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Real time solutions of Thermo-Hydro Mechanical problems with application to the design of Engineered Barriers via Reduced Order Methods

PhD Candidate: Arash Moaven

PhD Advisors:
Prof. Sergio Zlotnik
Prof. Thierry J. Massart

Acknowledgements

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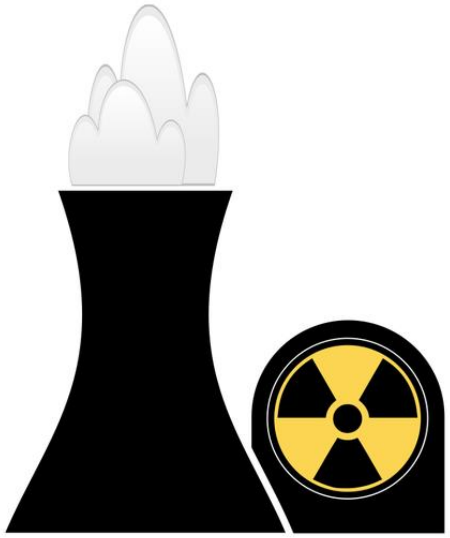
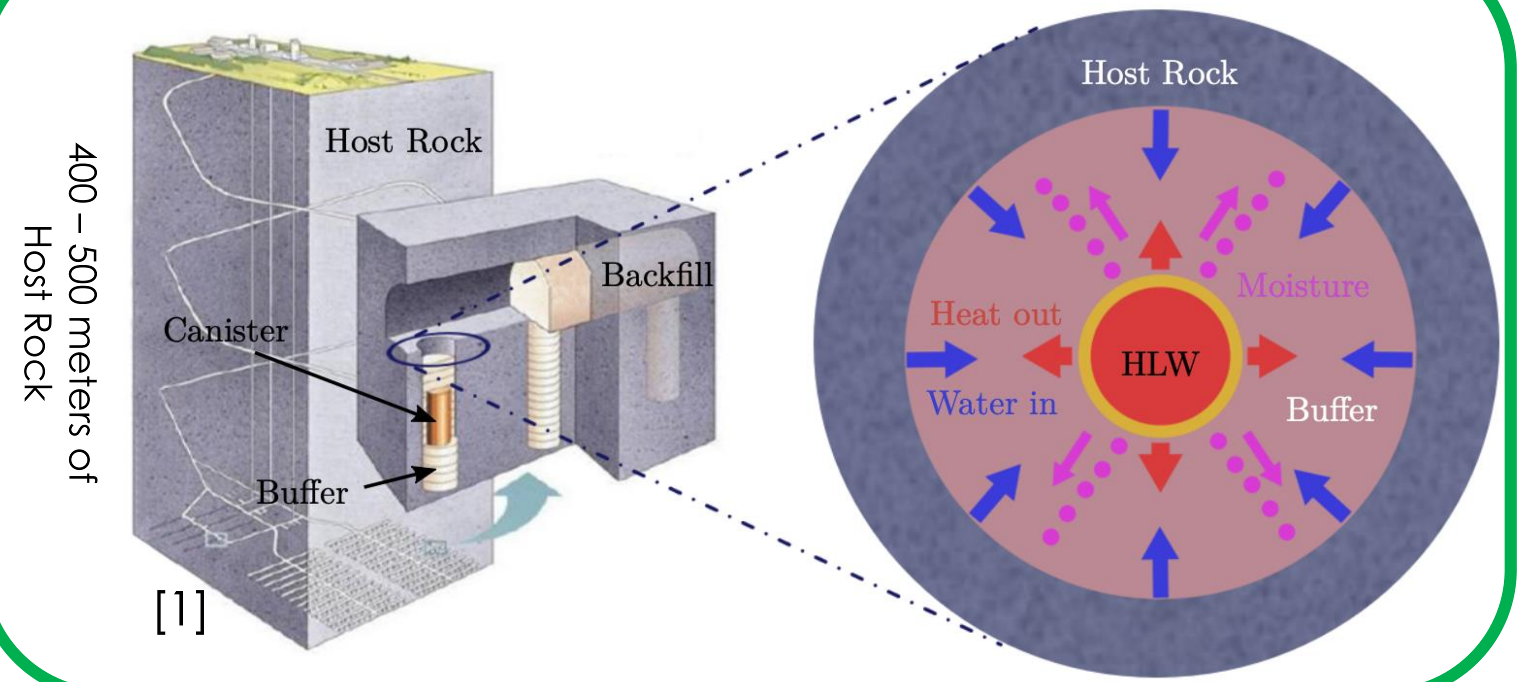
Motivation



Nuclear Power Plant

Isolating Radioactive High-Level Waste (HLW) With Deep Geological Repositories



THM problems

are parametric problem

We would like to provide: Generalized Solution

Proper Generalized Decomposition (PGD) is a Reduced Order Method (ROM) which is able to provide such a solutions

[1]- Toprak, E.; Mokni, N.; Olivella, S.: Pintado, X.: Thermo-Hydro-Mechanical Modelling of Buffer. Synthesis Report. August 2013

Problem Statement

- **Axisymmetric Rotational Framework**
- **Water saturation assumed**
- **Linear Elastic**
- $\Omega = \Omega_B \cup \Omega_{Bf} \cup \Omega_B \cup \Omega_C$

Governing Equations [2]

Heat Conservation

$$c_p^* \dot{T} - \nabla^T(\kappa \nabla T) = q$$

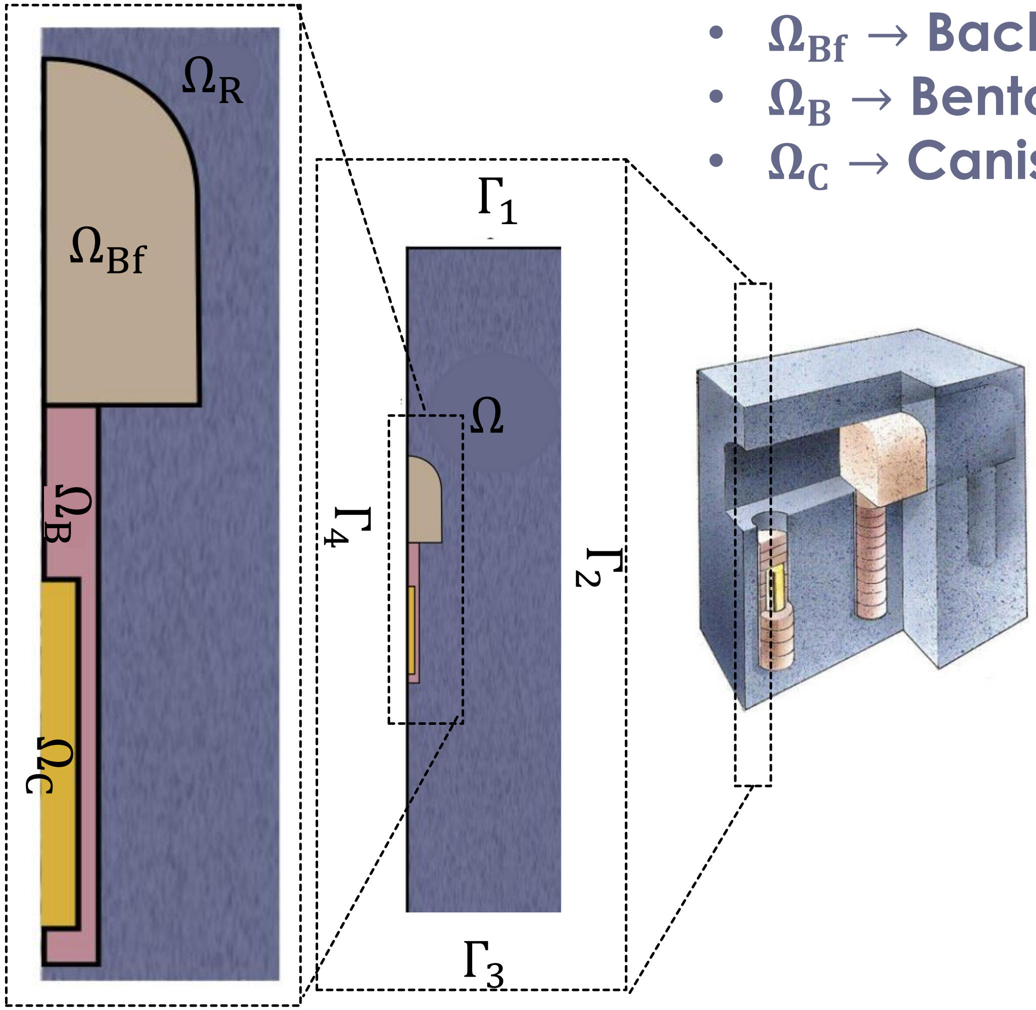
Fluid mass Conservation

$$-\nabla^T(K\nabla p) + \alpha \nabla \dot{u} + \left(\xi_1 + \frac{\xi_2}{E}\right)\dot{p} - \xi_3 \dot{T} = 0$$

Mechanical Equilibrium

$$-\nabla^T(\mathbf{C}\nabla \mathbf{u}) + \alpha \nabla p + \xi_4 E \nabla T = \mathbf{b}$$

Unknowns are	T, p and $\mathbf{u}$



- $\Omega_R \rightarrow$ Rock
- $\Omega_{Bf} \rightarrow$ Backfill
- $\Omega_B \rightarrow$ Bentonite
- $\Omega_C \rightarrow$ Canister

[2]- Selvadurai, A. P.S; Suvorov, A. P.: Thermo-Poroelasticity and Geomechanics. CAMBRIDGNE UNIVERSITY PRESS, 2017.

Discretization of the Problem

Spatially descritized system

Heat Conservation	$\mathbf{M}_t\dot{T} + \mathbf{K}_t T = f_q$
Fluid mass Conservation	$-\mathbf{M}_{pt}\dot{T} + \mathbf{K}_p\, p + \mathbf{G}_{pd}\dot{\mathbf{u}} = 0$
Mechanical Equilibrium	$\mathbf{G}_{dt} T + \mathbf{G}_{dp}\, p + \mathbf{K}_d \mathbf{u} = \mathbf{f_b} + \mathbf{f_{tr}}$

Time Discretization:

$$\dot{g} = f(g,t) \;\rightarrow\; \frac{g^{i+1} - g^{i}}{\Delta t} = (1-\theta)f^{i} + \theta f^{i+1}$$

Monolothic Solver

$$\mathbf{K_G}\boxed{\mathbf{U}^{i+1}} = \mathbf{F}_* + \mathbf{K}_*\boxed{\mathbf{U}^{i}}$$

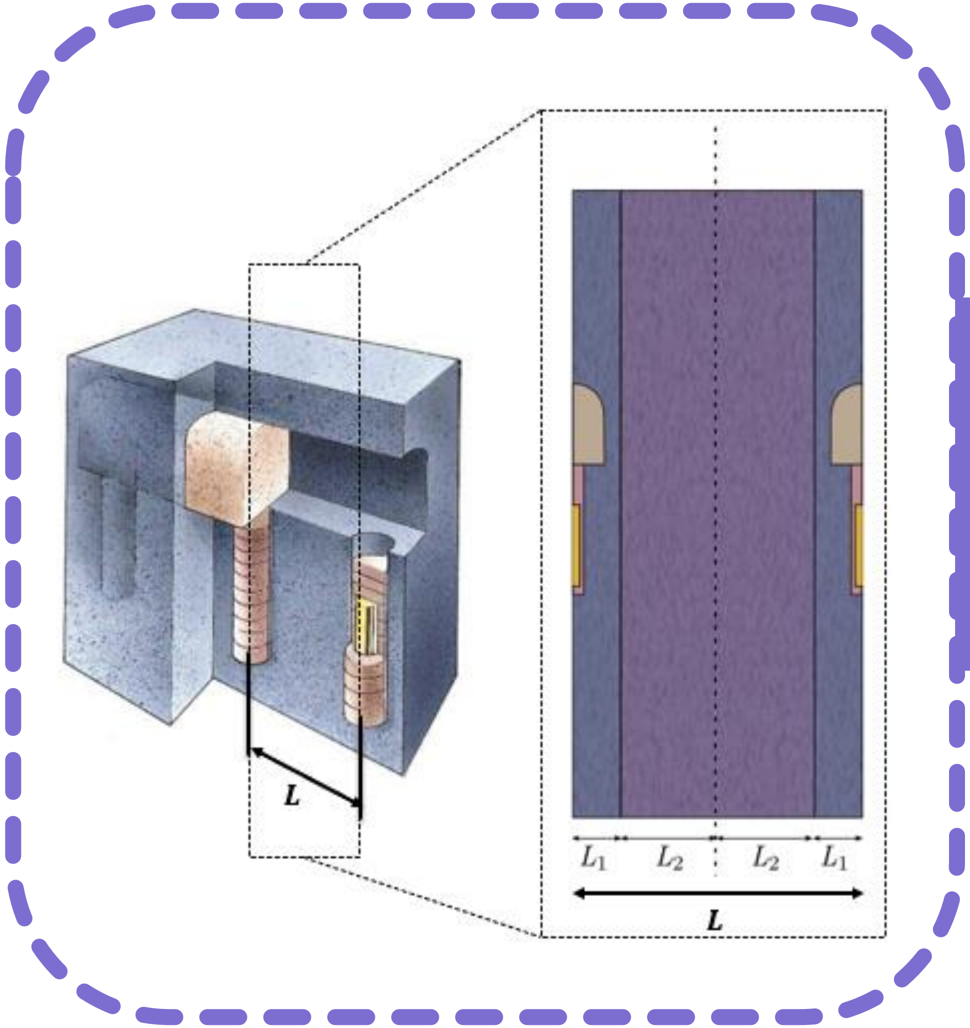
$$\mathbf{U}^{i+1} = \begin{bmatrix} \mathrm{T}^{i+1} \\ \mathrm{p}^{i+1} \\ \mathbf{u}^{i+1} \end{bmatrix}$$

$$\mathbf{U}^{i} = \begin{bmatrix} \mathrm{T}^{i} \\ \mathrm{p}^{i} \\ \mathbf{u}^{i} \end{bmatrix}$$

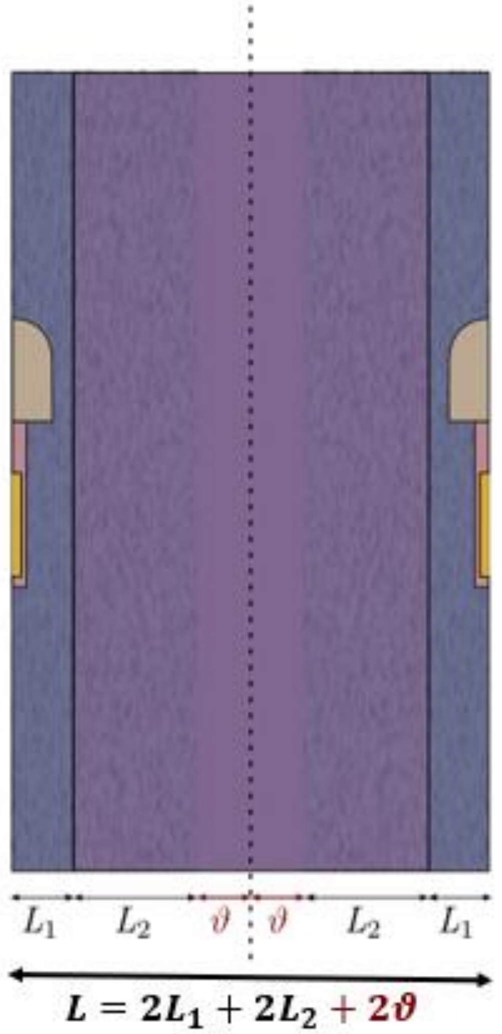
Definition of Parametric Problem

Three Material Parameters are considered uncertain	• κ (Heat Conductivty) • K (Hydraulic Conductivity) • E (Elastic Modulus)
Heat Conservation	$c_p^* \dot{\mathrm{T}} - \boldsymbol{\nabla}^{\mathrm{T}}(\kappa \boldsymbol{\nabla} \mathrm{T}) = \mathrm{q}$
Fluid mass Conservation	$-\boldsymbol{\nabla}^{\mathrm{T}}(K \boldsymbol{\nabla} \mathrm{p}) + \alpha \boldsymbol{\nabla} \dot{\mathbf{u}} + \left(\xi_1 + \frac{\xi_2}{\mathrm{E}}\right) \dot{\mathrm{p}} - \xi_3 \dot{\mathrm{T}} = 0$
Mechanical Equilibrium	$-\boldsymbol{\nabla}^{\mathrm{T}}(\mathbf{C}(\mathrm{E}, \upsilon) \boldsymbol{\nabla} \mathbf{u}) + \alpha \boldsymbol{\nabla} \mathrm{p} + \xi_4 \mathrm{E} \boldsymbol{\nabla} \mathrm{T} = \mathbf{b}$
Unknowns depend on material parameters	$\mathrm{T}(t, \Omega, \kappa, K, \mathrm{E})$, $\mathrm{p}(t, \Omega, \kappa, K, \mathrm{E})$ and $\mathbf{u}(t, \Omega, \kappa, K, \mathrm{E})$

Geometric Parameter ($\boldsymbol{\vartheta}$)



Geometric parameter ($\boldsymbol{\vartheta}$)
required distance between canisters



Unknowns also depend on geometric parameter

$\mathrm{T}(t, \Omega, \kappa, K, \mathrm{E}, \boldsymbol{\vartheta})$, $\mathrm{p}(t, \Omega, \kappa, K, \mathrm{E}, \boldsymbol{\vartheta})$ and $\mathbf{u}(t, \Omega, \kappa, K, \mathrm{E}, \boldsymbol{\vartheta})$

Generalized solution is high dimensional [3]

$$\mathrm{T}(t,\Omega,\kappa,K,\mathrm{E},\boldsymbol{\vartheta})\ ,\mathrm{p}(t,\Omega,\kappa,K,\mathrm{E},\boldsymbol{\vartheta})\ \text{and}\ \mathbf{u}(t,\Omega,\kappa,K,\mathrm{E},\boldsymbol{\vartheta})$$

$$\mathbf{U}(t,\underbrace{\Omega,\kappa,K,\mathrm{E},\boldsymbol{\vartheta}}_{\boldsymbol{\mu}}) = \begin{bmatrix} \mathrm{T}(t,\boldsymbol{\mu}) \\ \mathrm{p}(t,\boldsymbol{\mu}) \\ \mathbf{u}(t,\boldsymbol{\mu}) \end{bmatrix}$$

- **U** is six dimensional which is called high dimensional.
- Models defined in **high-dimensional** suffer from the so-called **curse of dimensionality**.

- **By using a standard mesh-based discretization technique, here Finite Element Method (FEM), wherein n_t, n_Ω, n_κ, n_K, n_E and n_ϑ are number of discretization for each dimension, the number of degrees of freedom for Generalized solution is:**

$$\boxed{\mathbf{n}_{\mathbf{Full}} = \mathbf{n}_t \times \mathbf{n}_\Omega \times \mathbf{n}_\kappa \times \mathbf{n}_\mathrm{K} \times \mathbf{n}_\mathrm{E}}$$

- FEM technique can become prohibitive with the **repetitive** solutions of PDEs

- In this work, **Encapsulated PGD** technique has been used to tackle this difficulty, with this technique the number of degrees of freedom for Generalized solution decreased to:

$$\mathbf{n}_{\mathbf{PGD}} = \mathbf{n}_t \times (\mathbf{n}_\Omega + \mathbf{n}_\kappa + \mathbf{n}_\mathrm{K} + \mathbf{n}_\mathrm{E})$$

[3]- Chinesta, F.; Keunings, R.; Leygue, A.: The Proper Generalized Decomposition for Advanced Numerical Simulation. Springer, 2014.

Encapsulated PGD [4]

- We seek a **Generalized solution** for $(\Omega, \kappa, K, \mathrm{E}, \vartheta) \in \Omega \times I_\kappa \times I_K \times I_\mathrm{E} \times I_\vartheta$ in each time step t.
- The **PGD** yields **an approximate solution** in the **separate form** for **each time step**:

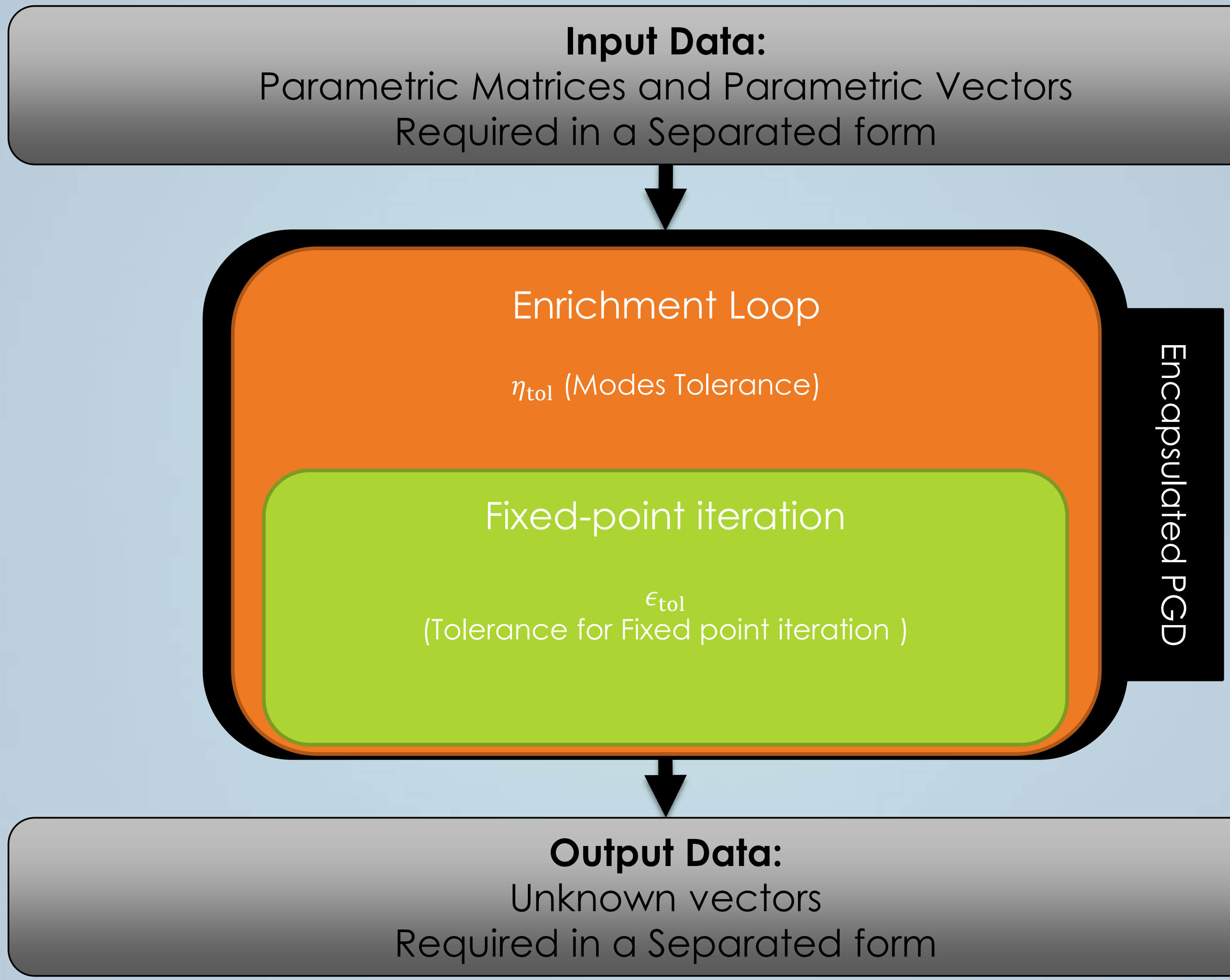
$$\mathbf{U}^{\boldsymbol{t}}_{\mathbf{PGD}}(\Omega, \kappa, K, \mathrm{E}, \vartheta) = \sum_{m=1}^{M} \mathbf{u}^m(\Omega) G_1^m(\kappa) G_2^m(K) G_3^m(\mathrm{E}) G_4^m(\vartheta)$$

- **PGD** contains **two inner loops** for computing enough terms (M) to approximate the **Generalized solution**
  - **Enrichment loop** (to compute successively terms of the solution)
  - **Fixed-point iteration** (to compute iteratively the modes in each term
- By using PGD method, the Stiffness Matrix and Force Vectors will be defined in separated formats (Monolothic Solver), and they are the main contribution of this work.

$$\mathbf{K}^{\boldsymbol{t}}_{\mathbf{PGD}}(\Omega, \kappa, K, \mathrm{E}, \vartheta) = \sum_{\widehat{m}=1}^{M_\phi} \mathbf{K}^{\widehat{m}}(\Omega) \phi_1^{\widehat{m}}(\kappa) \phi_2^{\widehat{m}}(K) \phi_3^{\widehat{m}}(\mathrm{E}) \phi_3^{\widehat{m}}(\vartheta)$$

$$\mathbf{F}^{\boldsymbol{t}}_{\mathbf{PGD}}(\Omega, \kappa, K, \mathrm{E}, \vartheta) == \sum_{\widetilde{m}=1}^{M_\psi} \mathbf{f}^{\widetilde{m}}(\Omega) \psi_1^{\widetilde{m}}(\kappa) \psi_2^{\widetilde{m}}(K) \psi_3^{\widetilde{m}}(\mathrm{E}) \psi_4^{\widetilde{m}}(\vartheta)$$

[4]- Diez, P.; Zlotnik, S.; Garcia-Gozalez, A.; Huerta, A.: Algebraic PGD for tensor separation and compression: An algoritmic approach. In: *Comptes Rendus Mecanique* 346 (2018), p. 501-514


Input Data:
Parametric Matrices and Parametric Vectors
Required in a Separated form
Enrichment Loop
η_{tol} (Modes Tolerance)
Fixed-point iteration
ϵ_{tol}
(Tolerance for Fixed point iteration)
Encapsulated PGD
Output Data:
Unknown vectors
Required in a Separated form

Numerical Results

First Example, Thermal Transient with Geometric and Material parameter.

- Domains
  - **Geometrical parameter**

$$\vartheta = [-5\text{ m} \quad 6\text{m}]$$

  - **Material parameter is Heat conductivity of the Rock ($\kappa_{\mathrm{R}} = \mu_{\kappa}$)**

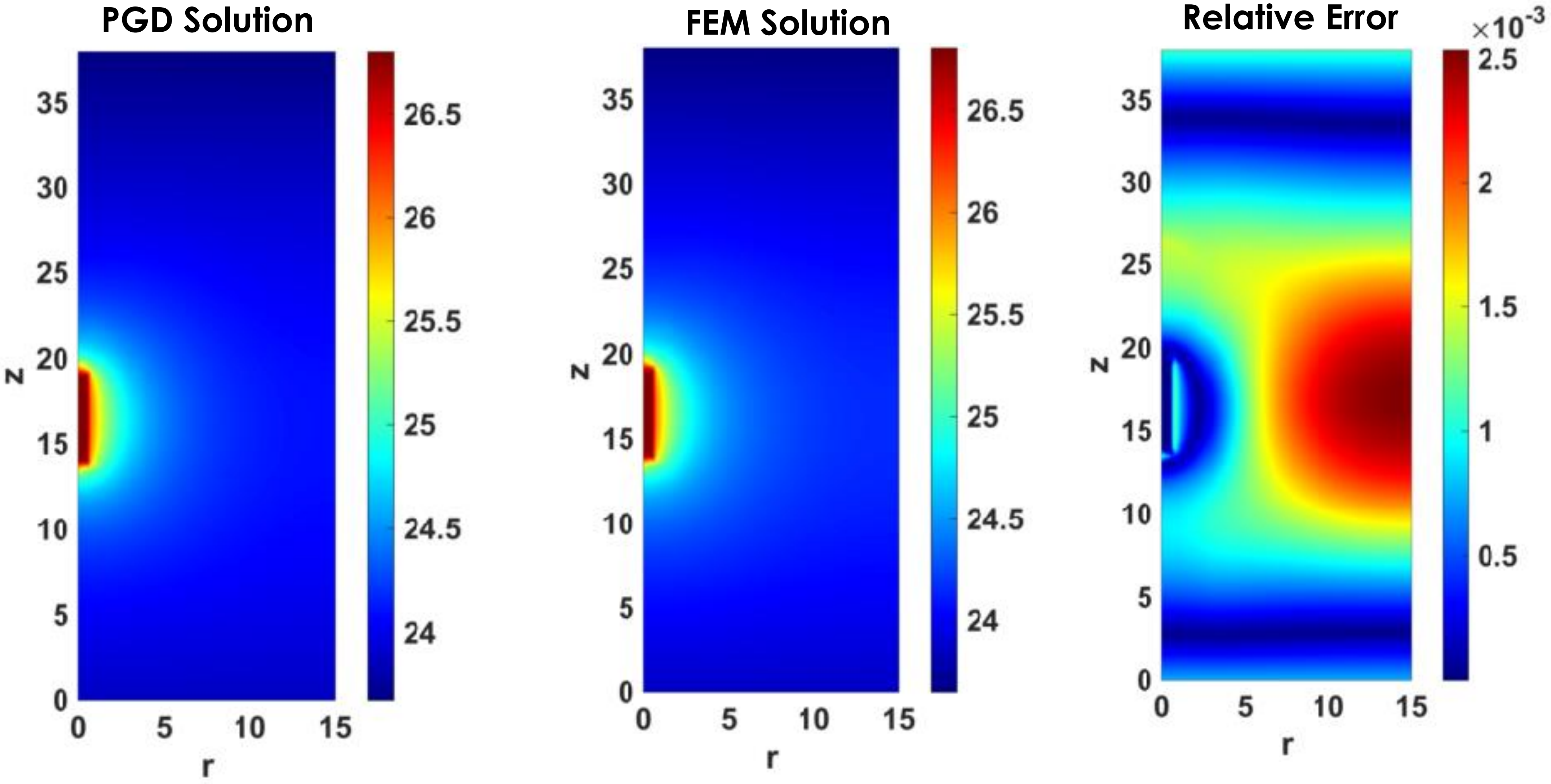
$$\mu_{\kappa} = [1\,\frac{\mathrm{W}}{\mathrm{m\,°K}} \quad 3\,\frac{\mathrm{W}}{\mathrm{m\,°K}}]$$

  - **Time domain**

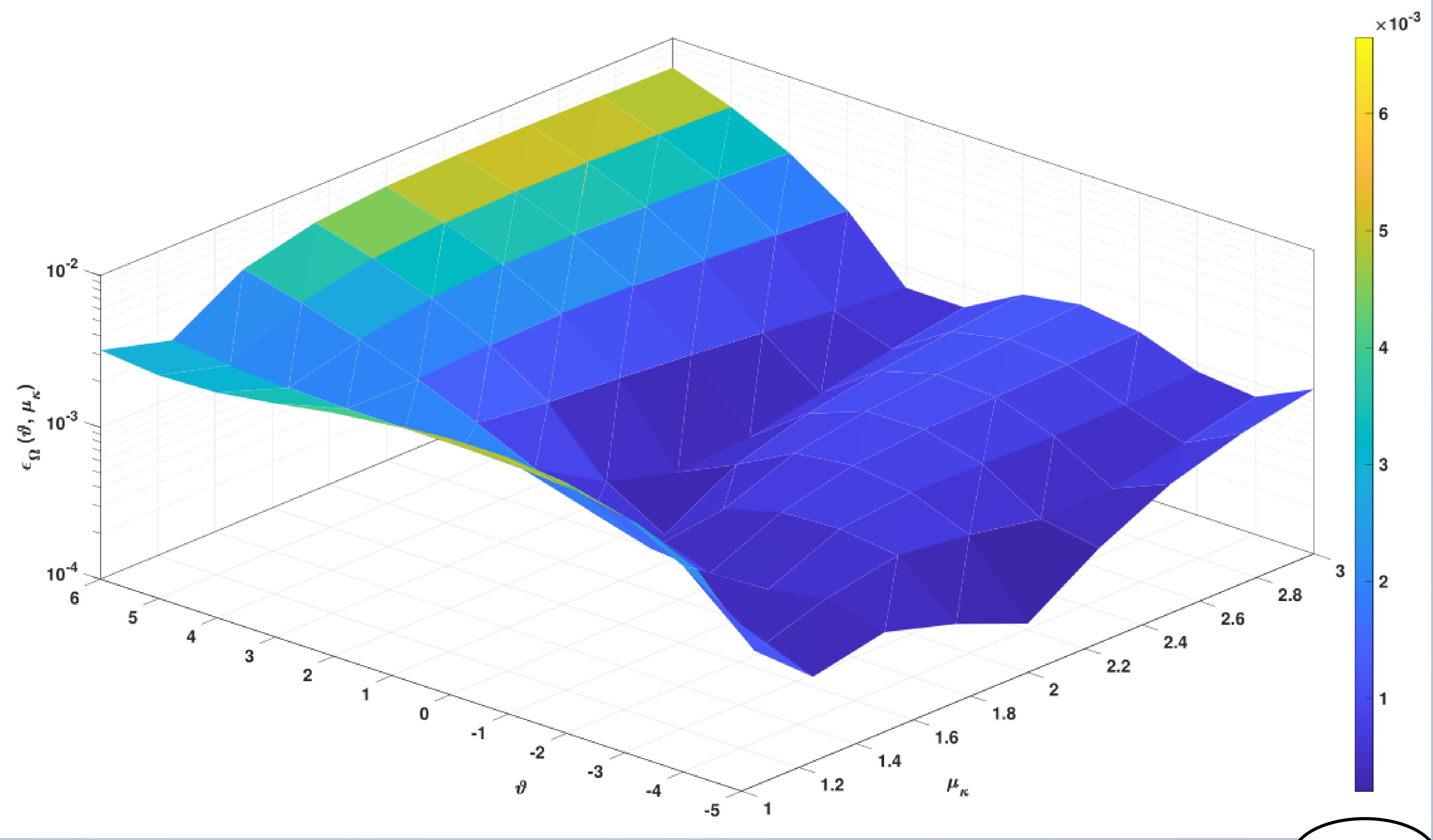
$$t = [0\; year \quad 1000\; year]$$

Encapsulated PGD vs FEM Solution for one point

$$\mu_\kappa = 2.61\,\frac{\mathrm{W}}{\mathrm{m}\,{}^\circ\mathrm{K}}, \vartheta = 6\ \mathrm{m}$$



3D Map of the Error integrated over Space at $t = 380$ year



$$\epsilon_\Omega(\mu_\kappa, \vartheta) = \frac{\|T_{FEM} - T_{PGD}\|_\Omega}{\|T_{FEM}\|_\Omega}$$

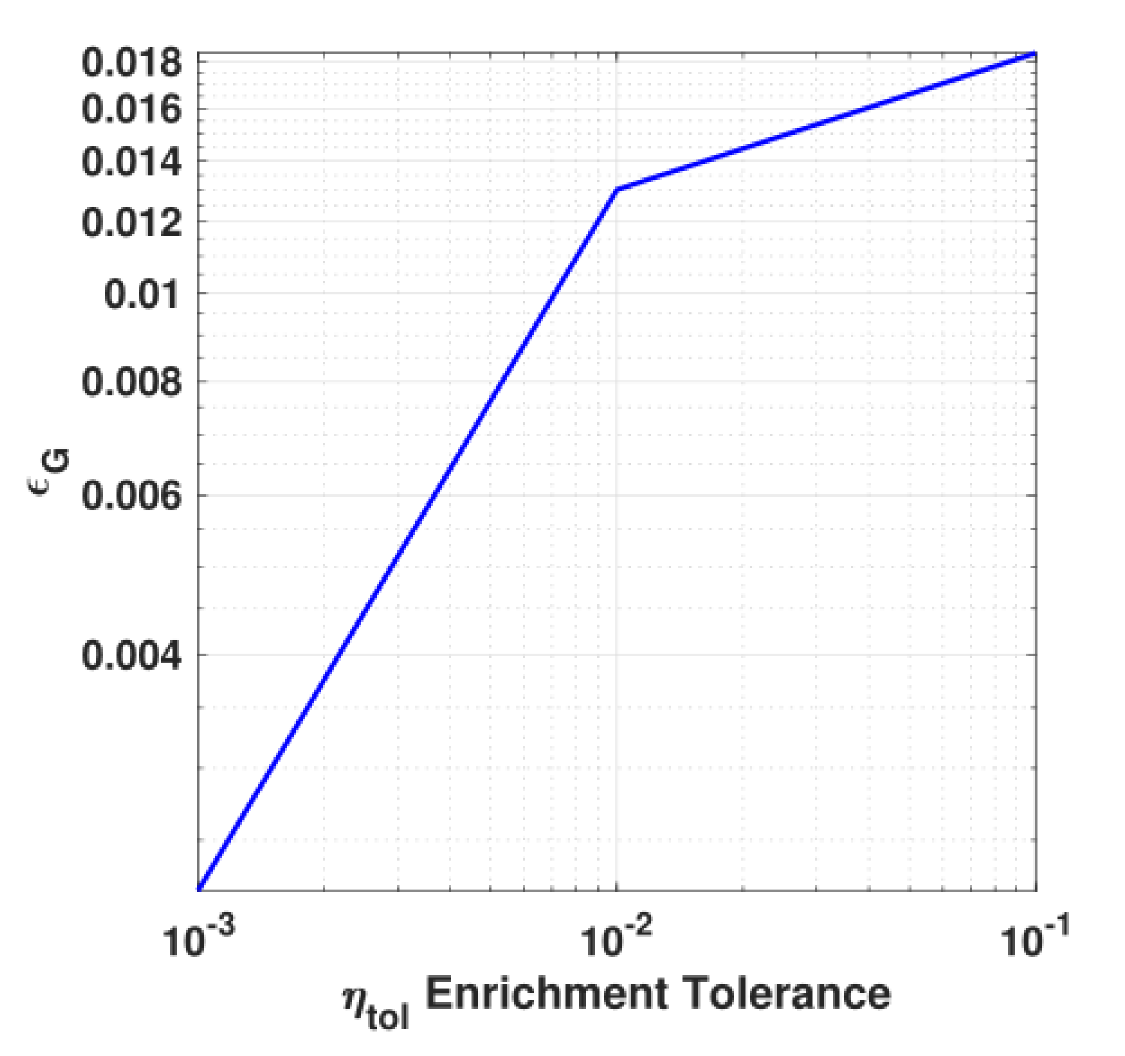
$\Omega \rightarrow$ Space

Average error integrated in time and parameters decreases with the enrichment tolerance

Global Error

$$\epsilon_G = \frac{\|U_{FEM} - U_{PGD}\|_{\Omega\times I_{\kappa_R}\times I_{\vartheta}}}{\|U_{FEM}\|_{\Omega\times I_{\kappa_R}\times I_{\vartheta}}}$$

$$\Omega \rightarrow \text{Space}$$
$$I_{\kappa_R} \in [1,3]$$
$$I_{\vartheta} \in [-5,6]$$
$$I_t \in [1,1000]$$



Based on following data:

- $\boldsymbol{\vartheta = -5:6}$
- $\boldsymbol{\kappa_R = 1:0.25:3}$
- $\boldsymbol{t = 1:1000}$
- $\textbf{Modes} = \mathbf{1:20}$

Numerical Results

Second Example, THM Steady State case with Geometric and Material parameters.

Three Material Parameters

- **Heat Conductivity of the Rock** $(\boldsymbol{\mu_1})$
- **Hydraulic Conductivity of the Rock** $(\boldsymbol{\mu_2})$
- **Elastic Modulus of the Rock** $(\boldsymbol{\mu_3})$

+

Geometric Parameter

- **required distance between canisters** (ϑ)

- Domains
  - **Geometrical parameter:**

$$\vartheta \in [-5\mathrm{m} \;\; 6\mathrm{m}]$$

  - **Material parameter:**

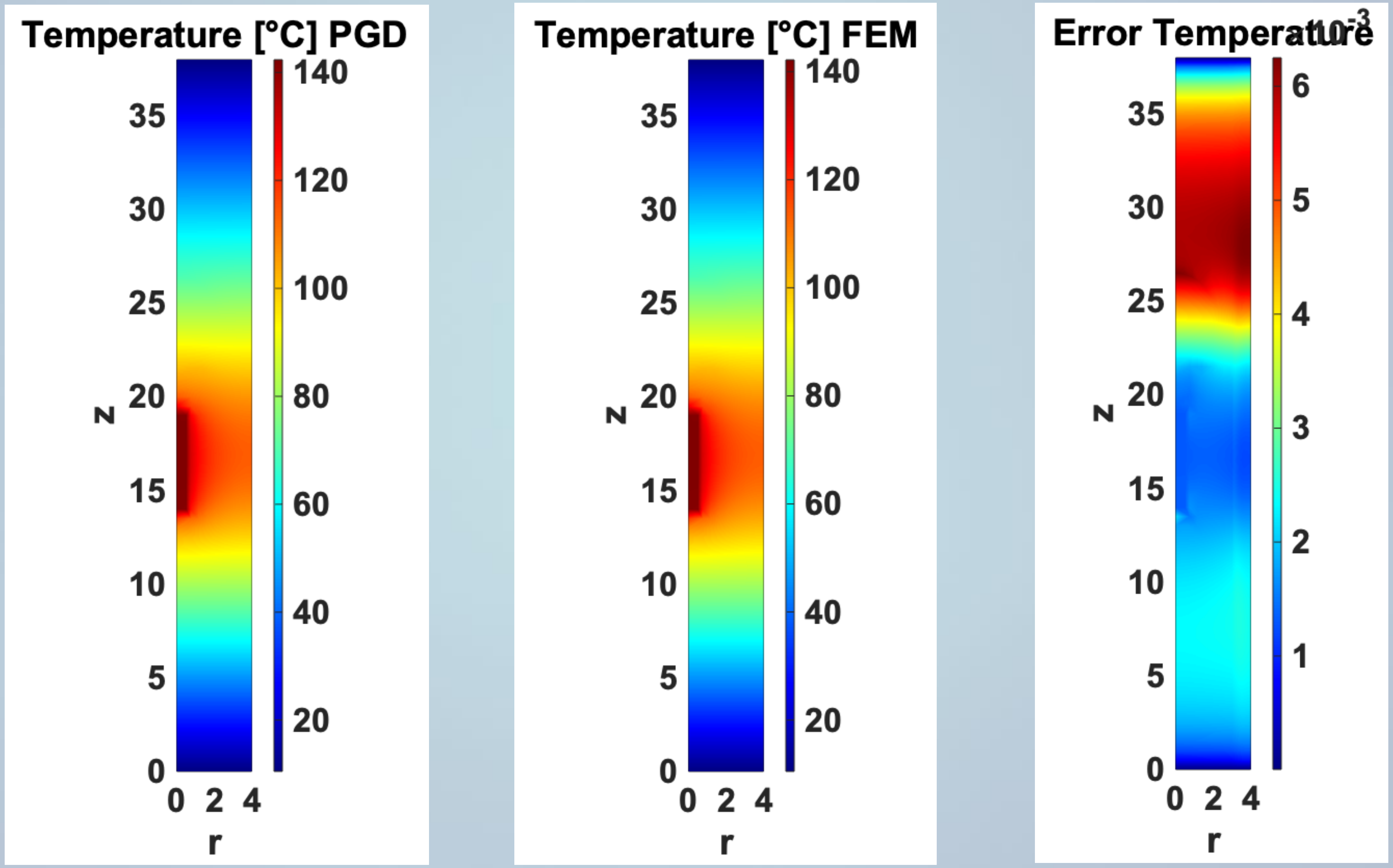
$$\mu_1 \in [1\frac{\mathrm{W}}{\mathrm{m}^\circ\mathrm{K}} \;\; \mathbf{3}\, \frac{\mathrm{W}}{\mathrm{m}^\circ\mathrm{K}}], \;\; \mu_2 \in [\, 2\times 10^{-13}\frac{\mathrm{m}}{\mathrm{s}} \;\; 1.02\times 10^{-11}\frac{\mathrm{m}}{\mathrm{s}}] \;\; \text{and} \;\; \mu_3 \in [55000\mathrm{MPa} \;\; 75000\mathrm{MPa}]$$

Encapsulated PGD vs FEM for one point

$\mu_1 = 2.61 \frac{\mathrm{W}}{\mathrm{m\ ^\circ K}}, \mu_2 = 1.52 \times 10^{-12}\ \frac{\mathrm{m}}{\mathrm{s}}$ and $\mu_3 = 65000\ \mathrm{MPa}$ and $\vartheta = -5\ \mathrm{m}$

Number of Modes

200

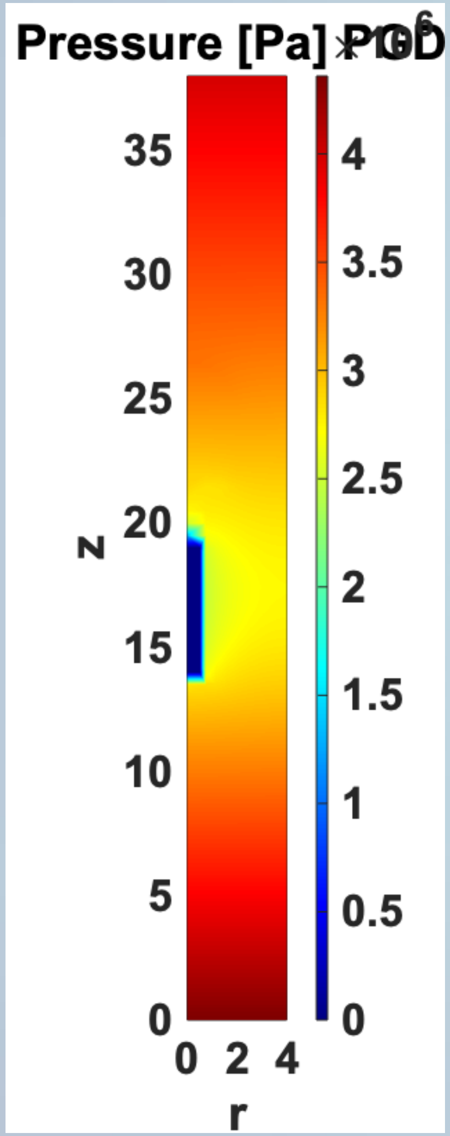


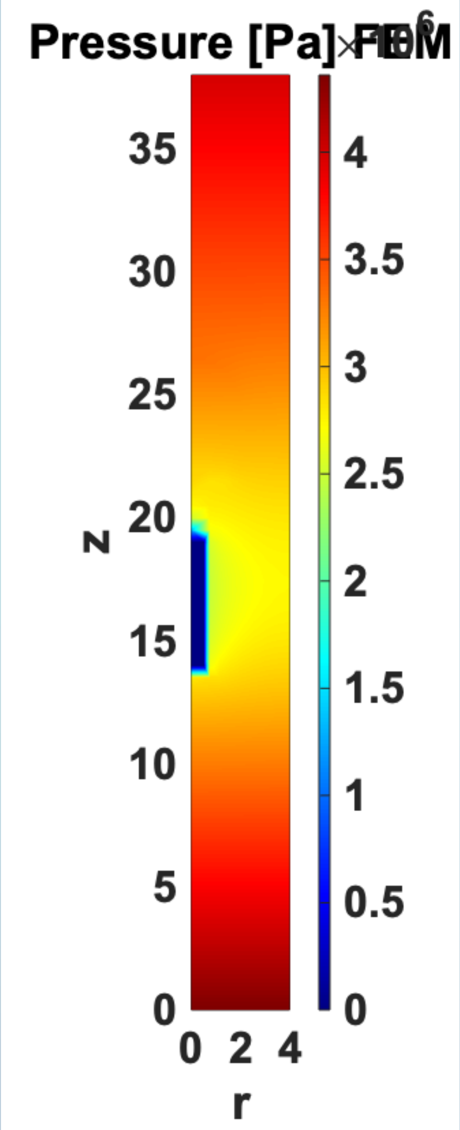
Encapsulated PGD vs FEM for one point

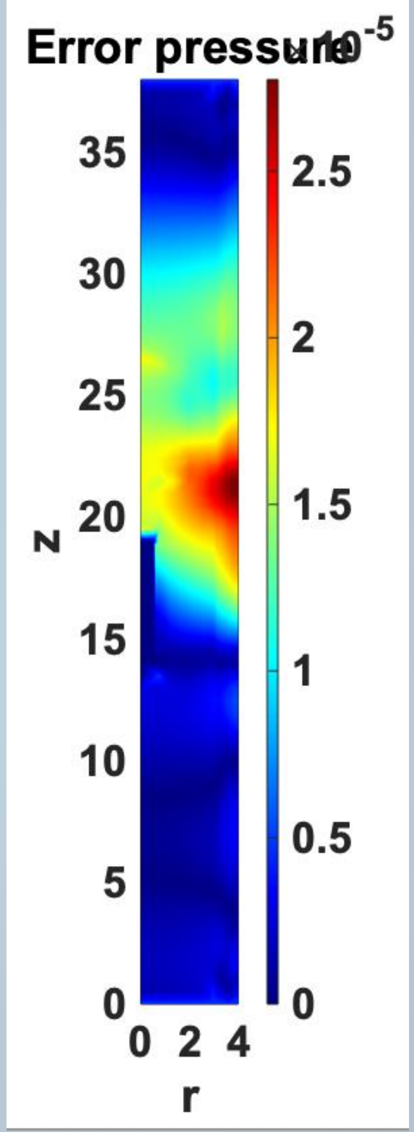
$\mu_1 = 2.61 \frac{\mathrm{W}}{\mathrm{m\,°K}}, \mu_2 = 1.52 \times 10^{-12}\ \frac{\mathrm{m}}{\mathrm{s}}$ and $\mu_3 = 65000\ \mathrm{MPa}$ and $\vartheta = -5\ \mathrm{m}$

Number of Modes

200





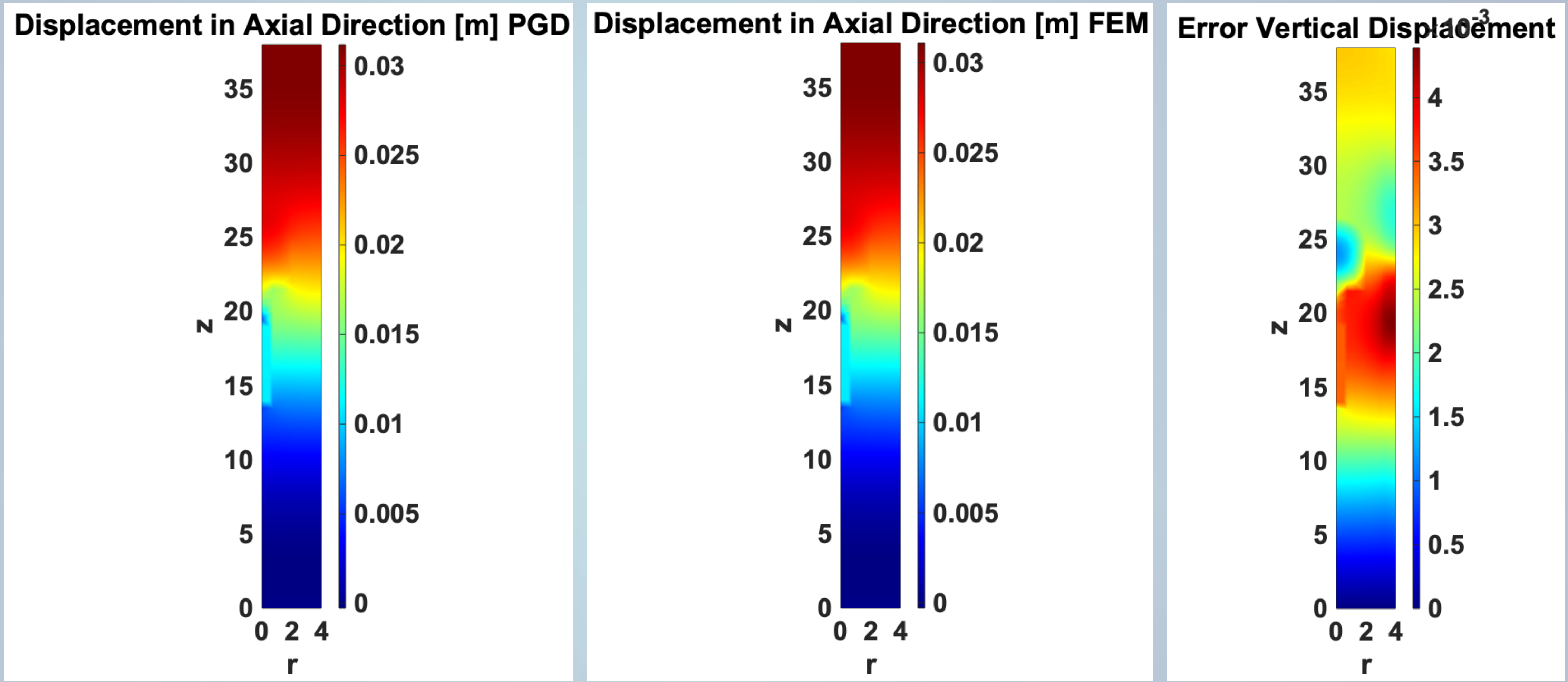


Encapsulated PGD vs FEM for one point

$$\mu_1 = 2.61\,\frac{\mathrm{W}}{\mathrm{m\ ^\circ K}}, \mu_2 = 1.52 \times 10^{-12}\,\frac{\mathrm{m}}{\mathrm{s}} \text{ and } \mu_3 = 65000\ \mathrm{MPa} \text{ and } \vartheta = -5\ \mathrm{m}$$

Number of Modes

200

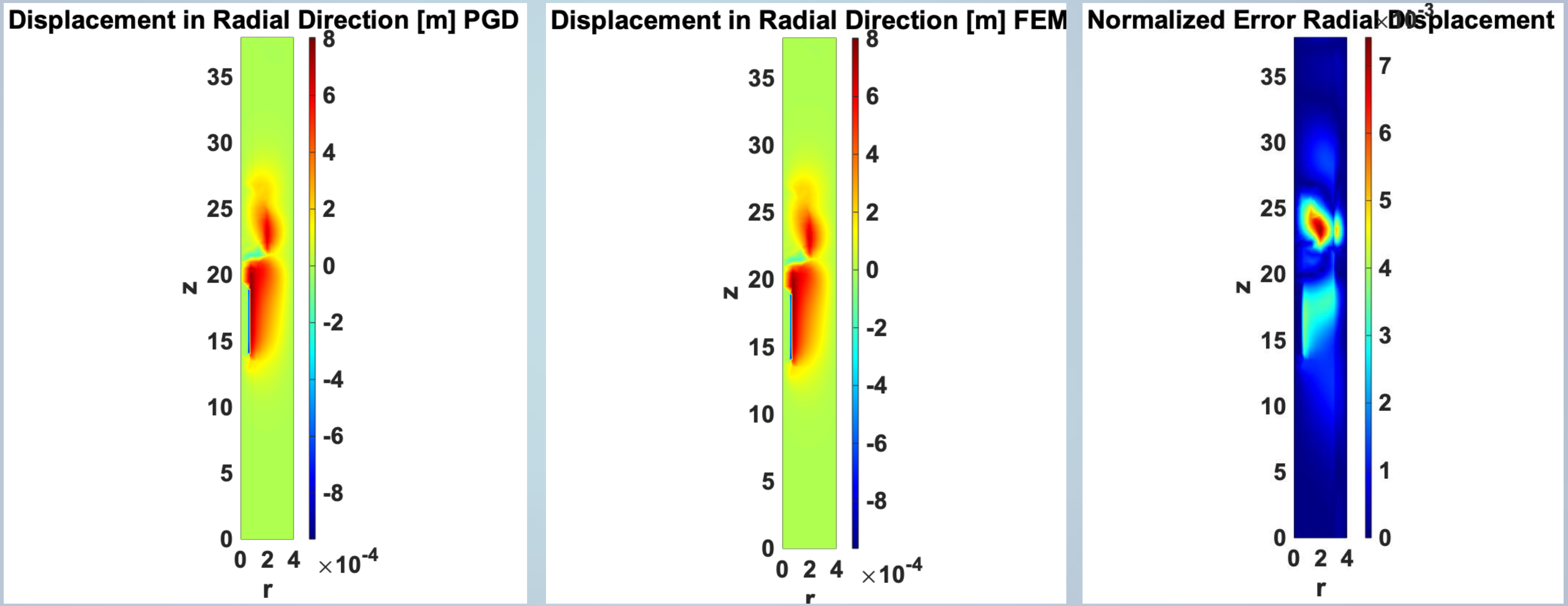


Encapsulated PGD vs FEM for one point

$\mu_1 = 2.61 \frac{\mathrm{W}}{\mathrm{m}\,^{\circ}\mathrm{K}}, \mu_2 = 1.52 \times 10^{-12}\ \frac{\mathrm{m}}{\mathrm{s}}$ and $\mu_3 = 65000\ \mathrm{MPa}$ and $\vartheta = -5\ \mathrm{m}$

Number of Modes

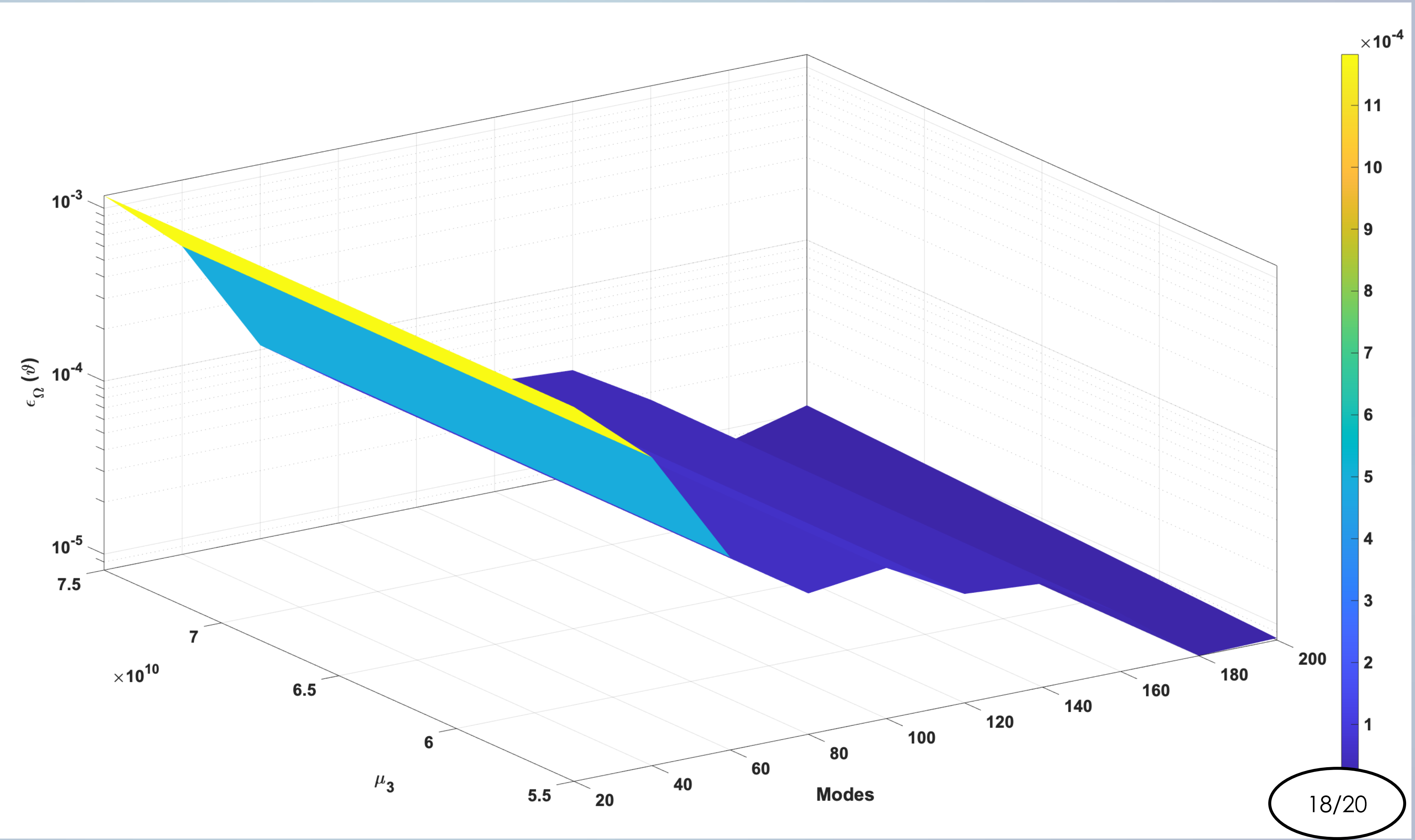
200



3D Map of the Error integrated over Space for a fixed input data value of $\vartheta = -5, \mu_1 = 2.61$ and $\mu_2 = 1.52 \times 10^{-12}$

$$\epsilon_\Omega(\mu_3) = \frac{\|U_{FEM} - U_{PGD}\|_\Omega}{\|U_{FEM}\|_\Omega}$$

$\Omega \rightarrow$ Space

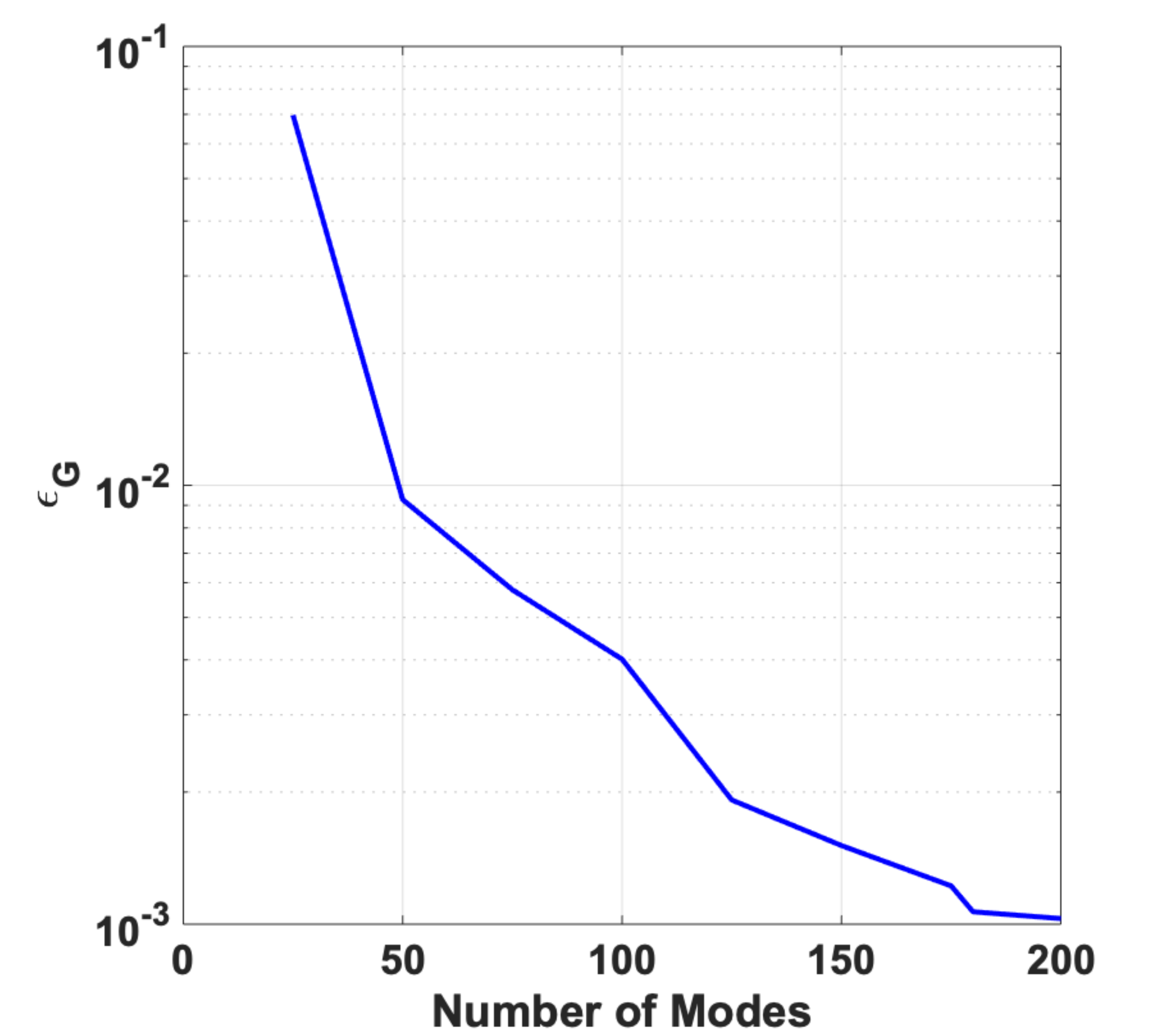


Average error integrated in time and parameters decreases with the Number of Modes

Global Error

$$\epsilon_G = \frac{\|U_{FEM} - U_{PGD}\|_{\Omega\times I_{\mu_1}\times I_{\mu_2}\times I_{\mu_3}\times I_\vartheta}}{\|U_{FEM}\|_{\Omega\times I_{\mu_1}\times I_{\mu_2}\times I_{\mu_3}\times I_\vartheta}}$$

$$\Omega \rightarrow \text{Space}$$
$$I_{\mu_1} \in [1,3]$$
$$I_{\mu_2} \in [2\times 10^{-13}, 1.02\times 10^{-11}]$$
$$I_{\mu_3} \in [5.5\times 10^{10}, 7.5\times 10^{10}]$$
$$I_\vartheta \in [-5,6]$$



Based on following data:

- $\boldsymbol{\vartheta} = [-5, -2.8088, -0.6066, 1.5956, 3.7978, 6]$
- $\boldsymbol{\mu_1} = [1, 1.4975, 1.9975, 2.4975, 3]$
- $\boldsymbol{\mu_2} = [0.002, 0.0219, 0.0419, 0.0619, 0.0819, 0.1020] \times 10^{-10}$
- $\boldsymbol{\mu_3} = [5.5, 5.9975, 6.4975, 6.9975, 7.5] \times 10^{10}$
- $\textbf{Modes} = [25, 50, 75, 100, 125, 150, 175, 180, 200]$

Conclusion and Outlook

Conclusion

- It has shown that PGD is numerical method able to provide generalized solutions of parametric problems.
- For finding Generalized Solution for such problems, PGD solver is much faster in comparison with FEM solver
- This presentation shows how ROM can provide real time solution to (simple) THM problems.

Outlook

- Final goal is finding Generalized Solution for Transient THM problem with both Geometric and Material Parameters.

Questions?

Thanks for your attention!