PRECONDITIONED FEM-BASED NEURAL NETWORKS FOR SOLVING INCOMPRESSIBLE FLUID FLOWS AND RELATED INVERSE PROBLEMS

Fabrice von der Lehr, Franziska Griese, Katharina Rauthmann, Philipp Knechtges
(SC-HPC, Cologne)

WAW Machine Learning 11

DLR

Motivation for Physics-Informed Neural Networks

Mechanistic modelling:

- Numerical simulations of partial differential equations (PDEs)
- Expensive, especially when PDEs have to be solved for several parameters
- Often infeasible in real-time applications / with limited computing capacity

➔ **Performant surrogate models needed**

Data-driven ML approaches:

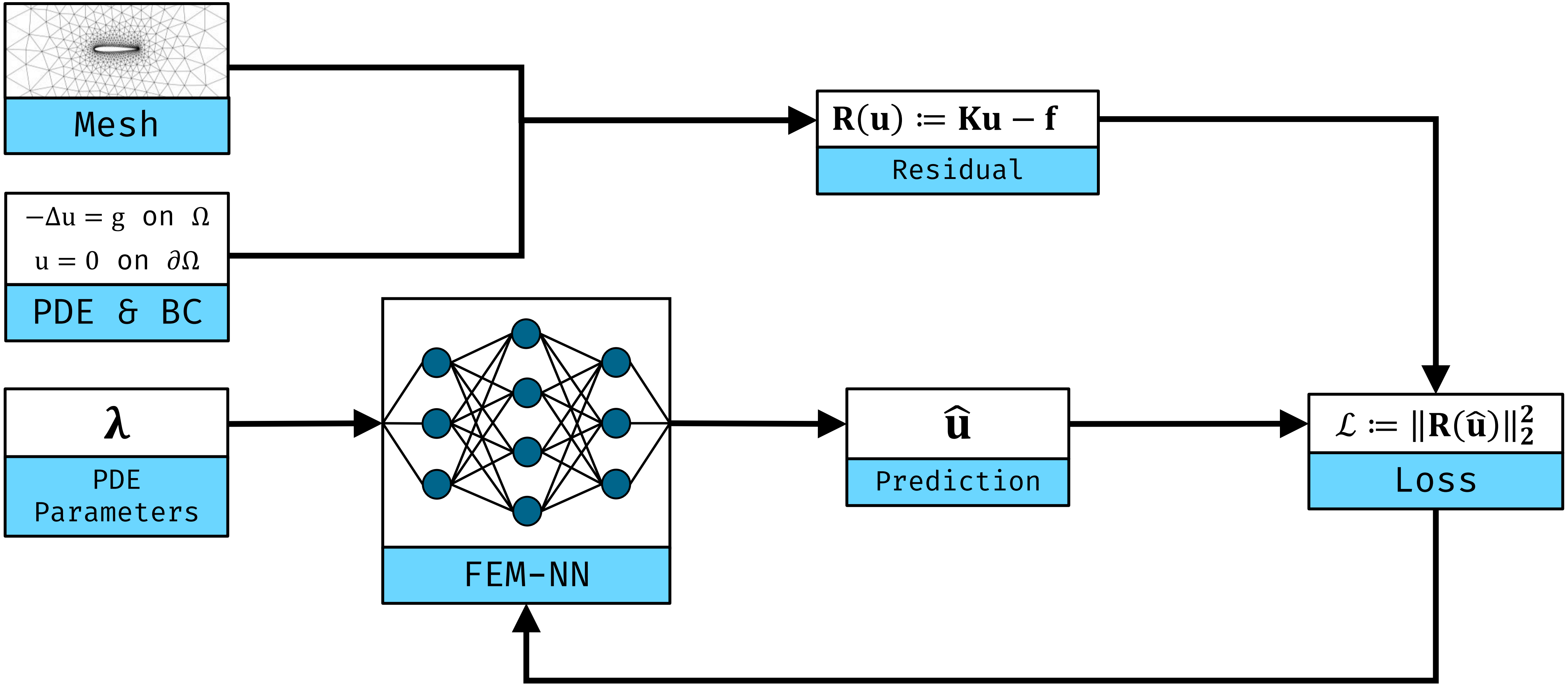
- Trained with data from simulations or real-world measurements
- Physical laws (e.g., conservation of energy) are not / only poorly considered

FEM-based Neural Networks

- Combining finite element method (**FEM**) with neural networks (**NNs**)
- Ideal outcome: **Uniting strengths** of both methods while **compensating their weaknesses**

FEM	NN
☹ No real-time capacity	☺ Fast prediction after training
☹ No cost amortization over multiple runs	☺ Parameterizable
☺ Sound mathematical foundation	☹ Black box model
☺ Numerical theory of errors	☹ Rudimentary convergence theory

FEM-based Neural Networks



Incompressible 2D Navier-Stokes Flow around an Airfoil

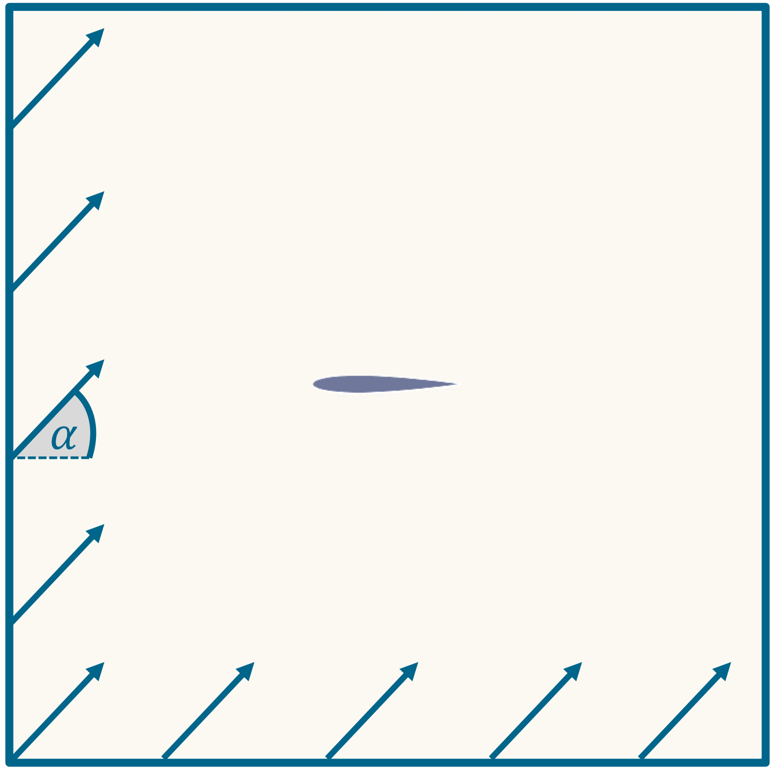
PDE:

$$-\eta\Delta u + \mathrm{u}\cdot\nabla u + \nabla p \;=\; 0,$$
$$\nabla\cdot u = \;0$$

with viscosity η, velocity u, and pressure p.

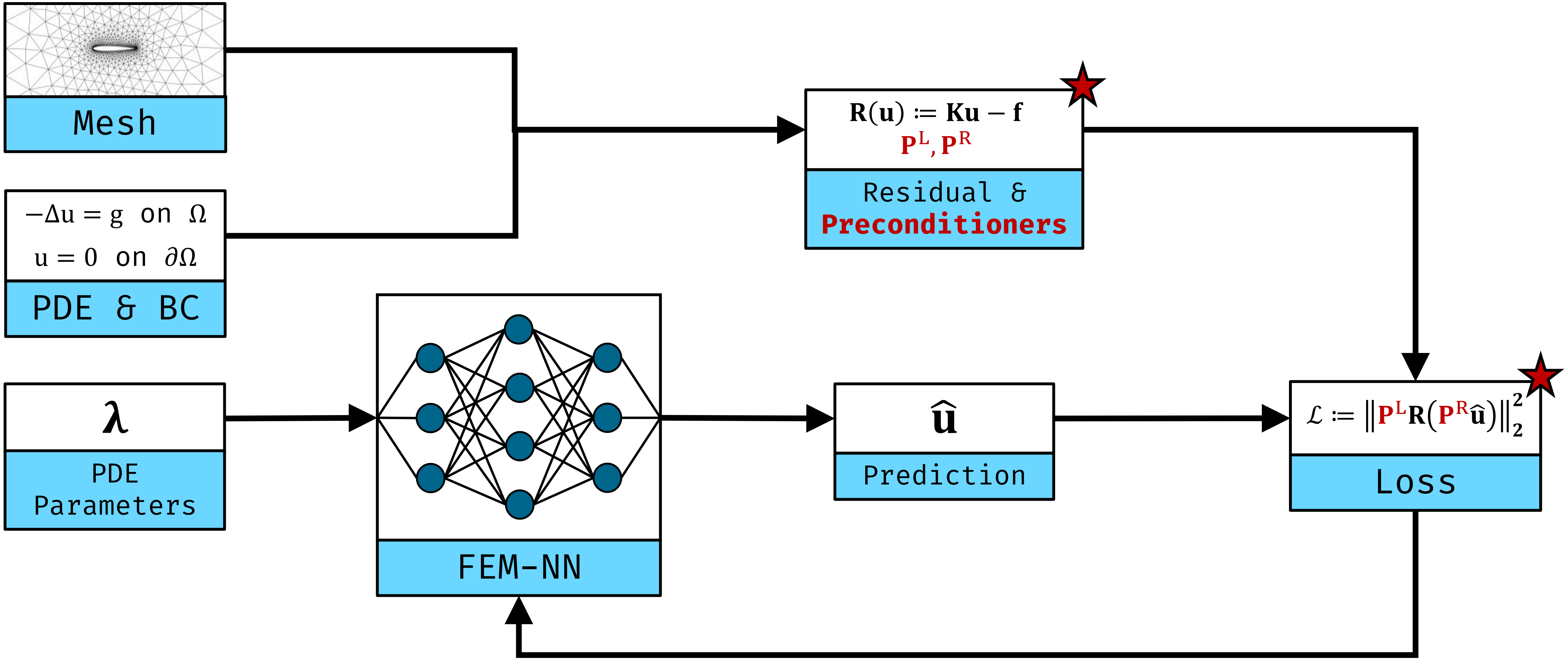
BC: Dirichlet at inflow (dependent on α), Neumann at outflow, no-slip at airfoil.

- Nonlinear saddle point problem
- Even for FEM hard, depending on η



Domain around NACA 0012 airfoil with an angle of attack α.

Preconditioned FEM-based Neural Networks



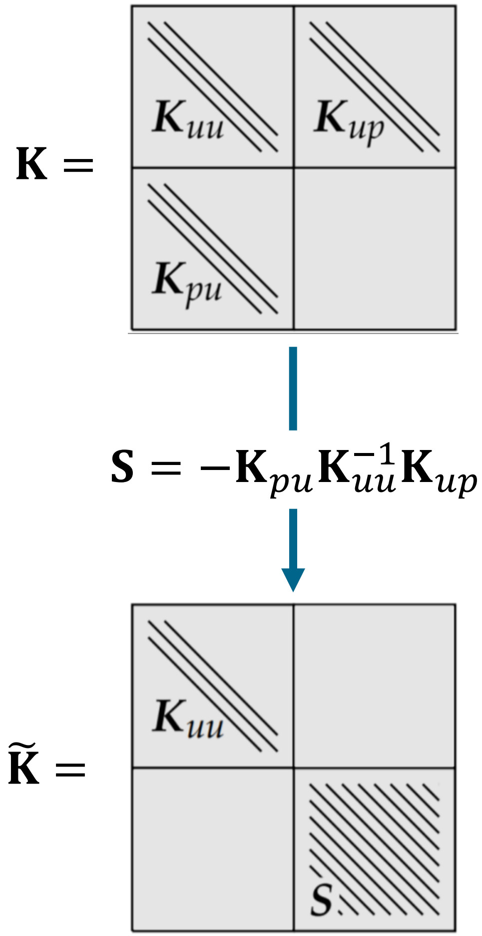
Preconditioning for Stokes and Navier-Stokes Problems

- Saddle point structure of the stiffness matrix $\mathbf{K}$ allows for **block-diagonal preconditioners** featuring the **Schur complement**

$$\mathbf{K} = \begin{bmatrix} \mathbf{K}_{uu} & \mathbf{K}_{up} \\ \mathbf{K}_{pu} & \mathbf{0} \end{bmatrix} \quad \rightarrow \quad \mathbf{S} = -\mathbf{K}_{pu}\mathbf{K}_{uu}{}^{-1}\mathbf{K}_{up}$$

$$\rightarrow \quad \mathbf{P}^{\mathrm{L}} := \begin{bmatrix} \mathbf{L}^{-1} & 0 \\ 0 & \mathbf{M}^{-1} \end{bmatrix}, \quad \mathbf{P}^{\mathrm{R}} := \begin{bmatrix} \mathbf{L}^{\mathrm{T}} & 0 \\ 0 & \mathbf{M}^{\mathrm{T}} \end{bmatrix}$$

- Here, $\mathbf{K}_{uu} = \mathbf{L}\mathbf{L}^{\mathrm{T}}$ and $-\mathbf{S} = \mathbf{M}\mathbf{M}^{\mathrm{T}}$ denote Cholesky decompositions, respectively

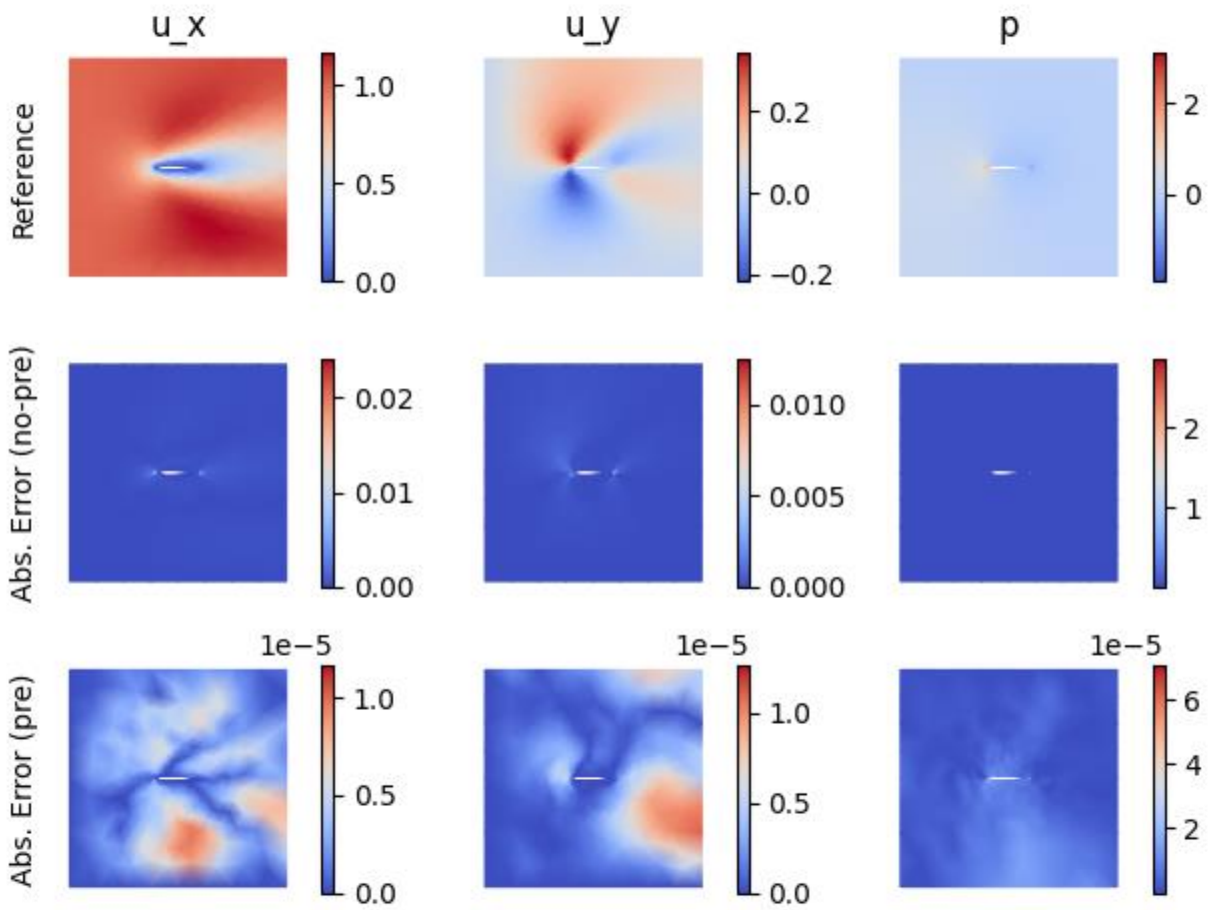


Results for 2D Navier-Stokes Equations

- Training with $\alpha = 1°,\ \eta = 0.1$, and 10k iterations (no-pre) / 250 iterations (pre) of L-BFGS
- Training time: 4 min (pre) / 9 min (no-pre)

→ Error improvement by >3 orders of magnitude

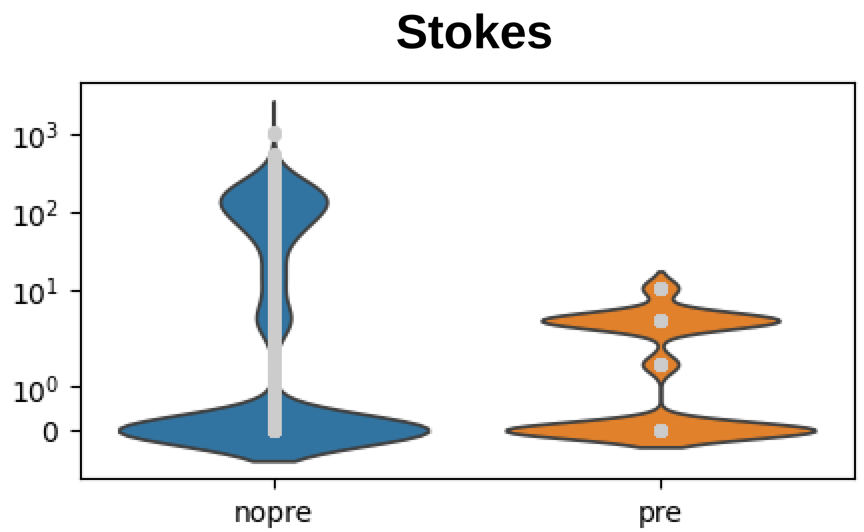
→ Speedup of x2

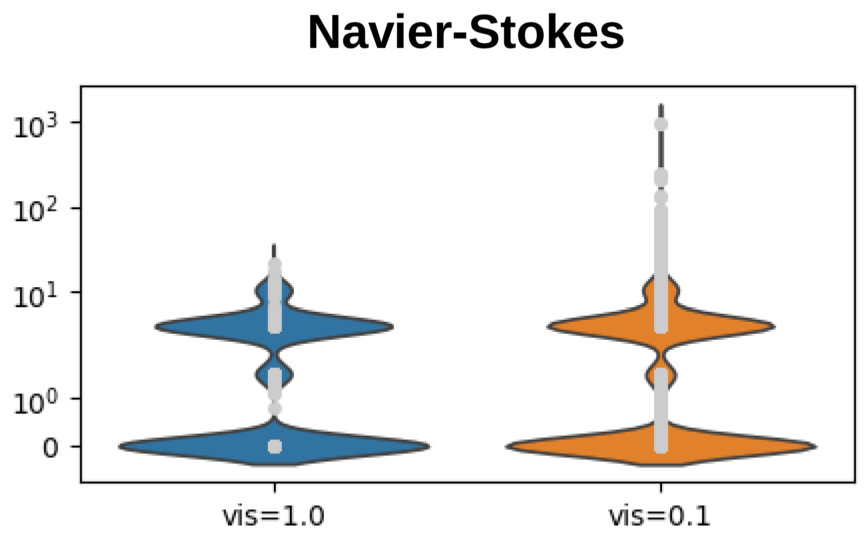


Eigenspectra of the Loss Hessian

- **Without preconditioning:** unclustered eigenspectrum, extending over several orders of magnitude
- **With preconditioning**: only few clusters at rather small eigenvalues

→ **Reduction of the condition number is transferred through the nonlinearity of the NN to its parameter space**





Conjugate Gradients (CG) on the Normal Equations

- Solving the least-squares problem

$$\min_{\mathbf{u}} ||\mathbf{K}\mathbf{u} - \mathbf{f}||_2^2$$

using BFGS is equivalent to applying CG to the normal equations

$$\underbrace{\mathbf{K}^T\mathbf{K}}_{\widetilde{\mathbf{K}}}\mathbf{u} = \underbrace{\mathbf{K}^T\mathbf{f}}_{\tilde{\mathbf{f}}}$$

- It is well known that **CG converges more quickly** if the **eigenspectrum** of the system matrix (here: $\widetilde{\mathbf{K}} = \mathbf{K}^T\mathbf{K}$) **has few clusters**

- This is the case if the **singular values** of the matrix $\mathbf{K}$ are well clustered

Implications for Preconditioning

- Classical preconditioners $\mathbf{P}$ are designed to **cheaply approximate the inverse $\mathbf{K}^{-1}$** and often guarantee a certain **clustering of eigenvalues**

- In our case, however, since $\mathbf{K}$ **is not necessarily symmetric** (e.g., Navier-Stokes), **its eigenvalues do generally not relate to its singular values**; in the worst case, such a near-inverse preconditioner could even **spread out the singular values further**

- By contrast, an **ideal left-preconditioner $\mathbf{P}^{\mathbf{L}}$ for the normal equations** is a **near-orthogonalizer**, i.e.,

$$\left(\mathbf{P}^{\mathbf{L}}\mathbf{K}\right)^{T}\left(\mathbf{P}^{\mathbf{L}}\mathbf{K}\right) \approx \mathbf{I},$$

as the singular values of an orthogonal matrix are all equal to 1

Orthogonalizing Preconditioners

- **LQ decomposition**

$$\mathbf{LQ} = \mathbf{K}$$

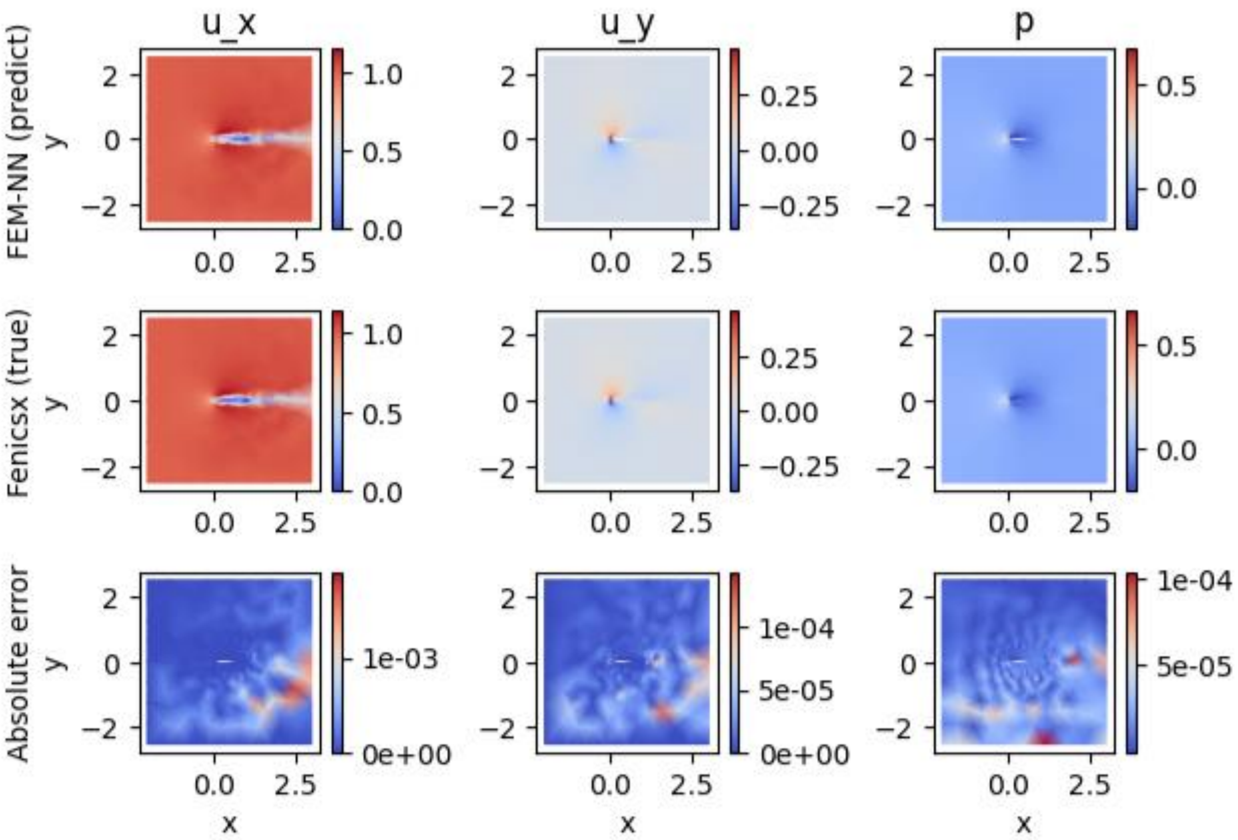
provides an **ideal orthogonalizing left-preconditioner** $\mathbf{P^L} = \mathbf{L}^{-1}$, but is expensive and has to be recomputed in the case of Navier-Stokes due to the nonlinear convection term

- **Cheaper incomplete LQ algorithms** and **data-driven preconditioners** have shown to cluster singular values **only insufficiently**

- Although the **set of all orthogonal matrices grows quadratically** with the matrix dimensionality, the design of cheaper orthogonalizing preconditioners has proven to be **difficult**

Results for 2D Navier-Stokes Equations (Low Viscosity)

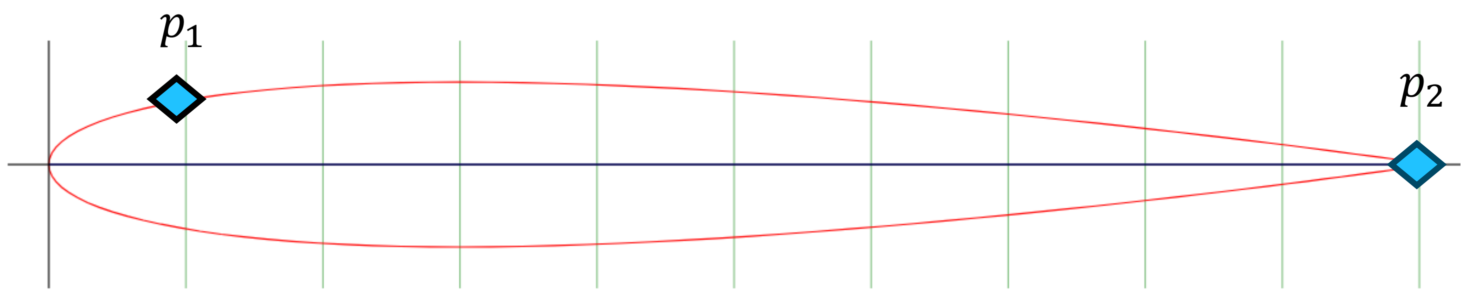
- **Continuation Method:** In order to compute the preconditioner $\mathbf{L}$ to $\mathbf{K}(\mathbf{u})$ for a viscosity η_k, we predict $\mathbf{u}$ using a FEM-NN previously trained for viscosity $\eta_{k-1} > \eta_k$
- This **iterative training process** is started by training w.r.t. the corresponding Stokes problem
- Accurate predictions are possible up to a **Reynolds number of 500** ($\eta = 0.02$, right figure)



Solving an Inverse Navier-Stokes Problem using FEM-NNs

Inverse problem:

Given noisy pressure measurements p_i at specific locations of the airfoil, infer the angle of attack α.

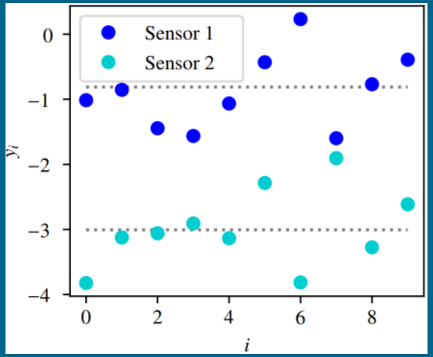


Solving an Inverse Navier-Stokes Problem using FEM-NNs

Inverse problem:

Given noisy pressure measurements p_i at specific locations of the airfoil, infer the angle of attack α.

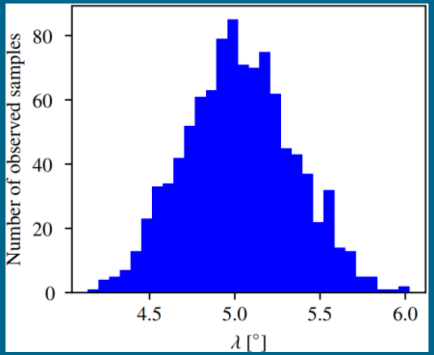
Input: Trained FEM-based NN, noisy measurements p_i



PYRO

Hamiltonian Monte Carlo (HMC)

Output: Distribution for angle of attack α



Fabrice von der Lehr, SC-HPC, DLR Cologne

Conclusion

- This talk presented **FEM-NNs** as performant **surrogate models** to solve **incompressible fluid flow problems**
- Since **efficient preconditioners** are **absolutely necessary, but difficult to obtain**, the method currently only performs well for **low to moderate Reynolds numbers** (10^2 to 10^3)
- The presented results have been created as part of the **DLR projects PISA (finished)** and **TIARA (ongoing)**