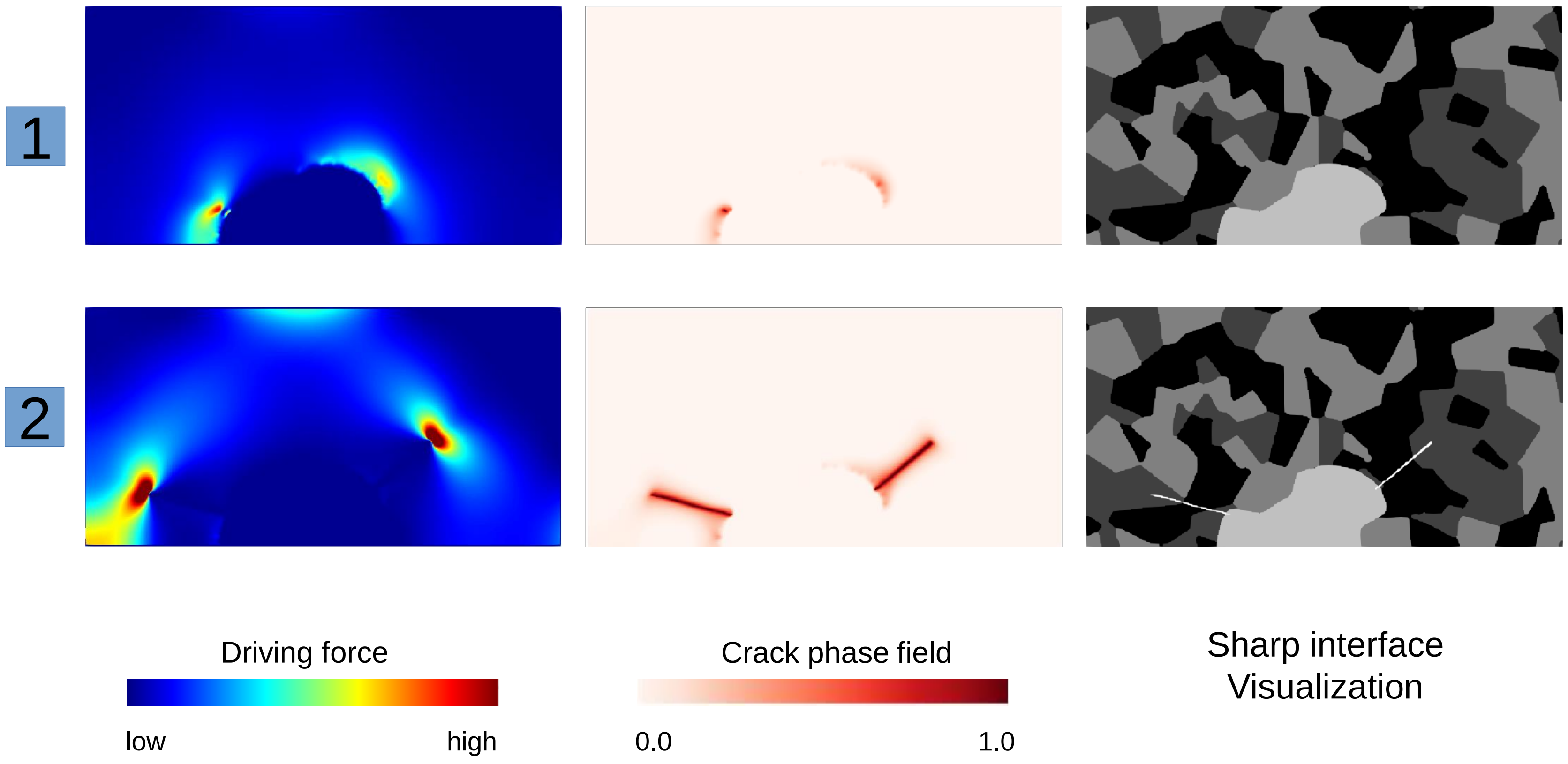




Pressure-induced cracks in corrosion pits

Pressure ramping





Data-driven Modeling and Simulation

Motivation

- Explosion in data from simulations & experiments
- Traditional analysis methods can’t keep up
- Need structured, scalable research data systems
- Foundation for AI, visualization & decision support

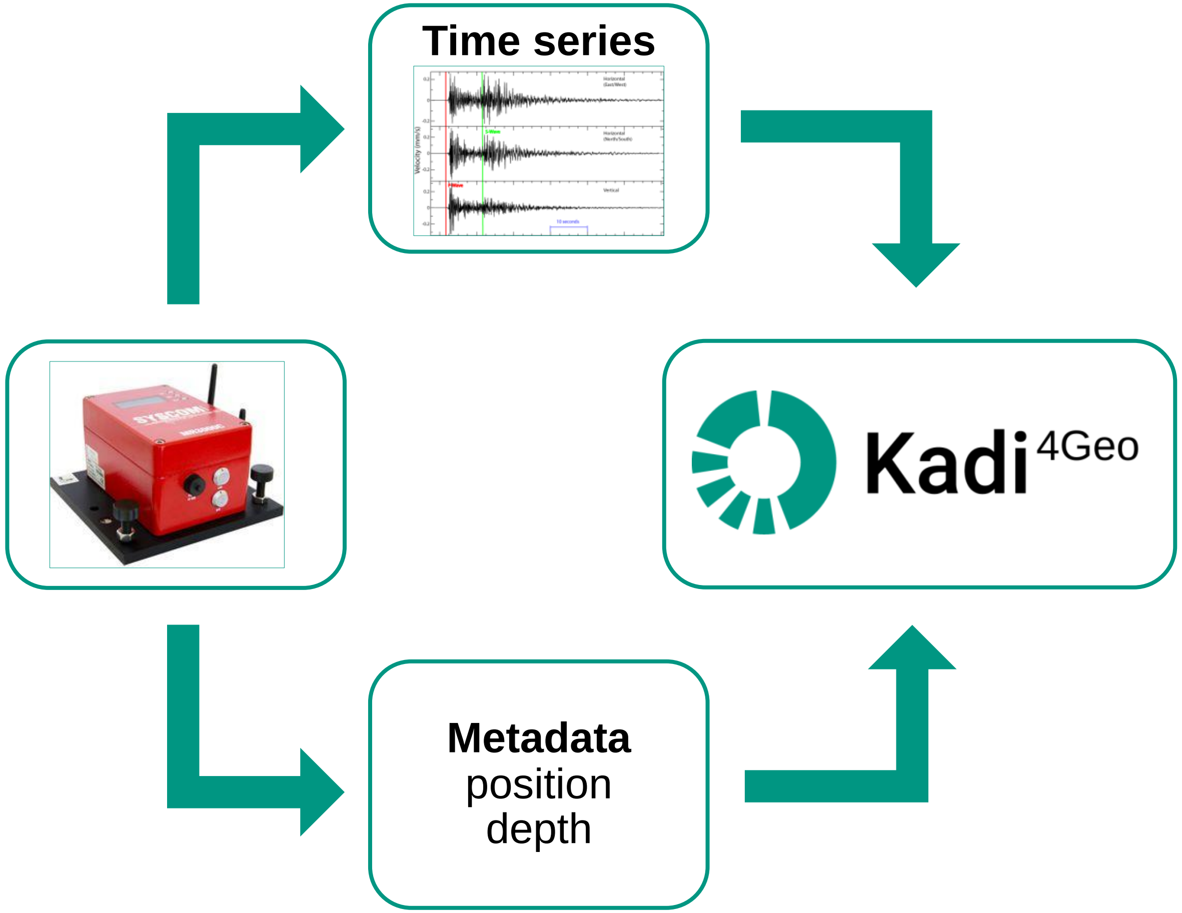
Research Data Infrastructure

Kadi 4Mat &Geo

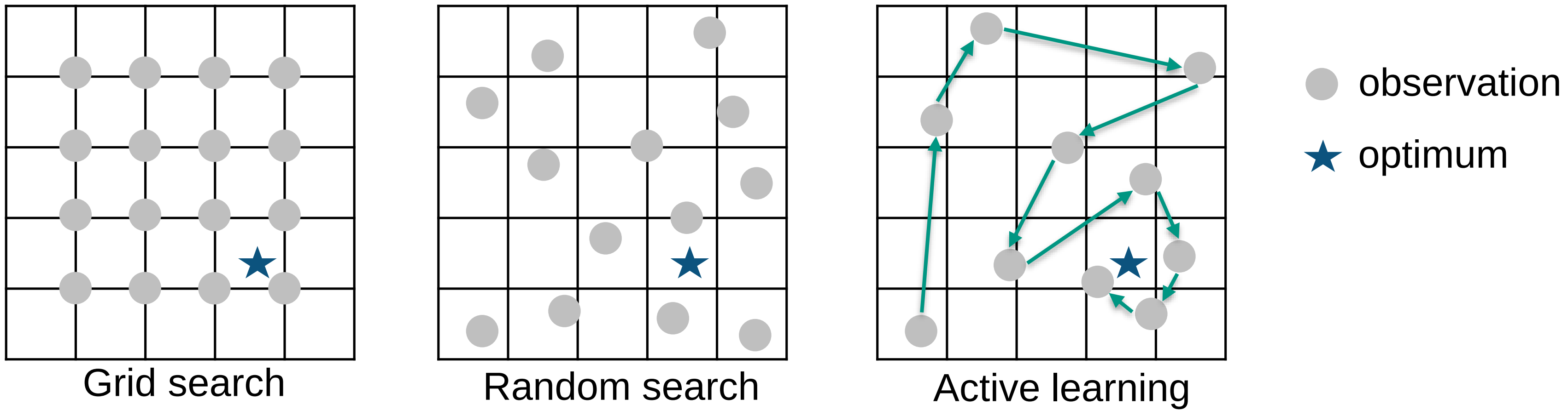
Karlsruhe Data Infrastructure
for Materials Science

Sensor Integration

- Store sensor metadata (e.g., position, depth)
- Collect time-series data continuously
- Stream data to Kadi4Geo in real time
- Enable fast querying & visualization



Active learning workflow for parameter identification



- Simulation parameters are costly to determine
- Active learning reduces experiments & runs
- It identifies simulation parameters systematically and efficiently

Active Learning with KadiStudio and KadiAI

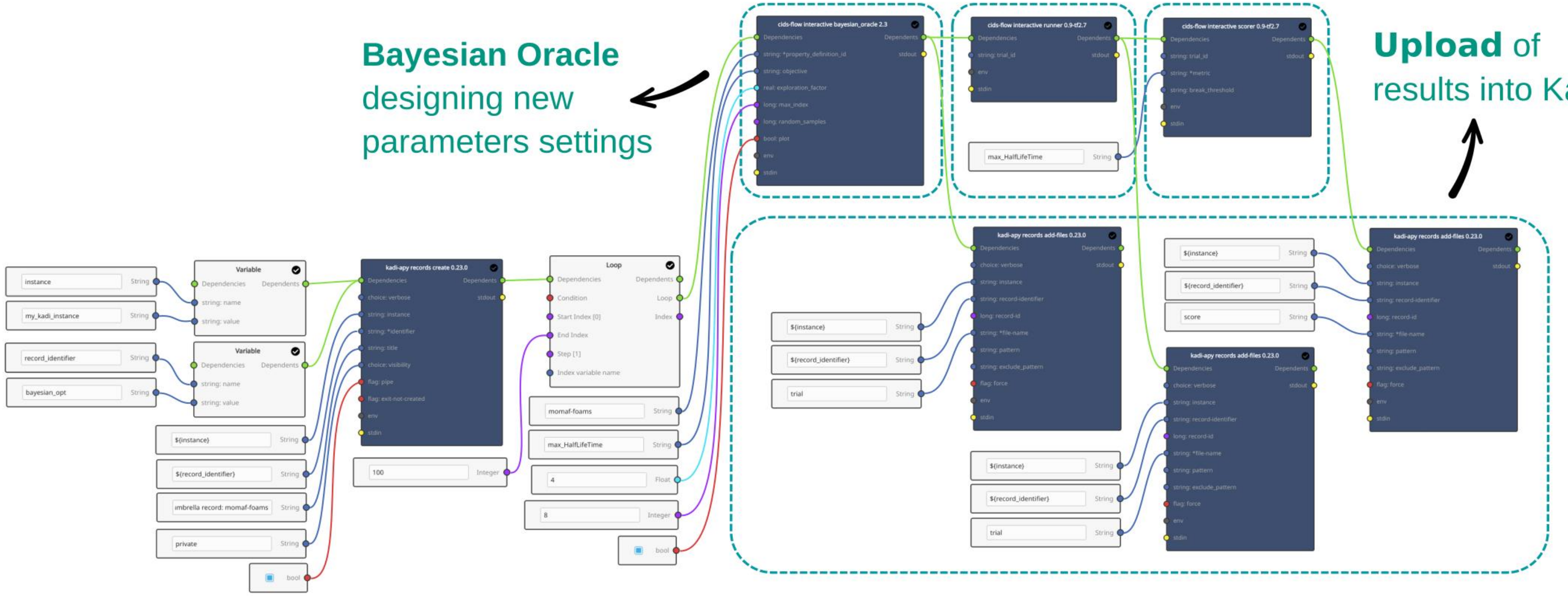
- Oracle workflow node
  - Perform Bayesian optimization in KadiStudio and link with Kadi4Mat

Execution of simulation/ experiment

Validation and score of the result

Bayesian Oracle designing new parameters settings

Upload of results into Kadi



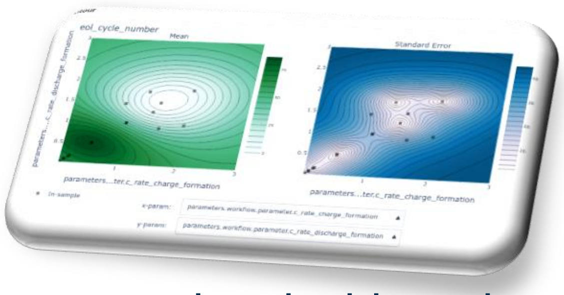
Oracle node for BO

Visualization of BO records

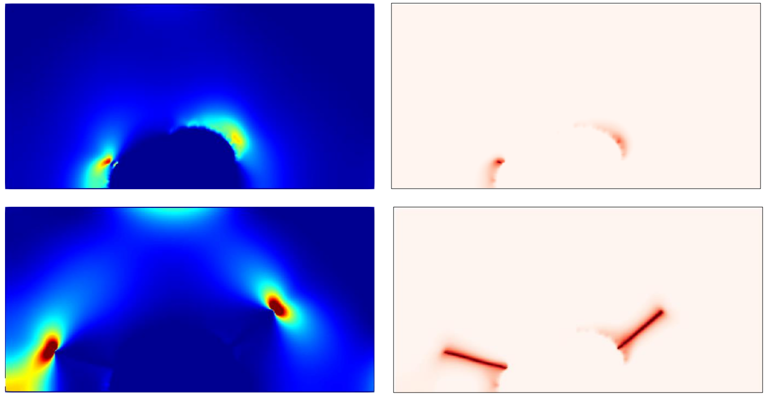
Tosato et al., KIT

Outlook: active learning agent for corrosion cracks

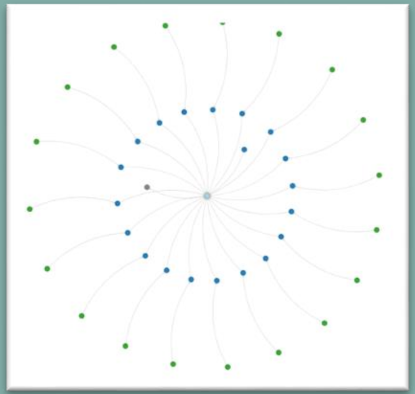
Active learning agent
- Design-of-simulations
- Parameter optimization



Interactive dashboards



Warm-data repository



KadiAIgent Plugin

PACE3D Plugin

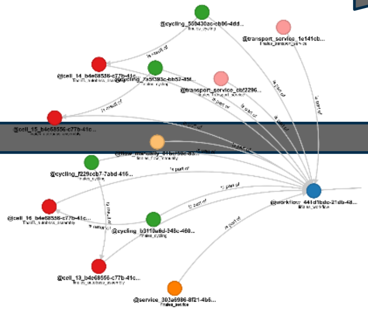
Send workflow request
- Automatically execute trial

PACE3D solver

HPC scheduling

Data uploader

Uploads results



Kadi4Mat

KadiAI

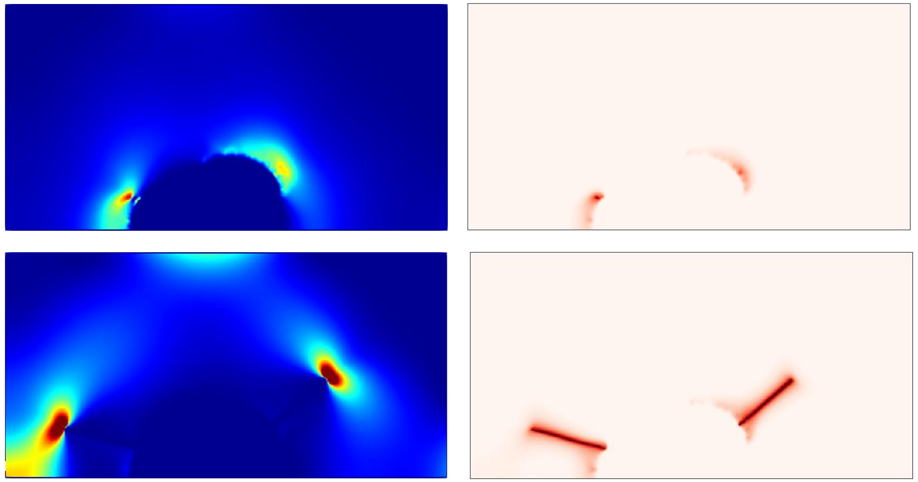
PACE 3D

KIT

Conclusion

Conclusion

- PACE3D enables high-fidelity corrosion simulations
- Kadi ecosystem supports structured, scalable workflows
- Active learning reduces cost and boosts efficiency
- AI agents are the future of autonomous simulation design



KadiAI Kadi4Mat&Geo PACE3D

KIT

Team @IAM-MMS (KIT) — Data-Driven Corrosion

Akash Kumar

Research associate (PhD Candidate), KIT

Dr. Nishant Prajapati

Group leader (Geo-modeling), KIT

Dr. Martin Reder

Group leader (Software developement), KIT

Dr. Arnd Koeppe

Group leader (AI / ML), KIT

Dr. Daniel Schneider

Group leader (Mechanics), KIT

Prof. Dr. rer. nat. Britta Nestler

Professor, KIT & HKA

Thanks for your attention !

Questions & Discussions

Appendix

What are research data?

- No fixed definition of research data
- “Research data are [...] digital and electronically storable data which arise in the course of a scientific project, e.g. through source research, experiments, measurements, surveys or questionnaires”

Translated from: https://www.dfg.de/download/pdf/foerderung/programme/lis/ausschreibung_forschungsdaten_1001.pdf, accessed 07.02.2020

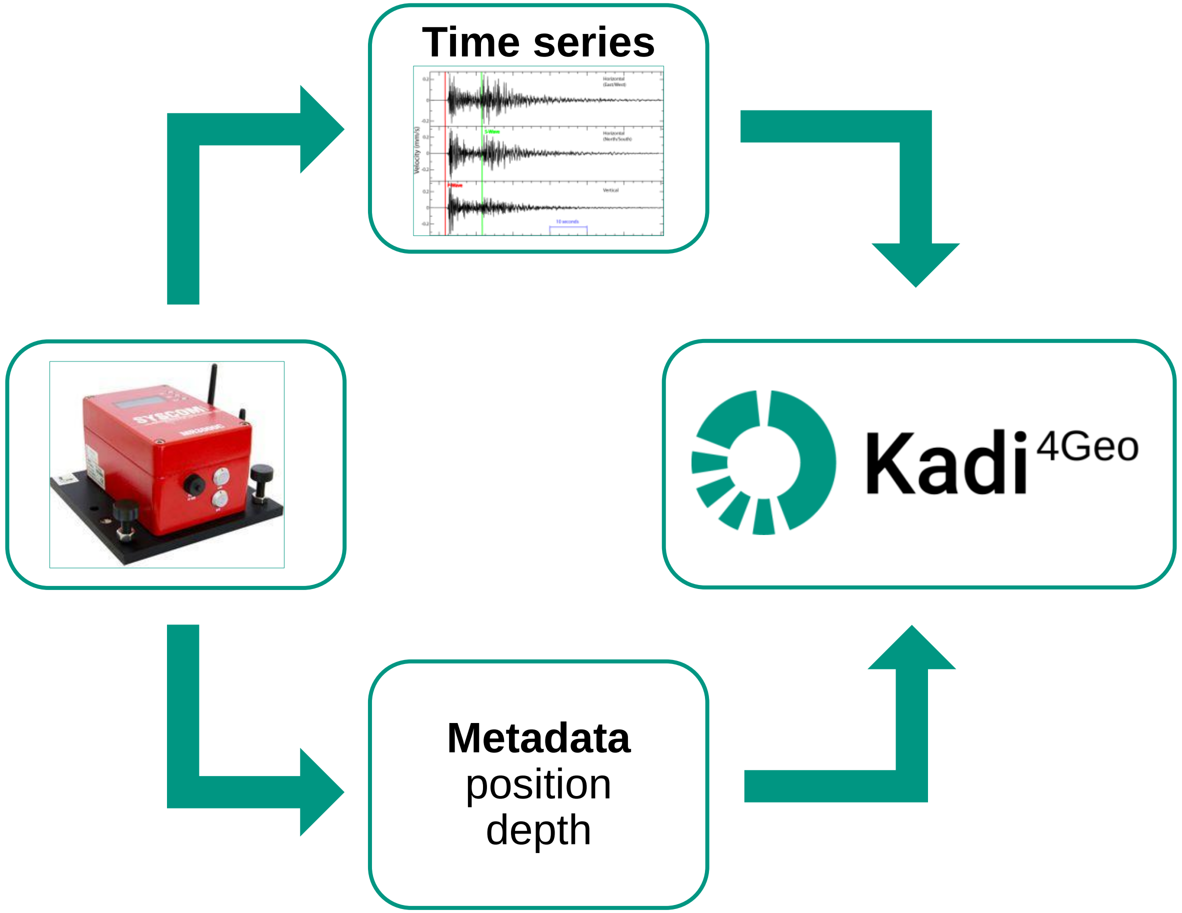
Motivation

- Without appropriate **data science methods**, it will no longer be possible to manage the ever-growing volumes of heterogeneous data from simulations and experiments

- An important aspect to be able to perform corresponding data analysis smoothly is the structured storage of research (meta)data with the help of a suitable **research data infrastructure**

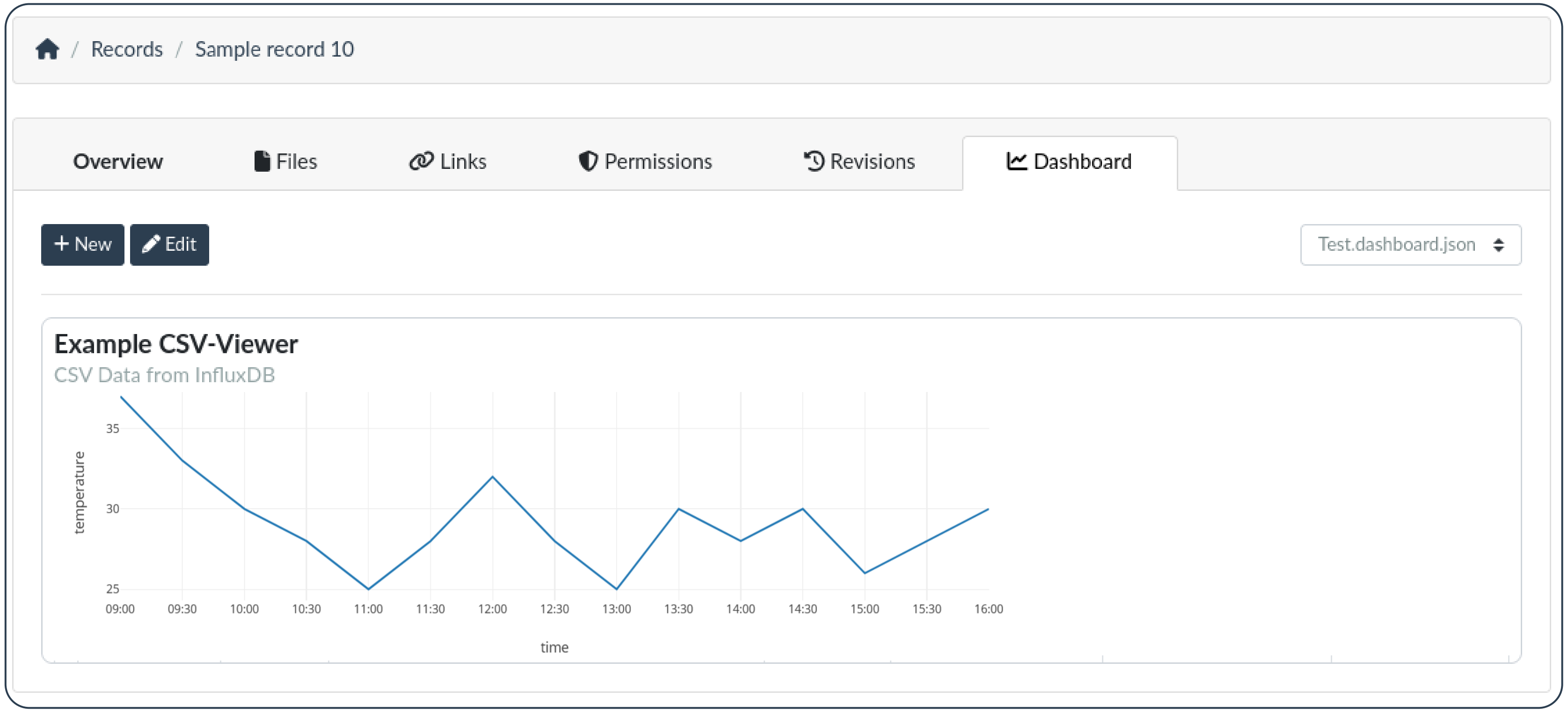
Sensor Integration

- Store **metadata** of sensors like geographic position / depth
- Collect **time series data** continuously via sensors and send it to Kadi4Geo
- Kadi4Geo allows storing large amounts of real-time data and **efficiently querying** it for **analyses** or **visualization**



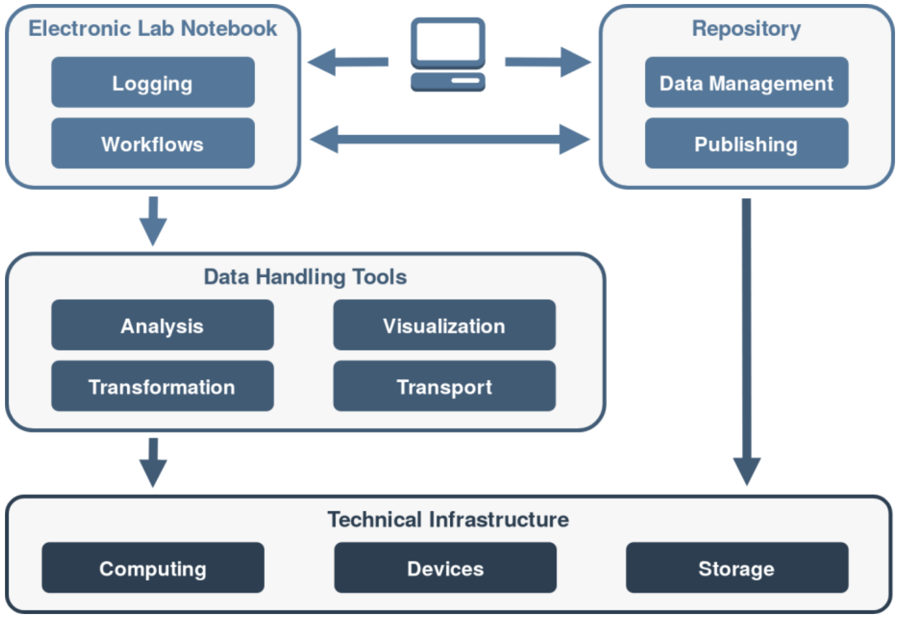
Sensor Monitoring (WIP)

- Monitor sensor data live with customizable **dashboards** inside of Kadi4Geo



Workflow with Kadi4Geo

- Automated **workflows** can be executed using different tools for data handling and data transport, the latter using the API of Kadi4Geo



Conceptual overview of the data infrastructure
https://kadi.iam-cms.kit.edu/

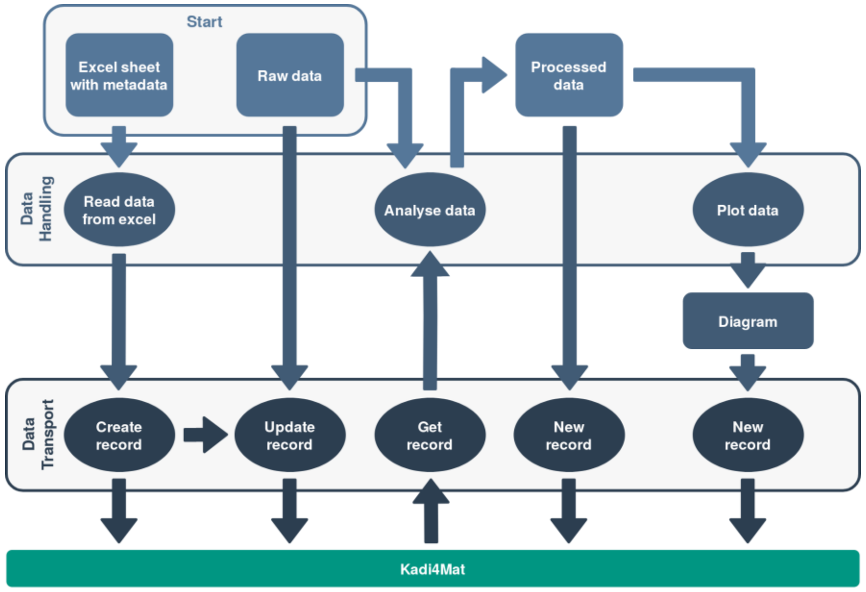


Figure source:
Ephraim Schoof and Nico Brandt, IAM-CMS, KIT