Scalable Graph Neural Networks for Mesh-Based Fluid Flow Modeling

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Data-Intensive Computing and AI/ML Applications at Scale
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Argonne NATIONAL LABORATORY

Interpretable Scientific Machine Learning for Mesh-Based Simulations with Graph Neural Networks

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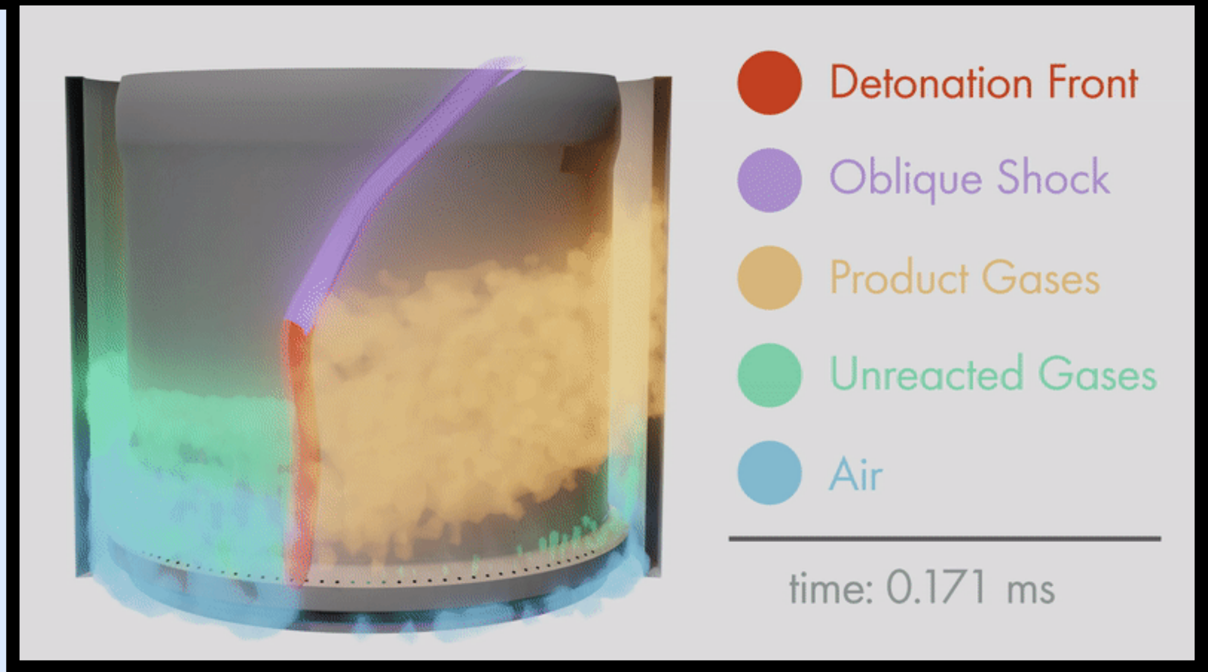
Research Objectives

Goal: surrogate models for **full-scale** unsteady fluid simulations (e.g., propulsion applications)

Objective 1: Enable complex geometry compatibility.



Solver: UMReactingFlow (APCL, UM)
Visualization: Michelle Lehmann (ORNL)

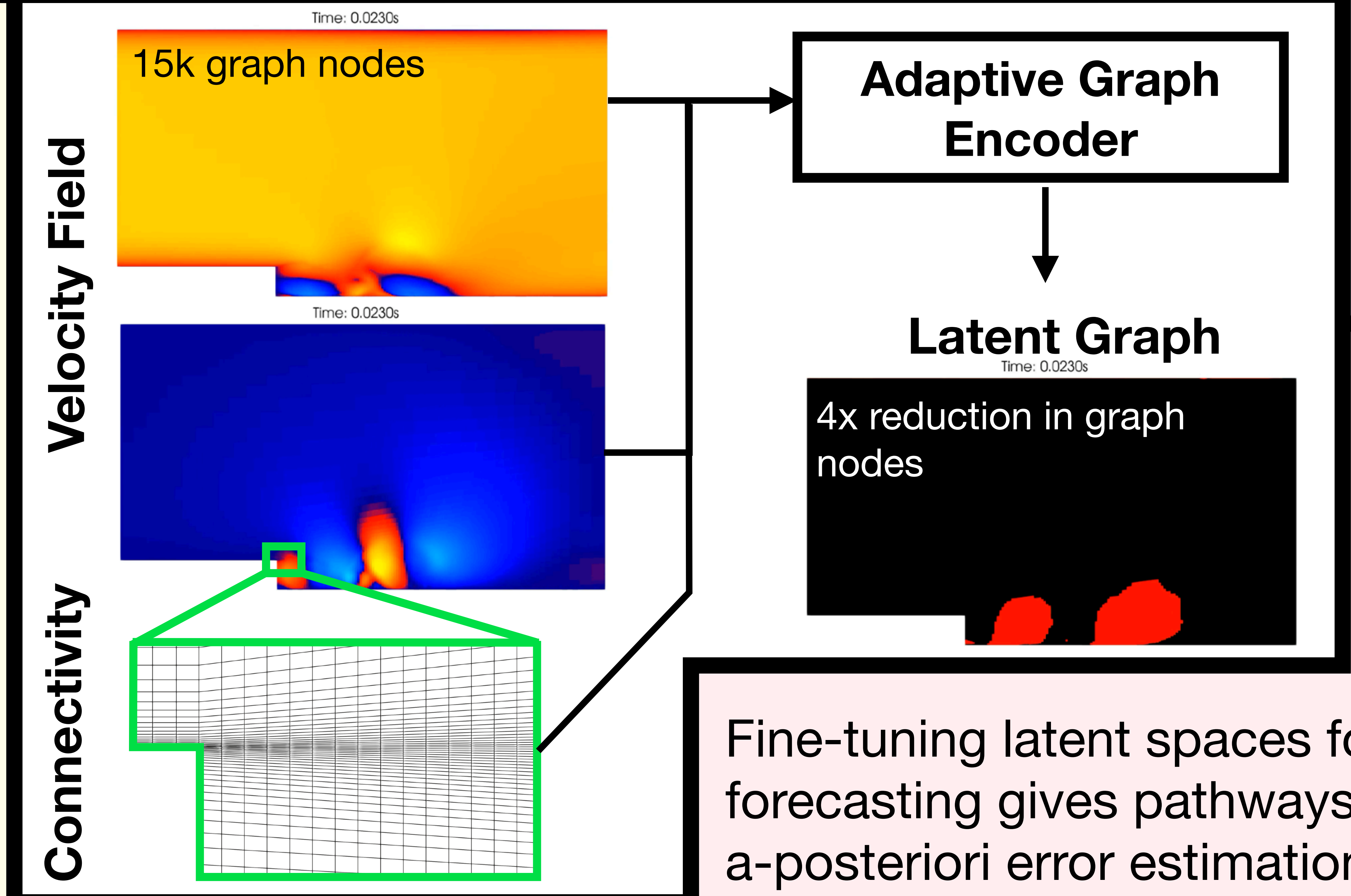
Objective 2: Ensure interpretable latent spaces, fine-tuned to modeling task (reconstruction, forecasting).

Objective 3: Develop scalable training and inference strategies.

Approach

Multiscale GNN layers: Employ **message passing** schemes at various grid resolutions to enable efficient propagation of information

Graph reduction: Top-K graph pooling strategy achieves reduction in input graph dimensionality using adaptive and learnable node subsampling



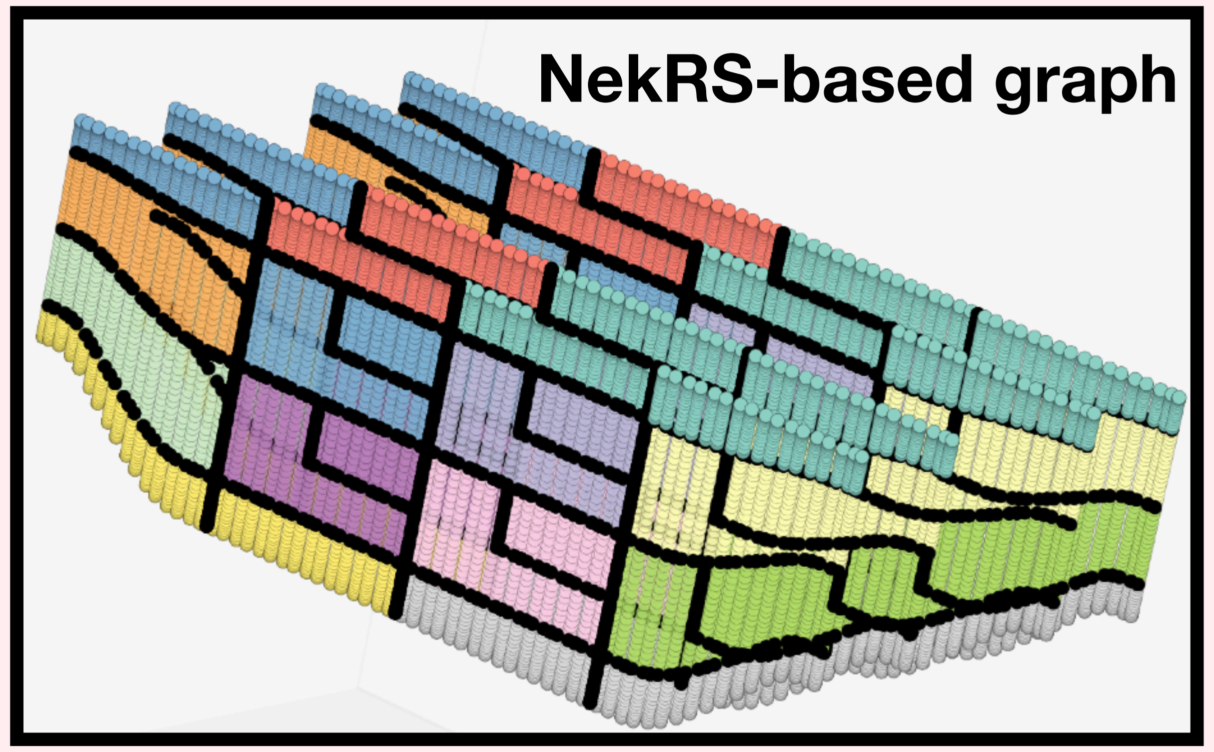
Domain decomposition: Leverage domain decomposition routines used in vetted exascale computational fluid dynamics codes (NekRS) to scale-up and train models on very large graphs

Impact & Ongoing Work

Interpretable GNN layers address key limitation in SOTA — latent spaces can now be accessed and mapped to physical phenomena.

Fine-tuning latent spaces for forecasting gives pathways for a-posteriori error estimation for surrogate models.

Ongoing work: distributed GNN operations using NekRS, and forecasting stability.



Scaling Up GNN Operations: Interfacing with NekRS

With: Romit Maulik, Riccardo Balin, Saumil Patel, Ramesh Balakrishnan, Venkat Vishwanath

NekRS

Boundary exchange information

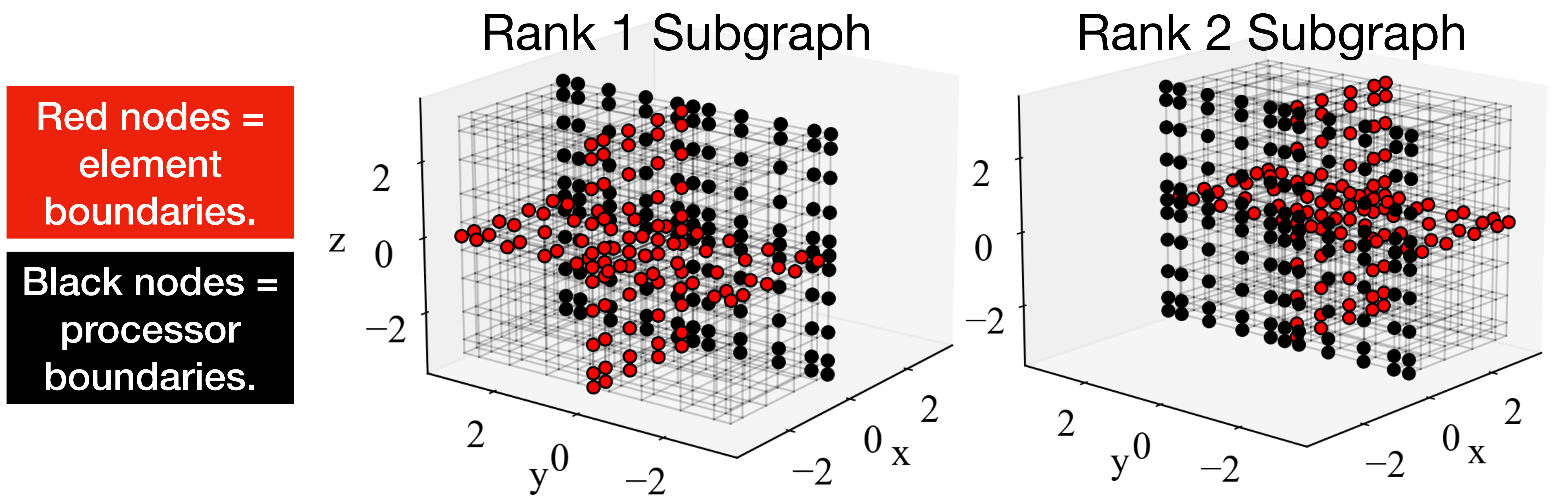
Local flowfield data

Graph representation of local CFD mesh

PyTorch Geometric

Parse NekRS meshes and feed into PyGeom

Partitioned NekRS-based graph



Graph Neural Network

Input Graph (Mesh-based flow field)

GLL node-based message passing

Loop over number of layers

Halo Swap

MP Layer

Output Graph (Mesh-based flow field)

GNN scope: node-level regression tasks (e.g., forecasting). Offline training demonstration in progress.