MMS Leibniz Days

Machine Learning for Simulation Intelligence in Composite Process Design

Research Group

Nonsmooth Variational Problems and Operator Equations

Head:
Michael Hintermüller

Accurate modelling of composites can be challenging due to the complex geometries of composite media and the presence of multiple scales with different physics. This requires computational grids with very fine resolution and imposes severe computational constraints on standard numerical solvers designed to solve the underlying equations (PDEs). Homogenization techniques are often used to overcome such difficulties and allow efficient extraction or upscaling of material properties from the microscale level for further use in macroscale simulations. In addition, enriching and improving classical composite design methods through machine learning is a promising research direction. We investigate the applicability of machine learning to composite design and the approximation of solutions to continuum media equations arising in this context.

ML4SIM research agenda

- The applications of machine learning to composite material design
- New mathematical architectures for approximating PDE solutions using a mixture of neural networks and standard numerical solvers.
- Discovering potential advantages, disadvantages, and future prospects of ML in the context of composite material modelling.
- New methodologies for multiscale simulation.
- Interdisciplinary exchange of ideas and experience between the partners.

Fluid flow in porous media

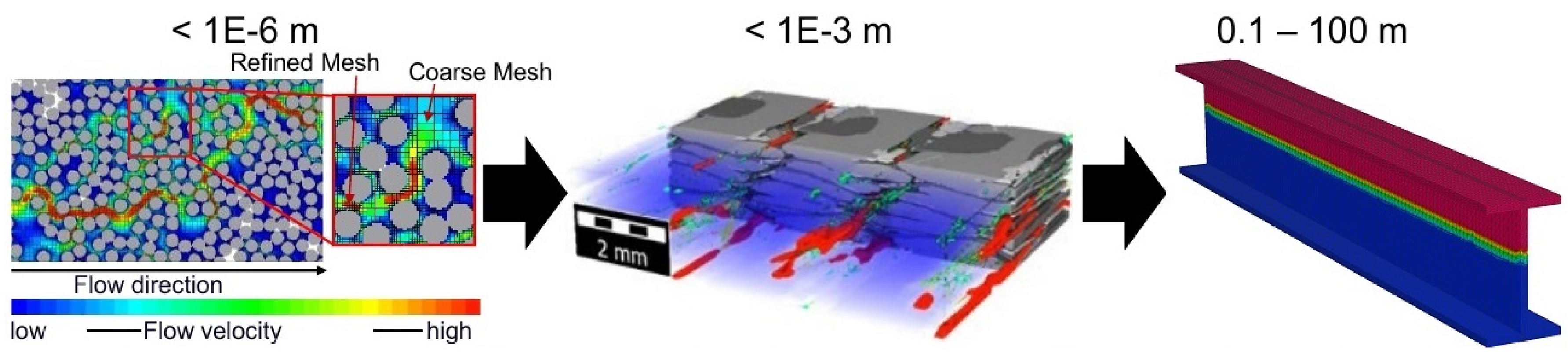


Illustration of physics at different scales for a liquid composite molding case: An adaptive grid in a microscopic flow simulation (2D) through a fiber bundle (left), mesoscopic flow simulation in a representative vol. element model of a textile (middle) and macroscopic simulation of part filling (right)

Physics-informed neural networks

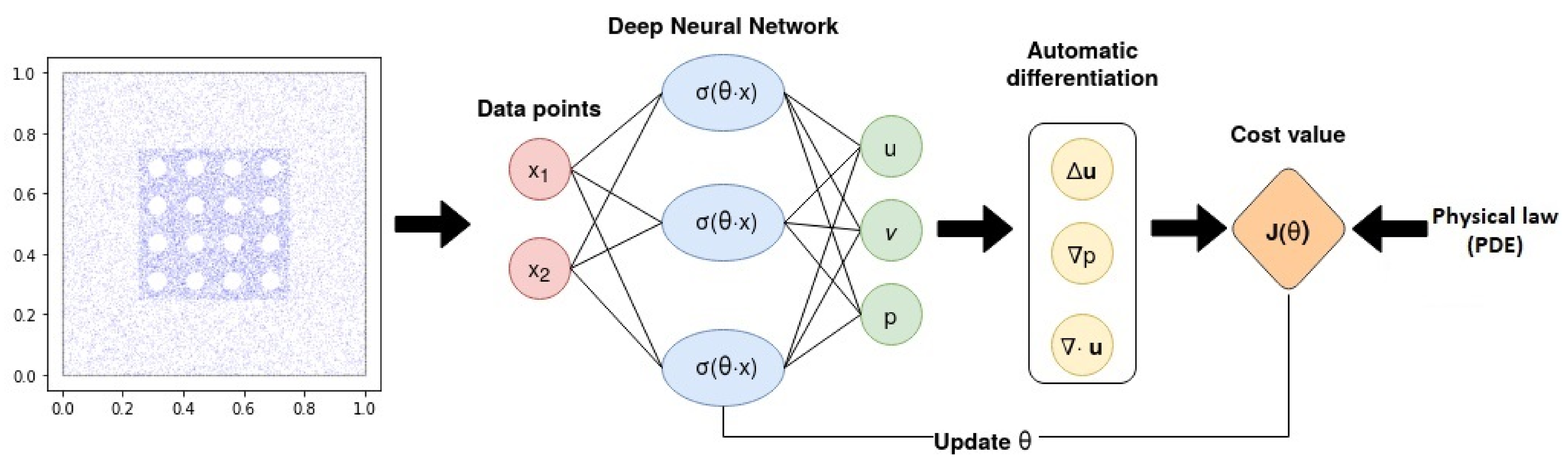
The knowledge of physics is built into a cost functional as the PDE residuals:

$$\mathcal{J}_\tau(\boldsymbol{u},p) := \|-\nu\Delta\boldsymbol{u} + \nabla p - \boldsymbol{f}\|^2_{[L^2(\Omega)]^2} + \tau_1\|\nabla\cdot\boldsymbol{u}\|^2_{L^2(\Omega)} + \tau_2\|\boldsymbol{u}-\boldsymbol{g}\|^2_{[L^2(\partial\Omega)]^2}$$

The least-squares problem over a class of neural networks $\mathfrak{N}_n$ is then solved:

$$\inf_{(u_{\boldsymbol{\theta}},p_{\boldsymbol{\theta}})\in\mathfrak{N}_n} \mathcal{J}_\tau(u_{\boldsymbol{\theta}},p_{\boldsymbol{\theta}})$$

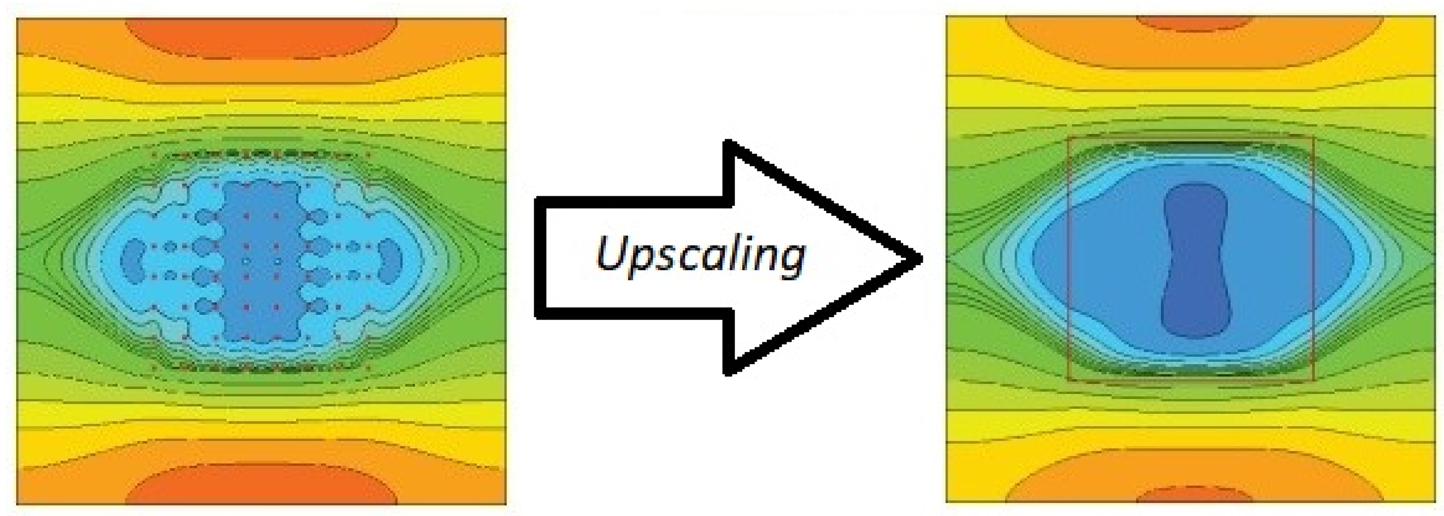
More details: Raissi, M., Perdikaris, P., Karniadakis, G.E., 2019. Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. Journal of Computational physics



- Physics-informed neural networks are meshless and are suitable for handling complex geometries of composite materials.
- The non-convex nature of the NN optimization often leads to difficulties and limitations and requires a certain delicacy in analytical and numerical handling

Governing equations

The Stokes-Brinkman-Darcy equations of fluid flow in porous media depend on the scale:



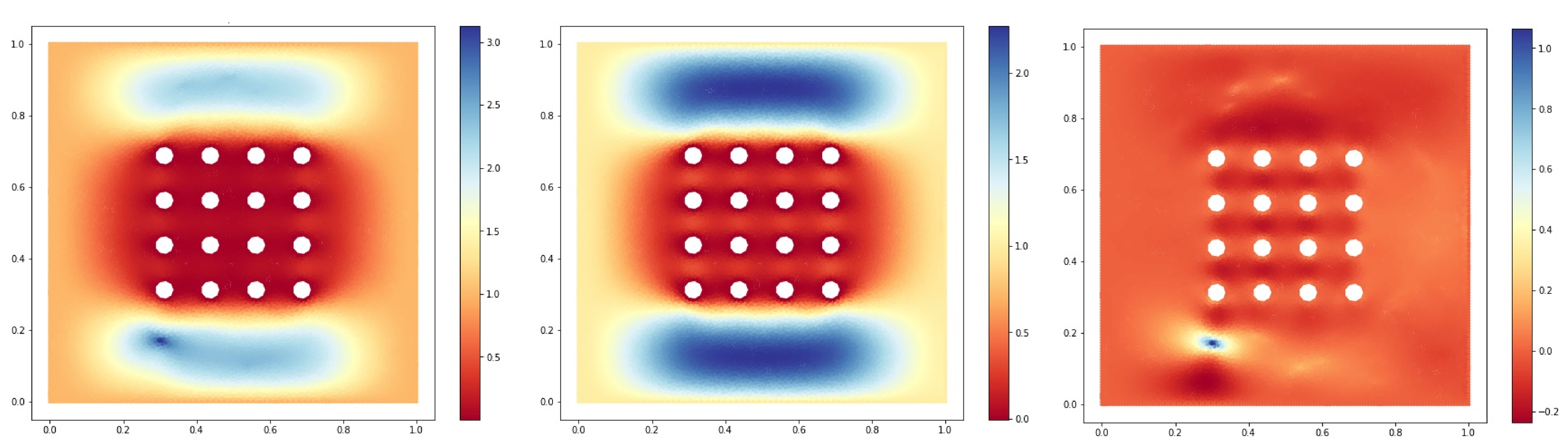
$$\begin{aligned} -\nu\Delta\boldsymbol{u} + \nabla p &= \boldsymbol{f} \text{ in } \Omega_\varepsilon,\\ \nabla\cdot\boldsymbol{u} &= 0 \text{ in } \Omega_\varepsilon,\\ \boldsymbol{u} = 0 \text{ on } \partial\Omega_\varepsilon^{ob},\ \boldsymbol{u} &= \boldsymbol{g} \text{ on } \partial\Omega_\epsilon^{w}. \end{aligned}$$

$$\begin{aligned} -\nu\Delta\boldsymbol{w} + \nabla\pi + \boldsymbol{K}^{-1}\boldsymbol{w} &= \boldsymbol{f} \text{ in } \Omega,\\ \nabla\cdot\boldsymbol{w} &= 0 \text{ in } \Omega,\\ \boldsymbol{w} &= \boldsymbol{g} \text{ on } \partial\Omega. \end{aligned}$$

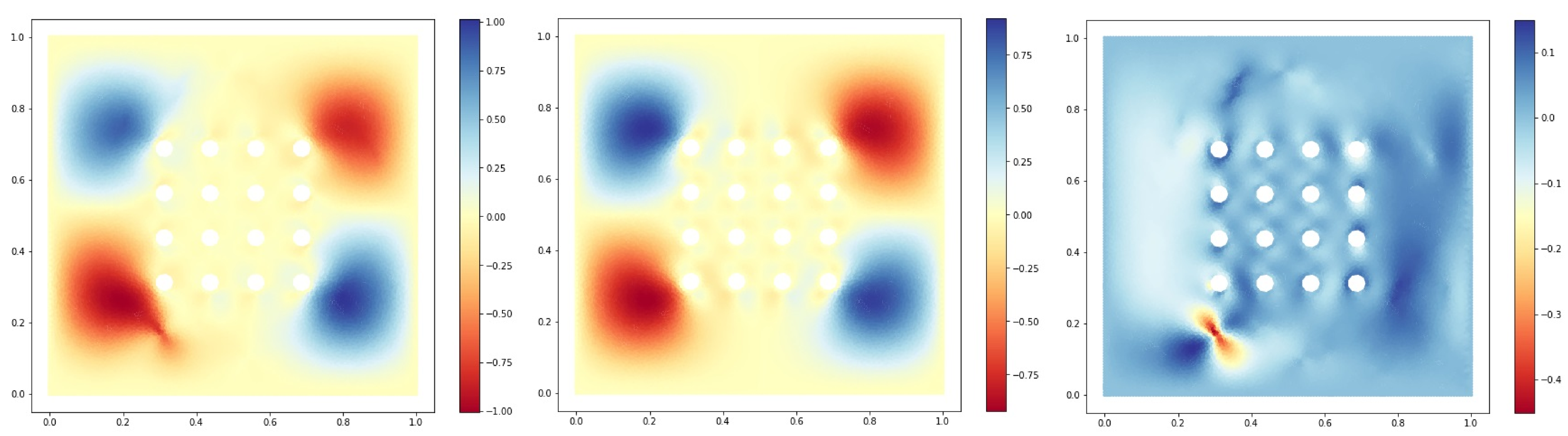
The permeability $\boldsymbol{K}$ is obtained by upscaling using Darcy's law from a few simulations of the Stokes problem:

$$\begin{pmatrix} \langle u^1\rangle & \langle u^2\rangle \\ \langle v^1\rangle & \langle v^2\rangle \end{pmatrix} = -\frac{1}{\nu}\begin{pmatrix} \langle\nabla p_x^1\rangle & \langle\nabla p_x^2\rangle \\ \langle\nabla p_y^1\rangle & \langle\nabla p_y^2\rangle \end{pmatrix}\begin{pmatrix} K_{xx} & K_{xy} \\ K_{yx} & K_{yy} \end{pmatrix}, \quad \langle\cdot\rangle = \frac{1}{|\Omega_\varepsilon^{ob}|}\int_{\Omega_\varepsilon^{ob}} \cdot\, dx$$

More details: Griebel, M, Klitz, M., 2010. Homogenization and numerical simulation of flow in geometries with textile microstructures. Multiscale Modeling and Simulation .



The horizontal velocity component u: PINN approximation (left), FEM approximation (center), pointwise error (right).



The vertical velocity component v: PINN approximation (left), FEM approximation (center), pointwise error (right).

Hybrid multiscale solver

The hybrid physics-informed neural network for numerical homogenization is formulated as an optimal control problem with PDE constraints:

$$\inf_{(\boldsymbol{u},p,\boldsymbol{w})} \mathcal{J}_{\tau,\delta}(\boldsymbol{u},p,\boldsymbol{w}) := \mathcal{J}_\tau(\boldsymbol{u},p) + \tau_3\mathcal{J}_D(\boldsymbol{u},\boldsymbol{w}),$$

subject to the Stokes-Brinkman equations :

$$\begin{aligned} \boldsymbol{K}^{-1}\boldsymbol{w} - \nu\Delta\boldsymbol{w} + \nabla\pi &= \boldsymbol{f} \text{ in } \Omega,\\ \nabla\cdot\boldsymbol{w} &= 0 \text{ in } \Omega,\\ &+ \text{boundary conditions.} \end{aligned}$$

The term $\mathcal{J}_D(\boldsymbol{u},\boldsymbol{w})$ measures the discrepancy between u and w and couples two scales:

$$\mathcal{J}_D(\boldsymbol{u},\boldsymbol{w}) := \|\boldsymbol{B}_\delta\boldsymbol{u} - \boldsymbol{w}\|^2_{[L^2(\Omega)]^2},\ \boldsymbol{B}_\delta\boldsymbol{u}(x) := \frac{1}{|B_\delta|}\int_{B_\delta}\boldsymbol{u}(y)dy,$$

where $B_\delta(z) := \{x : \|x-z\|_{R^2} \leq \delta\}$.

The combination of physics-informed neural networks with robust and efficient numerical solvers may be a possible way to mitigate the challenges of vanilla neural network approach

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