Modelling of radionuclide transport process using SHEMAT-Suite

1st URS PhD Workshop

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Chair of Methods for Model-based Development in Computational Engineering

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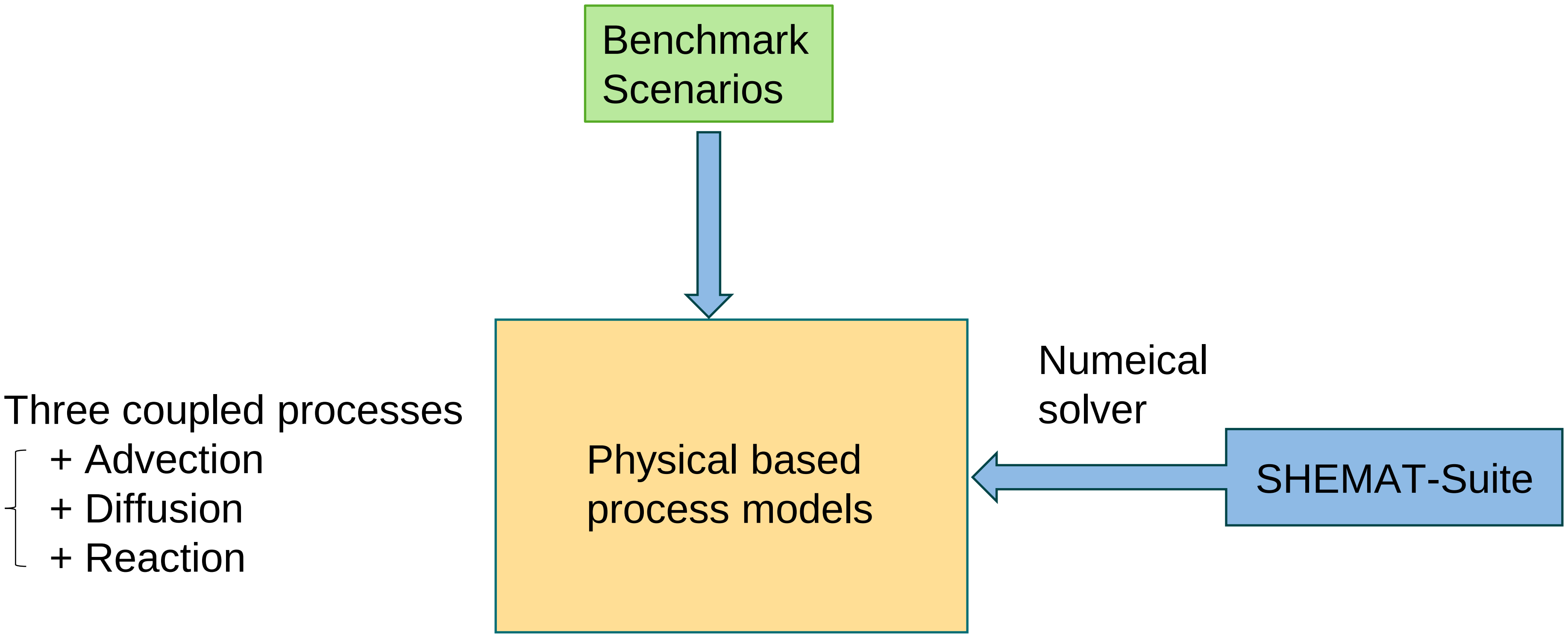
Motivation

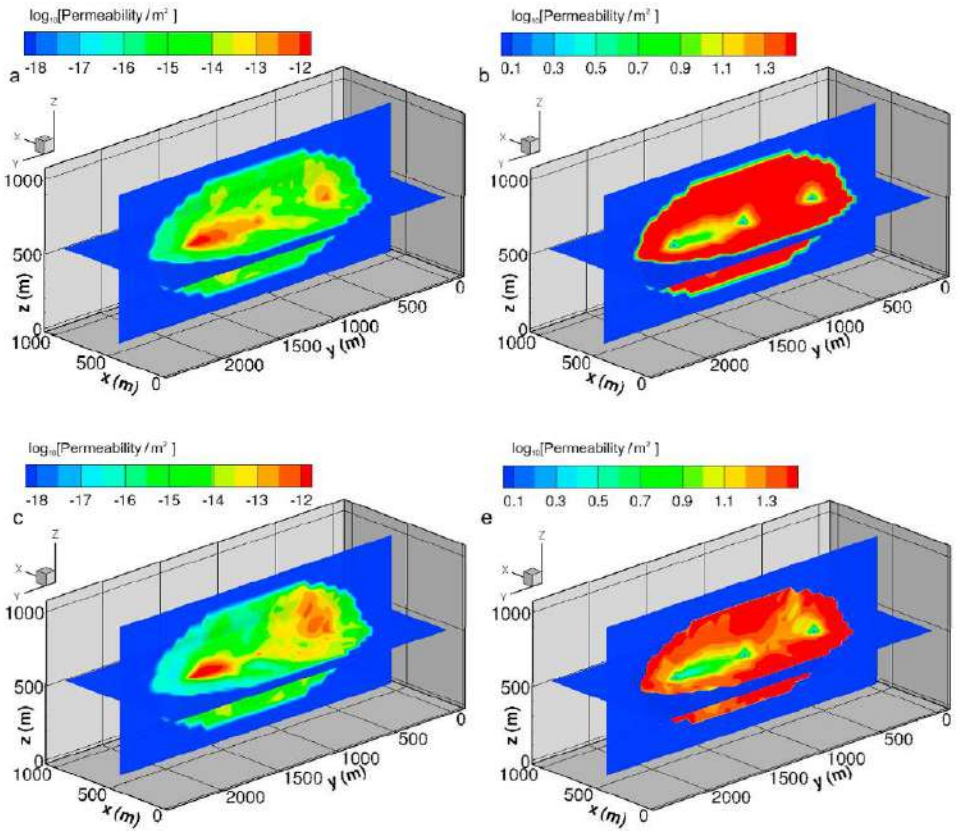

Benchmark Scenarios
Numeical solver
Three coupled processes
+ Advection
+ Diffusion
+ Reaction
Physical based process models
SHEMAT-Suite

Introduction

Open-source **SHEMAT-Suite (S**imulator for **HE**at and **MA**ss **T**ransport**)** is a numerical code for computing **flow**, **heat** and **species** transport equations in porous media. The code solves transient or steady-state, forward and inverse coupled problems in 1D, 2D, and 3D.

Governing Equations of SHEMAT-Suite:

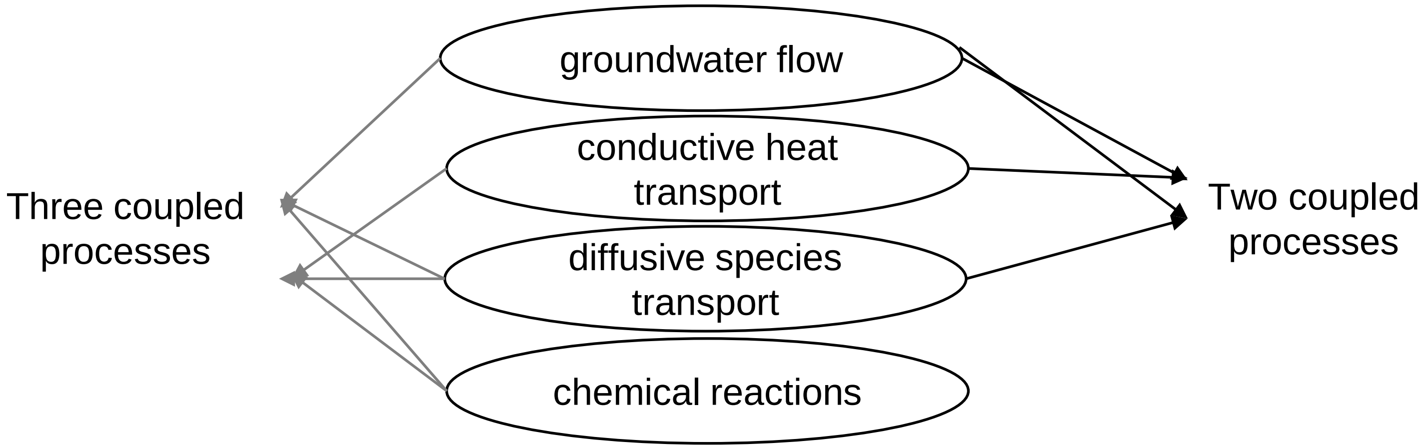
- Groundwater flow
- Heat transport
- Species transport



(Vogt, C., et al)

Introduction

SHEMAT-Suite can solve the following classes of problems:

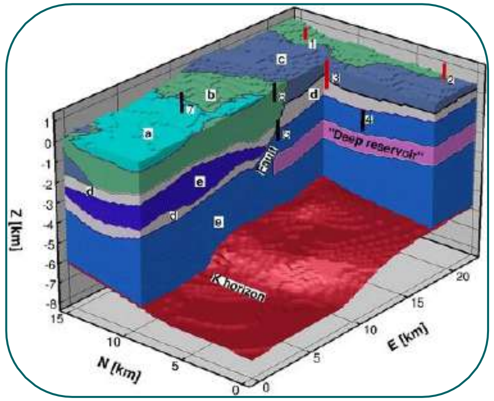


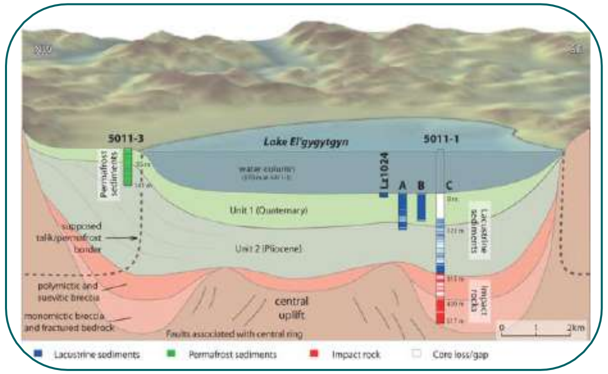
SHEMAT-Suite uses a finite difference method to solve the partial differential equations numerically.

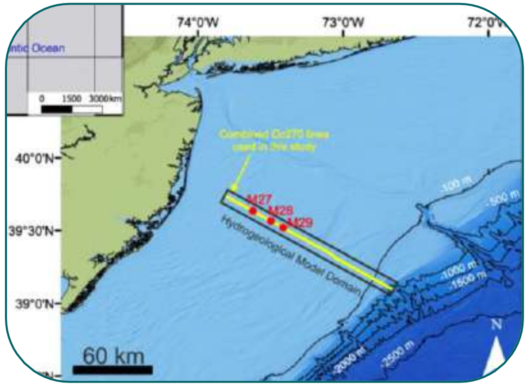
- Upwind Differencing Scheme
- Il'in Flux Blending Scheme
- Smolarkiewicz Advection Scheme

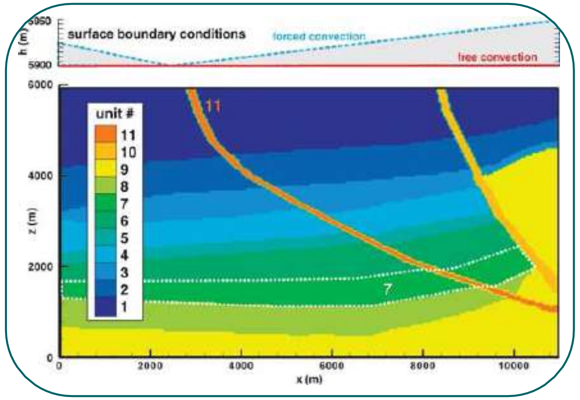
Important Application Areas

Four important **application areas** of SHEMAT-Suite:









- **Geothermics:**
- **Paleoclimate:**
- **Hydrogeology:**
- **Inverse method development:**

(Ebigbo, Anozie, et al.)

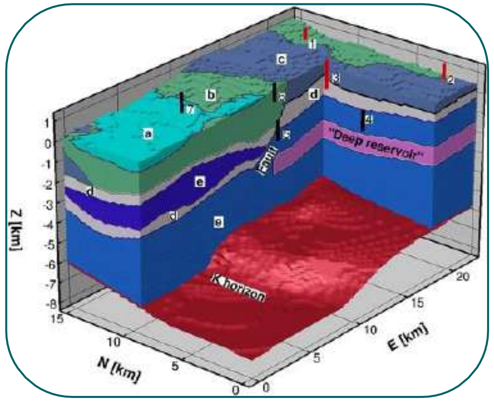
(D. Mottaghy et al.)

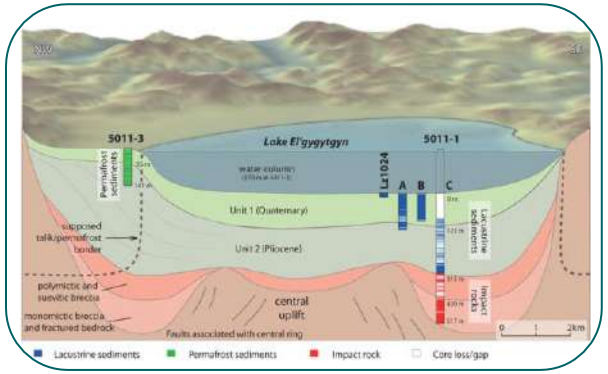
(Thomas, A. T., et al.)

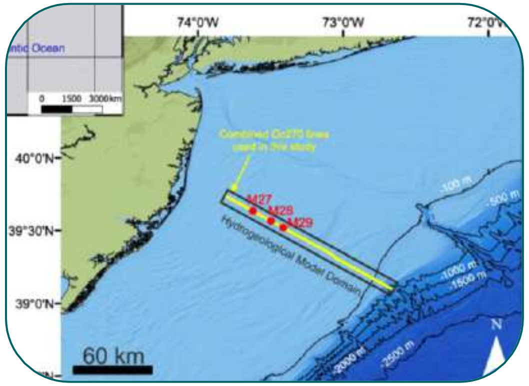
(Rath, V., A. Wolf, and H. M. Bücker.)

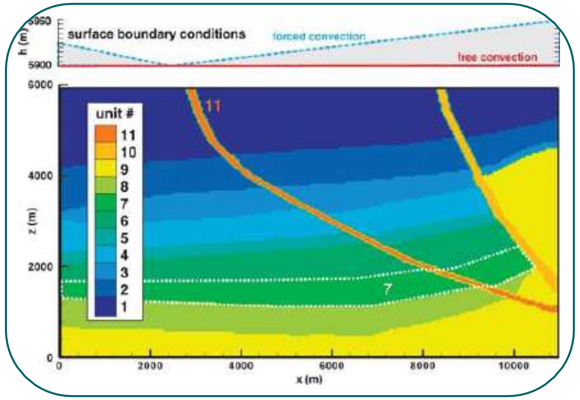
Important Application Areas

Four important **application areas** of SHEMAT-Suite:









- **Geothermics:**
  - ➢ Borehole heat exchanger and temperature sensor simulations
  - ➢ Deep geothermal reservoirs simulation
  - ➢ …

(Ebigbo, Anozie, et al.)

- **Paleoclimate:**
  - ➢ Property module for ice for simulating freezing and thawing processes in porous media.
  - ➢ …

(D. Mottaghy et al.)

- **Hydrogeology:**
  - ➢ Simulating the submarine groundwater discharge
  - ➢ Ensemble-based and rely on high-performance computing for the modern aquifer flow simulations
  - ➢ …

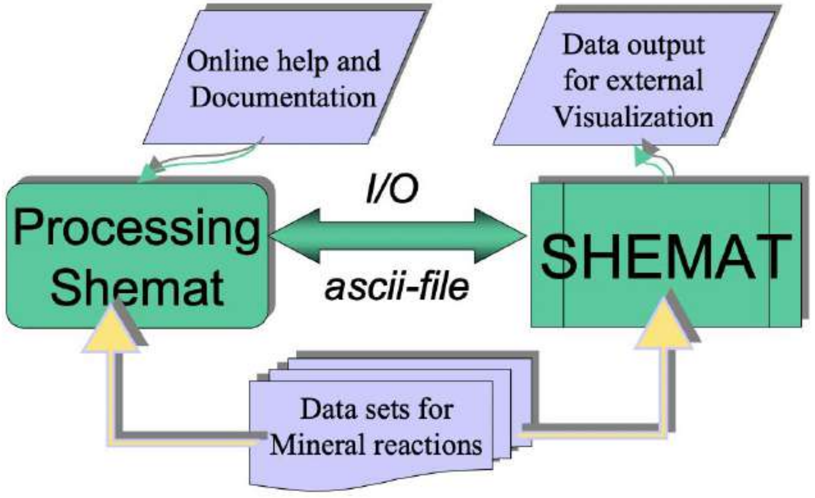
(Thomas, A. T., et al.)

- **Inverse method development:**
  - ➢ Three-dimensional inverse parameter estimation
  - ➢ Uncertainty quantification of expected geothermal energy usage
  - ➢ optimal experimental design
  - ➢ …

(Rath, V., A. Wolf, and H. M. Bücker.)

SHEMAT to SHEMAT-Suite

- SHEMAT (Fortran 77)



General structure of the simulation package SHEMAT / Processing SHEMAT (Clauser 2003)

- SHEMAT-Suite (Fortran 95)

Git:

❖ SHEMAT-Suite-open
Repository for code development for open-source SHEMAT-Suite.

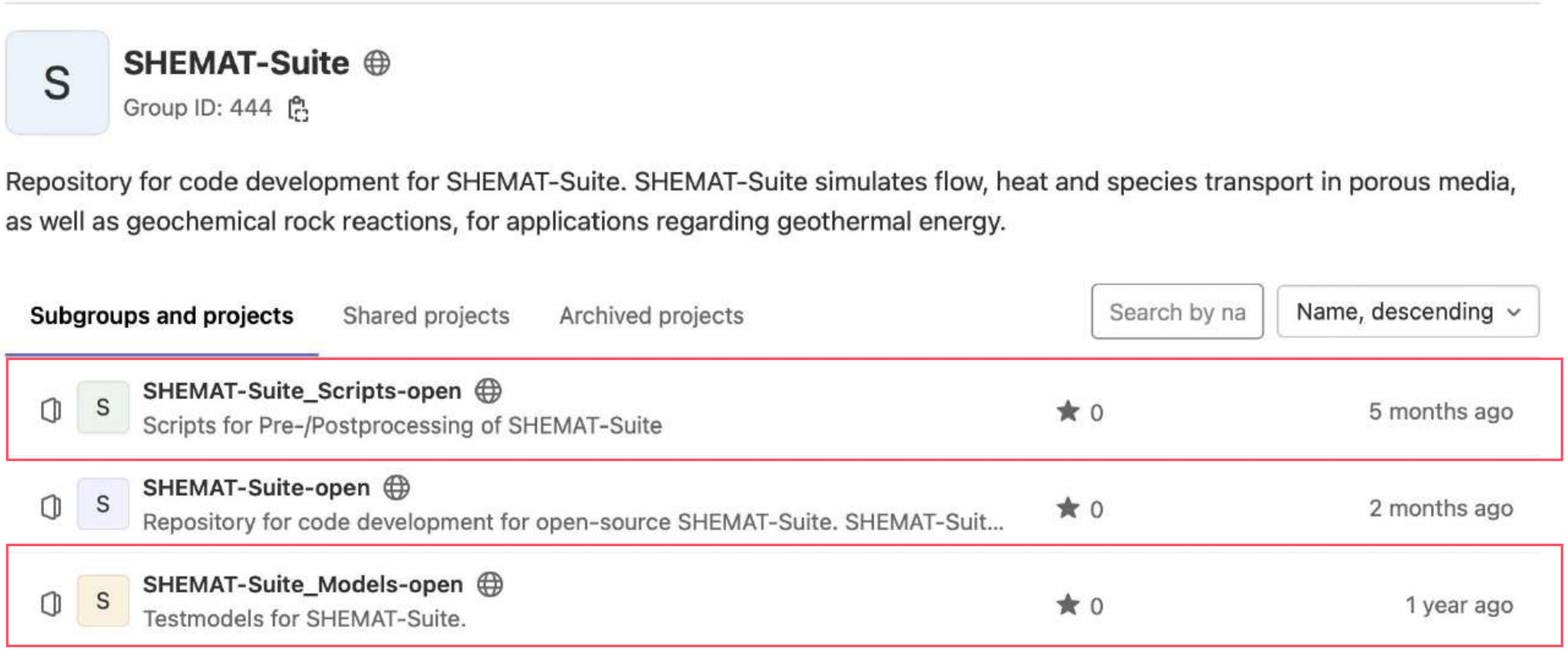
❖ SHEMAT-Suite_Models-open
Testmodels for SHEMAT-Suite.

❖ SHEMAT-Suite_Scripts-open
Scripts for Pre-/Postprocessing of SHEMAT-Suite.

Overview of current code version

- Current code version: v9.00
- Permanent link to code/repository: https://github.com/ElsevierSoftwareX/SOFTX_2020_135
- Operating environment: Linux OS

➢ Open source environment



SHEMAT-Suite _Models-open

S

SHEMAT-Suite_Models-open

Project ID: 41816

34 Commits 1 Branch 0 Tags 310.4 MB Project Storage

Testmodels for SHEMAT-Suite.

Benchmarks for SHEMAT-Suite	Source
`fw_basc_ElderProblem`	Elder, J., Numerical experiments with free convection in a vertical slot, Journal of Fluid Mechanics, 24(4), 823–843 (1966).
`fw_basc_HenryProblem`	Thomas, A. T., Reiche, S., Riedel, M., & Clauser, C., The fate of submarine fresh groundwater reservoirs at the new jersey shelf, usa, Hydrogeology Journal, 27(7), 2673–2694 (2019). http://dx.doi.org/10.1007/s10040-019-01997-y
`fw_const_DP`	Domenico, P. A., & Palciauskas, V. V., Theoretical analysis of forced convective heat transfer in regional ground-water flow, Geological Society of America Bulletin, 84(12), 3803 (1973). http://dx.doi.org/10.1130/0016-7606(1973)84<3803:taofch>2.0.co;2
`fw_const_HeatConduction1D`	simple analytical solution
`fw_const_Peclet`	simple analytical solution
...	...

https://git.rwth-aachen.de/SHEMAT-Suite/shemat-suite_models-open

Input and Output File

ASCII input files

Example →

SHEMAT-Suite

Output Files

- vtk (Paraview)
- plt (Tecplot)
- hdf (hdf5 software)
- txt

Input File 1: Input file of the THEIS model. (Keller, Johannes, et al.)

```
! # =====>>>>>   RUN INFO                          <<<<<===== # !
# title
theis
# linfo
2 3 2 3
# runmode
0
# active head
# PROPS = const
# USER = none
! # =====>>>>>   GRID                              <<<<<===== # !
# grid
69 69 1
# delx
3*160.0d0 1*80.0d0 1*40.0d0 3*20.0d0 3*10.0d0
5*5.0d0 5*2.0d0 11*1.0d0 2*1.0d0 1.0d0 2*1.0d0
11*1.0d0 5*2.0d0 5*5.0d0 3*10.0d0 3*20.0d0
1*40.0d0 1*80.0d0 3*160.0d0
# dely
3*160.0d0 1*80.0d0 1*40.0d0 3*20.0d0 3*10.0d0
5*5.0d0 5*2.0d0 11*1.0d0 2*1.0d0 1.0d0 2*1.0d0
11*1.0d0 5*2.0d0 5*5.0d0 3*10.0d0 3*20.0d0
1*40.0d0 1*80.0d0 3*160.0d0
# delz
20.d0
! # =====>>>>>   TIME STEP CONTROL                 <<<<<===== # !
# timestep control
1
1.0 1.0 1.0 0.0
# tunit
86400
# time periods, records=1
0.0  3.5  100 lin
! # =====>>>>>   SOLVER CONTROL                    <<<<<===== # !
# nlsolve
50 0
# lsolvef (linear solver control)
1.d-10 64 500
# nliterf (nonlinear iteration control)
1.0d-10 1.0d0
! # =====>>>>>   BOUNDARY AND INITIAL CONDITIONS   <<<<<===== # !
# head bcn, records=1, direction=0
35 35 1 -0.001d0 0
# head bcd, simple=right, value=init
# head bcd, simple=back, value=init
# head init
4761*20.0d0
# temp init
4761*20.0d0
! # =====>>>>>   PROPERTIES                        <<<<<===== # !
# fluid props
1000.0d0 5.0D-8 4218.0d0 0.65d0 1.0D-3 0.02d0
# units
0.1d0  1.d0  1.d0 1d-12 1.d-8  1.d0  1.d0  3.35d0  0.d0  2300000.d0  10d0  0.d0  0.d0
! # =====>>>>>   GEOMETRY                          <<<<<===== # !
# uindex
4761*1
! # =====>>>>>   OUTPUT                            <<<<<===== # !
# file output: vtk hdf
```

Input and Output File

ASCII input files → Example →

↓

SHEMAT-Suite

↓

Output Files
- vtk (Paraview)
- plt (Tecplot)
- hdf (hdf5 software)
- txt

Input File 1: Input file of the THEIS model. (Keller, Johannes, et al.)

Run Info

```
! # =====>>>>>   RUN INFO                    <<<<<===== # !
# title
theis
# linfo
2 3 2 3
# runmode
0
# active head
# PROPS = const
# USER = none
```

Grid

```
! # =====>>>>>   GRID                        <<<<<===== # !
# grid
69 69 1
# delx
3*160.0d0 1*80.0d0 1*40.0d0 3*20.0d0 3*10.0d0
5*5.0d0 5*2.0d0 11*1.0d0 2*1.0d0 1.0d0 2*1.0d0
11*1.0d0 5*2.0d0 5*5.0d0 3*10.0d0 3*20.0d0
1*40.0d0 1*80.0d0 3*160.0d0
# dely
3*160.0d0 1*80.0d0 1*40.0d0 3*20.0d0 3*10.0d0
5*5.0d0 5*2.0d0 11*1.0d0 2*1.0d0 1.0d0 2*1.0d0
11*1.0d0 5*2.0d0 5*5.0d0 3*10.0d0 3*20.0d0
1*40.0d0 1*80.0d0 3*160.0d0
# delz
20.d0
```

Time Step

```
! # =====>>>>>   TIME STEP CONTROL           <<<<<===== # !
# timestep control
1
1.0 1.0 1.0 0.0
# tunit
86400
# time periods, records=1
0.0  3.5  100 lin
```

Solver Control

```
! # =====>>>>>   SOLVER CONTROL              <<<<<===== # !
# nlsolve
50 0
# lsolvef (linear solver control)
1.d-10 64 500
# nliterf (nonlinear iteration control)
1.0d-10 1.0d0
```

Boundary conditions

```
! # =====>>>>>   BOUNDARY AND INITIAL CONDITIONS   <<<<<===== # !
# head bcn, records=1, direction=0
35 35 1 -0.001d0 0
# head bcd, simple=right, value=init
# head bcd, simple=back, value=init
```

Initial Values

```
# head init
4761*20.0d0
# temp init
4761*20.0d0
```

Parameters

```
! # =====>>>>>   PROPERTIES                  <<<<<===== # !
# fluid props
1000.0d0 5.0D-8 4218.0d0 0.65d0 1.0D-3 0.02d0
# units
0.1d0  1.d0  1.d0 1d-12 1.d-8  1.d0  1.d0  3.35d0  0.d0  2300000.d0  10d0  0.d0  0.d0
! # =====>>>>>   GEOMETRY                    <<<<<===== # !
# uindex
4761*1
```

Output

```
! # =====>>>>>   OUTPUT                      <<<<<===== # !
# file output: vtk hdf
```

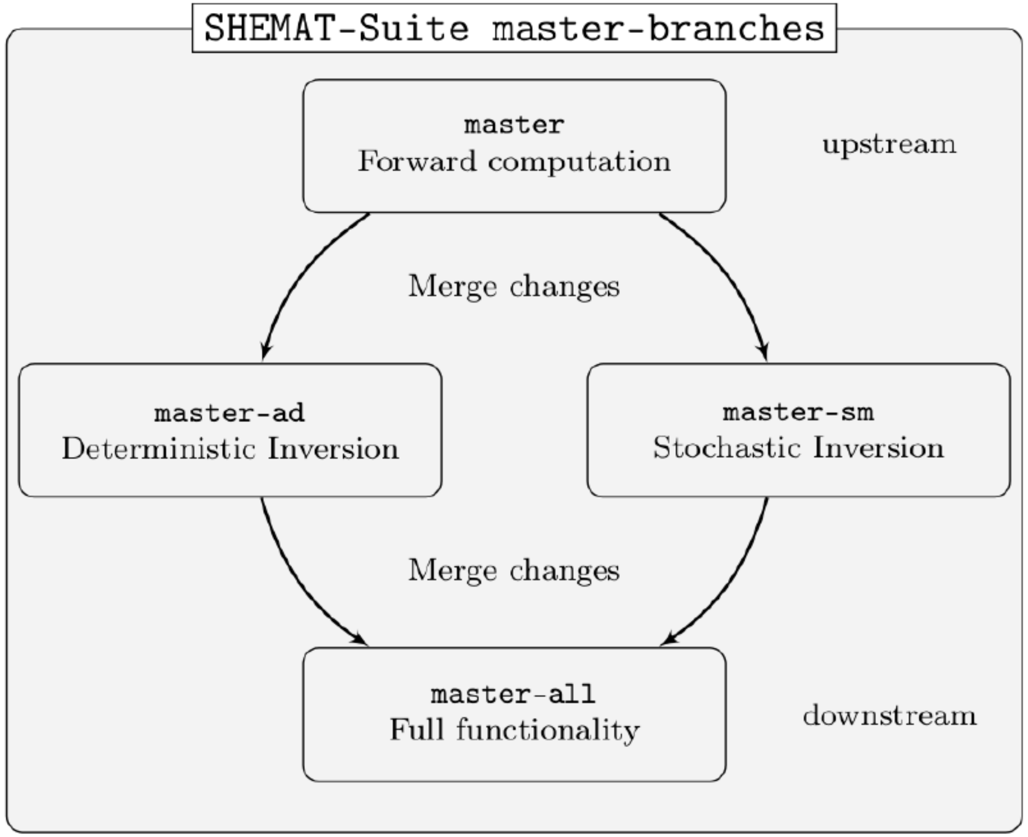
SHEMAT-Suite-Wiki →

- General information
- Tutorial
- Instructions

Software functionalities

The source code of SHEMAT-Suite is functioned in two levels: **1. The branch level** 2. The directory level.

- A **forward-mode** (*master*) for pure forward computation.
- An **automatic-differentiation-mode** (*master-ad*) for deterministic inverse computation.
- A **stochastic-mode** (*master-sm*) for geostatistical simulation and parameter estimation.
- *Master-all* compiling in all three modes.



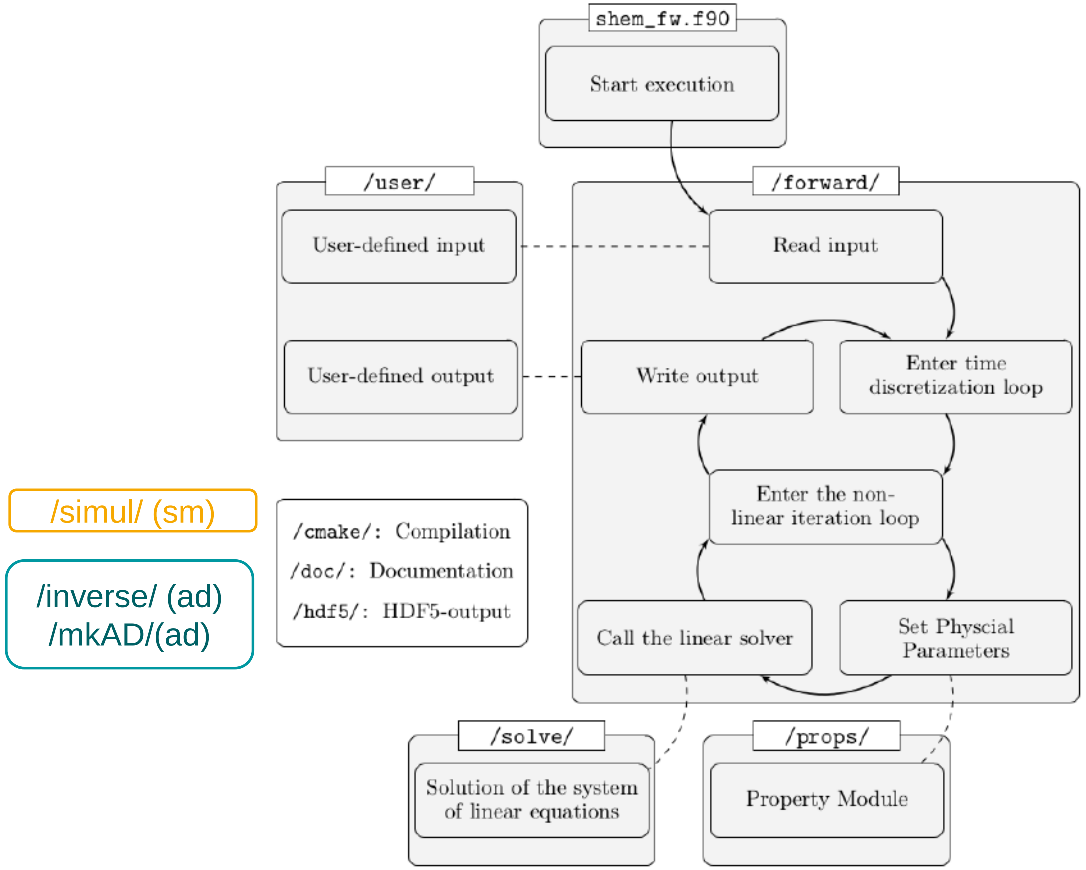
(Keller, Johannes, et al.)

Software architecture

The source code of SHEMAT-Suite is functioned in two levels: 1. The branch level **2. The directory level.**

The master branch contains the following directories:

- ***/forward/:*** forward computation
- ***/solve/:*** the solution of systems of linear equations.
- ***/props/:*** dynamic behavior and coupling of fluid and rock properties.
- ***/user/:*** user-defined input and out subroutines, a user-defined Fortran-module.
- ***/hdf5/:*** interfaces with the HDF5 library for input and output.
- ***/cmake/:*** compilation utilities using CMake tools.
- ***/doc/:*** input for generating the Doxygen documentation.



(Keller, Johannes, et al.)

Pre-/Postprocessing of SHEMAT-Suite

Compatible Python-based implementations:

pySHEMAT: Python wrapper for **SHEMAT** input and output files.
(https://github.com/flohorovicic/pyshemat)

❖ SHEMAT-Suite_Scripts-open

Pre-processing:
convert_to_hdf5.py : **can be used to convert some of the SHEMAT-Suite input arrays into hdf5-files.**
The user input for SHEMAT-Suite is provided in an ASCII-file. For reducing the reading time of larger input files, SHEMAT-Suite provides the option to readHDF5 input instead.

Post-processing:
pyshemkf: **Python environment for handling SHEMAT-Suite output of EnKF simulations**
pyshemkf can generate graphs and 2D-figures of variables and parameters provided by typical output of SHEMAT-Suite.
(https://github.com/jjokella/pyshemkf)

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Important code developments of SHEMAT-Suite

Table 1 (Keller, Johannes, et al.)

Newly implemented functionality	Key reference
Inverse parameter estimation based on automatic differentiation	Rath et al. 2006 [11]
Latent heat effects due to freezing and melting	Mottaghy and Rath, 2006 [34]
Monte Carlo techniques for uncertainty quantification and reduction	Vogt et al. 2010 [50]
Borehole heat exchanger module[b]	Mottaghy and Dijkshoorn, 2012 [51]
Shared-memory parallelization	Wolf, 2011 [7]
Data assimilation based on the ensemble Kalman Filter	Vogt et al. 2012 [31]
Multi-phase flow module using automatic differentiation[a]	Büsing et al. 2014 [27]
Distributed-memory parallelization[a]	Rostami and Bücker, 2014 [38]
Heat transfer model for plane thermo-active geotechnical systems[a]	Kürten et al. 2014 [52,53]
Anisotropic flow module using the full permeability tensor[a]	Chen et al. 2016 [54]
Supercritical water/steam module using automatic differentiation[a]	Büsing et al. 2016 [29]
Optimal borehole positioning with respect to reservoir characterization via optimal experimental design[c]	Seidler et al. 2016 [41]
Halite precipitation model in porous sedimentary rock adjacent to salt diapirs[a]	Li et al. 2017 [55]
Efficient two-phase flow in heterogeneous porous media using exact Jacobians[a]	Büsing, 2020 [28]

[a]Functionalities not available in the open-source package.
[b]Simplified functionality available in the open-source package.
[c]SHEMAT-Suite functionality available open-source, additional software required.

Why SHEMAT-Suite?

- Computing flow, heat and species transport equations in porous media.
- Git-branches for software development.
- Automatic differentiation (AD) for calculating exact Jacobian in inversions.
- Large variety of application fields and online test example.
- High performance computing capacities.
- Deterministic and stochastic inversion.

(Keller, Johannes, et al.)

References

1. Clauser, C., Bartels, J., Cheng, L., Ranalli, G., Chiang, W., & Pape, H. (2003). SHEMAT and Processing SHEMAT–Numerical simulation of reactive flow in hot aquifers.
2. Vogt, C., Marquart, G., Kosack, C., Wolf, A., & Clauser, C. (2012). Estimating the permeability distribution and its uncertainty at the EGS demonstration reservoir Soultz-sous-Forêts using the ensemble Kalman filter. Water Resources Research, 48(8).
3. Ebigbo, A., Niederau, J., Marquart, G., Dini, I., Thorwart, M., Rabbel, W., ... & Clauser, C. (2016). Influence of depth, temperature, and structure of a crustal heat source on the geothermal reservoirs of Tuscany: numerical modelling and sensitivity study. Geothermal Energy, 4(1), 1-29.
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5. Thomas, A. T., Reiche, S., Riedel, M., & Clauser, C. (2019). The fate of submarine fresh groundwater reservoirs at the New Jersey shelf, USA. Hydrogeology Journal, 27(7), 2673-2694.
6.Rath, V., Wolf, A., & Bücker, H. M. (2006). Joint three-dimensional inversion of coupled groundwater flow and heat transfer based on automatic differentiation: sensitivity calculation, verification, and synthetic examples. Geophysical Journal International, 167(1), 453-466.
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8. Wellmann, J. F., Croucher, A., & Regenauer-Lieb, K. (2012). Python scripting libraries for subsurface fluid and heat flow simulations with TOUGH2 and SHEMAT. *Computers & Geosciences*, *43*, 197-206.

Thank you for your attention