Imperial College London

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Surrogate Modelling of Fluid Dynamics within Various Vascular Geometries with Physics-Informed Neural Networks

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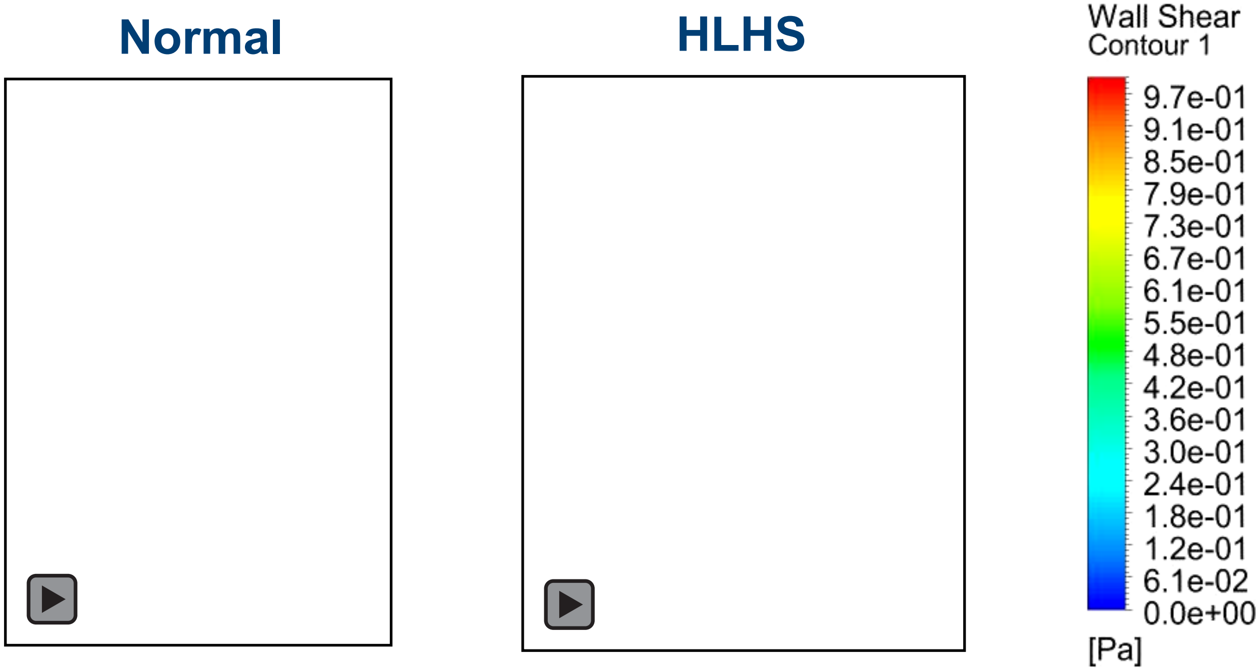
From CFD to PINN

- Huge alternations in flow dynamics are associated with the cardiovascular diseases (e.g., hypoplastic left-heart syndrome)
- *In-silico* fluid modelling is a powerful surrogate to the highly invasive clinical measurements



Wong, H S & **Li, B** *et al.* (2023)

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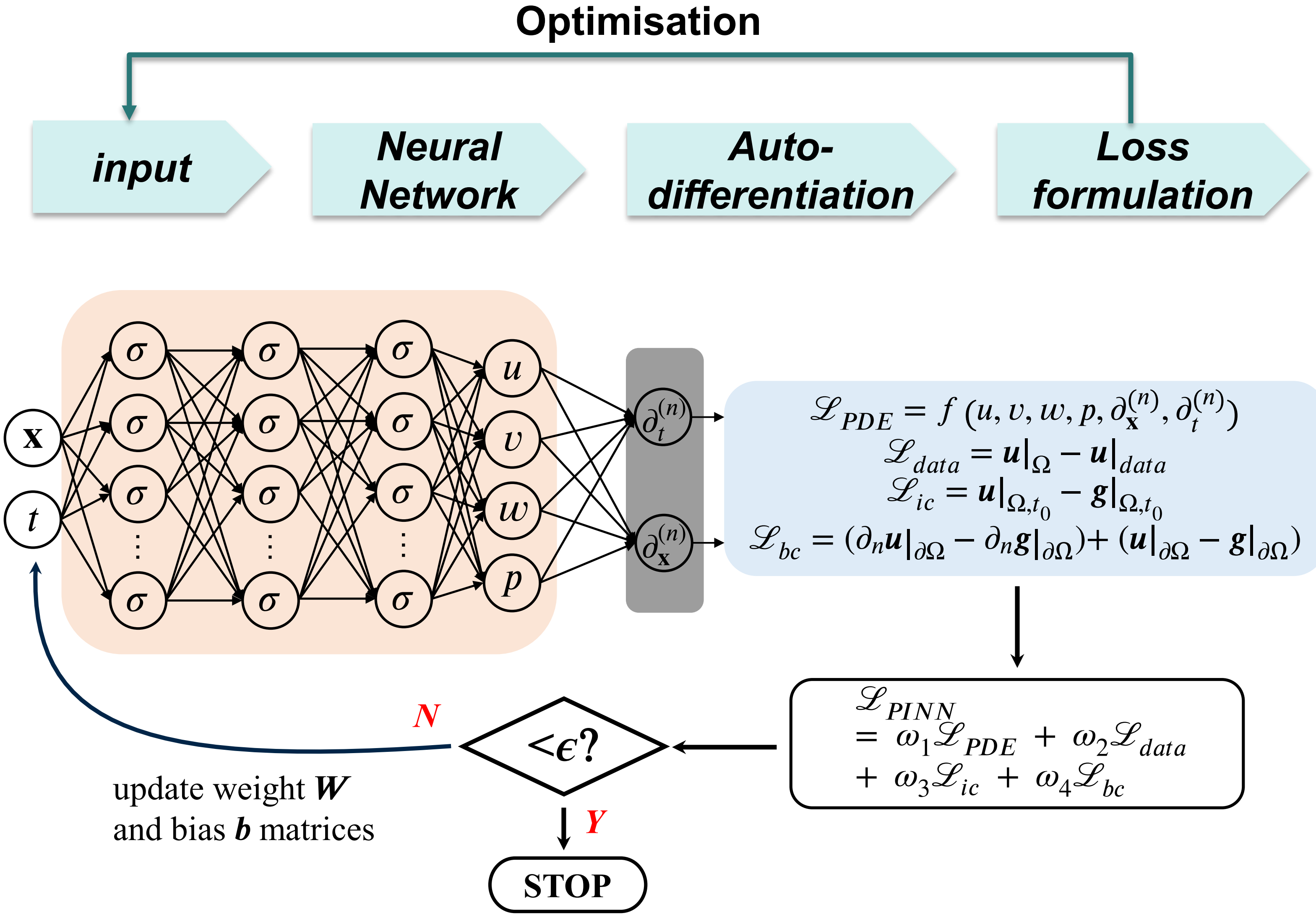
Numerical solvers (CFD, FSI)

- Accurate
- Long simulation time
- Tedious procedures

Physics-informed Neural Networks (PINN)

- Mesh-free
- Physics-constraint + data-assisted
- Diminutive model size
- Forward and inverse capability

Vanilla PINN for Fluid Simulation



Modified and reproduced based on Cai *et al.* (2021)

Physics Loss Formulation

$$\mathcal{L}_{PINN} = \omega_1 \mathcal{L}_{PDE} + \omega_2 \mathcal{L}_{data} + \omega_3 \mathcal{L}_{ic} + \omega_4 \mathcal{L}_{bc}$$

The N-S momentum eqns are raised from $\boldsymbol{F} = m\boldsymbol{a}$

$$\underbrace{\rho\left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u}\right)}_{m\ \mathbf{a}} = \underbrace{-\nabla p + \mu\nabla^2\mathbf{u} + \rho\mathbf{f}}_{\mathbf{F}}$$

Hence, $\boldsymbol{F} = m\boldsymbol{a} \Rightarrow m\boldsymbol{a} - \boldsymbol{F} = 0$ (for satisfying the conservation)

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u}\right) + \nabla p - \mu\nabla^2\mathbf{u} - \rho\mathbf{f} = 0$$

If $m\boldsymbol{a} - \boldsymbol{F} \neq 0$, the loss raises (formulated in the 2-norm fashion)

$$\mathcal{L}_{NS} = \left|\left|\rho\left(\frac{\partial \hat{\mathbf{u}}}{\partial t} + (\hat{\mathbf{u}}\cdot\nabla)\hat{\mathbf{u}}\right) + \nabla p - \mu\nabla^2\hat{\mathbf{u}} - \rho\mathbf{f}\right|\right|_2$$

$\hat{\mathbf{u}}$: trained (imperfect) result from the network

Overall objective

- Develop a physics-informed surrogate model to approximate the fluid dynamics within parameterized vascular geometries;
- Exploit the opportunity of predicting unseen fluid dynamics with a pre-trained model.

Benchmark I: Framework Realisation and Optimisation

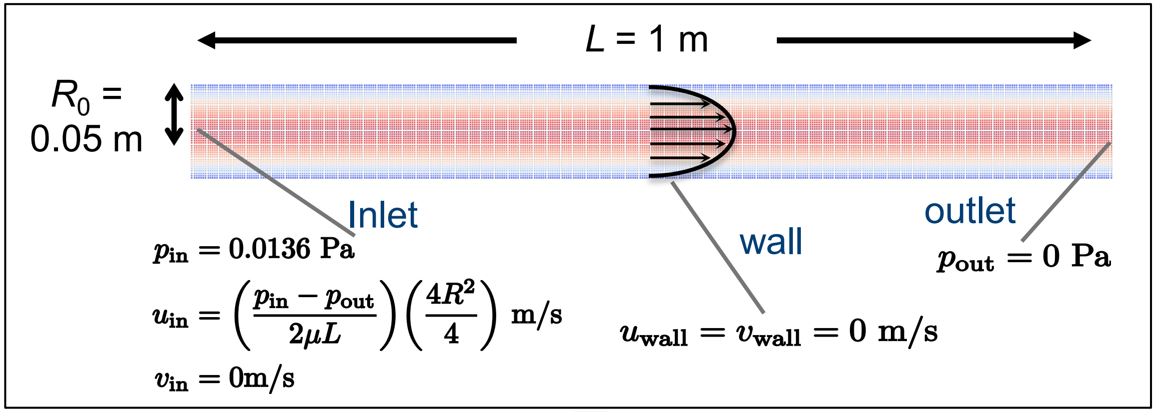
- Evaluate the feasibility of using performance-enhancing techniques: adaptive learning rate (ADR), hard boundary (HB), increase order (IO)

Benchmark II: Multi-Case Training and Prediction

- Implement the case hyper-network to simultaneously train multiple parametrised cases, and predict the unseen cases with the model

Problem Setup and Network Architecture

Fluid Mechanics & Geometry Transformation

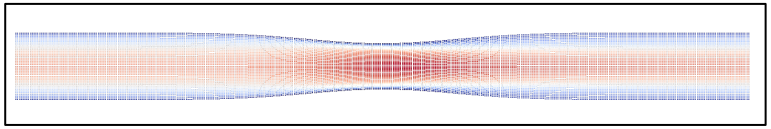


coordinate transformation

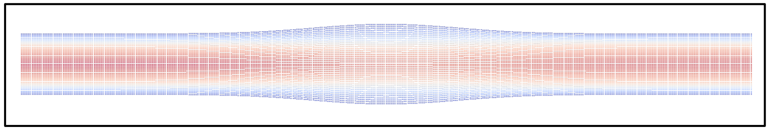
$$R(x) = R_0 - A\frac{1}{\sqrt{2\pi\sigma^2}}\exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

Adopted from Sun *et al.* (2020)

A = 0.004, stenosis



A = -0.004, aneurysm



Assumptions

- Steady flow
- Neglected body force
- Non-slip wall condition

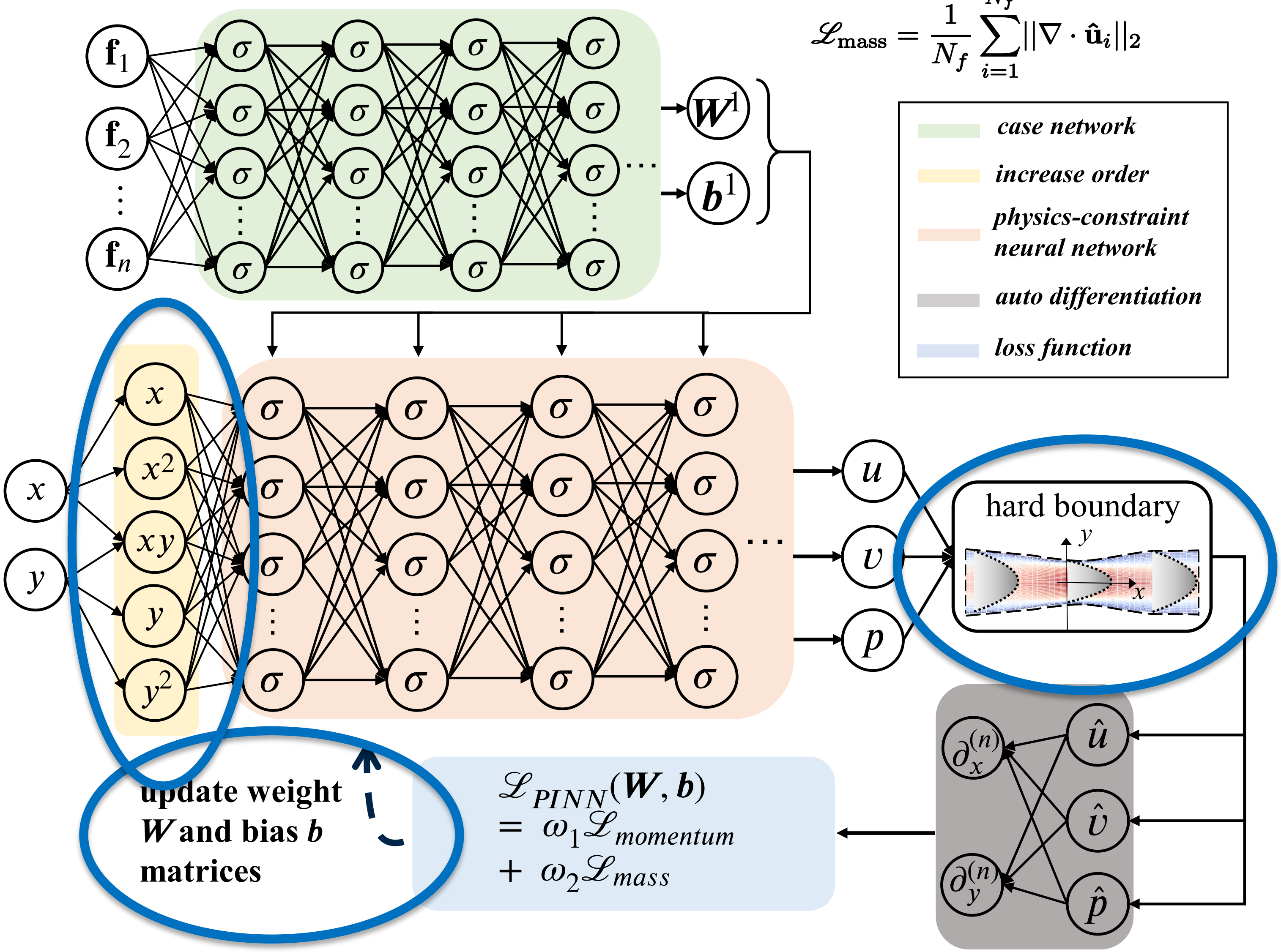
Key Parameters

- ρ = 1000 kg/m^3
- μ = 0.00185 kg/m s
- u_{max} = 9.25e-3 m/s
- Re = 500

Network architecture

$$\mathscr{L}_{\text{momentum}} = \frac{1}{N_f}\sum_{i=1}^{N_f}||(\hat{\mathbf{u}}_i \cdot \nabla)\hat{\mathbf{u}}_i + \nabla \hat{p}_i - \frac{1}{Re}\nabla^2 \hat{\mathbf{u}}_i||_2$$

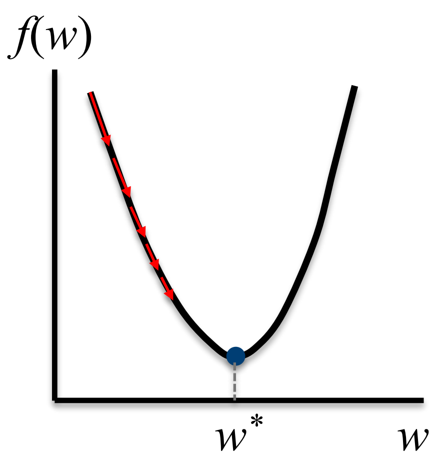
$$\mathscr{L}_{\text{mass}} = \frac{1}{N_f}\sum_{i=1}^{N_f}||\nabla \cdot \hat{\mathbf{u}}_i||_2$$



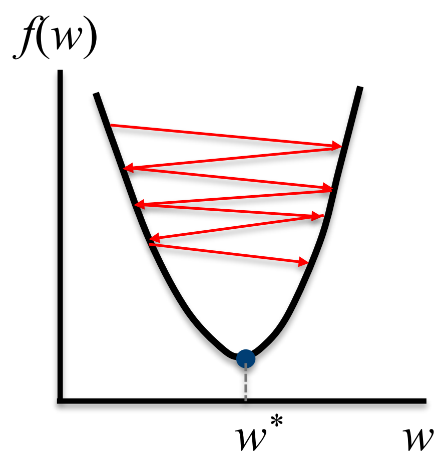
Performance-Enhancing Techniques

1- Adaptive Leaning Rate (ALR)

- ✗ The step-decay schedule cannot ensure the thorough the current convergence is;
- ✓ ALR continuously tracks the speed of convergence, decaying the LR when oscillations detected.



Slow convergence
with small LR



Local oscillation
with large LR

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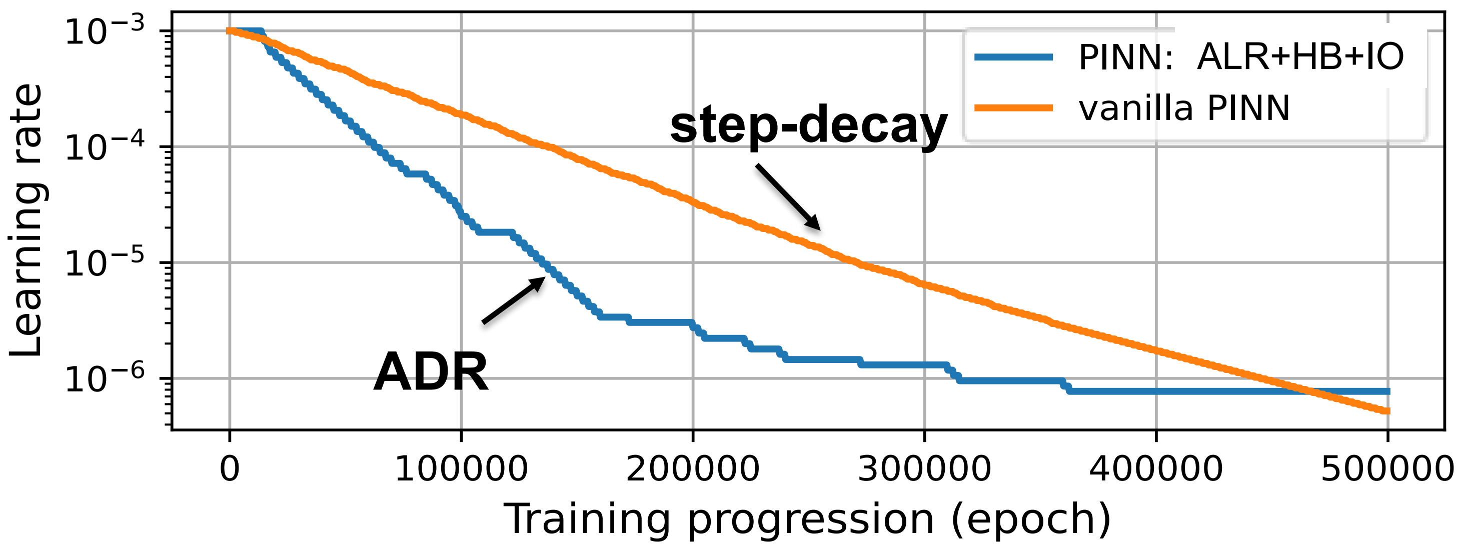

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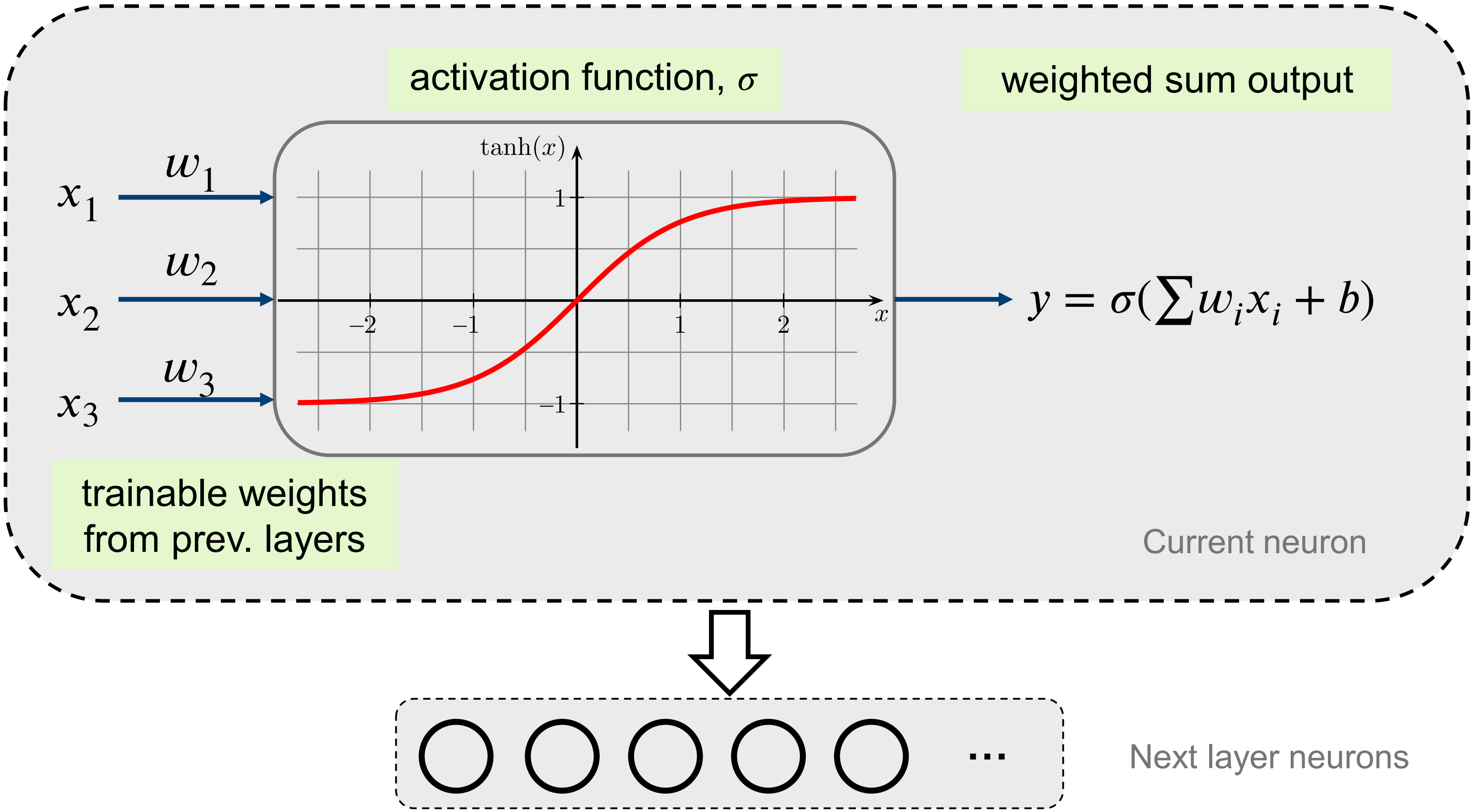
2- Hard Boundary (HB) Correction

✗ Constraining the boundary conditions in NN increases the DoF of NN;

✓ By using a hard boundary post layer, we can explicitly impose the desired boundary conditions to the domain.

Inside a Neuron



Q: can the `tanh` activate function model higher-order functions?

Performance-Enhancing Techniques

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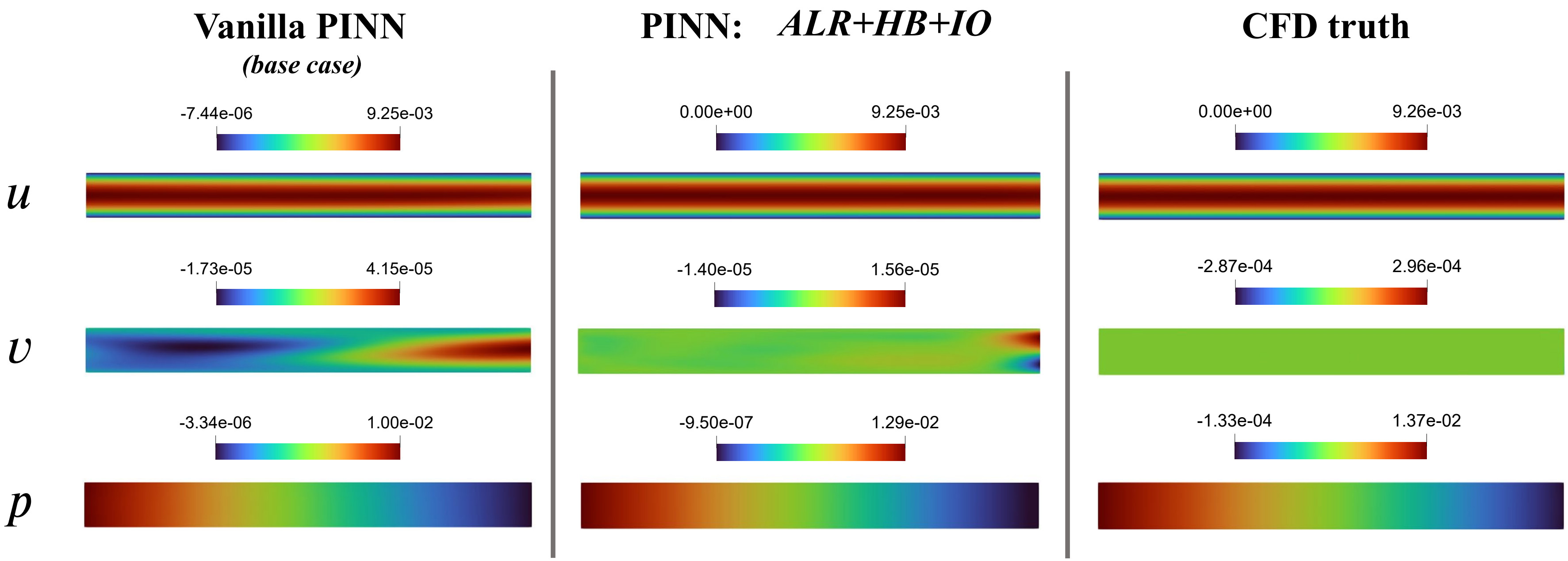
3- Increase Order (IO)

- ✗ `tanh` may not be able to model higher-order functions;
- ✓ Pre-compute the 2nd–order spatial coordinates may help NN better model the higher-order functions.

Results and Discussion

Framework Realisation and Optimisation



	$\varepsilon_{\mathbf{overall}}$ (%)	Avg. speed (iters/s)
Vanilla PINN	3.14	16.5
Modified PINN	0.48	3.75

Evaluation: % norm-2 error

$$\varepsilon = \frac{\sqrt{\sum_{i=1}^{N_f} |\mathbf{f}^i_{\mathrm{PINN}} - \mathbf{f}^i_{\mathrm{CFD}}|^2}}{\sqrt{\sum_{i=1}^{N_f} |\mathbf{f}^i_{\mathrm{CFD}}|^2}} \times 100\%$$

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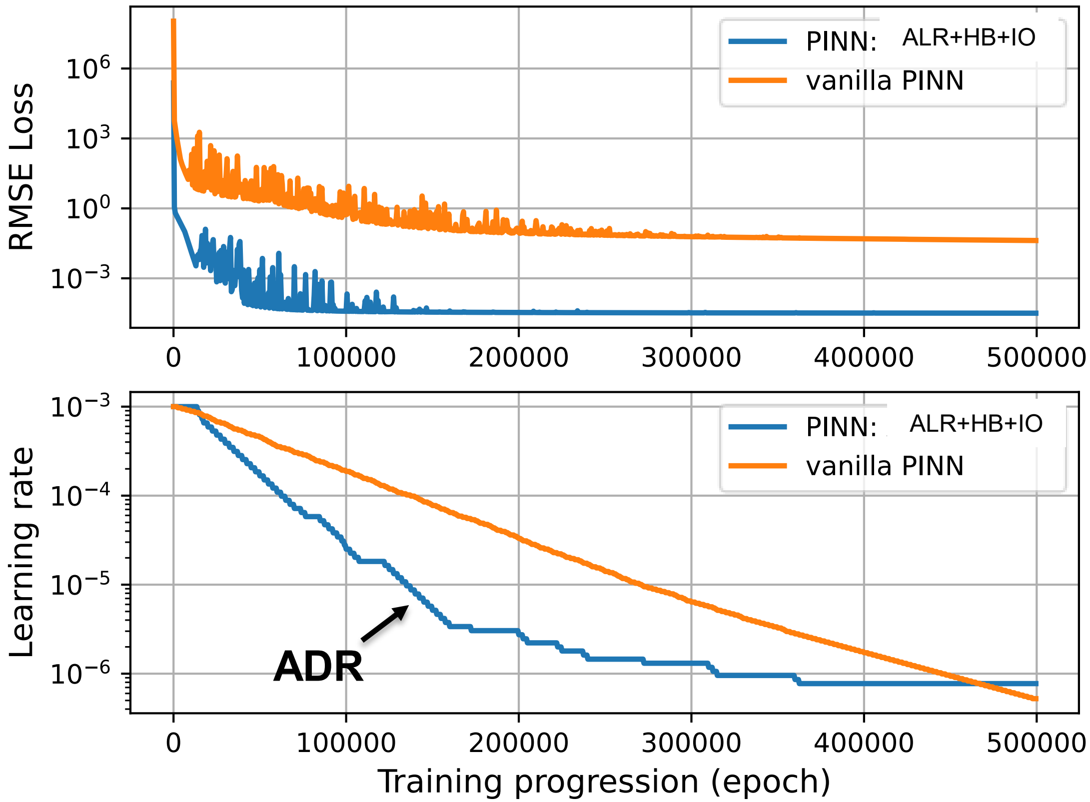

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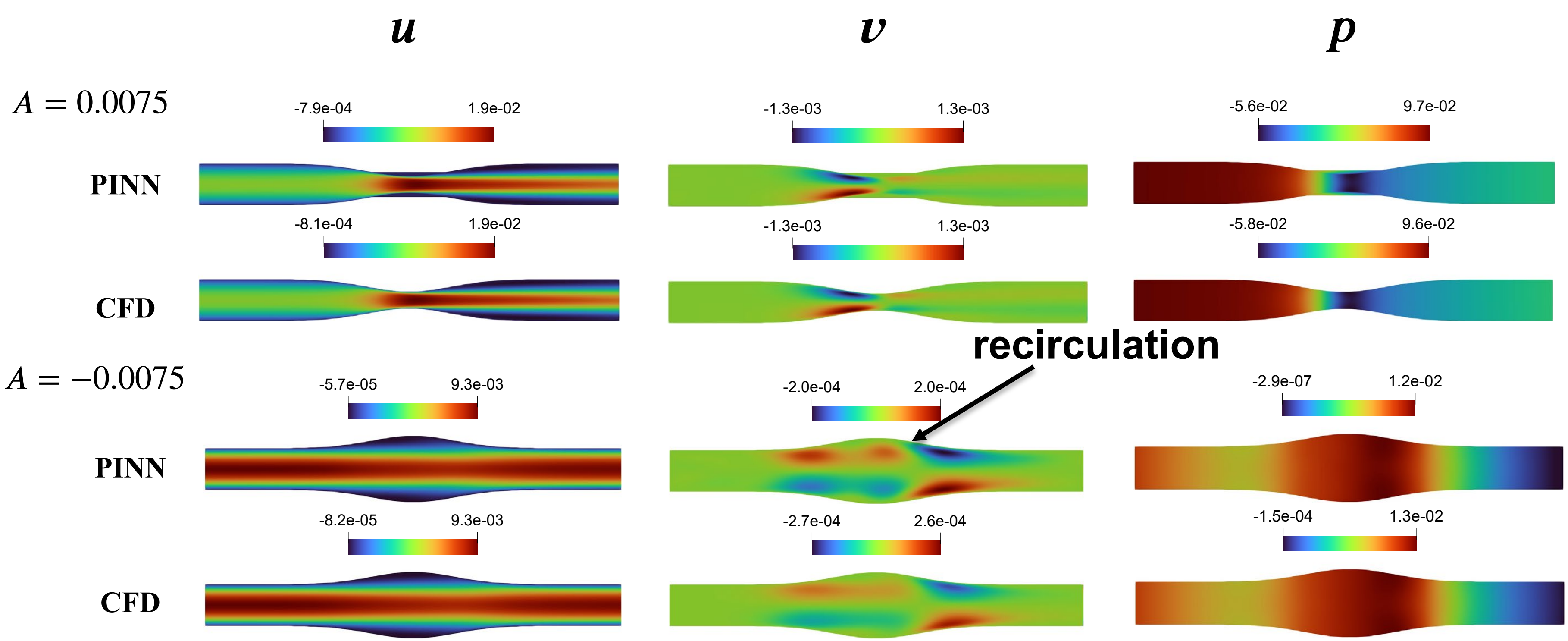
Stenosis & Aneurysm Cases

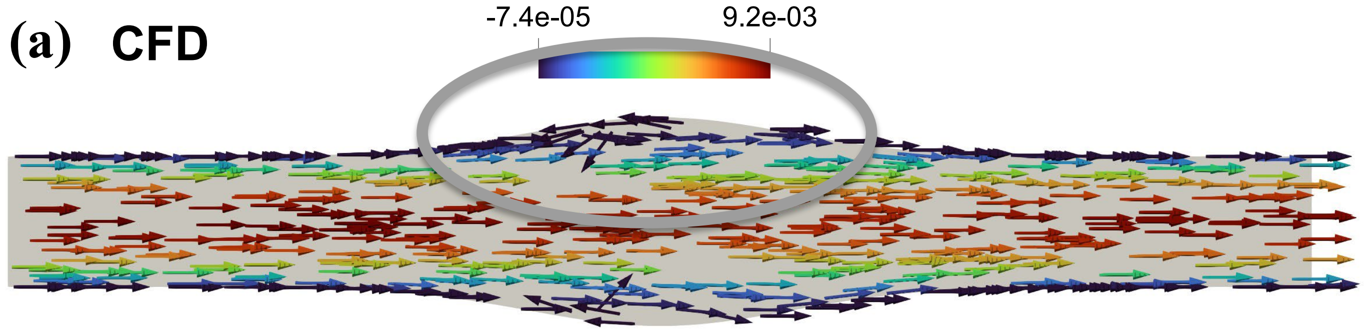


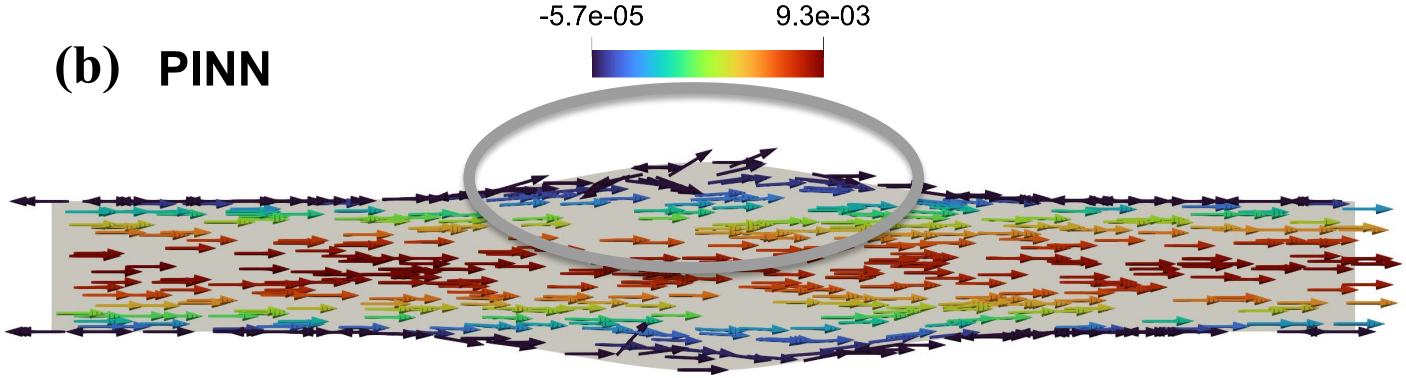
	Stenosis	Aneurysm
$\varepsilon_{\mathbf{overall}}$ (%)	2.90	4.77

Evaluation: % norm-2 error

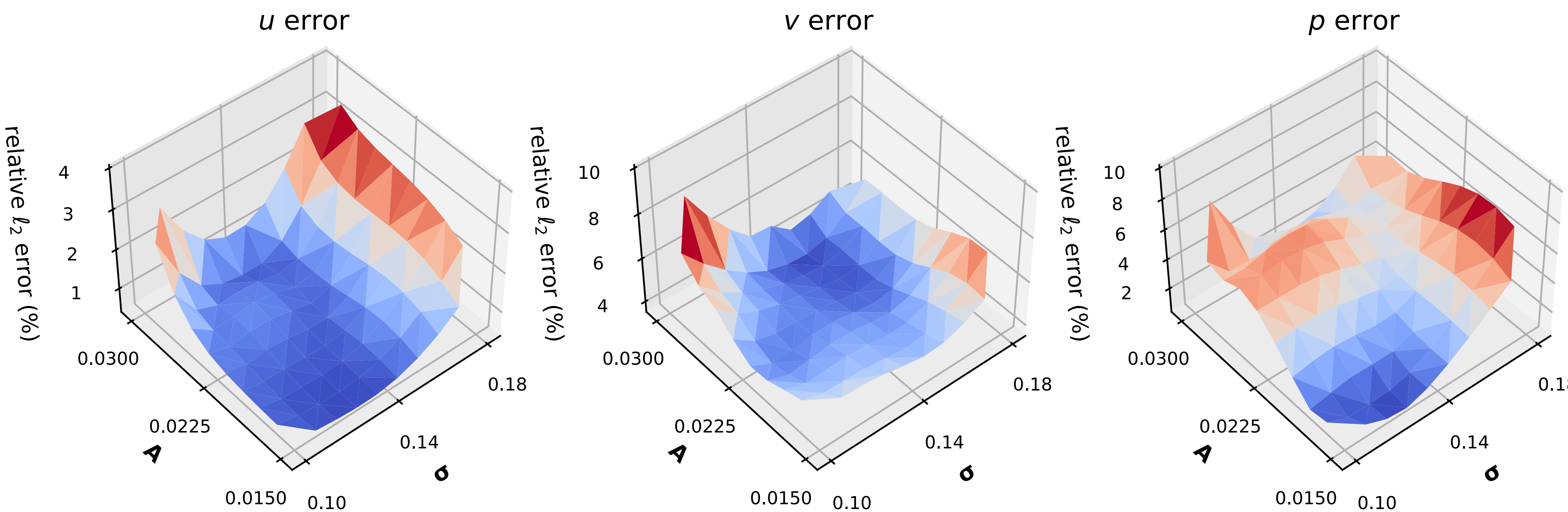
$$\varepsilon = \frac{\sqrt{\sum_{i=1}^{N_f} |\mathbf{f}_{\mathrm{PINN}}^{i} - \mathbf{f}_{\mathrm{CFD}}^{i}|^2}}{\sqrt{\sum_{i=1}^{N_f} |\mathbf{f}_{\mathrm{CFD}}^{i}|^2}} \times 100\%$$

Secondary Flow





Case Network



- 12 cases were trained, 96 unseen cases were predicted with feature parameters chosen between the training range.

$\varepsilon_{u,\max}$ (%)	$\varepsilon_{v,\max}$ (%)	$\varepsilon_{p,\max}$ (%)
3.39	8.35	7.25

- Generally, errors are low in the middle of the range, high around the range boundaries.

Summary

- Physics-informed neural networks are capable in accurately modelling the fluid dynamics for various geometries with the feasible performance-enhancing techniques.
- With a case hypernetwork, we unlocked the possibility of real-time prediction of the fluid dynamics without re-training the case.

Limitations

1. 2-D idealistic geometries with heavy assumptions
2. lacks well-defined procedures to control the outcome (hyper-params)
3. Unsteady flow compatibility?
4. **"Curse of dimensionality"** – how can we mitigate it?

Questions?

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- Wong HS, **Li B**, Chan WX, and Yap CH. *Pre-Training Varied Vascular Geometries with a Deep Learning Side Network in Physics-Informed Neural Network Simulations of Vascular Fluid Dynamics.* **ESBiomech23**

- Wong HS, Chan WX, **Li B**, and Yap CH. *Multicase Physics-Informed Neural Network for Biomedical Tube Flows.* In press