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Learning Reduced-Order Models for Blood Flow Simulations using Graph Neural Networks

Luca Pegolotti
Postdoctoral Researcher
Marsden Lab, Stanford University

Mathematical and Scientific Machine Learning
ICERM — Brown University
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NIH
National Institutes of Health

intel

L. Pegolotti, PhD

M. Pfaller, PhD

N. Rubio

K. Ding, PhD

R. Brugarolas, PhD

Prof. E. Darve

Prof. A. Marsden

Pegolotti et al. *Learning Reduced-Order Models for cardiovascular simulations with Graph Neural Networks. arXiv* https://arxiv.org/abs/2303.07310v1 (2023)

Why simulation

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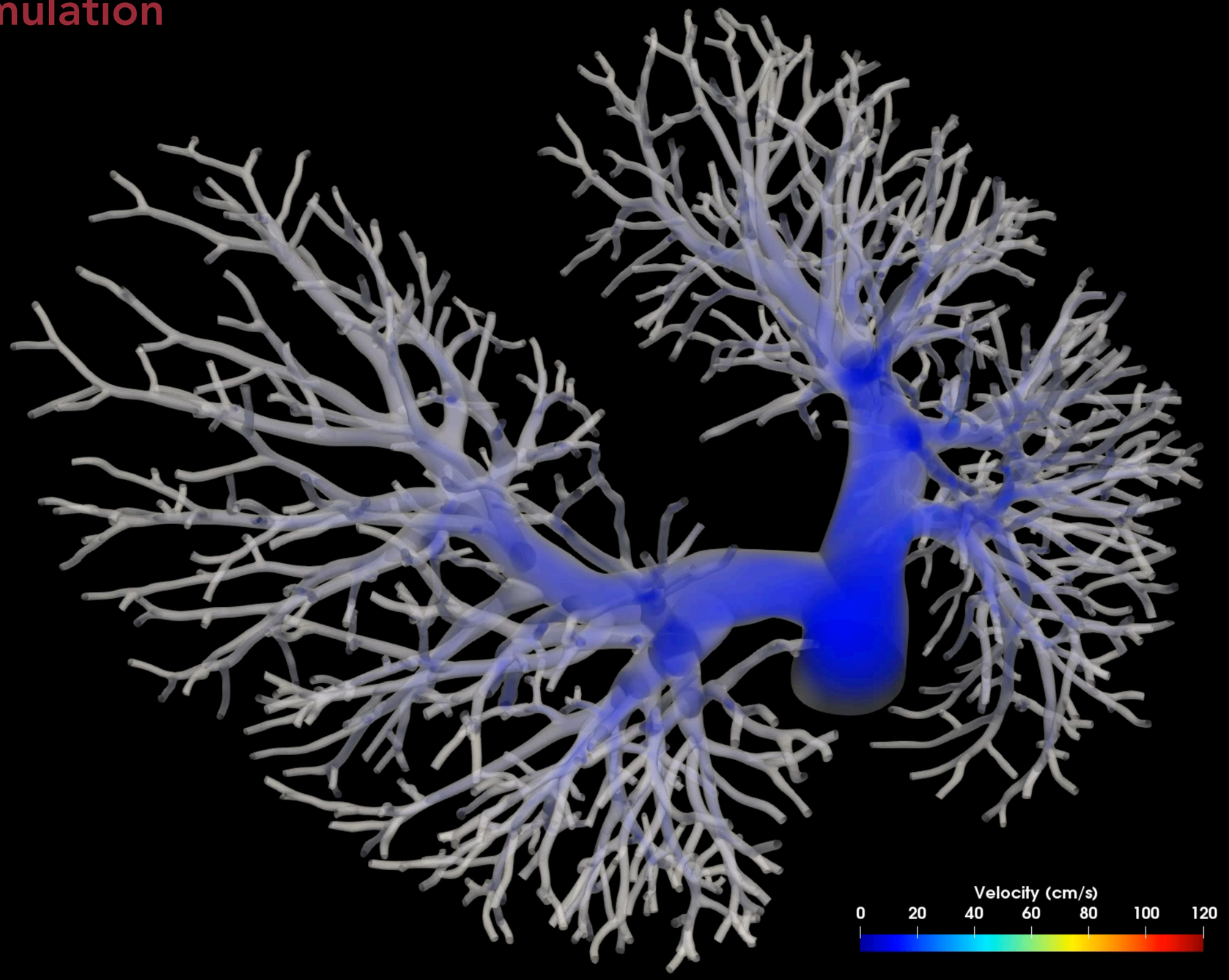

$O(10^6)$ elements

16 hours on 128 cores

Overview of Reduced-Order Models

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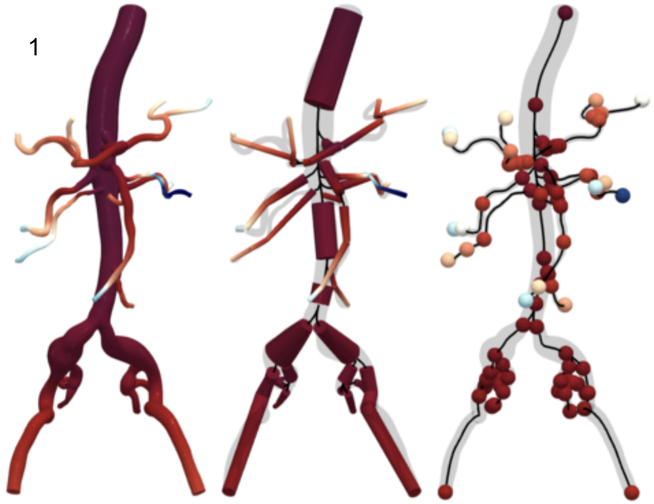
Reduced-Order Models

Physics-based models

1



3D 1D 0D

Data-driven models

2

Projection-based

3

Neural Network based

1. Pfaller et al. *Automated generation of 0D and 1D reduced-order models of patient-specific blood flow. Int. J. for Num. Met in Bio. Eng.* (2021)

2. Pegolotti et al. *Model order reduction of flow based on a modular geometrical approximation of blood vessels. Comp. Meth. in Appl. Mech. and Eng.* (2021)

3. Pegolotti et al. *Learning Reduced-Order Models for cardiovascular simulations with Graph Neural Networks. arXiv* https://arxiv.org/abs/2303.07310v1 (2023)

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Physics-based models

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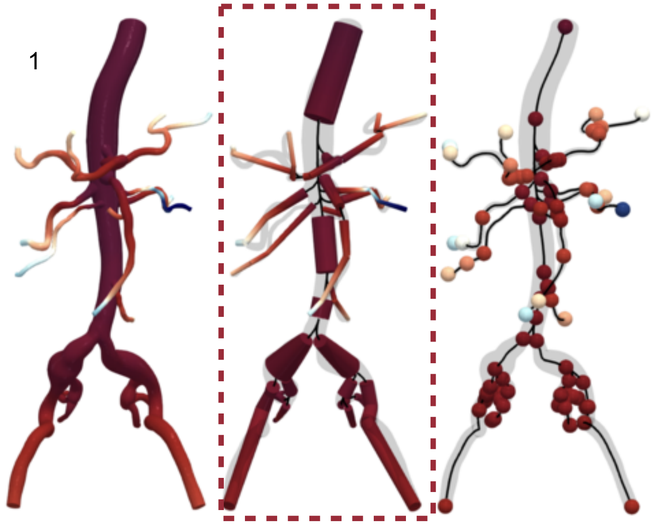

3D 1D 0D

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One-dimensional Reduced-Order Models

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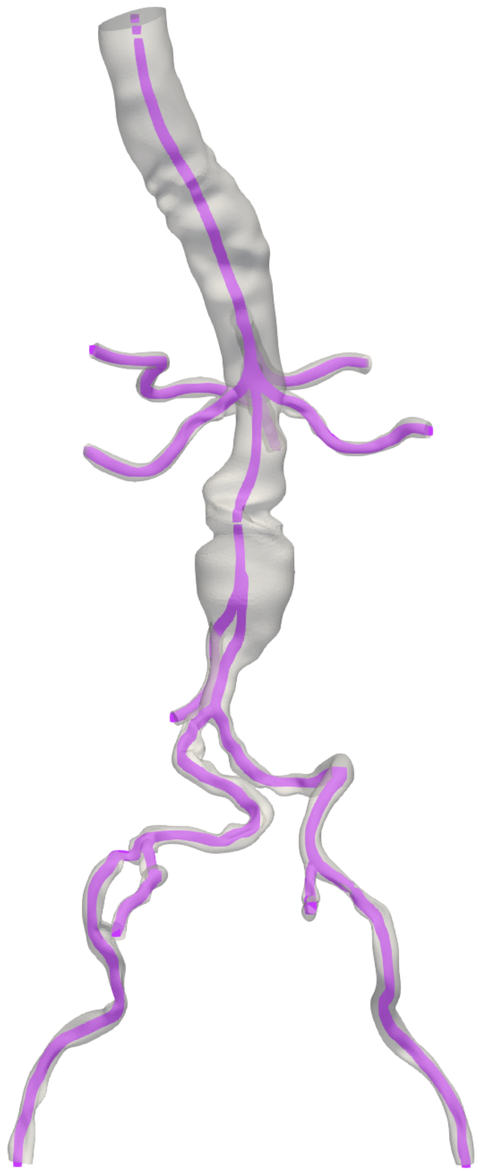
Equations:

$$\frac{\partial A}{\partial t} + \frac{\partial q}{\partial z} = 0$$

$$\frac{\partial q}{\partial t} + \frac{\partial}{\partial z}\left(\frac{4}{3}\frac{q^2}{A}\right) = -8\pi\nu\frac{q}{A} + \nu\frac{\partial^2 q}{\partial z^2} - \frac{A}{\rho}\frac{\partial p}{\partial z}$$

Constitutive Model:

$$p(z,t) = p_0(z) + \frac{4}{3}\left(k_1 e^{k_2 r_0(z)} + k_3\right)\left(1 - \sqrt{\frac{A_0(z)}{A(z,t)}}\right)$$



The problem

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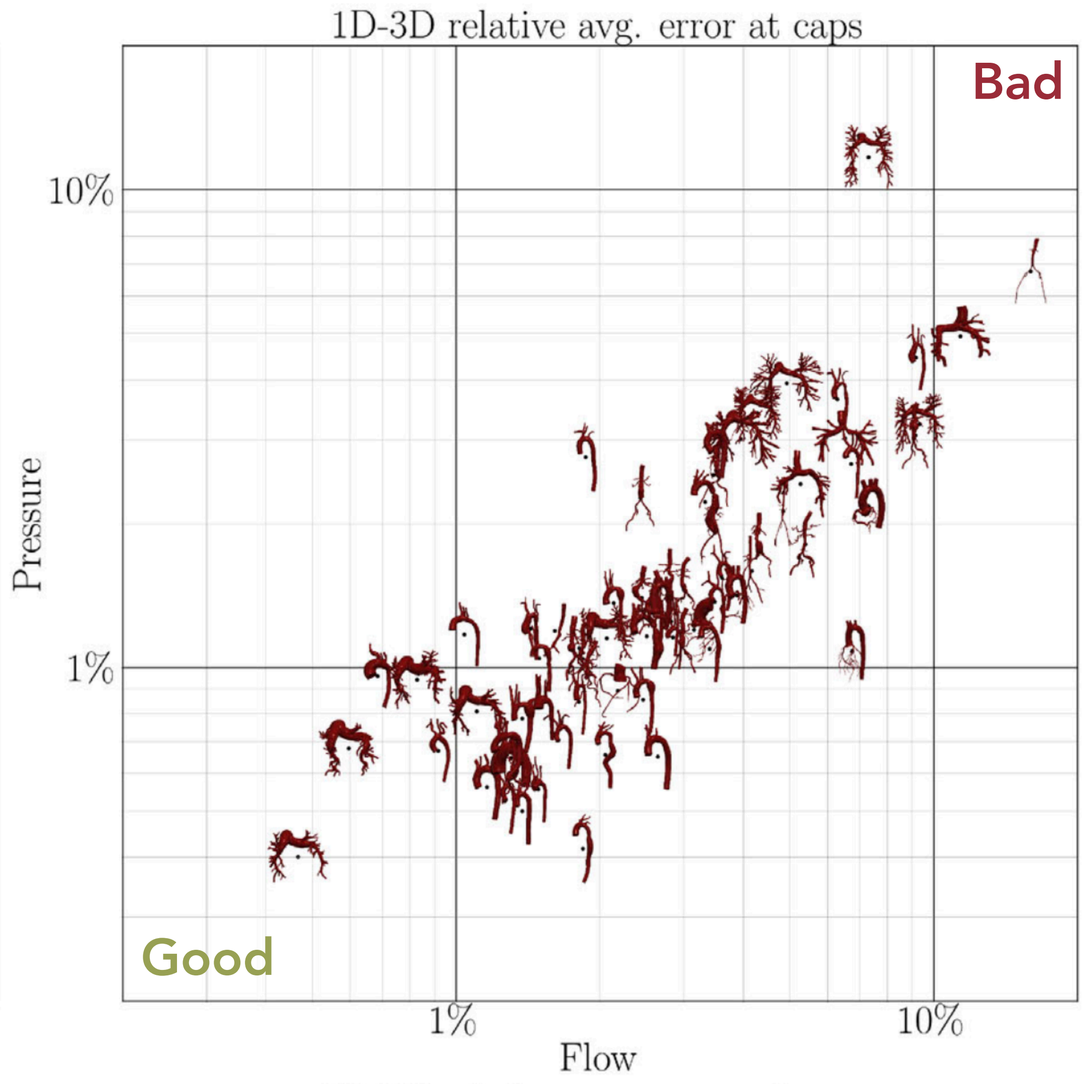

Pfaller et al. *Automated generation of 0D and 1D reduced-order models of patient-specific blood flow. Int. J. for Num. Met in Bio. Eng.* (2021)

The problem

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Physics-based zero/one-dimensional models may be inaccurate when (i) **multiple junctions** or (ii) **severe pathological conditions** are present.

Pfaller et al. *Automated generation of 0D and 1D reduced-order models of patient-specific blood flow. Int. J. for Num. Met in Bio. Eng.* (2021)

The Vascular Model Repository (VMR)

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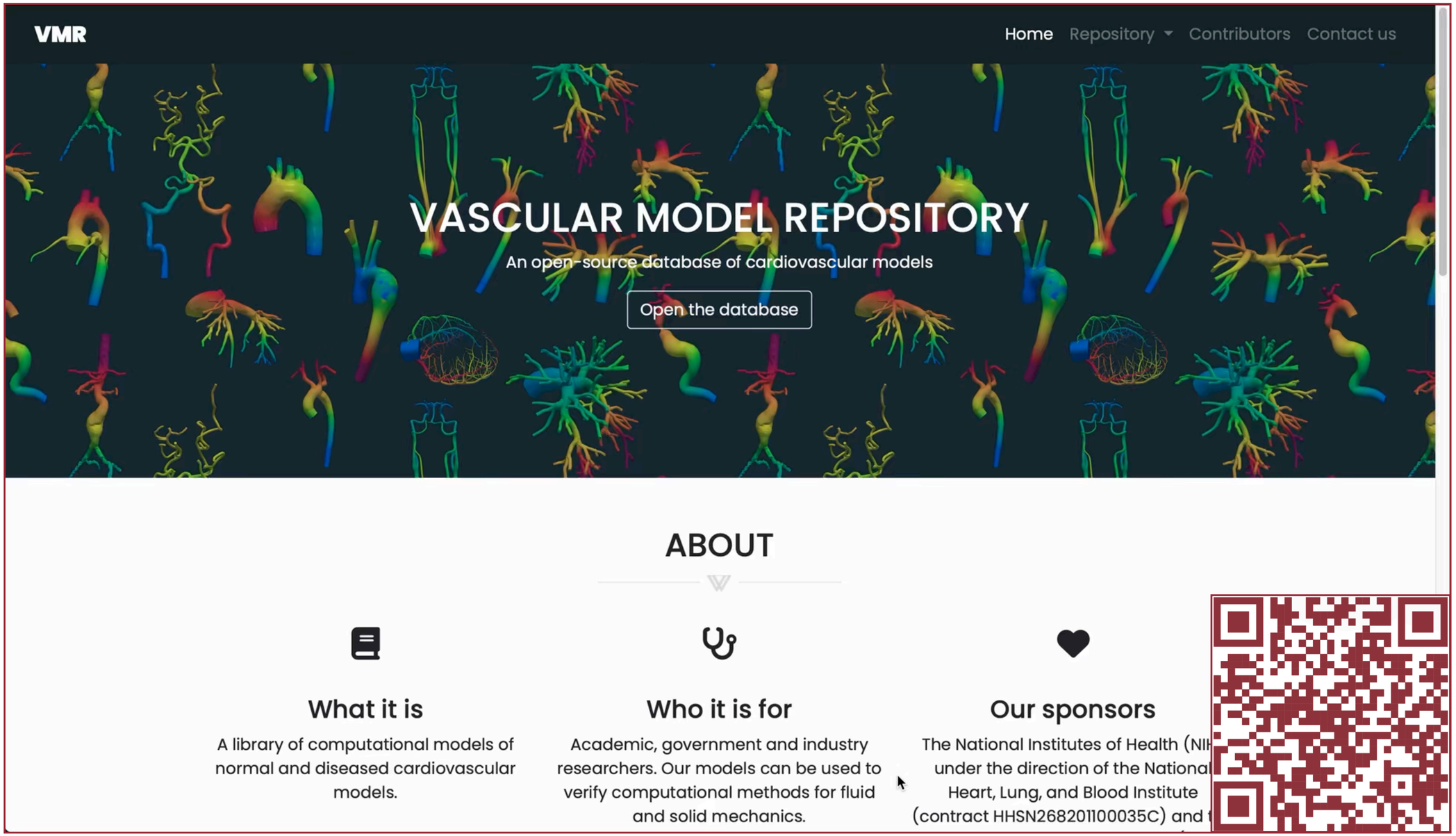
Available at **www.vascularmodel.com**



Requirements

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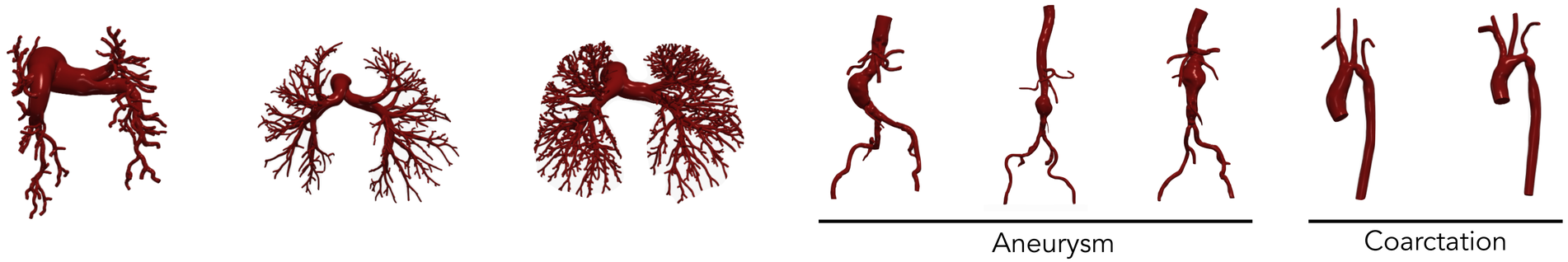
Data-driven treatment of **junctions** and **pathological conditions**



Requirements

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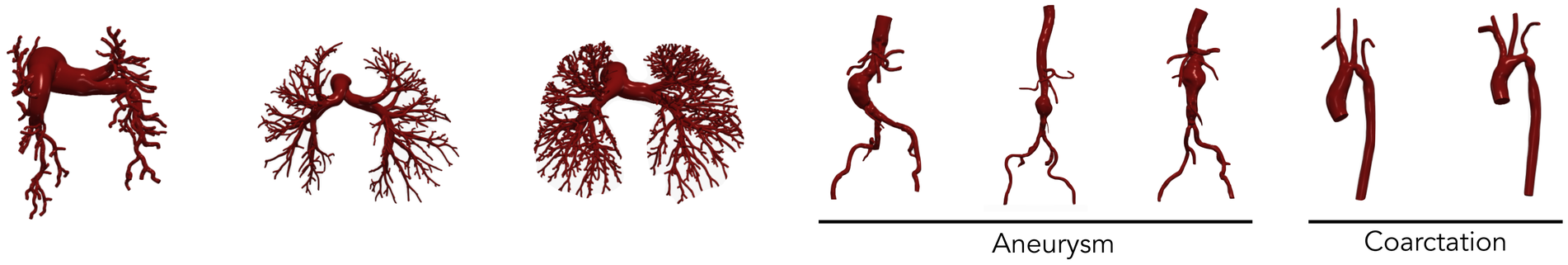
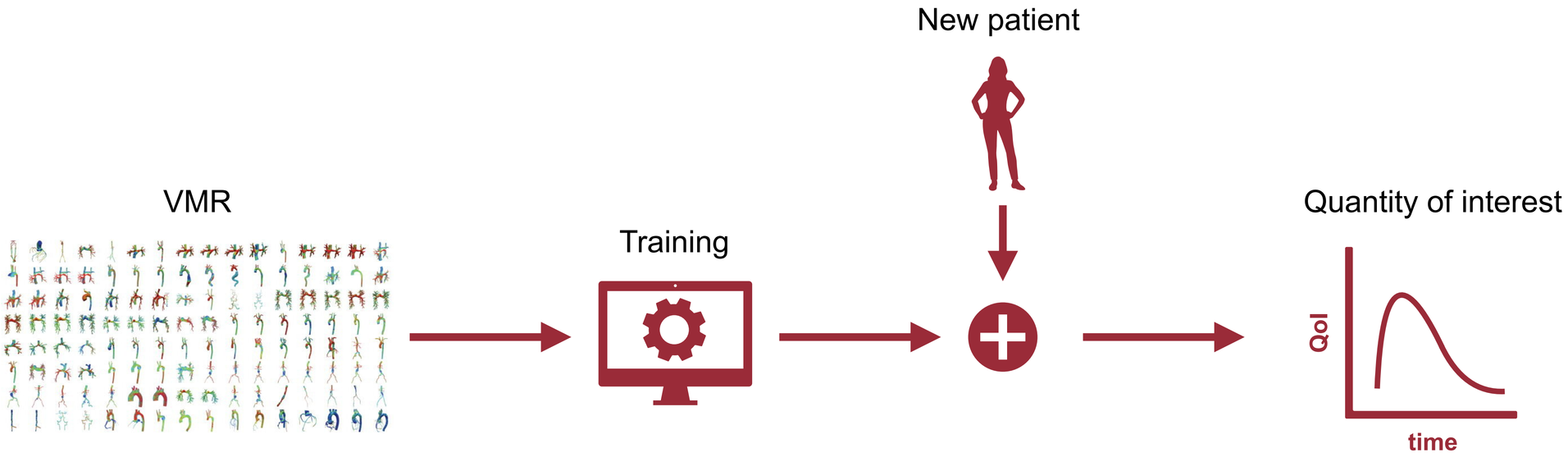
Data-driven treatment of **junctions** and **pathological conditions**



Flexibility with respect to geometry (**one trained ML model - many patients**)



Graph representation of vasculatures

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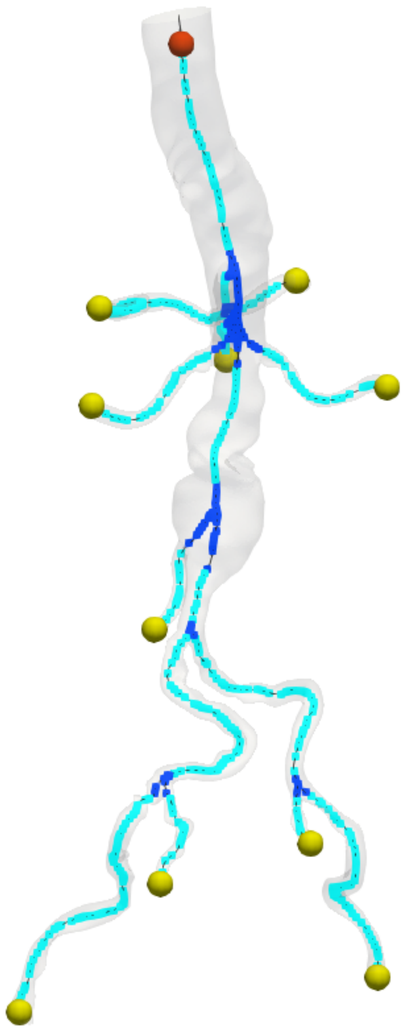

Centerline nodes = graph nodes

Associate features to each node and edge

Node feature	Definition
p_i^k	Pressure at time t^k
q_i^k	Flow rate at time t^k
A_i	Cross-sectional area
$\boldsymbol{\alpha}_i$	Nodal type
$\boldsymbol{\phi}_i$	Centerline tangent
T_{cc}	Cardiac cycle duration
p_{min}	Minimum pressure (across cardiac cycle)
p_{max}	Maximum pressure (across cardiac cycle)
$R_{i,p}$	R_p Parameter in RCR boundary conditions
C_i	C Parameter in RCR boundary conditions
$R_{i,d}$	R_d Parameter in RCR boundary conditions
l^k	Boolean load variable at time t^k

Table 1: Node features and their definitions.

Edge feature	Definition
$\mathbf{d}_{ij}^{\text{T}}/\lVert\mathbf{d}_{ij}\rVert$	Normalized vector distance between node i and j
z_{ij}	Shortest path length between node i and j
$\boldsymbol{\beta}_{ij}$	Edge type

Table 2: Edge features and their definitions.

MeshGraphNet

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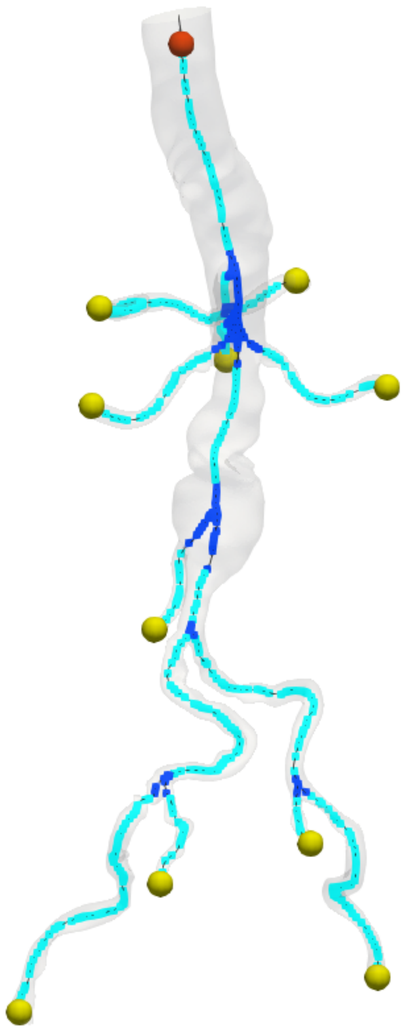
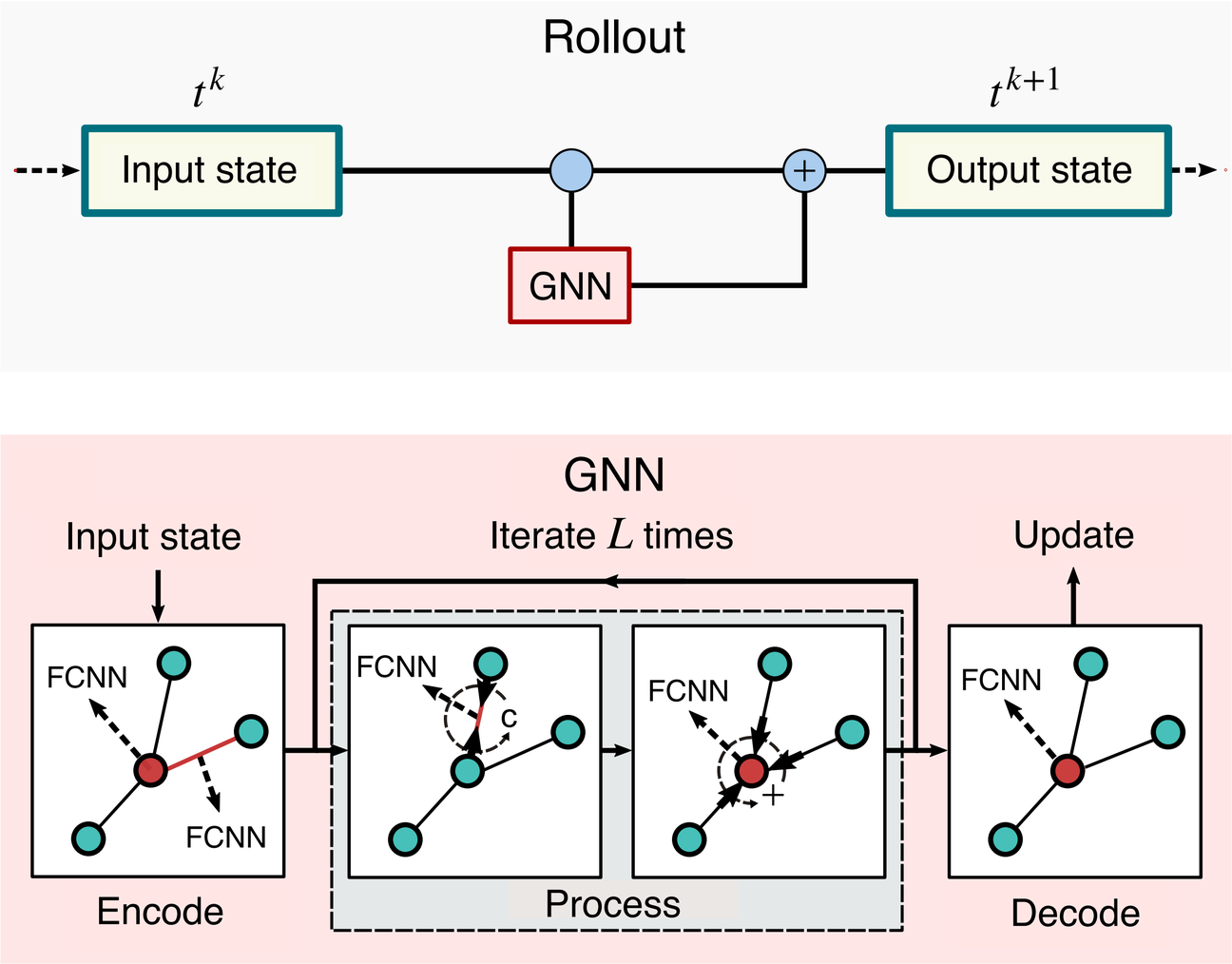


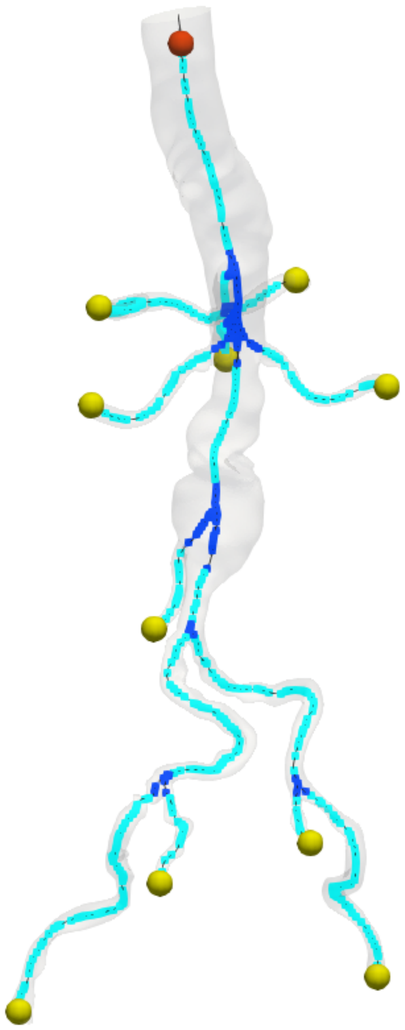


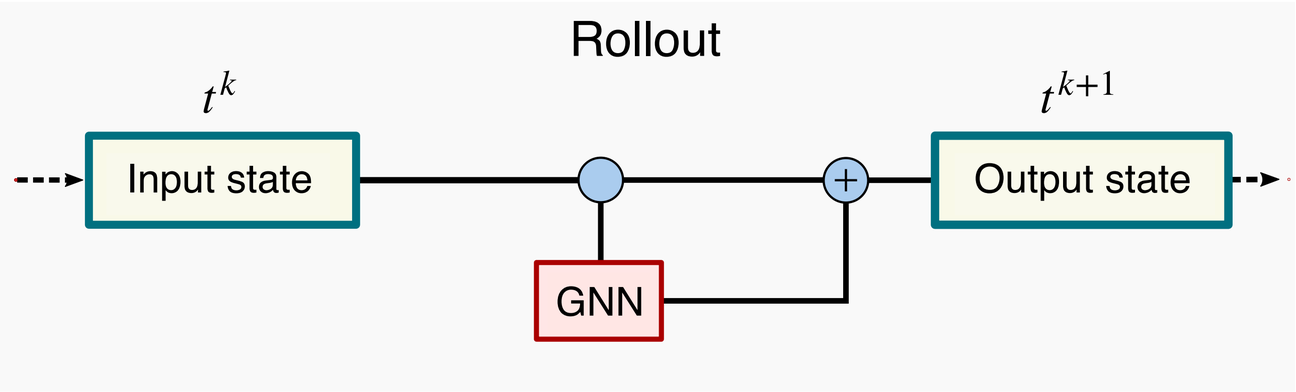
FCNN: fully-connected neural network

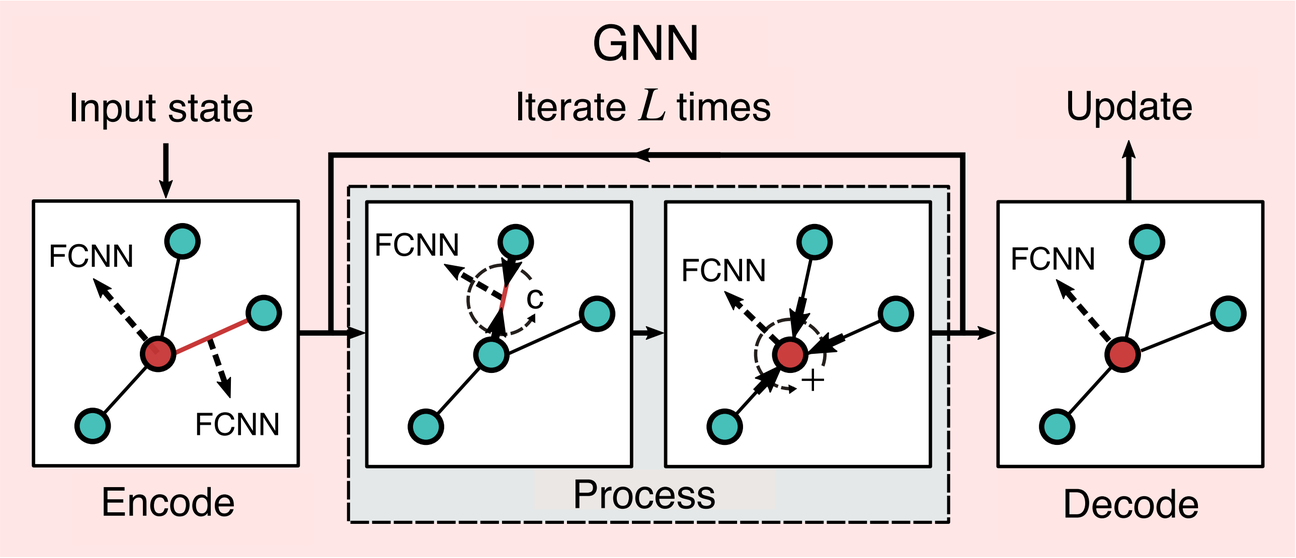
Pfaff et al. *Learning mesh-based simulation with Graph Networks.* ICLR (2021)

MeshGraphNet

Stanford







FCNN: fully-connected neural network

Process sub-steps

1. $\mathbf{w}_{ij}^{(l)} = \mathbf{f}(\mathbf{w}_{ij}^{(l-1)}, \mathbf{v}_i^{(l-1)}, \mathbf{v}_j^{(l-1)})$

2. $\mathbf{v}_j^{(l)} = \mathbf{f}(\mathbf{v}_j^{(l-1)}, \sum_{i:\exists e_{ij}} \mathbf{w}_{ij}^{(l)})$

Pfaff et al. *Learning mesh-based simulation with Graph Networks.* ICLR (2021)

Main modifications w.r.t. original MeshGraphNet (1)

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Add boundary edges

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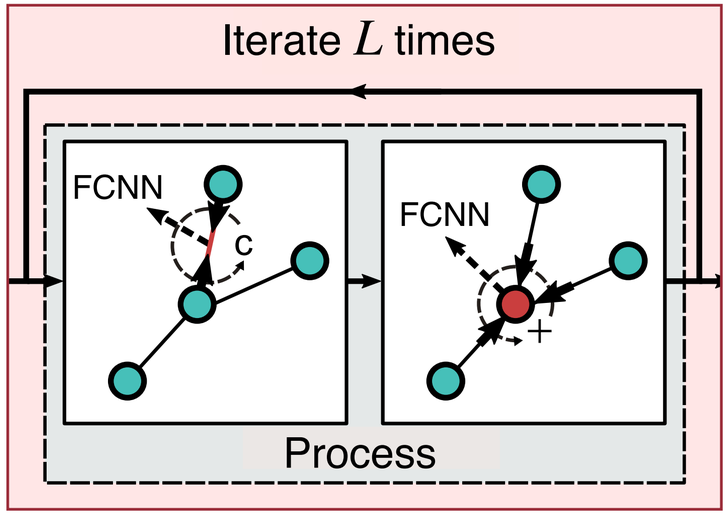
Add boundary edges

We want to keep L as small as possible



Main modifications w.r.t. original MeshGraphNet (2)

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Node feature	Definition
p_i^k	Pressure at time t^k
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A_i	Cross-sectional area
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Table 2: Edge features and their definitions.

Add application-specific features (: included in the original MeshGraphNet)

Main modifications w.r.t. original MeshGraphNet (2)

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Node feature	Definition
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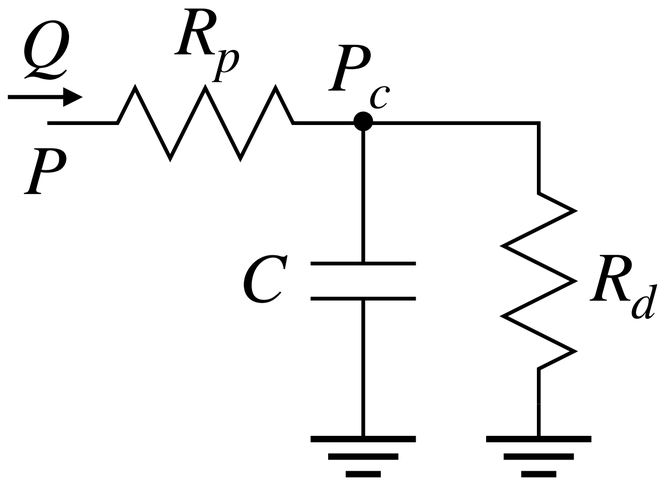

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Data generation pipeline

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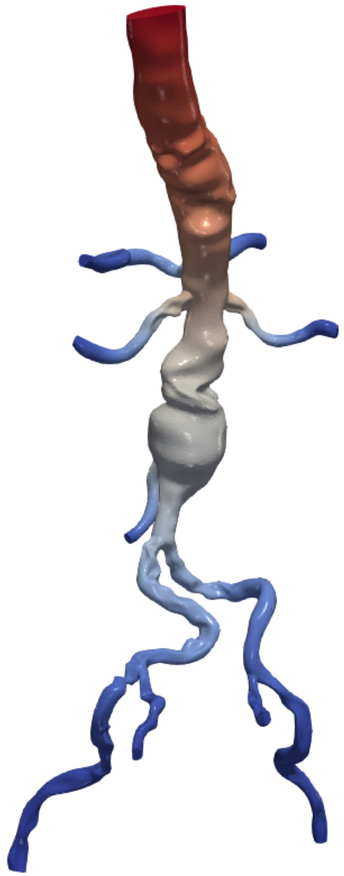
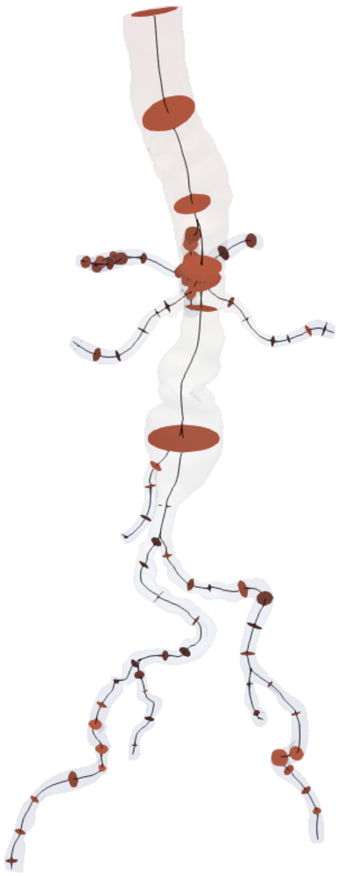
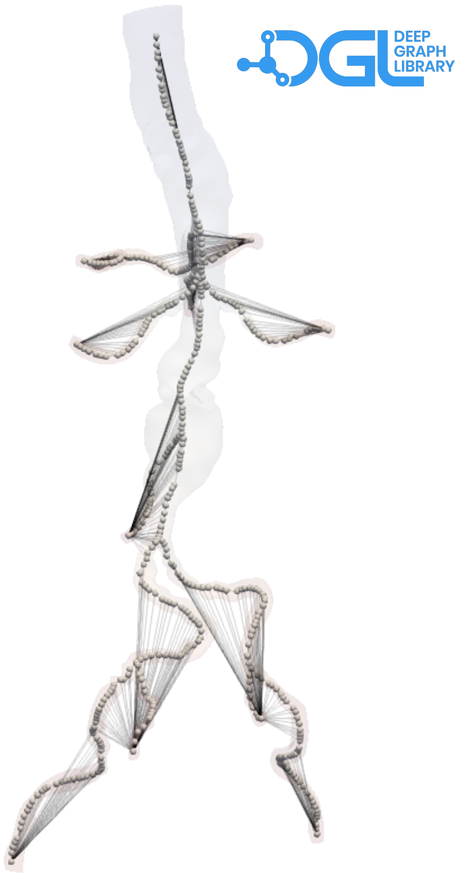
3D simulation



Integration over slices



Graph generation



Results (1)

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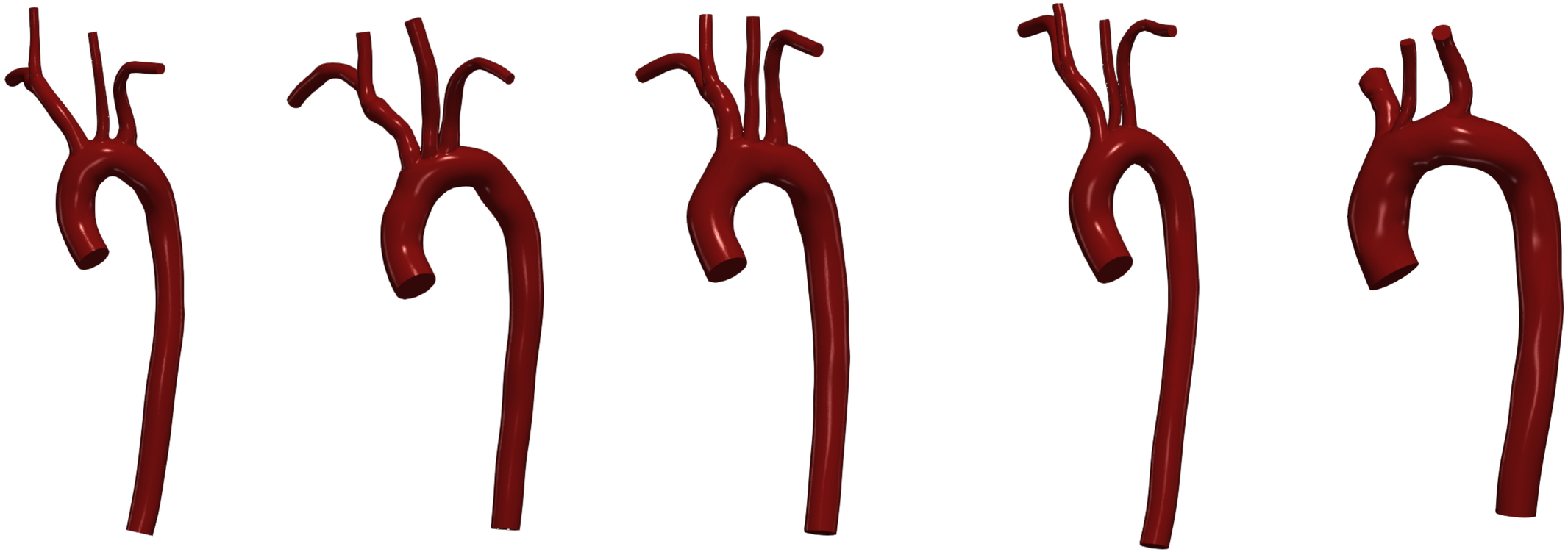
Goal: study error convergence as we consider more and more trajectories for training.



We performed 32 simulations with different boundary conditions for each of these geometries.

Convergence

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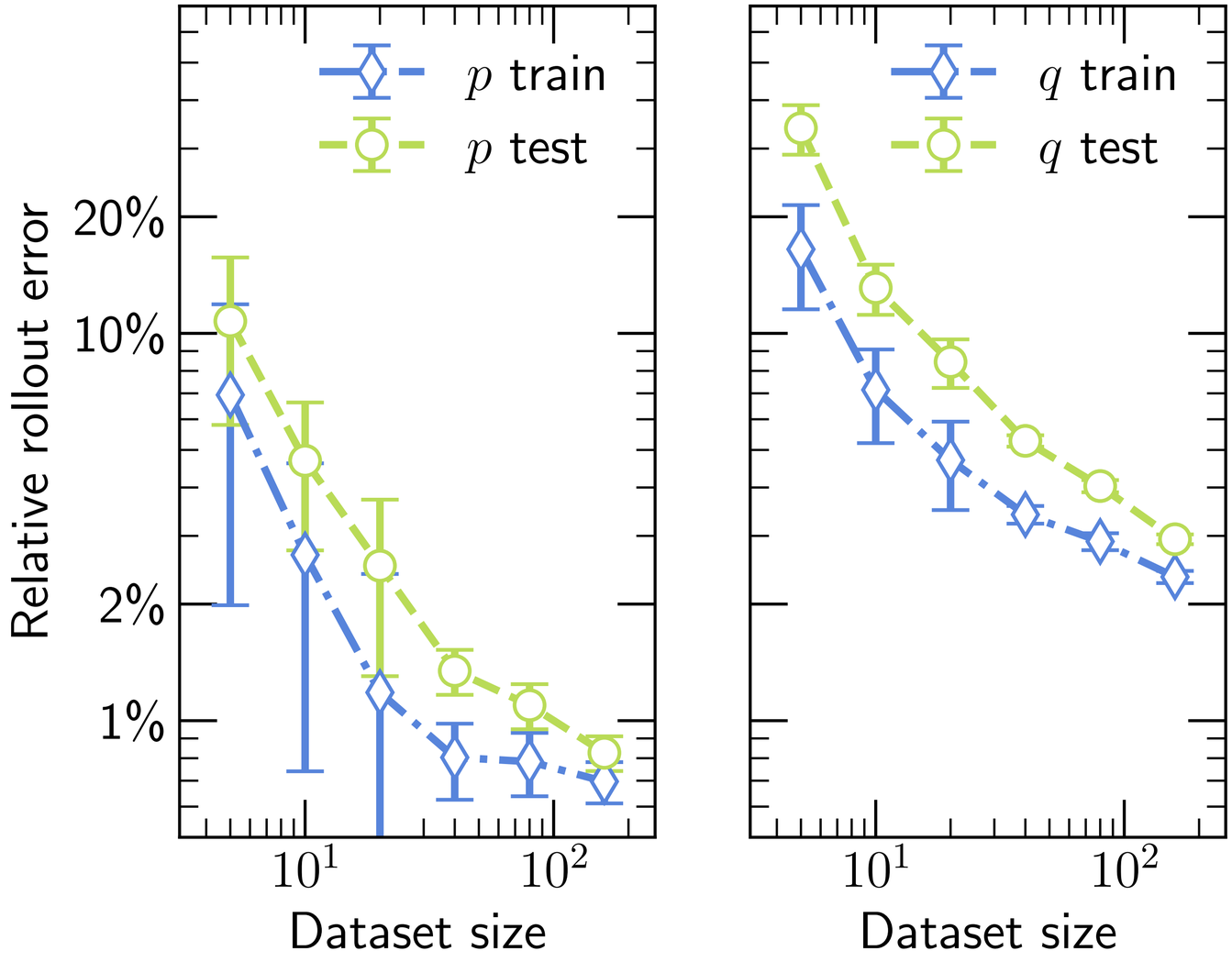
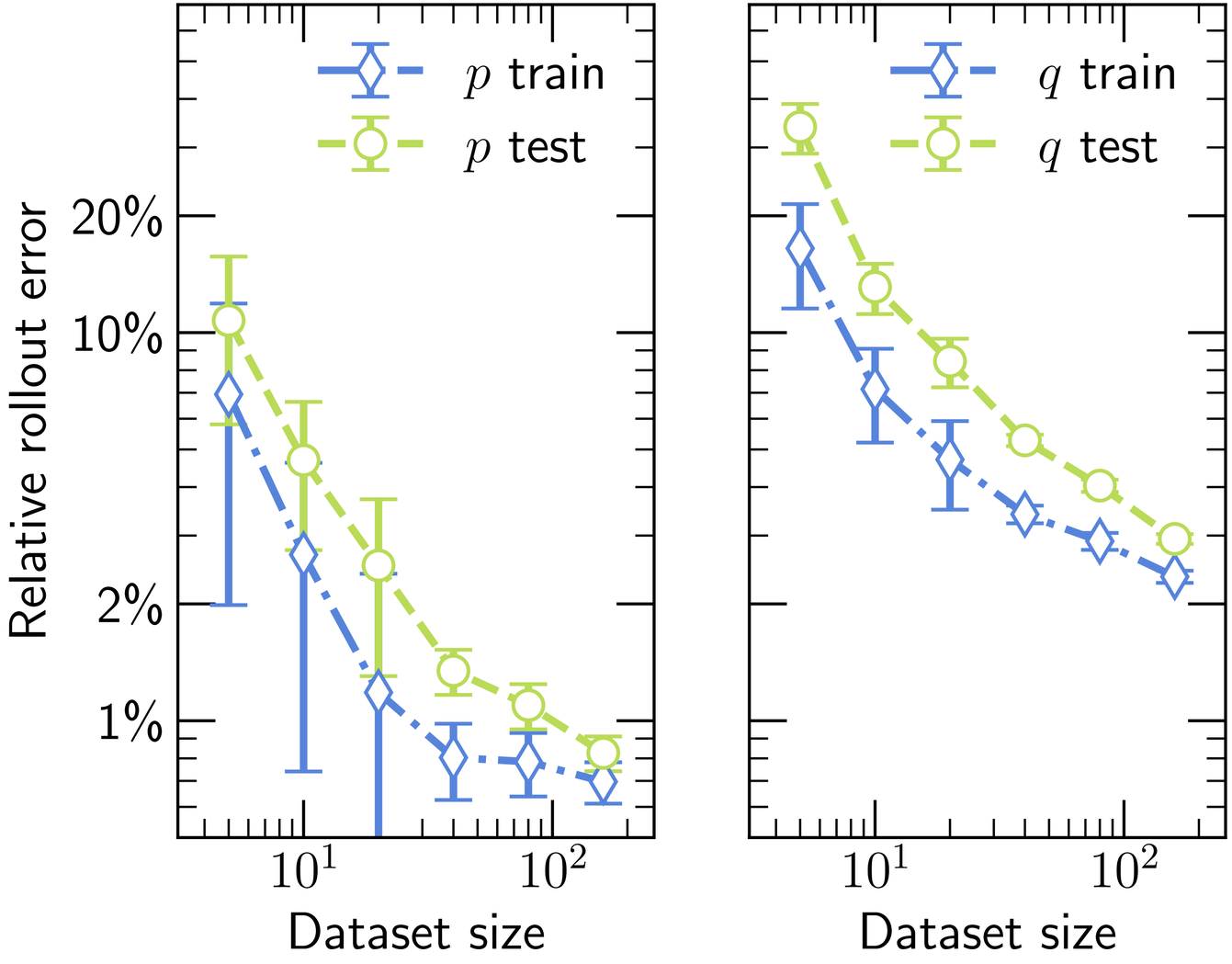


Convergence

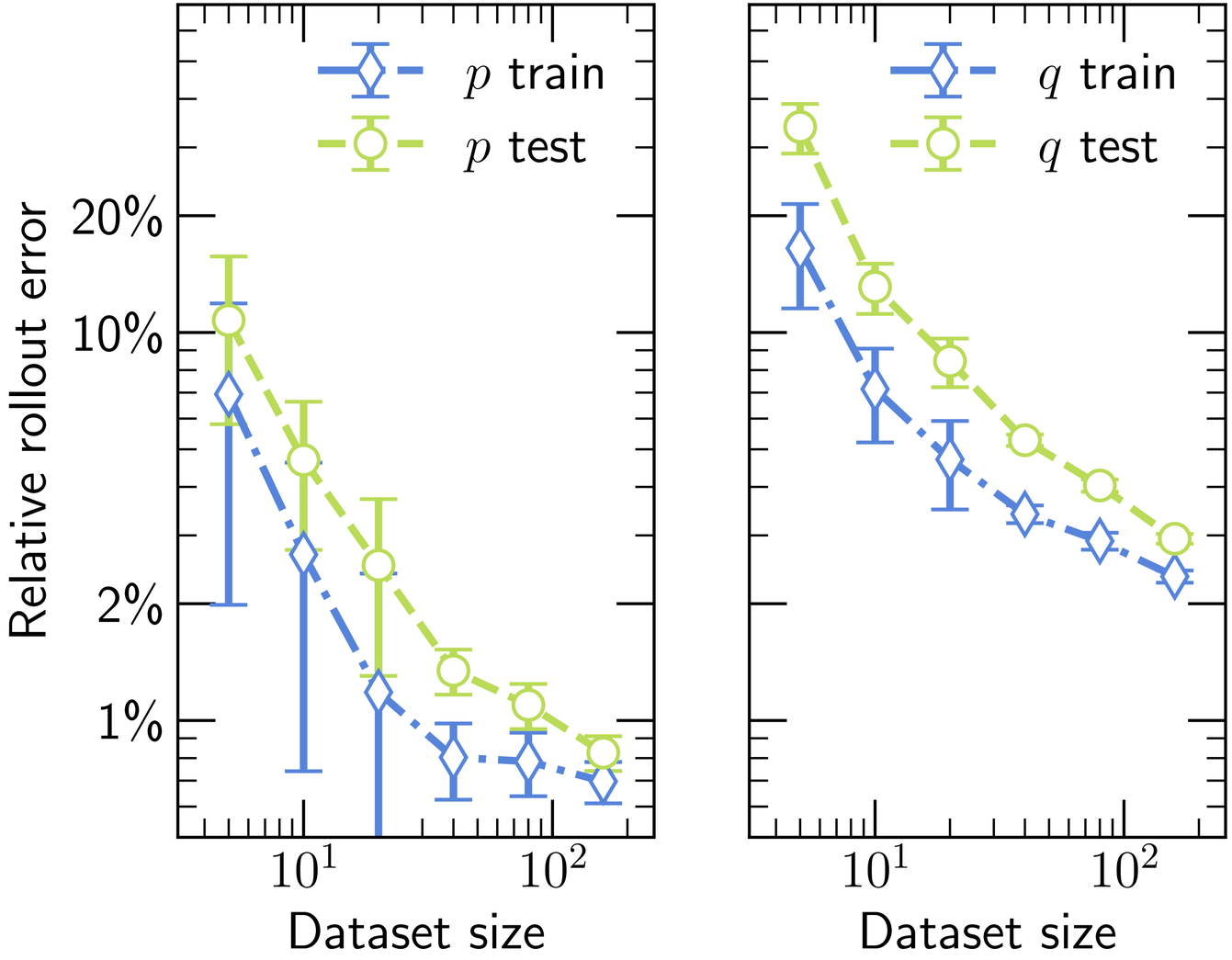
Stanford



Error decreases as dataset size increases

Convergence

Stanford



Error decreases as dataset size increases

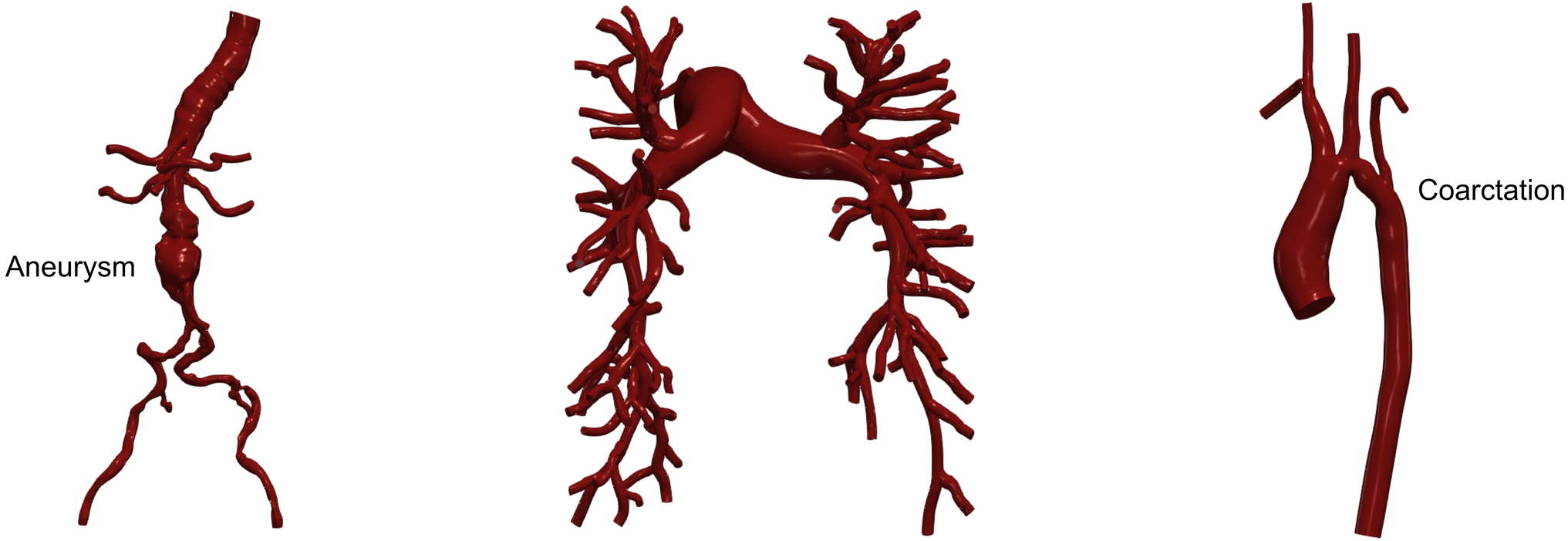
Generalization error decreases as dataset size increases

Results (2)

Stanford

Goal 1: train a single GNN on diverse anatomies.

Goal 2: compare performance against physics-based one-dimensional models.



We performed 50 simulations with different boundary conditions for each of these geometries.

3D vs GNN

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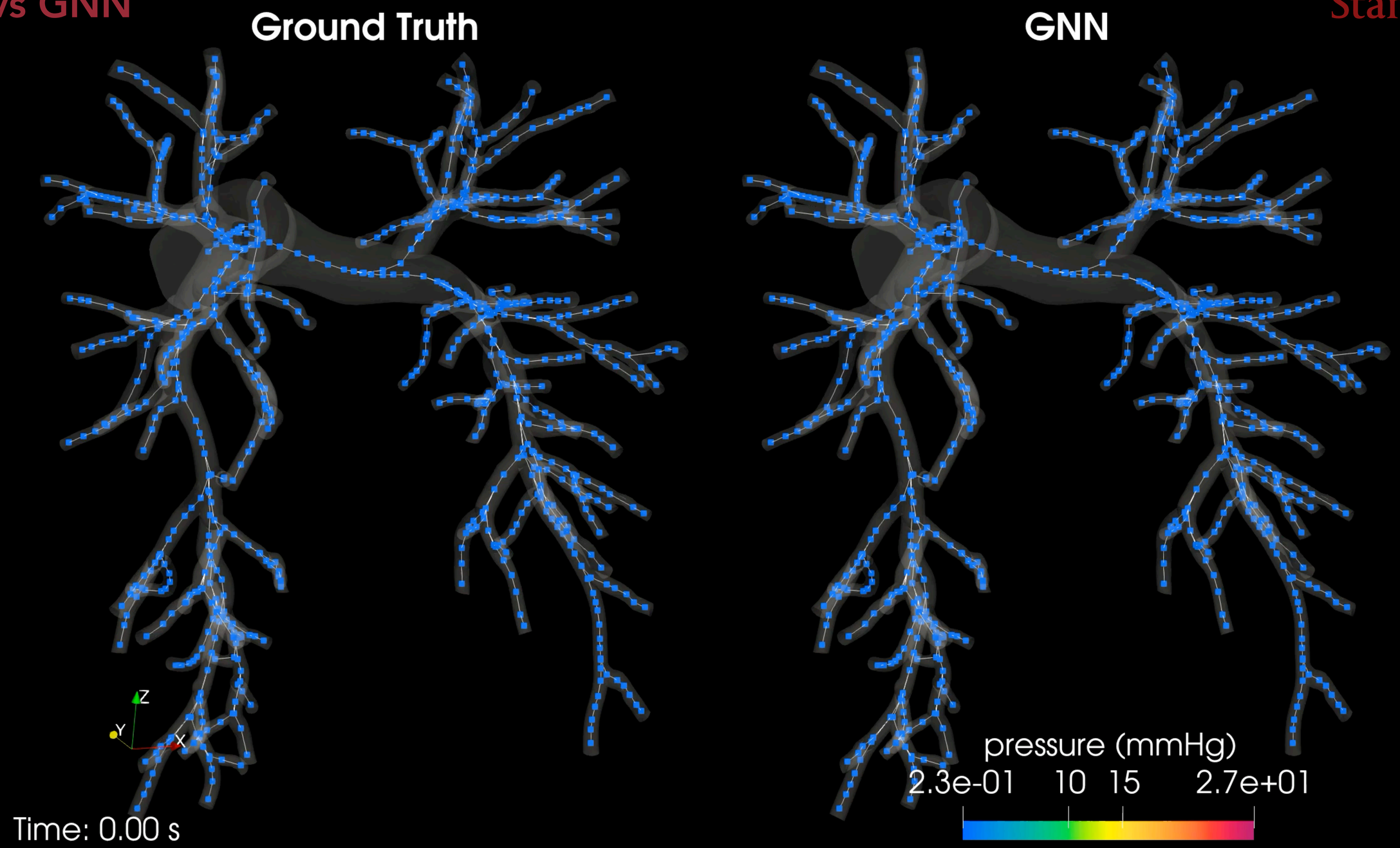
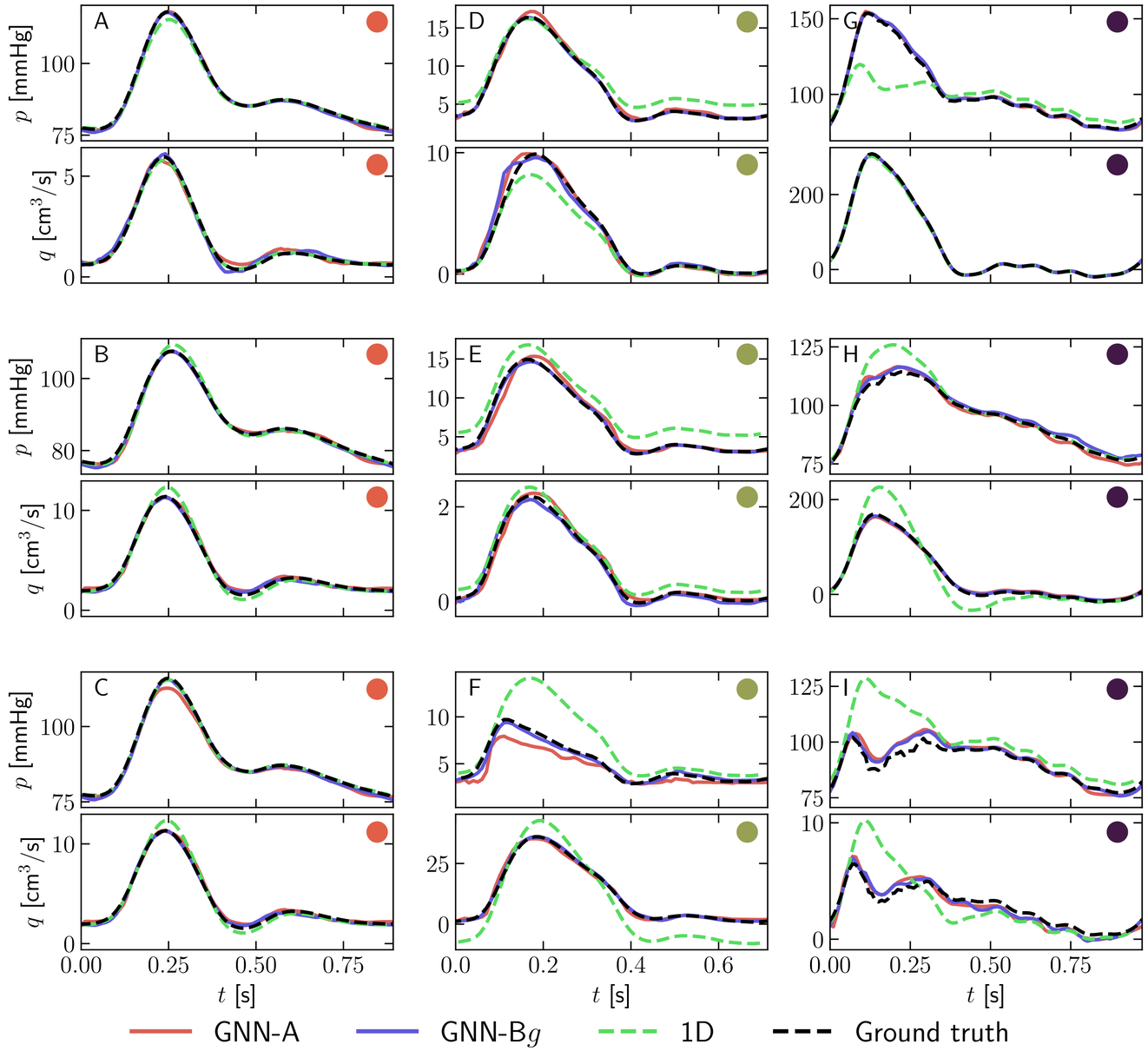
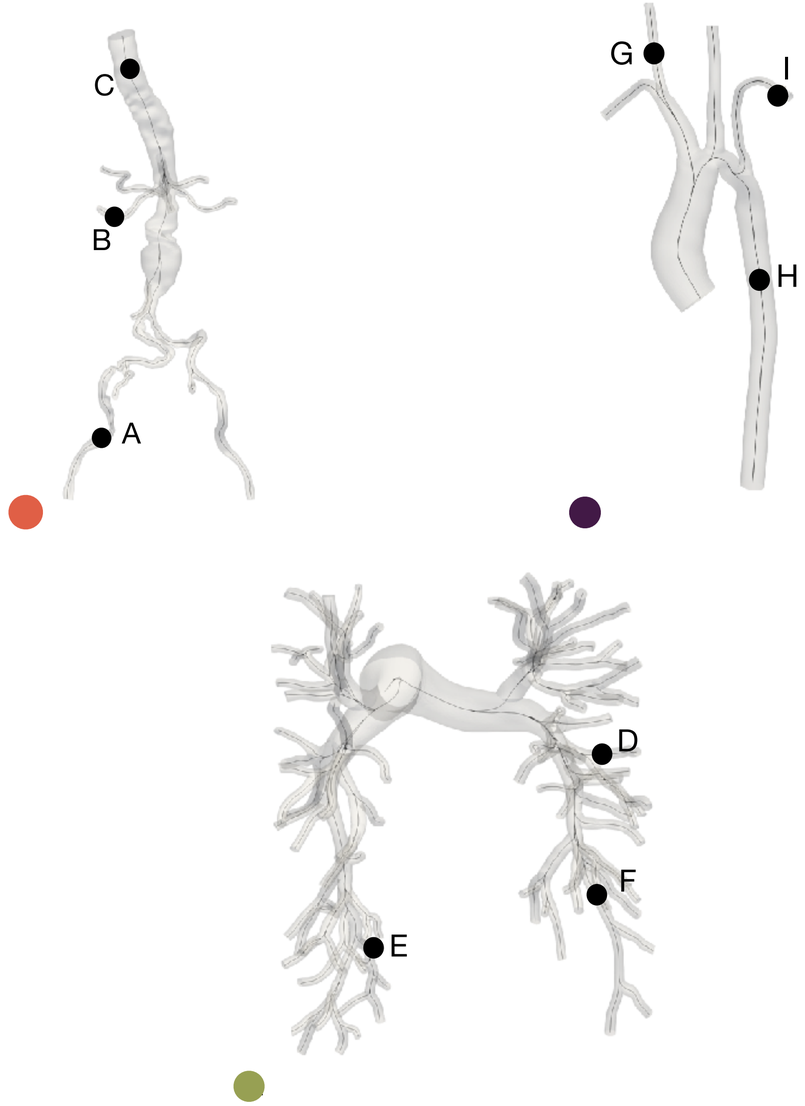


Qualitative results

Stanford Stanford

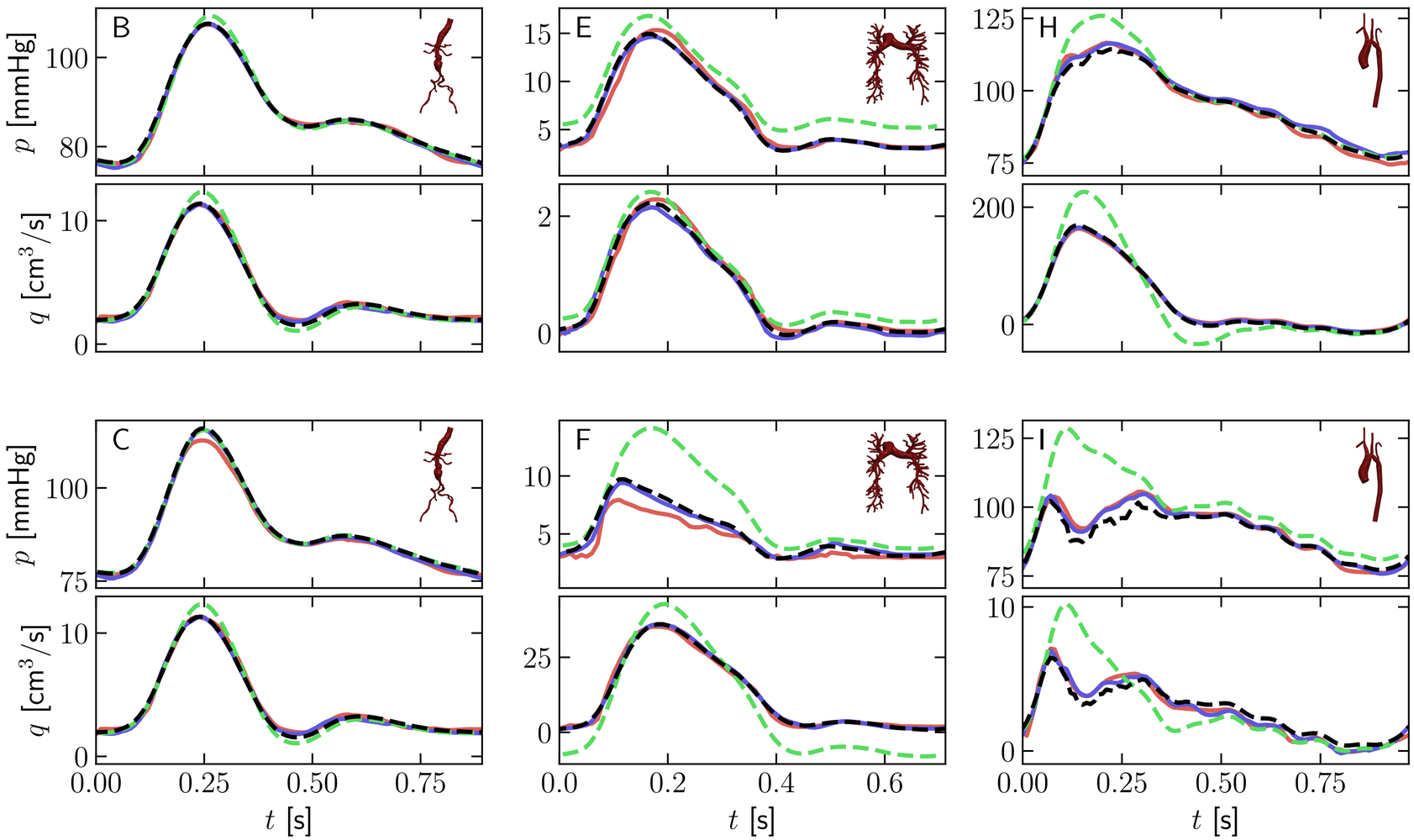




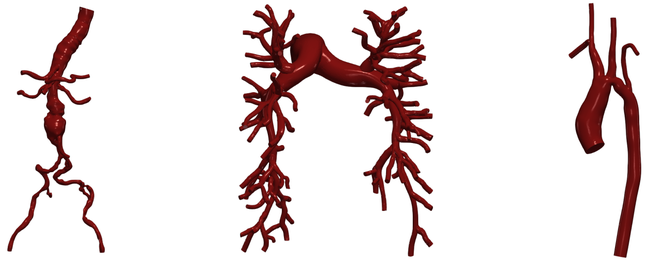
Qualitative results

Stanford Stanford

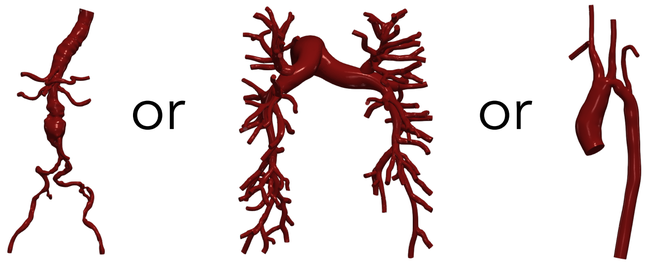
Goal 1: train a single GNN on diverse anatomies.



GNN-A: trained on



GNN-Bg: trained on



GNN-A GNN-Bg Ground truth

Qualitative results

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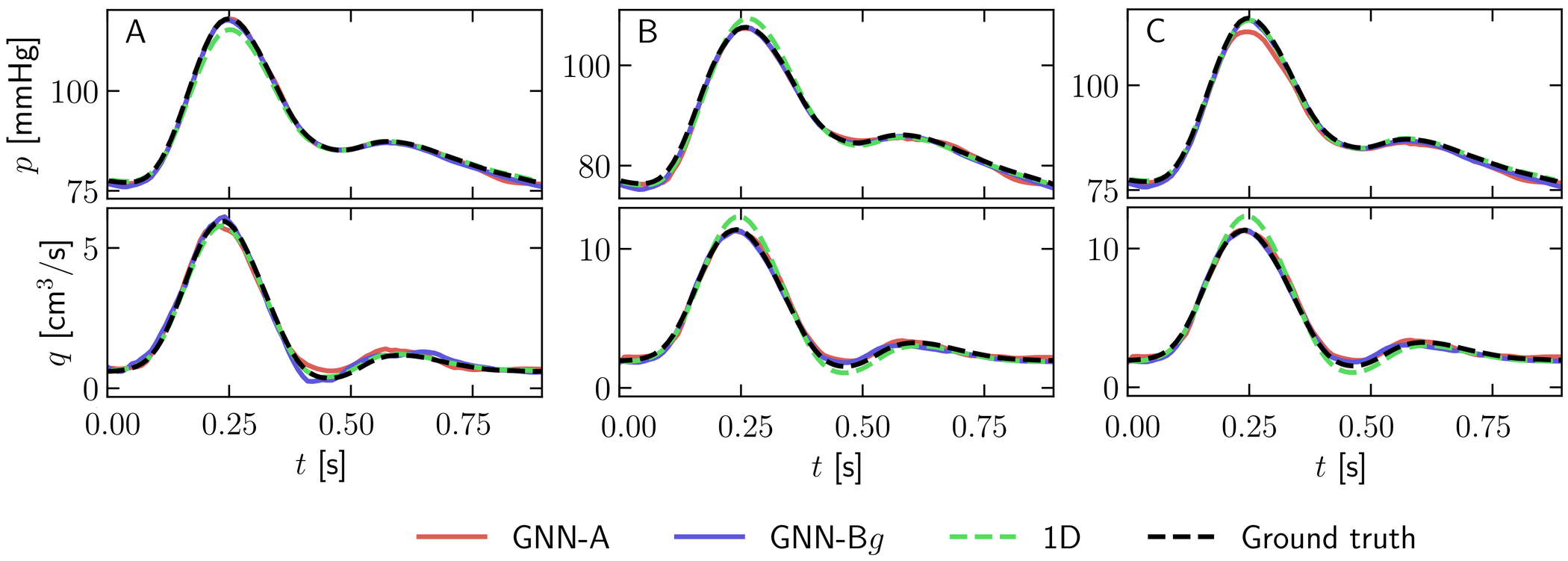
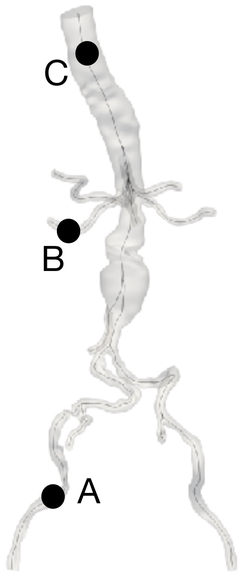
Goal 2: compare performance against physics-based one-dimensional models.





Good agreement on **aneurysm** model

Qualitative results

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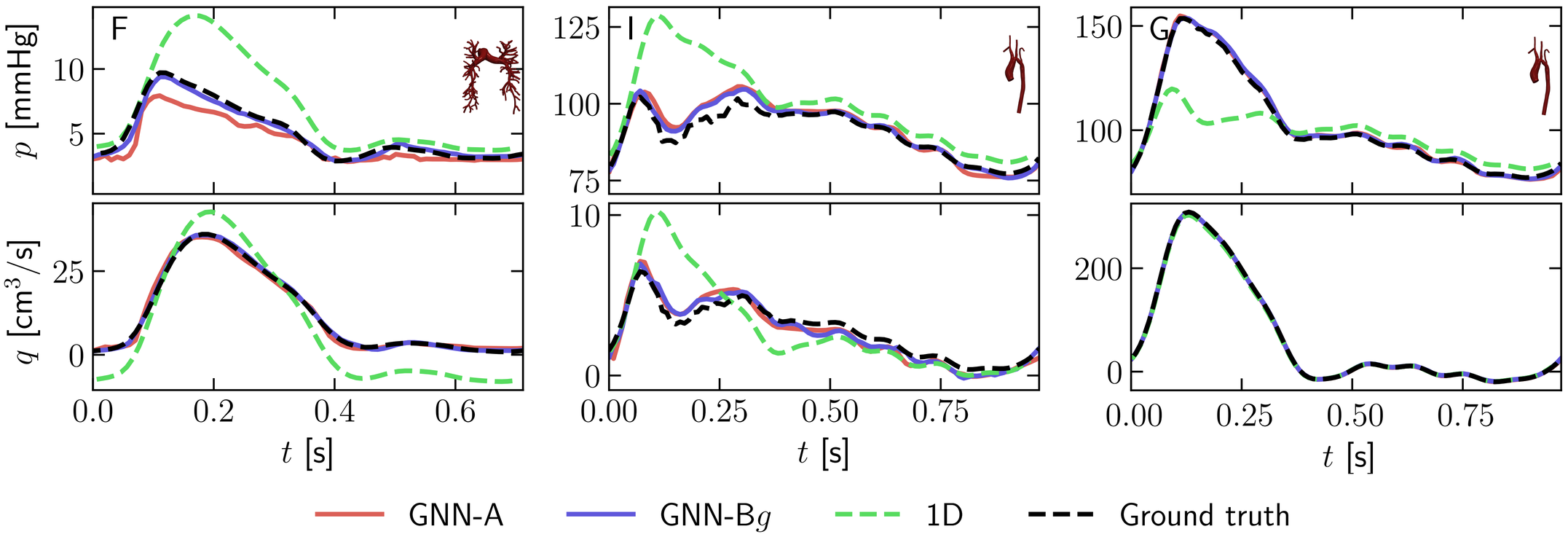
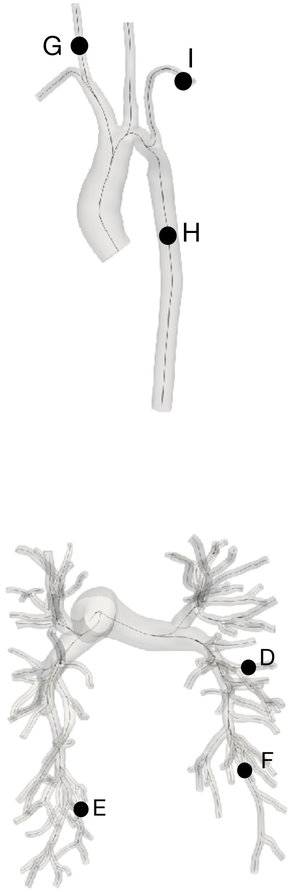
Goal 2: compare performance against physics-based one-dimensional models.





GNN superior on **pulmonary** and **coarctation models**

Ablation study

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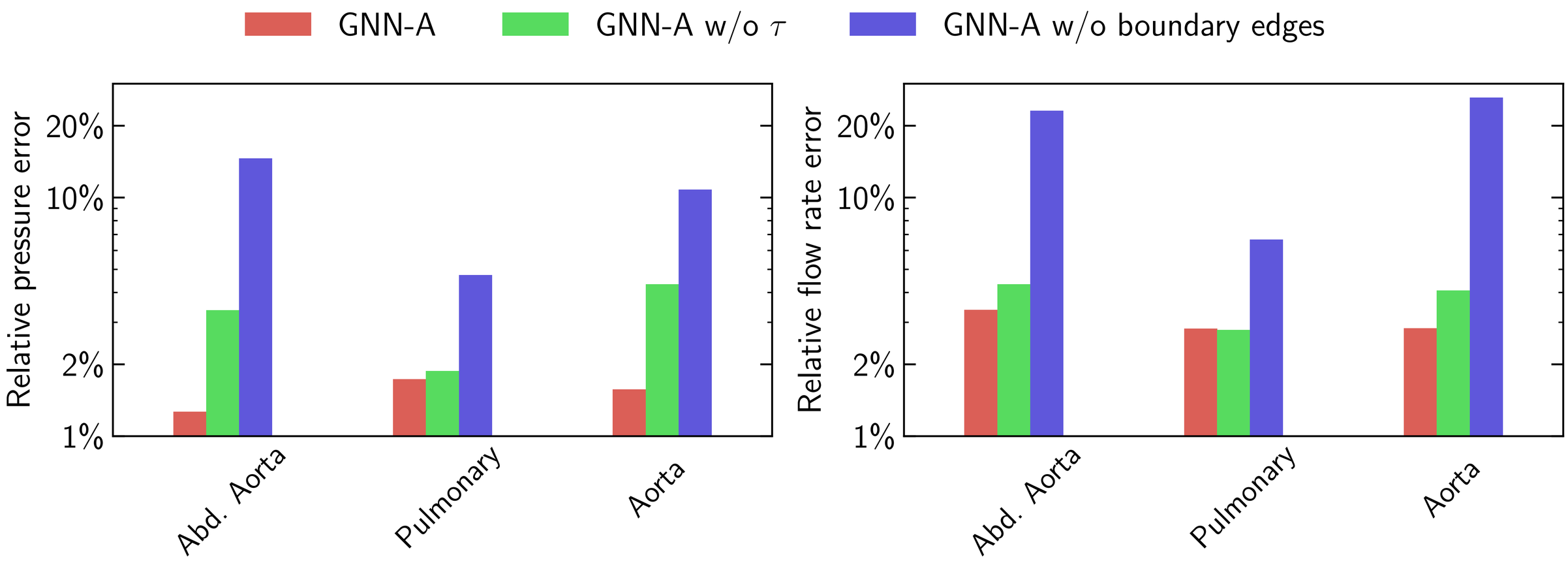

τ: application-specific features

Conclusions

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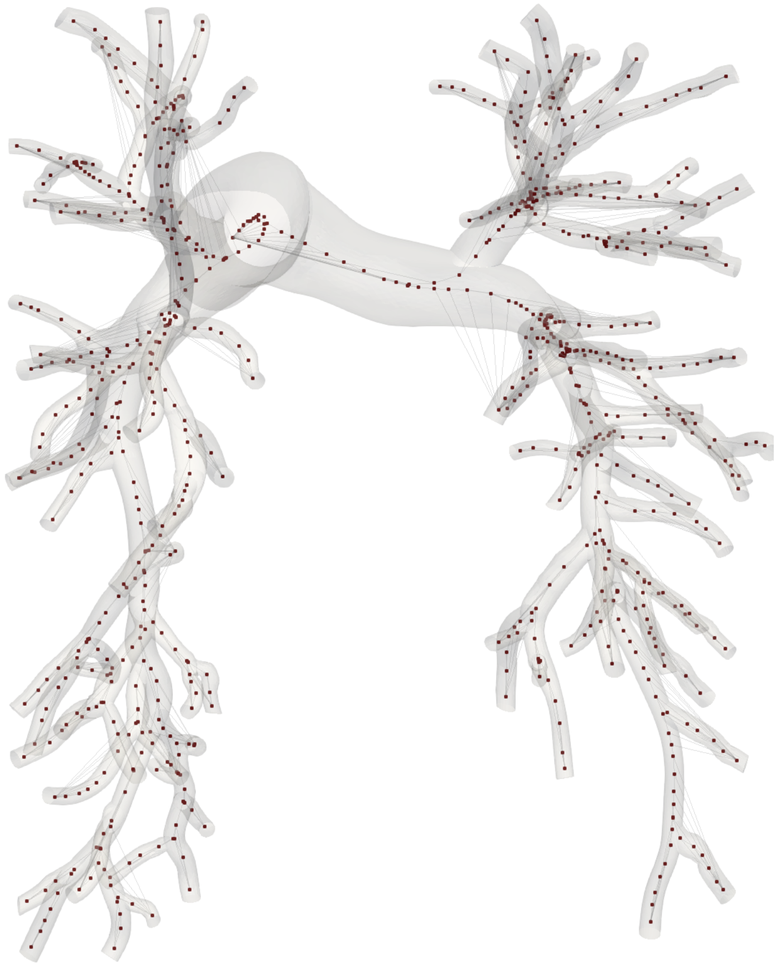
Graph Neural Networks can be used as **surrogate 1D models.**

They perform better than 1D models **when trained on sufficient data.**



arXiv paper

GitHub repository

Conclusions

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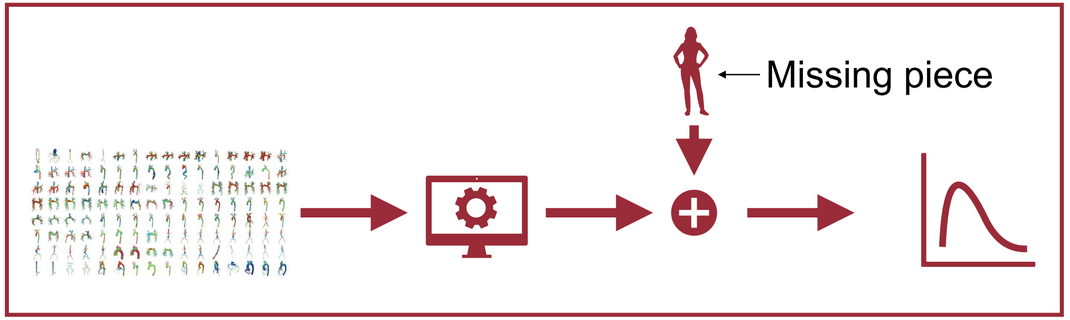
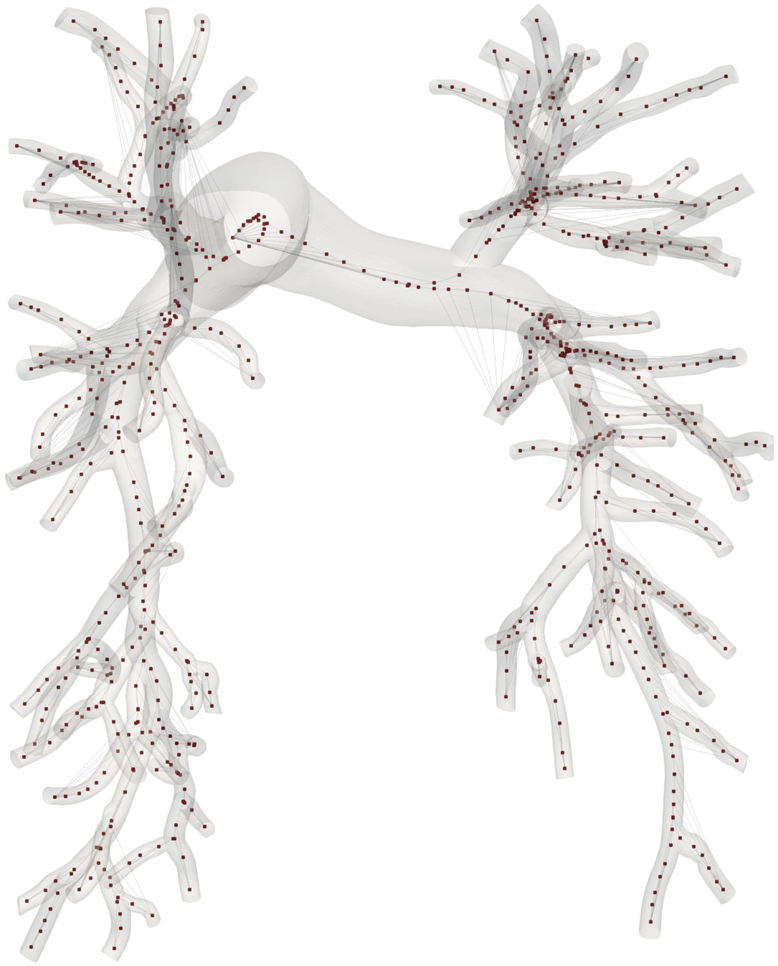
Graph Neural Networks can be used as **surrogate 1D models.**

They perform better than 1D models **when trained on sufficient data.**

Not there yet, but on the right track





arXiv paper

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