Geometry-aware framework for deep energy method: an application to structural mechanics with hyperelastic materials

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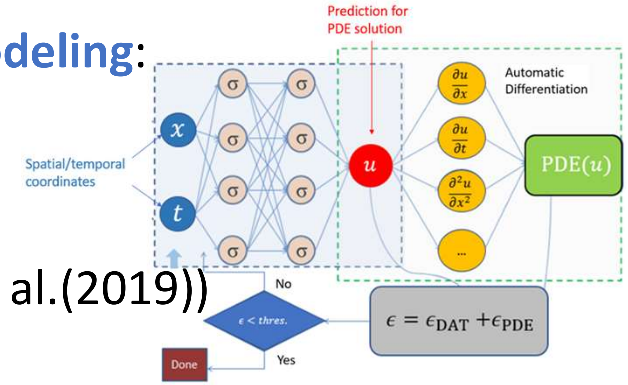
1. Context and background

Motivation

- **PINNs** (Raissi et al. (2019)) have gained much attention in **physical modeling**:
  - Uses a feedforward network as approximator
  - Integrates PDEs (strong form) as constraints in the loss function
  - Uses automatic differentiation to calculate the derivatives (at colocation points)



- **Deep energy method (DEM)** (Samaniego et al. (2019), Nguyen-Thanh et al.(2019))
  - Use the same principle of PINNs to solve the problems
  - Employ weak form of the physical system in the loss function

- However, **vanilla PINNs and DEM** are capable of inferring the solution on **only one configuration** (i.e. fixed IC/BCs, geometry, and other constraints).

Physics-informed neural operators

- Physics-informed DeepOnet (Li et al. (2021))
- Physics-informed Fourier Neural Operator (Wang et al. (2021))

➡ Inferring on **new PDE parameters, or new ICs / BCs.**

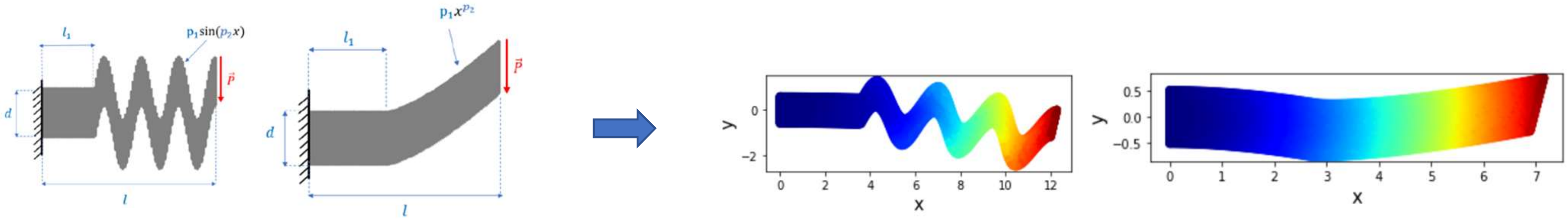
Geometry-aware framework

- PhyGeoNet (Gao et al. (2021))
- Physics-informed Point Net (Kashefi et al. (2022))
- Geometry-aware PINNs (Oldenburg et al. (2022))

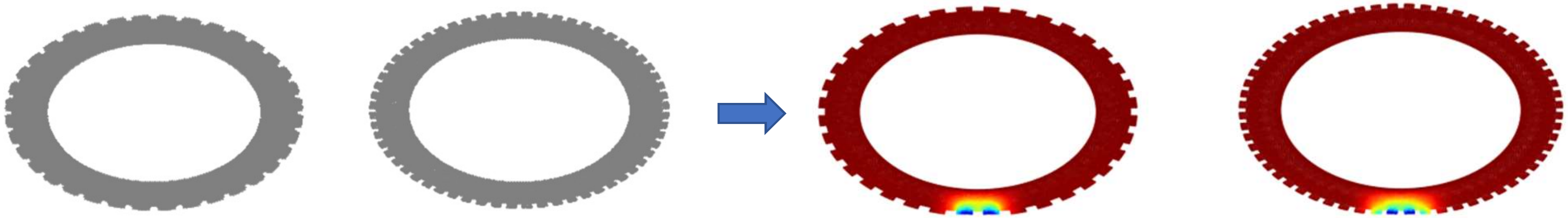
➡ Inferring on **new geometries.**

1. Context and background

- **Objective**: **infer the solution on various geometries for structural mechanical problems**.
    - An academic test case with reference solution produced by FEniCS.



- A more realistic industrial case with reference solution produced by an in-house solver.



- We propose novel **geometry-aware framework for physics-informed models**
    - Combing weak form of the physical system and shape encoding in the loss function.
    - Shape encoding: parametric encoding, PCA, VAE.
    - Extension with spatial coordinates or images to represent the geometry for real-world application.

Geometry-aware deep energy method (GADEM)

2. Solid mechanics: physical model

Problem: Find the displacement field $\boldsymbol{u}: \boldsymbol{\Omega} \rightarrow \boldsymbol{R}^{\boldsymbol{d}}$ and a constraint field $\mathbf{P}: \boldsymbol{\Omega} \rightarrow \boldsymbol{M}^{\boldsymbol{d}}$ such that:

Strong form

Constitutive law	$\mathbf{P} = \partial_{\boldsymbol{F}} W(\boldsymbol{F})$	in	$\boldsymbol{\Omega}$
Equations of motion	$\mathrm{Div}\, \mathbf{P} + \mathbf{f_0} = \mathbf{0}$	in	$\boldsymbol{\Omega}$
Boundary conditions	$\boldsymbol{u} = \boldsymbol{u}_{\boldsymbol{d}}$	on	$\boldsymbol{\Omega}_{\mathbf{D}}$
	$\mathbf{PN} = \mathbf{f_2}$	in	$\boldsymbol{\Omega}_{\mathbf{N}}$

- Very complex systems of PDEs.
- Hard to solve using classical PINNs as involving many high order differentiations.

Weak form

Potential energy
(at minimum in the equilibrium state)

$$\Pi(\boldsymbol{\phi}) = \int_{\boldsymbol{\Omega}} W dV - \int_{\boldsymbol{\Omega}} \boldsymbol{f}_{\mathbf{0}} . \boldsymbol{\phi} dV - \int_{\boldsymbol{\Omega}_{\mathbf{N}}} \boldsymbol{f}_{\mathbf{2}} . \boldsymbol{\phi} dA$$

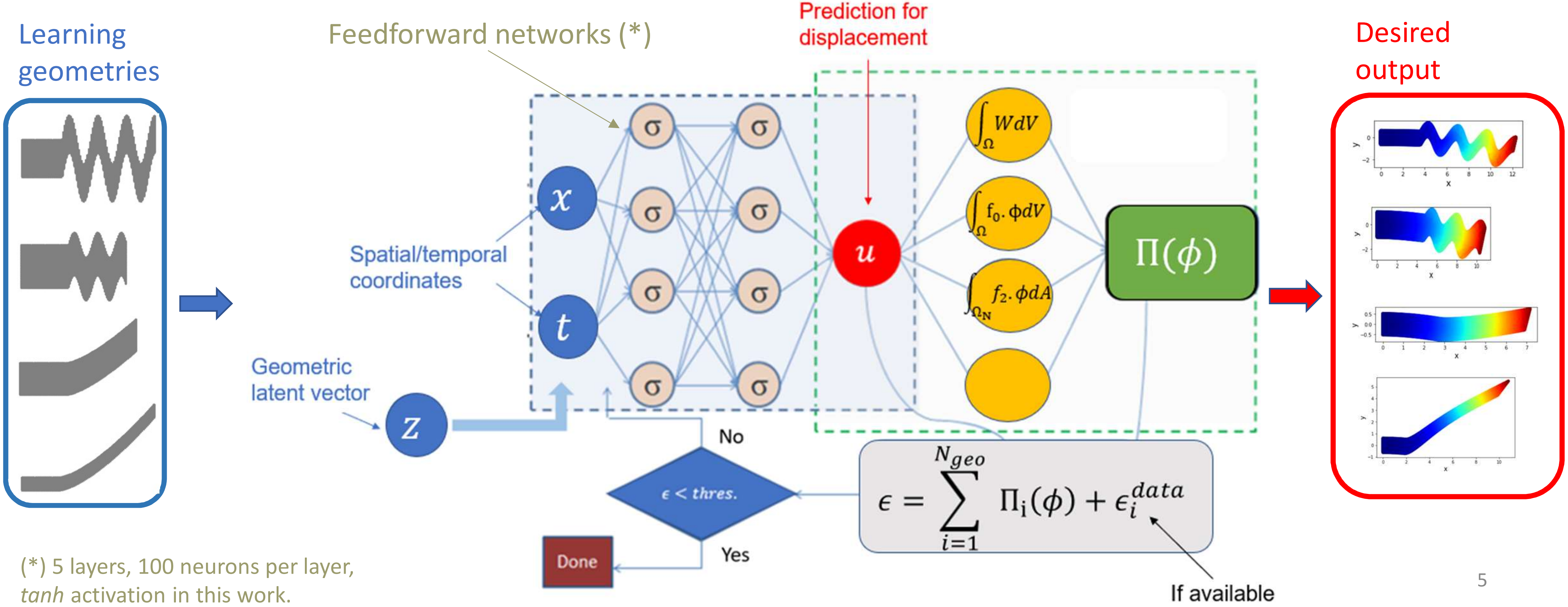
where $\boldsymbol{\phi}$ is a trial function and the displacement $\boldsymbol{u}$ fulfills the boundary condition *a priori*.

- Using only first-order differentiations.
- ➡ Small computational cost and fast training time.
- Reduce dependencies on PDEs of the base function.

3. Geometry-aware deep energy method (GADEM)

GADEM is based on the same principle of DEM, and:

- Encodes the geometric knowledge into the model.
- The potential energy of the systems over all geometries are minimized.

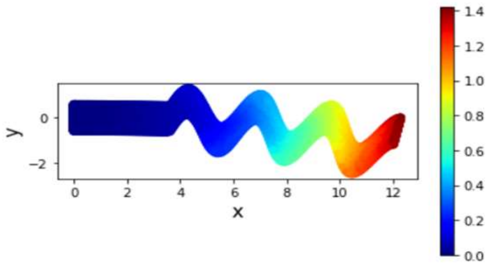


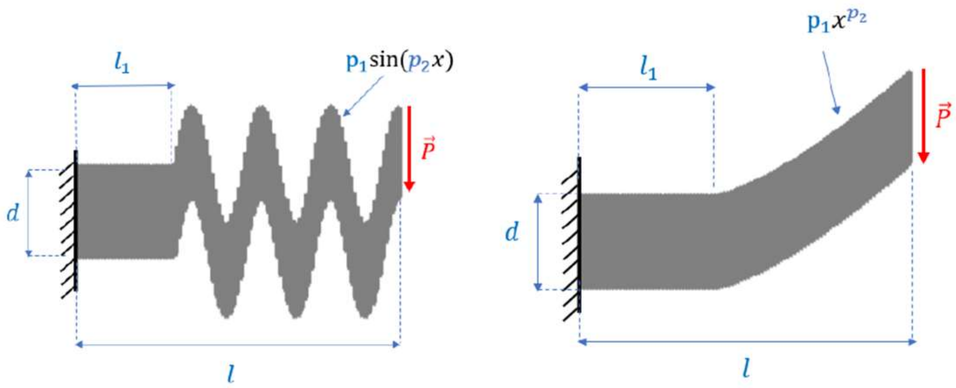
(*) 5 layers, 100 neurons per layer, *tanh* activation in this work.

4. Academic experimental design

Linear elasticity problem (small deformation):

- **Input:** The geometry depends on five parameters l, d, l_1, p_1, p_2.
- **Configuration:** The left side is clamped and the right side is subjected to a traction $\vec{P} = (0, -0.1)N$. Homogeneous, isotropic beams with Young's modulus $E = 1000N/m^2$, and Poisson's ratio $\nu = 0.3$.
- **Desired output:** The reference solution with FEniCS by Finite Element Method (FEM)



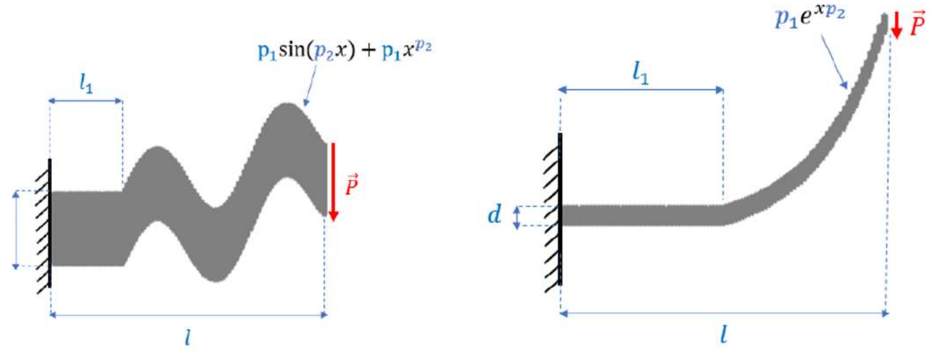


(a) Training set 1

(b) Training set 2

	Nb. geometries	Shape	Interval of parameters l, d, p_1, p_2, p
Train	50	$p_1 sin(p_2 x)$	$[4, 12], [1, 3], [1, 2], [0.5, 1.5], [0.25, 0.5]$
	50	$p_1 x^{p_2}$	$[4, 12], [1, 3], [0.1, 1], [1, 1.5], [0.25, 0.5]$
Test 1	10	$p_1 sin(p_2 x)$	$[4, 12], [1, 3], [1, 2], [0.5, 1.5], [0.25, 0.5]$
	10	$p_1 x^{p_2}$	$[4, 12], [1, 3], [0.1, 1], [1, 1.5], [0.25, 0.5]$
Test 2	10	$p_1 sin(p_2 x)$	$[12, 14], [3, 4], [2, 2.5], [0.25, 0.5], [0.5, 0.6]$
	10	$p_1 x^{p_2}$	$[2, 4], [0.5, 1], [0.05, 0.1], [1.5, 2], [0.1, 0.25]$
Test 3	20	$p_1 sin(p_2 x) + p_1 x^{p_2}$	$[4, 12], [1, 3], [1, 2], [0.5, 1.5], [0.25, 0.5]$
Test 4	20	$p_1 \exp(p_2 x)$	$[4, 12], [1, 3], [1, 2], [0.5, 1.5], [0.25, 0.5]$

Table 1: *Configuration for the geometries in training and testing sets.*

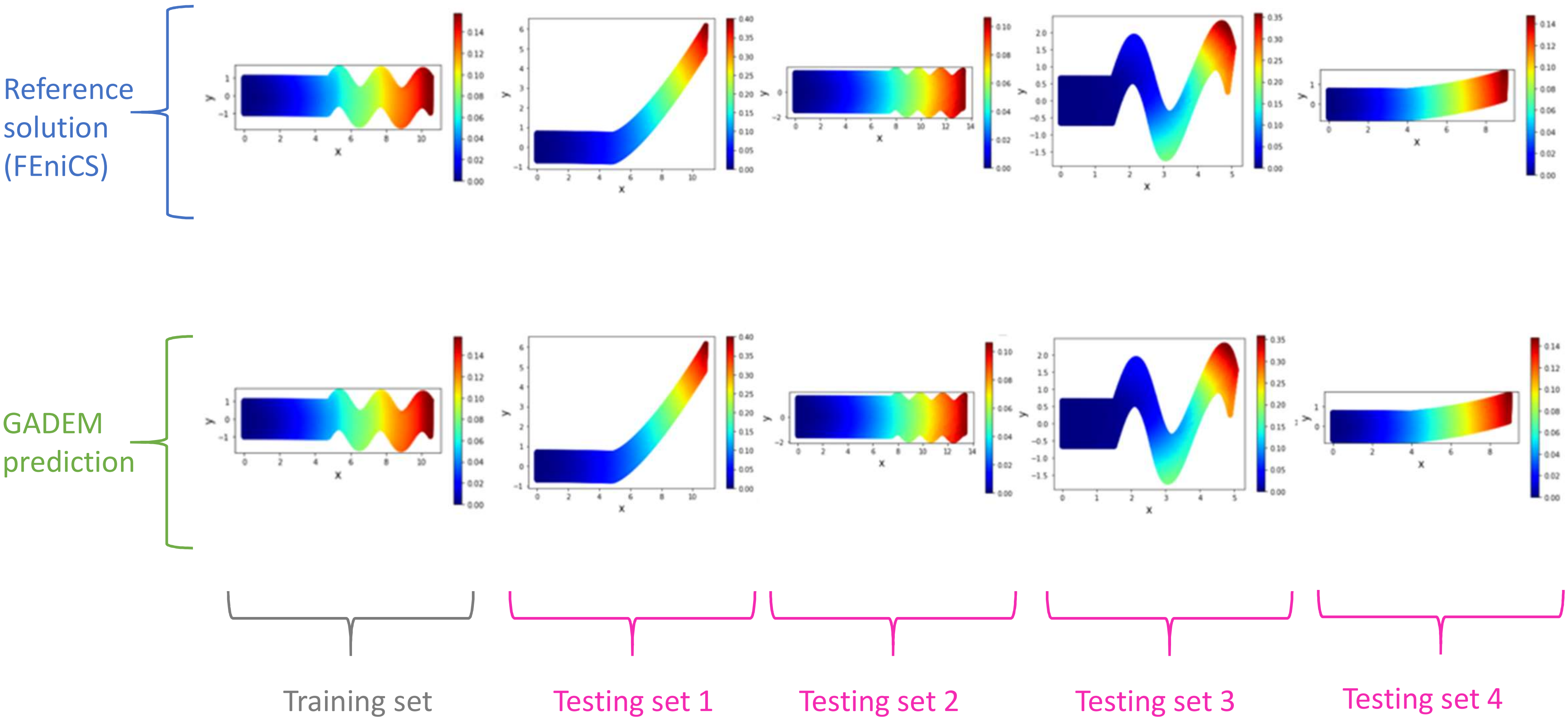


(a) Testing set 3

(b) Testing set 4

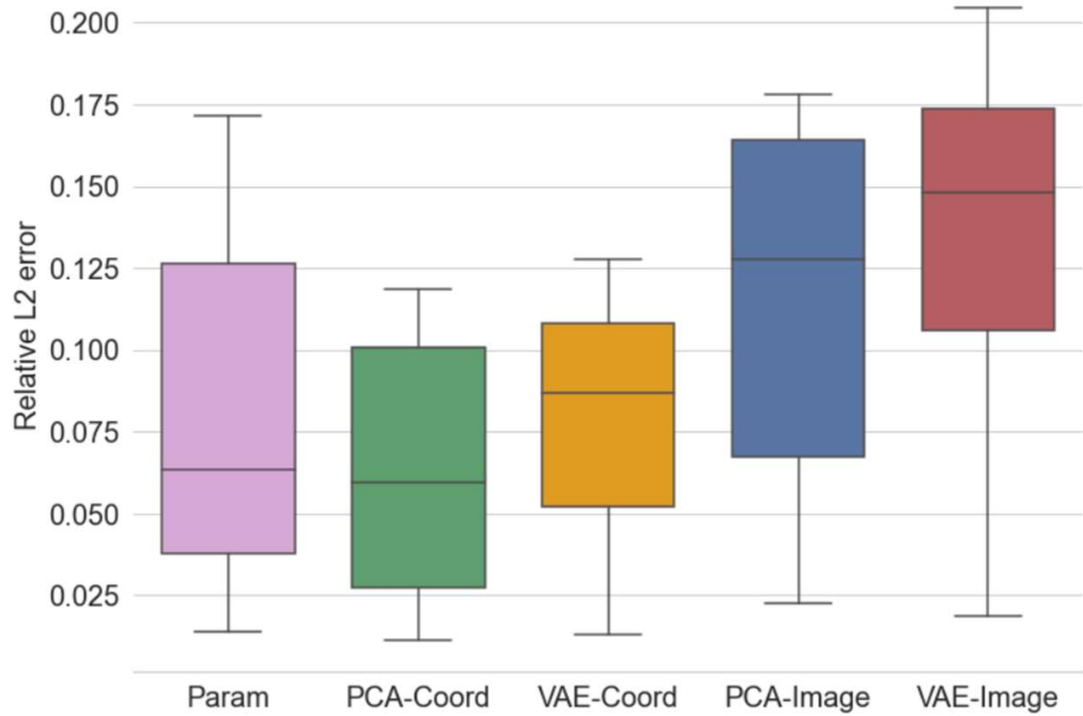
4. Academic experimental design

Illustration of GADEM prediction:

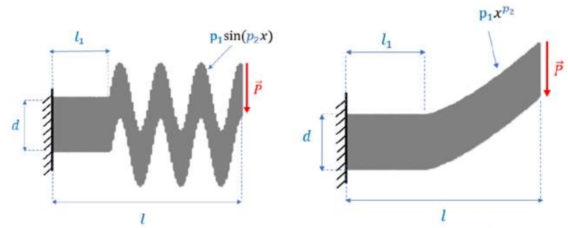


4. Geometric encoding for GADEM: comparison

Performance on training set:



Error of the prediction for all geometries in the **training set**



(a) Training set 1 (b) Training set 2

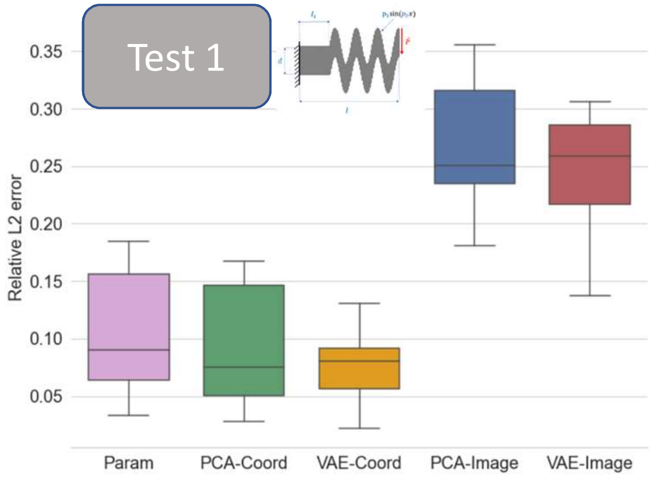
- **Parametric encoding**: geometric parameters (if available).
- **PCA-Coord**: spatial coordinates to represent the geometries and PCA to encode the geometries.
- **VAE-Coord**: spatial coordinates to represent the geometries and VAE to encode the geometries.
- **PCA-Image**: images to represent the geometries and PCA to encode the geometries.
- **VAE-Image**: images to represent the geometries and VAE to encode the geometries.

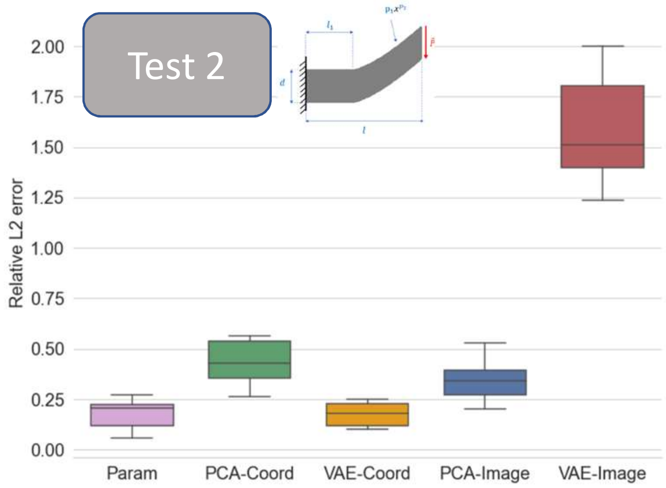
Size of latent vector is fixed $k = 5$.

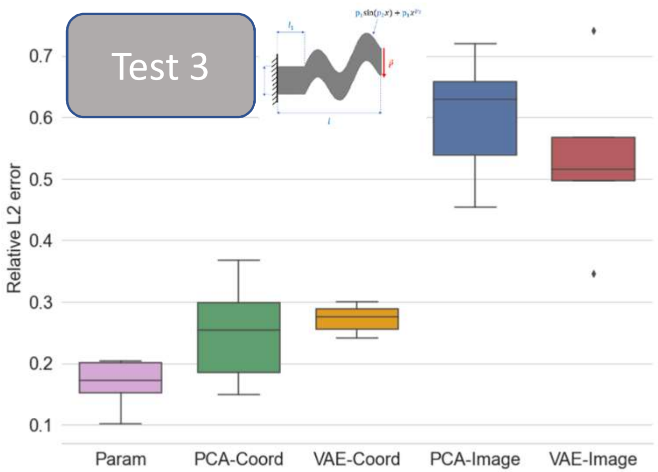
- GADEM approaches provides good prediction for the solutions (errors vary from 1%-20%)
- The approaches using spatial coordinates performs better than the approaches using images.

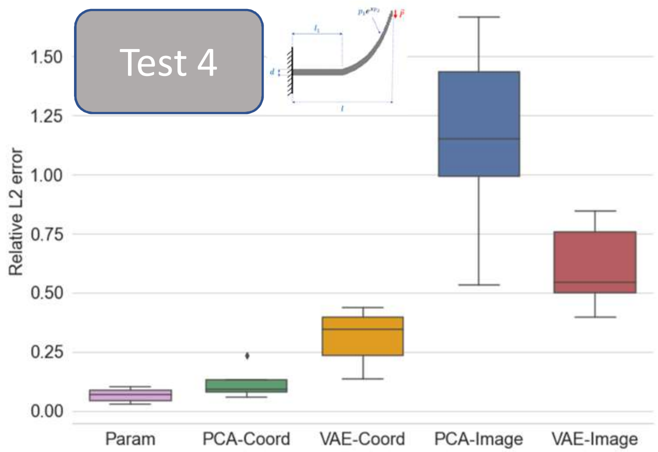
4. Geometric encoding for GADEM: comparison

Performance on testing set









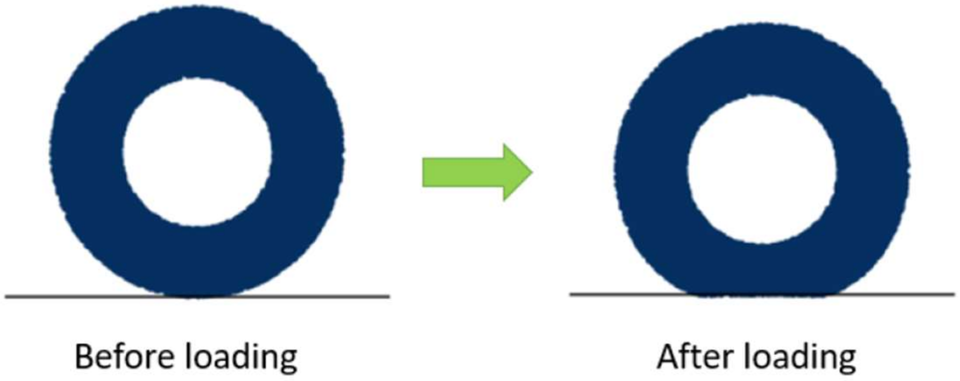
- The approaches using spatial coordinates perform better than the approaches using images.
- On the same shapes of geometries as training (test 1 and test 2), VAE-Coord provides better prediction than PCA-Coord.
- On new shapes of geometries (test 3 and test 4), PCA-Coord provides better prediction than VAE-Coord.

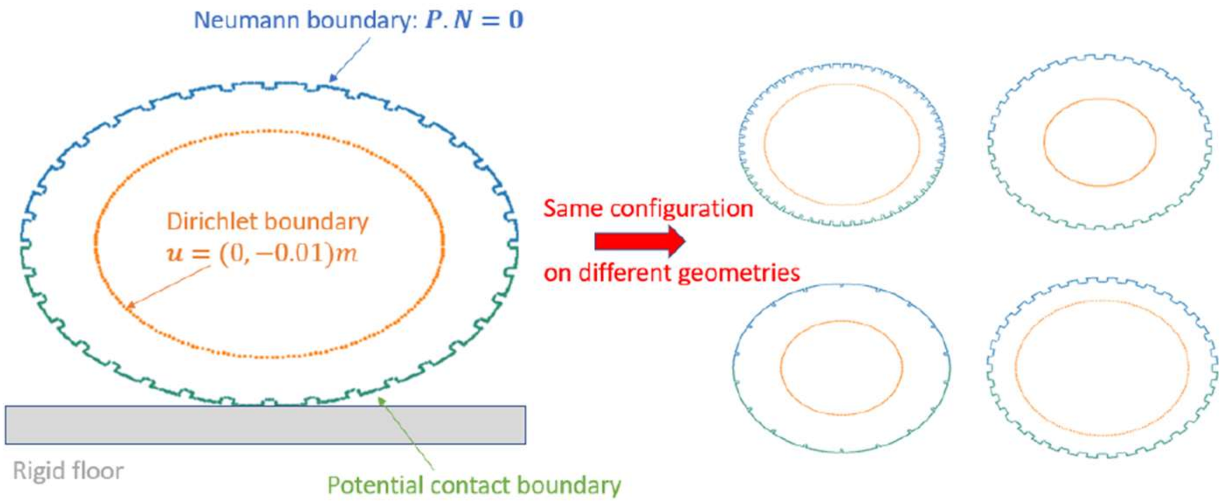
5. Toy industrial use case

Tire loading simulation (large deformation with contact)

- We consider the tires (made of rubber, incompressible material) loading simulation, which follow the Saint-Venant Kirchhoff hyperelastic model.

- The problem involves contact constraints, which results additional inequalities.





- As we do not dispose of the geometric parameters which control the shape of tires, we consider the following approaches:
  - PCA-Coord, VAE-Coord
  - PCA-Image, VAE Image

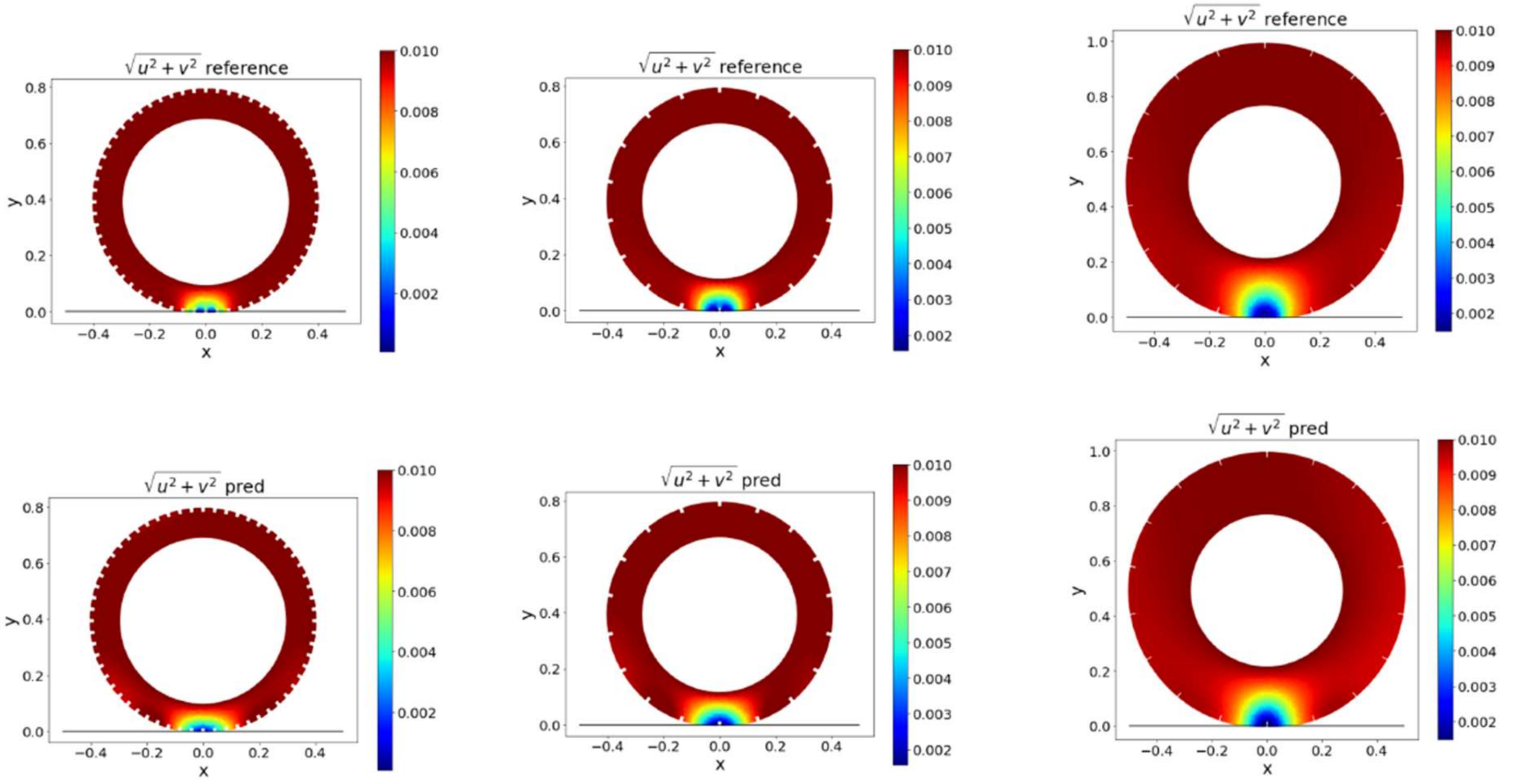
Size of latent vector is fixed $k = 5$.

5. Tire loading simulation

Illustration of GADEM prediction:

Reference solution (in-house solver)

GADEM prediction



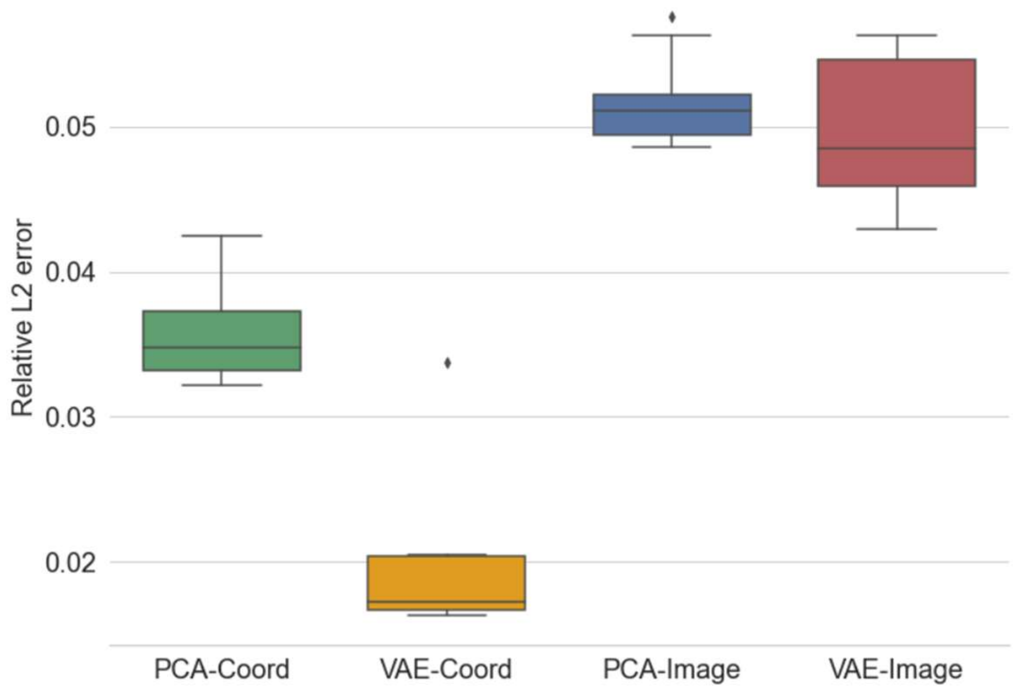
Training set

Testing set

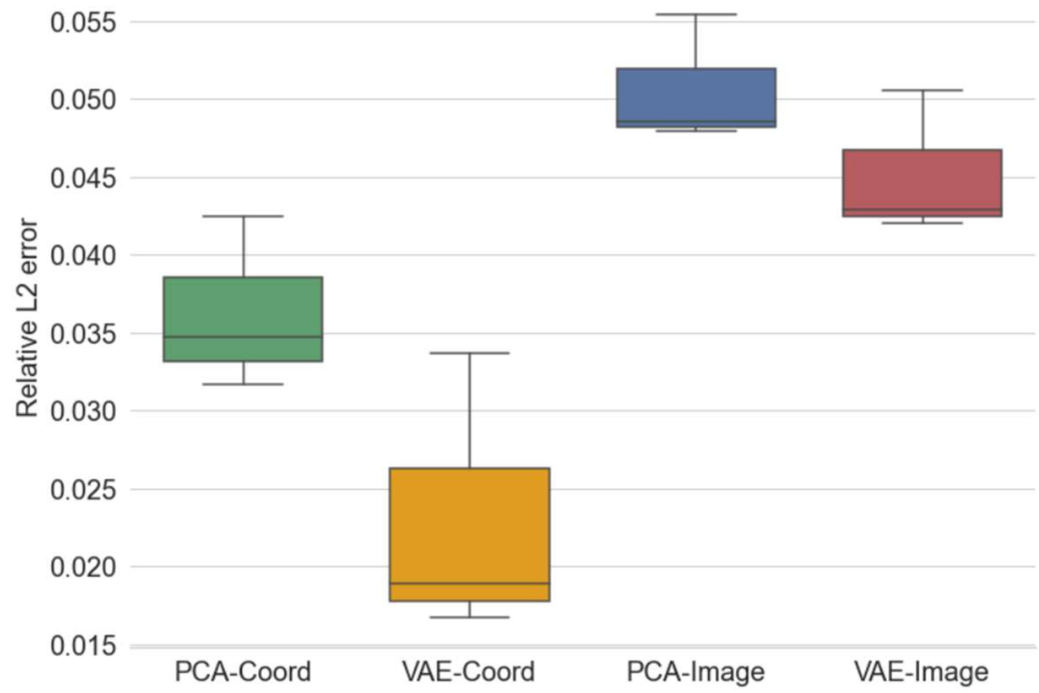
Testing set

5. Tire loading simulation

Geometric encoding comparison:



Error of the prediction in the **training set**



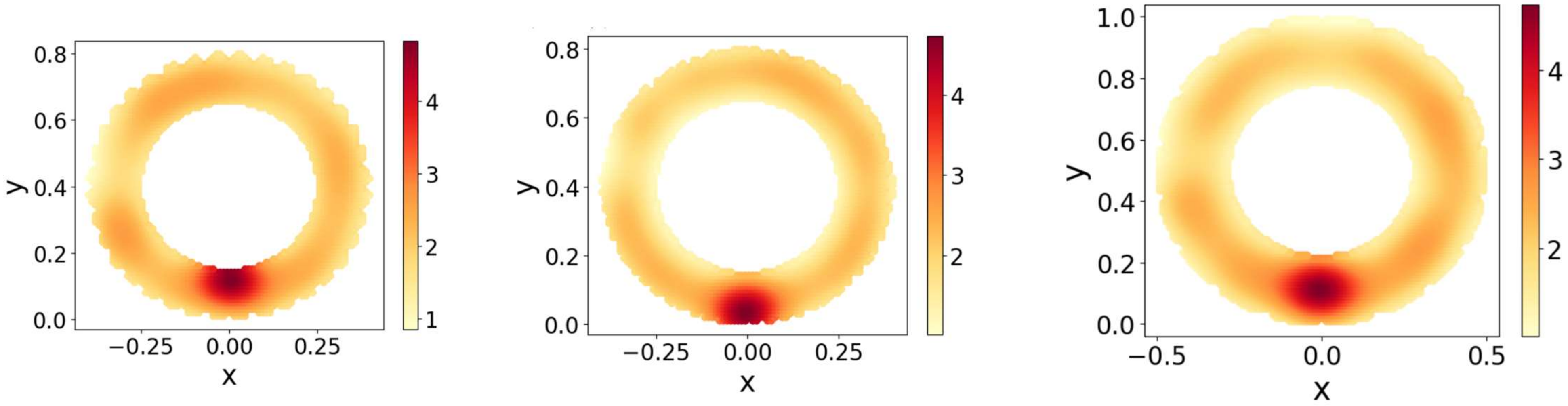
Error of the prediction in the **testing set**

- GADEM approaches provide good predictions for the displacements (errors vary from 1-5%)
- VAE-Coord outperforms the others.
- The approaches using spatial coordinates perform better than the approaches using images.

5. Tire loading simulation

Accuracy enhancement with FBOAL

- We apply FBOAL to infer the position of collocation points based on the potential energy.
- After each 100k epochs, we add and remove 1% of training points.



Density of collocation points for different tires

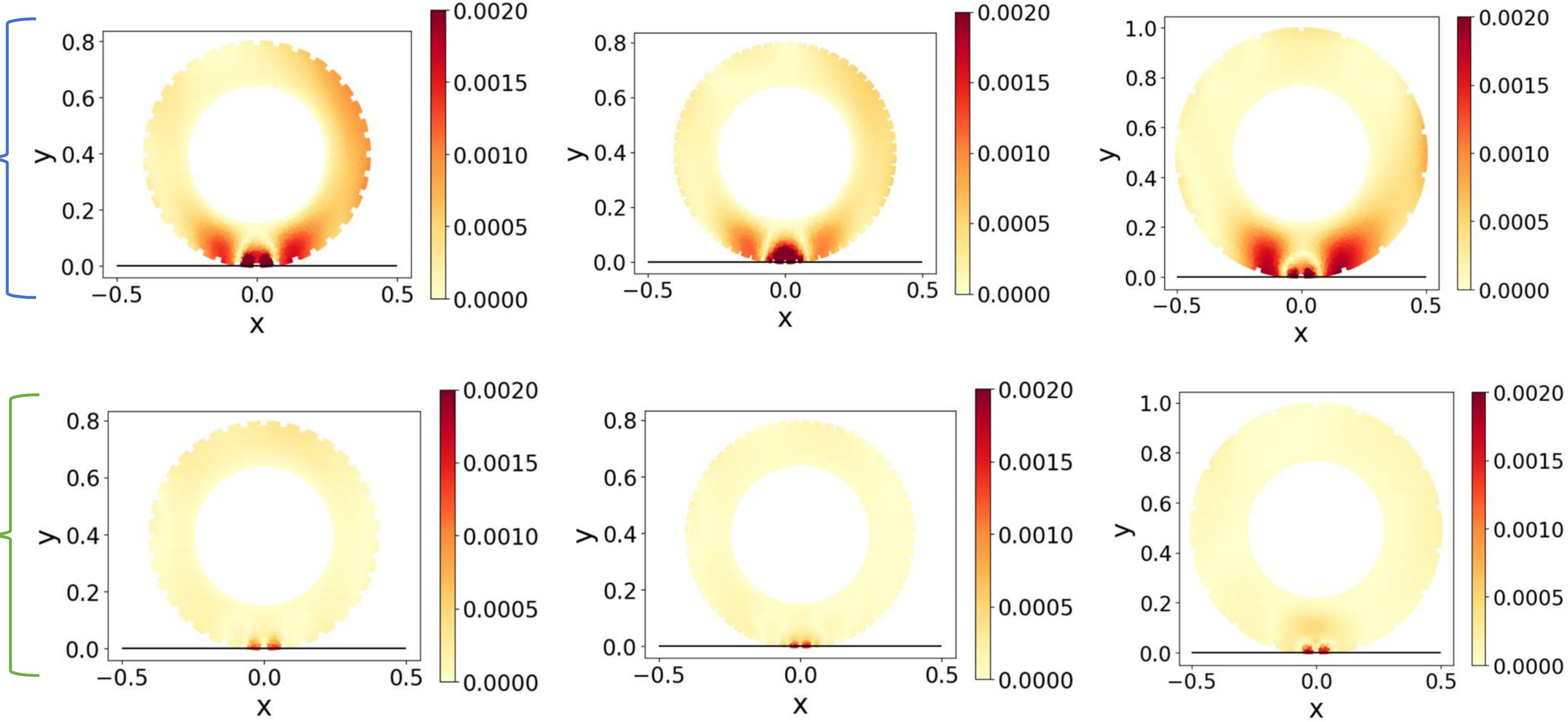
- FBOAL adds more points near the contact zones.

5. Tire loading simulation

Accuracy enhancement with FBOAL

Error without FBOAL

Error with FBOAL



○ The error is significantly reduced with FBOAL, especially at the contact zone.

5. Conclusion and perspectives

- **GADEM:** a geometry-aware framework for deep energy method.
- **GADEM** is capable of inferring the solution on **various geometries**, even on **new geometries** that are not included in the training.
- Using **spatial coordinates** to represent the geometries provides **better accuracy** than using **images**.
- **PCA** and **VAE** encoding can provides **same performance** as **parametric encoding.**
- **FBOAL** helps to **reduce significantly the prediction errors.**

Perspectives:

- Apply GADEM with different IC/BCs.

Related work:

- Nguyen, T.N.K., Dairay, T., Meunier, R., Millet, C. and Mougeot, M., 2023. Fixed-budget online adaptive learning for physics-informed neural networks. Towards parameterized problem inference. *International Conference of Computational Science.*
- Nguyen, T.N.K., Dairay, T., Meunier, R. and Mougeot, M., 2022. Physics-informed neural networks for non-Newtonian fluid thermo-mechanical problems: An application to rubber calendering process. *Engineering Applications of Artificial Intelligence*, *114*, p.105176.