PAUL SCHERRER INSTITUT

PSI

Wir schaffen Wissen – heute für morgen

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Reactive transport with OGS-GEMS: OGS-GEMS

OGS-GEMS
is using a subset of the available functionality of OGS to calculate:

- Groundwater flow
- Multi-species mass transport
- Chemical reactions (including feedback on porosity for precipitation and dissolution of minerals)

Coupling to Richards flow module (partial saturation) is in preparation
Coupling to heat transport is also possible

Parallel version available: Good speedup already for small problems due to parallel execution of the GEMS chemical solver.

Coupling between processes is performed by simple sequential execution of

Groundwater flow,
Mass transport, (for each independent component in GEMS)
Chemistry (GEMS)

for each time step.

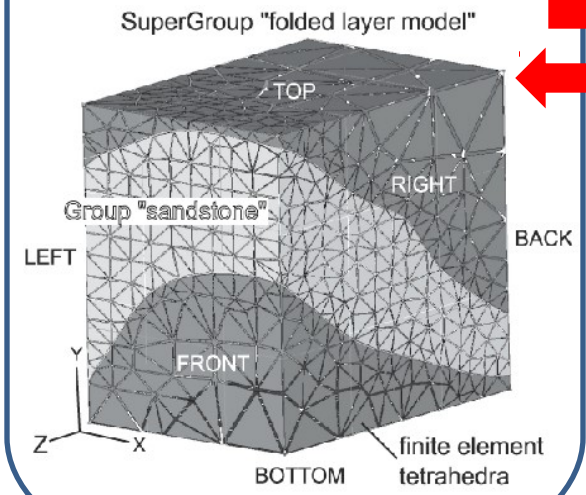
Advantage:
Simple to implement and to extend

Disdavantage:
One has to use small time steps → eventually very long calculation times

Coupled Reactive Transport Calculations

Conceptual Model

- Fractured porous rock
- Finite elements/ volumes



Chemical Model

-Rock chemistry
-Fluid X
-Thermodyn. database
-Interaction parameters
-Kinetic laws

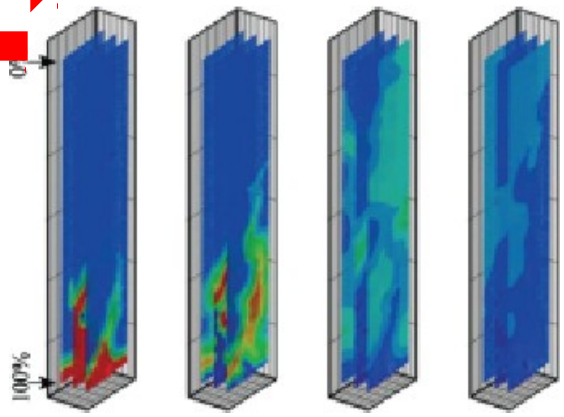
site specific

general

GEMS

Transport Model

- Continuity eq.
- Momentum eq.
- Energy eq.

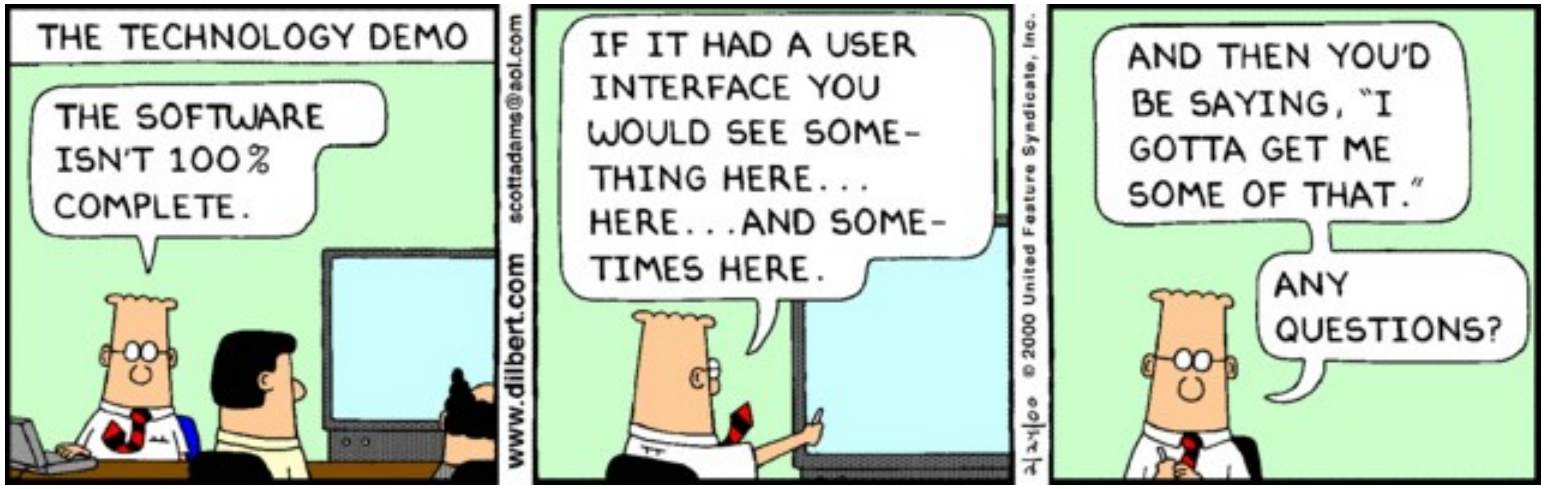


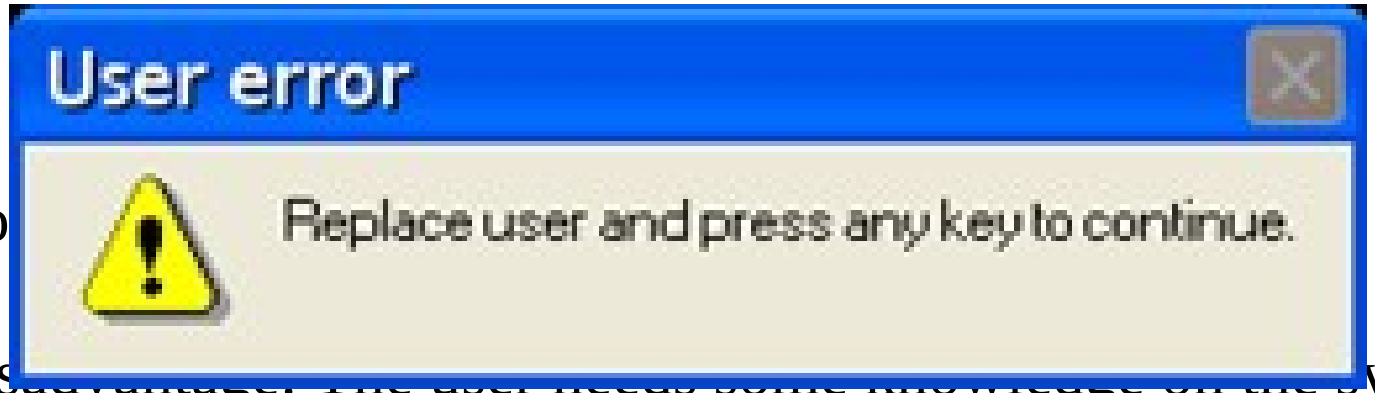
Tracer propagation in a heterogeneous Fractured network (Kalbacher 2007)

Chemical setup should be done with GEM-SELEKTOR v3

We need GEMS records for the different boundary conditions, and initial conditions for the whole domain including boundary nodes.

The porosity is calculated from the initial conditions assigned to each node and then interpolated to the elements for each time step. → That is why the correct solid/liquid ratio has to be chosen in the GEMS records. Eventually an inert solid has to be defined in order to get the correct porosity.





No

Disadvantage: The user needs some knowledge on the syntax.

Advantage: It runs on HPC computers (parallel version) and can be run in the background for several month if necessary (linux version of course :-)

To create an OGS-GEMS setup from scratch you either

- Copy a benchmark example

- Create a “normal setup” for Groundwater_flow and Mass_transport with the “normal” OGS (-GUI) version.

The following slides explain how you need to modify an existing set of input files.

We assume that we have a correct mesh and that all geometric objects we need for initial and boundary conditions are already defined in the GLI input file (ending .gli).

Normally we have to edit the following files:

Process definitions (ending .pcs)
Component properties (ending .mcp)
Material properties (ending . mmp)
Intial conditions (ending .ic)
Boundary conditions (ending .bc)
Output format (ending .out)
Time stepping (ending .tim)
OGS-GEMS specific settings (ending .gem)

Process definitions (ending .pcs)

We need first one definition for the Groundwater_flow process and N definitions for (mobile) mass transport processes

N is the number of independent components (size of the so called B vector in GEMS) including charge

If one has created file templates with GEMS2GRSF one could look up the number in the .out or .mcp file. The transported independent components are numbered in their name and the last one is always the charge zzz.

```
GeoSys-PCS: Processes ------------------------------------------------
#PROCESS
 $PCS_TYPE
 GROUNDWATER_FLOW
 $NUM_TYPE
   NEW
 $ELEMENT_MATRIX_OUTPUT
  0
 $RELOAD
  1 100   ; write restart file every 100th timestep

#PROCESS  ;1
 $PCS_TYPE
  MASS_TRANSPORT
 $NUM_TYPE
   NEW
 $ELEMENT_MATRIX_OUTPUT
  0
 $RELOAD
  1 100  ; write restart file every 100th timestep

#PROCESS    ;8
 $PCS_TYPE
  MASS_TRANSPORT
 $NUM_TYPE
   NEW
 $ELEMENT_MATRIX_OUTPUT
  0
 $RELOAD
  1 100  ; write restart file every 100th timestep

#STOP
```

Groundwater flow process

First transport process

Here are some entries missing

Last transport process

```
GeoSys-PCS: Processes ------------------------------------------------
#PROCESS
 $PCS_TYPE
 GROUNDWATER_FLOW
 $NUM_TYPE
   NEW
 $ELEMENT_MATRIX_OUTPUT
  0
 $RELOAD
  1 100   ; write restart file every 100th timestep

#PROCESS  ;1
 $PCS_TYPE
  MASS_TRANSPORT
 $NUM_TYPE
   NEW
 $ELEMENT_MATRIX_OUTPUT
  0
 $RELOAD
  1 100  ; write restart file every 100th timestep
```

Option to write restart files, good for long calculations and if you need to start a simulations with specific spatially heterogeneous distributions.

0 no restart files
1 100 ; (over) write restart file every 100 time steps
2 100 ; read restart file at the beginning
3 250 ; read restart file at the beginning and (over) write restart file every 250 time steps

Problem: Restart files do not include time information. Simplest solution is to synchronize VTK output with writing of the restart file (e.g. give out VTK and restart files every 100 time steps).

Component properties (ending .mcp)

Simply replace the old (or insert into) the old .mcp file with the template from GEMS2GSRF.

```
#COMPONENT_PROPERTIES ; comp1
 $NAME
  1-C
 $MOBILE
  1;  MOBILE-Flag: 0=imMOBILEe, 1=MOBILEe/transported
 $DIFFUSION
  1  1.0e-10

#COMPONENT_PROPERTIES ; comp2
 $NAME
  2-Ca
 $MOBILE
  1;  MOBILE-Flag: 0=imMOBILEe, 1=MOBILEe/transported
 $DIFFUSION
  1  1.0e-10



#COMPONENT_PROPERTIES ; comp8
 $NAME
  8-Zz
 $MOBILE
  1;  MOBILE-Flag: 0=imMOBILEe, 1=MOBILEe/transported
 $DIFFUSION
  1  1.0e-10

#STOP
```

Each transport process gets a component definition.

If you would like to calculate diffusive transport in media with variable porosity you should replace the default diffusion law by

9 1.0e-9 2.0

Diffusion following Archie's law
Pore diffusion coefficient
Exponent

Setting the exponent to 1.0 is identical to the default diffusion law.

```
#COMPONENT_PROPERTIES ; comp1
 $NAME
  1-C
 $MOBILE
  1;  MOBILE-Flag: 0=imMOBILEe, 1=MOBILEe/transported
 $DIFFUSION
  1  1.0e-10

#COMPONENT_PROPERTIES ; comp2
 $NAME
  2-Ca
 $MOBILE
  1;  MOBILE-Flag: 0=imMOBILEe, 1=MOBILEe/transported
 $DIFFUSION
  1  1.0e-10



#COMPONENT_PROPERTIES ; comp8
 $NAME
  8-Zz
 $MOBILE
  1;  MOBILE-Flag: 0=imMOBILEe, 1=MOBILEe/transported
 $DIFFUSION
  1  1.0e-10

#STOP
```

If you would like to calculate diffusive transport in media with variable porosity you should replace the default diffusion law by law no. 9.
Setting the exponent to 1.0 (9 1.0e-9 1.0) is identical to the default diffusion law (1 1.0e-9)

except that the calculation of effective Diffusion coefficients is based on harmonic mean (instead of arithmetic averaging) between neighboring nodes.

Medium properties (.mmp)

```
GeoSys-MMP  Material Medium Properties ----------------------------------
#MEDIUM_PROPERTIES
 $GEOMETRY_DIMENSION
  1
 $GEOMETRY_AREA
  1.000000e+000
 $POROSITY
  15  0.32
 $TORTUOSITY
  1   1.000000e+000
 $PERMEABILITY_TENSOR
  ISOTROPIC  1.15700e-6
 $MASS_DISPERSION
  1  0.0067  0.00067
 $DENSITY
  1  1800.0
 #STOP
```

Make sure this is 15 for all material definitions. Important, otherwise transport might be calculated with wrong porosities.

Boundary definitions (.bc)

For each different boundary condition you should create a GEMS record, export it to GEMS2GSRF and save the .bc template.

Concentration BC are normally given in mol/m^3 of the total dissolved independent component. If you convert the GEMS record with GEMS2GSRF this is correctly done.

```
GeoSys-BC: Boundary Conditions
------------------------------------------
#BOUNDARY_CONDITION
 $PCS_TYPE
  GROUNDWATER_FLOW
 $PRIMARY_VARIABLE
  HEAD
 $GEO_TYPE
  POINT POINT1
 $DIS_TYPE
  CONSTANT 10.0     ; this is at least 1 Bar

#BOUNDARY_CONDITION
 $PCS_TYPE
  MASS_TRANSPORT
 $PRIMARY_VARIABLE
  1-C
 $GEO_TYPE
  POINT POINT0
 $DIS_TYPE
  CONSTANT  9.97048719427360e-06
```

For the flow boundary set at least a reference pressure of 10 m water head (which is ~ 1 Bar)

Insert templates from GEMS2GSRF and adjust the GEO_TYPE according to the definitions in the .gli file.

```
GeoSys-BC: Boundary Conditions
------------------------------------------------

#POINTS
0  0.0   0.0 0.0 0.0 0.0 0.0 0.0 $NAME POINT0
1  0.5  0.0 0.0 0.0 0.0 0.0 0.0 $NAME POINT1
2  .25   0        0


#POLYLINE
 $NAME
  OUT_LINE
 $EPSILON
  1.0e-4
 $POINTS
  0
  1
#STOP
```

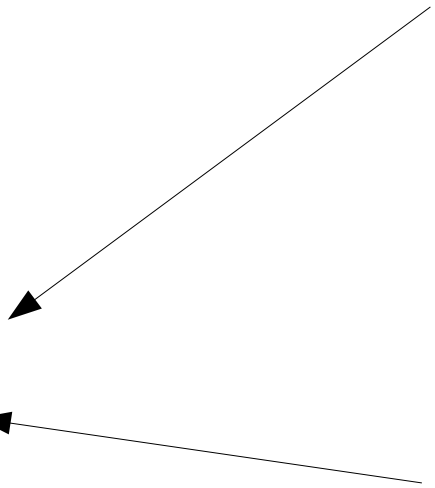
```
GeoSys-IC  Initial Conditions
-------------------------------------------------
#INITIAL_CONDITION
 $PCS_TYPE
  GROUNDWATER_FLOW
 $PRIMARY_VARIABLE
  HEAD
 $GEO_TYPE
  DOMAIN
 $DIS_TYPE
  CONSTANT 0.0

#INITIAL_CONDITION
 $PCS_TYPE
  MASS_TRANSPORT
 $PRIMARY_VARIABLE
  1-C
 $GEO_TYPE
  DOMAIN
 $DIS_TYPE
  CONSTANT  1.15377792658303e-01

#INITIAL_CONDITION
 $PCS_TYPE
  MASS_TRANSPORT
 $PRIMARY_VARIABLE
  2-Ca
 $GEO_TYPE
  POINT POINT0
 $DIS_TYPE
  CONSTANT  1.15377792658303e-01
```

For each part of the domain – including boundaries – add the corresponding sniplets from the GEMS2GSRF initial conditions and adjust the GEO_TYPE definition.
Later entries overwrite earlier ones!
Possible GEO_TYPES:
DOMAIN
POINT *name*
POLYLINE *name*
SURFACE *name*
VOLUME *name*

For the .out file simply replace the existing file with the GEMS2GSRF version and adjust for which time-steps you need for post processing.

In the .tim file make sure that the time step size is small enough to obey the Courant- and Neumann-criteria for advective and diffusive transport, respectively.

```
#OUTPUT
 $NOD_VALUES
  1-C
  2-Ca
  3-Cl
  4-H
  5-Mg
  6-O
  7-Sn
  8-Zz
 $ELE_VALUES
  POROSITY
 $GEO_TYPE
  DOMAIN
 $DAT_TYPE
  VTK
 $TIM_TYPE
   STEPS 10
#STOP
```



Only VTK format is supported with full output of the chemical system!

Output every X time steps. Adjust X to match the output of restart files (or vice versa).

VTK output contains:
Concentrations of dissolved independent components (normally in mol/m3 of liquid)

Total mole amounts of the independent components (normally per m^3) → can be used to investigate a specific node more closely with GEM-SELEKTOR v3.

Mole amount of the dependent components (dissolved species, gases, solids...normally per m^3)

Some other geochemical properties (pH, eh, pe...)

Node volumes, node porosity, volume changes ..

The .gem file is only needed for the OGS-GEMS version and contains some specific settings for the coupled version:

```
OpenGeoSys-GEMS definitions ----------------------------------
#GEM_PROPERTIES
  $GEM_INIT_FILE
    BC-dat.lst    ; only file name, no path
  $FLAG_POROSITY_CHANGE
    1    ; 0-not coupled;1=coupled;
  $MIN_POROSITY
    1.e-10
  $MAX_POROSITY
    1.0
  $FLAG_COUPLING_HYDROLOGY
    1    ; 0-not coupled;1=coupled;
  $TEMPERATURE_GEM
    298.15       ; temperature for GEMS in degree Celsius
  $TRANSPORT_B
     1 ; 1: do transport of b vector
#STOP
```

Choose here one of the records exported from GEMS ...the four files should be in the same directory as the OGS-GEMS input files

```
OpenGeoSys-GEMS definitions ----------------------------------------
#GEM_PROPERTIES
  $GEM_INIT_FILE
    BC-dat.lst    ; only file name, no path
  $FLAG_POROSITY_CHANGE
    1    ; 0-not coupled;1=coupled;
  $MIN_POROSITY
    1.e-10
  $MAX_POROSITY
    1.0
  $FLAG_COUPLING_HYDROLOGY
    1    ; 0-not coupled;1=coupled;
  $TEMPERATURE_GEM
    298.15        ; temperature for GEMS in degree Celsius
  $TRANSPORT_B
     1 ; 1: do transport of b vector
#STOP
```

Porosity changes according to precipitation/dissolution of solids.

Porosity of zero will kill the transport/flow solver!

If porosity changes the fluid volume is adjusted via source/sinks in the flow solver.

Set here the default temperature for GEMS...pressure is taken from flow solver!

Possible problems if the GEMS kernel does not work:

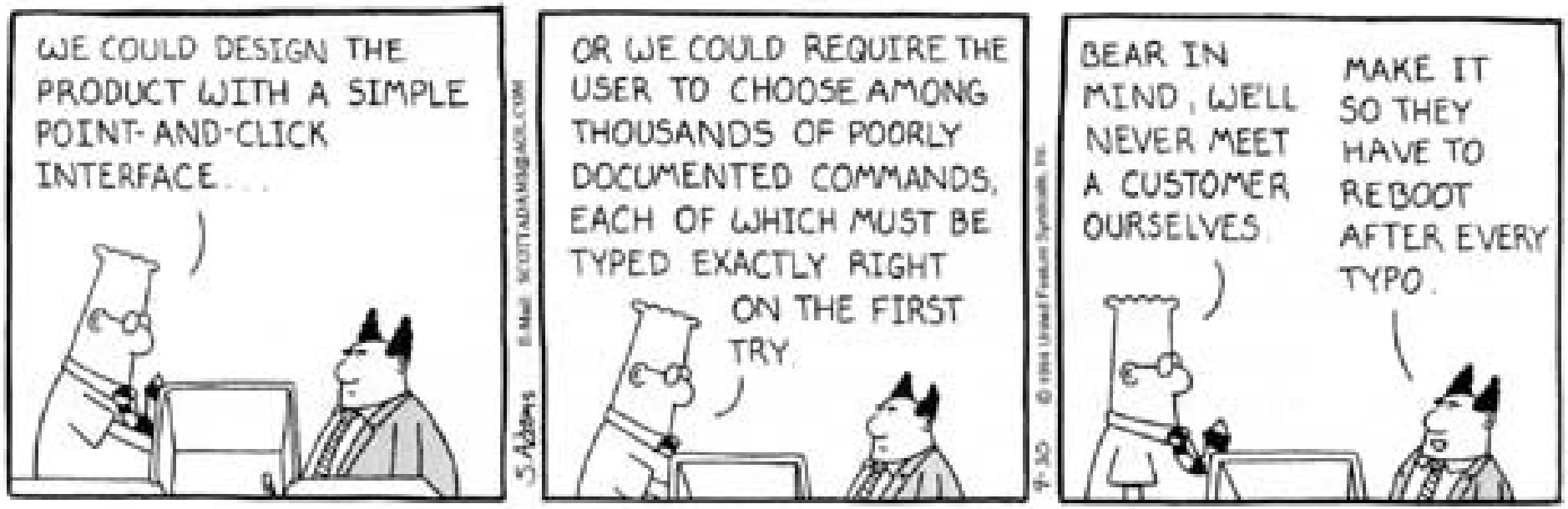
During initialization:

- Wrong GEM configuration file name in .gem file
- Mistake in .ic (or .bc) definitions
  - pressure of GROUNDWATER_FLOW (water head) is outside the range defined in the GEMS setup → (GEMS failed see ipmlog.txt)
  - temperature in .gems does not match the temperature of the GEMS setup

After initialization

- Oscillations in transport solver (concentrations) → adjust time stepping and or check GEMS setup for redox buffer
- Problems in the numerical settings of GEMS ...contact the GEMS mailing list!

Thanks to Dimitrii Kulik for the excellent work on improving GEMS-PSI and to Haibing Shao and the OGS-community for the OGS-GEMS coupling.


WE COULD DESIGN THE PRODUCT WITH A SIMPLE POINT-AND-CLICK INTERFACE...
OR WE COULD REQUIRE THE USER TO CHOOSE AMONG THOUSANDS OF POORLY DOCUMENTED COMMANDS, EACH OF WHICH MUST BE TYPED EXACTLY RIGHT ON THE FIRST TRY.
BEAR IN MIND, WE'LL NEVER MEET A CUSTOMER OURSELVES.
MAKE IT SO THEY HAVE TO REBOOT AFTER EVERY TYPO.