Predicting CO2 Plume Migration in Carbon Storage Projects using Graph Neural Networks

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Disclaimer

- This work is done in collaboration with NETL: **Chung Yan Shih, Paul Holcomb and others** (Energy Analysis | netl.doe.gov) using NVIDIA Modulus

- This project is part of Department of Energy (DOE) **Science-informed Machine Learning for Accelerating Real-Time Decisions in Subsurface Applications (SMART) Initiative** led by team at NETL and work is partially presented at GTC.

NVIDIA Modulus

Framework to build and customize Physics-ML models

Multi-domain support

Build physics-ml models for CFD, Heat Transfer, Structural, Electromagnetics, Molecular Dynamics

Optimized Training

Accelerate training and throughput by parallelizing the model and the training data across multi-node.

SOTA Model Architectures

Easily explore physics-ml model architectures – Neural Operators, PINNs, GNNs, Diffusion Models.

Support

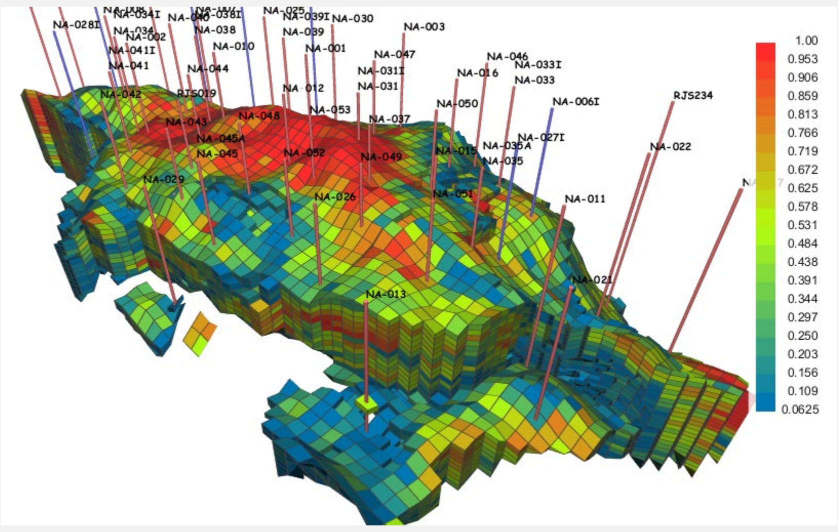
NVIDIA AI Enterprise and experts by your side to keep projects on track

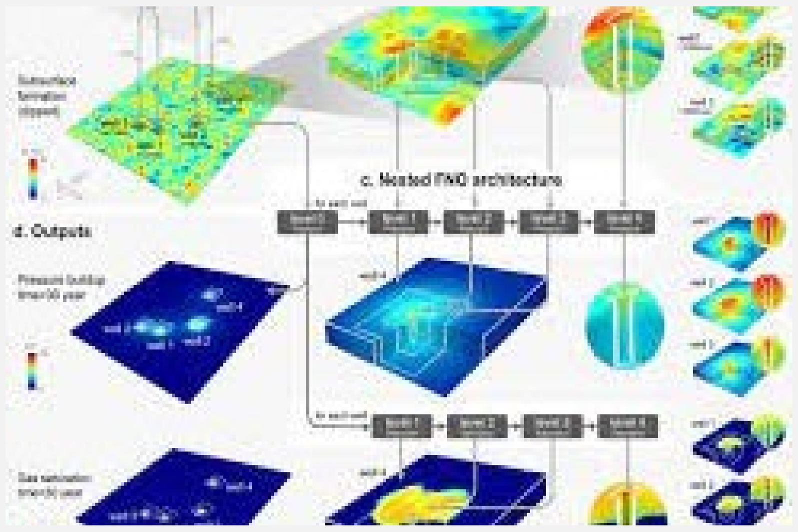
General Availability – Part of NV AIE (Starting NV AIE 4.0)

NVIDIA Modulus

Various simulation domains and case-studies

Energy





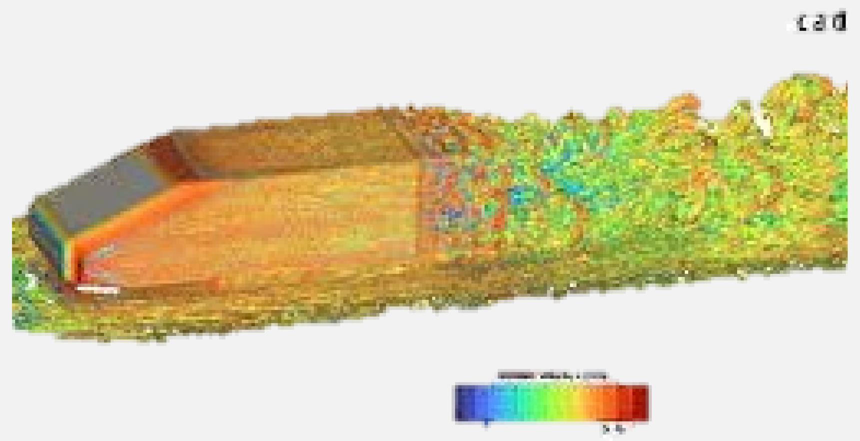
Applications like sub-surface flows for oil reservoirs or carbon storage, turbulent flows around wind turbine or power generation systems that require physics-ml surrogate models

Climate and Weather

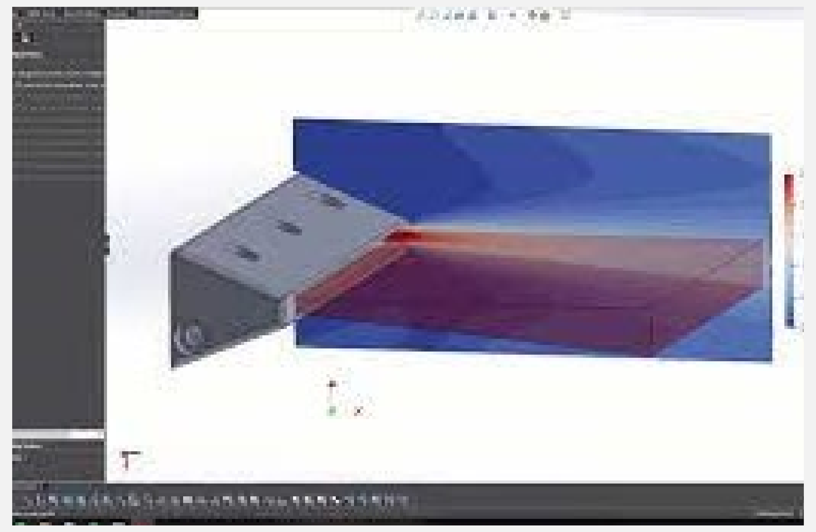
Physics ML surrogates for simulating weather and climate at various scales – global to local

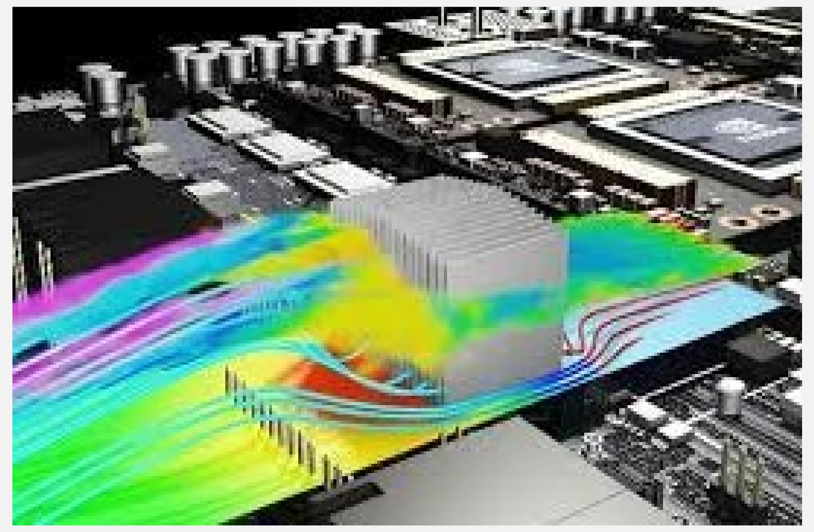
Industrial HPC

Physics ML surrogates for accelerating traditional simulation-based design workflows



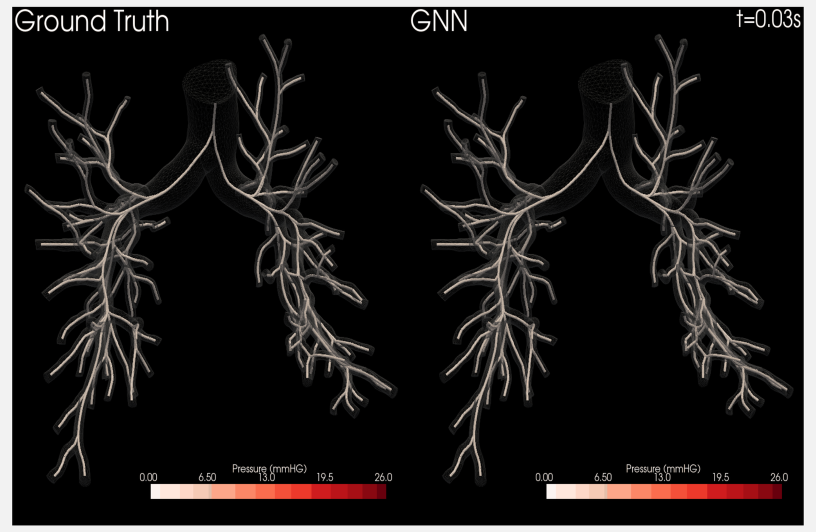
Design Optimization

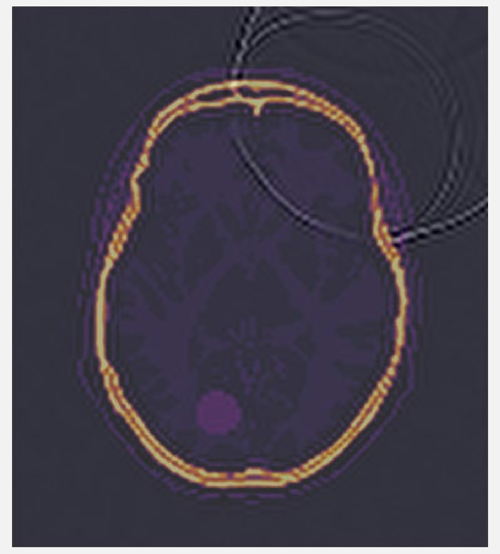




Physics ML surrogates to explore the design space characterized by physical parameters

Healthcare



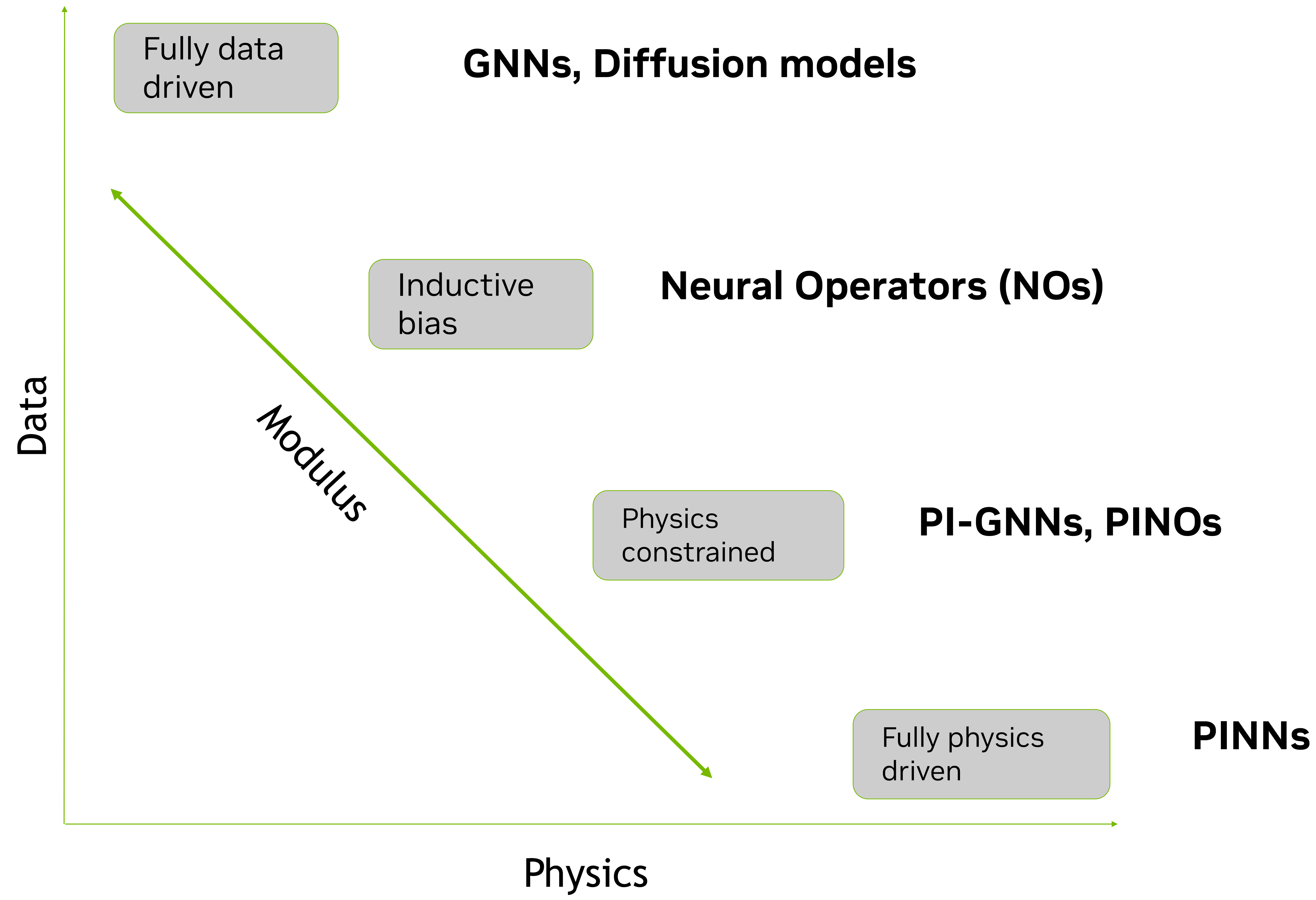


Physics ML surrogates for accelerating traditional simulation-based design workflows

Open-Source AI Toolkit for Physics-based ML

SOTA architectures for ML training

- Bringing novel AI architectures that have demonstrated success for engineering and science problems
- Using case studies as reference starting points



Modulus Model Zoo - Diverse Physics-ML approaches:

- fully Physics driven AI models
- fully data driven AI models
- hybrid (data + Physics) AI models

Neural Operators:

- Fourier Neural Operator family (FNO, AFNO, PINO)
- DeepONet
- Transformer Neural Operator

GNNs:

- GraphCast
- MeshGraphNet ..

Diffusion Models:

- DDPM++
- NCSN++
- ADM ..

Physics informed Neural Networks (PINNs):

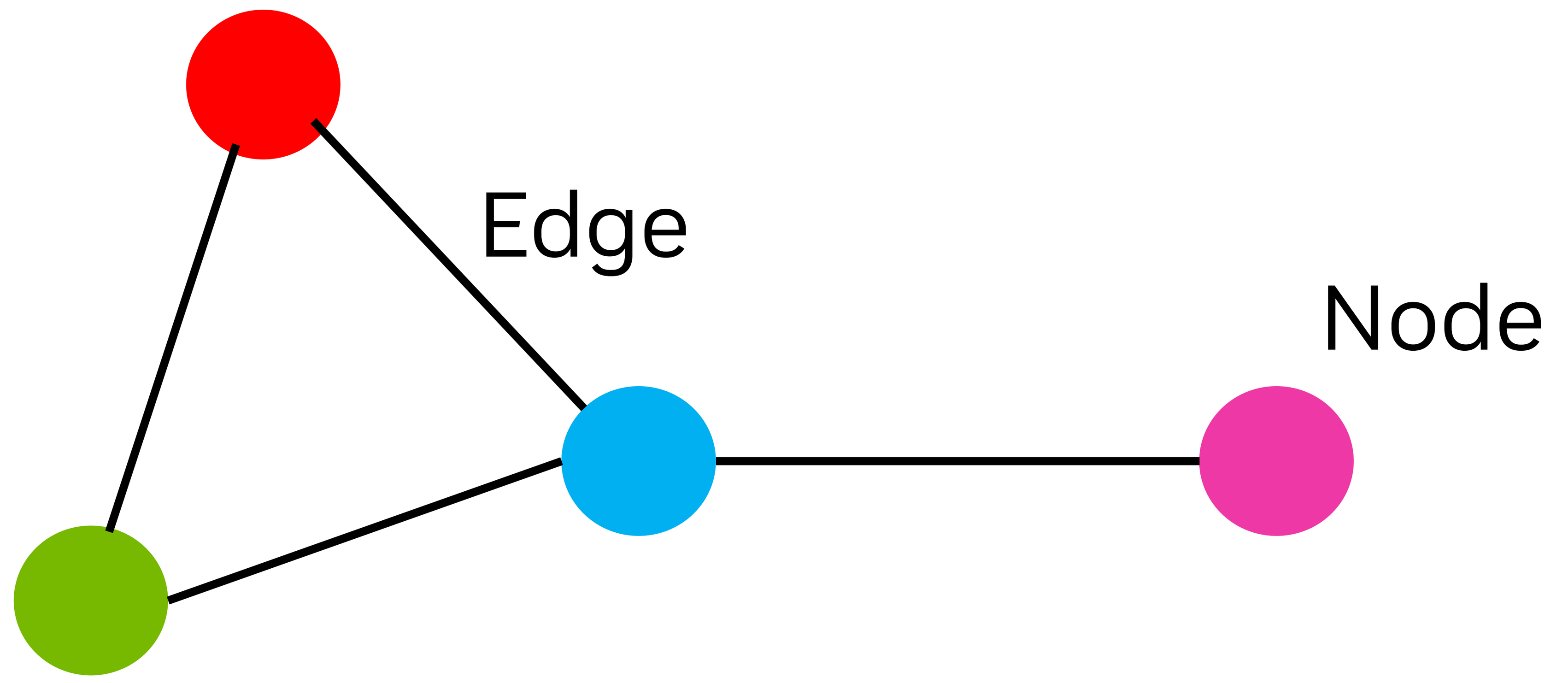
- Fourier Feature Network
- Spatial-temporal Fourier Feature Networks
- Super Resolution Net …

What are Graph Neural Networks (GNNs) ?

Node, Edge and Global features

- GNN is a deep learning framework that operates on graph type objects
- Examples of graphs : social networks, molecular structure, communication network, traffic networks, citation networks, meshes etc.
- GNNs can be leverage the graph structure to perform three type of prediction tasks:

1) Node level : predicting unknown quantities for graph nodes
2) Edge level : predicting the existence of missing links b/w nodes
3) Graph or Global level : predicting unknowns for entire graph



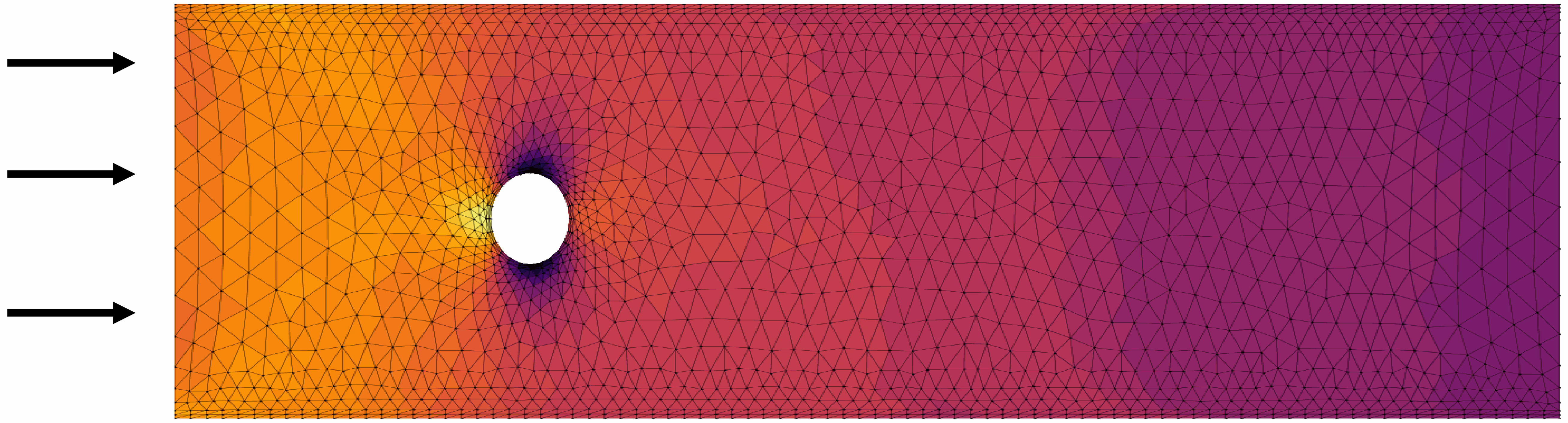
A Graph

Graph Neural networks for mesh-based simulation

Fluid Flow

Flow past cylinder

Wall

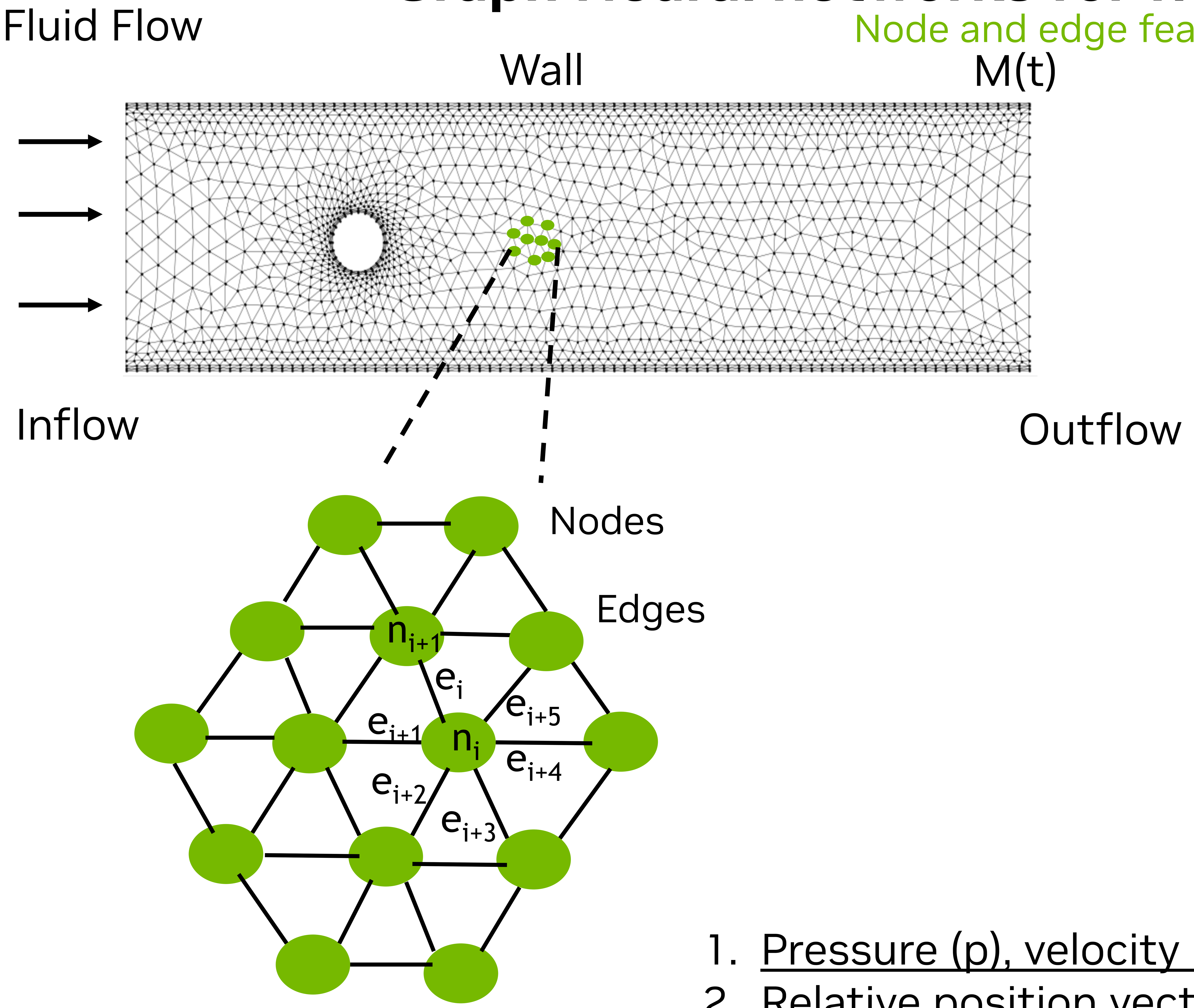


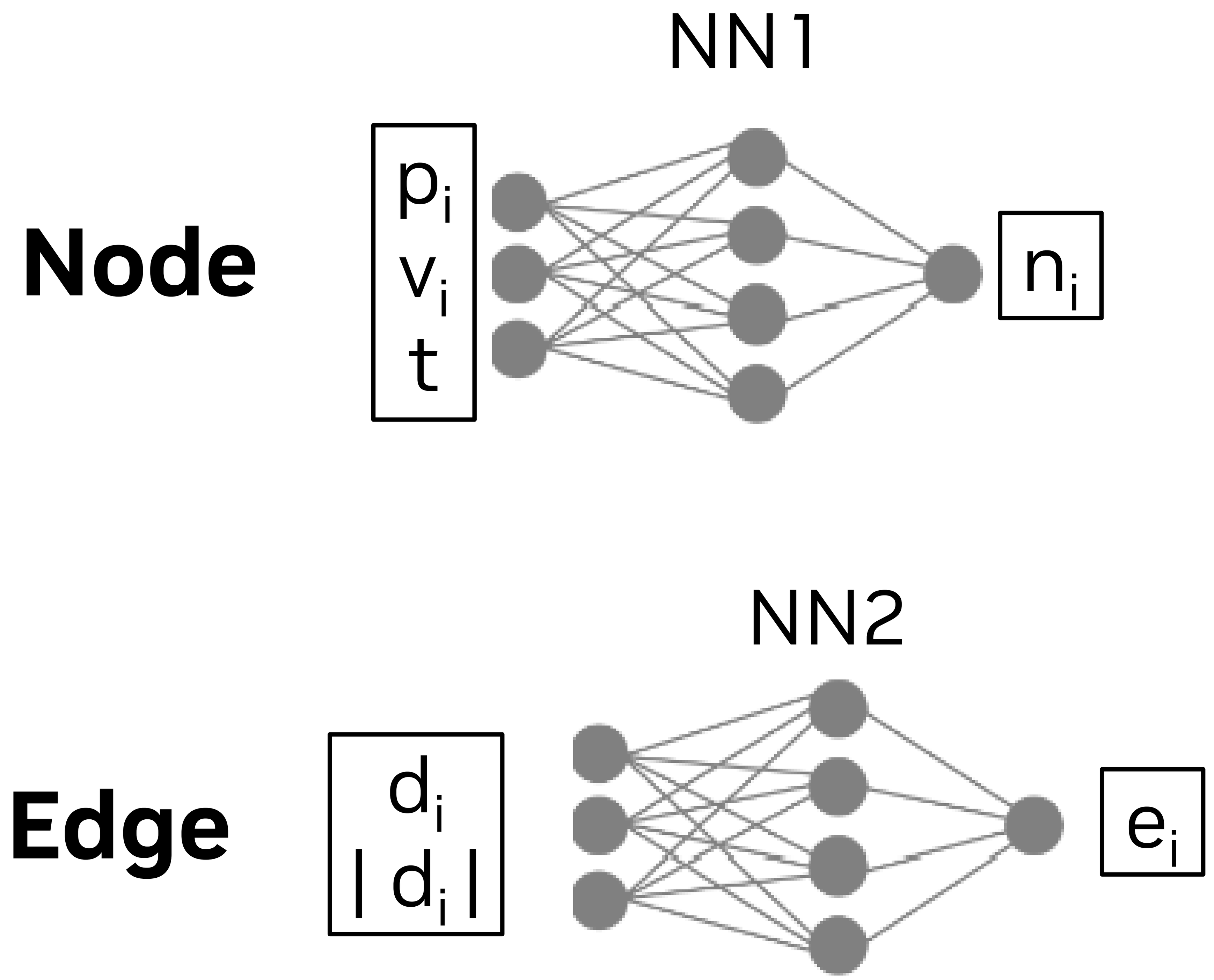
Inflow

Outflow

Graph Neural networks for flow past cylinder: Encoding

Node and edge feature encoding





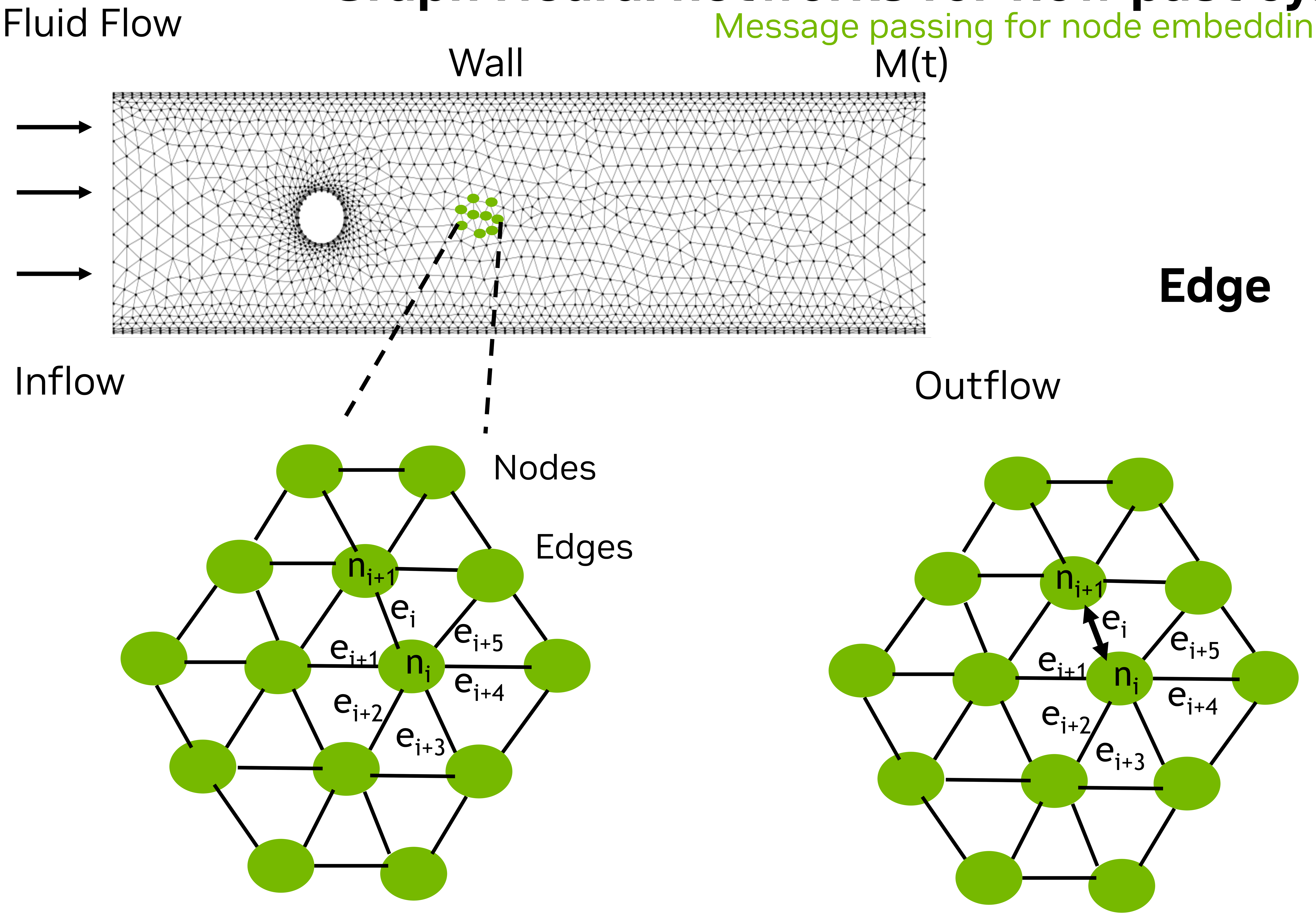
1. Pressure (p), velocity (v), node type (t) as input **node features.**
2. Relative position vector (d) and its norm (|d|) as input **edge features**

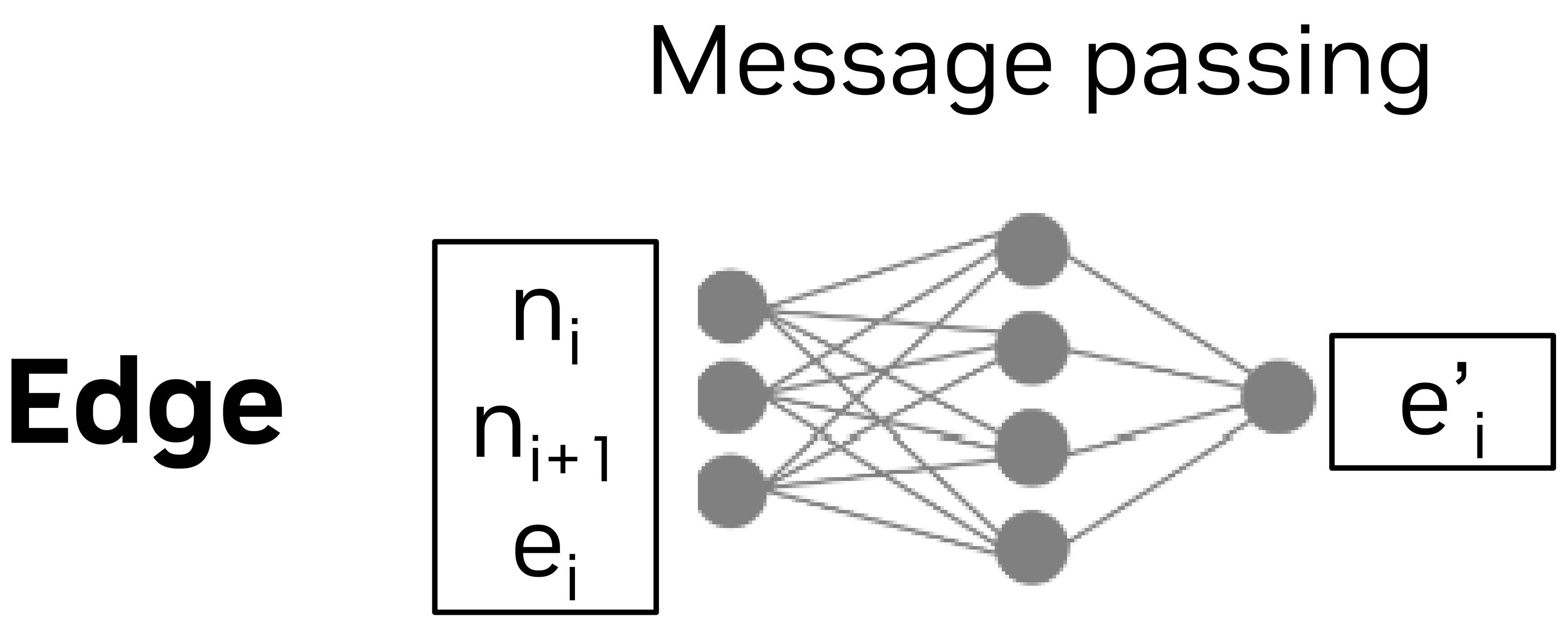
Graph Neural networks for flow past cylinder: Processing

Message passing for node embeddings

Graph Neural networks for flow past cylinder: Processing

Message passing for node embeddings

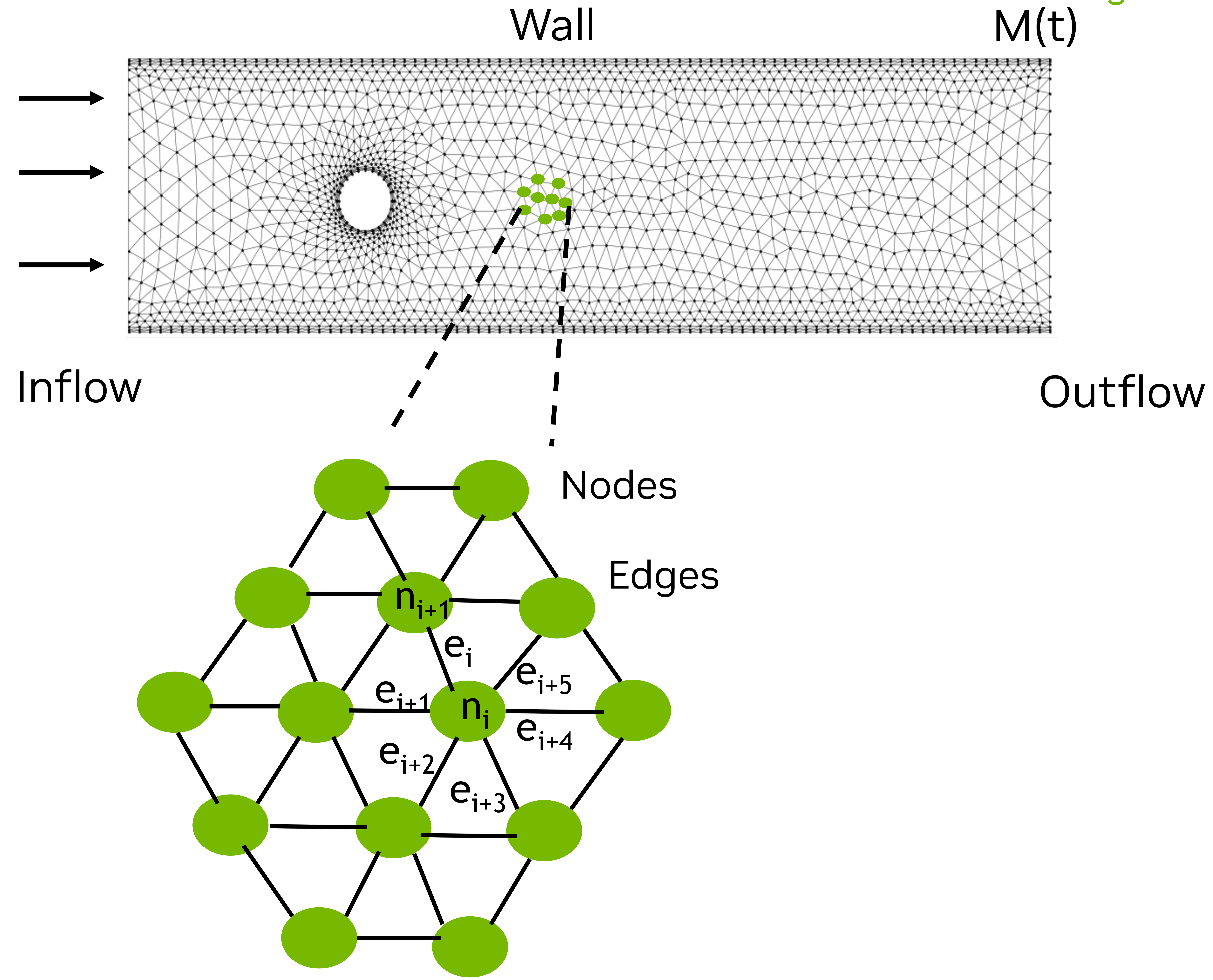


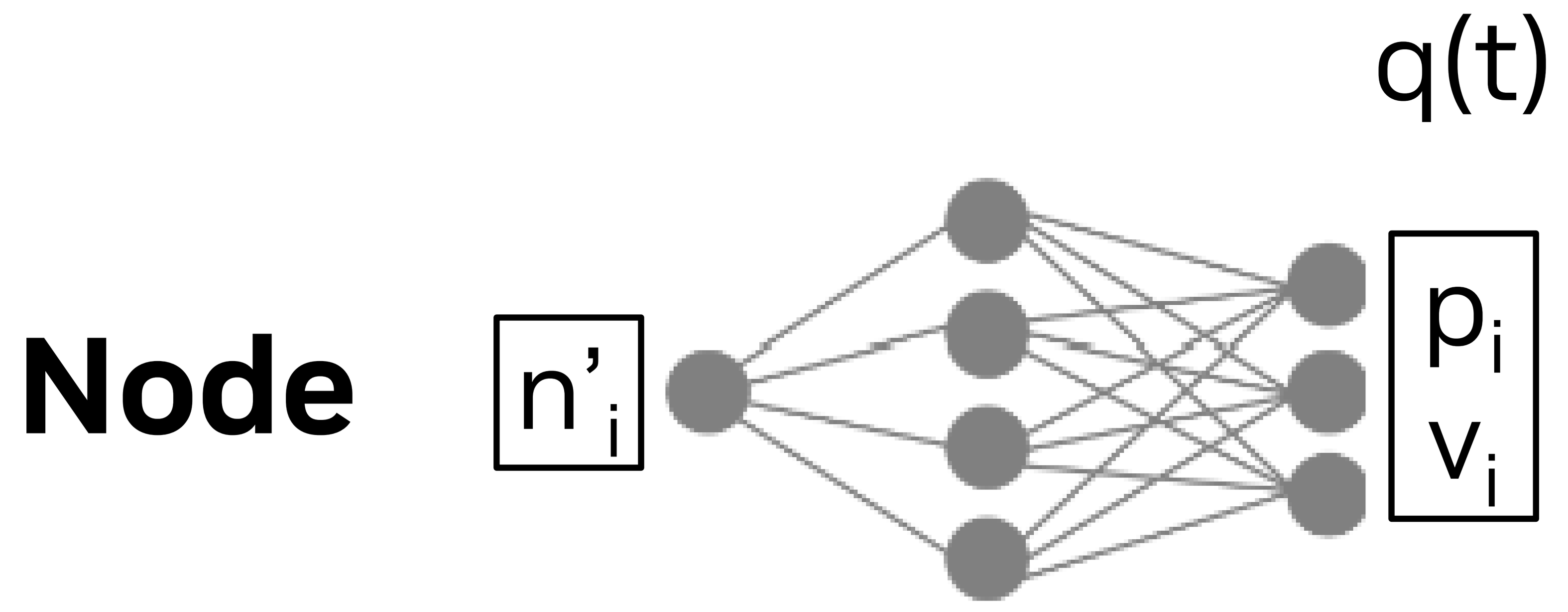


Graph Neural networks for flow past cylinder: Decoding

Node and edge feature encoding

Fluid Flow





Graph Neural networks for flow past cylinder

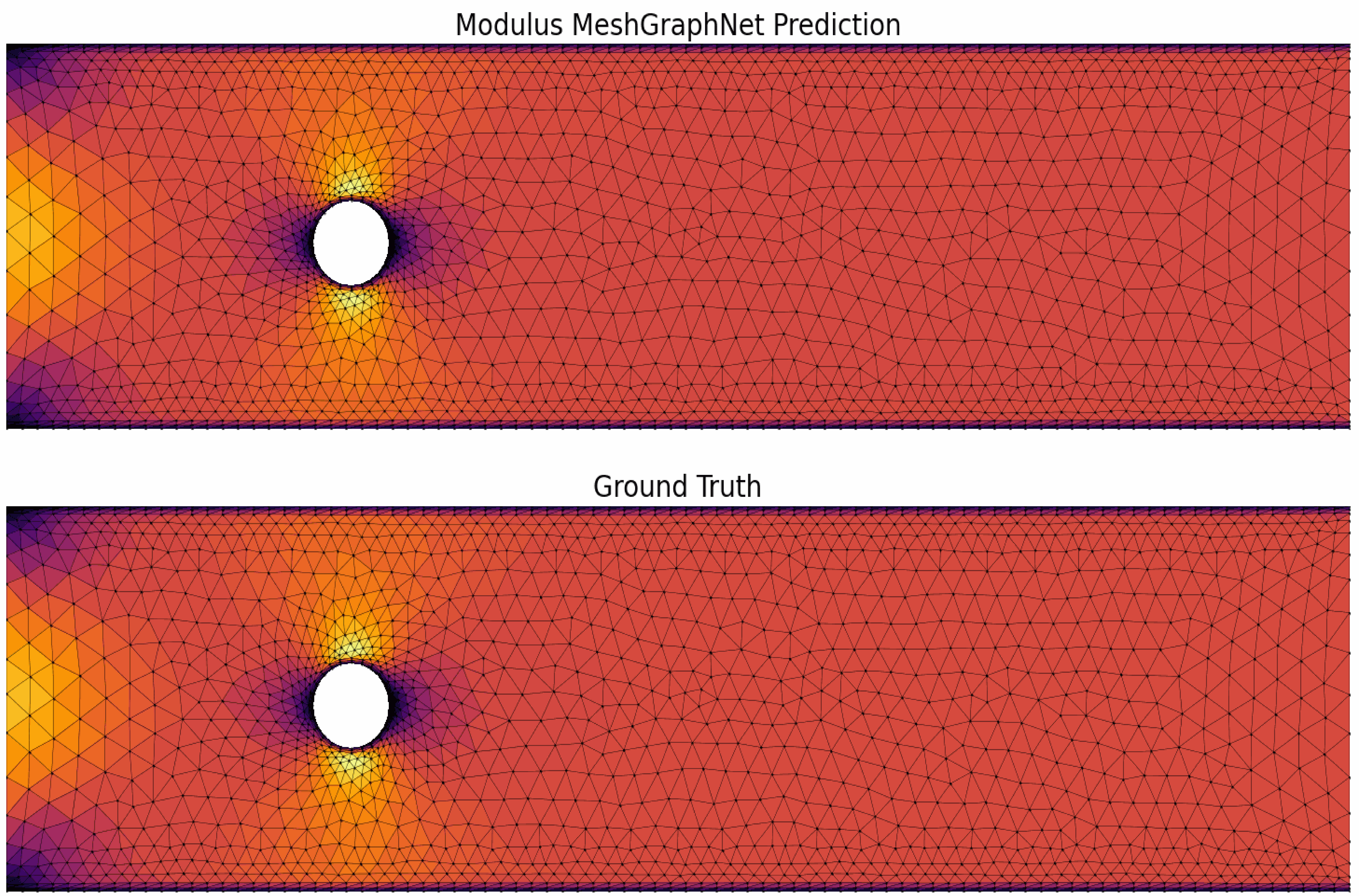
Step 1: **Encoding**: encode features as node and edge embeddings

Step 2: **Processing**: Update node and edge embeddings using message-passing

Step 3 **Decoding**: Generate updated feature from new edge and node embeddings

Graph Neural networks for flow past cylinder

- Why use Graph Neural Networks or Meshgraphnets
  - Can handle structured and unstructured grids, mesh deformities, discontinuities etc
  - Generalization over meshes, boundary conditions, material properties
  - Parameter sharing in GNNs helps to learn transient simulations better



National Climate Task Force Goals

Why it is important for NETL and NVIDIA ?

REDUCING U.S. GREENHOUSE GAS EMISSIONS

50-52%

BELOW 2005 LEVELS

IN

2030

REACHING

100%

CARBON POLLUTION-FREE ELECTRICITY

BY

2035

ACHIEVING A

NET-ZERO

EMISSIONS ECONOMY

BY

2050

DELIVERING

40%

OF THE BENEFITS FROM FEDERAL INVESTMENTS IN CLIMATE AND CLEAN ENERGY TO

DISADVANTAGED COMMUNITIES

Established by President Joe Biden to reduce emissions, increase resilience, advance environmental justice, and achieve true energy security

IBDP: Illinois Basin Decatur Project (IBDP)

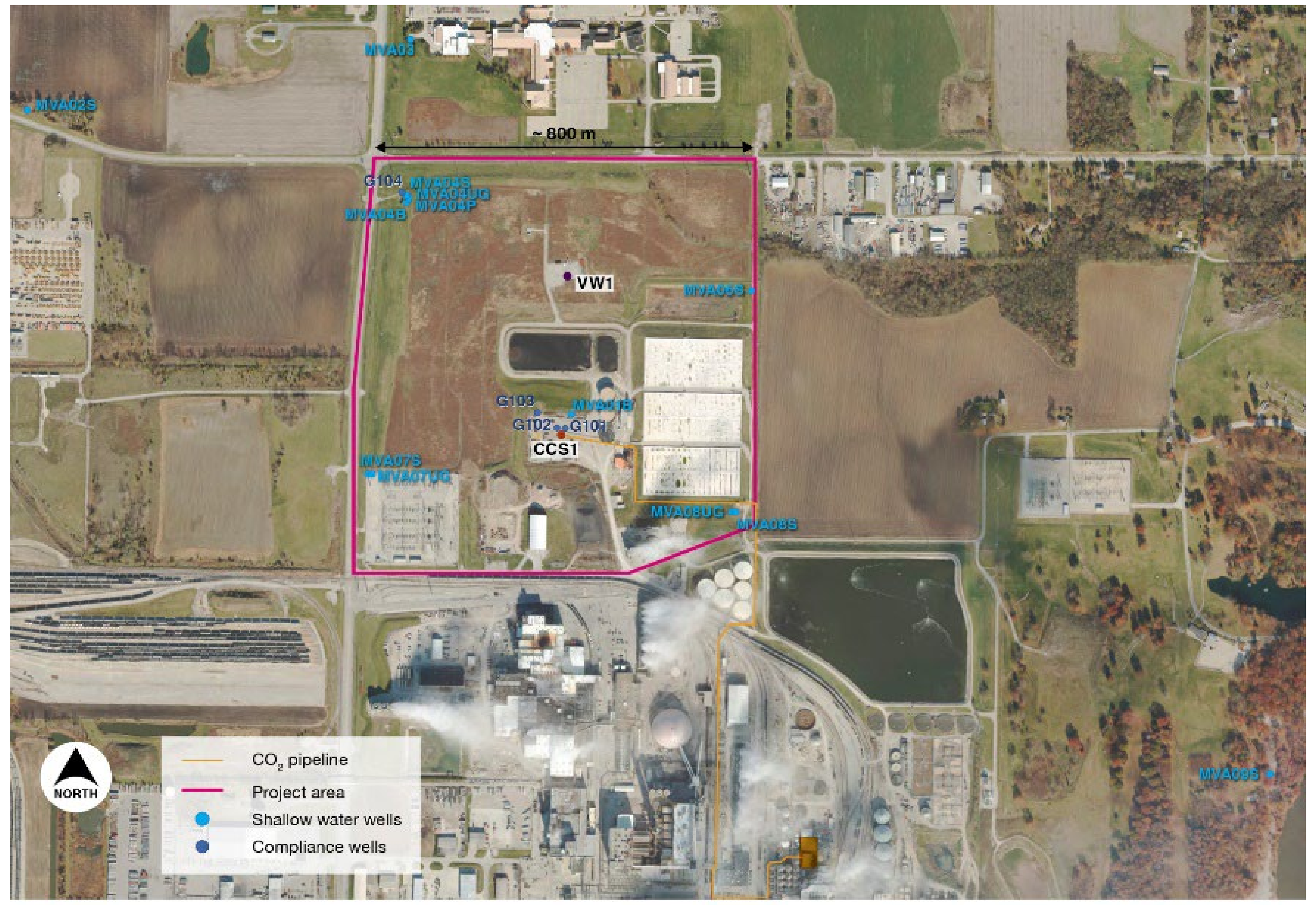
Demonstrated the feasibility of Carbon Capture and Storage as a Critical path

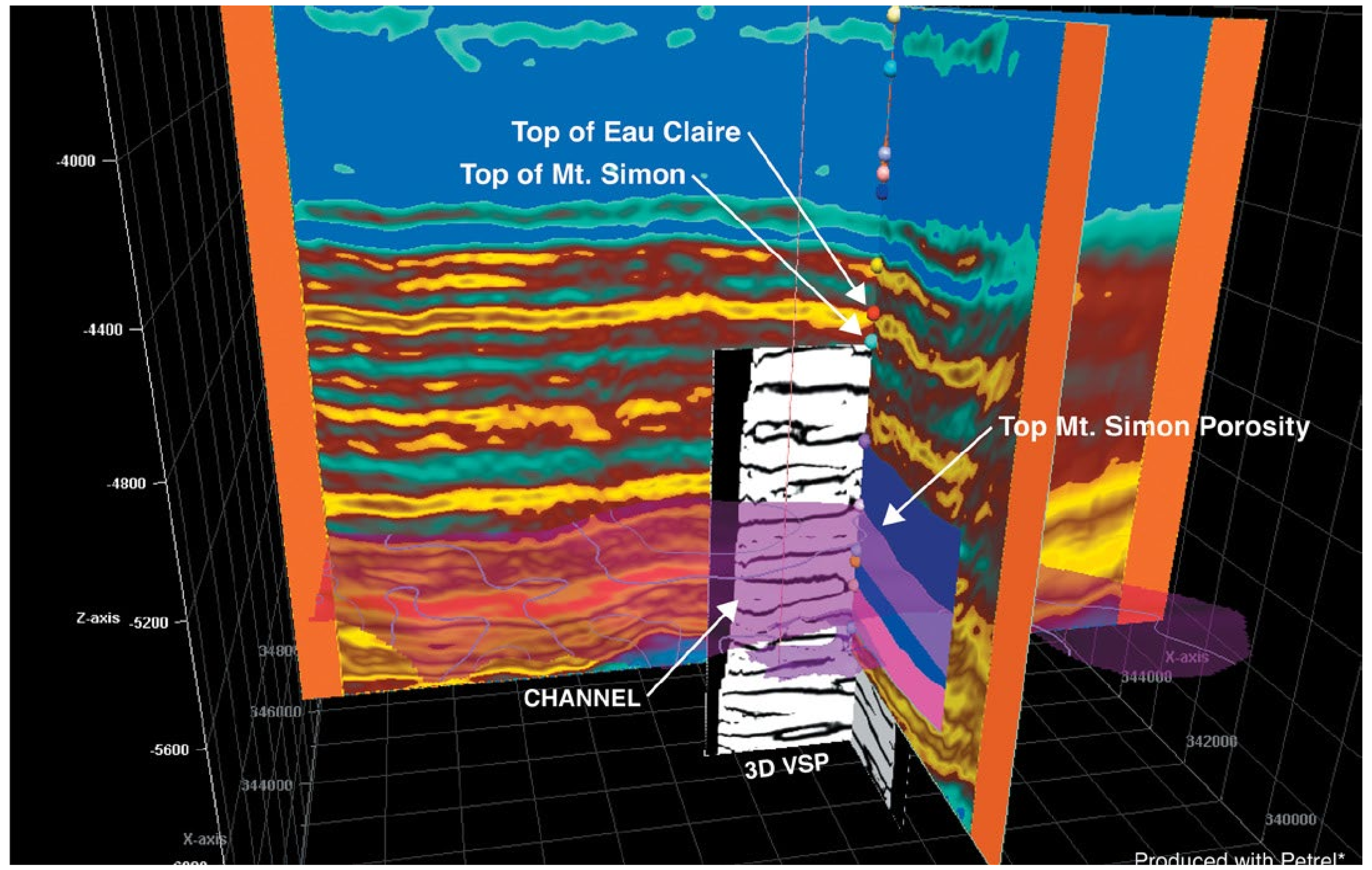
- Safely and effectively demonstrate the full carbon capture, utilization, and storage (CCUS) value chain in a saline reservoir

- Project stored CO2 from ADM's ethanol fermentation plant. Operations consist of a compression/dehydration facility, a delivery pipeline, one injection well, one deep observation/verification well, and a geophysical test well, all developed on the ADM-owned site

- 1 million metric tons of CO2 have been injected into an extensive reservoir with no difficulties.

- One of the first EPA Underground Injection Control Class VI permits (CO2 storage well).



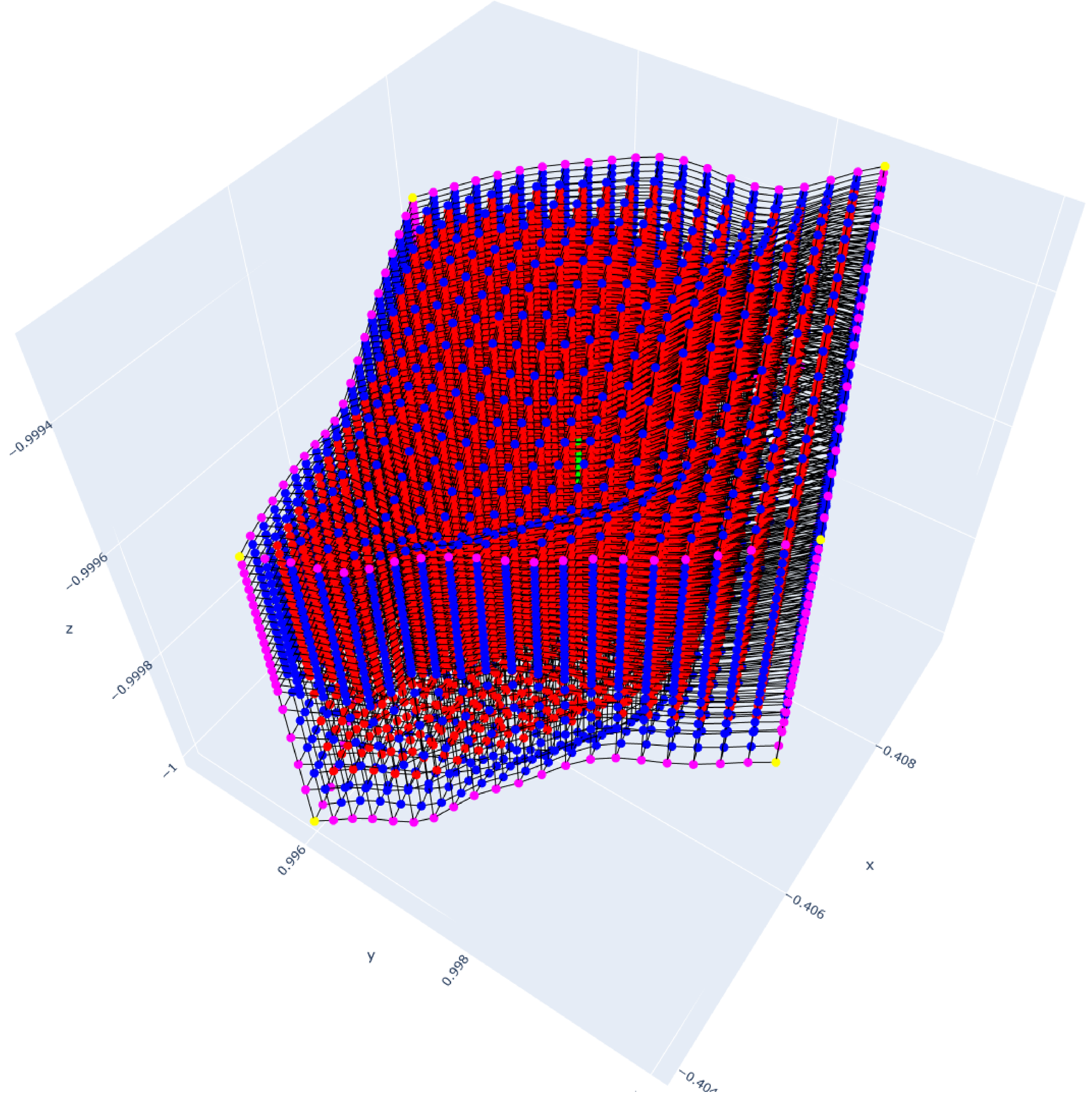


IBDP Dataset

Update blue node from initial state to the next state

Name	IBDP Model
Source	Phase 2 WP 2C.3
Inputs	Porosity, permeability, fault transmissivity modifiers, horizons (or formation indexes) @ 1M tons / 30-year rate
Outputs	Pressure, Saturation
Injection Wells	1
Grid Size	9.7 mile x 9.3 mile
Timestep	3 years injection, 1 year post-injection
Samples	100

IBDP Grid



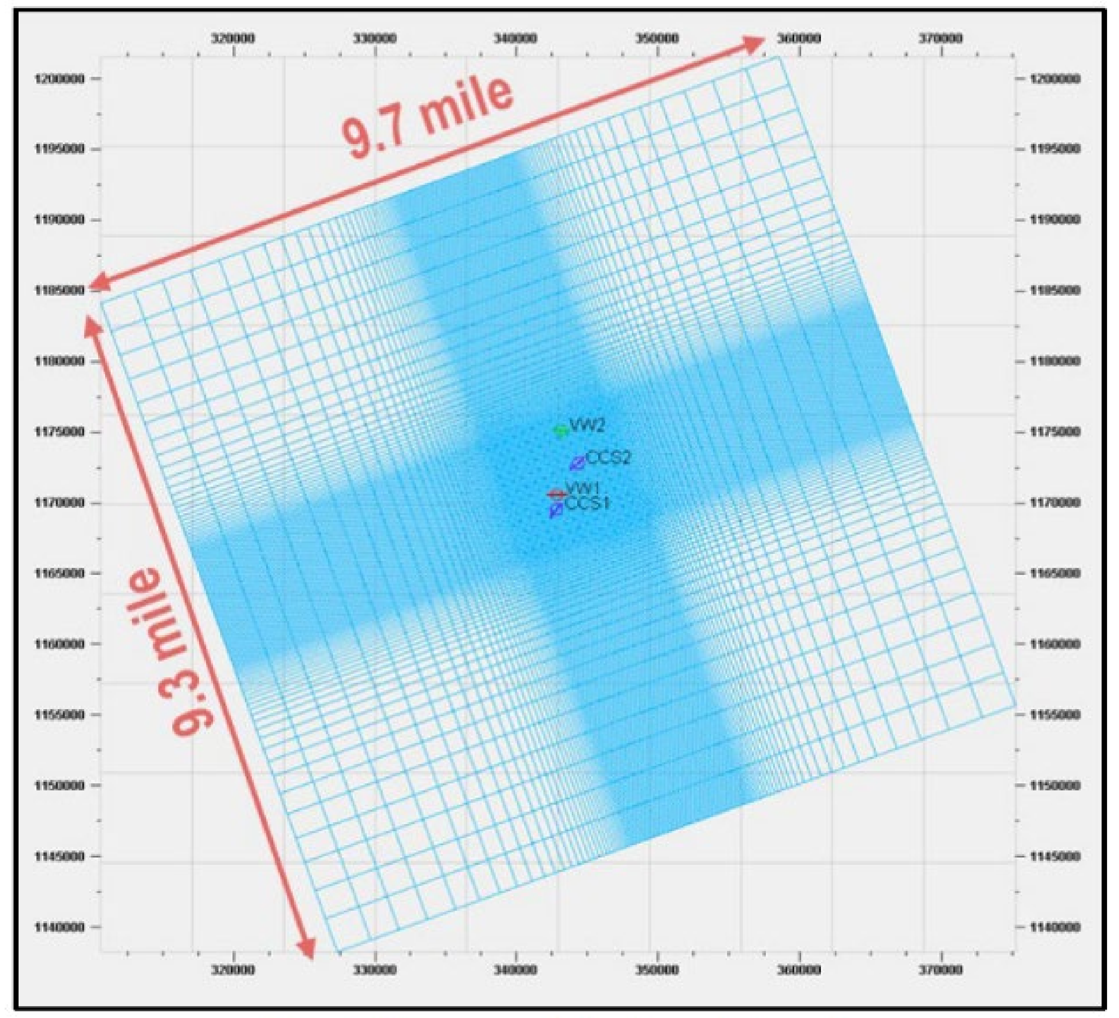
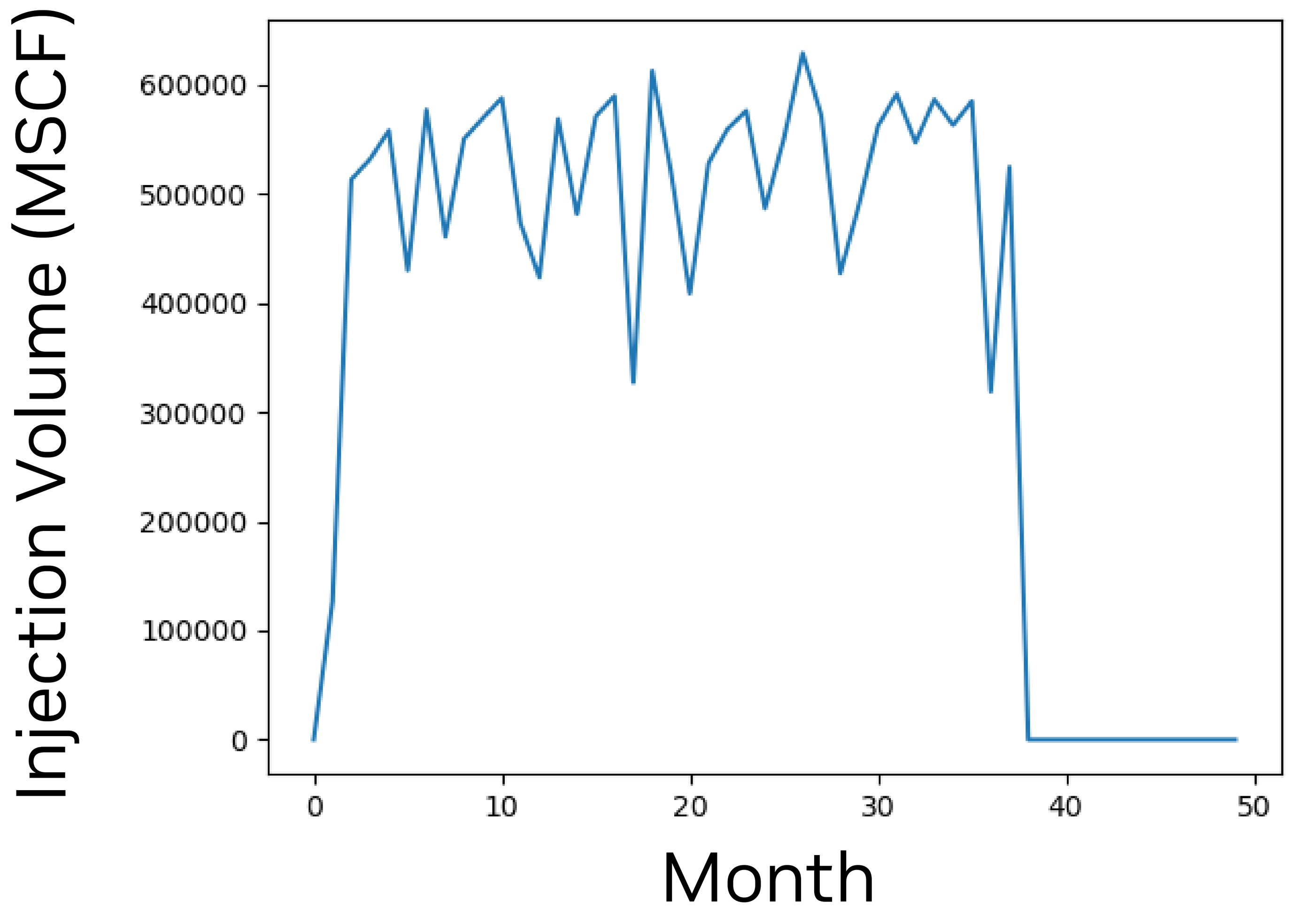
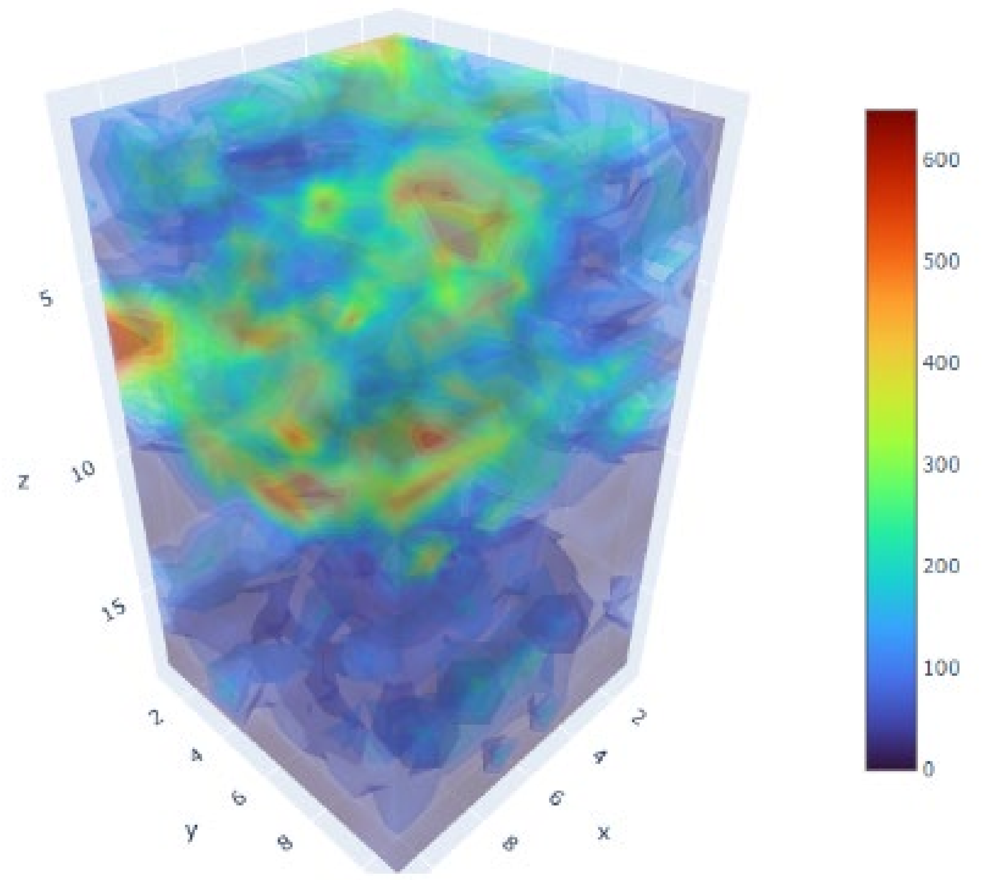


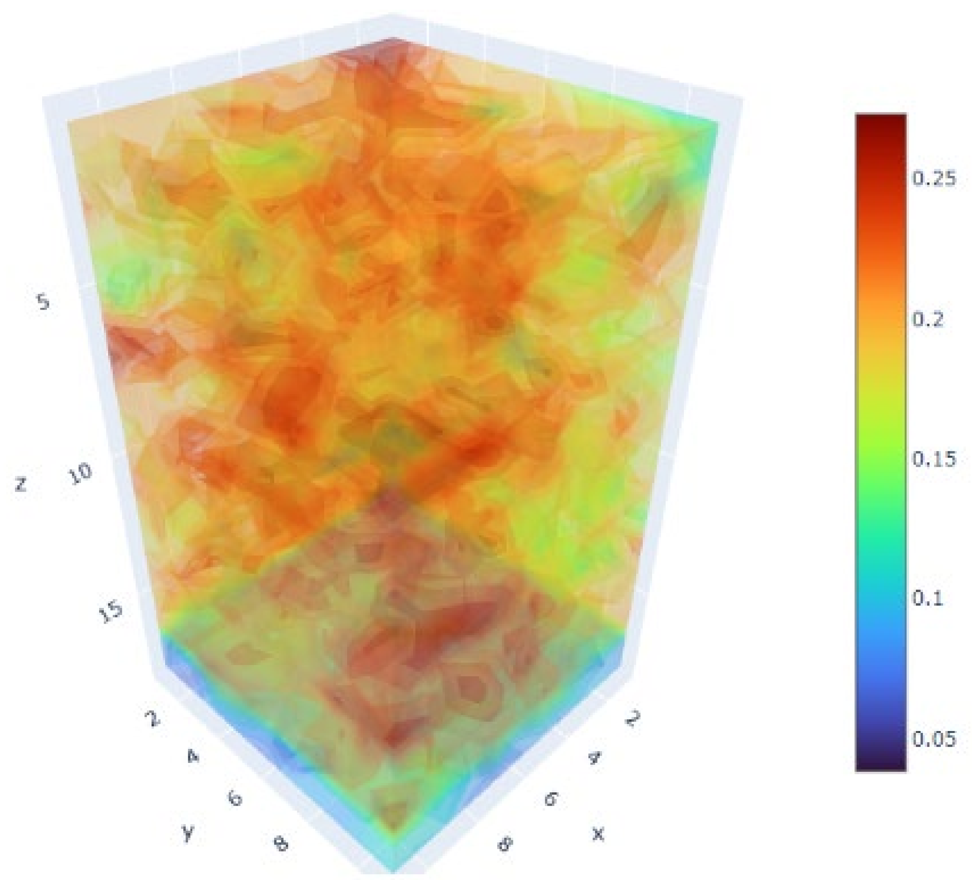
Figure 67. Dynamic model domain and tartan grid.



Avg. Permeability



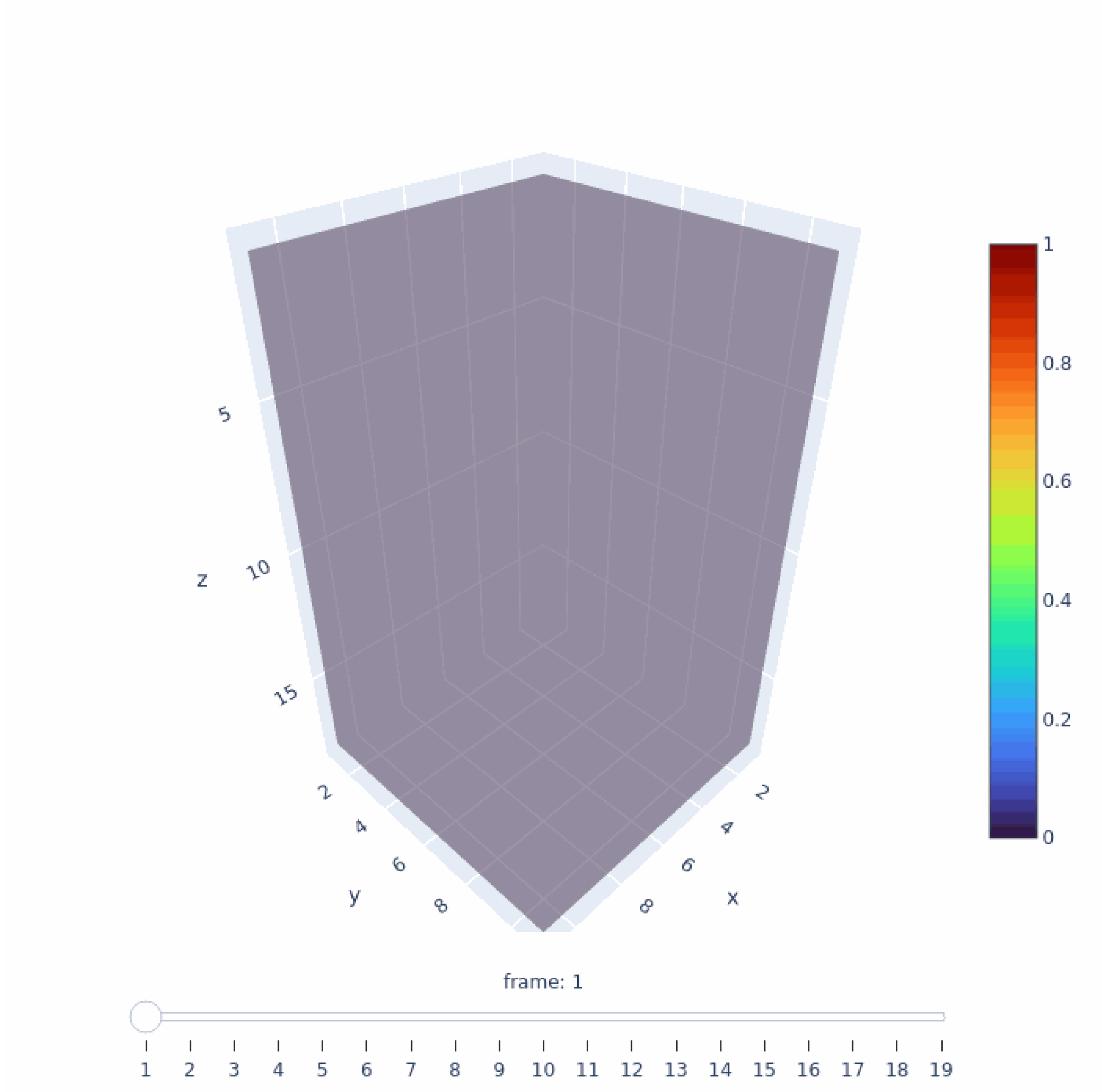
Avg. Porosity



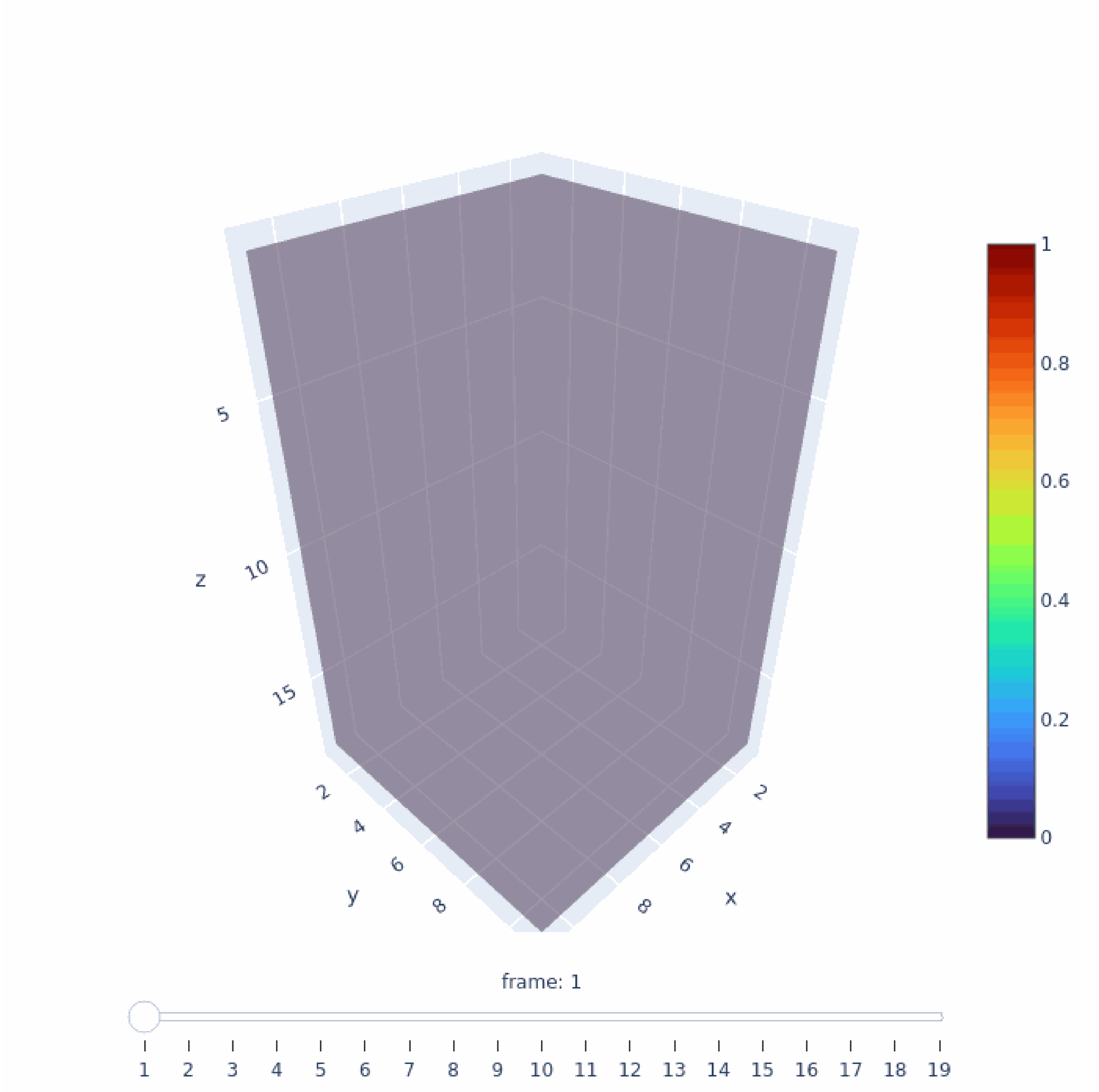
Saturation Prediction (1-36 months)

Trained on 12 months dataset

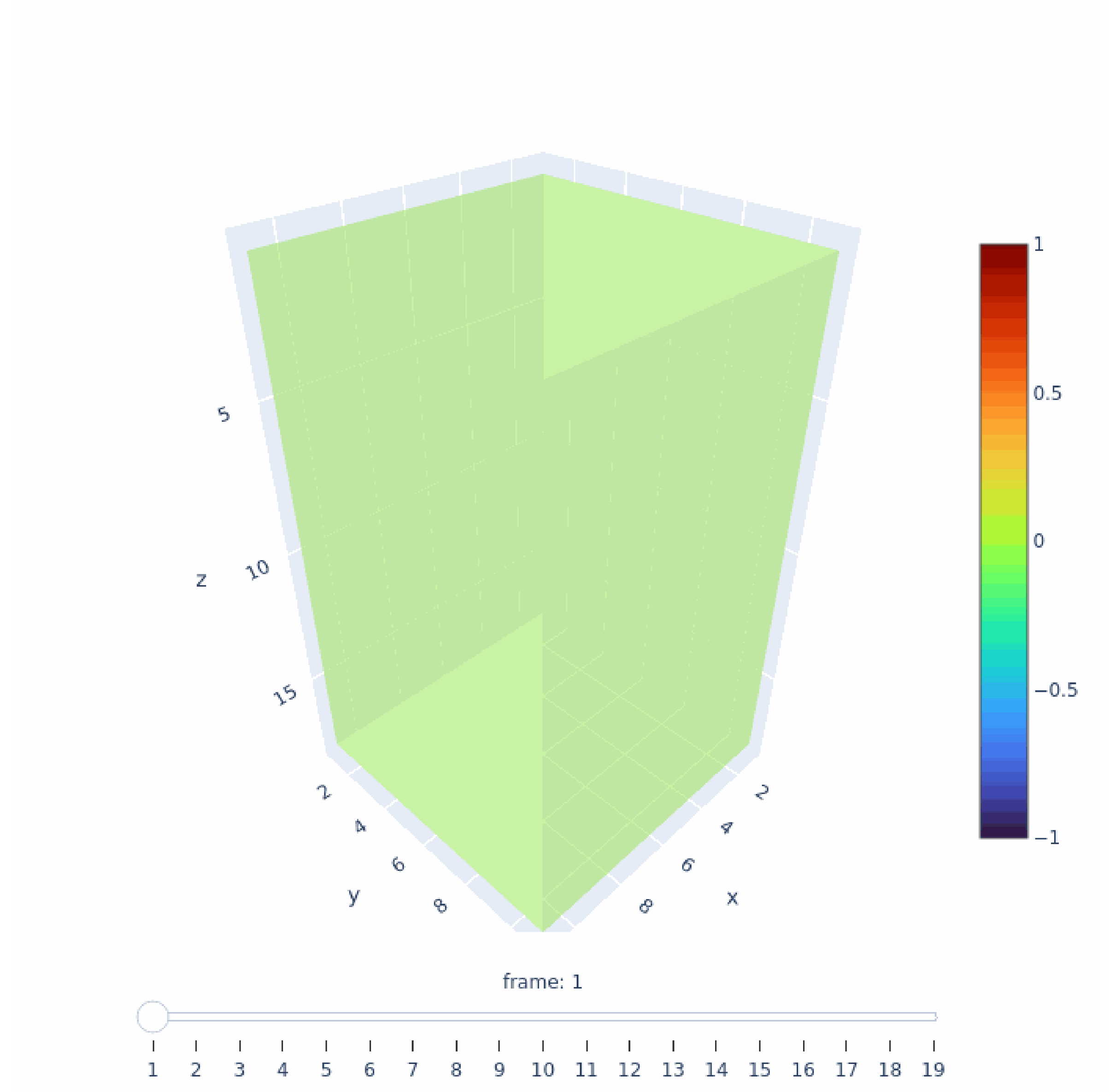
Ground Truth



Prediction



Difference

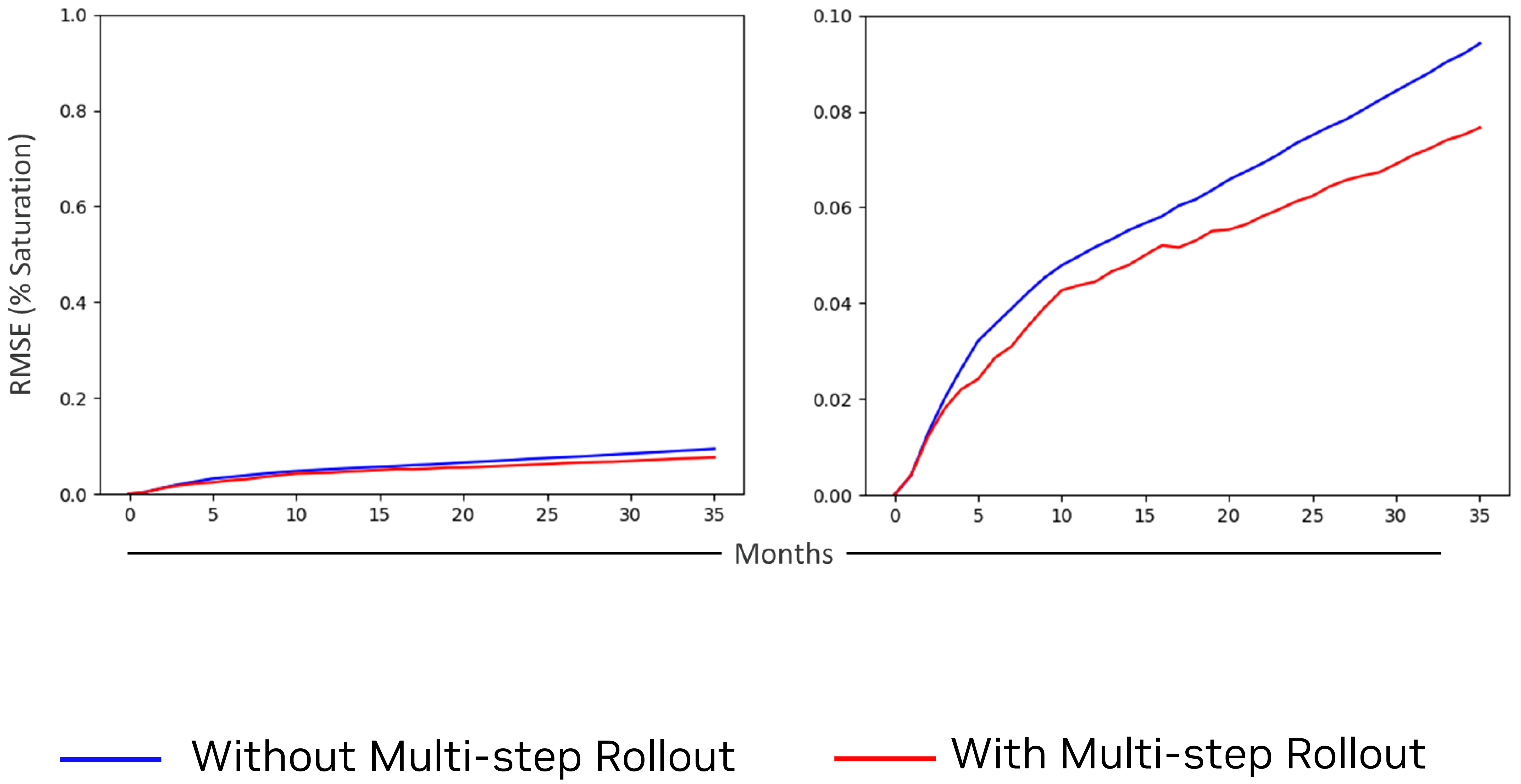


Saturation RMSE

Trained on 12 months dataset

- Predicting multiple steps performs slightly better than predicting single step in GNN with 93% accuracy

- More advanced models: **Graph Transformer** are giving much better results with **98% accuracy**



Conclusion

- GNNs can learn complex physical system interactions **such as in CCS simulations**

- GNNs offer generalization over different meshes, boundary conditions, material properties, unstructured data, mesh discontinuities etc.

- The results from the latest model will be shared after getting approval from DOE/NETL **at GTC 2025** or other relevant conferences