Multiscale Modeling of CO2 Flow and Storage in Pre-Salt Reservoirs: Perspectives and Challenges

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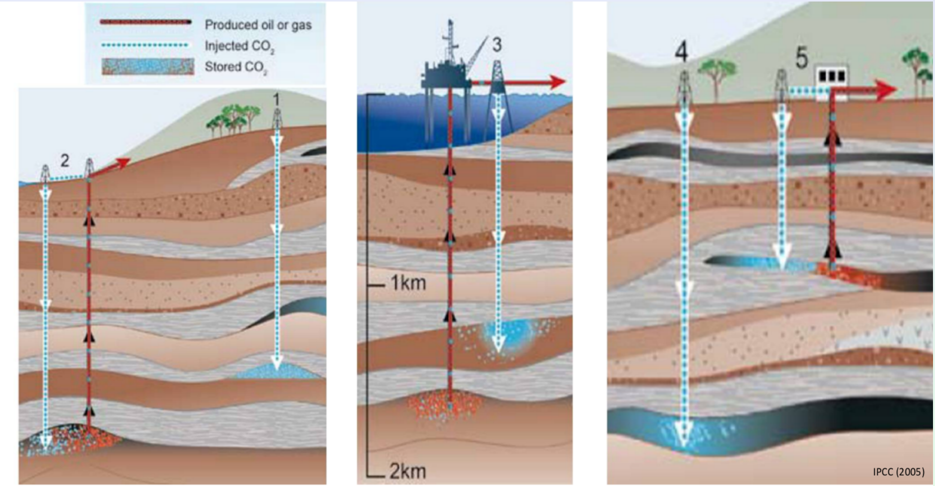
OUR MAIN TARGET

Feasibility of Vuggy Carbonates (Pre-Salt) as Potential Storage Sites for CO2 Storage



➢ **<u>Oil fields</u>**

1- Depleted reservoirs (gas/oil)

2- Enhanced oil recovery

➢ **Saline Aquifers;**

3- Deep unused saline water-saturated reservoir rocks.

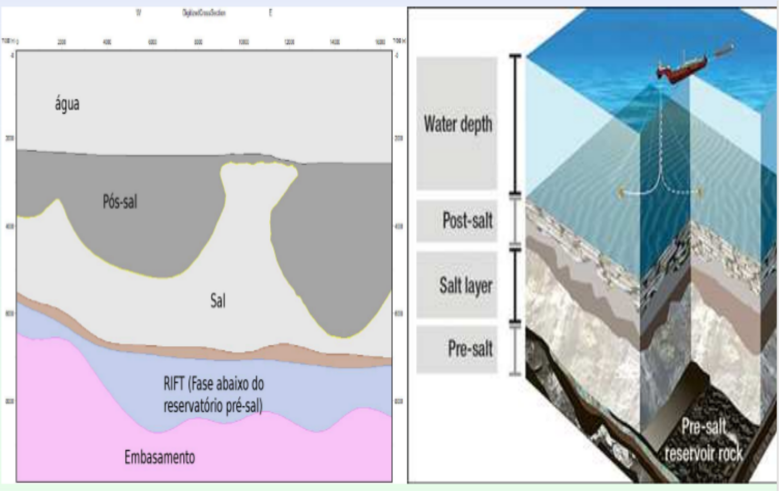
➢ **Coal layers.**

4- Deep Unmineable coal

5- ECBM Recovery

Possible Choices for Storage Sites

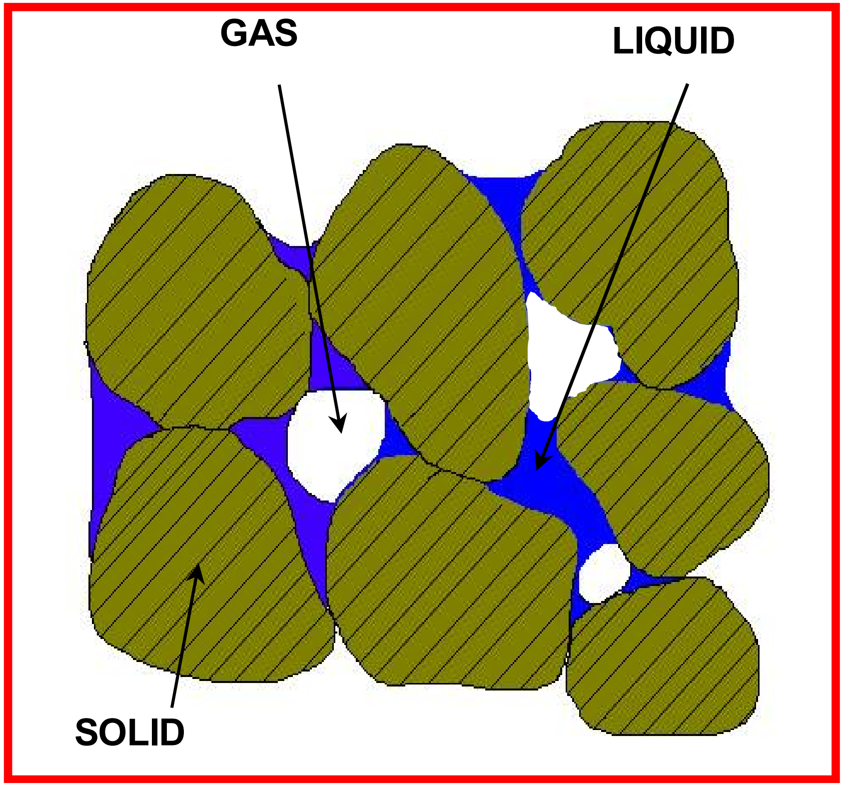
Carbonate Underneath the Salt Layer or Rock Salt



OUTLINE OF THE LECTURE

- Pros and Cons
  - Storage Site: Carbonate underneath the Salt Layer
    - Review of CO_2-properties at the Subsurface
    - CO_2 movement and Driving Forces
    - Thermodynamics
    - Geochemistry
  - Review of the Main Trapping Mechanims in the Subsurface
    - Stratigraphic, Residual,
    - Solubility, Mineral
  - Drawbacks: (Ongoing Research)
    - Geomechanical Issues
    - Apperance of High Permeability Pathways - Conduits
  - Storage Site: Salt Layer
- Concluding Remarks on Feasibility of CO_2 Storage in the Pre-Salt

Multiphase multispecies approach



The species are:

- mineral (-) : main mineral
- water (*w*) : as liquid or evaporated in the gas phase
- air (*a*) : dry air, as gas or dissolved in the liquid phase
- chemical species : interacting (reactive) species

The three phases are:

- gas (*g*) : mixture of dry air and water vapour
- liquid (*l*) : water + air dissolved + dissolved chemical species
- solid (*s*) : main mineral + absorbed cations + precipitated minerals

Reactive transport equations

$$\frac{\partial}{\partial t}(\phi S_w \rho_w c_i) + \nabla \cdot \mathbf{j}_i = R_i \quad (i = 1, \dots, N)$$

Total Flow:

Chemical reactions

$$\mathbf{j}_i = \rho_w c_i \mathbf{q}_w + \mathbf{D}_w \nabla c_i + \phi S_w \rho_w c_i \dot{\mathbf{u}}$$

Advective

Non-advective
(dispersion and diffusion)

Solid velocity

Reactive transport equations

$$\frac{\partial}{\partial t}(\phi S_w \rho_w c_i) + \nabla \cdot \mathbf{j}_i = R_i \quad (i = 1, \ldots, N)$$

- CHEMICAL INTERACTION OF *N* INTERACTING SPECIES
  - Slow reactions: kinetics controlled
  - Fast reactions: equilibrium controlled
- PHENOMENA CONSIDERED
  - Homogeneous reactions
    - Aqueous complex formation
    - Acid/base reactions
    - Oxidation/reduction reactions
  - Heterogeneous reactions
    - Cation exchange
    - Dissolution/precipitation of minerals (equilibrium and kinetics)
  - Other reactions
    - Radioactive decay
    - Linear sorption

Reactive transport equations

$$\frac{\partial}{\partial t}(\phi S_l \rho_l c_i) + \nabla \cdot \mathbf{j}_i = R_i \quad (i = 1,\ldots,N)$$

- CHEMICAL INTERACTION OF *N* INTERACTING SPECIES

- Slow reactions: kinetics controlled
  - Rate of species production in kinetics-controlled reactions

$$r_m = A_m k_m \left| \Omega_p{}^r - 1 \right|^n$$

$$\Omega_p = \frac{Q_m}{K_m} \quad ; \quad Q_m = \prod_{j=1}^{N_c} a_j^{v_{mj}}$$

$$k_m = k_{25} \exp\left[\frac{-E_a}{R}\left(\frac{1}{T} - \frac{1}{298.15}\right)\right]$$

- Fast reactions: equilibrium controlled
  - A chemical equilibrium model is uses based on the minimization of Gibbs free energy

$$\underset{n_j^c, n_i^x}{minimize} \quad G = \sum_{j=1}^{N_c} \mu_j^c n_j^c + \sum_{i=1}^{N_x} \mu_i^x n_i^x$$

$$n_j^U = n_j^c + \sum_{i=1}^{N_x} \nu_{ij} n_i^x \quad (j = 1,\ldots,N_c)$$

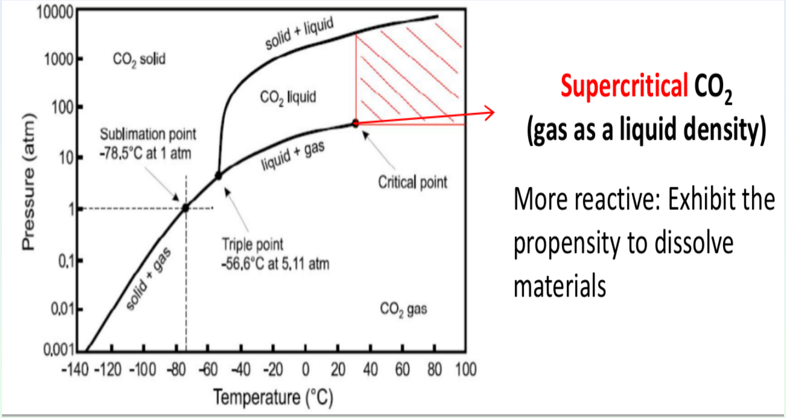
$$n_i^x \geq 0 \quad (i = 1,\ldots, N_x)$$

$$n_j^c \geq 0 \quad (j = 1,\ldots, N_c)$$

  - Newton-Raphson algorithm
  - Lagrange multipliers to incorporate the restrictions of the system

Thermodynamics: Supercritical State

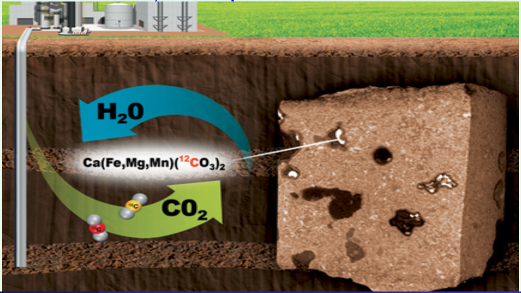
Temperature: $31.1C$, Pressure 7.38 MPa: Geothermal gradients $25C/KM, z = 800m$.

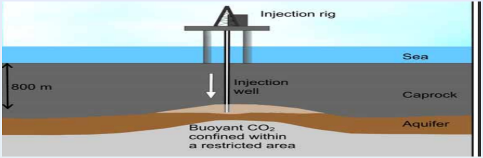


- In the long-term behaves as a separate phase with much lower Volume

Desirable Properties for a Successful Injectivity

- Efficient Trapping Mechanics
- Host formation not impermeable
- Deep enough to maintain Co_2 in superctitical state
- High areal extent of the cap rock
- Avoidance of Geomechanical Structural Damage
- After Long Term Dissolution/Precipitation remains in a Mineralized state

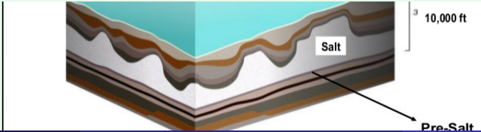




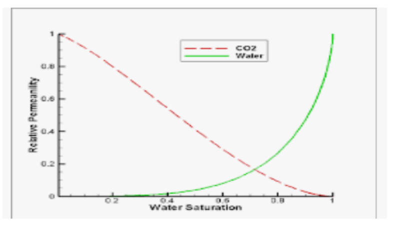
Two-Phase Flow in Porous Media. Buoyant Forces

$$
\begin{aligned}
\mathbf{v}_T &= -KK_r(S)(\nabla P - \rho \mathbf{g}) \\
\phi \frac{\partial S}{\partial t} &+ \nabla \cdot (\mathbf{v}_T f(S)) = 0 \\
f_{=} f_w &(1 - \alpha(Kg(\rho_w - \rho_g))
\end{aligned}
$$

Salt (Halite and Dolomite) – Excellent non-reactive Impermeable Medium.



Also referred to as capillary trapping



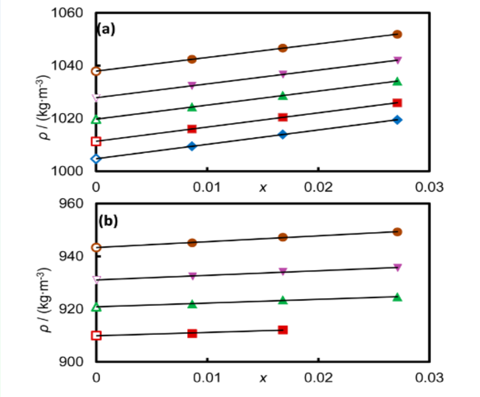
[Relative Permeability Curves

$$\mathbf{v}_T = -\frac{K}{\mu} K_r(S)(\nabla P - \rho \mathbf{g}), \qquad \phi \frac{\partial S}{\partial t} + \nabla \cdot (\mathbf{v}_T f(s)) = 0$$

- A fraction of the CO_2 is left behind as a disconnected phase

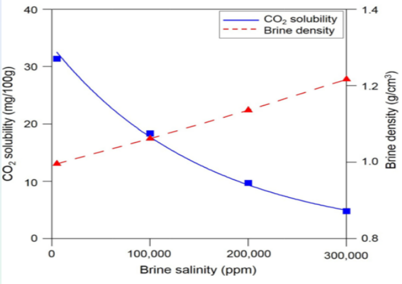
Increase in Brine Density

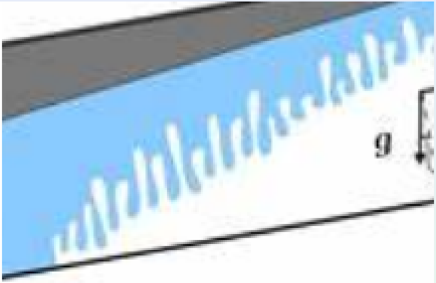
$$\rho = \rho_{water}(1 - X) + X\rho_{CO2}, \qquad X - -\textbf{mass fraction}\, C_{O2}$$



Top T= 296 K: Bottom T= 449 K

Increase in Brine Density – Gravitational stability, $\rho_w = \rho_w(C_{CO2})$





- Moves in the Opposite DIrection of the Free Gas.
- Sinks towards the bottom of the host formation
- Mass fraction – Convective-Diffusion Reaction Equation

$$\phi\frac{\partial\phi(\rho_w X_i)}{\partial t} + \nabla\cdot(\rho_w X_i \mathbf{v}_D) = \nabla\cdot(D_i\nabla(\rho_w X_i)) + F_i, \qquad i = CO_2, water$$

Trapping Mechanisms: iv) Mineral Trapping

- Solubility $\rightarrow\rightarrow$ Acidification $\rightarrow\rightarrow$ Weak carbonic acid

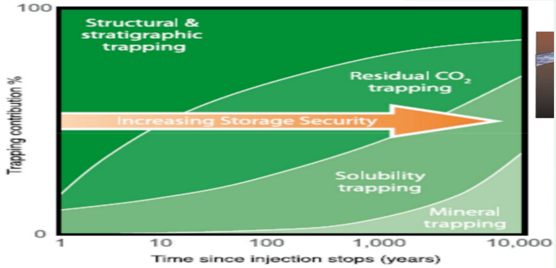
$$CO_2 + H_2O = HCO_3^- + H^+$$

(water acidification)

- Trigger Dissolution – Precipitation Geochemical Reactions

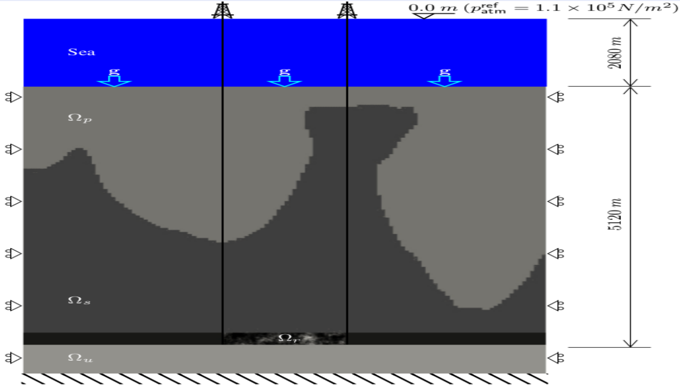
$$CaCO_3\,(s) + H_2CO_3\,(aq) \rightleftharpoons Ca^{2+}\,(aq) + HCO_3^-\,(aq)$$
$$\Uparrow$$
$$CO_2\,(g) + H_2O\,(l)$$

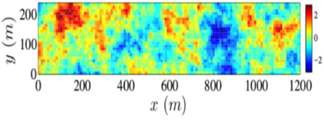
Time Scales



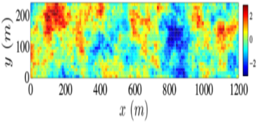
Drawbacks: Structural Geomechanics

i) Integrity of the Cap Rock





(b) Log-permeability



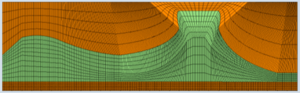
(a) Log-porosity

Hydro-Mechanical Multi-Physics Coupled Model

- Two-Phase Flow, Elasticity of the Host Rock,
- Viscoelasticity of the Cap Rock Salt

Fixed Stress Split: Creep of the Rock Salt)

$$\begin{aligned} \operatorname{div} \boldsymbol{\sigma}_e &= -\rho_s^{POS}\mathbf{g} \\ \boldsymbol{\sigma}_e &= \boldsymbol{\mathcal{C}}\mathbb{E}_e + \boldsymbol{\sigma}^0 \\ \mathbb{E}_e &= \frac{1}{2}\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^T\right) \end{aligned} \quad \text{in } \Omega_{POS}$$

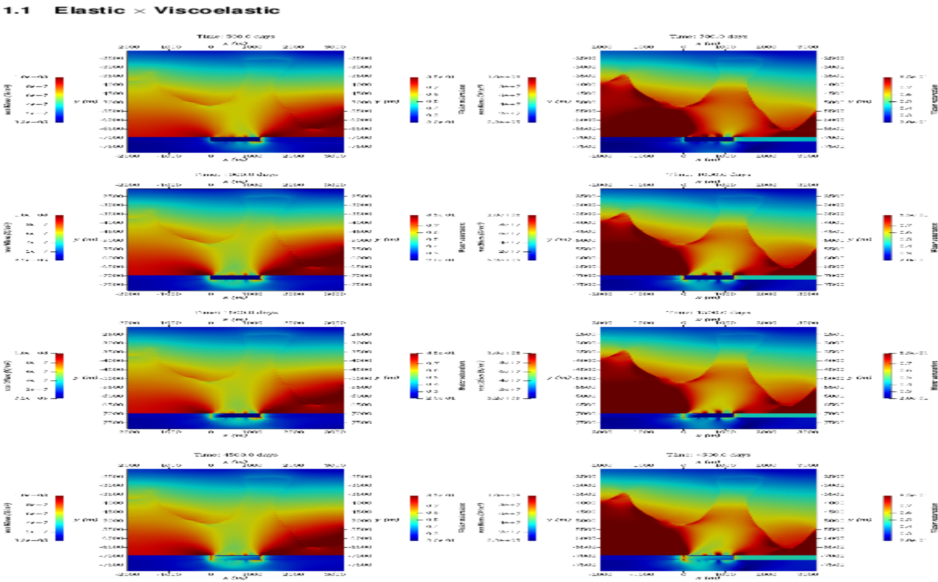


$$\begin{aligned} \operatorname{div} \boldsymbol{\sigma}_e &= -\rho_s^{DOMO}\mathbf{g} \\ \boldsymbol{\sigma}_e &= \boldsymbol{\mathcal{C}}\mathbb{E}_e + \boldsymbol{\sigma}^0 \\ \mathbb{E} &= \nabla^s\mathbf{u} \\ \mathbb{E}_e &= \mathbb{E} - \mathbb{E}_v \\ \mathbf{S} &= 2G\mathbf{P}_{dev}\mathbb{E}_e \\ \dot{\mathbb{E}}_v &= \dot{\gamma}\frac{\partial \sigma_V}{\partial \sigma} = \dot{\gamma}\sqrt{\frac{3}{2}}\frac{\mathbf{S}}{\|\mathbf{S}\|} \\ \dot{\gamma} &= \mathcal{E}_R^*\left(\frac{\sigma_V}{\sigma_R}\right)^N \qquad \sigma_V = \sqrt{\frac{3}{2}}\|\mathbf{S}\| \end{aligned} \quad \text{in } \Omega_{SALT}$$

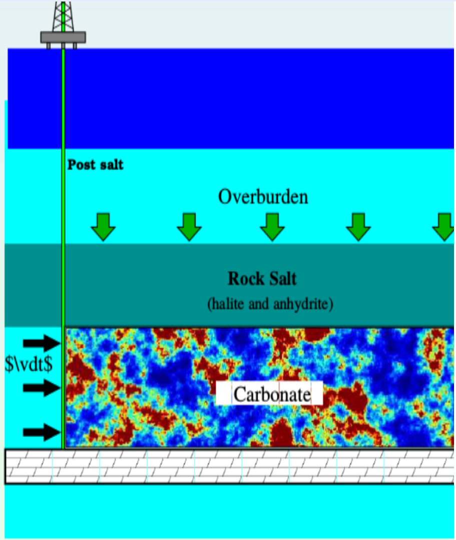
$$\begin{aligned} &\operatorname{div} \boldsymbol{\sigma}_e = \nabla p - \Big(\big(S_w\rho_w + (1-S_w)\rho_o\big)\phi + \rho_s^{RES}(1-\phi)\Big)\mathbf{g} \\ &\boldsymbol{\sigma}_e = \boldsymbol{\mathcal{C}}\mathbb{E}_e + \boldsymbol{\sigma}^0, \qquad \mathbb{E}_e = \frac{1}{2}\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^T\right) \\ &\beta\frac{\partial p}{\partial t} + \operatorname{div} \mathbf{v}_{Dt} = -\beta\frac{\partial\tilde{\sigma}}{\partial t} \\ &\mathbf{v}_{Dt} = -\lambda_t(S_w)K(\phi)(\nabla p + \mathbb{E}) \\ &\frac{\partial(S_w\phi)}{\partial t} + \operatorname{div}\Big(\lambda_w(S_w)\big(\mathbf{v}_{Dt} - \boldsymbol{\eta}k_{ro}\big)\Big) = 0 \end{aligned} \quad \text{in } \Omega_{RES}$$

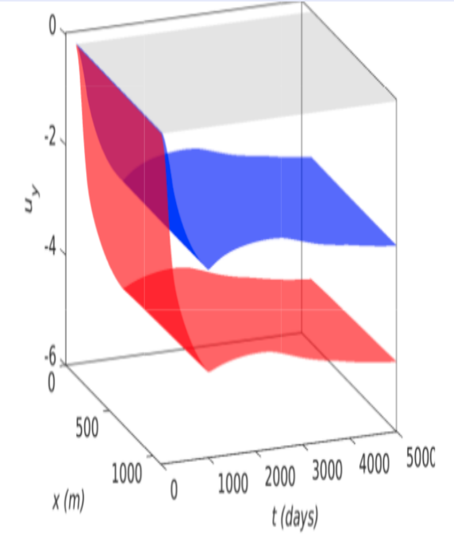
Saturation and Von-Mises Stress

Elastic x Viscoelastic



Surface Uplift

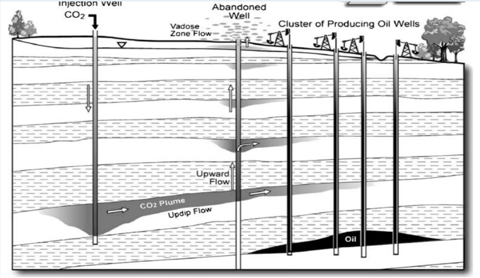




Structural Geomechanical Issues

ii) Leakage through Abandoned Wells

- Saline Aquifers; Do not suffer from this possibility
- Oil fields. Anthropogenic activity.



- Preexisting Abandoned wells penetrating caprock
- Potential leakage high-permeability pathways for buoyant CO_2

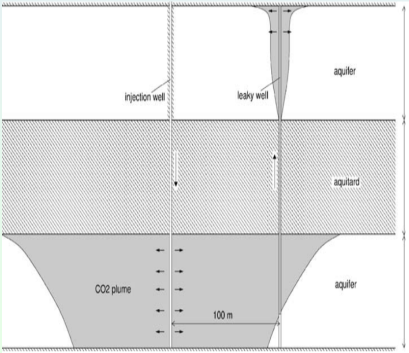
Structural Geomechanical Issues

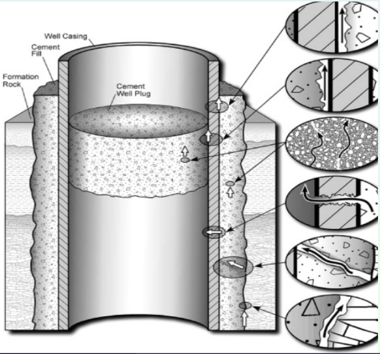
ii) Leakage through Abandoned Wells

Two-Phase Flow (Celia et al 2013)

$$\phi \frac{\partial \rho_g S_g}{\partial t} - \nabla \cdot (\rho_g \lambda_g \boldsymbol{K}(\nabla P - \rho_g \mathbf{g}) = 0$$

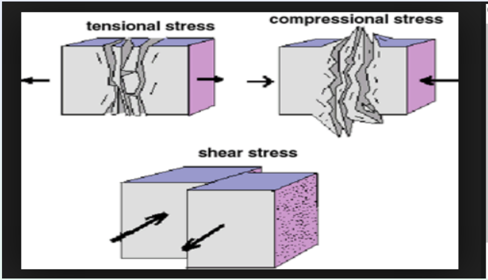
$$\phi \frac{\partial S_w}{\partial t} - \nabla \cdot (\lambda_w \boldsymbol{K}(\nabla P - \rho_w \mathbf{g}) = 0$$

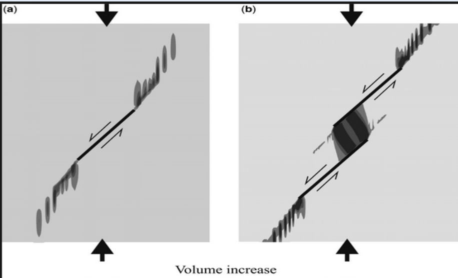




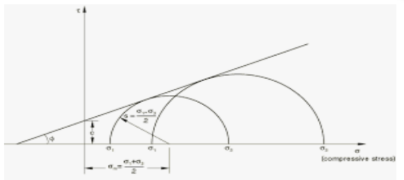
Structural Geomechanics

iii) Fault Activation due to Fluid Over-Pressurization





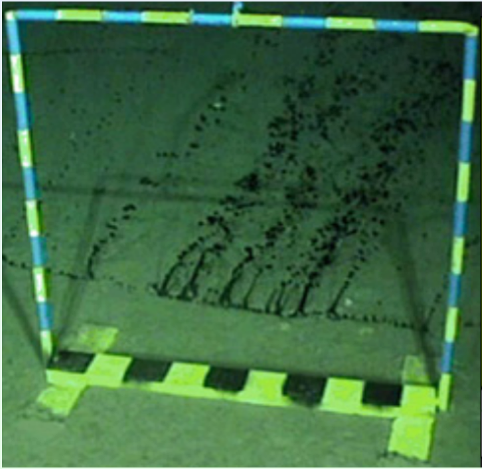
Localized Leaking: Plasticity. Mohr Coulomb Function. $\dot{\varepsilon}_p = \lambda \, \partial F(\boldsymbol{\sigma}) / \partial \boldsymbol{\sigma}$

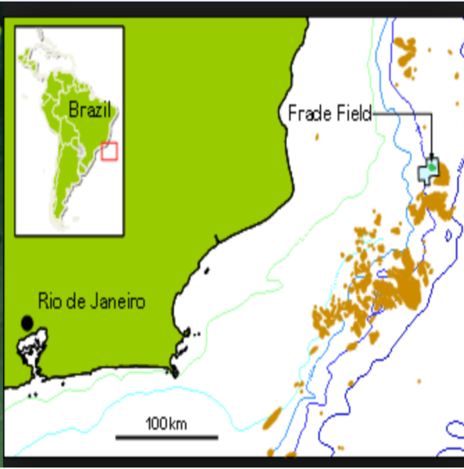


Structural Geomechanics

iii) Fault Activation

- Frade Field Oil Spill Incident

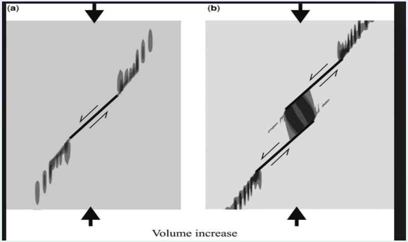




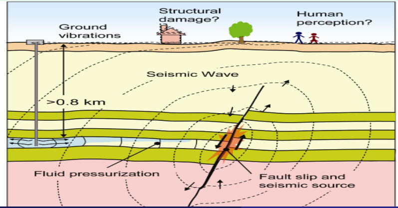
iii) Fault Activation

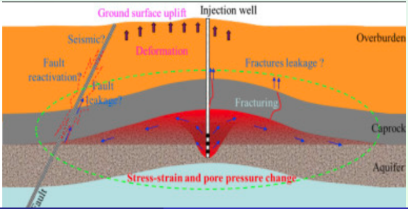
Dilatancy: Increase in Permeability

$$\frac{\partial \phi \rho_G}{\partial t} + \nabla \cdot (\rho_G \mathbf{v}_D) = 0, \qquad \mathbf{v}_d = -K(\nabla p - \rho_G \mathbf{g})$$



Injection-Fault-Activation → Ground Surface Uplift and Induced Siesmicity



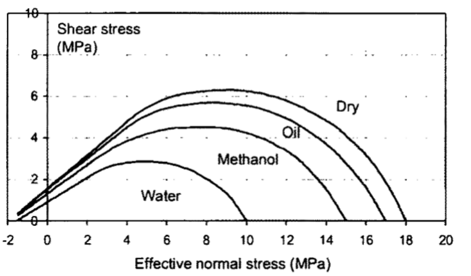


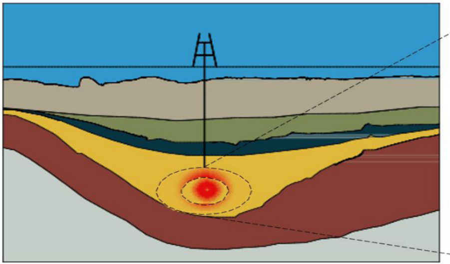
Injectivity Index

$$II = \frac{\textbf{Injection Flow Rate}}{P_{inj} - P_{res}}$$

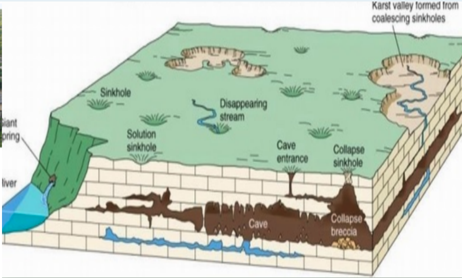
Low pH triggers dissolution/precipitation reactions new the injector
Geomechanics: Poroplasticity: Decrease strength of the rock bonds.

$$\nabla \cdot \boldsymbol{\sigma} - \nabla P = 0, \qquad \boldsymbol{\sigma} = C(\mathcal{E}(u) - \mathcal{E}_p)$$
$$\dot{\mathcal{E}}_p = \lambda \partial F(\boldsymbol{\sigma}, S)/\partial \boldsymbol{\sigma}$$



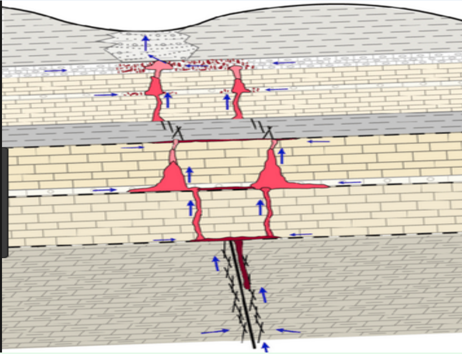


- Fractured Corridors. Enlarged due to Dissolution Collapse

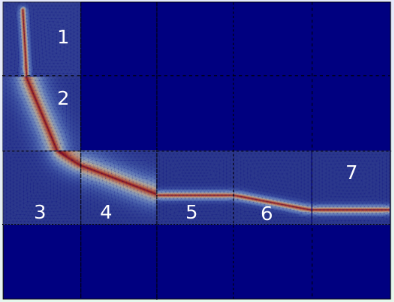


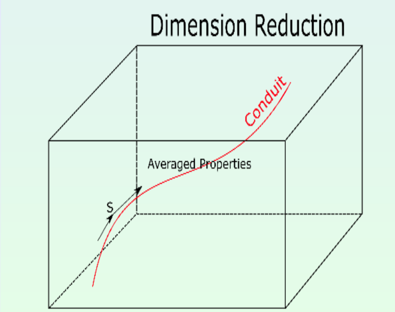
Presence of a Cave Network

Karst Conduits



Coupled 3D - 1D Model





$$\beta_r \frac{\partial P_r}{\partial t} + \nabla \cdot \mathbf{v}_d = KI(P_r - P_c)\delta_\Delta \quad \text{in} \quad \Omega$$

$$\mathbf{v}_d = -\boldsymbol{K} \nabla P_r$$

Coupled System

$$\beta_c \frac{\partial P_c}{\partial t} + \frac{dv_c}{ds} = -\frac{KI}{A_c}(P_r - P_c)$$

$$v_c = -K \frac{dp_c}{ds} \quad \text{in} \quad \Gamma_c$$

Summary - High-Fidelity (Fine-Scale) Model

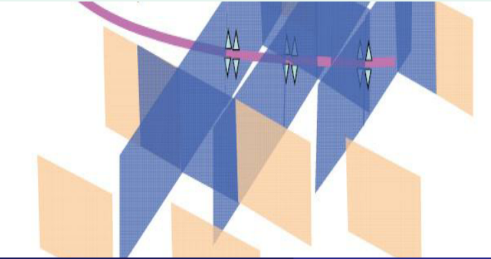
$$\beta_m \frac{\partial P_m}{\partial t} - \nabla \cdot (K_m \nabla P_m) = KI(P_m - P_c)\delta_\Delta \quad \Omega \subset \mathbb{R}^3$$

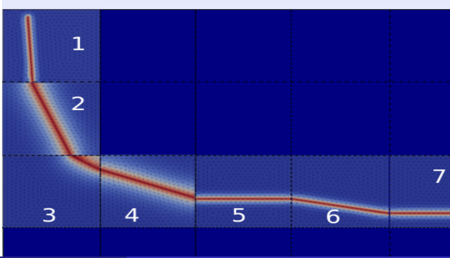
$$\beta_f \frac{\partial P_f}{\partial t} - \nabla_\tau \cdot (K_f \nabla_\tau P_f) = (\mathbf{v}_m^+ - \mathbf{v}_m^-) \cdot \boldsymbol{n} \quad \Gamma \subset \mathbb{R}^2$$

$$\beta_c \frac{\partial P_c}{\partial t} + \frac{dv_c}{ds} = -\frac{KI}{A_c}(P_r - P_c)$$

$$v_c = -K_c \frac{dp_c}{ds} \quad \text{in} \quad \gamma_c \quad \mathbb{R}^1$$

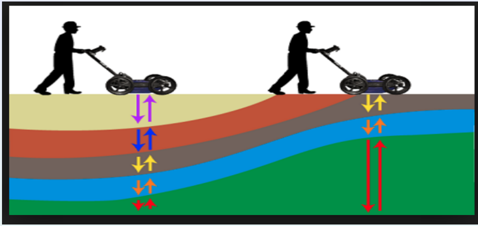
δ_Δ – Dirac line source



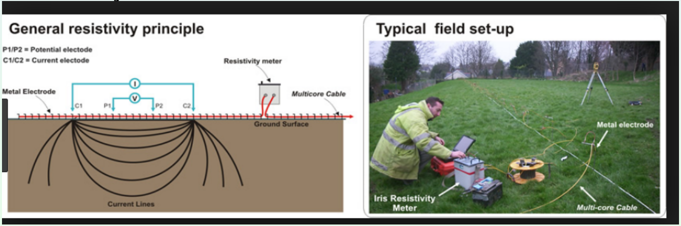


III Incorporate Outcrop Data

- GPR – Elecro-Magnetic Waves   Near-Surface Seismic Acustic Waves

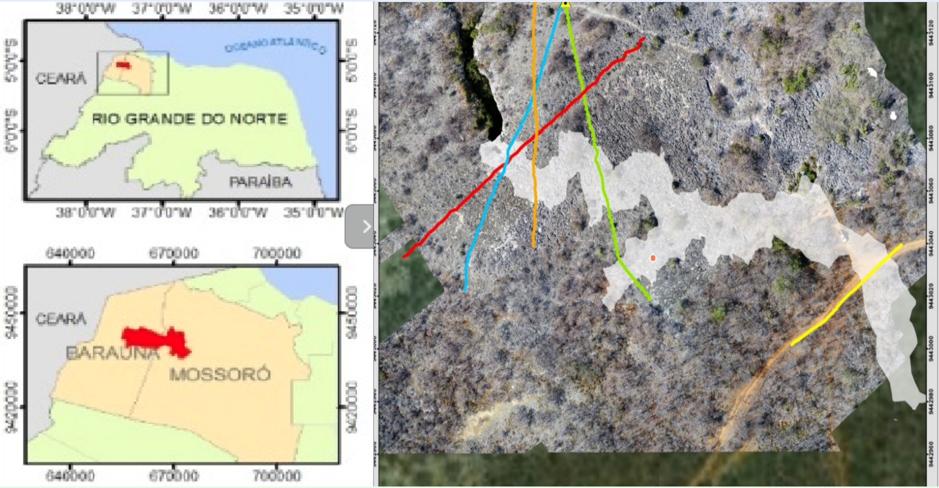


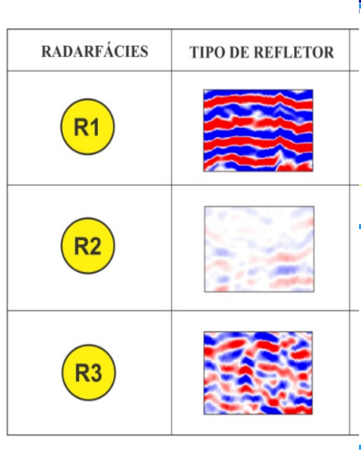
- Electro-Resistivity – Electric Current – Electrodes



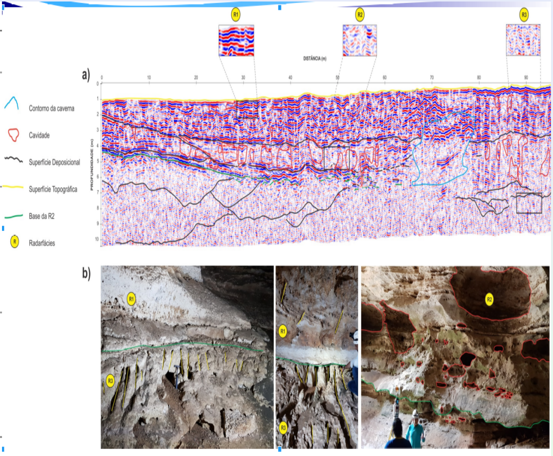
- – Joint Work with F Hilario Bezerra and F Pinheiro (UFRN)

Outcrop FURNA FEIA



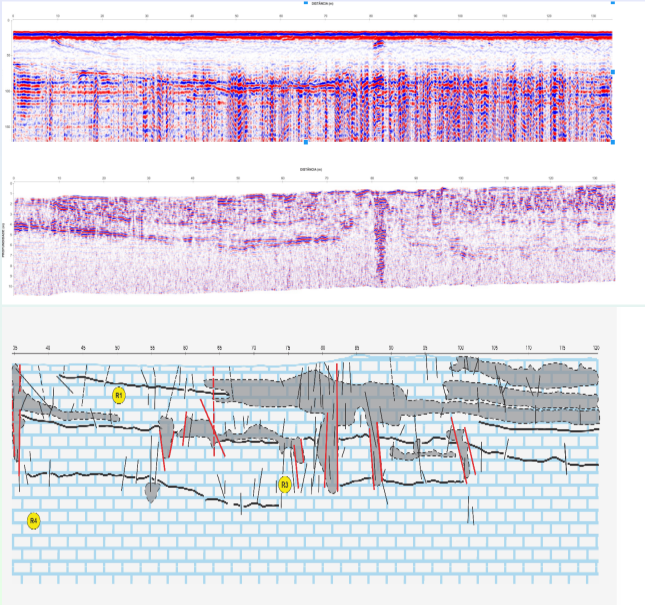


RADARFÁCIES
TIPO DE REFLETOR
R1
R2
R3

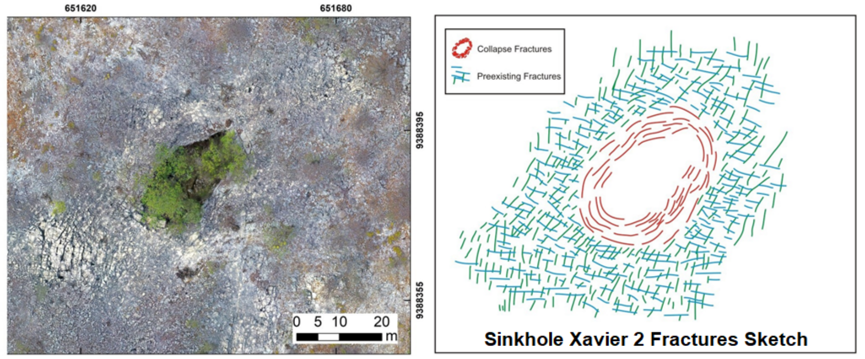


a)
DISTÂNCIA (m)
PROFUNDIDADE (m)
R1
R2
R3
Contorno da caverna
Cavidade
Superfície Deposicional
Superfície Topográfica
Base da R2
Radarfácies
b)

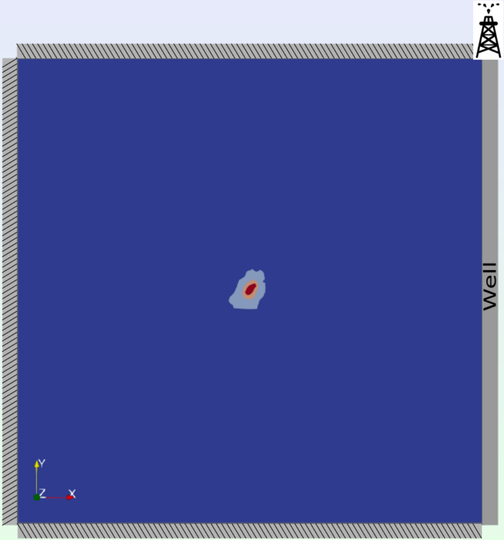
IMAGE PROCESSING



Sinkhole Xavier 2



Sinkhole Xavier 2



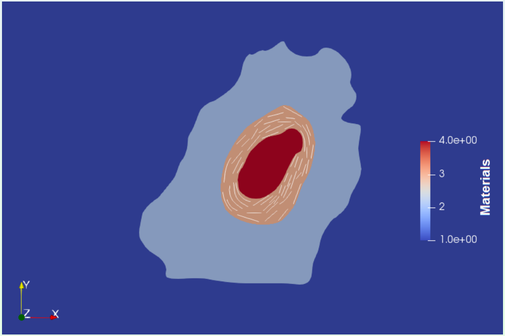
Sinkhole Xavier 2 - Materials

Material	**Description**	**Permeability** $[m^2]$
1	Intact Rock	$K_x = K_y = 2.96076 \times 10^{-13}$
2	Intact Rock + Micro fractures (estimated via ODA)	$K_x = 3.07392 \times 10^{-13}$ $K_y = 3.08085 \times 10^{-13}$
3	Intact Rock + Micro fractures (estimated via ODA) + discrete fractures	$K_x = 3.07392 \times 10^{-13}$ $K_y = 3.08085 \times 10^{-13}$
4	Sinkhole	$K_x = K_y = 1.0 \times 10^{-8}$
White Lines	Discrete Fractures	$K_f = 8.333 \times 10^{-10}$ (aperture $= 1.0 \times 10^{-4}$ m)

Estimating ODA:

Micro-Fractures Permeability
$K_f = 8.333 \times 10^{-10}$ m^2

Micro-Fractures Aperture
$d = 1.0 \times 10^{-4}$ m



Input Parameters: Sinkhole Xavier 2

Parameters	Values
Domain	500m $\times$ 500m
Rock Permeability (Horizontal)	$K_x = 3.2433 \times 10^{-13}$ m^2
Rock Permeability (Vertical)	$K_y = 3.2815 \times 10^{-13}$ m^2
Initial Pressure	56 MPa
Well Pressure	55 MPa
Sinkhole Pressure	55 MPa
Karst Index	7.370811×10^{-13} m^3
Total Simulation Time	4×10^5 s
Time Step	2000 s

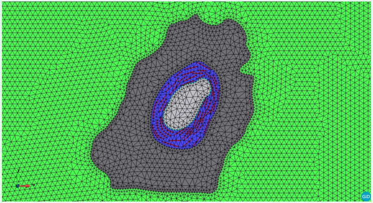
Sinkhole Xavier 2

Two simulations were performed:

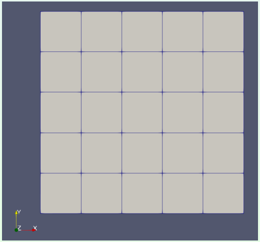
- High Fidelity Simulation
- Macro Scale Simulation using Karst Index

Simulation	High Fidelity	Macro Scale
Number of Elements	578412 (triang.)	25 (quad.)
Number of Nodes	290107	36
Processing time	7 minutes	1.42 seconds

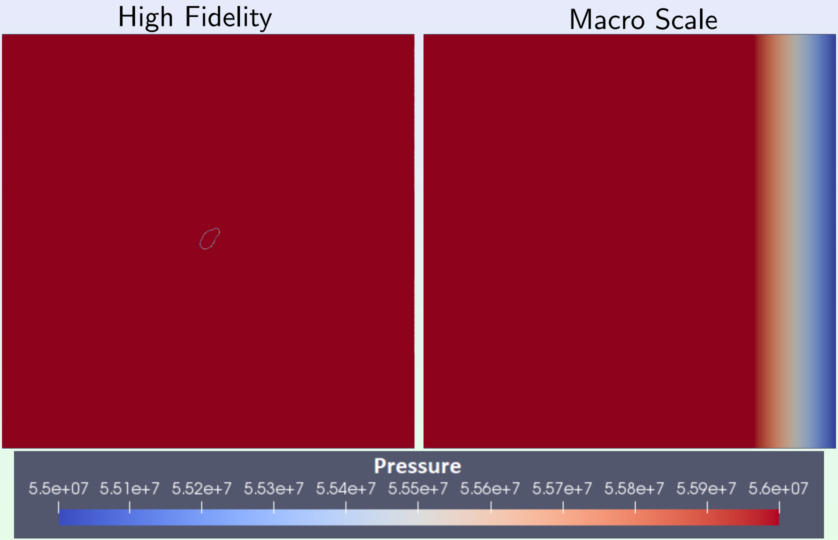
High Fidelity Mesh (zoom)



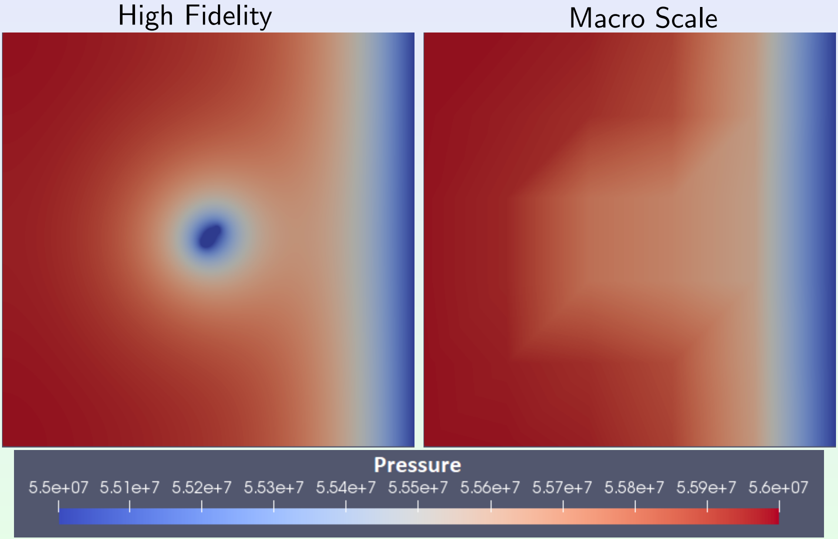
Macro Scale Mesh



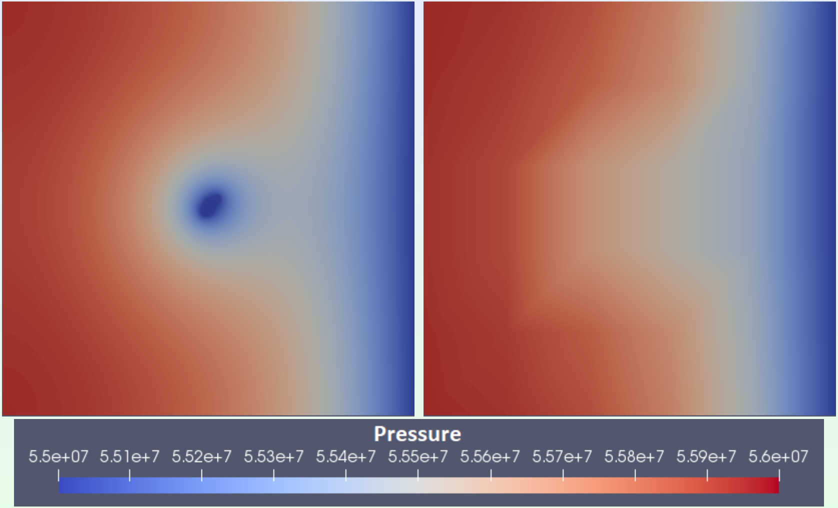
Sinkhole Xavier 2



Sinkhole Xavier 2

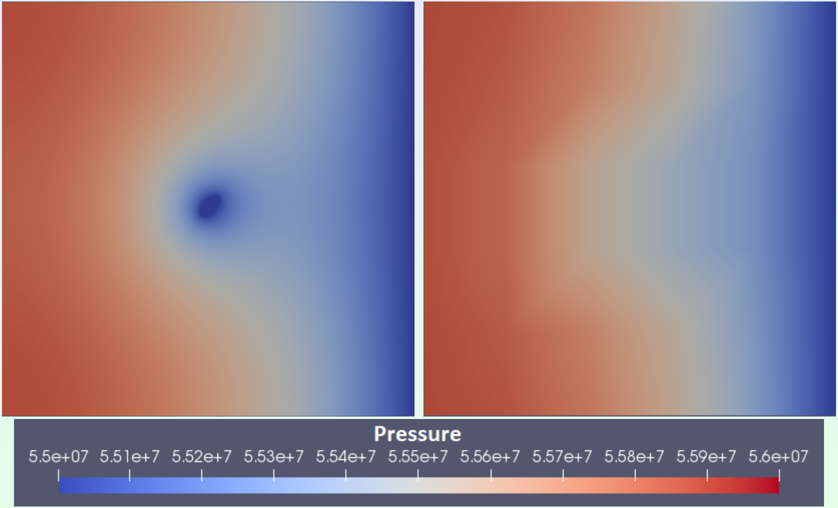


High Fidelity | Macro Scale



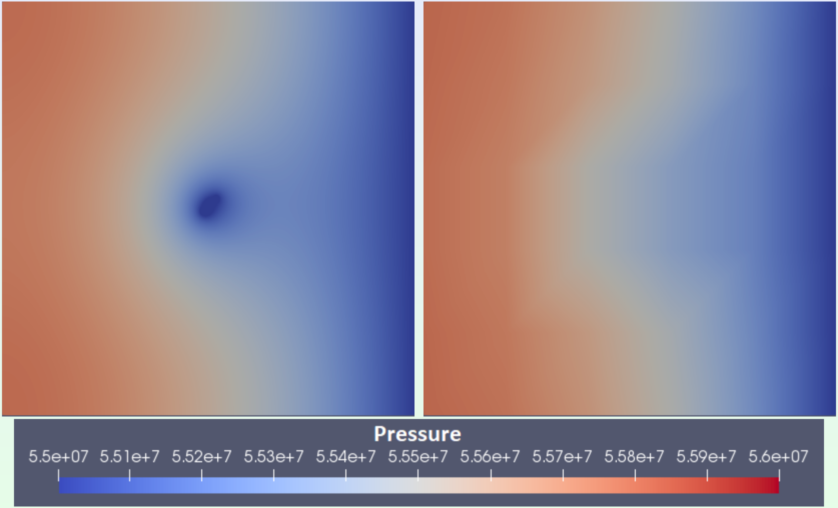
Sinkhole Xavier 2

High Fidelity   Macro Scale

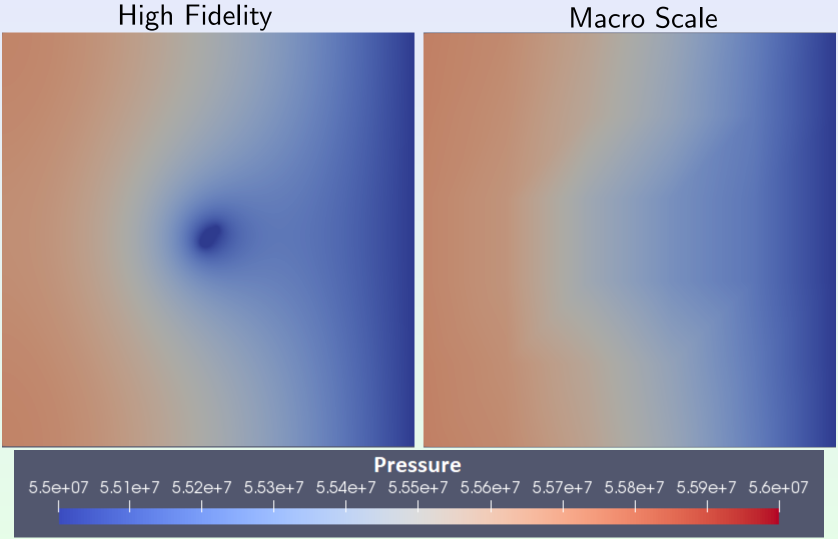


Sinkhole Xavier 2

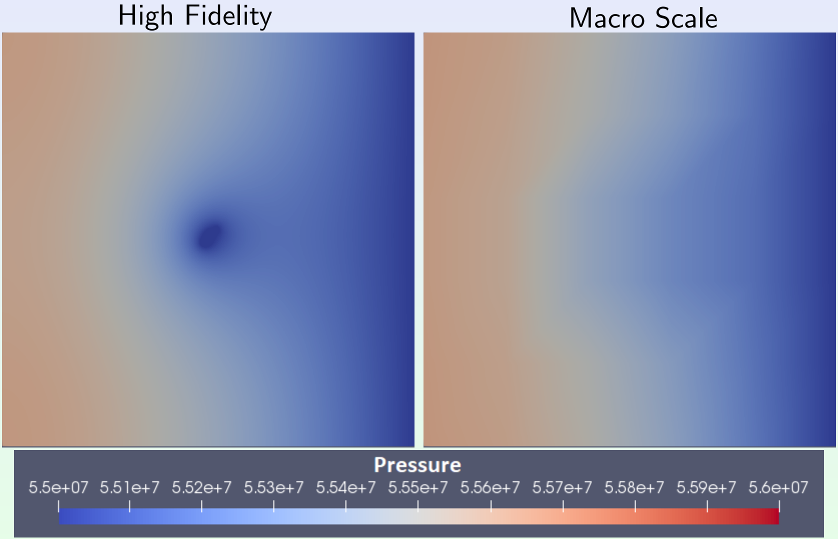
High Fidelity   Macro Scale



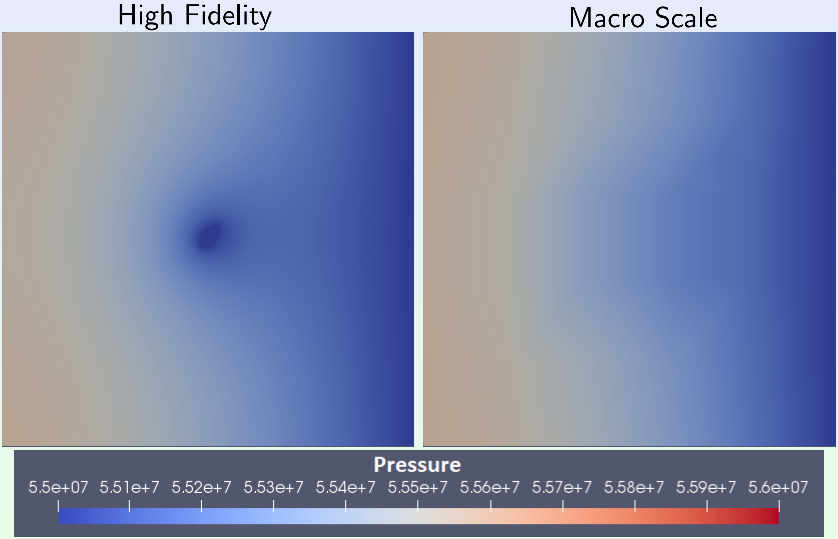
Sinkhole Xavier 2



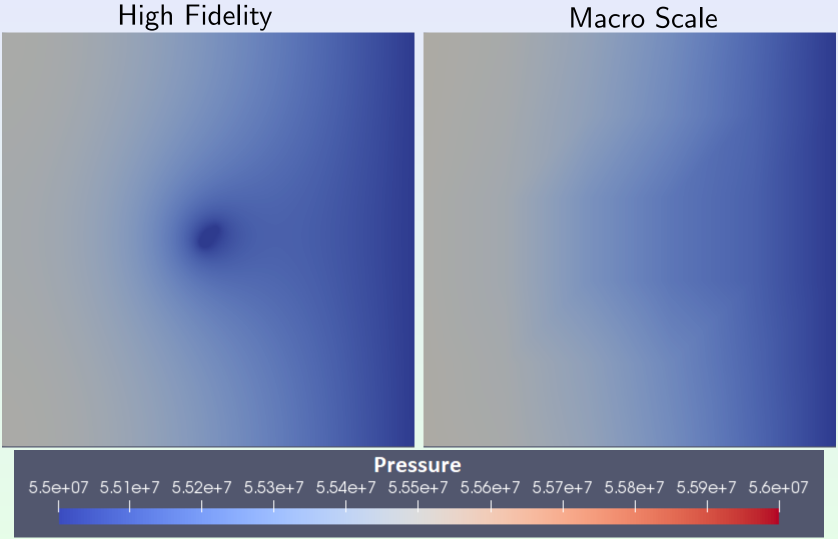
Sinkhole Xavier 2



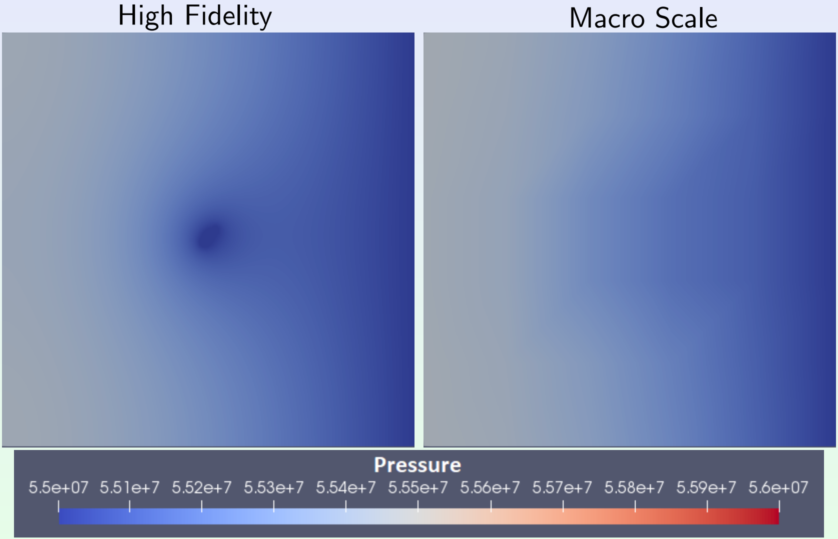
Sinkhole Xavier 2



Sinkhole Xavier 2

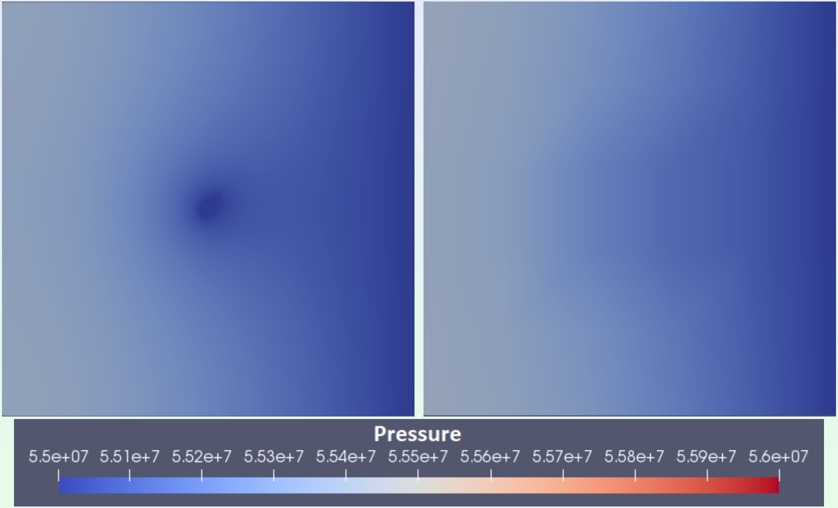


Sinkhole Xavier 2

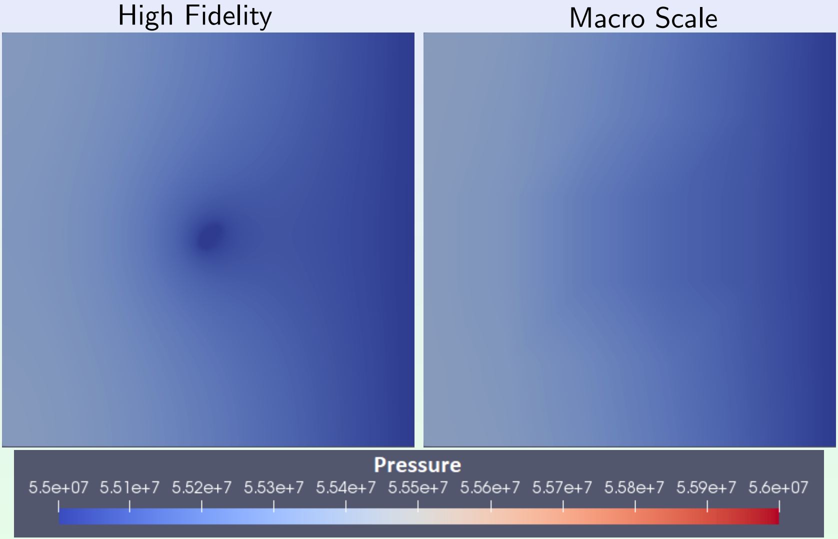


Sinkhole Xavier 2

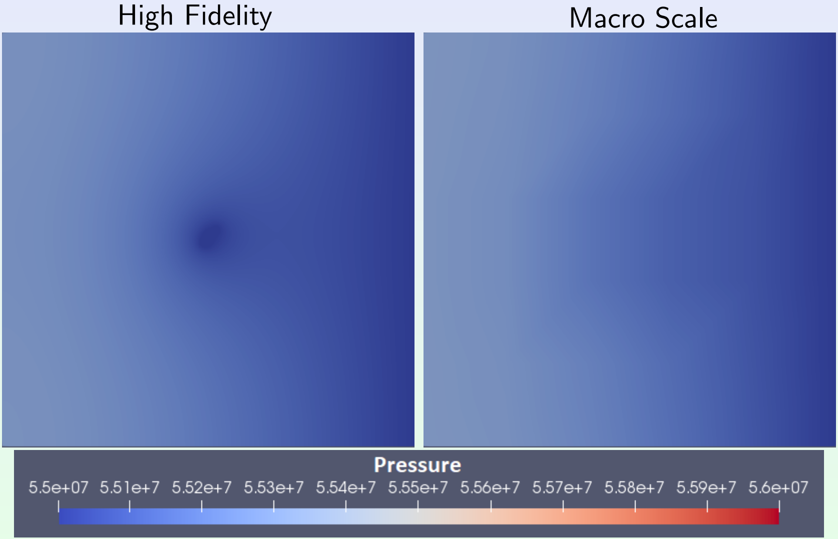
High Fidelity | Macro Scale



Sinkhole Xavier 2



Sinkhole Xavier 2



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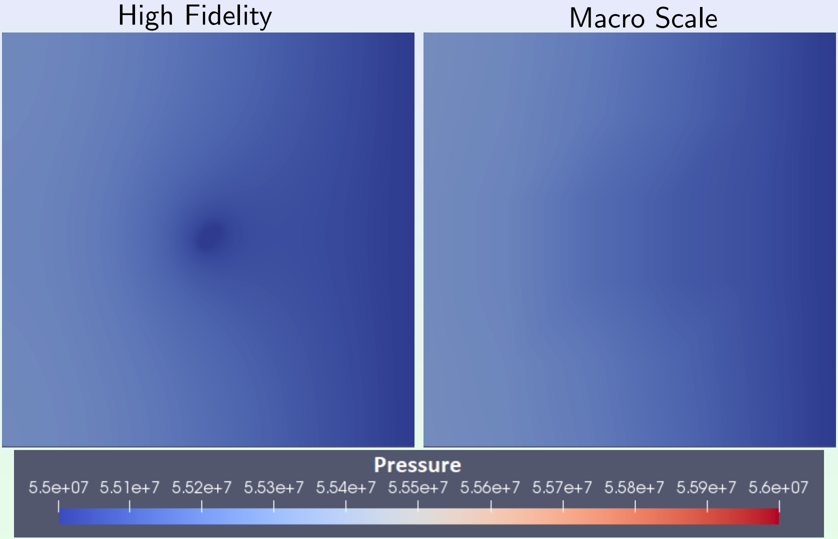
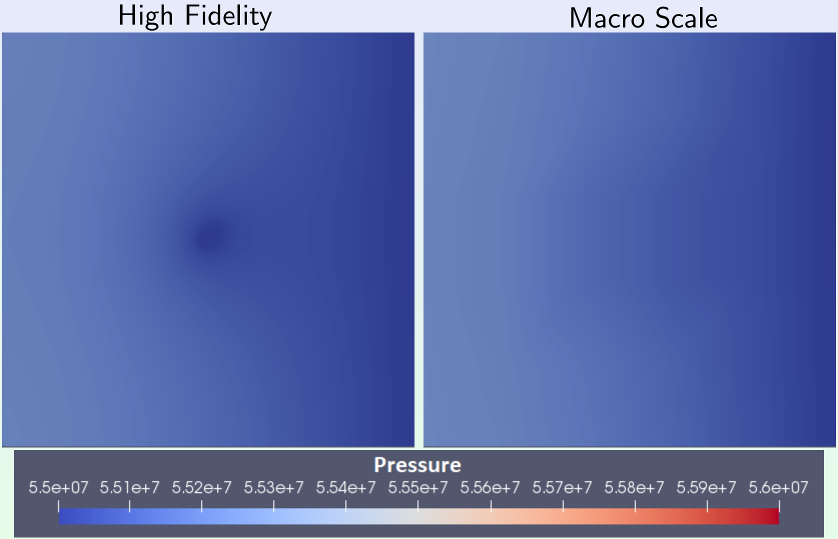
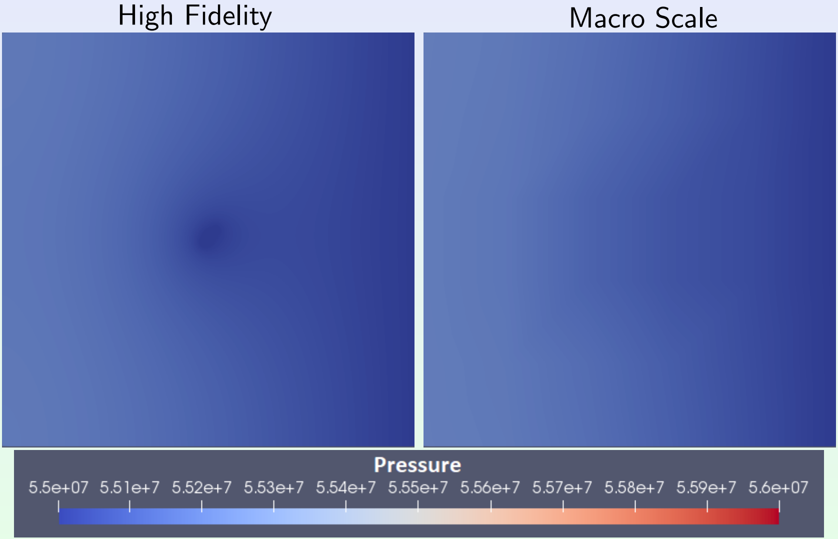


Sinkhole Xavier 2



Sinkhole Xavier 2



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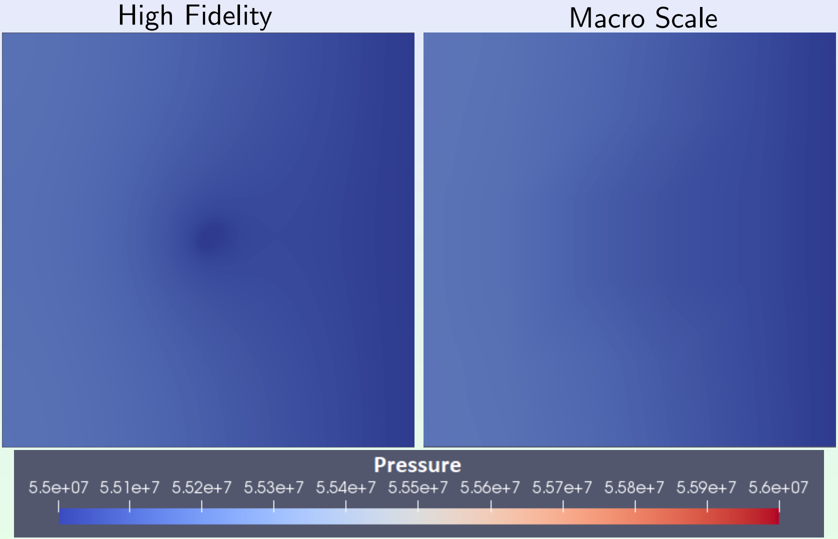
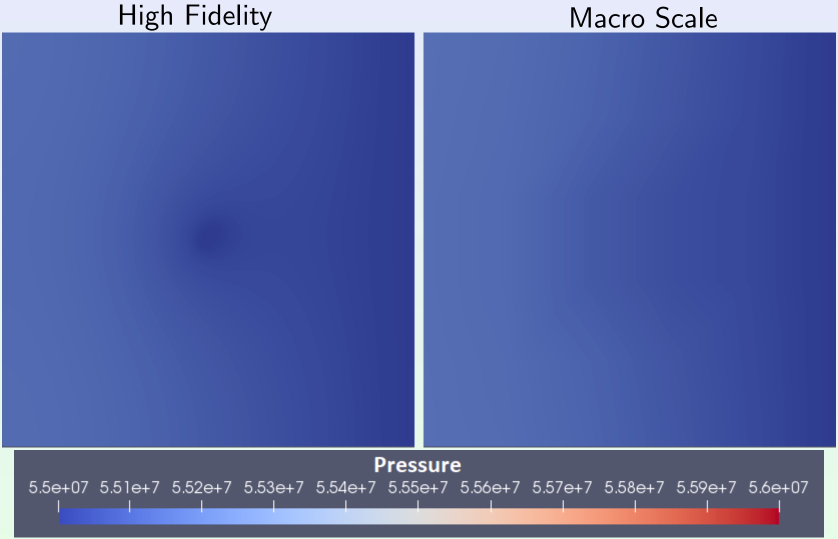
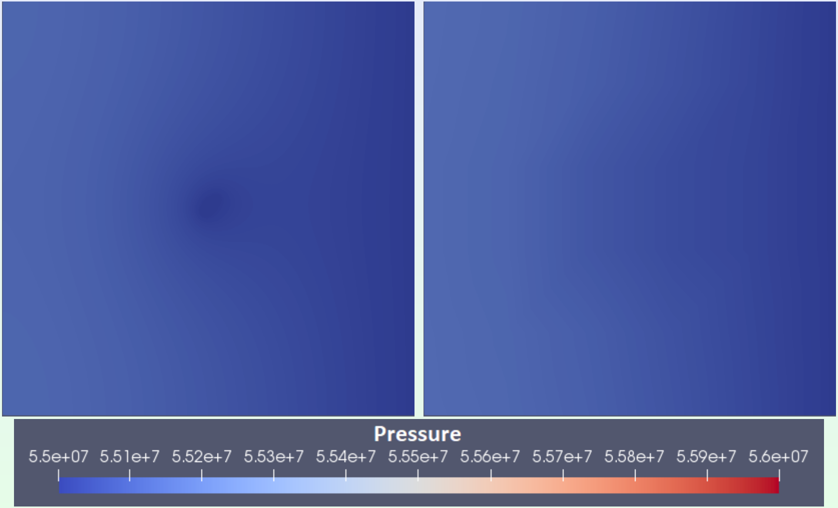


Sinkhole Xavier 2

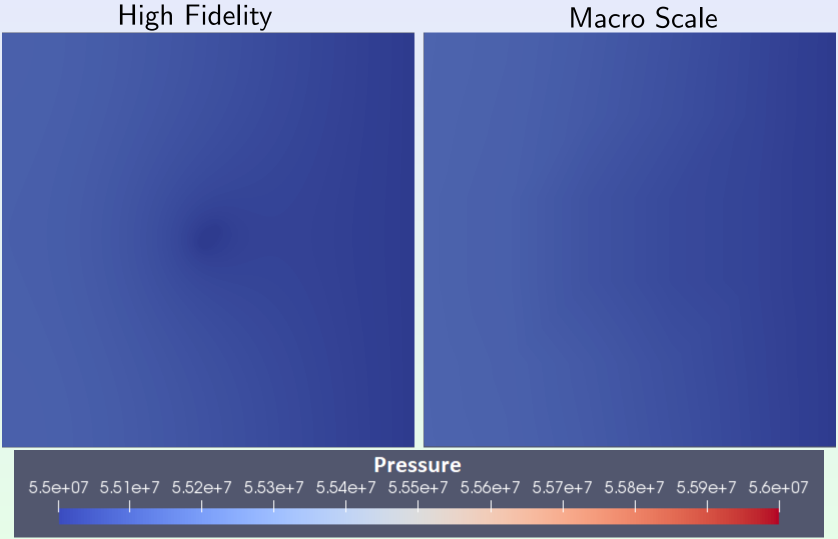


Sinkhole Xavier 2

High Fidelity Macro Scale



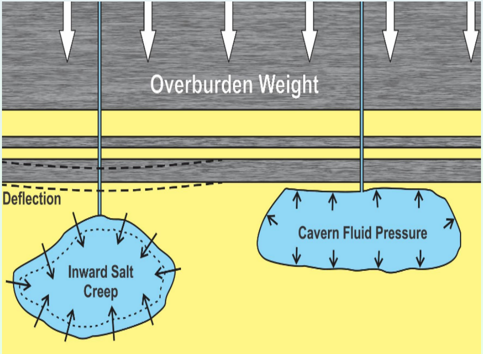
Sinkhole Xavier 2



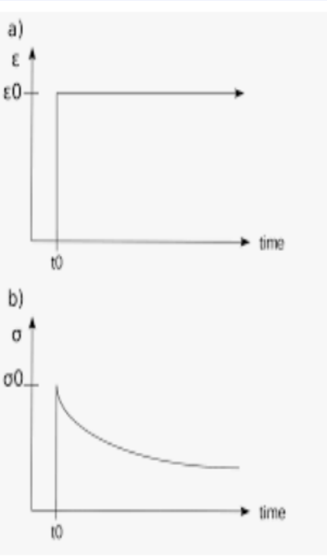
Storage in Salt Dome Caverns

Efficient underground repository

- Inject Fresh Water; withdraw brine dissolving the salt
- Create a stable large Cavity. Salt is chemically inert to CO_2
- Also potental sites for energy storage using highly compressible gases
- Creep. Salt tends to fill the holes gradually moving towards the cavern

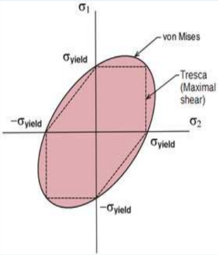


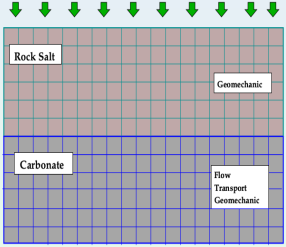
Creep Model for Halite



Geomechanics: Von Mises Stress – Distortional Energy

$$\boldsymbol{\sigma} = -p\mathbf{I} + \mathbf{s}, \qquad Q = \sqrt{\frac{3}{2} s_{ij} s_{ji}} \qquad \frac{\partial \mathcal{E}_c}{\partial t} = \epsilon_0 \left(\frac{Q}{\sigma_0} \right)^{N} \sqrt{\frac{3}{2}} \frac{\mathbf{s}}{\|\mathbf{s}\|}$$





Viscoelastic Model for the Rock Salt

Q – Energy that triggers creep in the saline cap rock

CONCLUDING REMARKS

- Great Opportunity for CO_2-storage in Pre-Salt
- Salt Layer
  - Self-Healing due to Creep
  - Chemically Inert to CO_2
  - Impermeable Geological Formation

Energy: WAG – Water Alternate Gas Injection for OIl Recovery