Scalable, adaptive, and explainable scientific machine learning with applications to computational fluid dynamics

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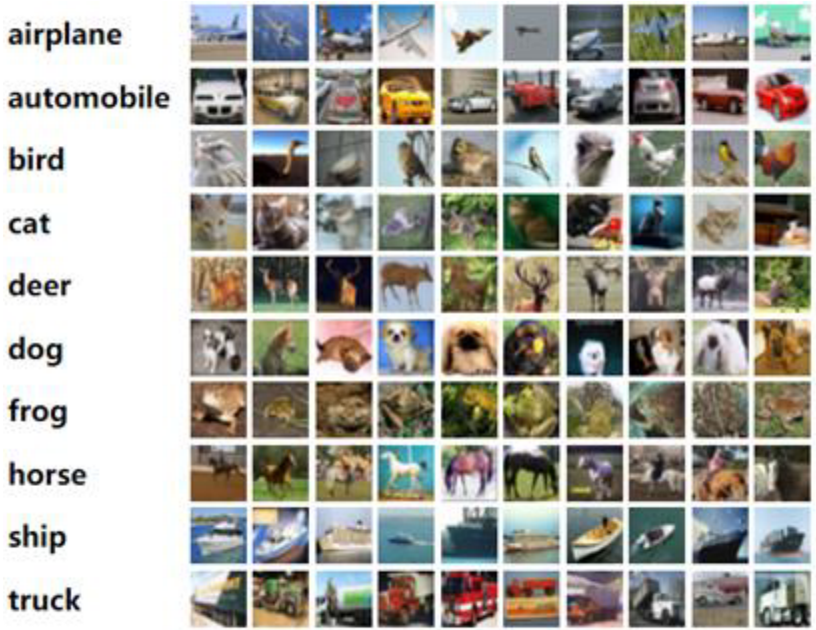
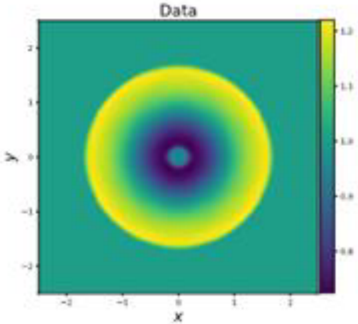
PennState

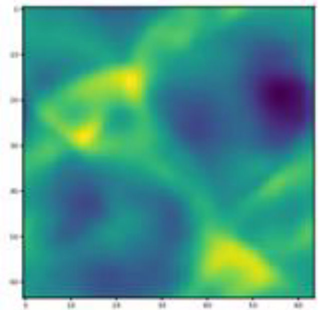
Machine learning and benchmarks

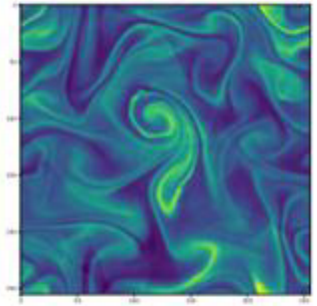


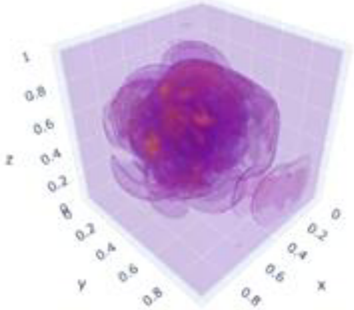
Machine learning algorithms have been revolutionized through community-based benchmarks and annual competitions: PASCAL-VOC challenge, ImageNet, etc.

Typical benchmarks for data-driven modeling





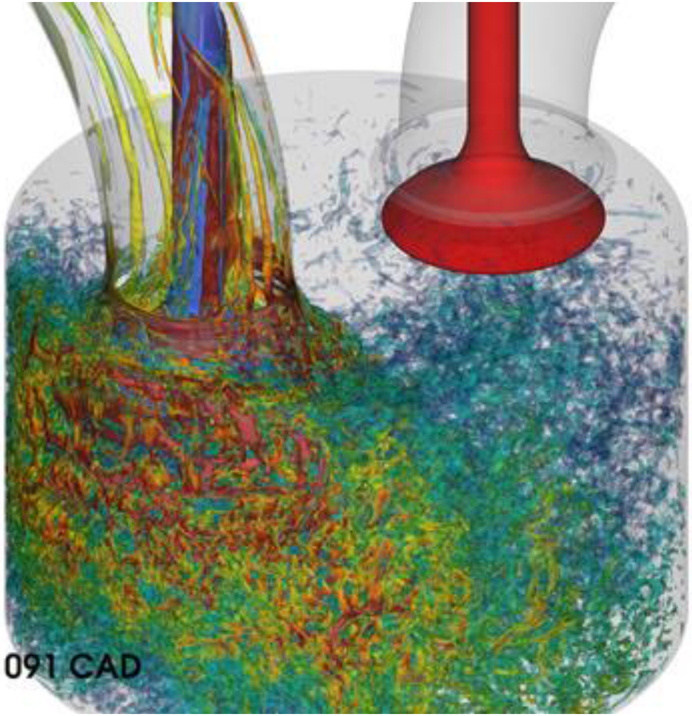




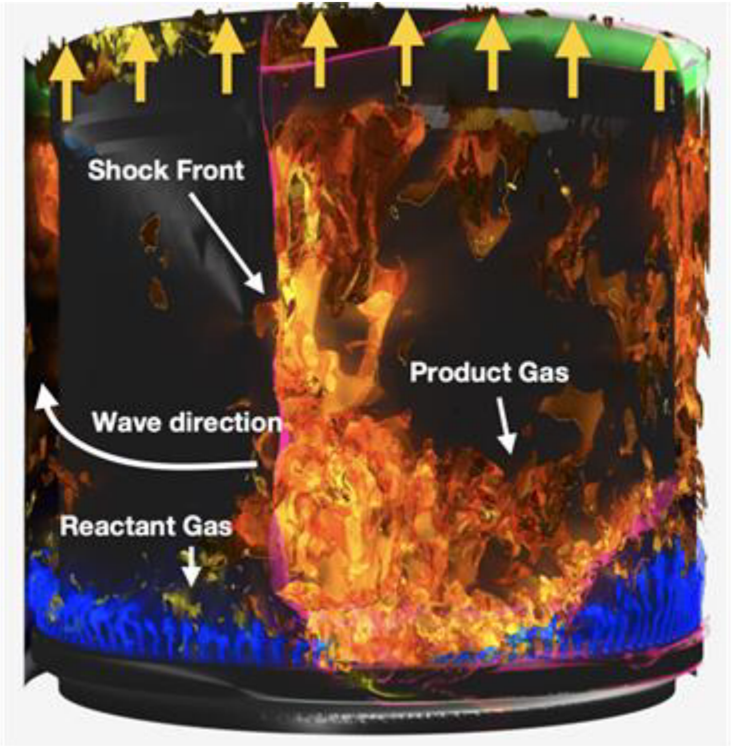
PDE	N_d	Time	N_s
advection	1	yes	1 024
Burgers'	1	yes	1 024
diffusion-reaction	1	yes	1 024
diffusion-reaction	2	yes	128×128
diffusion-sorption	1	yes	1 024
compressible Navier-Stokes	1	yes	1 024
compressible Navier-Stokes	2	yes	512×512
compressible Navier-Stokes	3	yes	$128 \times 128 \times 128$
incompressible Navier-Stokes	2	yes	256×256
Darcy flow	2	no	128×128
shallow-water	2	yes	128×128

Pros: Easy to share data, easy to interface with ML ecosystem (structured grids), easy to reproduce.
Cons: There is a tendency to develop specialized algorithms that do not "scale"
Image and table courtesy: PDEBench, NeurIPS, 2022

Realistic scientific computing

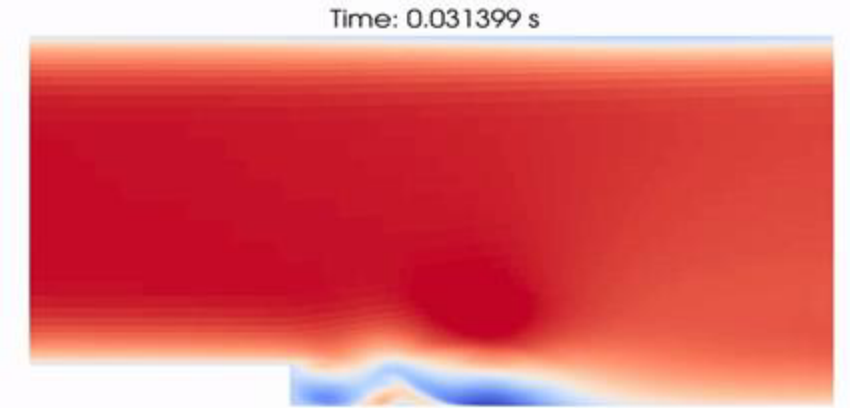


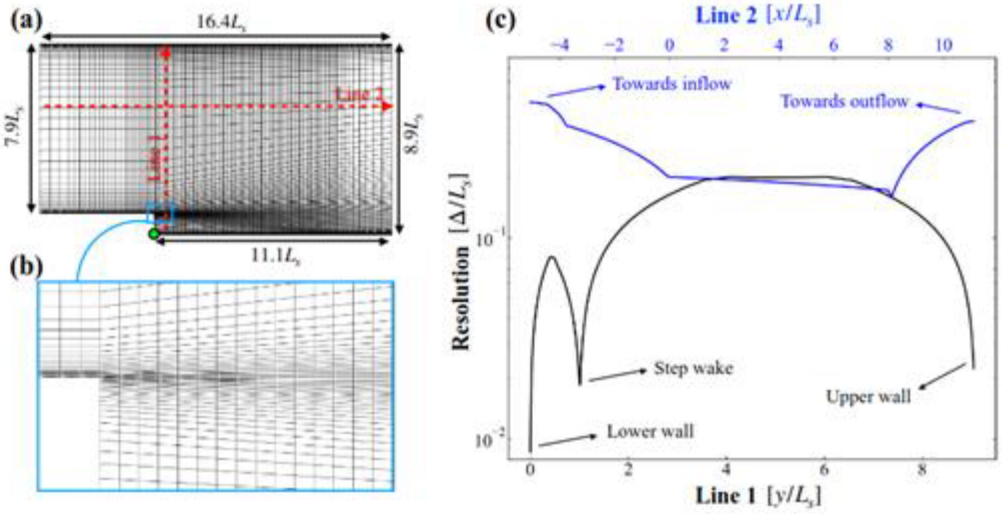
Saumil Patel and Nek5000 team, ANL

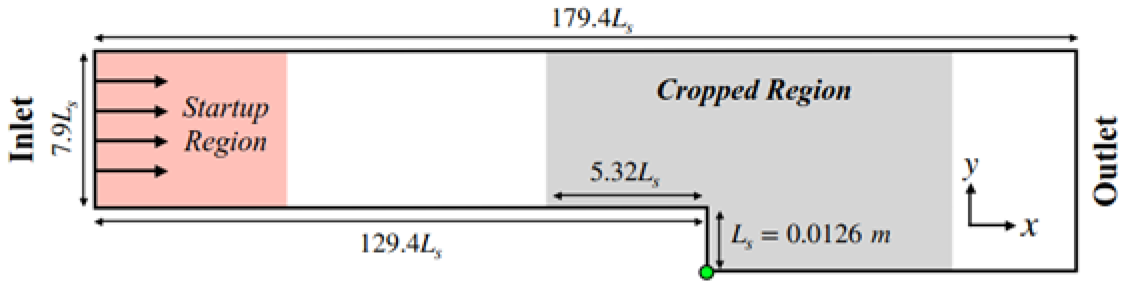


UMReactingFlow solver, APCL group, University of Michigan (PI: Venkat Raman)" and this paper: "Bielawski, R., Barwey, S., Prakash, S. and Raman, V., *Computers & Fluids (Accepted)*

A prototypical CFD problem







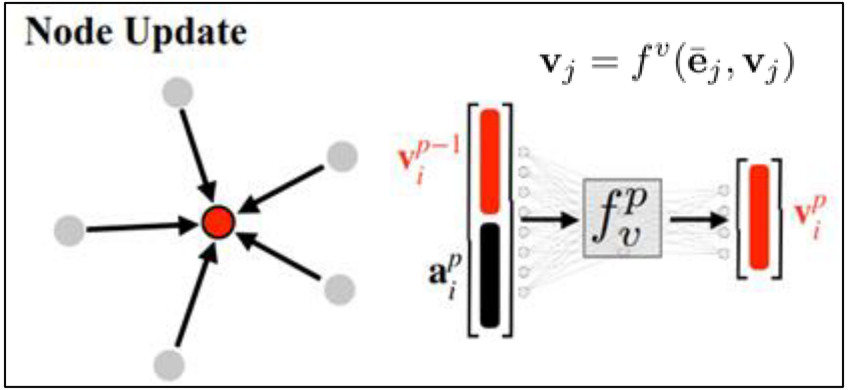
Flow over a backward facing step:

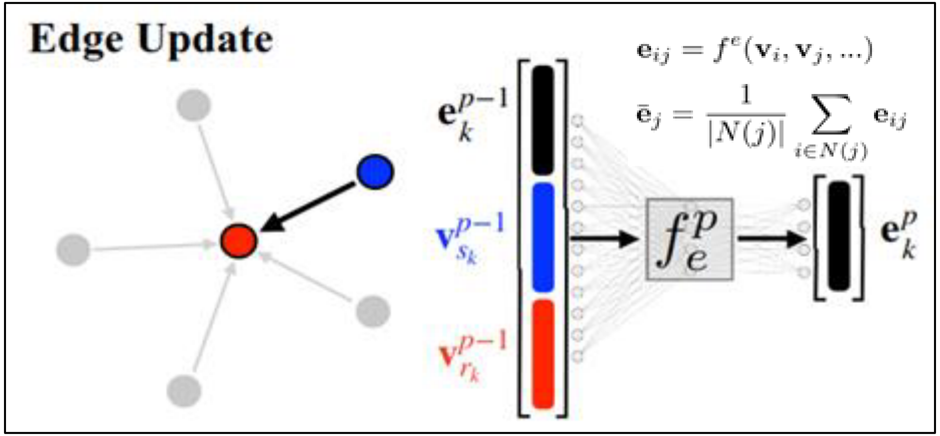
- Experimental data available.
- Mesh available (NASA LARC)
- Prototypical for *several* applications.

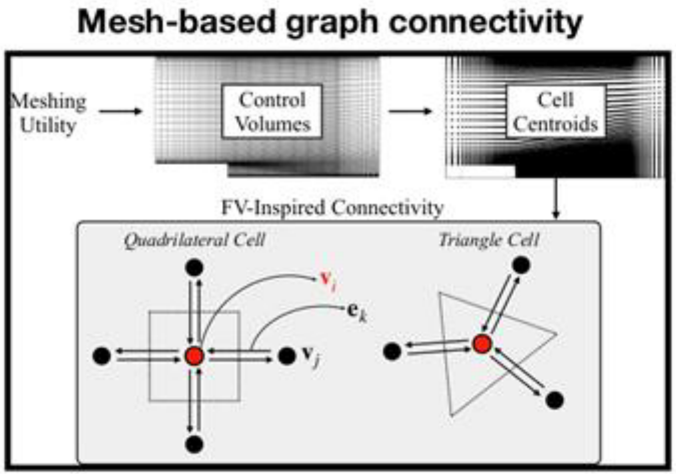
We propose

A scalable and interpretable deep learning paradigm for unstructured computational fluid dynamics datasets

Geometric deep learning for unstructured data

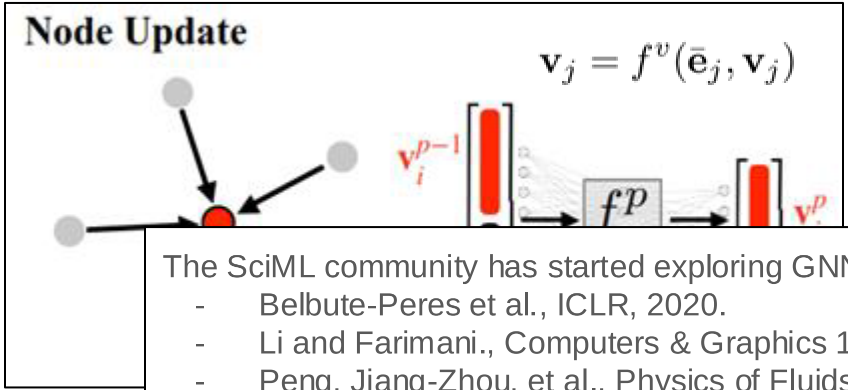


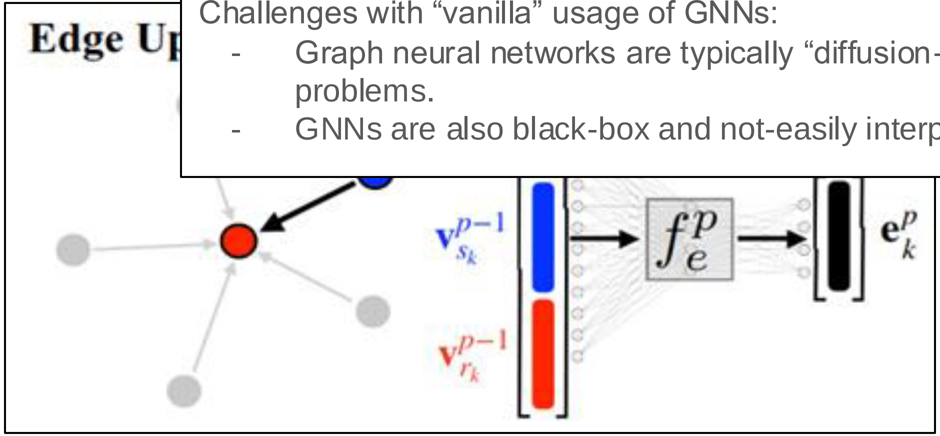


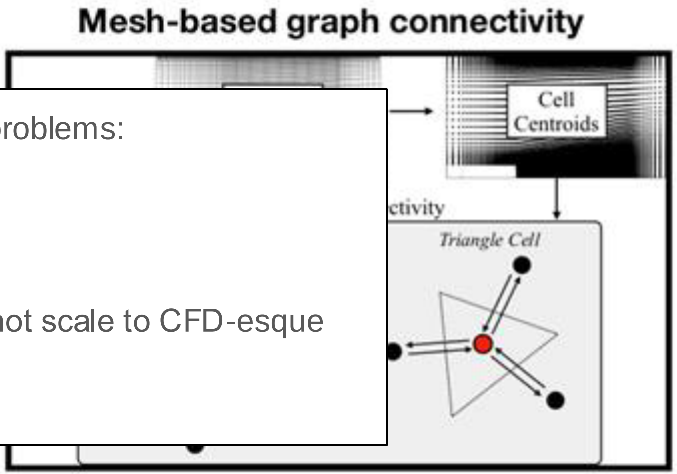


Parallels between function approximation on CFD meshes and message passing in graph neural networks. For a finite-volume code - the nodes are cell-center values, the edges are fluxes and some notion of distance.

Geometric deep learning for unstructured data







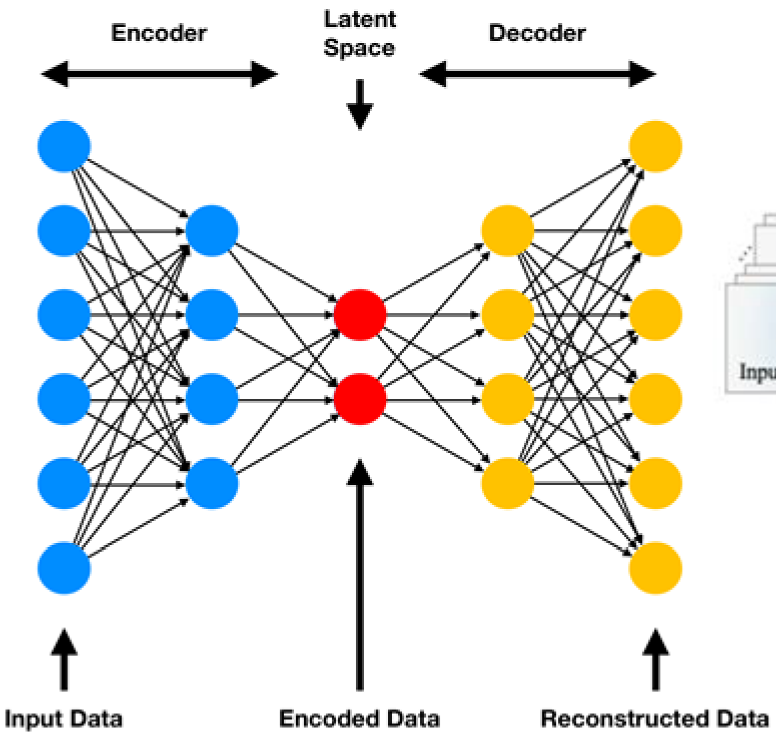
The SciML community has started exploring GNNs for realistic CFD problems:

- Belbute-Peres et al., ICLR, 2020.
- Li and Farimani., Computers & Graphics 103 (2022): 201-211.
- Peng, Jiang-Zhou, et al., Physics of Fluids 35.8 (2023).

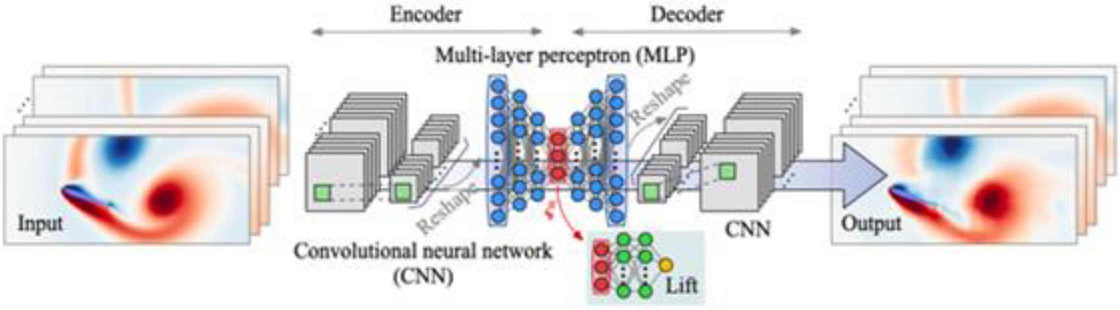
Challenges with “vanilla” usage of GNNs:

- Graph neural networks are typically “diffusion-driven” and cannot scale to CFD-esque problems.
- GNNs are also black-box and not-easily interpreted.

Autoencoders - a primer

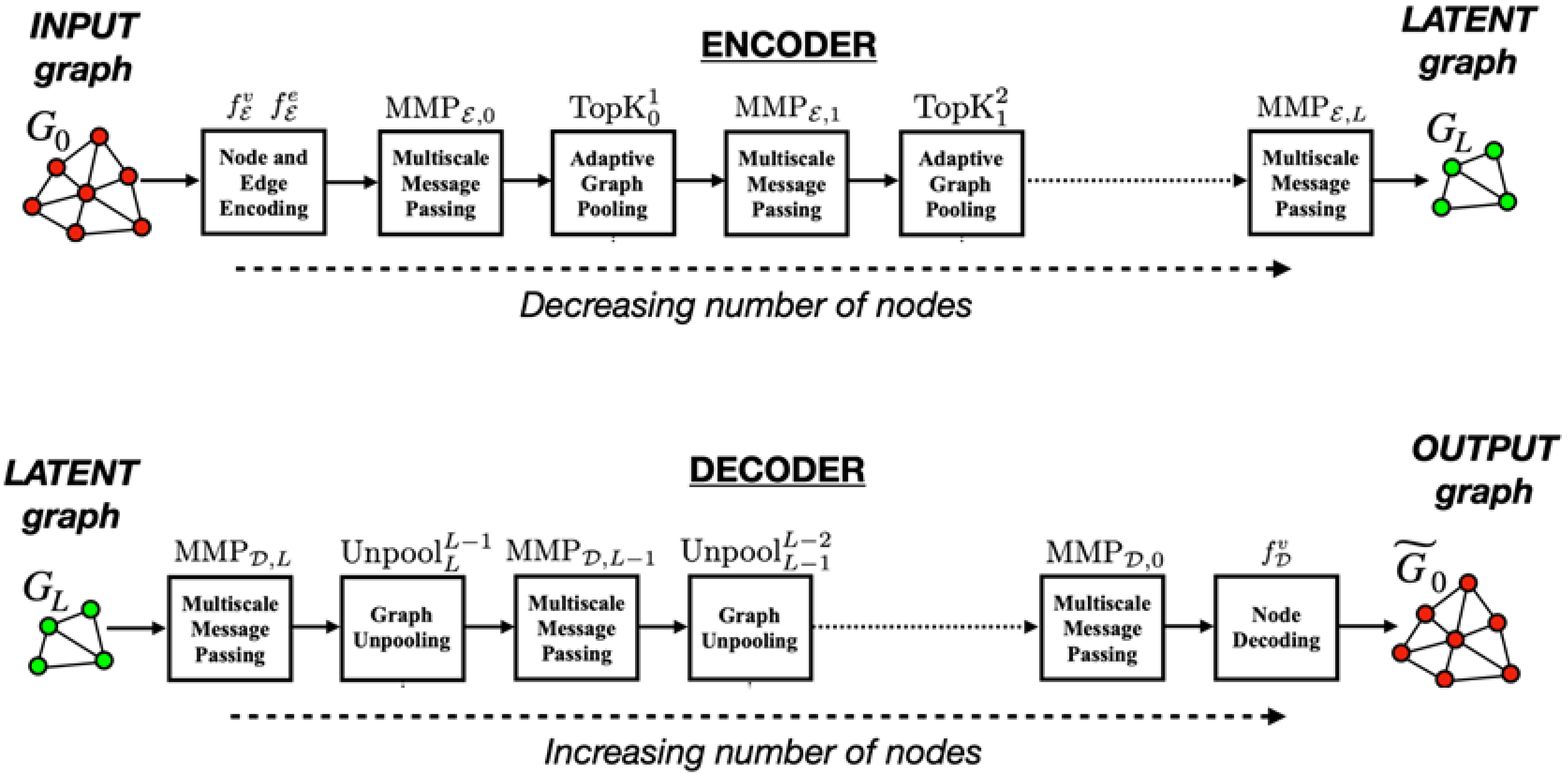


SciML models frequently use compression to accelerate function approximation and inference. We will leverage autoencoders to do the same.

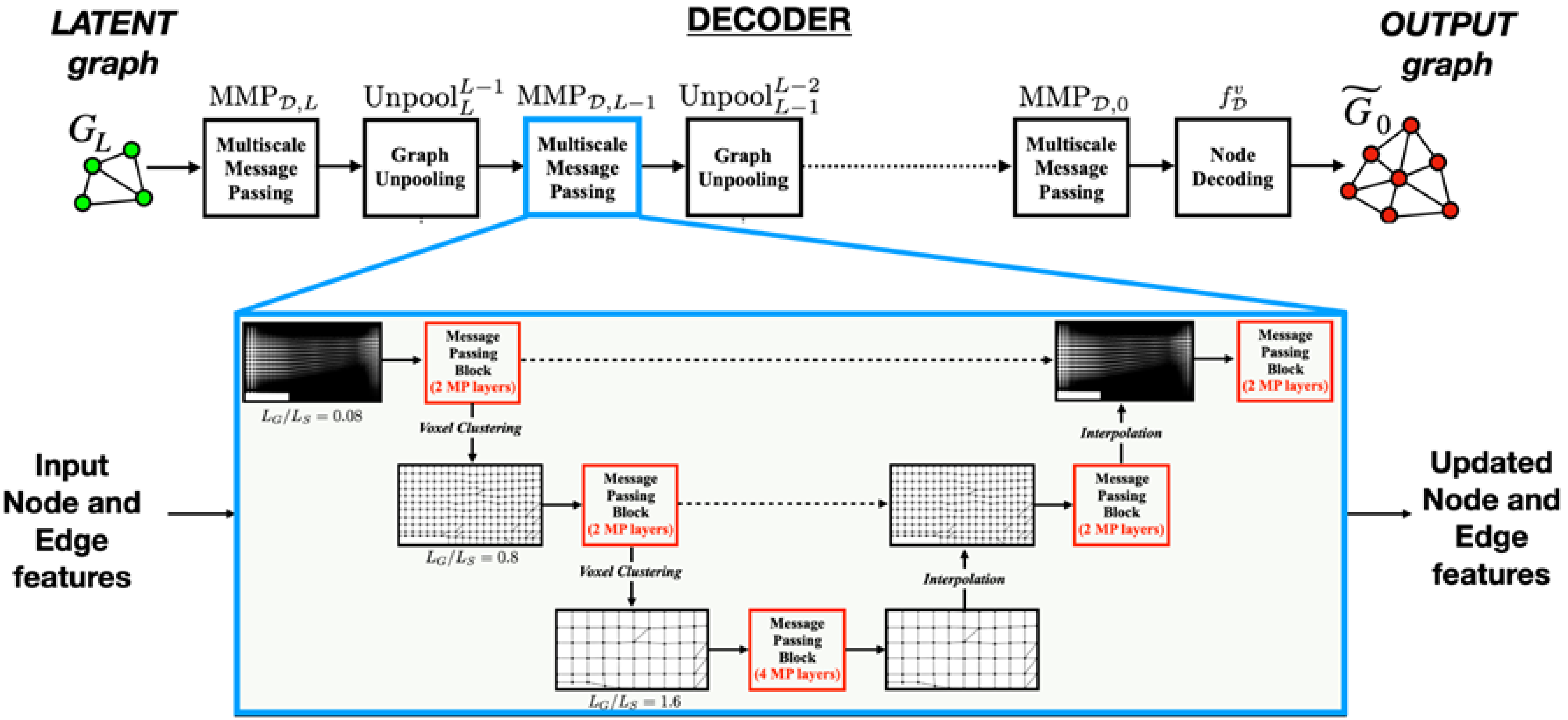


Autoencoders have been used to efficiently compress high-dimensional flow-fields and build reduced-order models. **Criticism**: The compression is not easily interpretable. **Image courtesy - Taira Lab, UCLA.**

A graph neural network autoencoder



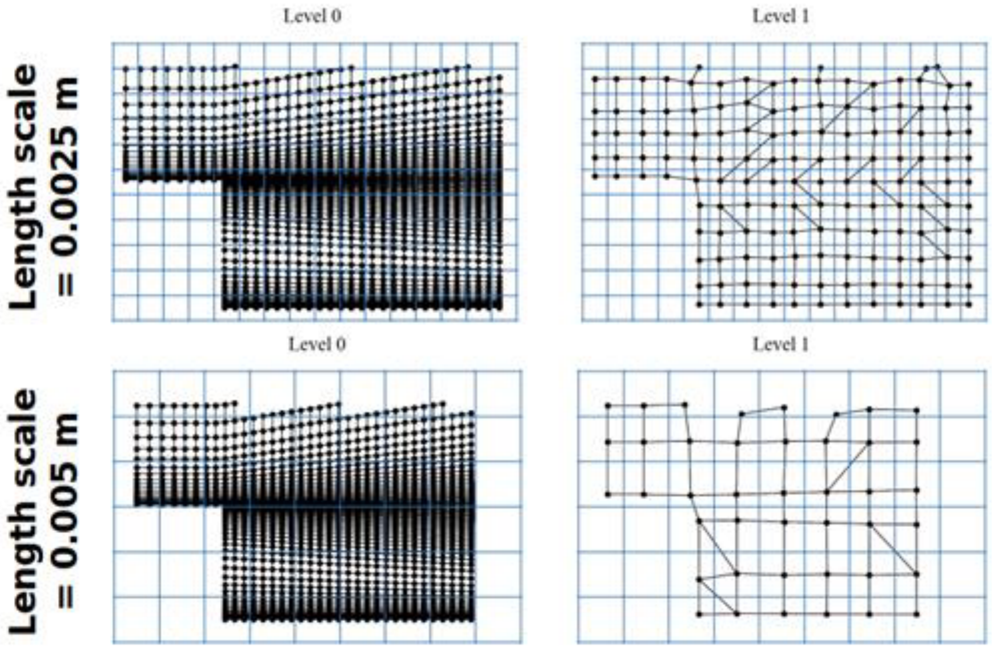
Scalability via multiscale message passing



Gao, Hongyang, and Shuiwang Ji. "Graph u-nets." ICML, 2019.

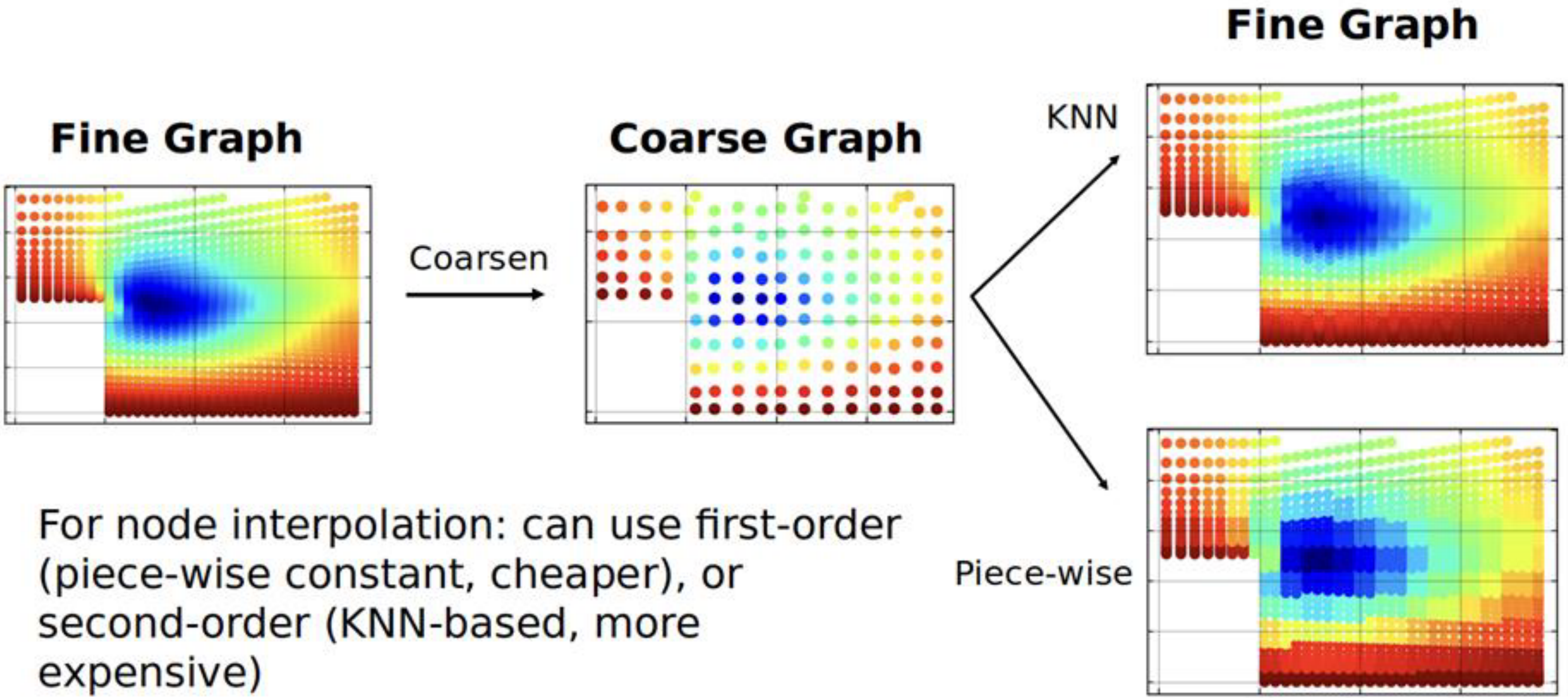
Scalability via multiscale message passing

- Voxel-based clustering (Coarse mesh is still unstructured)
- Step 1: prescribe a target length scale
- Step 2: create a structured mesh at this target length scale
- Step 3: identify node-cell ownership
- Step 4: coarsen
  - For nodes: coarse node comes from mean of fine nodes within cell
  - For edges: coarse edge comes from mean of fine edges intersecting cells



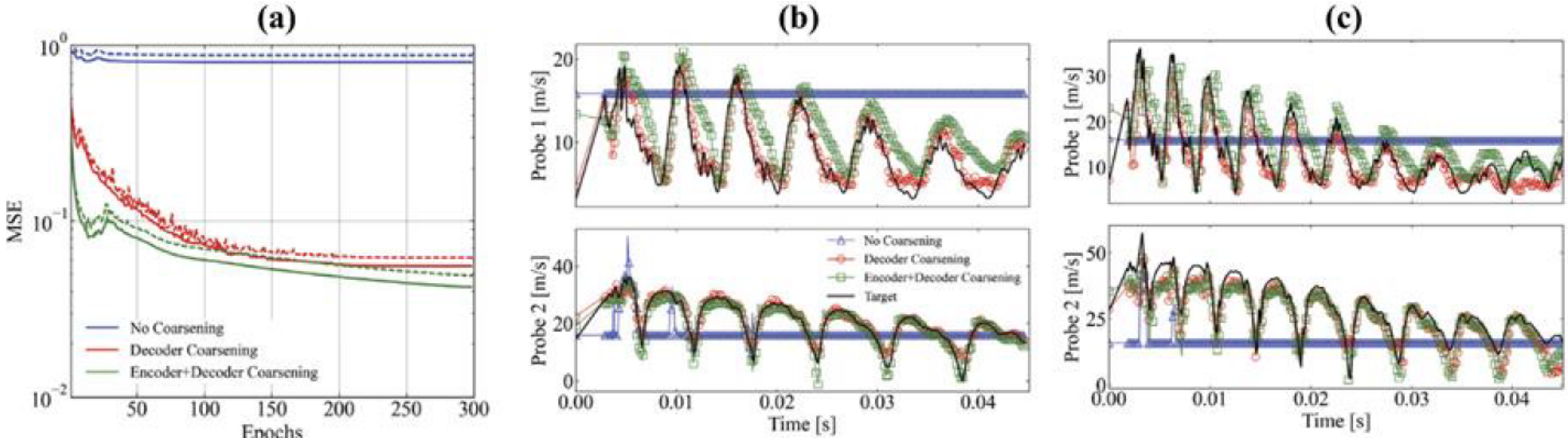
Adaptive selection of length scales for latent space possible - "Length scale discovery"?

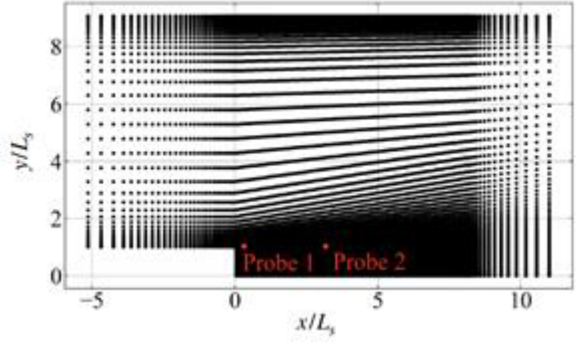
Scalability via multiscale message passing



For node interpolation: can use first-order (piece-wise constant, cheaper), or second-order (KNN-based, more expensive)

Scalability via multiscale message passing

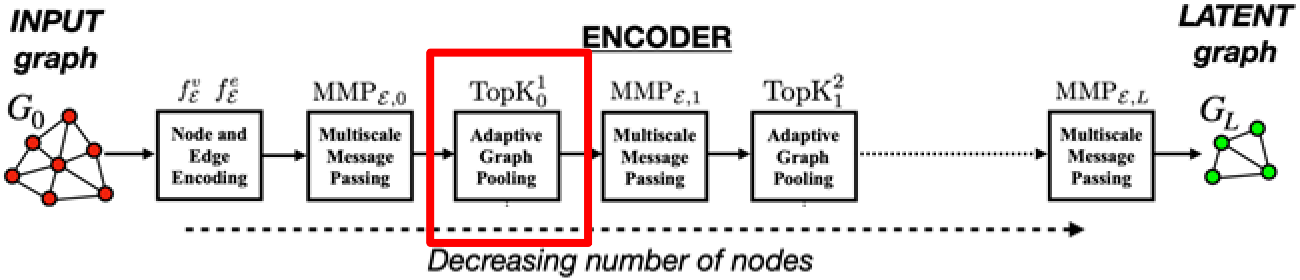




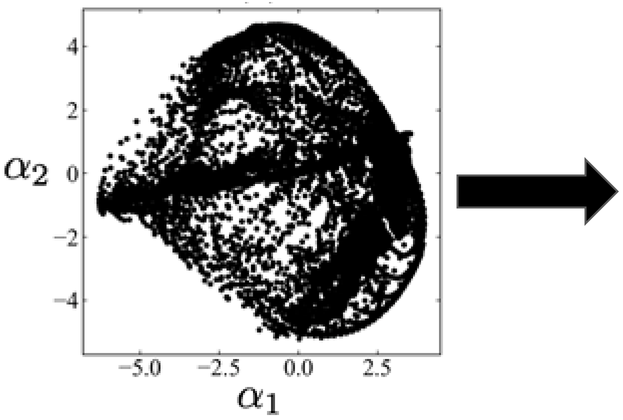
The multiscale message passing layer addresses the "flatlining" of the standard graph neural network for a **compression application.**

Interpretability via adaptive subsampling

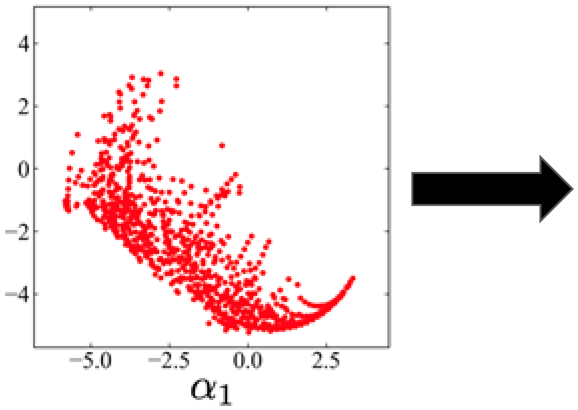
Node downsampling occurs using learnable projection vector. **Top-K projection.**



Input Node Features

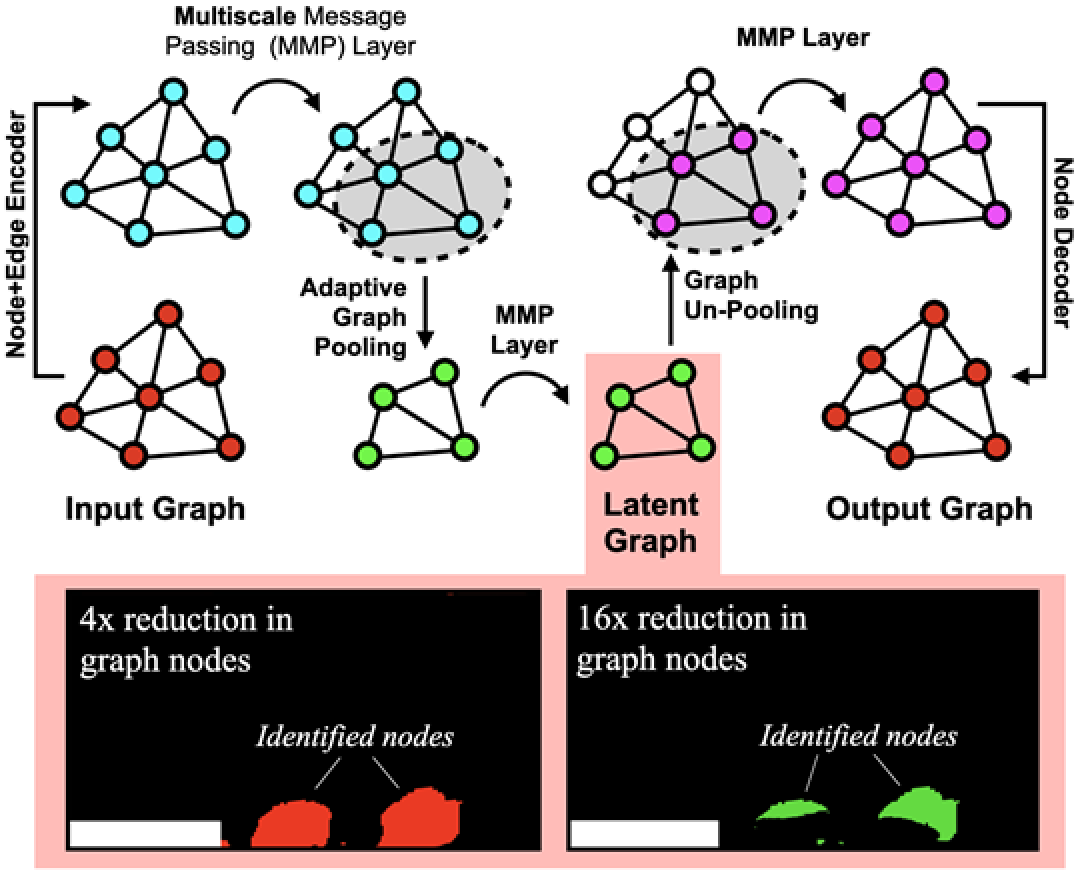


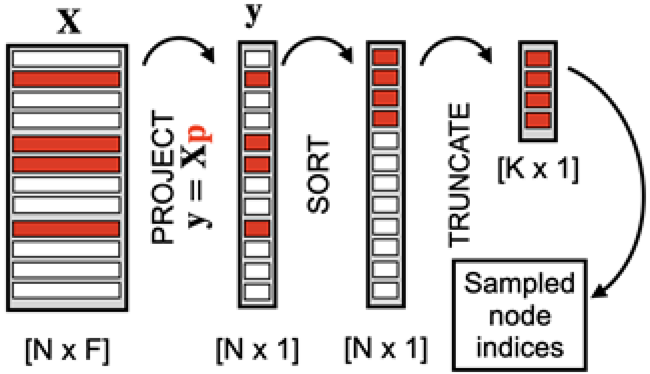
Sub-sampled nodes



Masked Field

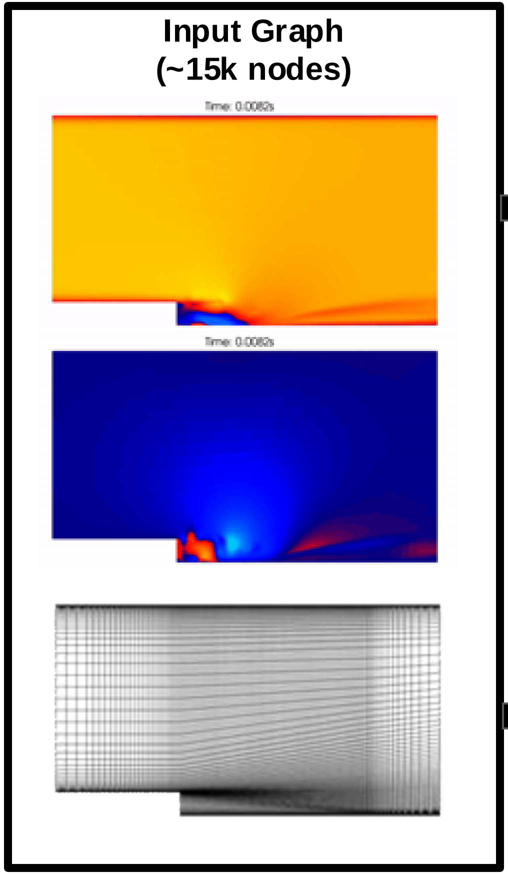
Interpretability via adaptive subsampling





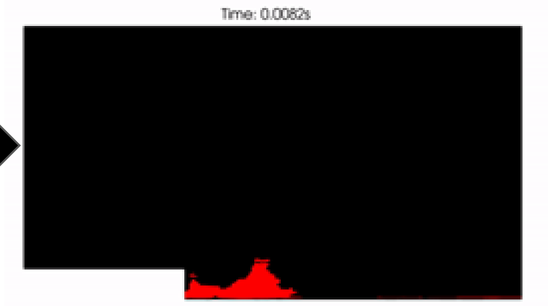
During training - the GNN learns what nodes must be retained (ergo “important”) to promote accuracy!

Interpretability via adaptive subsampling



16x reduction in nodes

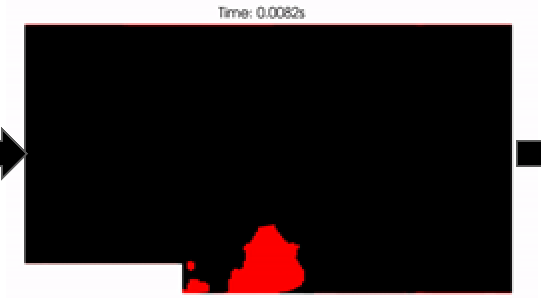
Latent space



In progress: Building a “Lagrangian” reduced-order model in the latent space.

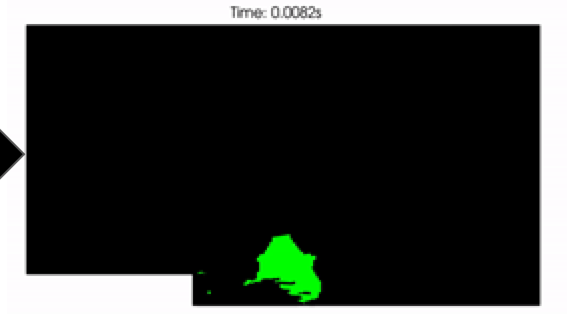
4x

Hidden layer 1



4x

Latent space



In conclusion

We have thus far:

1. An ability to deal with advection dominated datasets and realistic benchmarks.
2. An ability to deal with large unstructured meshes.
3. An ability to visualize and interpret what happens *within* a neural network.

Barwey S, Shankar V, Viswanathan V, **RM**. Multiscale graph neural network autoencoders for interpretable scientific machine learning. Journal of Computational Physics. 2023 Dec 15;495:112537.

A larger version of this talk

1. Builds an interpretable surrogate model for **forecasting** on this dataset.
2. Introduces **a-posteriori** indicator of spatial error.