Enriching continuous Lagrange finite element approximation spaces using neural networks

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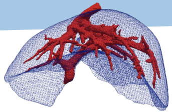
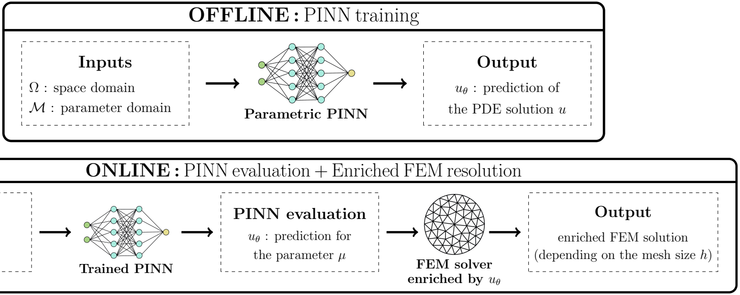
Scientific context



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 $\boldsymbol{e}_y = (0,1)$.
Find the velocity $\boldsymbol{u} = (u, v)$, the pressure p and the temperature T such that

$$\begin{cases} (\boldsymbol{u}\cdot\nabla)\boldsymbol{u} + \nabla p - \mu\Delta\boldsymbol{u} - g(\beta T + 1)\boldsymbol{e}_y = 0 \ \text{ in } \Omega & \text{(momentum)} \\ \nabla\cdot\boldsymbol{u} = 0 \ \text{ in } \Omega & \text{(incompressibility)} \\ \boldsymbol{u}\cdot\nabla T - k_f\Delta T = 0 \ \text{ in } \Omega & \text{(energy)} \\ + \text{ suitable BC} & \end{cases} \qquad (\mathcal{P})$$

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 $\boldsymbol{\mu} = (\mu, k_f) \in \mathcal{M} = [0.01, 0.1]^2$.

Stationary incompressible Navier-Stokes equations (with buoyancy and gravity) :
We consider $\boldsymbol{x} = (x, y) \in \Omega$ and $\boldsymbol{e}_y = (0, 1)$.
Find $\boldsymbol{U} = (\boldsymbol{u}, p, T) = (u, v, p, T)$ such that

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

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Boundary Conditions:

- $\boldsymbol{u} = 0$ on $\partial\Omega$
- $T = 1$ on the left wall ($x = -1$) and $T = -1$ on the right wall ($x = 1$)
  $\dfrac{\partial T}{\partial n} = 0$ on the top and bottom walls ($y = \pm 1$, denoted by Γ_{ad})

Physics-informed neural network (PINN)

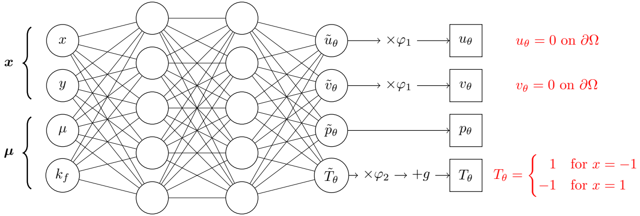
The PINN is parametrized by the $\boldsymbol{\mu}$ parameter.

Neural Network considered

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

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

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 $\theta^\star$, such that

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

where the different cost functions[1] are defined by

adiabatic condition

$$\boxed{J_{ad}(\theta) = \int_{\mathcal{M}} \int_{\Gamma_{\text{ad}}} \left| \frac{\partial T_\theta(\boldsymbol{x},\boldsymbol{\mu})}{\partial n} \right|^2 d\boldsymbol{x} d\boldsymbol{\mu},}$$

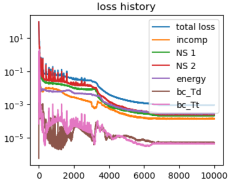
3 residual losses

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

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

Network - MLP	
layers	$40, 60, 60, 60, 40$
σ	sine

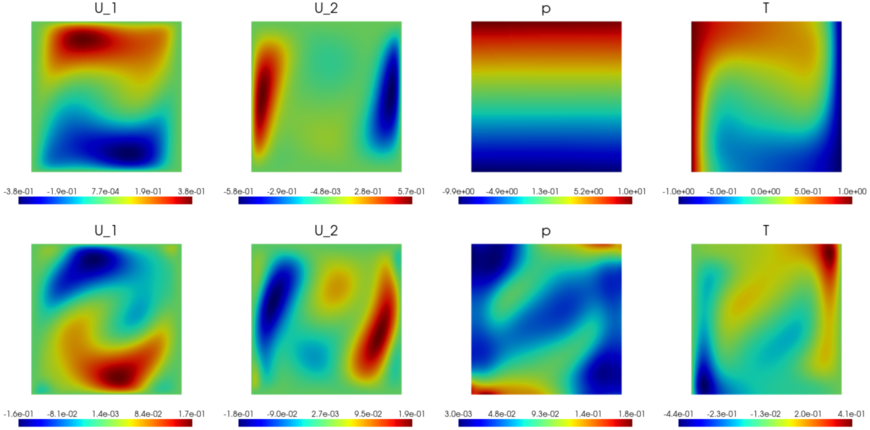
Training (ADAM / LBFGs)			
lr	7e-3	N_{col}	40000
n_{epochs}	10000	N_{bc}	30000



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

PINN solution

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



TODO : renommer figure $u_\theta \dots$ (solutions et erreurs) + ajouter erreurs L2

Finite element method (FEM)

The $\boldsymbol{\mu}$ parameter is fixed in the FE resolution.

Discrete weak formulation I

We consider a mixed finite element space $\boxed{M_h = [V_h^0]^2 \times Q_h \times W_h}$ and

$$\left.\begin{array}{ccccccc} \boldsymbol{u}_h & \in & [V_h^0]^2 & \subset & [H_0^1(\Omega)]^2 & : & \mathbb{P}_2 \\ p_h & \in & Q_h & \subset & L_0^2(\Omega) & : & \mathbb{P}_1 \end{array}\right\} \text{(Taylor–Hood spaces)}$$

$$\begin{array}{ccccccc} T_h & \in & W_h & \subset & W & : & \mathbb{P}_1 \end{array}$$

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

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

Weak problem : Find $U_h = (\boldsymbol{u}_h, p_h, T_h) \in M_h$ s.t., $\forall (\boldsymbol{v}_h, q_h, w_h) \in M_h^0$,

$$\begin{aligned} &\int_\Omega (\boldsymbol{u}_h \cdot \nabla)\boldsymbol{u}_h \cdot \boldsymbol{v}_h \, d\boldsymbol{x} + \mu \int_\Omega \nabla \boldsymbol{u}_h : \nabla \boldsymbol{v}_h \, d\boldsymbol{x} \\ &\qquad - \int_\Omega p_h \nabla \cdot \boldsymbol{v}_h \, d\boldsymbol{x} - g \int_\Omega (1 + \beta T_h)\boldsymbol{e}_y \cdot \boldsymbol{v}_h \, d\boldsymbol{x} = 0, \qquad \text{(momentum)} \\ &\int_\Omega q_h \nabla \cdot \boldsymbol{u}_h \, d\boldsymbol{x} + 10^{-4} \int_\Omega q_h \, p_h \, d\boldsymbol{x} = 0, \qquad \text{(incompressibility + pressure penalization)} \\ &\int_\Omega (\boldsymbol{u}_h \cdot \nabla T_h) \, w_h \, d\boldsymbol{x} + \int_\Omega k_f \nabla T_h \cdot \nabla w_h \, d\boldsymbol{x} = 0, \qquad \text{(energy)} \end{aligned} \qquad (\mathcal{P}_h)$$

where $M_h^0 = [V_h^0]^2 \times Q_h \times W_h^0$ with $W_h^0 \subset \{w \in H^1[\Omega],\ w|_{x=\pm 1} = 0\}$.

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:

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

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

$$\vec{u} = (u_i)_{i=1}^{N_u} \in \mathbb{R}^{N_u}, \quad \vec{v} = (v_i)_{i=1}^{N_u} \in \mathbb{R}^{N_u},$$

$$\vec{p} = (p_j)_{j=1}^{N_p} \in \mathbb{R}^{N_p} \text{ and } \vec{T} = (T_k)_{k=1}^{N_T} \in \mathbb{R}^{N_T}.$$

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 $F : \mathbb{R}^{N_h} \to \mathbb{R}^{N_h}$ 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 $F : \mathbb{R}^{N_h} \to \mathbb{R}^{N_h}$ 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 algorithm [Aghili et al., 2025]

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

for $n \geq 0$ **do**

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

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

end

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  Update $\vec{U}_k^{(n+1)} = \vec{U}_k^{(n)} + \delta_k^{(n+1)}$;
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:
  $$\vec{U}_{k,0} = \left(\mathbf{0}_{N_u}, \mathbf{0}_{N_u}, \mathbf{0}_{N_p}, \vec{T}_0\right)$$
  where for $i = 1, \ldots, N_T$,
  $$(\vec{T}_0)_i = g(\boldsymbol{x}^{(i)}) = 1 - (x^{(i)} + 1)$$
  with $\boldsymbol{x}^{(i)} = \left(x^{(i)}, y^{(i)}\right)$ 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 [Odot et al., 2021].
  Considering a fixed parameter with $k \in \{1,2,3\}$, we can use the following initialization for $i = 1, \dots, N_h$,

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

  with $\boldsymbol{x}^{(i)} = \left(x^{(i)}, y^{(i)}\right)$ the i-th dofs coordinates of M_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 $\boldsymbol{\mu}^{(k-1)}$.
  - We interpolate the coarse solution to the current mesh.
  - We use it as an initialization for the Newton method, i.e.

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

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 $\boldsymbol{\mu}^{(k-1)}$.

Enriched finite element method using PINN

Enriched space using PINN

Considering the PINN prior $U_\theta = (\boldsymbol{u}_\theta, p_\theta, T_\theta)$, we define the mixed finite element space additively enriched by the PINN as follows:

$$\boxed{M_h^+ = \left\{U_h^+ = U_\theta + C_h^+, \quad C_h^+ \in M_h^0\right\}}$$

with $M_h^0 = [V_h^0]^2 \times Q_h \times W_h^0$, $U_h^+ = (\boldsymbol{u}_h^+, p_h^+, T_h^+) \in M_h^+$ and $C_h^+ = (\boldsymbol{C}_{h,\boldsymbol{u}}^+, C_{h,p}^+, C_{h,T}^+)$.

We can then define the three finite element subspaces of M_h^+ as follows:

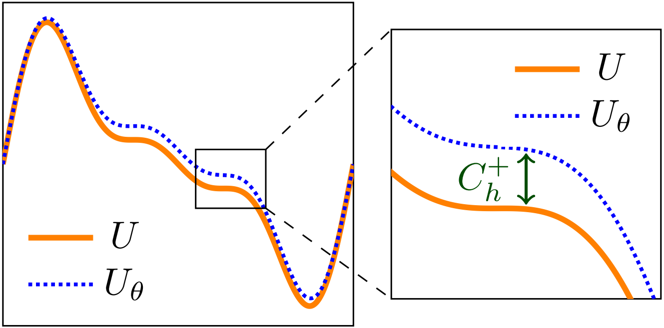
$$\begin{aligned}
\boldsymbol{V}_h^+ &= \left\{\boldsymbol{u}_h^+ = \boldsymbol{u}_\theta + \boldsymbol{C}_{h,\boldsymbol{u}}^+, \ \boldsymbol{C}_{h,\boldsymbol{u}}^+ \in [V_h^0]^2\right\}, \quad \text{(vectorial)}\\
Q_h^+ &= \left\{p_h^+ = p_\theta + C_{h,p}^+, \ C_{h,p}^+ \in Q_h\right\},\\
W_h^+ &= \left\{T_h^+ = T_\theta + C_{h,T}^+, \ C_{h,T}^+ \in W_h^0\right\},
\end{aligned}$$

where $C_{h,\boldsymbol{u}}^+$, $C_{h,p}^+$ and $C_{h,T}^+$ becomes the unknowns of the problem.

à ajouter : dans quoi vit U_θ ?

??

Schématisation en 1D de la correction... à voir comment présenter.



Weak formulation - Additive approach

Weak problem : Find $C_h^+ = (\boldsymbol{C}_{h,\boldsymbol{u}}^+, C_{h,p}^+, C_{h,T}^+) \in M_h^0$ s.t., $\forall(\boldsymbol{v}_h, q_h, w_h) \in M_h^0$,

$$
(\mathcal{P}_h^+)
\begin{cases}
\displaystyle\int_\Omega \left[(\boldsymbol{u}_\theta\cdot\nabla)\boldsymbol{u}_\theta + (\boldsymbol{u}_\theta\cdot\nabla)\boldsymbol{C}_{h,\boldsymbol{u}}^+ + (\boldsymbol{C}_{h,\boldsymbol{u}}^+\cdot\nabla)\boldsymbol{u}_\theta + (\boldsymbol{C}_{h,\boldsymbol{u}}^+\cdot\nabla)\boldsymbol{C}_{h,\boldsymbol{u}}^+\right]\cdot\boldsymbol{v_h}\,d\boldsymbol{x} \\
\quad - \mu\left(\displaystyle\int_\Omega \Delta\boldsymbol{u}_\theta\boldsymbol{v}_h\,d\boldsymbol{x} - \int_\Omega \nabla\boldsymbol{C}_{h,\boldsymbol{u}}^+ : \nabla\boldsymbol{v}_h\,d\boldsymbol{x}\right) + \left(\int_\Omega \nabla p_\theta\cdot\boldsymbol{v}_h\,d\boldsymbol{x} - \int_\Omega C_{h,p}^+\nabla\cdot\boldsymbol{v}_h\,d\boldsymbol{x}\right) \\
\quad - g\displaystyle\int_\Omega (1+\beta(T_\theta + C_{h,T}^+))\boldsymbol{e}_y\cdot\boldsymbol{v}_h\,d\boldsymbol{x} = 0, \text{ (momentum)} \\
\displaystyle\int_\Omega q_h\left[\nabla\cdot\boldsymbol{u}_\theta + \nabla\cdot\boldsymbol{C}_{h,\boldsymbol{u}}^+\right]d\boldsymbol{x} + 10^{-4}\int_\Omega q_h\,(p_\theta + C_{h,p}^+)\,d\boldsymbol{x} = 0, \text{ (incompressibility + penal)} \\
\displaystyle\int_\Omega \left[\boldsymbol{u}_\theta\cdot\nabla T_\theta + \boldsymbol{u}_\theta\cdot\nabla C_{h,T}^+ + \boldsymbol{C}_{h,\boldsymbol{u}}^+\cdot\nabla T_\theta + \boldsymbol{C}_{h,\boldsymbol{u}}^+\cdot\nabla C_{h,T}^+\right]w_h\,d\boldsymbol{x} \\
\quad - k_f\left(\displaystyle\int_\Omega \Delta T_\theta w_h\,d\boldsymbol{x} - \int_\Omega \nabla C_{h,T}^+\cdot\nabla w_h\,d\boldsymbol{x} + \int_{\Gamma_{\text{ad}}}\frac{\partial C_{h,T}^+}{\partial n}w_h\,d\boldsymbol{s}\right) = 0, \text{ (energy)}
\end{cases}
$$

with $U_\theta = (\boldsymbol{u}_\theta, p_\theta, T_\theta)$ the PINN prior.

Parler des BC modifiés pour l'approche add ?

Newton method - Additive approach

We want to solve the non linear system:

$$F_\theta(\vec{C}) = 0$$

with $F_\theta : \mathbb{R}^{N_h} \to \mathbb{R}^{N_h}$ the non linear operator associated to the weak problem $(\mathcal{P}_h^+)$ and $\vec{C} \in \mathbb{R}^{N_h}$ the correction vector (unknown).

Algorithm 2: Newton algorithm [Aghili et al., 2025]

Initialization step: set $\vec{C}^{(0)} = 0$;
for $n \geq 0$ **do**
  Solve the linear system $F_\theta(\vec{C}^{(n)}) + F'_\theta(\vec{C}^{(n)})\delta^{(n+1)} = 0$ for $\delta^{(n+1)}$;
  Update $\vec{C}^{(n+1)} = \vec{C}^{(n)} + \delta^{(n+1)}$;
end

Advantage compared to DeepPhysics[1]: Appendix 1

u_θ is not required to live in the same discrete space as C_h^+.

[1] The additive approach is exactly the same as DeepPhysics if we take U_θ in the same space as C_h^+.

Numerical results

Numerical results

TODO

Conclusion

TODO

Parler du papier en linéaire et dire que dans ce cadre on a des résultats théoriques de convergence.

References

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Appendix 1 : DeepPhysics / Additive approach

A1 – ??