

## ENVINF-Retreat 2025, Day 1

### Work Group Hydroinformatics

- FZ: Is a Germany-wide model sensible?
  - Good for PR reasons.
  - plan: combine individual catchment models
- JB: mesh convergence check with huge models?
  - plausibility tests, no strict convergence analysis
- PS: which aquifers are used?
  - in Germany model there is only one aquifer. It is confined.
- OK: Good example for cross-department collaboration at UFZ.
- Plans for 2025
  - Coupling to DroughtMAS
  - model verification
- Preparation phase for programme defense
  - who is the customer? → e.g. water resource management
  - when does this stop to be a toy model?
  - Lausitz model...
    - \* model still has deficits in mining areas

### Work Group Software

- OK: Workflow manager efforts deserve more visibility
- TK: WFM are game changer in way of work (2nd game changer: HPC)
- TK: difference snakemake vs. Aiida?
  - snakemake → implicit (rules), Aiida → explicit (Python script)
  - snakemake usually the better choice
  - Aiida better multi platform support
  - Aiida → data provenance graph
- TK: Adding third-party libs might create platform dependencies. Avoid? Mark?
  - Try to minimize dependencies.
- CL: make selected research simulations reproducible?
  - could be done
- OK: create research projects that use/highlight workflows. Push visibility.

### Work group visualization

- OK: Work group is on the forefront of digitalization
- OK: Berufungskommission TUDD “Serious Games for City Planning”

## Work group Geothermal/RTP

- OK: Depending on 3rd party funding (EasyQuart+)
- OK: POF-V dependence

## Konates overview

- Future: OGS in Neptune project?
- OK: Konates-II? (maybe incl. in BGE/BGR project?)
- Malm aquifer (Munich)
- Geothermal lithium

## OpenWorkFlow

- TK: make profile sharper
- PS: distinguish better between OGS and OWF
  - OWF was chosen to avoid “OGS”
- JB: expertise building (Journal Club)

## Pitch – Jörg

- Model uncertainties (e.g. as expert opinion for BGE)
- Where could experimental data come from?
- OK: Switzerland → TH2/TH2M/TRM comparison (similar to FE minibenchmarks)
  - ThEDi is delicate
  - funding needed
- TN: cf. Vinay split structural water and mineral water
  - thermal fluid pressurization is directly linked to integrity criteria

## Pitch – Norbert

- Gas production (LILW)
- Transport equation in TH2M for Tritium
- TN: Maybe follow-up studies of Michel Pitz’s or Eike’s PhD work.
- FV: Prio? H2 in high level waste?
  - geochemistry is too complicated (code too slow then)

## Pitch - Mostafa

- CO2 sequestration

- TH2M+PF
- JB: TH2M+PF is very resource intensive. Is application scale possible?
  - difficult
- DN: very many parameters
- TK: How to verify?
  - e.g. via geothermal efficiency
  - e.g. via fault activation/earth quakes
- OK: ML models might help with acceleration
  - proposal would be worthwhile
- CC: different phases: fracturing/stable operation
  - MG: apply phase field to compute material properties for different materials
    - \* MM: non-propagating fractures are faster to simulate

## Pitch - Afid

- JB: training of ML model. What is the goal?
  - TK: MHM can use global climate models, we want to do similar things
- TK: machine learning for calibration (MHM is much faster than OGS)
- MJä: FINAM coupling for heat transport BHE for more flexibility when coupling e.g. to BHE models (time step control)

## Pitch – Philipp

- Local mass conservation
- HS: mass loss/gain due to reaction. will that change the conservation properties?
- DN: which FE families would be interesting to explore? MFEM? DG?
  - make an informed choice before starting...
  - more tomorrow
- Lagrangian approach
- consistent velocity field needed
- DN: perfect for GPU

## ENVINF-Retreat 2025, Day 2

### DN – OGS Overview

- DN: Customization points needed for ad hoc developments
- OK: Use DUNE/MOOSE/Fenics in OWF?
- Next big steps?
  - Modularization of constitutive relations
  - Better testing necessary
  - Shape functions from Fenics

## TM – SUTOGS

- OK: Link to projects?
  - Success measure e.g.: 10 students. Ask if OGS is easy to use.
- TN: DigBen hierarchical testing
- FK: Do not close way to new users by restricting OGS as “expert software”.
- OK: Will there be many new processes?

## FZ – OGSTools

- JH: Mirror OGS tools in Python?
  - for one liners
- MJo: Connection to OGS’s modularity issues?
  - increases modularity

## FK – Documentation

- DN: ChatGPT with OpenGeoSys knowledge might be an option.
- OK: Documentation for repository modelling is necessary.
- Lot of arguments in favour of large language models
- TN: develop use cases together with existing/prospective users
- DN: Python/Jupyter to lower the entrance threshold
- DN: Writing good documentation is something different than writing code.  
For a developer the functionality is clear.
- OK: regular courses “getting started”
- MM: Cf. ChatGPT-Fenics
- WW: Link in user guide to parameter documentation

## TF – HPC

- JB: Is GPU a general trend in HPC? Only GPUs in the future?
  - JSC is experimental → Exascale
  - But GPU fraction is likely to grow.
- TK: Who has problems for 100 cores and more
  - HS (maybe), MM
- HS: PINN, useable for RTP (acceleration)
  - huge amount of GPU resources not needed
- JB: potential for TH2M assembly optimizations
- PS: approximate Jacobians
  - or other assembly schemes for Jacobians

## KR – Digital Twins

- CL: Data management is a key point.

- OS: What to put into the vis study?
  - e.g. vertical stress, because it has a large visual impact
  - previews in ParaView
  - which simulated parameters are interesting to visualize?
- further meta data: responsible person, publications, ...
- MJä: run surrogate models from digital twin?
- JH: Python as a tool? OGSTools functionalities missing?
  - OS: Unity does not use Python naturally, but for VTK based visualizations it might be an option
- MJo: Include VTK web based vis in OGSTools?

## **TN – TUBAF projects**

- regularization similar to phase field
- Sandwich → Digital Twin, OWF, ...

## **WW - Pitch Locking**

- JB: Any preferred scheme? Higher order elements already chosen?
  - Pros/Cons for all schemes
- DN: What is the mesh sensitivity problem for higher order elements?
  - To be clarified.

## **PS – Pitch Mix/Hybrid FEM/DG/FVM**

- Preferred method?
  - Particle tracking need consistent velocity field.
  - vertex centered FVM might be worthwhile
- OK: Test methods in existing tool and port to OGS if it works?
  - would be an option.

## **MG – Adaptive meshing**

- JB: useful, but a lot of effort required → proposal needed
- DN: maybe try with another software first

## **MJä – Time integration**

- DN: Maybe add Crank-Nicholson again
- PS: RK4 might lead to some issues
- other schemes interesting: Newmark, SDIRK, ...