Parametrization Technique for Reactive Multiphase Flow and Transport

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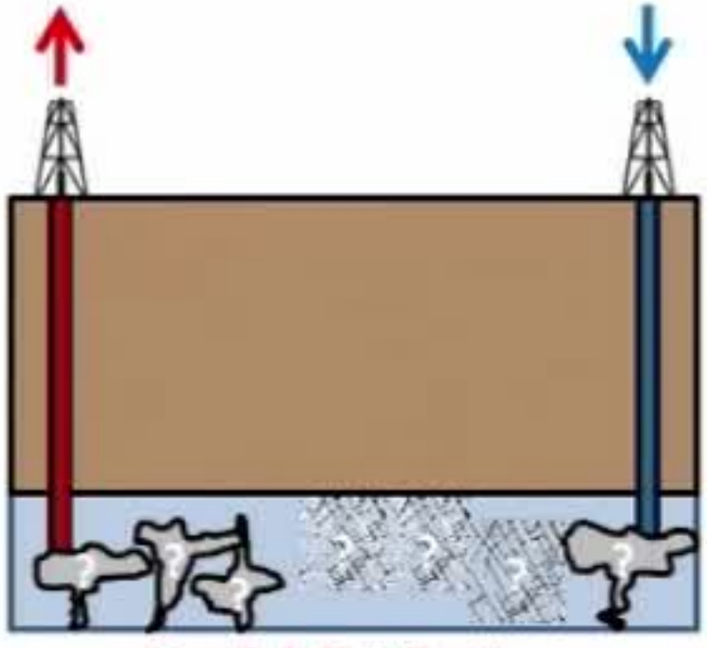
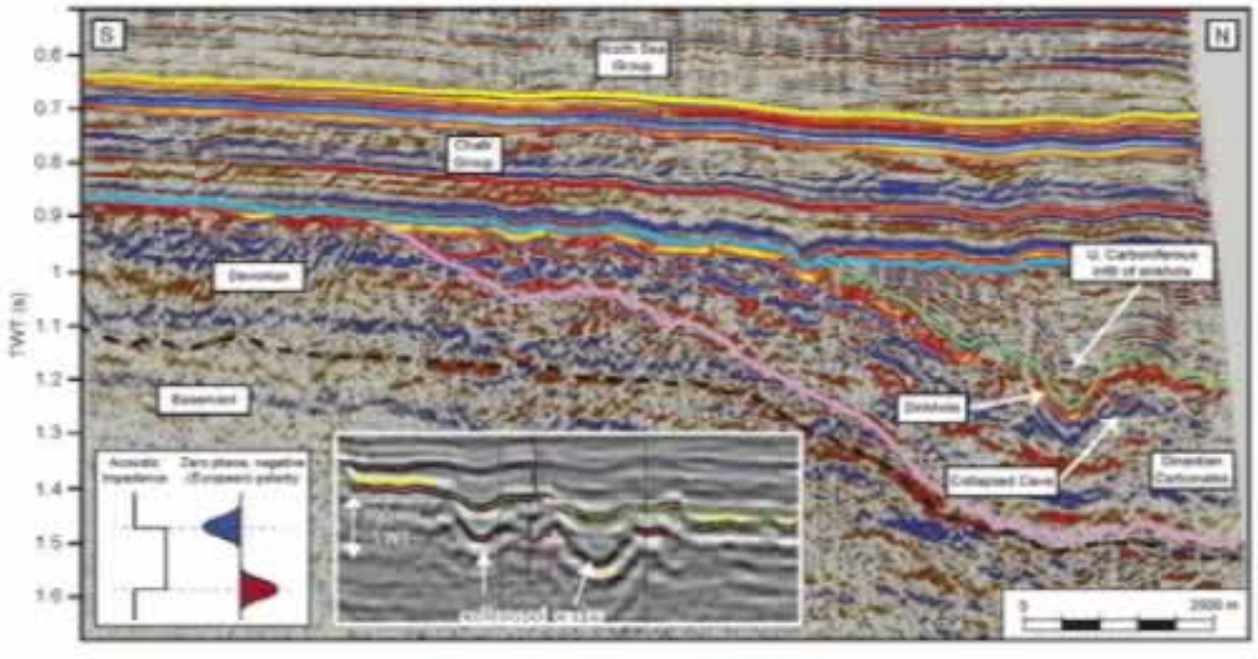
Motivation

- **Hydrocarbon** and **Geothermal** energy potential in (pre-salt) carboniferous carbonates
- Difficult reservoir characterization, large uncertainty in spatial distribution of discontinuity networks → unpredicted hazards



Spatial distribution uncertain!

Heavily fractured and karstified!



Reijmer et al. (2017)

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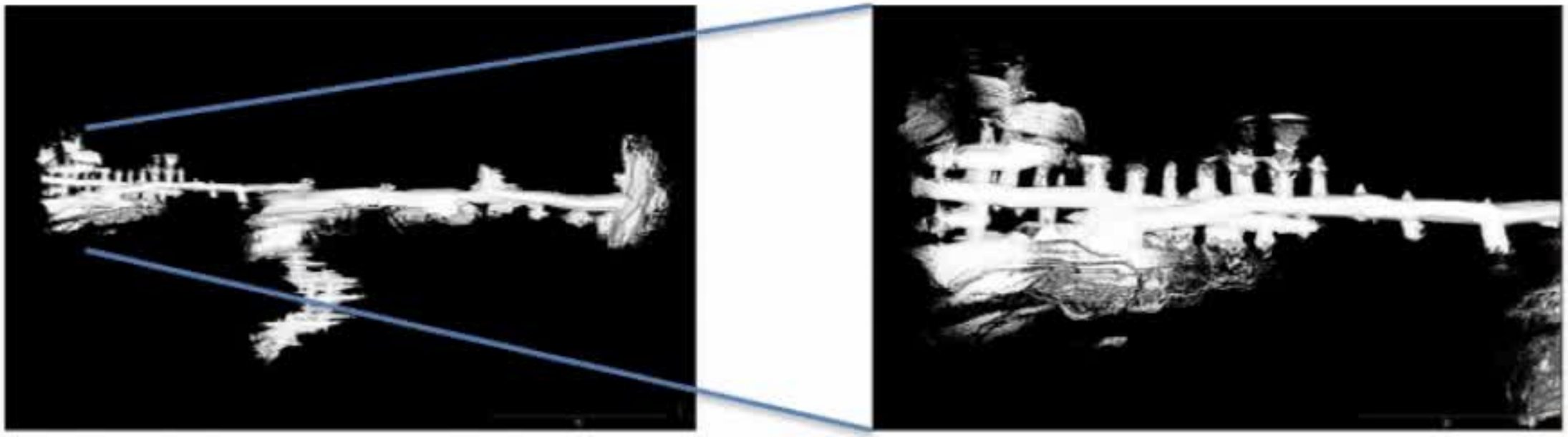
Objective

Reduce risks of subsurface applications by improving the geomodeling workflow of fractured & karstified reservoirs. This requires integration of coupled flow and reactive transport in porous media with outcrop and lab data.

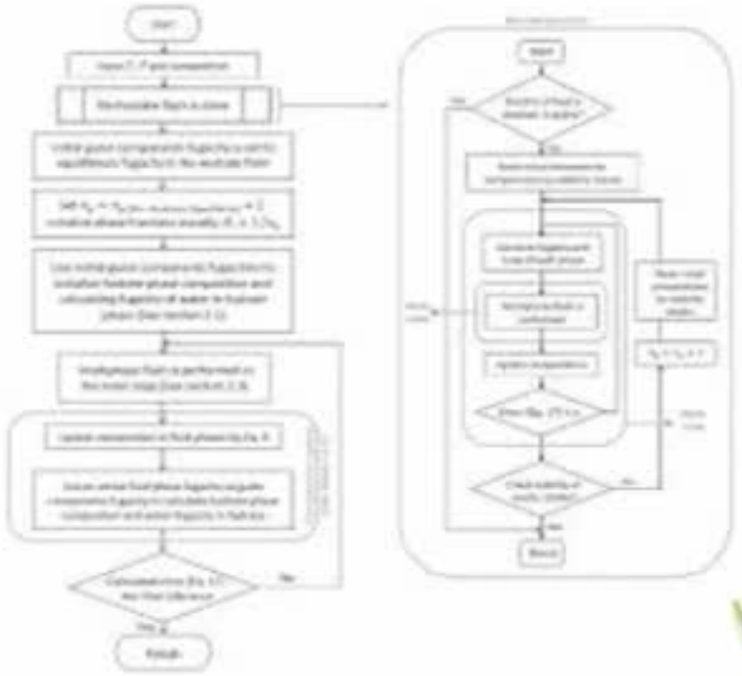


Linearization

- Implementation depends on a
  - nonlinear formulation
  - number of phases and components
  - fluid and rock properties
  - etc…
- Involves huge volumes of code

The most difficult part to design and optimize (especially for new hardware architectures)

Which data involved in simulation?



SGOF

0	0	1	0
0.001	0	1	0
0.02	0	0.997	0
0.05	0.005	0.98	0
0.12	0.025	0.7	0
0.2	0.075	0.35	0
0.25	0.125	0.2	0
0.3	0.19	0.09	0
0.4	0.41	0.021	0
0.45	0.6	0.01	0
0.5	0.72	0.001	0
0.6	0.87	0.0001	0
0.7	0.94	0	0
0.88	0.98	0	0

$$\beta_c(\omega) = \sum_{j=1}^{n_p} x_{cj}^l \rho_j^l \frac{k_{rj}^l}{\mu_j^l}.$$

$$p = \frac{RT}{v-b} - \frac{a}{v(v+b)+b(v-b)}$$

$$\left[(\mu-\mu^0)\,\xi_T + 10^{-4}\right]^{1/4} = a_0 + a_1\rho_{pr} + a_2\rho_{pr}^2 + a_3\rho_{pr}^3 + a_4\rho_{pr}^4$$

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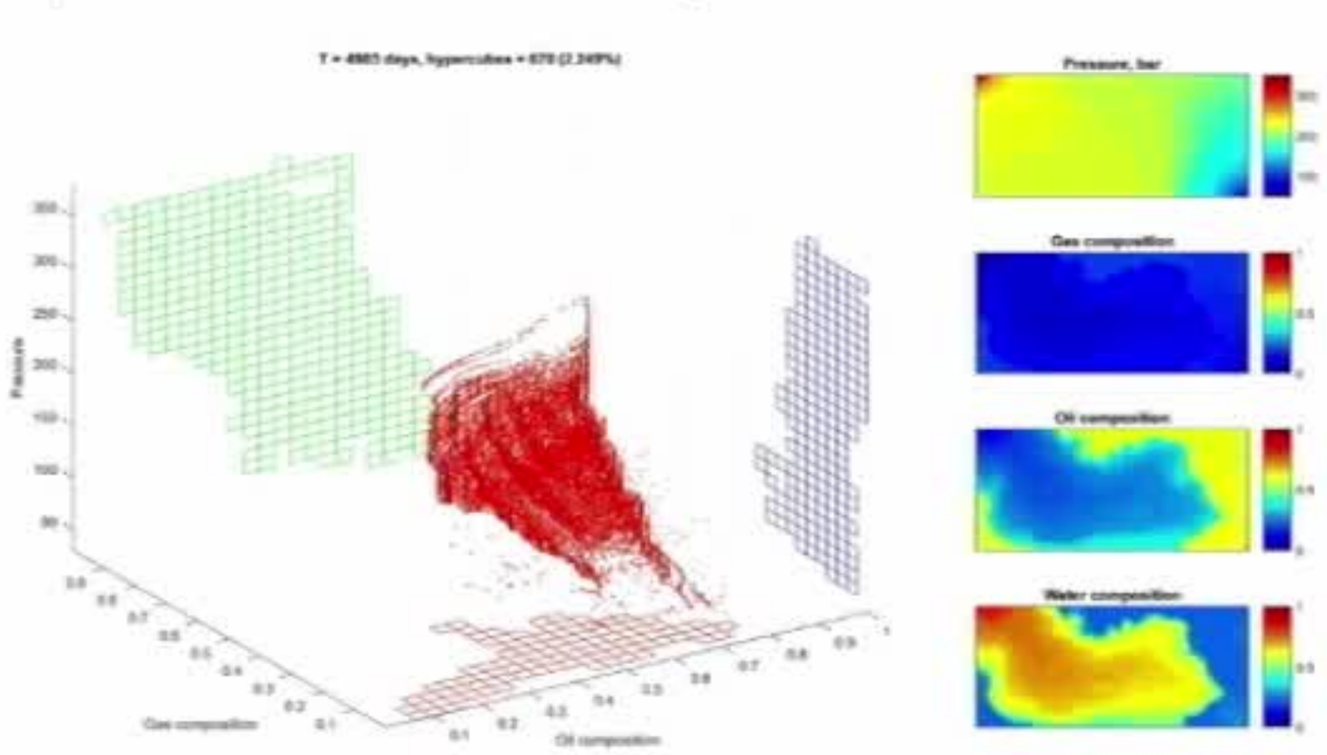
Simulation framework for inversion

Delft Advanced Research Terra Simulator

- Discretization in space, time and **physics** (OBL)
- C++/CUDA implementation of performance-critical kernels + **open-source** Python interfaces
- Validated for various geothermal and petroleum applications
- Adaptive parametrization in space of unknowns



More information at https://darts.citg.tudelft.nl/

Compositional simulation with reactions

Reducing number of mass balance equations:

- Aris and Mahi, 1963: Reaction invariants
- Rubin, 1983: Tenads
- Lichtner, 1985 & 1996: Primary species
- Molins et al., 2004: Components
- Fan et al., 2012: Elements

Multiphase thermal multicomponent reactive transport (Sequential or Fully Implicit schemes):

- TOUGHREACT (Xu et al., 2012)
- PFLOTRAN (Lichtner et al., 2015)
- DUMUX (Flemisch et al., 2011)
- AD-GPRS (Farshidi, 2016)

Equilibrium reactions with OBL

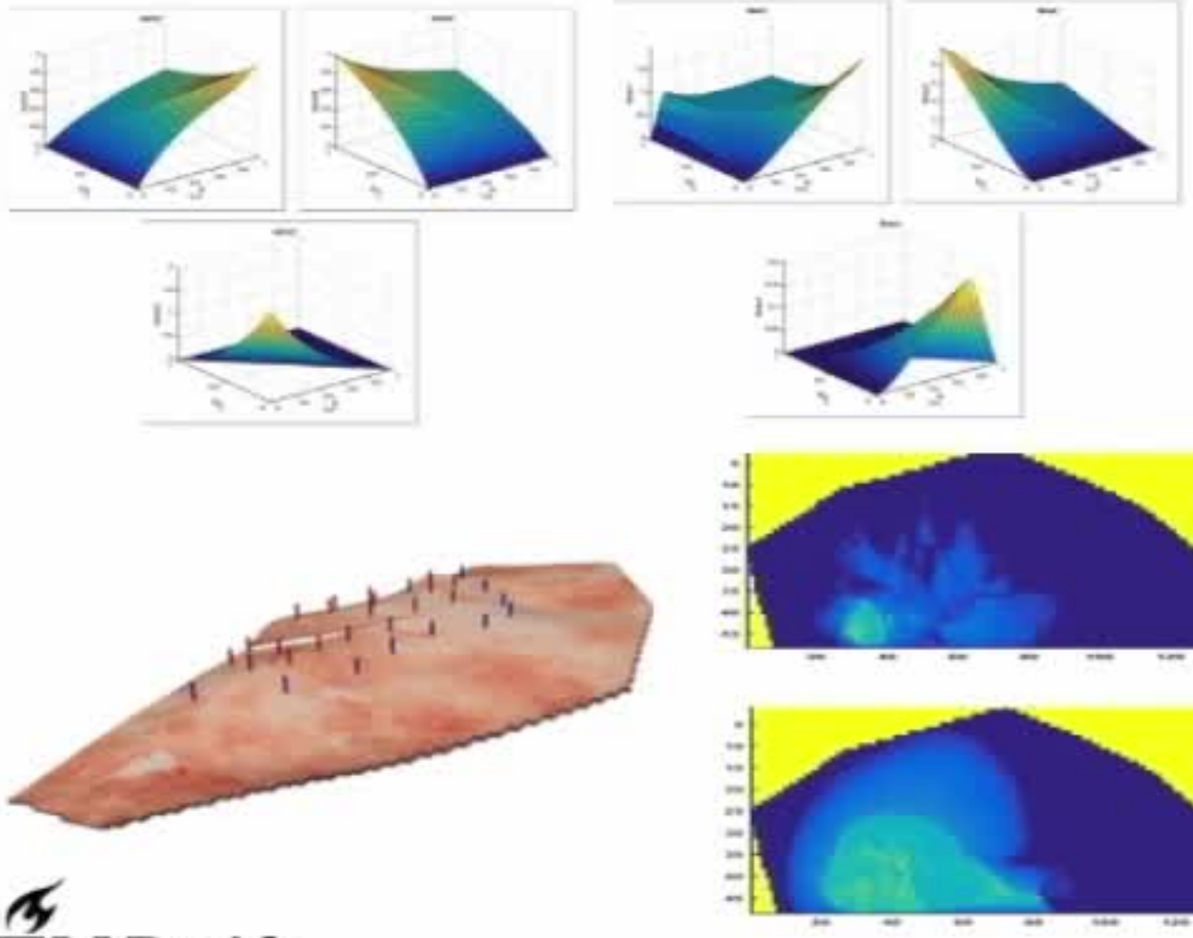
$$\boldsymbol{E}\times\ \frac{\partial}{\partial t}(\phi\rho_t z_c)+\mathrm{div}(l_c)=\sum_{q=1}^{n_q} v_{cq}r_q \quad\Rightarrow\quad \frac{\partial}{\partial t}\left(\phi^T\rho_t^E z_i^E\right)+\mathrm{div}(\boldsymbol{e_i l})=0$$

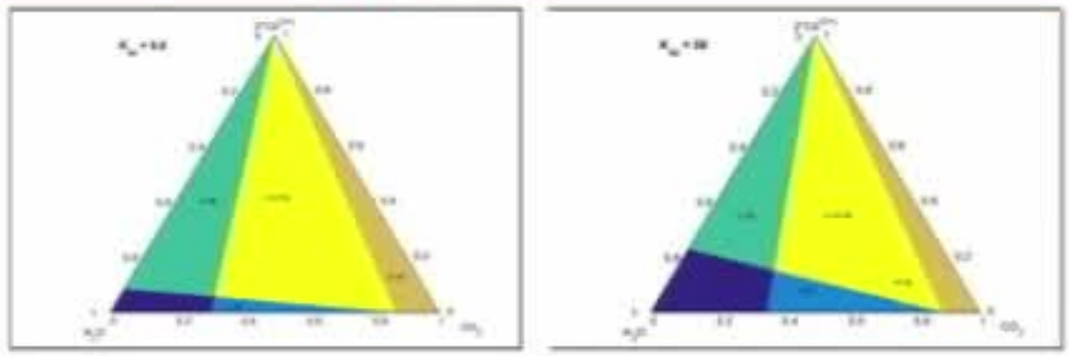
$$\boldsymbol{\omega}=\{p,\boldsymbol{z^E}\}\rightarrow\begin{cases}\alpha_i(\boldsymbol{\omega})=c(p)\rho_t^E z_i^E\\ \beta_i(\boldsymbol{\omega})=\boldsymbol{e_i}\sum_{j=1}^{n_p}\boldsymbol{x_j}\rho_j\frac{k_{rj}}{\mu_j}\end{cases}$$

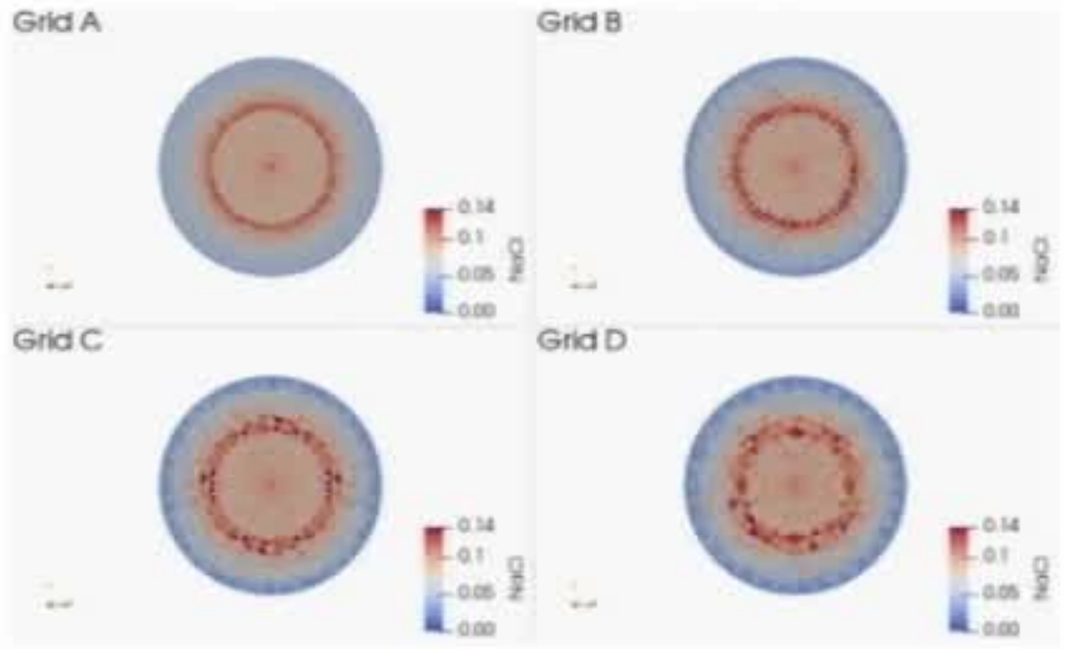
$$\prod_{c=1}^{n_c} a_c^{v_{cq}}-K_q=0$$

$$\rho_t^E=\rho_t\sum_{i=1}^{n_e}\boldsymbol{e_i z}$$

$$\boldsymbol{z^E}\sum_{i=1}^{n_e}\boldsymbol{e_i z}-\boldsymbol{Ez}=0$$

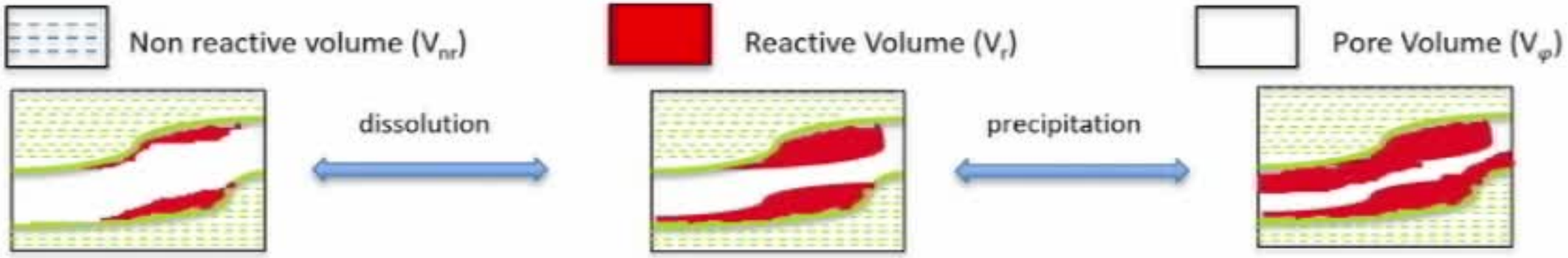






Kala and Voskov (2018)

Porosity-permeability treatment



- Bulk volume is a sum of reactive (V_r), non reactive (V_{nr}) and pore volume (V_φ).

$$V_b = V_\varphi + V_r + V_{nr}$$

- We introduce the concept of total porosity which is defined as

$$\varphi^T = \varphi_r + \varphi$$

- Fluid porosity can be calculated using the mineral saturation values

$$\varphi^{n+1} = \varphi^T \left(1 - \sum_i^{n_m} S_i^{n+1}\right)$$

- Power law transmissibility multiplier using upstream fluid porosity

$$T^M(\varphi^{n+1}) = \left(\frac{\varphi_{n+1}}{\varphi^T}\right)^A = \left(1 - \sum_i^{n_m} S_i^{n+1}\right)^A$$

- In this way, $T^M \in [0, 1]$, i.e. at any time: $T = \Gamma^{max} T^M$

Operator form of equations

$$a(\xi)\left(\alpha_c(\omega) - \alpha_c(\omega_n)\right) + \sum_l b(\xi,\omega)\beta_c(\omega) - c(\xi)\gamma_c(\omega) = 0$$

- $a(\xi) = \phi_0(\xi)V(\xi),$
- $b(\xi,\omega) = \Delta t \Gamma^{l,max}(\xi)(p - p^l)$
- $c(\xi) = \Delta t V(\xi),$

$$\alpha_c(\omega) = \left(1 + c_r\left(p - p_{ref}\right)\right)\sum_{j=1}^{n_p} x_{cj}\rho_j s_j,$$

$$\beta_c(\omega) = \sum_{j=1}^{n_p} T^M x_{cj}^l \rho_j^l \frac{k_{rj}^l}{\mu_j^l},$$

$$\gamma_c(\omega) = \sum_{k=1}^{n_k} \nu_{ck} r_k$$

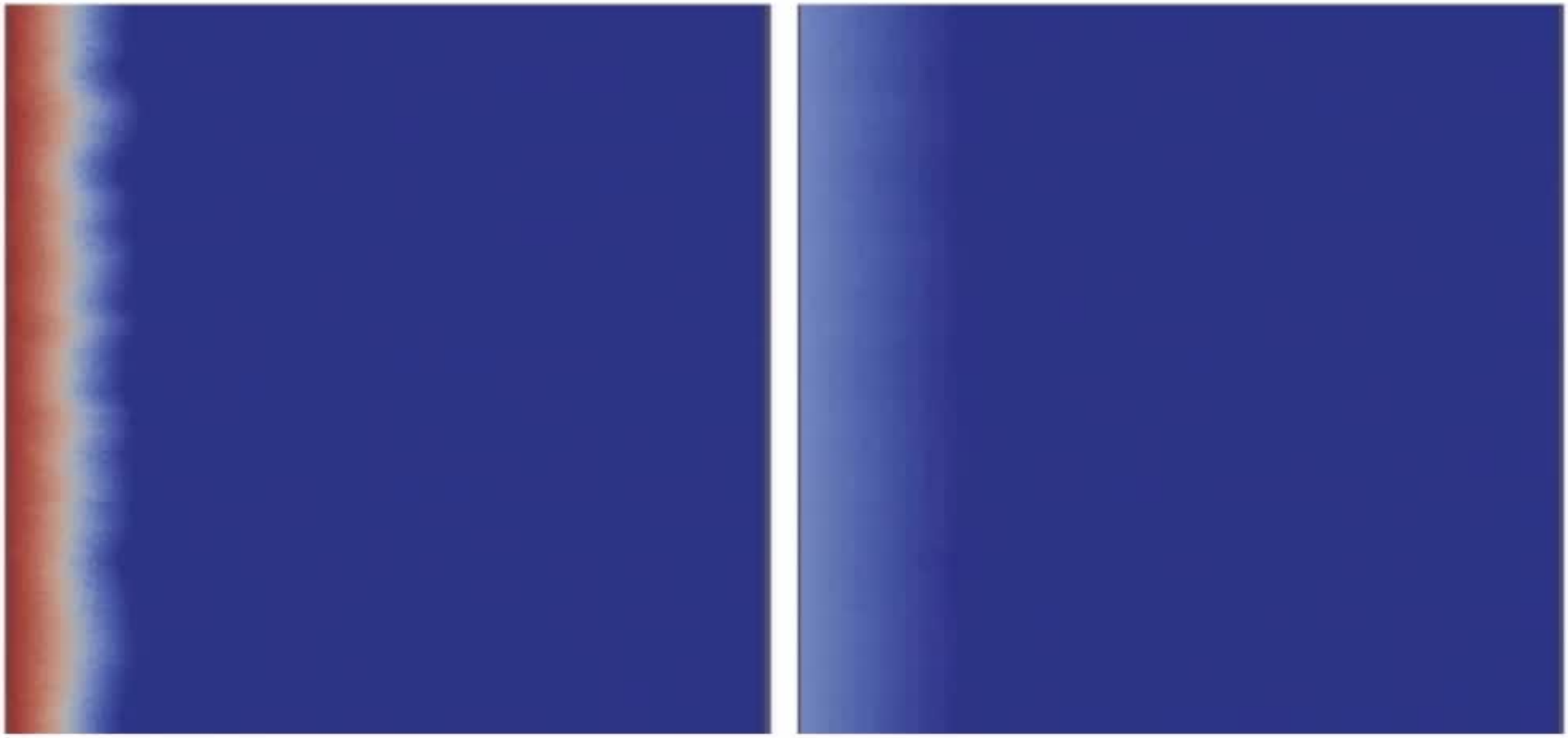
Example for a single kinetic reaction:

$CaCO_3 \rightarrow Ca^{+2} + CO_3^{-2}$

$$\gamma_c(\omega) = \nu_c k A_s \left(1 - \frac{Q}{K}\right) z_{CaCO3}$$

Slower kinetic rates

L_{res} = 100 [m]; H_{res} = 10 [m]; Q_{inj} = 1 [m^3/day] → v_{avg} = 0.001 [m/day]



k_{rate} = 0.0005 [1/day] → Da ~ 0.5

k_{rate} = 0.00001 [1/day] → Da ~ 0.01

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Conclusion and future work

- Parametrization approach extended for kinetic and equilibrium reactions
- Flexibility of the OBL framework helps in implementation of complex physics

On-going work

- Validate simulation results with reactions
  - CO_2 sequestration
  - Gas-hydrates
  - Geothermal scaling
  - Chemical EOR
- Add diffusion operators
- Apply framework to fracture network
- Link to real cave data and laboratory experiments

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Wormholes in different discretizations

L_{res} = 100 [m]; H_{res} = 10 [m]; Q_{inj} = 1 [m^3/day] → v_{avg} = 0.001 [m/day]

Kinetic reactions with OBL

$$\frac{\partial}{\partial t}(\varphi^T \rho^T z_c) + \mathrm{div} \sum_{j=1}^{n_p} x_{cj} \rho_j \overrightarrow{u_j} - \sum_{k=1}^{n_k} \nu_{ck} r_k - \sum_{q=1}^{n_q} \nu_{cq} r_q = 0$$

$$(V\varphi^T \rho^T z_c)^{n+1} - (V\varphi^T \rho^T z_c)^n - \Delta t \sum_{l \in L} \sum \left(x_{cj} \rho_j \lambda_j \Gamma^{max} T^M\right)^l (p - p^l)$$

$$-\Delta t \left(V \sum_{k=1}^{n_k} \nu_{ck} r_k \right)^{n+1} = 0$$

$$a(\xi)\left(\alpha_c(\omega) - \alpha_c(\omega_n)\right) + \sum_l b(\xi, \omega)\beta_c(\omega) - c(\xi)\gamma_c(\omega) = 0$$