A neural network approach to learning solutions of a class of elliptic variational inequalities

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November 21, 2025

Warm up ... on PINNs

Plain vanilla partial differential equation (PDE): The Poisson problem:

Given $f \in H^{-1}(\Omega)$, find $u \in H_0^1(\Omega)$, $\Omega \subset \mathbb{R}^n$, such that

$$-\Delta u = f \text{ in } H^{-1}(\Omega).$$

Weak form of PDE:

$$\int_\Omega \nabla u \cdot \nabla \phi \, dx = \langle f, \phi \rangle_{H^{-1},H_0^1} \quad \forall \phi \in H_0^1(\Omega).$$

Classical P^1 globally continuous finite element ansatz $u_h(x) = \sum_{i=1}^{n_h} u_i b_i(x)$, $x \in \Omega$ and basis elements $b_i \in H_0^1(\Omega)$, $i = 1, \dots, n_h$, yields the problem: Given $\mathbf{f} \in \mathbb{R}^{n_h}$, find $\mathbf{u} = (u_1, \dots, u_{n_h})^\top \in \mathbb{R}^{n_h}$ such that

$$\mathbf{L}\mathbf{u} = \mathbf{f}.$$

Physics-informed Neural Network (PINN) ansatz: Parametrize u by neural network ansatz yielding $u_\theta \in H^1(\Omega)$ and solve

$$\mathfrak{f}(\Theta) = \min \frac{1}{2} \| -\Delta u_\theta - f \|_{H^{-1}}^2 \text{ over } \theta \in \mathbb{R}^{n_{|\theta|}} \text{ s.t. } u_\theta = 0 \text{ on } \partial\Omega.$$

Warm up ... on PINNs

Feedforward neural network (FFN) ansatz for u_θ:

$$u_\theta(x) := T_{\mathfrak{d}+1} \circ \sigma \circ \ldots \circ \sigma \circ T_0(x)$$

with depth $\mathfrak{d} \in \mathbb{N}$, activation function σ (e.g., $\tanh(\cdot)$, $\max(0,\cdot)$,...), and

$$T_\ell(z) = A_\ell z + b_\ell, \quad \ell = 0, \ldots, \mathfrak{d}+1.$$

Let $\theta = (A_{\mathfrak{d}+1}, b_{\mathfrak{d}+1}, \ldots, A_0, b_0)$.

Aspects.

- FE ansatz: (sparse) linear system; unique solution
- PINN:
  - $\to$ Nonlinear, possibly nonsmooth minimization problem
  - $\to$ Constraints (e.g., b.c.) delicate
  - $\to$ Norm in the objective problematic $\Rightarrow$ requires higher regularity of u to become practical

Selected literature on PINNs

- Pioneered in [Lagaris, Likas, Fortiadis]; see also [Raissi, Perdikaris, Karniadakis].
- Inverse problems [Chen, Lu, Karniadakis, Dal Negro], [Mishra, Molinaro].
- Advanced solvers [Moseley, Markham, Nissen-Meyer], [Jagtap, Karniadakis]
- Nonconvexity handling [Wang, Teng, Yu, Perdikaris]
- Problematic for high frequencies, multiscales [Wang, Teng, Yu, Perdikaris]

- Deep Ritz for variational problems [E, Yu], [Dondl, Müller, Zeinhofer]
- Discrete weak formulations [Brevis, Muga, van der Zee]

A class of elliptic VIs

Given a Lipschitz, coercive operator $A : K \subset V \to V^*$, and $f \in H$, consider:

$$\text{Find } u \in K : \langle Au - f, v - u \rangle_{V^*,V} \geq 0 \quad \text{for all } v \in K,$$

with, e.g., $\Omega \subset \mathbb{R}^n$, $H = L^2(\Omega)$, $V = H^1(\Omega)$ and, for given $\psi \leq h$ on $\partial\Omega$,

$$K := \left\{ u \in H^1(\Omega) \mid u \geq \psi \text{ in } \Omega, u = h \text{ on } \partial\Omega \right\},$$

Many applications:

- Contact problems – potentially complex geometry, composite materials
- Option pricing – high dimension
- Multiphase demixing of alloys, fluids, species... (via phase field ansatz) – many phases yield high dimensional VI
- ...

Literature: ProxNets [Schwab, Stein]

Saddle point formulation

For simplicity, here for given $b \in L^\infty(\Omega)^n$, $c \in L^\infty(\Omega)$:

$$A := -\Delta + b \cdot \nabla + c\,\mathrm{id}, \qquad \text{(non-symmetric).}$$

Define $L\colon V \times V \to \mathbb{R}$ as

$$L(u, v) := \langle Au - f, u - v \rangle.$$

Note that $L(\cdot, v)$ is convex and $L(u, \cdot)$ is concave for fixed $u, v \in V$. If (u, v) is a saddle point then it satisfies

$$L(u, v) = \min_{\tilde{u} \in K} \sup_{\tilde{v} \in K} L(\tilde{u}, \tilde{v}) = \max_{\tilde{v} \in K} \inf_{\tilde{u} \in K} L(\tilde{u}, \tilde{v}).$$

Moreover, L has a saddle point if and only if the second equality holds.

Note:

- If $u \in K$ solves VI, then (u, u) is saddle point of L on $K \times K$; conversely, if (u, v) is saddle point of L on $K \times K$, then $u = v$ and u solves VI.
- Definition of L reminiscent of weak form associated with $Au - f$.

Min-max approach via regularized gap function

Assumption. Let u^* solve VI, and let sets X, Y satisfy

(i) $u^* \in X \cap Y$,

(ii) $K \cap X \subset K \cap Y$,

(iii) $K \cap Y$ is convex and closed.

Examples:

- $X = Y = V = H^1(\Omega)$.
- $Y = \overline{B}^{H^2}(0; r)$ with appropriate $r > 0$, some $X \subset Y$ suitably chosen: Requires $u^* \in H^2(\Omega)$ which is true under data regularity.

For $\gamma > 0$, define $L_\gamma \colon V \times V \to \mathbb{R}$ by

$$L_\gamma(u, v) := L(u, v) - \frac{1}{2\gamma}\|u - v\|_V^2,$$

Min-max approach via regularized gap function

and the generalized regularized gap function $G_\gamma \colon V \to \mathbb{R}$ given by

$$G_\gamma(u) := \sup_{v \in K \cap Y} L_\gamma(u, v) = \sup_{v \in K \cap Y} \left(L(u, v) - \frac{1}{2\gamma} \|u - v\|_V^2 \right).$$

Then G_γ has the following properties:

(i) G_γ is finite everywhere on V,

(ii) $G_\gamma(u) \geq 0$ for $u \in K \cap X$,

(iii) $u \in K \cap X$ satisfies $G_\gamma(u) = 0$ if and only if u solves the VI,

(iv) $G_\gamma \colon K \cap X \subset V \to \mathbb{R}$ is lower semicontinuous.

Hence, to find a solution to the VI, we can solve

$$\min_{u \in K \cap X} G_\gamma(u) \equiv \min_{u \in K \cap X} \sup_{v \in K \cap Y} L_\gamma(u, v) \equiv \min_{u \in K \cap X} \max_{v \in K \cap Y} L_\gamma(u, v)$$

with the latter due to strong convexity of $-L_\gamma(u, \cdot)$ and closedness of $K \cap Y$.

Min-max approach via regularized gap function

Let $C_a > 0$ denote the coercivity constant of A. Then

$$\left(C_a - \frac{1}{2\gamma}\right) \|u - u^*\|_V^2 + \langle Au^* - f, u - u^* \rangle \leq G_\gamma(u) \qquad \forall u \in V.$$

If $u \in K$, the duality product can be omitted.

From now on, we assume

$$\gamma > \frac{1}{2C_a}.$$

Relaxation via penalization. A generalized problem can be posed as

$$\min_{u \in X^{\mathrm{s}}} \max_{v \in X^{\mathrm{t}}} L_\gamma(u, v) + R_1(u) - R_2(v)$$

where $R_1(u)$ incorporates a penalty for violations of $u \in K$ and / or $u = h$ on $\partial\Omega$; similarly for $R_2(v)$, and X^{s} and X^{t} are corresponding, suitable sets.

Neural network approach

Let $\mathcal{F} := \mathcal{F}(\mathfrak{d}, \mathfrak{w}, \sigma)$, layer width $\mathfrak{w} \in \mathbb{N}$, denote the set of neural network functions.

Homogeneous boundary conditions: Let $v \in \mathcal{F}$ and $\eta \in C^1(\overline{\Omega})$ with $\eta|_{\partial\Omega} = 0$. Then $v\eta = 0$ on $\partial\Omega$. We write $v\eta \in \mathcal{F}_{0,\eta}$.

More generally: Given an operator $M : C^1(\overline{\Omega}) \to C^1(\overline{\Omega})$, let

$$\mathcal{F}(\mathfrak{d}, \mathfrak{w}, \sigma, M) := \{M \circ u \; : \; u \in \mathcal{F}(\mathfrak{d}, \mathfrak{w}, \sigma)\}.$$

Lemma. Let $u \in \mathcal{F}(\mathfrak{d}, \mathfrak{w}, \sigma, M)$. If $\sigma \in C^1(\mathbb{R})$ and M is continuous. Then $\theta \mapsto u_\theta(\cdot)$ is continuous from $\mathbb{R}^{\mathfrak{m}}$, with $\mathfrak{m} = |\theta|$, to $C^1(\overline{\Omega})$.

Consequence.

$$\mathcal{F}(\mathfrak{d}, \mathfrak{w}, \sigma, M) \subset C^1(\overline{\Omega}) \subset H^1(\Omega).$$

For ReLU, i.e., $\sigma(\cdot) = \max(0, \cdot)$, also $\mathcal{F}(\mathfrak{d}, \mathfrak{w}, \sigma) \subset H^1(\Omega)$.

NN approximation

For simplicity, $A = -\Delta + k\mathrm{Id}$, $k \geq 0$, generating the pairing

$$\langle Au, u - v \rangle = \int_\Omega \nabla u \cdot \nabla(u - v) + ku(u - v).$$

Take a set of collocation points $\{x_i\}_{i=1}^N$ and define $\hat{L}\colon C^1(\overline{\Omega}) \times C^1(\overline{\Omega}) \to \mathbb{R}$ by

$$\begin{aligned}\hat{L}(u, v) :=& \frac{|\Omega|}{N} \sum_{i=1}^N [\nabla u(x_i) \cdot (\nabla u(x_i) - \nabla v(x_i)) + ku(x_i)(u(x_i) - v(x_i))] \\ &- \frac{|\Omega|}{N} \sum_{i=1}^N f(x_i)(u(x_i) - v(x_i)).\end{aligned}$$

Similarly, the discrete version of L_γ is $\hat{L}_\gamma\colon C^1(\overline{\Omega}) \times C^1(\overline{\Omega}) \to \mathbb{R}$ given by

$$\hat{L}_\gamma(u, v) := \hat{L}(u, v) - \frac{|\Omega|}{2\gamma N} \sum_{i=1}^N \left[(u(x_i) - v(x_i))^2 + |\nabla u(x_i) - \nabla v(x_i)|^2\right].$$

NN approximation

Let $\mathcal{X}^s$ and $\mathcal{X}^t$ be arbitrary subsets of $C^1(\bar{\Omega}) \cap \mathcal{F} \cap B(0;\rho)$, $\rho > 0$ sufficiently large (respectively with potentially different widths, depths and activations, etc., cf. the Petrov–Galerkin method).

Discretised version of penalty problem:

$$\min_{u \in \mathcal{X}^s} \max_{v \in \mathcal{X}^t} \hat{L}_\gamma(u, v).$$

In general, $\mathcal{X}^s$ and $\mathcal{X}^t$ need not be subsets of K. Hence, we consider the penalized version:

$$\min_{u \in \mathcal{X}^s} \max_{v \in \mathcal{X}^t} \hat{L}_\gamma(u, v) + \hat{R}_1(u) - \hat{R}_2(v)$$

Define the discrete version of ”gap function” $\hat{G}_\gamma \colon \mathcal{X}^s \to \mathbb{R}$ by

$$\hat{G}_\gamma(u) := \max_{v \in \mathcal{X}^t} \hat{L}_\gamma(u, v) + \hat{R}_1(u) - \hat{R}_2(v).$$

If $\hat{L}_\gamma(u, u) + \hat{R}_1(u) - \hat{R}_2(u) \geq 0$ and $\mathcal{X}^s \subseteq \mathcal{X}^t$, then $\hat{G}_\gamma(u) \geq 0$ for all $u \in \mathcal{X}^s$.

NN approach: remarks on existence

Sets of neural network functions may neither be closed nor convex. Work around via quasi-minimization: $\bar{u} \in U \subset X$, X a Hilbert space, is *quasi-minimizer* of $J : U \to \mathbb{R}$ if it satisfies $J(\bar{u}) \leq \inf_{u \in U} J(u) + \epsilon$ for some $\epsilon > 0$.

Weaken notion of global minmax points for a function $\mathfrak{f} : X \times Y \to \mathbb{R}$. Define a *quasi-minimax point* as a point (x^*, y^*) that satisfies

$$\mathfrak{f}(x^*, y) - \epsilon \leq \mathfrak{f}(x^*, y^*) \quad \forall y \in Y \quad \text{and} \quad \max_{y \in Y} \mathfrak{f}(x^*, y) \leq \max_{y \in Y} \mathfrak{f}(x, y) + \epsilon \quad \forall x \in X$$

for some $\epsilon > 0$, and then study the associated theory. NOT THE FOCUS HERE!

Rather consider the general min-max problem (over NN fctns)

$$\min_{u \in \mathcal{X}^s} \max_{v \in \mathcal{X}^t} \hat{\ell}(u, v)$$

NN approach: remarks on existence

Assumptions. Let $\hat{\ell}\colon C^1(\overline{\Omega}) \times C^1(\overline{\Omega}) \to \mathbb{R}$ be a given map and assume

$$\mathcal{X}^s \subset \mathcal{F}(\mathfrak{d}^s, \mathfrak{w}^s, \sigma^s, M^{\mathrm{s}}), \quad \mathcal{X}^t \subset \mathcal{F}(\mathfrak{d}^t, \mathfrak{w}^t, \sigma^t, M^{\mathrm{t}}),$$

with associated parameter spaces $\Theta^{\mathfrak{s}}$ and $\Theta^{\mathfrak{t}}$, respectively. Furthermore,

(i) $\hat{\ell}\colon C^1(\overline{\Omega}) \times C^1(\overline{\Omega}) \to \mathbb{R}$ is continuous,

(ii) $M^{\mathrm{s}}, M^{\mathrm{t}} \in C^0(C^1(\overline{\Omega}), C^1(\overline{\Omega}))$,

(iii) $\Theta^{\mathfrak{s}}, \Theta^{\mathfrak{t}}$ are non-empty and compact.

Perspective here: *solution* to min-max problem (over NN fctns) associated with solving the finite-dimensional problem

$$\min_{\theta \in \Theta^{\mathfrak{s}}} \max_{\vartheta \in \Theta^{\mathfrak{t}}} \hat{\ell}(u(\theta, \cdot), v(\vartheta, \cdot)).$$

Proposition. The above problem admits a solution $\hat{u} \in \mathcal{X}^s$.

Result carries over to penalized problem above with $\hat{L}_\gamma$.

Error analysis

Let $\hat{u}_A$ be an approximate (numerical) solution. We have

$$\left(C_a - \frac{1}{2\gamma}\right) \|\hat{u}_A - u^*\|_V^2 \leq G_\gamma(\hat{u}_A) - G_\gamma(u^*) - \langle Au^* - f, u^* - \hat{u}_A \rangle.$$

Since $\hat{u}$ solution of discrete penalty problem: $\hat{G}_\gamma(\hat{u}) \leq \hat{G}_\gamma(u) \quad \forall u \in \mathcal{X}^s$.

Let $H_\gamma : V \to \mathbb{R}$ be continuous version of $\hat{G}_\gamma$, i.e.,

$$H_\gamma(u) := \max_{v \in \mathcal{X}^t} L_\gamma(u, v) + R_1(u) - R_2(v),$$

For arbitrary $\bar{u} \in \mathcal{X}^s$, we have

$$\begin{aligned} G_\gamma(\hat{u}_A) - G_\gamma(u^*) \leq &\underbrace{G_\gamma(\hat{u}_A) - H_\gamma(\hat{u}_A)}_{I} + \underbrace{H_\gamma(\hat{u}_A) - \hat{G}_\gamma(\hat{u}_A) + \hat{G}_\gamma(\bar{u}) - H_\gamma(\bar{u})}_{II} \\ &+ \underbrace{\hat{G}_\gamma(\hat{u}_A) - \hat{G}_\gamma(\hat{u})}_{III} + \underbrace{H_\gamma(\bar{u}) - H_\gamma(u^*)}_{IV} + \underbrace{H_\gamma(u^*) - G_\gamma(u^*)}_{V} \end{aligned}$$

Error analysis

We get

$$\left(C_a - \frac{1}{2\gamma}\right) \|\hat{u}_A - u^*\|_V^2 \leq \xi_{\text{app}} + 2\xi_{\text{stat}} + \xi_{\text{opt}}$$
$$+ H_\gamma(u^*) - G_\gamma(u^*) + \langle Au^* - f, u^* - \hat{u}_A\rangle - R_1(\hat{u}_A)$$

with the *approximation error*

$$\xi_{\text{app}} := \max_{v \in K \cap Y} \min_{w \in \mathcal{X}^t} K_1\|w - v\|_V + K_2\|w - v\|_{L^2(\Omega)} + K_3\|w - v\|_{L^2(\partial\Omega)}$$
$$+ \inf_{u \in \mathcal{X}^s} \big(K_4\|u - u^*\|_V + K_5\|u - u^*\|_{L^2(\Omega)} + K_6\|u - u^*\|_{L^2(\partial\Omega)}\big)$$

related to how well the spaces $\mathcal{X}^s$ and $\mathcal{X}^t$ approximate u^* and the set $K \cap Y$ respectively; the *statistical error*

$$\xi_{\text{stat}} := \sup_{\substack{u \in \mathcal{X}^s \\ v \in \mathcal{X}^t}} |L_\gamma(u, v) + R_2(u) + R_1(v) - (\hat{L}_\gamma(u, v) + \hat{R}_2(u) + \hat{R}_1(v))|,$$

measuring the error from numerically approximating the integrals; and the *optimization error*

$$\xi_{\text{opt}} := \hat{G}_\gamma(\hat{u}_A) - \hat{G}_\gamma(\hat{u}).$$

Error analysis

The quantity $\xi_K := \langle Au^* - f, u^* - \hat{u}_A \rangle - R_1(\hat{u}_A)$ is due to the presence of K and satisfies for $\epsilon > 0$

$$\xi_K \le \epsilon \quad \text{for penalty weights } w \ge \frac{1}{4\epsilon} \|Au^* - f\|^2_{L^2(\Omega)}.$$

The error $\xi_S := H_\gamma(u^*) - G_\gamma(u^*)$ is due to the approximating spaces and satisfies for $\epsilon > 0$ and sufficiently large penalty parameters

$$\xi_S \le \epsilon - \frac{1}{2\gamma} \|u^* - v^*\|^2_V - R_2(v^*),$$

where $v^* \in \operatorname{argmax}\{L_\gamma(u^*, w) - R_2(w) : w \in H^1(\Omega)\}$.

Error analysis

For estimating the approximation error we need that there exists a neural network architecture $\mathcal{F}^s$ with activation function σ^s satisfying: for every $w \in H^2(\Omega)$ and every $\epsilon > 0$, there exists $\mathfrak{d}^s, \mathfrak{w}^s \in \mathbb{N}$ and $u \in \mathcal{F}^s(\mathfrak{d}^s, \mathfrak{w}^s, \sigma^s)$ such that

$$\|u - w\|_V \leq \epsilon.$$

Similarly for $\mathcal{F}^t$. Moreover, we need the existence of $\bar{R}$ such that

$$\|v\|_V \leq \bar{R} \quad \forall v \in K \cap Y.$$

These two properties hold indeed true for Ω of class $C^{1,1}$, $h \in H^{3/2}(\partial\Omega)$, $\psi \in H^2(\Omega)$ and $\bar{R} \geq \|u^*\|_V$. As a consequence: For any $\epsilon > 0$ there exist NN architectures such that

$$\xi_{\text{app}} \leq \epsilon.$$

[Gühring, Raslan]

For estimating the statistical error we need the concept of Rademacher complexity...

...measures richness of a class of sets w.r.t. a probability distribution.

Error analysis

Rademacher complexity. Let $\mathcal{F}$ be a family of functions from Ω into $\mathbb{R}$ and let P be a distribution over Ω and $\{X_i\}_{i=1}^N$ be independent identically distributed (iid) samples from P. The *Rademacher complexity* of $\mathcal{F}$ associated with the distribution P and sample size N is defined as

$$\mathcal{R}(\mathcal{F}) := \mathbb{E}_{\{X_i\}_{i=1}^N} \mathbb{E}_{\{\sigma_i\}_{i=1}^N} \left[\sup_{u \in \mathcal{F}} \frac{1}{N} \sum_{i=1}^N \sigma_i u(X_i) \right],$$

where $\{\sigma_i\}_{i=1}^N$ are iid random variables such that $\mathbb{P}[\sigma_i = 1] = \mathbb{P}[\sigma_i = -1] = \frac{1}{2}$.

Covering number. Given $\varepsilon > 0$, we say that $\mathcal{A} \subset \mathbb{R}^n$ is an ε*-cover of* $\mathcal{B} \subset \mathbb{R}^n$ *with respect to a metric* ρ if for all $v' \in \mathcal{B}$, there exists $v \in \mathcal{A}$ such that $\rho(v, v') \leq \varepsilon$. The ε*-covering number of* $\mathcal{B}$, denoted as $\mathfrak{C}(\varepsilon, \mathcal{B}, \rho)$, is the minimum cardinality among all ε-covers of $\mathcal{B}$ with respect to the metric ρ.

Lemma. Assume that the collocation points $\{x_i\}_{i=1}^N$ are iid drawn from $U(\Omega)$. Then

$$\sup_{\substack{u \in \mathcal{F}^s \\ v \in \mathcal{F}^t}} |L_\gamma(u,v) + R_1(u) - R_2(v) - (\hat{L}_\gamma(u,v) + \hat{R}_1(u) - \hat{R}_2(v))| \leq 2|\Omega| \sum_{i=1}^{10} \mathcal{R}(\mathcal{F}_i),$$

Error analysis

$$
\begin{aligned}
&\mathcal{F}_1 = \{\|\nabla u\|^2 : u \in \mathcal{F}^s\}, && \mathcal{F}_2 = \{\nabla u \cdot \nabla v : u \in \mathcal{F}^s, v \in \mathcal{F}^t\},\\
&\mathcal{F}_3 = \{ku^2 : u \in \mathcal{F}^s\}, && \mathcal{F}_4 = \{kuv : u \in \mathcal{F}^s, v \in \mathcal{F}^t\},\\
&\mathcal{F}_5 = \{fu : u \in \mathcal{F}^s\}, && \mathcal{F}_6 = \{fv : v \in \mathcal{F}^t\},\\
&\mathcal{F}_7 = \left\{\frac{1}{2\gamma}(u-v)^2 : u \in \mathcal{F}^s, v \in \mathcal{F}^t\right\}, && \mathcal{F}_8 = \left\{\frac{1}{2\gamma}|\nabla u - \nabla v|^2 : u \in \mathcal{F}^s, v \in \mathcal{F}^t\right\}\\
&\mathcal{F}_9 = \{w_{o_1}|(\psi - u)^+|^2 : u \in \mathcal{F}^s\}, && \mathcal{F}_{10} = \{w_{o_2}|(\psi - v)^+|^2 : u \in \mathcal{F}^t\}.
\end{aligned}
$$

Theorem. Let $f \in C^0(\Omega) \cap L^\infty(\Omega)$, the activation function $\sigma \in C^1(\mathbb{R}) \cap L^\infty(\mathbb{R})$ be Lipschitz and Θ be bounded. Then we have for a constant $K(\eta, f) > 0$

$$
\mathbb{E}_{\{x_i\}_{i=1}^N}[\xi_{\text{app}}] \le \frac{K(\eta, f) n^{\frac{3}{2}} \mathfrak{m} \sqrt{\sum_{k=0}^{2\mathfrak{d}} 2^k}\, 2^{\frac{9\mathfrak{d}-2}{2}} \mathfrak{w}^{7\mathfrak{d}+3} \bar{C}^{14\mathfrak{d}+9} \sqrt{C_\Omega}}{N^{\frac{1}{4}}}.
$$

The precise form of the estimate is due to a Deep Ritz Residual NN, but for FFNs the bound is similar.

Extension: PINN-based multi-complexity solver

(with D. Korolev)

Application motivation

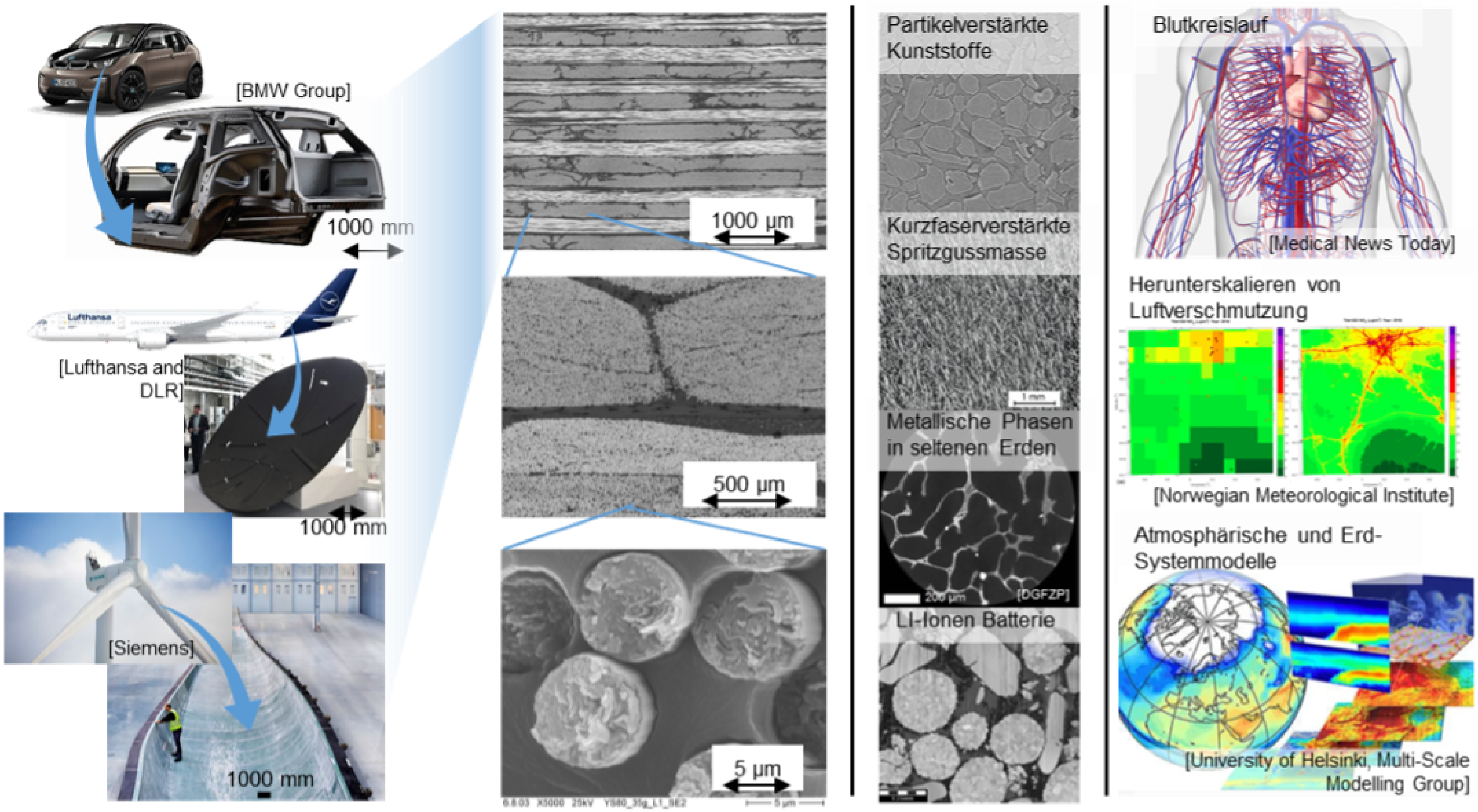


Figure: Fiber composites (left); further examples from material sciences (middle); other societal relevant areas (right).

Industrial context

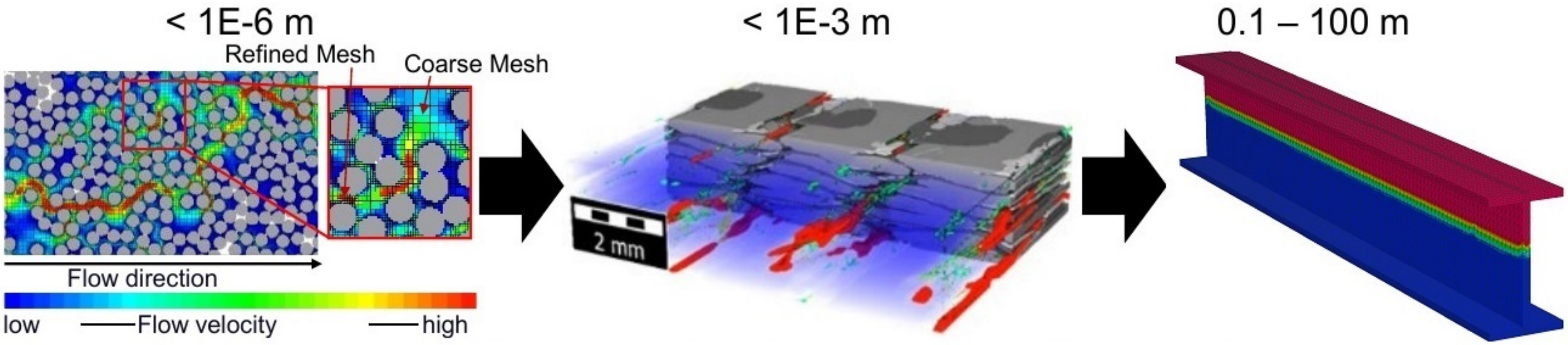


Figure: Liquid composite molding (LCM) simulation.

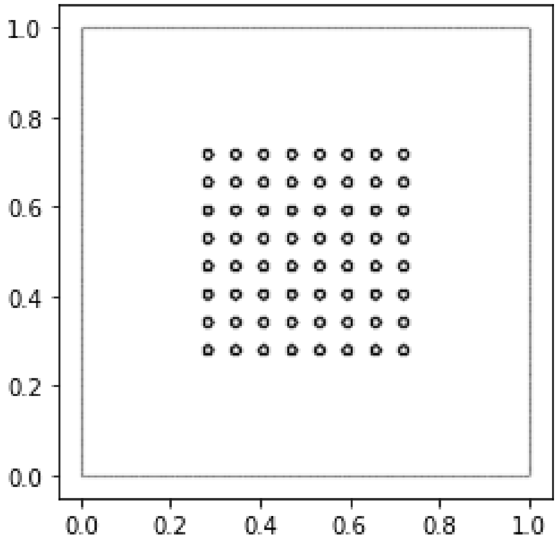
Challenges in LCM modelling:

- The presence of different physics at multiple scales.
- Large-scale computations using numerical homogenization.
- Complicated geometries at the microscale level.

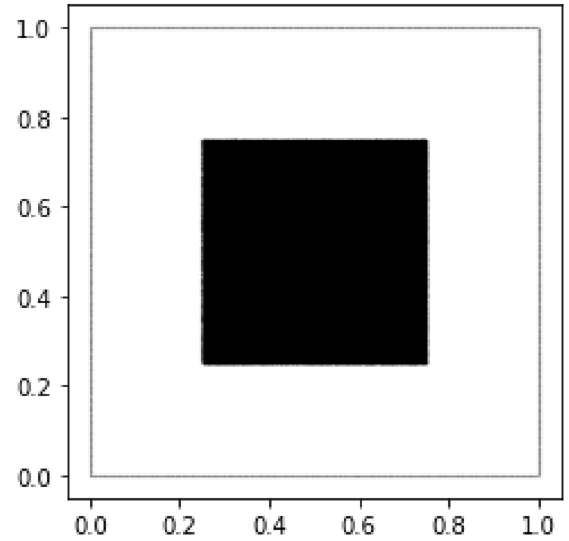
Goals:

- Develop approximation schemes enriched by DL for speed up.
- Improve accuracy of permeability prediction.

Simple example: Fluid flow in porous media



Micro-scale domain Ω_ϵ



Meso-scale domain Ω

Stokes equation on Ω_ϵ:

$$-\nu\Delta\boldsymbol{u} + \nabla p = \boldsymbol{f}$$
$$\nabla\cdot\boldsymbol{u} = 0$$

Stokes-Brinkman equation on Ω:

$$-\nu\Delta\boldsymbol{w} + \nabla\pi + \boldsymbol{K}_\varepsilon^{-1}\boldsymbol{w} = \boldsymbol{f}$$
$$\nabla\cdot\boldsymbol{w} = 0$$

Numerical homogenization

Given $\Omega_\epsilon,\ \Omega \subset \mathbb{R}^2$, find $\{\boldsymbol{u}^i, p^i\}$ and $\{\boldsymbol{w}^i, \pi^i\}$, $i = 1, 2$ from

$$\begin{aligned} -\nu \Delta \boldsymbol{u}^i + \nabla p^i &= \boldsymbol{e}^i \text{ on } \Omega_\epsilon \\ \nabla \cdot \boldsymbol{u}^i &= 0 \text{ on } \Omega_\epsilon \\ \boldsymbol{u}^i &= 0 \text{ on } \partial\Omega_\epsilon^{ob} \\ \boldsymbol{u}^i,\ p^i &\text{ are } \Omega_\epsilon - \text{periodic} \end{aligned}$$

$$\begin{aligned} -\nu \Delta \boldsymbol{w}^i + \nabla \pi^i + \boldsymbol{K}_\epsilon^{-1} \boldsymbol{w}^i &= \boldsymbol{e}^i \text{ on } \Omega \\ \nabla \cdot \boldsymbol{w}^i &= 0 \text{ on } \Omega \\ \boldsymbol{w}^i,\ \pi^i &\text{ are } \Omega - \text{periodic} \end{aligned}$$

Numerical homogenization

Given $\Omega_\epsilon,\ \Omega \subset \mathbb{R}^2$, find $\{\boldsymbol{u}^i, p^i\}$ and $\{\boldsymbol{w}^i, \pi^i\}$, $i = 1, 2$ from

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$$\begin{aligned} -\nu\Delta\boldsymbol{w}^i + \nabla\pi^i + \boldsymbol{K}_\epsilon^{-1}\boldsymbol{w}^i &= \boldsymbol{e}^i \text{ on } \Omega \\ \nabla\cdot\boldsymbol{w}^i &= 0 \text{ on } \Omega \\ \boldsymbol{w}^i,\ \pi^i &\text{ are } \Omega - \text{periodic} \end{aligned}$$

Darcy's law $\left(\boldsymbol{u} = -\frac{\boldsymbol{K}_\epsilon}{\nu}\nabla p\right)$ links two scales:

$$\begin{pmatrix} \langle u_x^1\rangle_p & \langle u_x^2\rangle_p \\ \langle u_y^1\rangle_p & \langle u_y^2\rangle_p \end{pmatrix} = -\frac{1}{\nu}\underbrace{\begin{pmatrix} K_{xx} & K_{xy} \\ K_{yx} & K_{yy} \end{pmatrix}}_{\boldsymbol{K}_\epsilon}\begin{pmatrix} \langle\partial_x p^1\rangle_p & \langle\partial_x p^2\rangle_p \\ \langle\partial_y p^1\rangle_p & \langle\partial_y p^2\rangle_p \end{pmatrix},$$

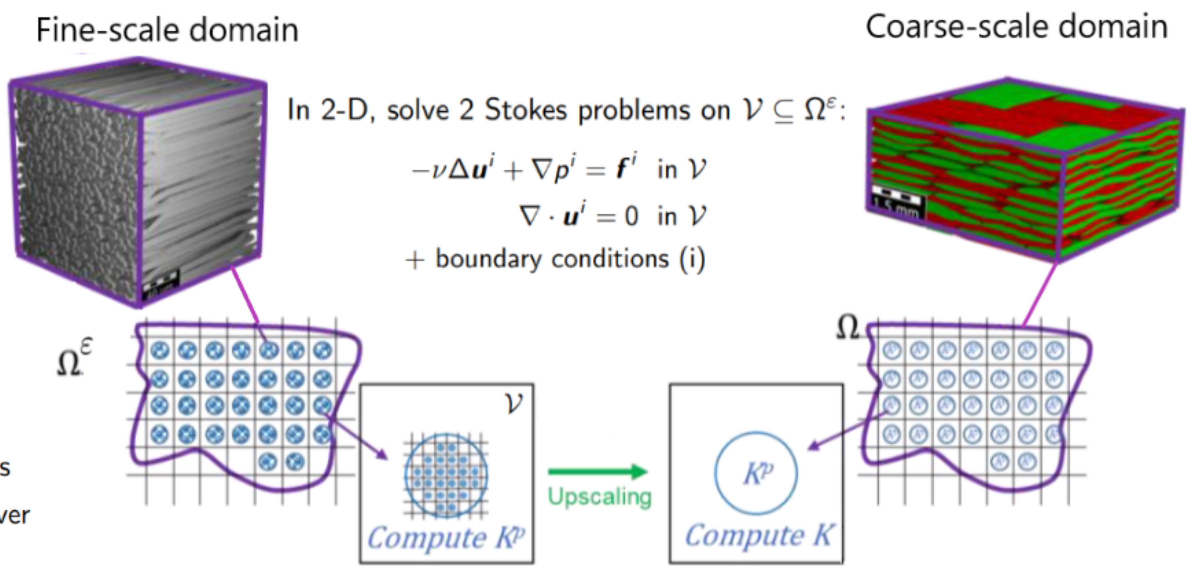
where $\langle\,\cdot\,\rangle_p = \frac{1}{|\Omega_\epsilon^p|}\int_{\Omega_\epsilon^p} \cdot\, dx$ is the averaging over the obstacle region $\Omega_\epsilon^p \subset \Omega_\epsilon$.

Challenges:

- Complex fine-scale geometries
- Repetitive and expensive computations
- Quality of models on the microscale

Our approach:

- Use PINNs on the fine-scale
- Use multiscale structure to improve PINNs
- Derive a hybrid PINN-FEM multiscale solver



Darcy's law for $\boldsymbol{K}^p$ (2-D version), $\boldsymbol{u}^i = (u^i, v^i)$, $1 \leq i \leq 2$:

$$\begin{pmatrix} \langle u^1\rangle_{\mathcal{V}} & \langle u^2\rangle_{\mathcal{V}} \\ \langle v^1\rangle_{\mathcal{V}} & \langle v^2\rangle_{\mathcal{V}} \end{pmatrix} = -\frac{1}{\nu} \begin{pmatrix} \langle \partial_x p^1\rangle_{\mathcal{V}} & \langle \partial_x p^2\rangle_{\mathcal{V}} \\ \langle \partial_y p^1\rangle_{\mathcal{V}} & \langle \partial_y p^2\rangle_{\mathcal{V}} \end{pmatrix} \underbrace{\begin{pmatrix} K^p_{11} & K^p_{12} \\ K^p_{21} & K^p_{22} \end{pmatrix}}_{\boldsymbol{K}^p}$$

Upscaling: PINN - FEM connection

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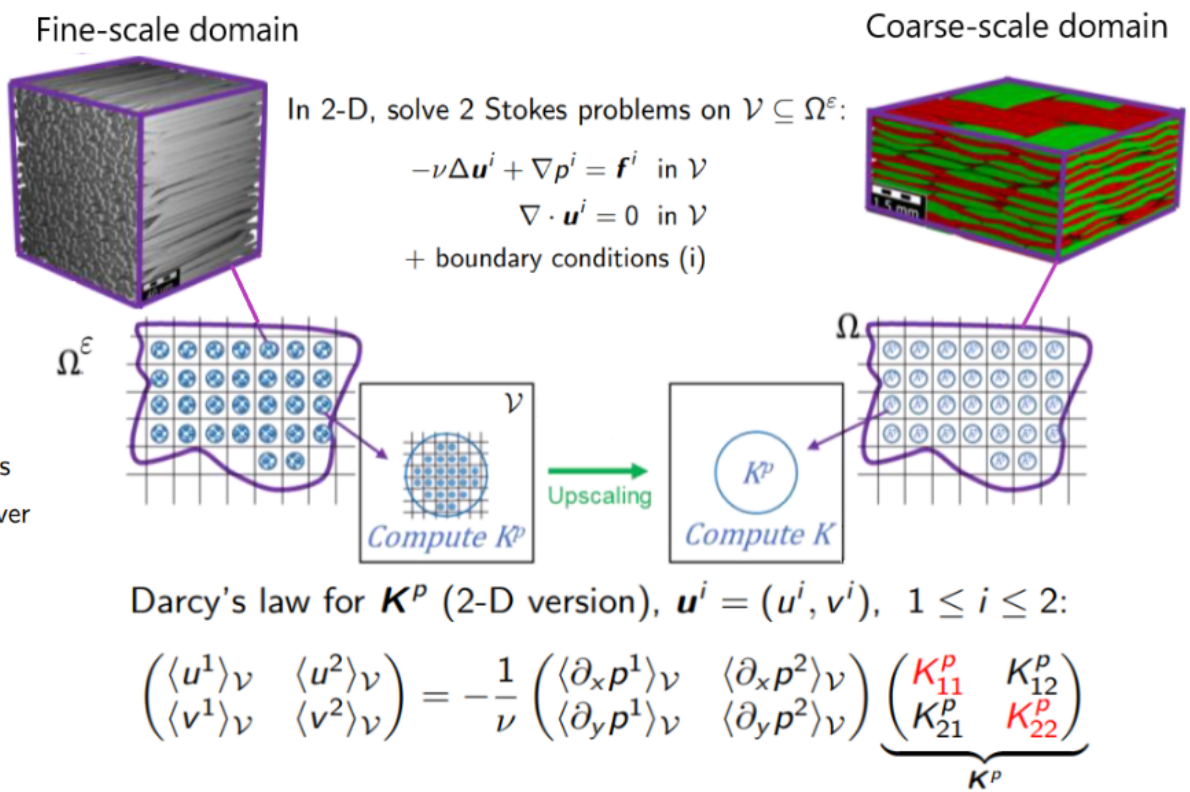

Lit. on multiscale: [Allaire], [E], [Enquist], [Efendiev], [Vanden-Eijnden],...

PINN-based ansatz

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- Interpret $u_{\boldsymbol{\theta},n}$ as control, y as state.

Numerical test

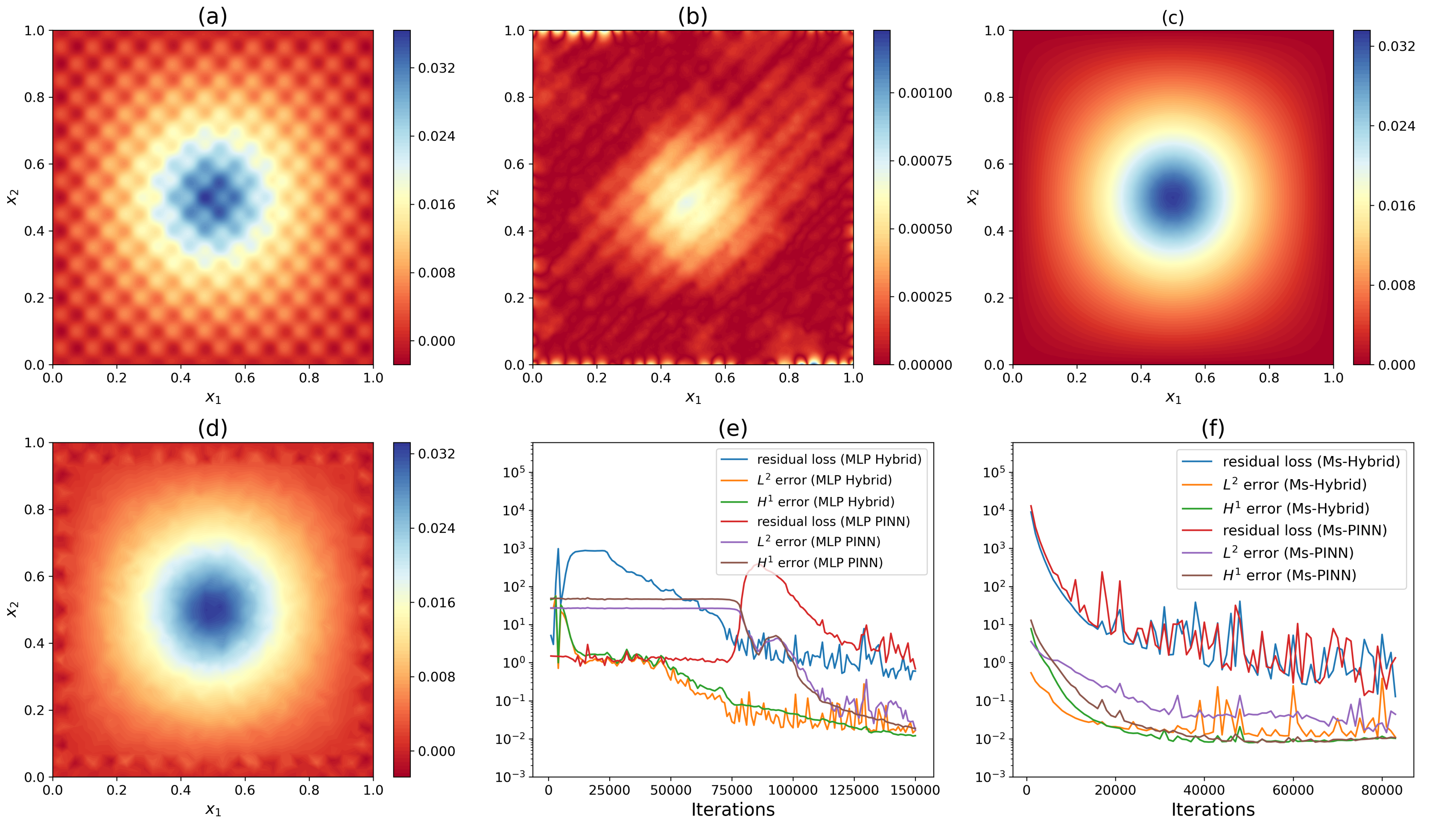

Figure: Results for $\varepsilon = 0.1$: **(a)** Hybrid MLP-based fine-scale solution u^{ε}_{HNN}, **(b)** Pointwise error $|u^{\varepsilon}_{HNN}(x) - u^{\varepsilon}_{h}(x)|$, **(c)** Predicted state $y_h(u^{\varepsilon}_{HNN})$, **(d)** Compression $\bar{Q}_{\delta} u^{\varepsilon}_{HNN}$, **(e)** PDE residual losses and relative L^2 and H^1 errors vs iterations for MLP-based hybrid solver and MLP PINN, **(f)** PDE residual losses and relative L^2 and H^1 errors vs iterations for Ms-PINN-based hybrid solver and Ms-PINN.

Outlook

- Expand approach to genuine multi (i.e. beyond two level) complexity model
- Use variational / deep Ritz formulation to lower regularity requirement for PINN model
- 2nd-order optimality analysis, perturbation stability, and error estimates (NN / FEM)
- Design dedicated optimization solver allowing inexact subproblem solves
- Admit constraints on y, u_θ such as pointwise constraints
- Extend to more general equilibrium problems (VIs, QVIs, games)
- Lowering NN regularity — towards ReLU activation
- ...

Thank you for your attention!