

Enriching continuous Lagrange finite element approximation spaces using neural networks

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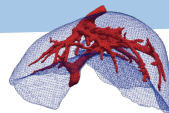
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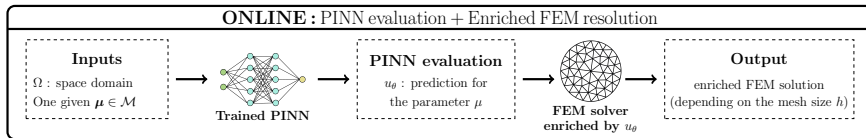
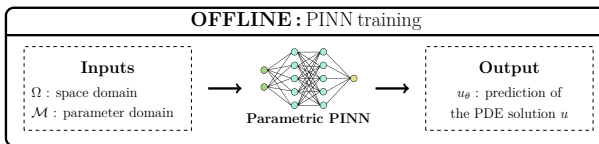
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Scientific context



Context : Create real-time digital twins of an organ (e.g. liver).

Objective : Develop an hybrid finite element / neural network method.
accurate quick + parameterized



Problem considered

Stationary incompressible Navier-Stokes equations (with buoyancy and gravity) :

We consider $\Omega = [-1, 1]^2$ a squared domain and $\mathbf{e}_y = (0, 1)$.

Find the velocity $\mathbf{u} = (u, v)$, the pressure p and the temperature T such that

$$\left\{ \begin{array}{ll} (\mathbf{u} \cdot \nabla) \mathbf{u} + \nabla p - \mu \Delta \mathbf{u} - g(\beta T + 1) \mathbf{e}_y = 0 & \text{in } \Omega \quad (\text{momentum}) \\ \nabla \cdot \mathbf{u} = 0 & \text{in } \Omega \quad (\text{incompressibility}) \\ \mathbf{u} \cdot \nabla T - k_f \Delta T = 0 & \text{in } \Omega \quad (\text{energy}) \\ + \text{suitable BC} & \end{array} \right. \quad (\mathcal{P})$$

with $g = 9.81$ the gravity, $\beta = 0.1$ the expansion coefficient, μ the viscosity and k_f the thermal conductivity. [Coulaud et al., 2024]

Problem considered

Objective: Simulate the flow for a range of $\mu = (\mu, k_f) \in \mathcal{M} = [0.01, 0.1]^2$.

Stationary incompressible Navier-Stokes equations (with buoyancy and gravity) :

We consider $\mathbf{x} = (x, y) \in \Omega$ and $\mathbf{e}_y = (0, 1)$.

Find $\mathbf{U} = (\mathbf{u}, p, T) = (u, v, p, T)$ such that

$$\begin{cases} R_{mom}(\mathbf{U}; \mathbf{x}, \mu) = 0 & \text{in } \Omega & \text{(momentum)} \\ R_{inc}(\mathbf{U}; \mathbf{x}, \mu) = 0 & \text{in } \Omega & \text{(incompressibility)} \\ R_{ener}(\mathbf{U}; \mathbf{x}, \mu) = 0 & \text{in } \Omega & \text{(energy)} \\ + \text{suitable BC} \end{cases} \quad (\mathcal{P})$$

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Boundary Conditions:

- $\mathbf{u} = 0$ on $\partial\Omega$
- $T = 1$ on the left wall ($x = -1$) and $T = -1$ on the right wall ($x = 1$)
- $\frac{\partial T}{\partial n} = 0$ on the top and bottom walls ($y = \pm 1$)

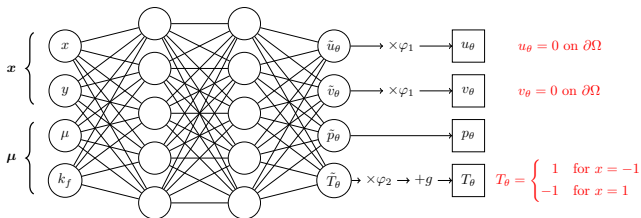
Physics-informed neural network (PINN)

Neural Network considered

We consider a parametric NN with 4 inputs and 4 outputs, defined by

$$U_{\theta}(\mathbf{x}, \boldsymbol{\mu}) = (u_{\theta}, v_{\theta}, p_{\theta}, T_{\theta})(\mathbf{x}, \boldsymbol{\mu}).$$

The Dirichlet boundary conditions are imposed on the outputs of the MLP by a **post-processing** step. [Sukumar and Srivastava, 2022]



We consider two levelsets functions φ_1 and φ_2 , and the linear function g defined by

$$\varphi_1(x, y) = (x - 1)(x + 1)(y - 1)(y + 1),$$

$$\varphi_2(x, y) = (x - 1)(x + 1) \quad \text{and} \quad g(x, y) = 1 - (x + 1).$$

PINN training

Approximate the solution of (\mathcal{P}) by a PINN : Find the optimal weights θ^* , such that

$$\theta^* = \underset{\theta}{\operatorname{argmin}} \left(J_{inc}(\theta) + J_{mom}(\theta) + J_{ener}(\theta) + J_{ad}(\theta) \right), \quad (\mathcal{P}_\theta)$$

where the different cost functions¹ are defined by

adiabatic condition

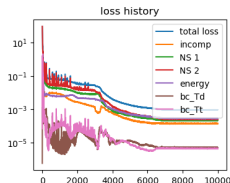
$$J_{ad}(\theta) = \int_{\mathcal{M}} \int_{\partial\Omega|_{y=\pm 1}} \left| \frac{\partial T_\theta(\mathbf{x}, \boldsymbol{\mu})}{\partial n} \right|^2 d\mathbf{x} d\boldsymbol{\mu},$$

3 residual losses

$$J_\bullet(\theta) = \int_{\mathcal{M}} \int_{\Omega} |R_\bullet(U_\theta(\mathbf{x}, \boldsymbol{\mu}); \mathbf{x}, \boldsymbol{\mu})|^2 d\mathbf{x} d\boldsymbol{\mu},$$

with U_θ the parametric NN and \bullet the PDE considered (i.e. *inc*, *mom* or *ener*).

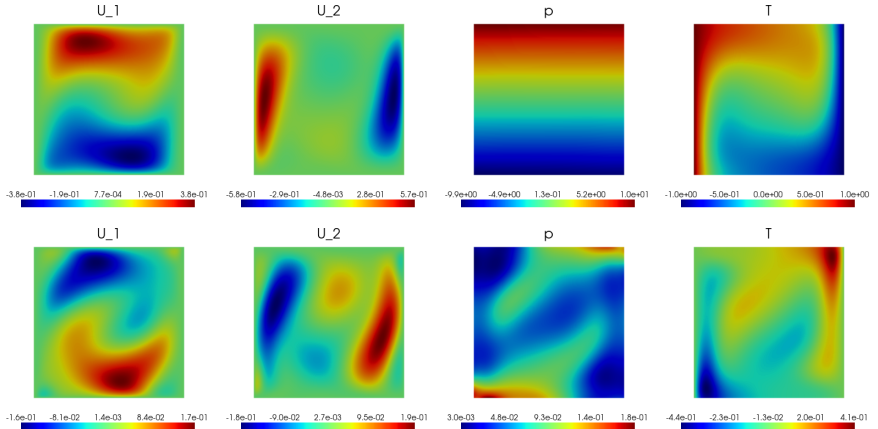
Network - MLP		Training (ADAM / LBFGS)			
<i>layers</i>	40, 60, 60, 60, 40	<i>lr</i>	7e-3	<i>N_{col}</i>	40000
<i>σ</i>	sine	<i>n_{epochs}</i>	10000	<i>N_{bc}</i>	30000



¹ Discretized by a random process using Monte-Carlo method.

PINN solution

$$\mu^{(1)} = (0.1, 0.1), \mu^{(2)} = (0.05, 0.05) \text{ and } \mu^{(3)} = (0.01, 0.01)$$



TODO : renommer figure u_θ . . . (solutions et erreurs) + ajouter erreurs L2

Finite element method (FEM)

Discrete weak formulation I¹

Find $U_h = (\mathbf{u}_h, p_h, T_h) \in [V_h^0]^2 \times Q_h \times W_h$ s.t., $\forall (\mathbf{v}_h, q_h, w_h) \in [V_h^0]^2 \times Q_h \times W_h^0$,

$$\begin{aligned}
 & \int_{\Omega} (\mathbf{u}_h \cdot \nabla) \mathbf{u}_h \cdot \mathbf{v}_h \, dx + \mu \int_{\Omega} \nabla \mathbf{u}_h : \nabla \mathbf{v}_h \, dx \\
 & \quad - \int_{\Omega} p_h \nabla \cdot \mathbf{v}_h \, dx - g \int_{\Omega} (1 + \beta T_h) \mathbf{e}_y \cdot \mathbf{v}_h \, dx = 0 \quad (\text{momentum}) \\
 & \int_{\Omega} q_h \nabla \cdot \mathbf{u}_h \, dx = 0 \quad (\text{incompressibility}) \\
 & \int_{\Omega} (\mathbf{u}_h \cdot \nabla T_h) w_h \, dx + \int_{\Omega} k_f \nabla T_h \cdot \nabla w_h \, dx = 0 \quad (\text{energy})
 \end{aligned} \tag{P_h}$$

with

$$\left. \begin{aligned}
 \mathbf{u}_h & \in [V_h^0]^2 \subset [H_0^1(\Omega)]^2 : \mathbb{P}_2 \\
 p_h & \in Q_h \subset L_0^2(\Omega) : \mathbb{P}_1 \\
 T_h & \in W_h \subset W : \mathbb{P}_1
 \end{aligned} \right\} \quad (\text{Taylor-Hood spaces})$$

and

$$W = \{w \in H^1(\Omega), w|_{x=-1} = 1, w|_{x=1} = -1\}.$$

¹The μ parameter is fixed in the FE resolution.

Discrete weak formulation I¹

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$$\begin{aligned}
 & \int_{\Omega} (\mathbf{u}_h \cdot \nabla) \mathbf{u}_h \cdot \mathbf{v}_h \, dx + \mu \int_{\Omega} \nabla \mathbf{u}_h : \nabla \mathbf{v}_h \, dx \\
 & \quad - \int_{\Omega} p_h \nabla \cdot \mathbf{v}_h \, dx - g \int_{\Omega} (1 + \beta T_h) \mathbf{e}_y \cdot \mathbf{v}_h \, dx = 0 \quad (\text{momentum}) \\
 & \int_{\Omega} q_h \nabla \cdot \mathbf{u}_h \, dx + 10^{-4} \int_{\Omega} q_h p_h \, dx = 0 \quad (\text{incompressibility} + \text{pressure penalization}) \\
 & \int_{\Omega} (\mathbf{u}_h \cdot \nabla T_h) w_h \, dx + \int_{\Omega} k_f \nabla T_h \cdot \nabla w_h \, dx = 0 \quad (\text{energy})
 \end{aligned} \tag{P_h}$$

with

$$\left. \begin{aligned}
 \mathbf{u}_h & \in [V_h^0]^2 \subset [H_0^1(\Omega)]^2 : \mathbb{P}_2 \\
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 \end{aligned} \right\} \quad (\text{Taylor-Hood spaces})$$

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Discrete weak formulation II

Considering $(\phi_i)_{i=1}^{N_u}$, $(\psi_j)_{j=1}^{N_p}$ and $(\eta_k)_{k=1}^{N_T}$ the basis functions of the finite element spaces V_h^0 , Q_h and W_h respectively, we can write the discrete solutions as:

$$\mathbf{u}_h(\mathbf{x}) = \sum_{i=1}^{N_u} \begin{pmatrix} u_i \\ v_i \end{pmatrix} \phi_i(\mathbf{x}), \quad p_h(\mathbf{x}) = \sum_{j=1}^{N_p} p_j \psi_j(\mathbf{x}) \quad \text{and} \quad T_h(\mathbf{x}) = \sum_{k=1}^{N_T} T_k \eta_k(\mathbf{x}),$$

with the unknown vectors for velocity, pressure and temperature defined by

$$\begin{aligned} \vec{u} &= (u_i)_{i=1}^{N_u} \in \mathbb{R}^{N_u}, \quad \vec{v} = (v_i)_{i=1}^{N_u} \in \mathbb{R}^{N_u}, \\ \vec{p} &= (p_j)_{j=1}^{N_p} \in \mathbb{R}^{N_p} \quad \text{and} \quad \vec{T} = (T_k)_{k=1}^{N_T} \in \mathbb{R}^{N_T}. \end{aligned}$$

Considering $N_h = 2N_u + N_p + N_T$, we can define the global vector of unknowns as:

$$\vec{U} = (\vec{u}, \vec{v}, \vec{p}, \vec{T}) \in \mathbb{R}^{N_h}.$$

and $F : \mathbb{R}^{N_h} \rightarrow \mathbb{R}^{N_h}$ the nonlinear operator associated to the weak formulation (\mathcal{P}_h).

Newton method

We consider the following three parameters:

$$\boldsymbol{\mu}^{(1)} = (0.1, 0.1), \boldsymbol{\mu}^{(2)} = (0.05, 0.05) \text{ and } \boldsymbol{\mu}^{(3)} = (0.01, 0.01).$$

We want to solve the non linear system:

$$F(\vec{U}_k) = 0$$

with $F : \mathbb{R}^{N_h} \rightarrow \mathbb{R}^{N_h}$ a non linear operator and $\vec{U}_k \in \mathbb{R}^{N_h}$ the unknown vector associated to the k -th parameter $\boldsymbol{\mu}^{(k)}$ ($k = 1, 2, 3$).

Algorithm 1: Newton's algorithm [Aghili et al., 2025]

Initialization step: set $\vec{U}_k^{(0)} = \vec{U}_{k,0}$;

for $j \geq 0$ **do**

 Solve the linear system $F(\vec{U}_k^{(j)}) + F'(\vec{U}_k^{(j)})\delta_k^{(j+1)} = 0$ for $\delta_k^{(j+1)}$;

 Update $\vec{U}_k^{(j+1)} = \vec{U}_k^{(j)} + \delta_k^{(j+1)}$;

end

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end

How to initialize the Newton solver?

3 types of initialization

- **Natural initialization :**
- **DeepPhysics initialization :**
- **Incremental initialization.**

3 types of initialization

- **Natural initialization** : Using constant or linear function.

Considering a fixed parameter with $k \in \{1, 2, 3\}$, we can use the following initialization:

$$\vec{U}_{k,0} = (\mathbf{0}_{N_u}, \mathbf{0}_{N_u}, \mathbf{0}_{N_p}, \vec{T}_0)$$

where for $i = 1, \dots, N_T$,

$$(\vec{T}_0)_i = g(\mathbf{x}^{(i)}) = 1 - (x^{(i)} + 1)$$

with $\mathbf{x}^{(i)} = (x^{(i)}, y^{(i)})$ the i -th dofs coordinates of W_h .

- **DeepPhysics initialization** :
- **Incremental initialization**.

3 types of initialization

- **Natural initialization** : Using constant or linear function.
- **DeepPhysics initialization** : Using PINN prediction [Odote et al., 2021].
 Considering a fixed parameter with $k \in \{1, 2, 3\}$, we can use the following initialization for $i = 1, \dots, N_h$,

$$(\vec{U}_{k,0})_i = U_\theta(\mathbf{x}^{(i)}, \boldsymbol{\mu}^{(k)})$$

with $\mathbf{x}^{(i)} = (x^{(i)}, y^{(i)})$ the i -th dofs coordinates of $[V_h^0]^2 \times Q_h \times W_h$ and U_θ the PINN.

- **Incremental initialization.**

3 types of initialization

- **Natural initialization** : Using constant or linear function.
- **DeepPhysics initialization** : Using PINN prediction [Odot et al., 2021].
- **Incremental initialization.** Using a coarse FE solution of a simpler parameter.
 - We consider a fixed parameter with $k \in \{2, 3\}$.
 - We consider a coarse grid (16×16 grid) and compute the FE solution of (\mathcal{P}_h) for the parameter $\mu^{(k-1)}$.
 - We interpolate the coarse solution to the current mesh.
 - We use it as an initialization for the Newton method, i.e.

$$\vec{U}_{k,0} = (\vec{u}_{k-1}, \vec{v}_{k-1}, \vec{p}_{k-1}, \vec{T}_{k-1})$$

where $\vec{u}_{k-1}, \vec{v}_{k-1}, \vec{p}_{k-1}$ and \vec{T}_{k-1} are the FE solutions for the parameter $\mu^{(k-1)}$.

Enriched finite element method using PINN

Newton method - Additive approach

TODO

Numerical results

Numerical results

TODO

Conclusion

TODO

References

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