MUFITS
Training Course

Day 4

BINMIXT module; LGR; Onshore/offshore; Crossflow

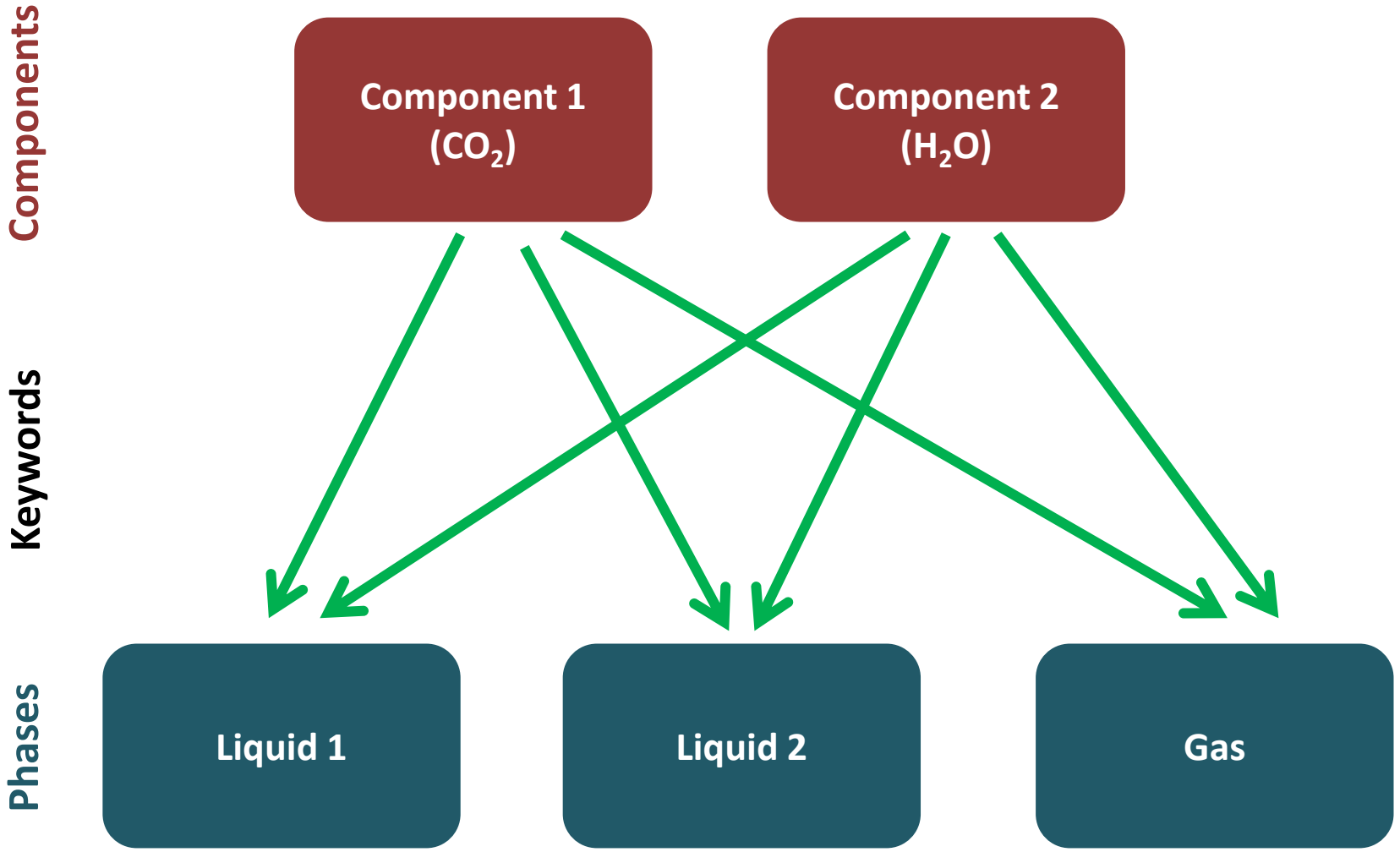
Program

- BINMIXT module
- Local grid refinements (LGRs)
- Boundary conditions at Earth surface (onshore/offshore)
- Crossflow

BINMIXT module

EOS module BINMIXT

T≠const



Options vs. EOS modules

	SIMPLMOD	T2EOS1	BINMIXT	BLACKOIL	GASSTORE
CAPPRES	Yes	No	No	Yes	Yes
HCROCK	Yes	Yes	Yes	No	Yes
HCFLUID	No	Yes	No	No	No
ISOTHERM	Yes	Yes	No	No	Yes
ADDPHASE	Yes	Not tested	Yes	Not tested	Not tested
EQL-ENDEQL (initial equilibration)	No	No	No	Yes	Yes
EOSNUM regions	Yes	No	No	Yes	No

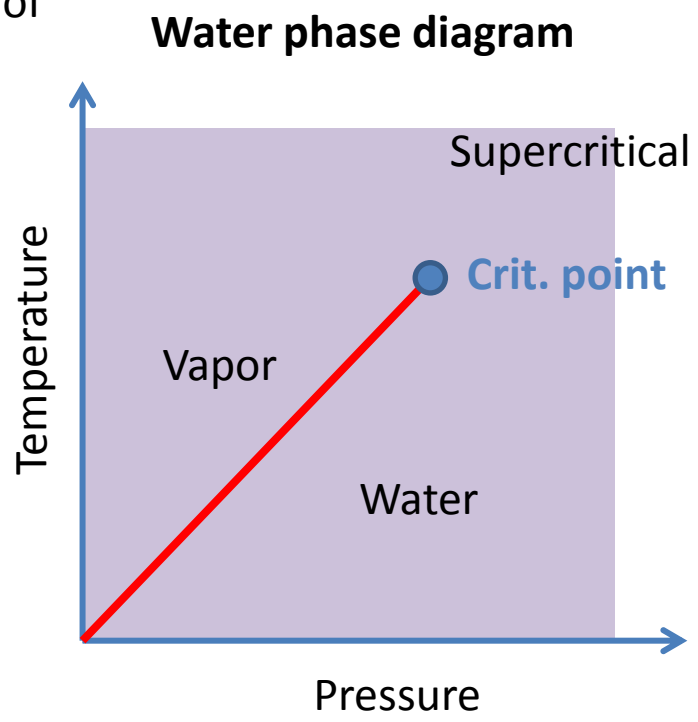
EOS module description

BINMIXT module is designed for nonisothermal modelling of multiphase flows of binary mixture in a wide range of pressures and temperatures and under near critical thermodynamic conditions.

The module is capable of modelling three-phase flows of binary mixture.

BINMIXT is the default module of the simulator.

This courses covers application of the module for CO_2-H_2O flows. The available range of pressures is <0.01 bars to >1500 bars. The available range of temperatures is 0 °C to >900 °C.



Primary variables

For robust hydrodynamic simulations in the vicinity of critical conditions, a non-classic variables must be used: pressure-enthalpy-composition.

classic approach

P, T, x

pressure, temperature, composition

"Flash" calculation (evaluation of thermodynamic equilibrium). Cubic equation of state is used

Only 1- and 2-phase states of the mixture:

liquid (H_2O) | **gas** ($sc.CO_2$)

possible phases

the proposed approach

P, h, x

pressure, enthalpy, composition

A generalization of classic "flash" calculation

1-, 2- and **3-phase** states of the mixture:

liquid (H_2O) | **liquid** ($l.CO_2$) | **gas** ($g.CO_2$)

possible phases

Mathematical model

Balance equation

$$\frac{\partial}{\partial t}\left(m\sum_{i=1}^{3}\frac{M_{(j)}x_{i(j)}}{v_i}s_i \right) + \qquad \text{- mass conserv.}$$

$$+\operatorname{div}\left(\sum_{i=1}^{3}\frac{M_{(j)}x_{i(j)}}{v_i}\mathbf{w}_i \right) = 0, \quad j = 1,2$$

$$\frac{\partial}{\partial t}\left(m\sum_{i=1}^{3}\frac{e_i}{v_i}s_i + (1-m)\frac{e_s}{v_s} \right) + \qquad \text{- energy conserv.}$$

$$+\operatorname{div}\left(\sum_{i=1}^{3}\frac{h_i}{v_i}\mathbf{w}_i - \lambda\mathbf{grad}T \right) = 0$$

$$\mathbf{w}_i = -K\frac{f_i}{\mu_i}\left(\mathbf{grad}P - \frac{M_i}{v_i}\mathbf{g} \right) \qquad \text{- Darcy correlation}$$

Equations are in molar variables

+

Equations for prediction

$$\sigma_t = \sum_{i=1}^{3}\sigma_i V_i \to \max,$$

$$\sigma_i = \sigma\left(P, h_i, x_i\right), \qquad \sum_{i=1}^{3} V_i = 1$$

$$\sum_{i=1}^{3} h_i V_i = h_t, \qquad \sum_{i=1}^{3} x_i V_i = x_t$$

$$0 \le V_i \le 1$$

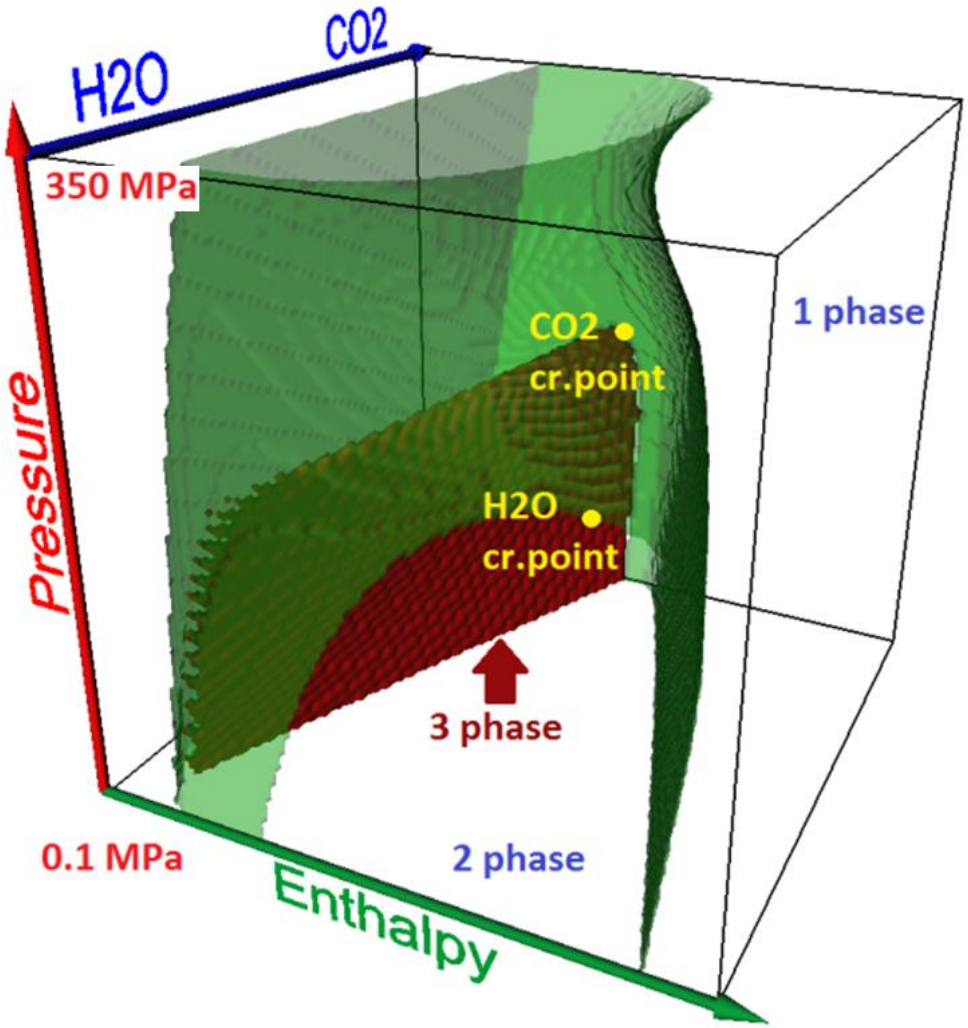
$j = 1$ – CO_2

$j = 2$ – H_2O

P – pressure, h – enthalpy

x – composition, σ – entropy

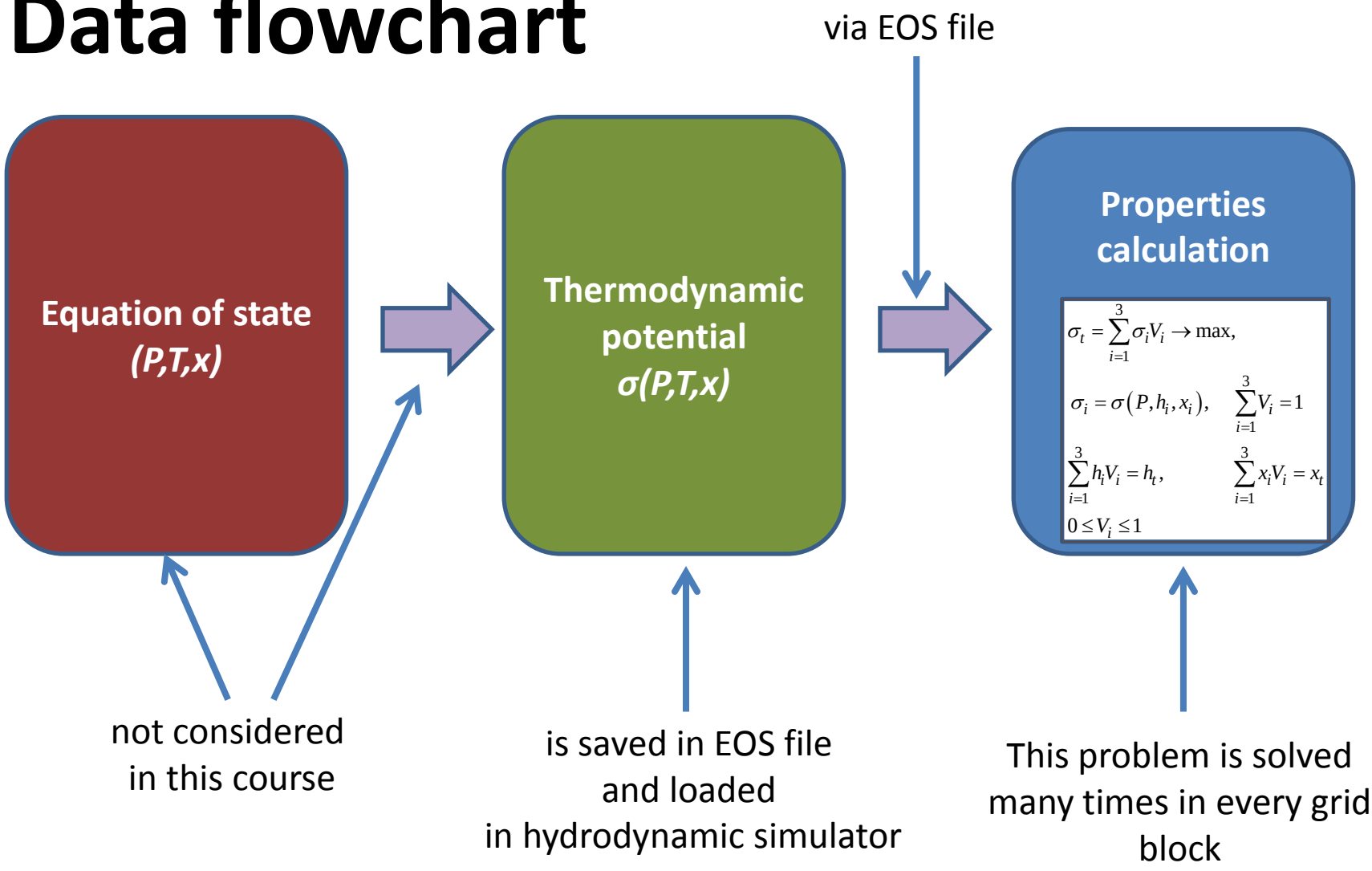
CO_2-H_2O phase diagram



Phase diagram in pressure-enthalpy-composition variables

Outside green surface - single-phase states, inside green and outside red surface – two-phase states, inside red surface – three-phase states.

Data flowchart



LOADEOS keyword

The EOS-file contains the thermodynamic potential of the mixture which was calculated in advance. The file should be copied in INCLUDE folder. The file must be loaded by the **LOADEOS** keyword in **PROPS** section.

LOADEOS syntax

```
1 -- in PROPS section
2
3 LOADEOS
4    filename /
5
6 ================================================================================
7
8    filename - name of EOS file.
```

Additional mnemonics

Mnemonic	Description
ENTHT	Total molar enthalpy (kJ/mol)
COMP1T	Total molar fraction of the 1st component (CO_2)
COMP2T	Total molar fraction of the 2nd component (H_2O)
SGASINIT	Initial gas saturation
SLIQINIT	Initial liquid saturation

Initial conditions

Initial conditions options:

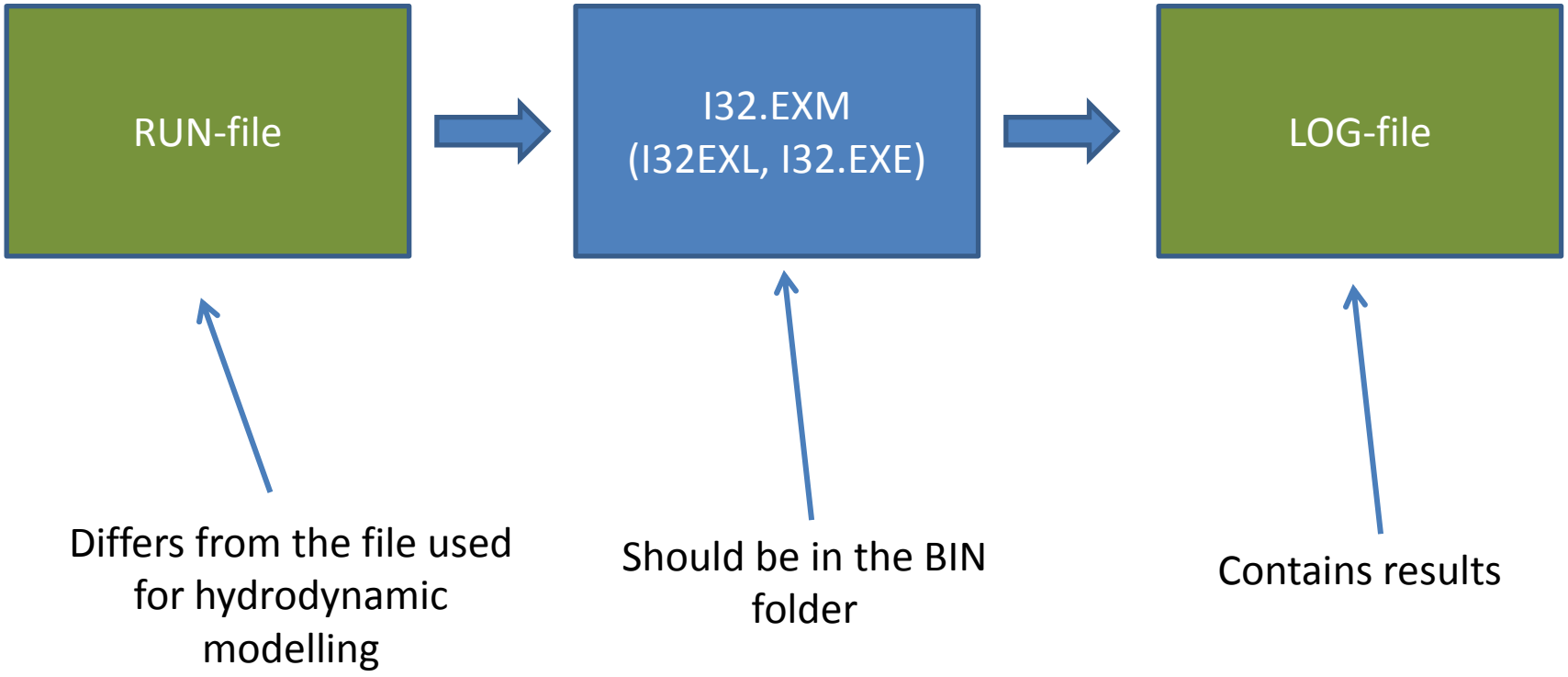
a) Pressure (PRES), Temperature (TEMP or TEMPC), Composition (COMP1T or COMP2T) [priority 1];

b) Pressure (PRES), Enthalpy (ENTHT), Composition (COMP1T or COMP2T) [priority 2].

For two-phase states defined by a) and b) the saturations of phases can be redefined by the SLIQINIT and SGASINIT mnemonics. Note, that in this case, the total enthalpy (ENTHT) and total compositions (COMP1T or COMP2T) are altered to satisfy the conditions for saturation, however the thermophysical properties of each phase (density, viscosity, etc.) are not altered.

PVT program

PVT-program allows to calculate properties of the binary mixture for a given parameters (e.g., pressure, temperature, etc.). The calculation reports are outputted in LOG-file.



Properties for a given P and T

The properties for a given pressure, temperature and composition can be calculated by the **PHEQPTX** keyword.

PHEQPTX syntax

```
PHEQPTX
  pres1  temp1  comp1t1 comp2t1 /
  pres2  temp2  comp1t2 comp2t2 /
  pres3  temp3  comp1t3 comp2t3 /
  ...
/

================================================================================

  pres#   - pressure;
  temp#   - temperature (degrees of Kelvin);
  comp1t# - total molar fraction of the 1st component;
  comp2t# - total molar fraction of the 2nd component.
```

PVT program (exercise)

Exercise: Calculate thermodynamic equilibriums for :

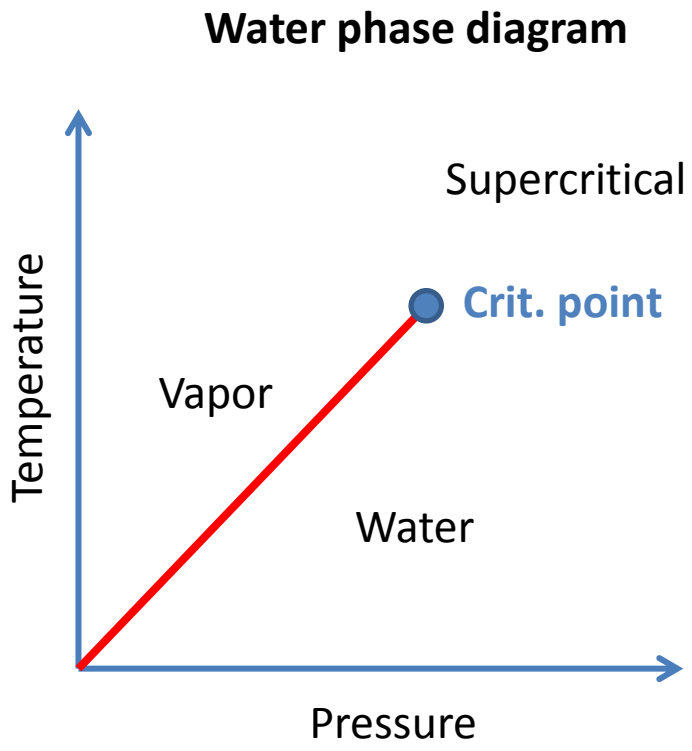
1) PRES=10MPa, TEMPC=100C, COMP1T=0
2) PRES=10MPa, TEMPC=200C, COMP1T=0.7

1. **Open RUN-file in text editor**
2. **Run the simulation**
3. **Open LOG-file to see results**

PHASES keyword

When moving around the critical point in the phase diagram there is no strict boundary between liquid phase and gaseous phase.

The PHASES keyword defines characteristic parameters of phases which can be used to output from hydrodynamic simulation the phases saturations, phases densities, viscosities etc.



PHASES keyword

PHASES syntax

```
-- in PROPS section

PHASES
   name1  pres1  entht1  comp1t1  comp2t1 /
   name2  pres2  entht2  comp1t2  comp2t2 /
   name3  pres3  entht3  comp1t3  comp2t3 /
   ...
/

================================================================================

   name#   - phase name (4-byte character);
   pres#   - pressure;
   entht#  - total molar enthalpy;
   comp1t# - total molar fraction of the 1st component;
   comp2t# - total molar fraction of the 2nd component.
```

Note, that the enthalpy for a phase definition can be calculated for a given temperature using PVT program.

The recommended parameters of phases (for H_2O subcritical conditions) are

- H_2O-rich phase: PRES= 1 MPa, ENTHT=5 kJ/mol, COMP1T=0
- CO_2-rich phase: PRES= 10 MPa, ENTHT=10 kJ/mol, COMP1T=1

PHASES keyword

The PHASES keyword creates the following mnemonics:

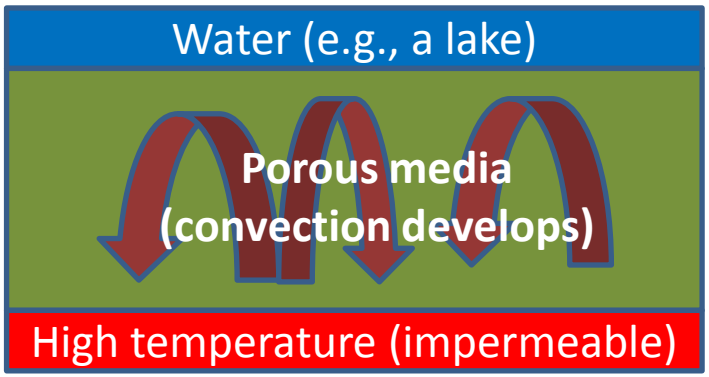
Mnemonic	Description
SAT#name	Saturation
DEN#name	Density
VIS#name	Viscosity
…	See Reference manual

Here, ‘name’ is the phase name defined by the PHASES keyword.

Scenario 10

Scenario 10

interpretation

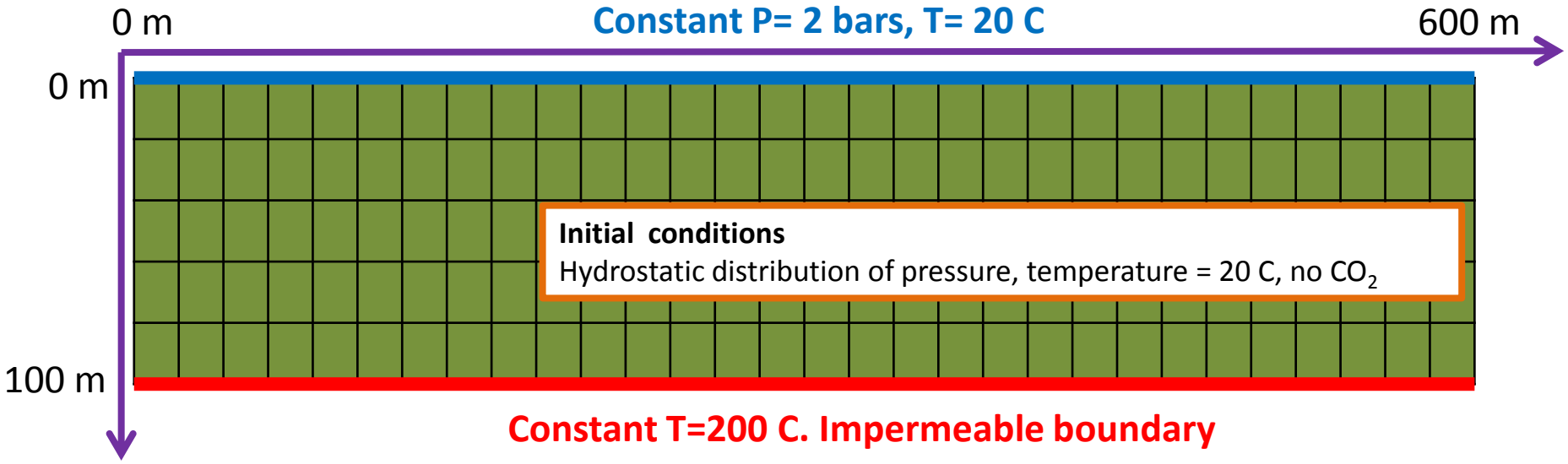


Simulate scenario up to 100000 days reporting distributions every 1000 days

Grid: 30*5. EOS-module: BINMIXT

Rock properties:
Porosity = 0.25;
Permeability = 100 mD ;
Rock density = 2900 kg/m^3;
Heat capacity = 0.84 kJ/kg/K;
Heat conduct. = 2 W/m/K.

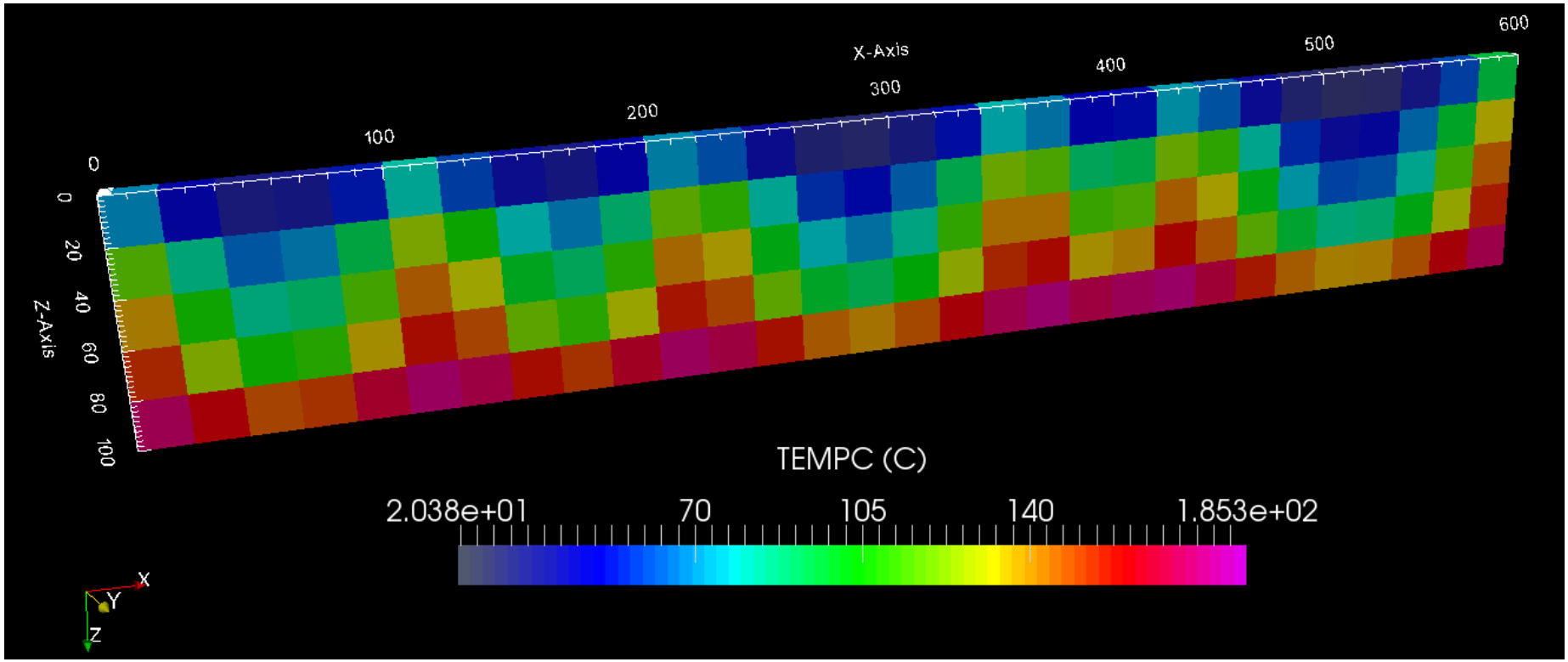
Rel. perm:
Brooks & Corey, smin =0.2
smax =0.95



RUN-file (scenario 10)

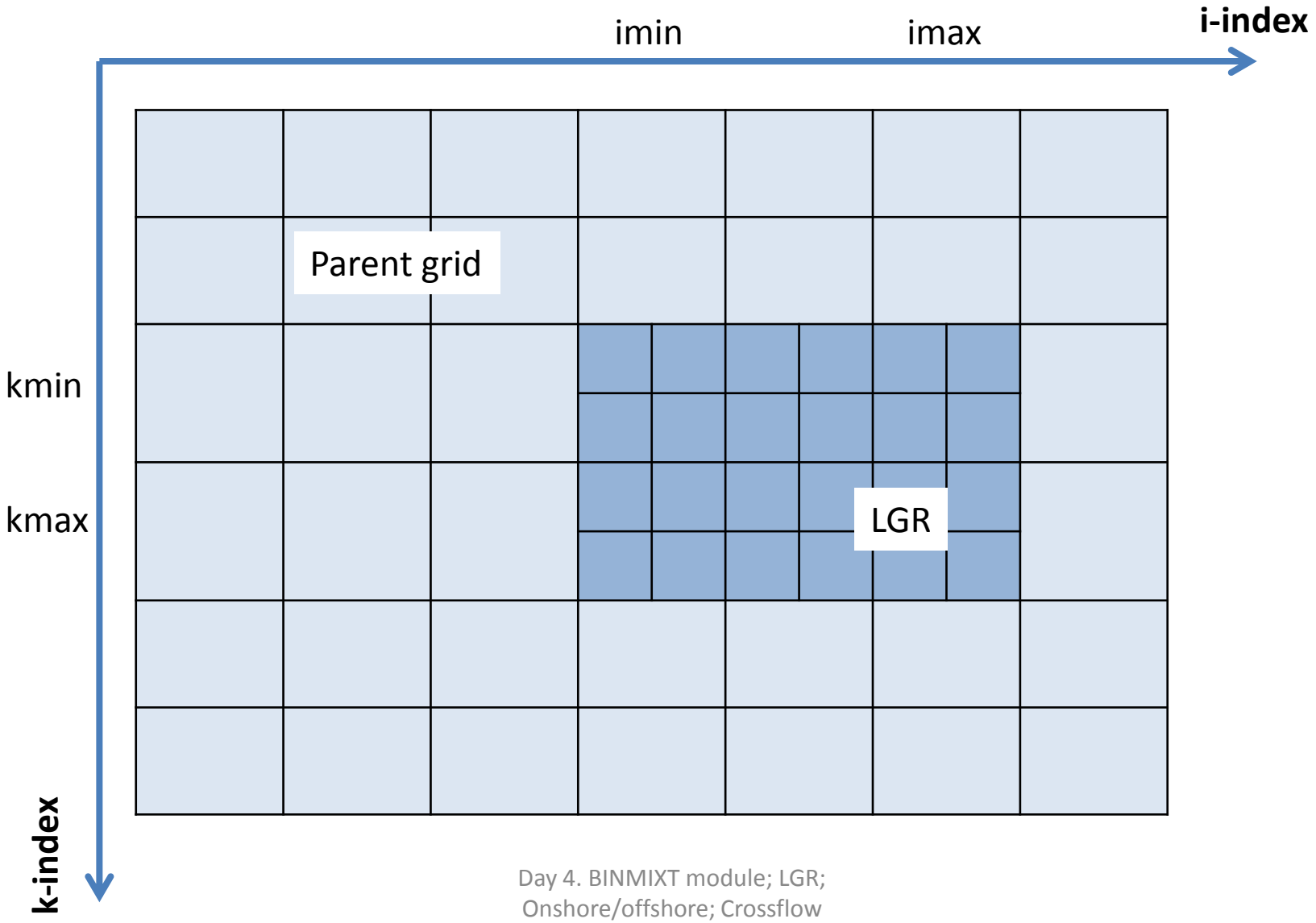
1. Open RUN-file in text editor
2. Run the simulation
3. Open results in ParaView

Result (scenario 10)



Local grid refinements (LGRs)

Local grid refinements



CARFIN keyword

The **CARFIN** keyword defines local grid refinements

CARFIN syntax

```
-- within MAKE-ENDMAKE brackets

CARFIN
  name  imin imax  jmin jmax  kmin kmax  nx ny nz  parent /

================================================================================

     name      - name of the refined grid;
     imin/imax - the boundaries of the refined grid along i-index direction
                 in the parent grid;
     jmin/jmax - the boundaries of the refined grid along j-index direction
                 in the parent grid;
     kmin/kmax - the boundaries of the refined grid along j-index direction
                 in the parent grid;
     nx        - the number of grid blocks in the refined grid along i-index
                 direction;
     ny        - the number of grid blocks in the refined grid along j-index
                 direction;
     nz        - the number of grid blocks in the refined grid along k-index
                 direction;
     parent    - the parent grid name.

```

REFINE & ENDFIN keywords

Keyword **REFINE** selects a grid to be active. It affects the **BOX** keyword and arrays loading. After the keyword **CARFIN** the created grid is active.

REFINE syntax

```
1 -- in every section except RUNSPEC and POST
2
3 REFINE
4    gridname  resname /
5
6 ================================================================================
7
8     gridname - grid name (8-byte character);
9     resname  - the name of reservoir in which the grid is defined.
```

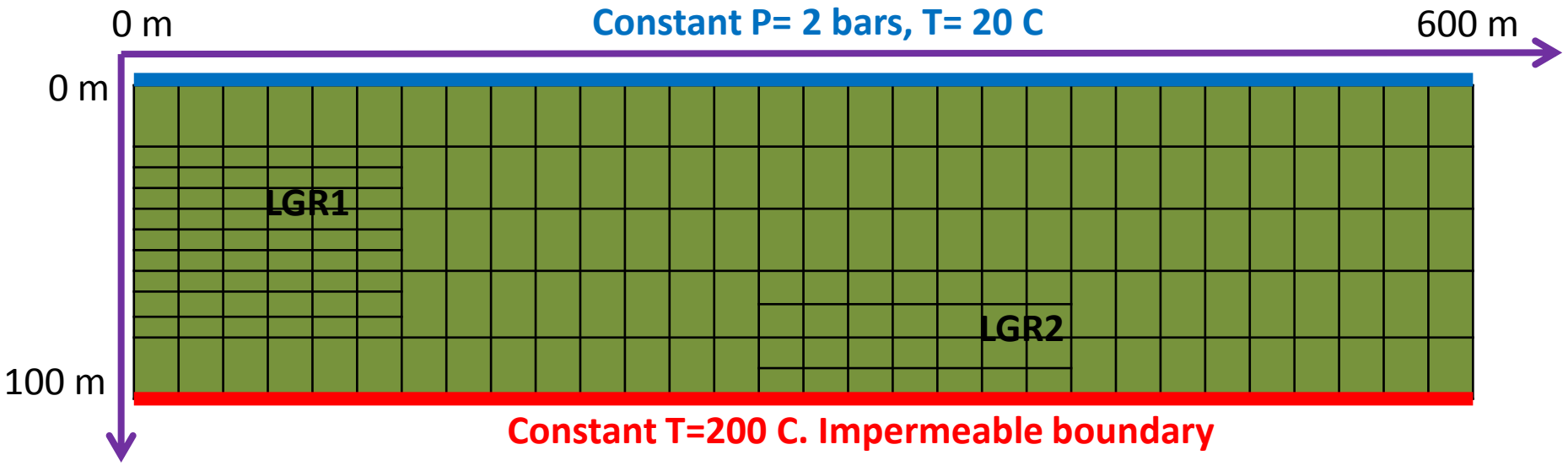
Keyword **ENDFIN** resumes the active grid to the initial grid encompassing the whole reservoir

ENDFIN syntax

```
1 -- in every section except RUNSPEC and POST
2
3 ENDFIN
```

Local grid refinements

Exercise: Re-simulate scenario 10 using the following grid.



Answer

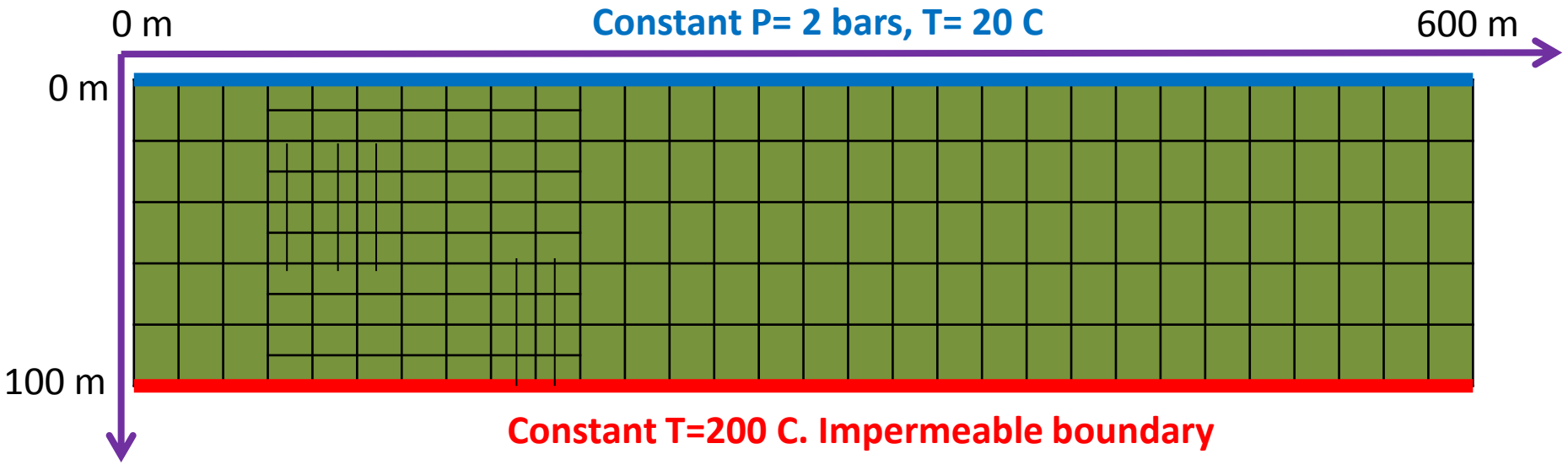
Day 4. Answer

```
-- within MAKE-ENDMAKE brackets

CARFIN
  LGR1   1  6  1 1  2 4     6  1  9 /
CARFIN
  LGR2  15 21  1 1  4 5     7  1  4 /
ENDFIN
```

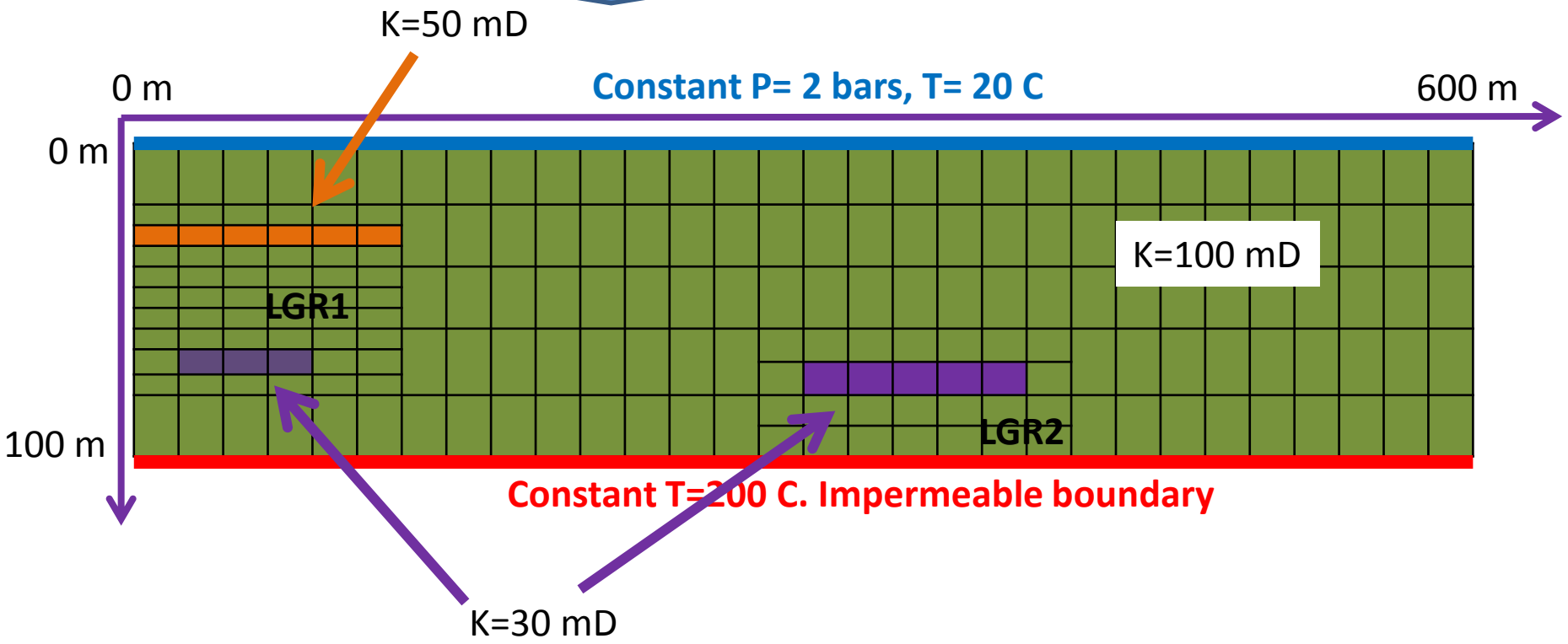
Nested LGRs

Exercise: Re-simulate scenario 10 using the following grid.



LGRs; Arrays loading

Exercise: Re-simulate scenario 10 using the following permeability distribution.



LGRs; Arrays loading (answer)

Day 4. Answer

```
-- in GRID section

ENDFIN
EQUALS
   PERMX 100 /
/
REFINE
  LGR1 /
EQUALS
   PERMX 50   4*       2*2 /
   PERMX 30   2 4 2*   2*8 /
/
REFINE
  LGR2 /
EQUALS
   PERMX  30  2 6 2*   2*2 /
/
ENDFIN
COPY
  PERMX PERMZ /
/
```

Local grid refinements

Exercise: Re-simulate scenario 10 using twice as more refined grid as the initial grid. Do not change the MAKE keyword.

More complicated LGRs

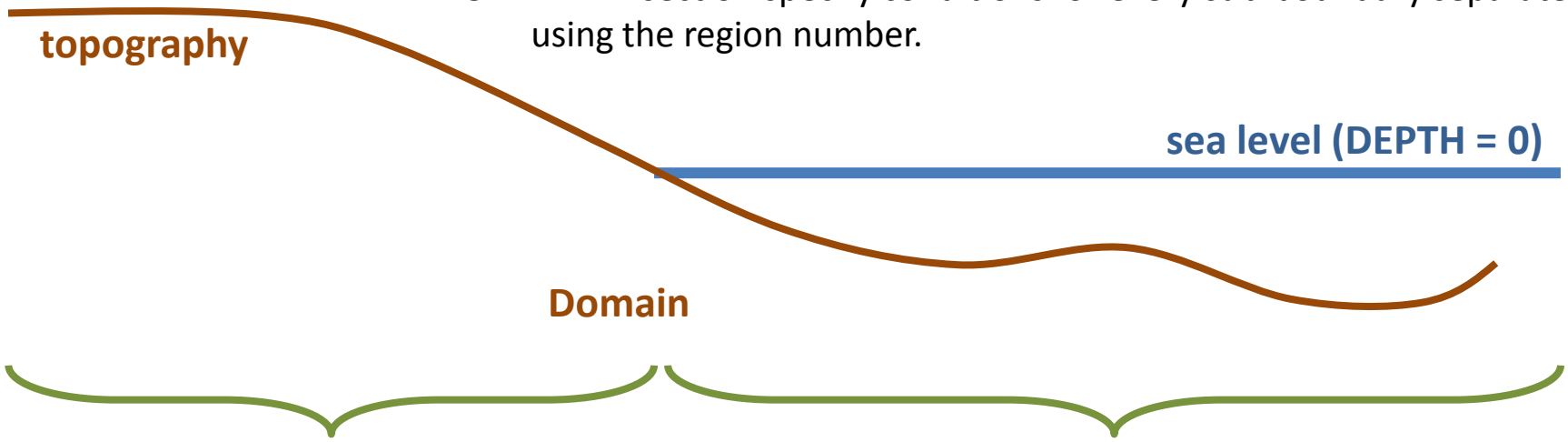
More complicated LGRs can be created using HXFIN, HYFIN, HZFIN, NXFIN, NYFIN, NZFIN keywords (see the Reference manual).

Scenario 11
(Onshore/offshore boundary conditions)

Onshore/offshore conditions

To model the boundary conditions:

1. Create the boundary grid blocks for the top surface of the domain using the BOUNDARY keyword;
2. Divide the boundary into two sub-boundaries (onshore and offshore) using the DEPTH property. Use a region number (e.g., INCONUM) to distinguish the sub-boundaries.
3. In INIT section specify conditions for every sub-boundary separately using the region number.



At the top surface of the domain: air (we use CO_2 instead), P=1 Bar, T=20°C

At the top surface of the domain: water, P = hydrostatic in water, T=20°C (or other value).

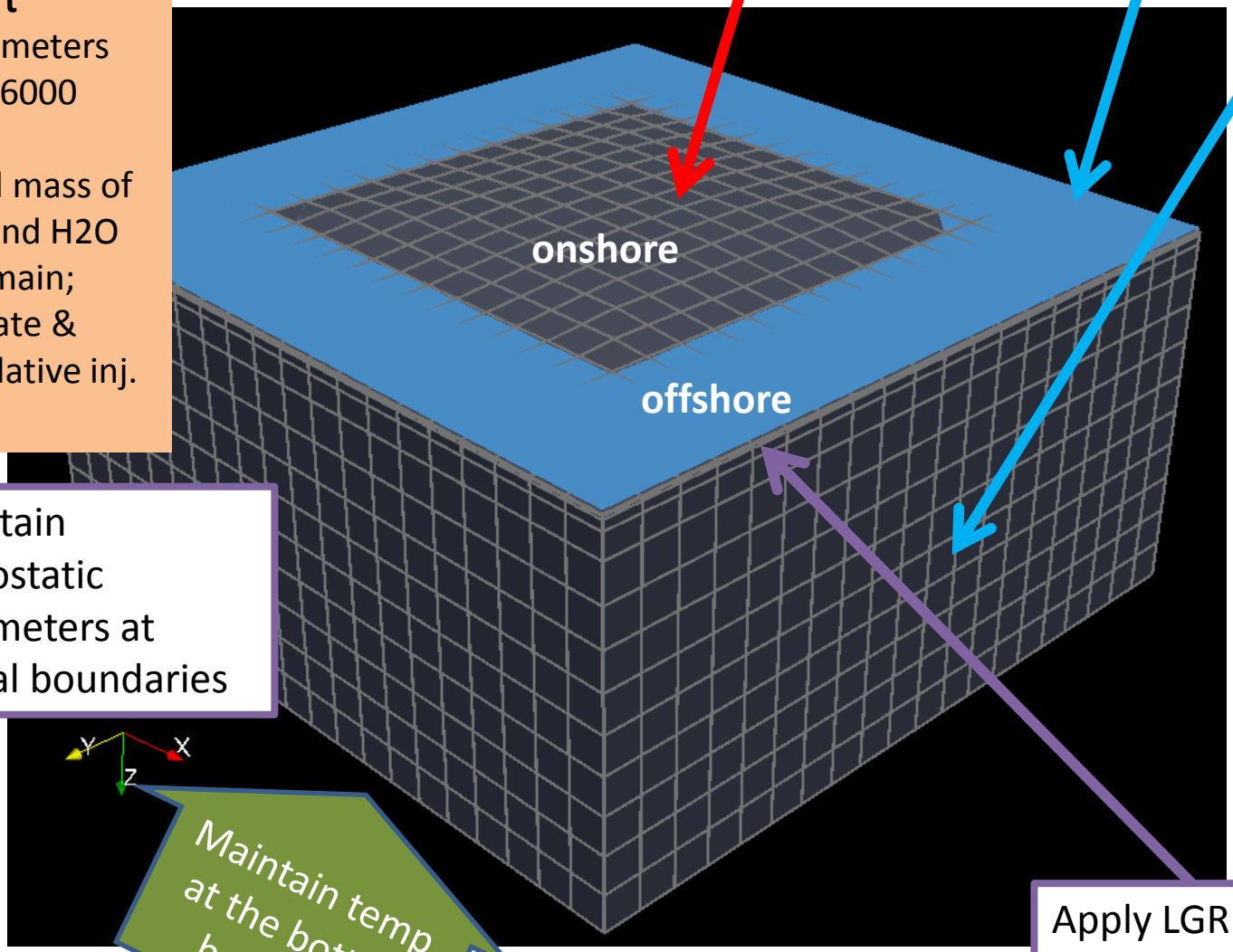
Simulate using 3 (or 2) cores

Scenario 11

"Square" island ☺
P=0.1 Mpa, T=20 C
Pure CO_2

Pressure hydrostatic
Geoth. Grad 2.5 C/100m
Pure water

Report
- parameters up to 6000 days;
- total mass of CO2 and H2O in domain;
- Inj. rate & cumulative inj. rate.



Maintain hydrostatic parameters at lateral boundaries

Maintain temp. at the bottom boundary

Grid file is provided.
Porosity =0.2
X-Perm=20 mD
Z-Perm=10 mD
RockDen=2900 kg/m3
RockHC =1 kJ/kg/K
RockHCcf=2W/m/K
Rel.Perm see in RUN.

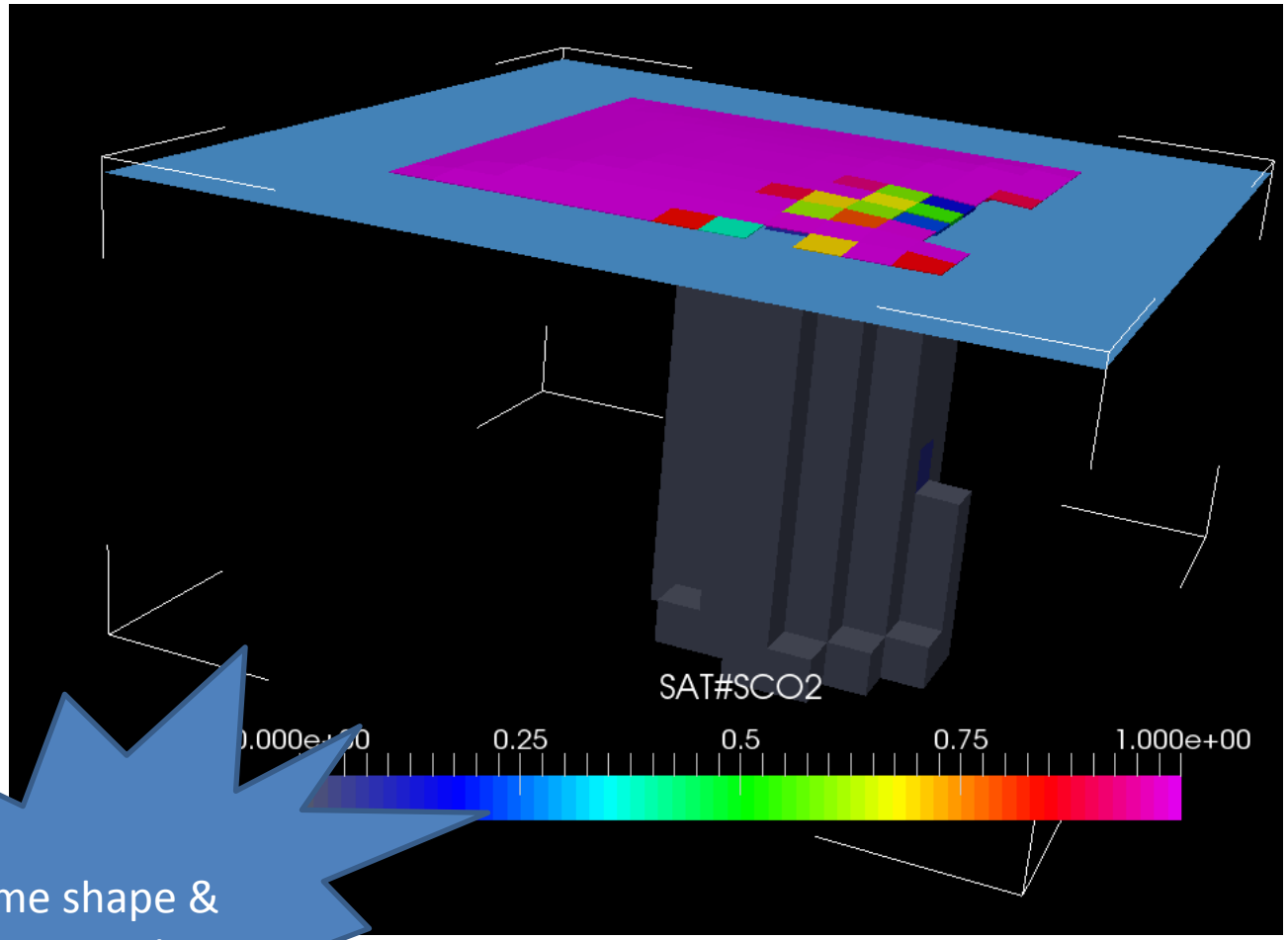
Model influx of hot magmatic fluid in block (13,12,10).
Fluid T=400C at P=10MPa,
CO2 mol. frac.=50%.
Rate= 500 t/day.

Apply LGR near surface

RUN-file (scenario 11)

1. Open RUN-file in text editor
2. Run the simulation
3. Open results in ParaView

Results (scenario 11)

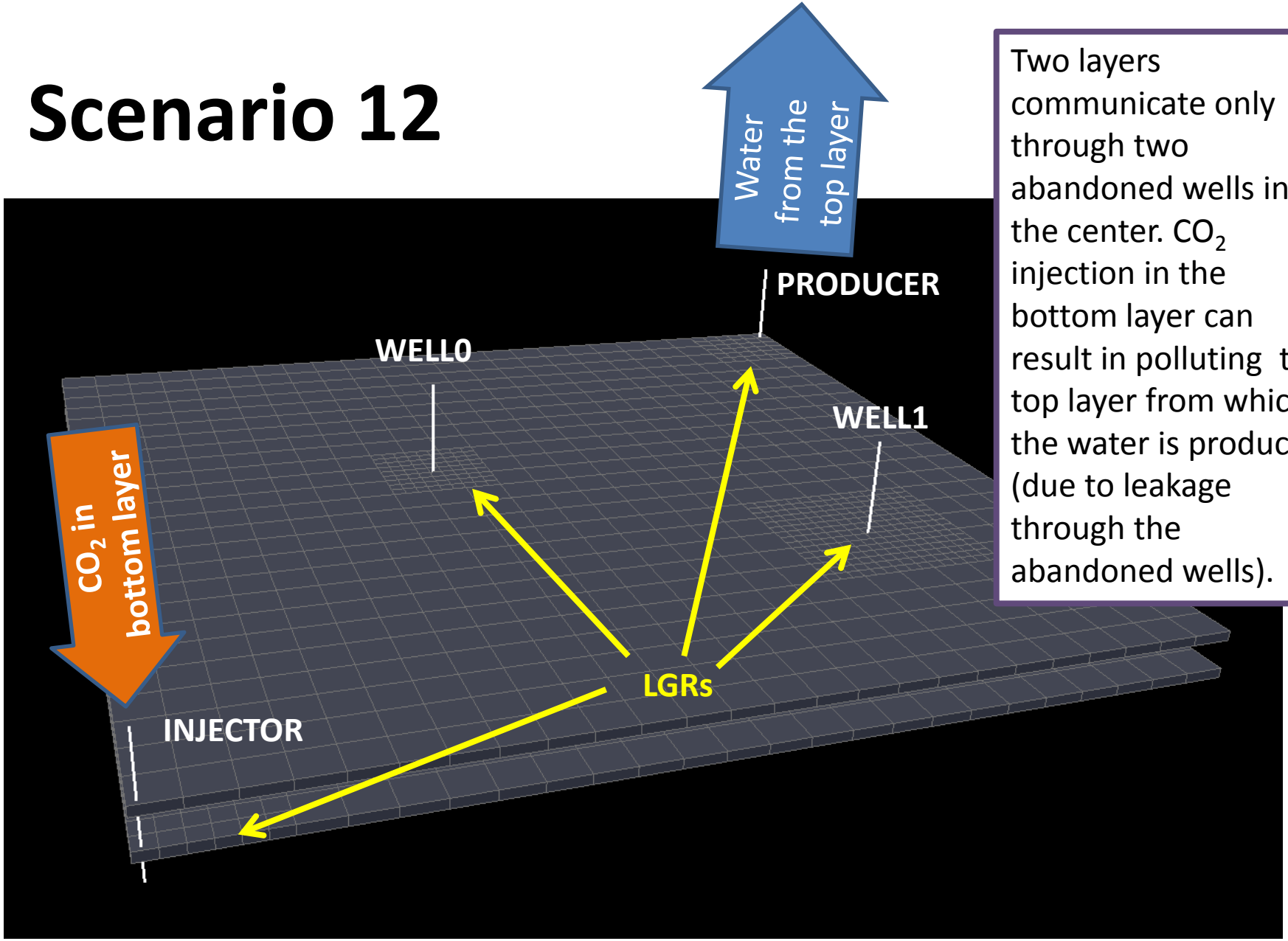


Plume shape & CO_2 saturation

Scenario 12

(simulations with both LGRs and Wells)

Scenario 12

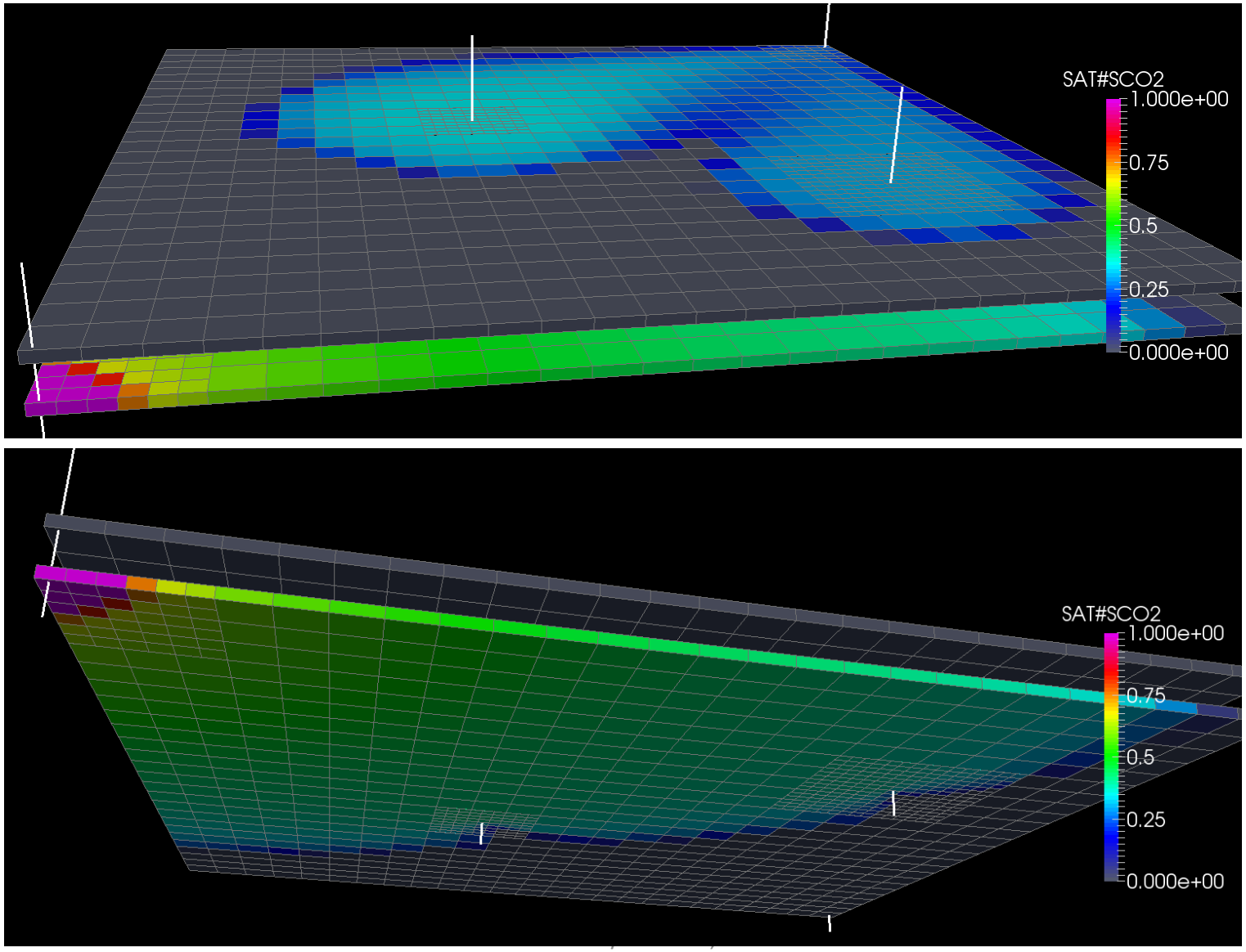


Two layers communicate only through two abandoned wells in the center. CO_2 injection in the bottom layer can result in polluting the top layer from which the water is produced (due to leakage through the abandoned wells).

RUN-file (scenario 12)

1. Open RUN-file in text editor
2. Run the simulation
3. Open results in ParaView

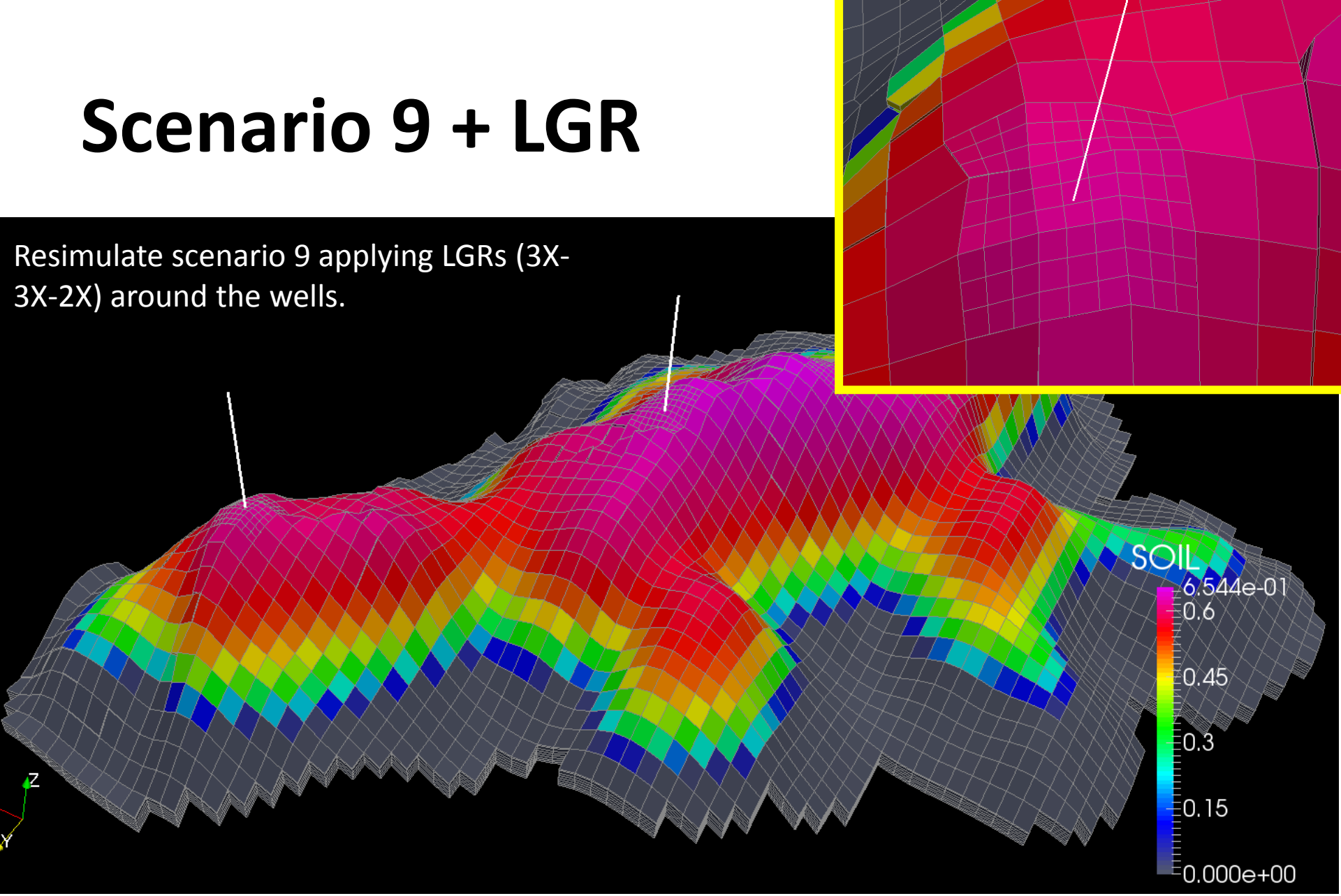
Results (scenario 12)



Back to Scenario 9

Scenario 9 + LGR

Resimulate scenario 9 applying LGRs (3X-3X-2X) around the wells.



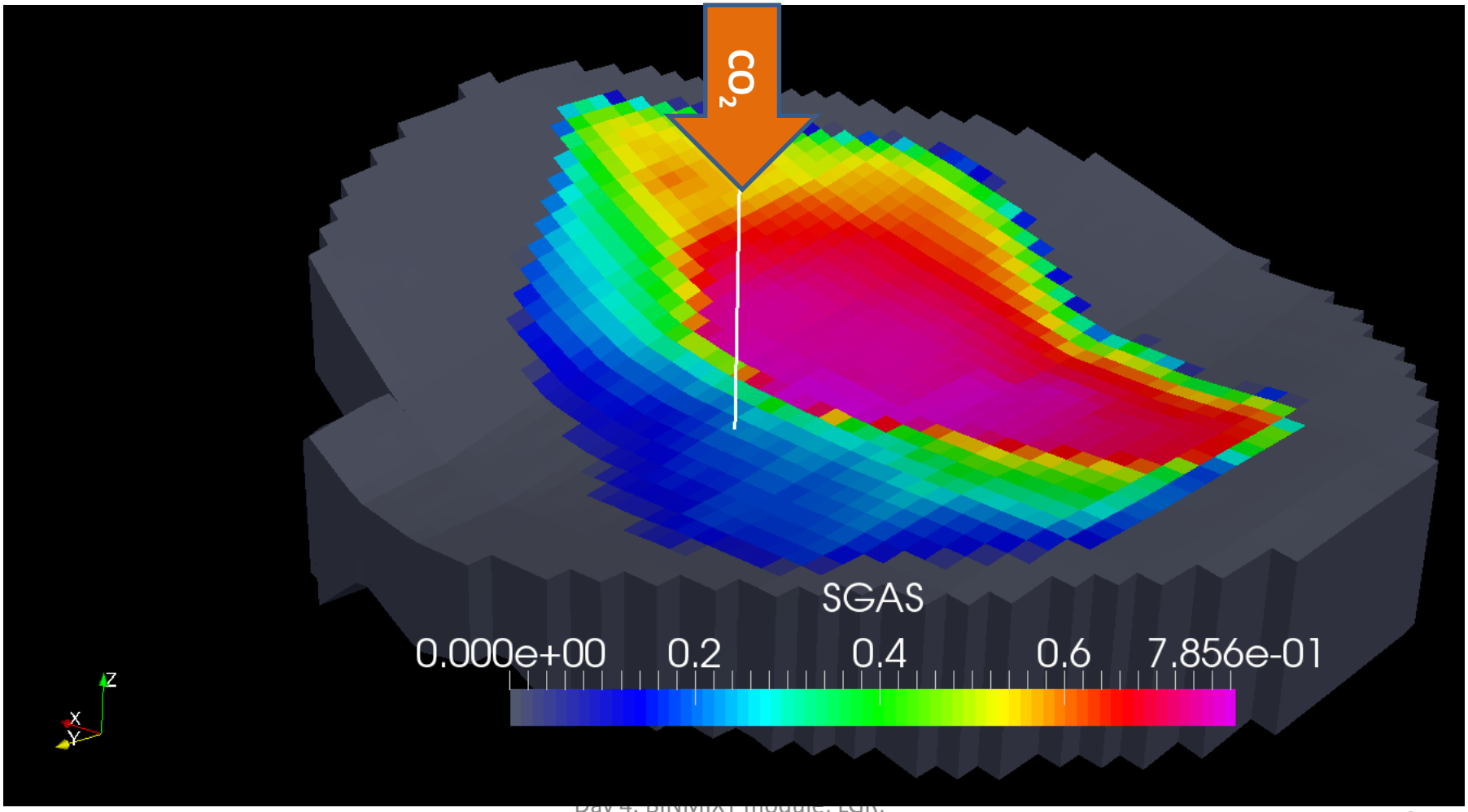
Scenario 9 (LGR)

1. Open RUN-file in text editor
2. Run the simulation
3. Open results in ParaView

Back to Scenario 8

Back to Scenario 8

Resimulate scenario 8 using BINMIXT module:



Scenario 8 (BINMIXT)

1. Open RUN-file in text editor
2. Run the simulation
3. Open results in ParaView

Next day

- A 2D radial problem;
- Recommendations for tuning of the simulator;
- More complicated scenarios with the GASSTORE and BLACKOIL modules