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Presentation >> Final | 13 Sept 2024

Rapid modelling of ATES using ML

MSc Independent Research Project (IRP 2024)

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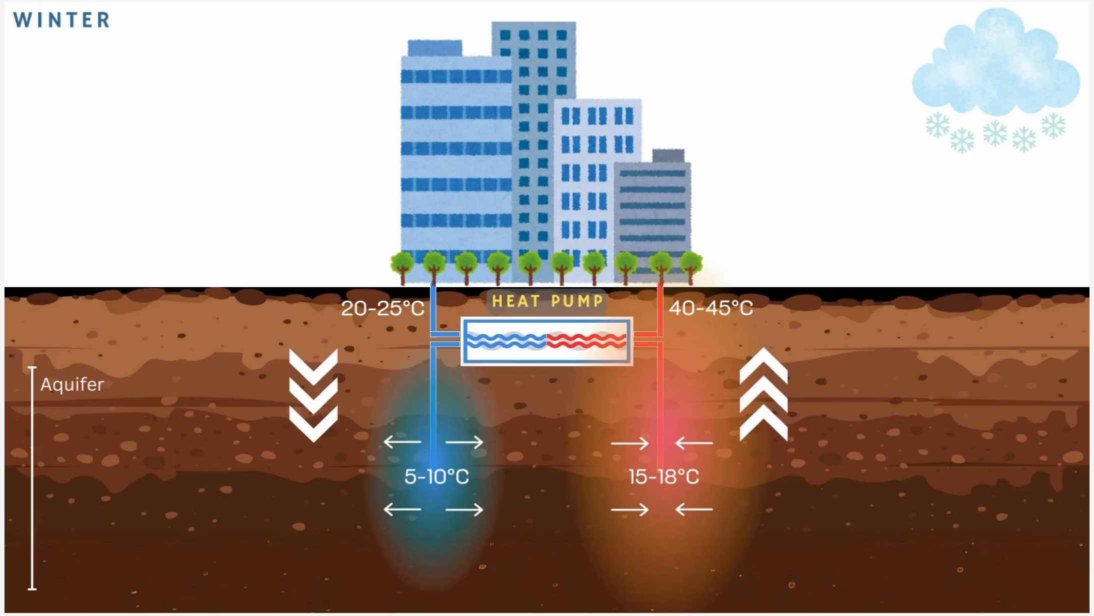
Rapid modelling of ATES using ML

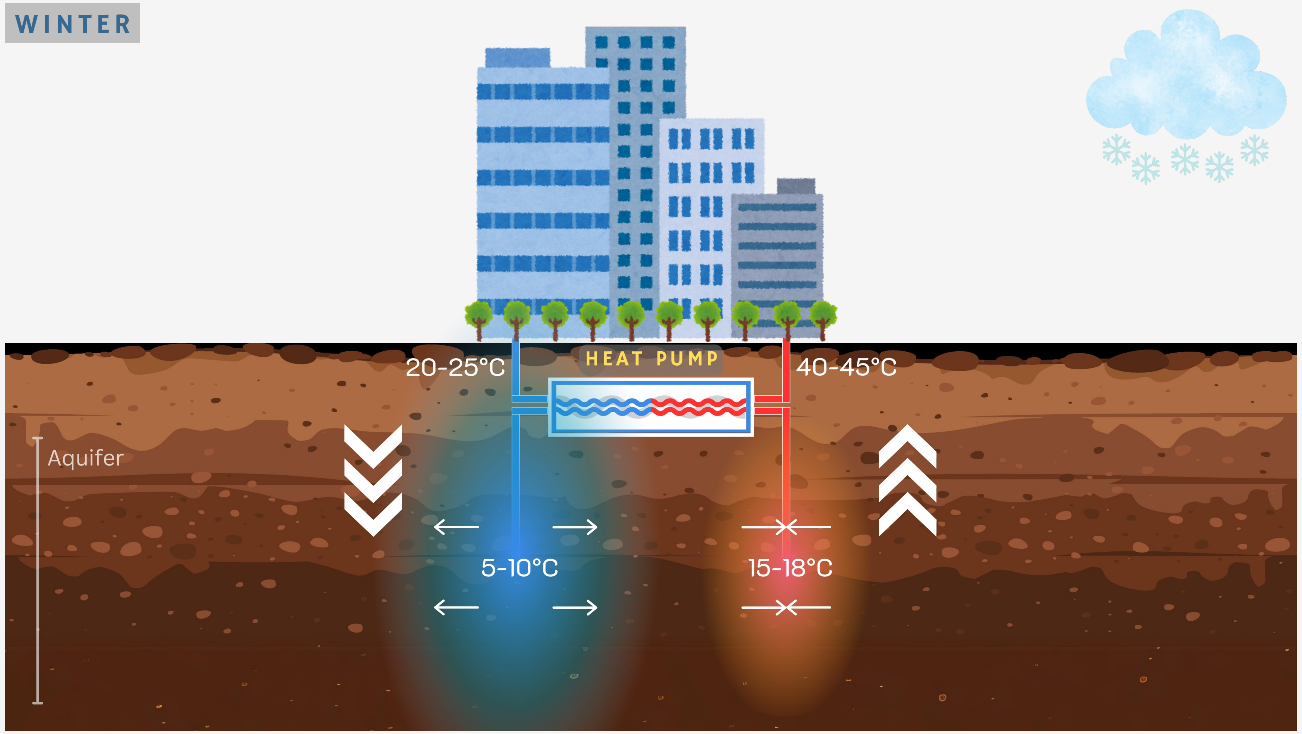
Aquifer Thermal Energy Storage (ATES)

provides a low carbon technology solution to regional heating and cooling at the heart of energy transition.



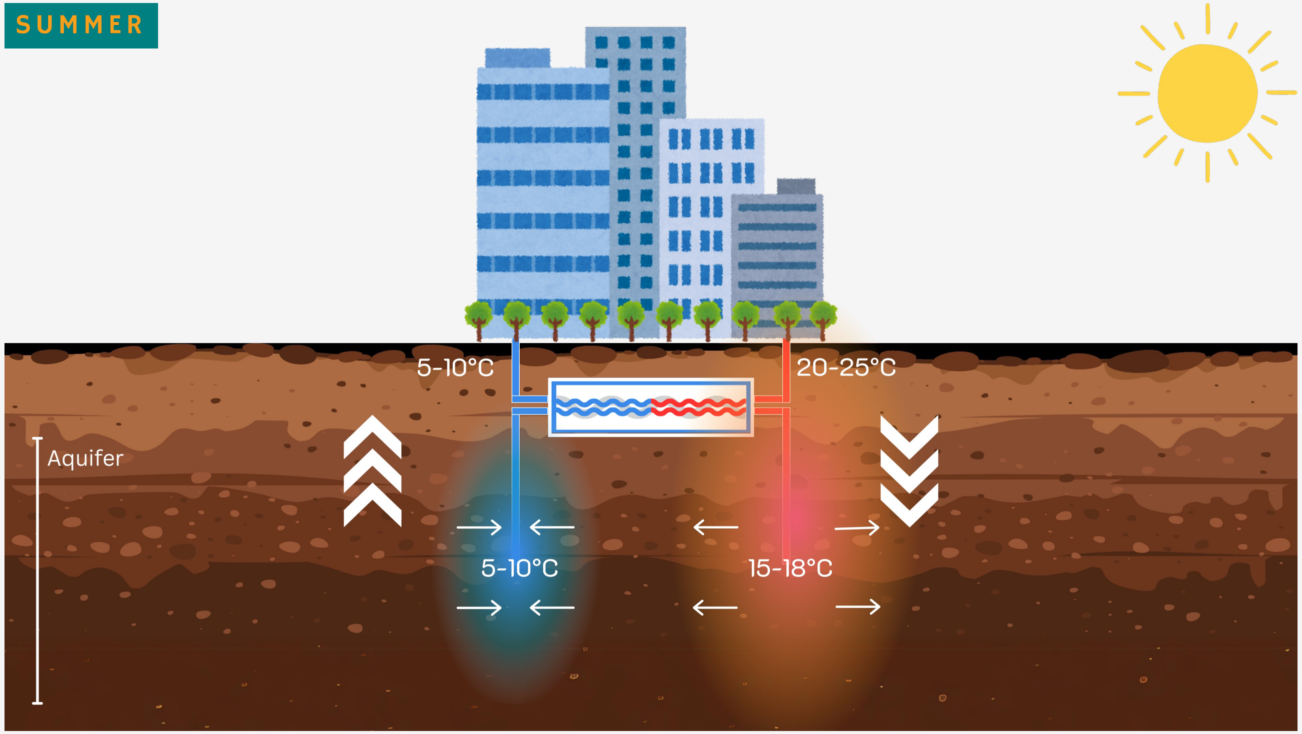
Capture and store the waste heat / cool over the season and extract for heating / cooling in the next season.

Aquifer Thermal Energy Storage (ATES)



- Capture and store waste cool
- Produce stored heat from underground reservoir to provide heating via heat pump

Aquifer Thermal Energy Storage (ATES)



- Capture and store waste heat
- Produce stored cool from underground reservoir to provide cooling

Project introduction

IC-FERST

Imperial College Finite Element Reservoir Simulator

- Numerical simulation of multiphase flow and transport in complex geological reservoirs.

Input → **IC - FESRT** → **Output**

Input:

- x 1 | .msh | Mesh
- x 1 | .mpml | Text file
- x 2 | .bdf | Well 1 &2

Output:

- x 240 | .vtu | unstructured mesh data
- x 1 | .csv | outflux

IC-FERST

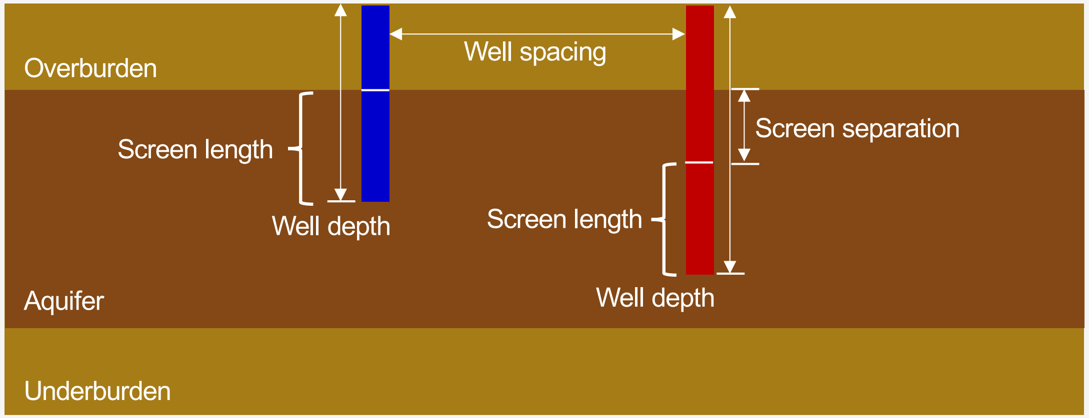
- Heat plume expand and contract alternately across seasons
- Summer : inject waste heat to warm well

>> heat plume expand in warm well

- Adaptive Meshing on irregular grid

Scenarios in simulations

Reservoir Configurations (Mesh)



Key variables across scenarios

- Well spacing
- Well depth (Well 1 & 2)
- Screen Length
- Screen separation
- Vertical permeability (Kz)

840 scenarios in dataset

Rapid modelling of ATES using ML

Problem Description

Numerical simulations : Computational expensive

- Involve the solving of coupled PDEs
- High resolution spatial mesh and small timesteps >> ensure accuracy

Project Purpose

ML approach : Retain accuracy & spatial resolution while increasing efficiency

- Pure data-driven (no pre-informed physics)
- scalability by hardware acceleration (GPU parallelization)

IC - FESRT ❯❯❯❯❯ ***FAST PROXY*** ❯❯❯❯❯ **ML models**

> 24 hours*

< 30 minutes

*Without mesh adaptivity

Significance of work

- Scalable acceleration on numerical simulations
- Transferable approach to create a fast proxy for other fields
- Energy Transition : Rapid modelling of ATES for instant insight

IC - FESRT → *FAST PROXY* → ML models

> 24 hours*

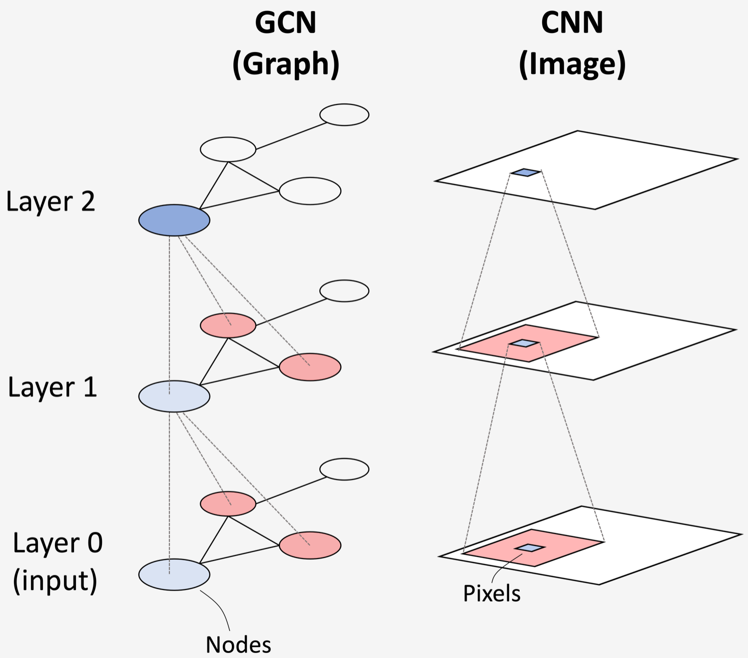
< 30 minutes

Objectives

Input → ML models → Output

- Captures spatial-temporal features in unstructured graph data
- Captures the physics and replicate the simulation results

GNN vs CNN

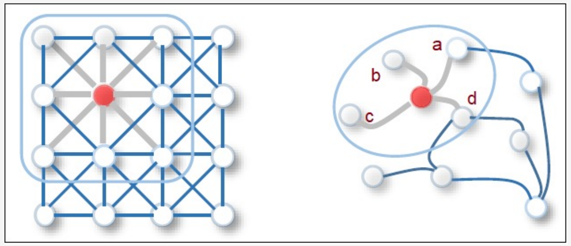


Graph Neural Networks (GNNs) ✓

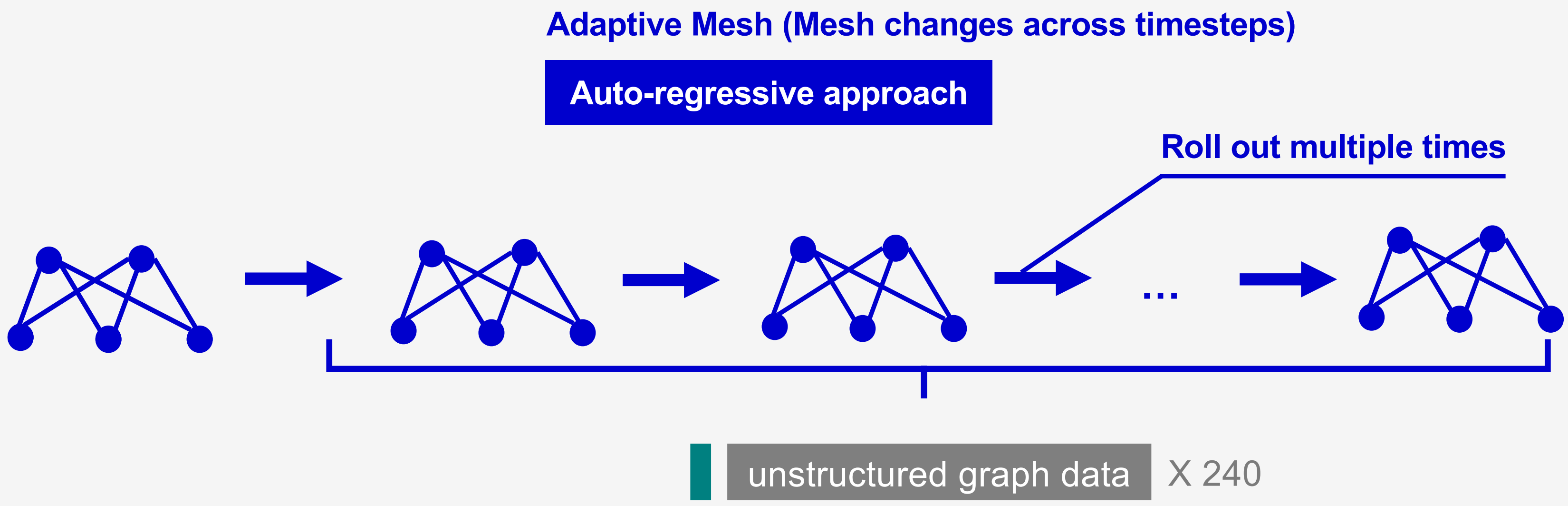
- Work well with **irregular mesh**
- Permutation invariance
- Proven to work well even with faulted Reservoir

Convolution Neural Networks (CNNs)

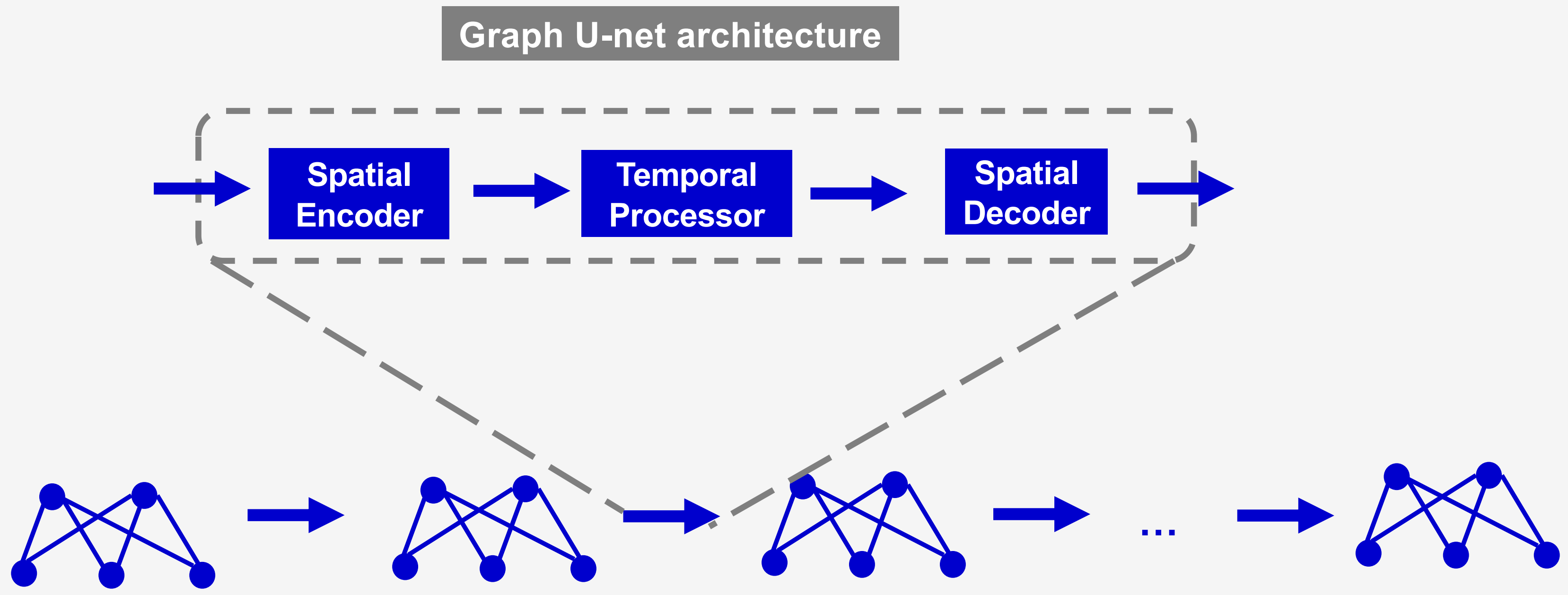
- Regular grid ONLY
- Permutation equivariance



Approach


Adaptive Mesh (Mesh changes across timesteps)
Auto-regressive approach
Roll out multiple times
...
unstructured graph data
X 240

Approach


Graph U-net architecture
Spatial Encoder
Temporal Processor
Spatial Decoder
...

Pre-processing

Check and load pre-processed data

Read csv, vtu and bdf

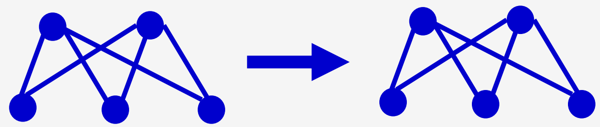
Pre-processing into PyG

- Injection strategy (Sequence Generation)
- Graph Construction (From vtu, bdf and csv)
- Mesh Projection (Forward / Backward)

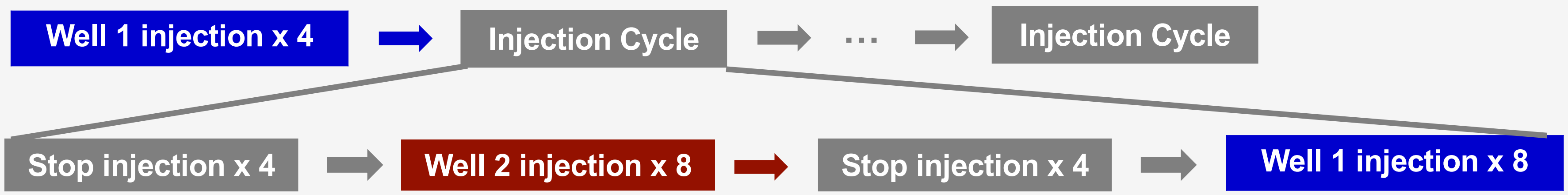
Standardization (temperature / pressure)

Save pre-processed data (.pt)

Dataset >> Dataloader



Pre-processing



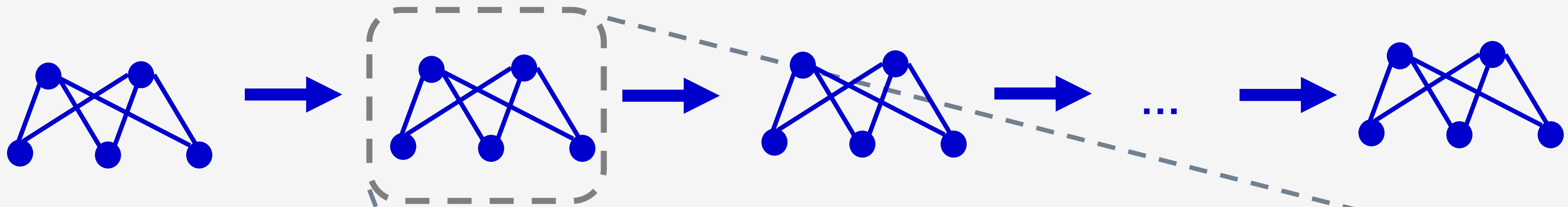
Injection strategy (Sequence Generation)

- ❖ Initial well 1 injection followed by cycles of alternate injection phase and stationary phase
- ❖ Encoded into an integer list of injection sequence

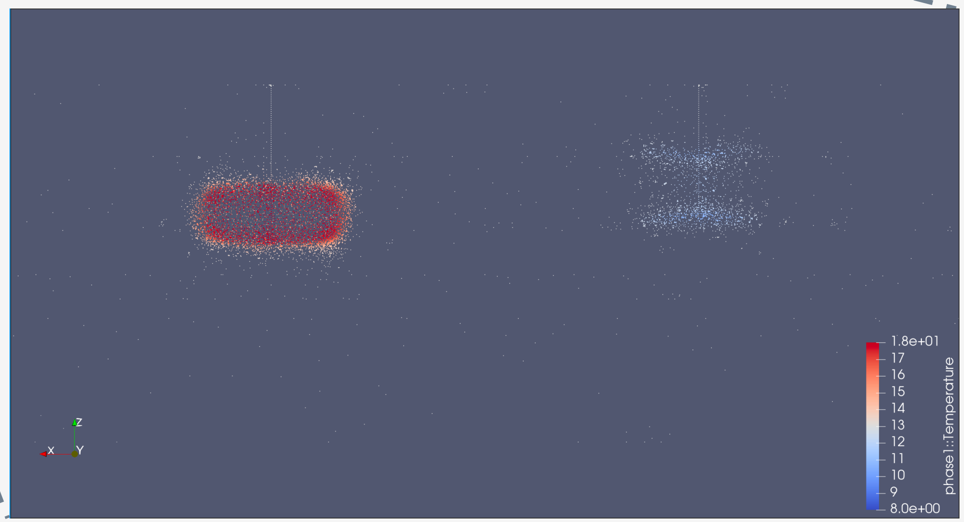
>> node feature : (1) Current injection phase (2) Next injection phase

Pre-processing

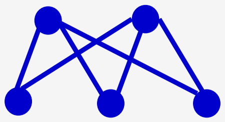
Graph Construction
(From vtu, bdf and csv)



Node Feature (Input state)
Phase 1 Temperature
Phase 1 Pressure
X-coordinates
Y-coordinates
Z-coordinates
Vertical Permeability (Kz)
Current injection phase
Next injection phase

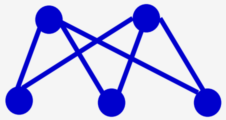


Data availability



Input

Auto-regressive approach



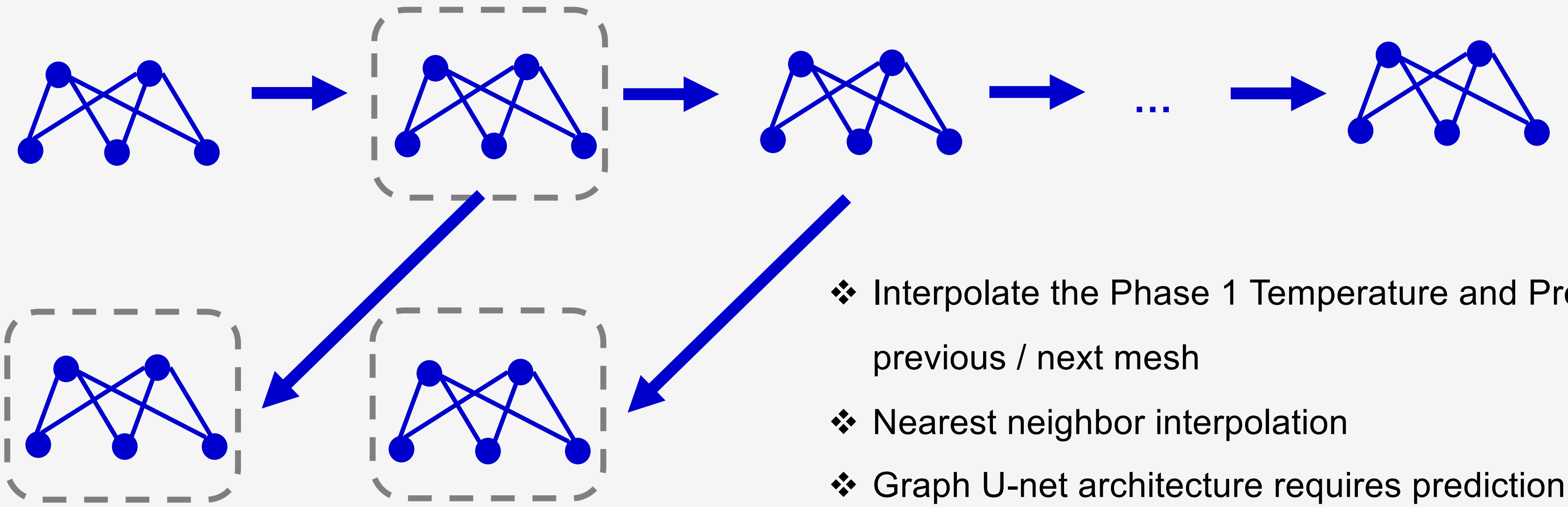
Output

Node Feature
Phase 1 Temperature
Phase 1 Pressure
Vertical Permeability (Kz)
Current injection phase
Next injection phase

Node Feature
Phase 1 Temperature
Phase 1 Pressure

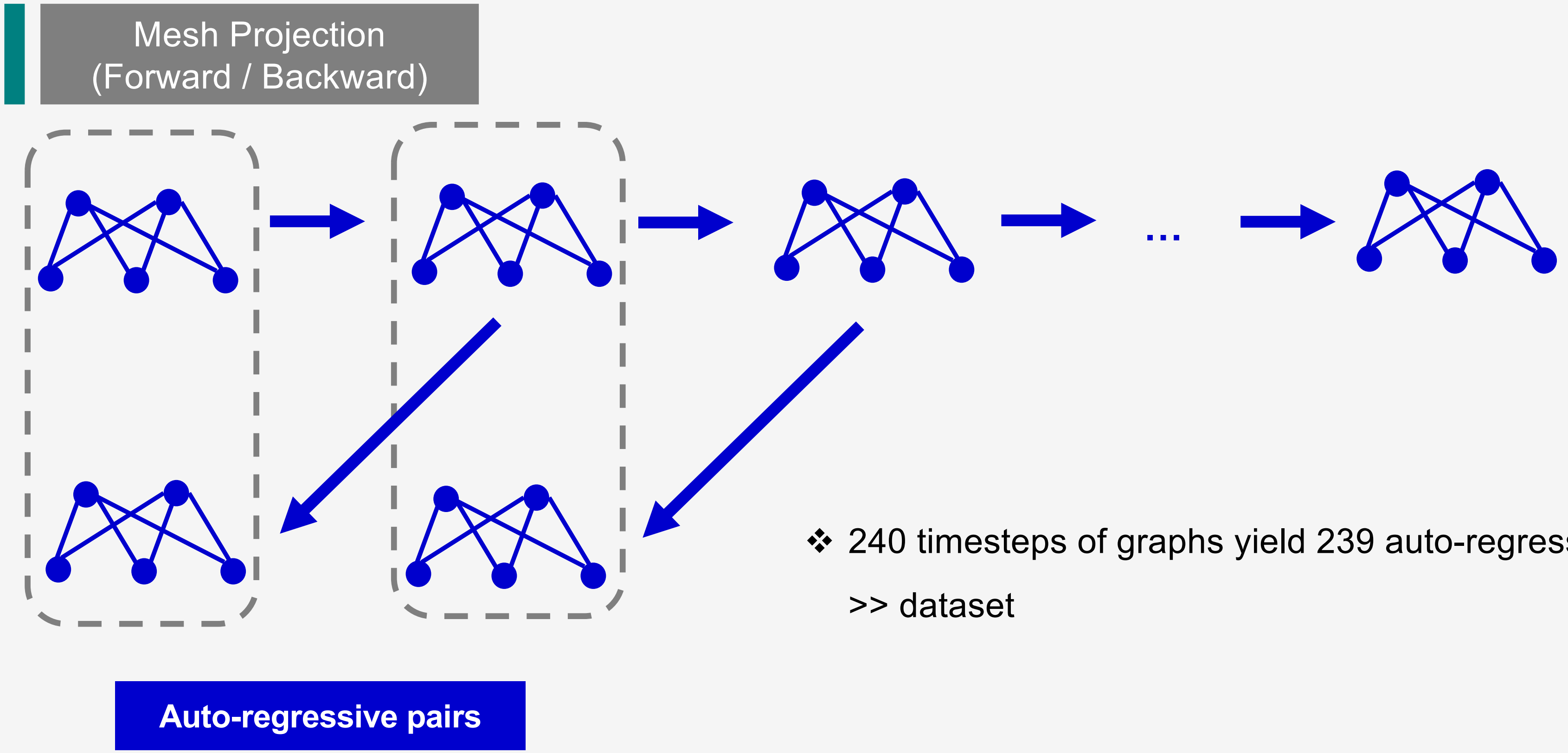
Pre-processing

Mesh Projection
(Forward / Backward)



- Interpolate the Phase 1 Temperature and Pressure to previous / next mesh
- Nearest neighbor interpolation
- Graph U-net architecture requires prediction on the same mesh

Pre-processing

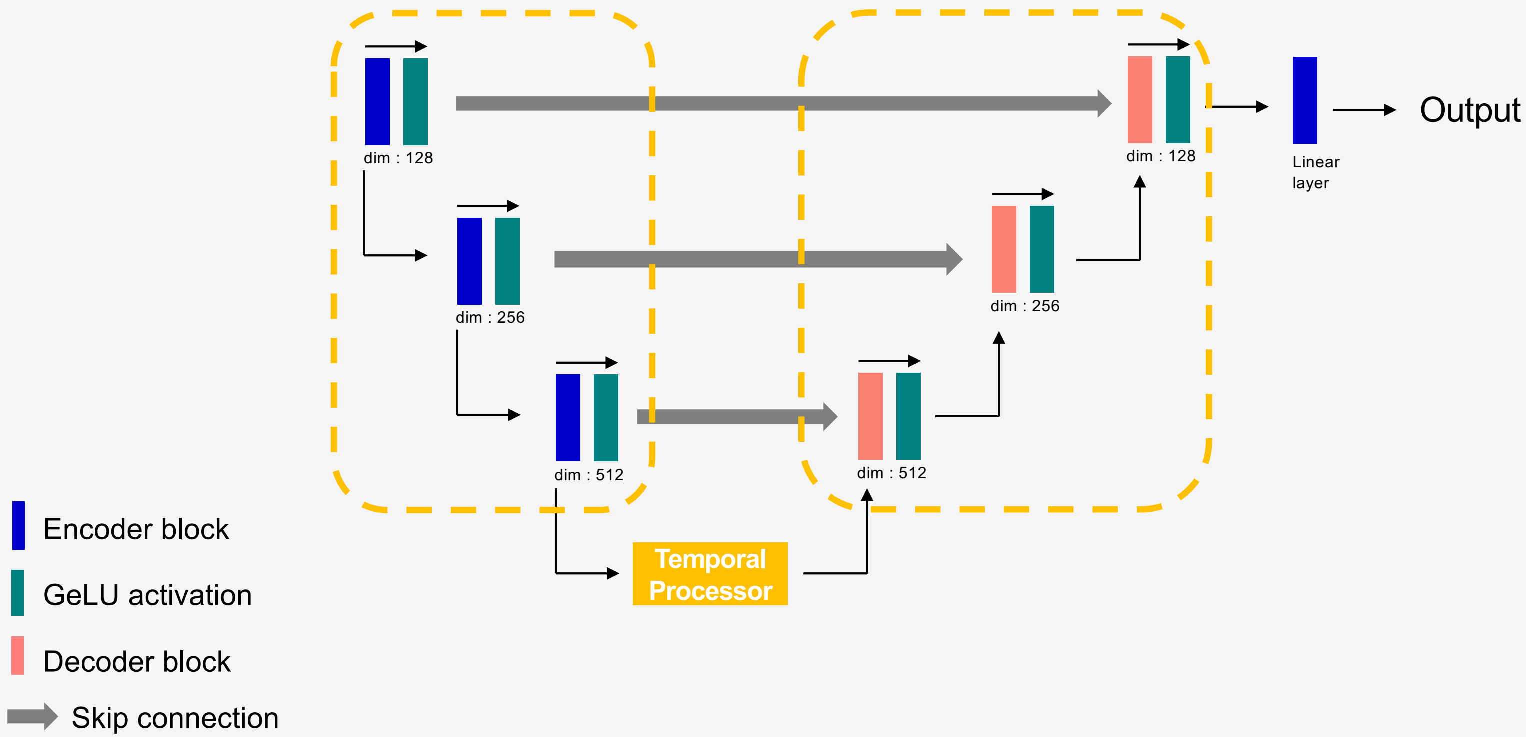


- 240 timesteps of graphs yield 239 auto-regressive pairs

  >> dataset

Model Architecture

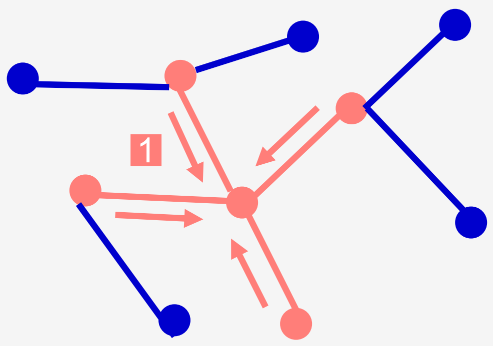
Auto-regressive **Graph U-net architecture**



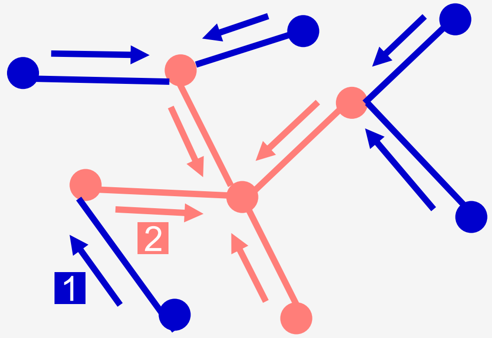
Model Architecture

Encoder & Decoder block
GCNConv
Hybrid (GCNConv | GATConv)
Multi-hop GCNConv (K > 1)

Temporal Processor block
Temporal Convolution
Temporal attention
RNN cell / LSTM

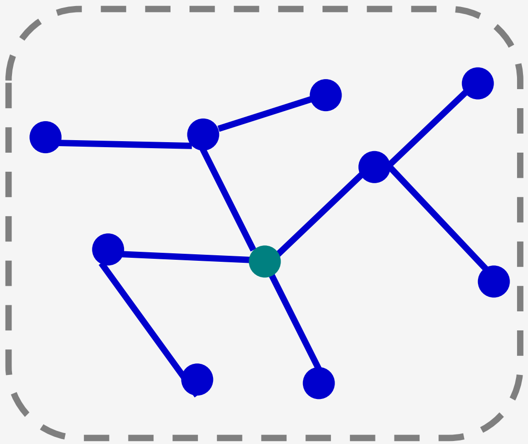


GCNConv :
1- hop aggregation



2 - hop GCNConv :
2 - hop aggregation

Relative importance of nodes

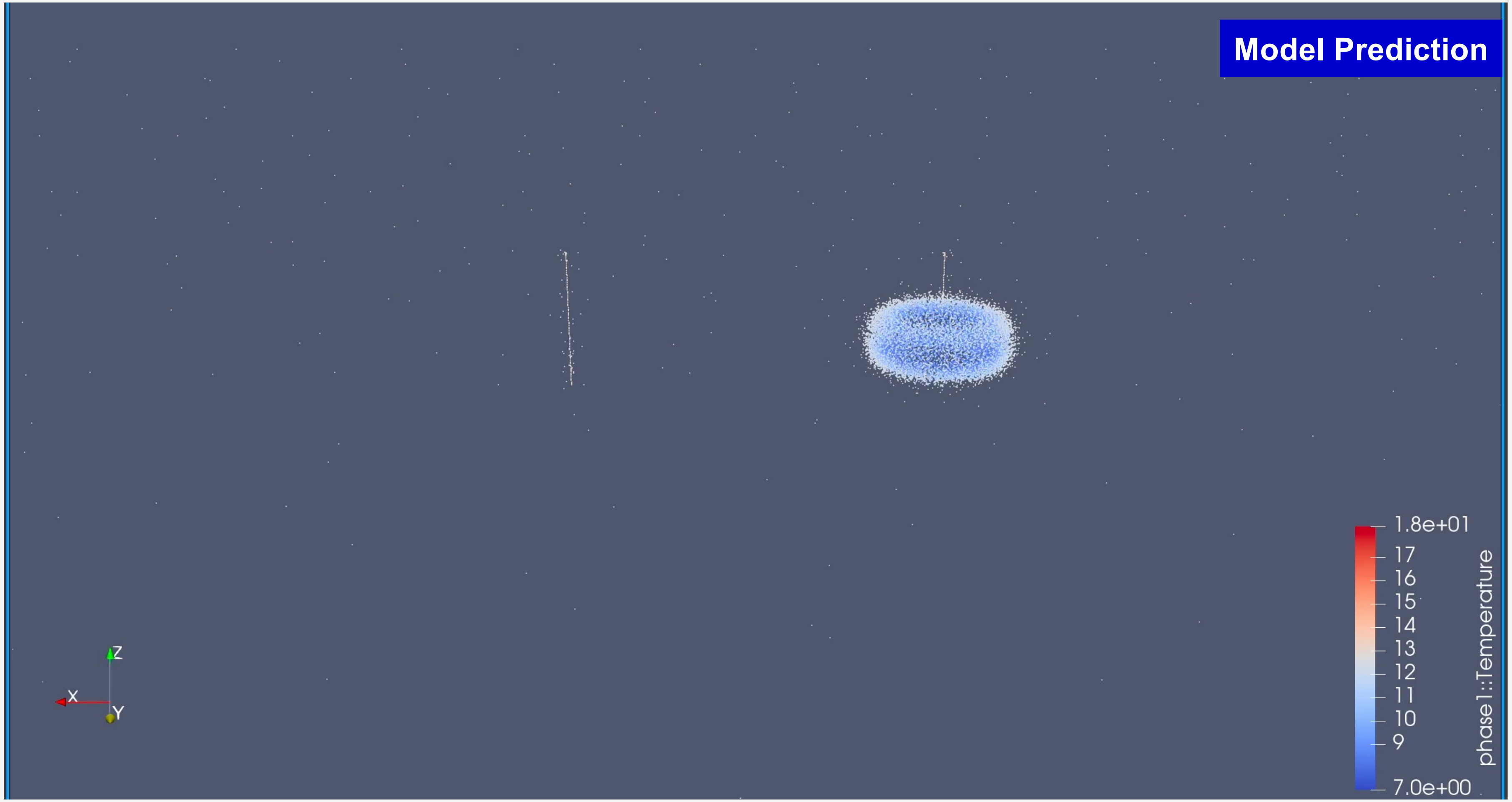


GATConv

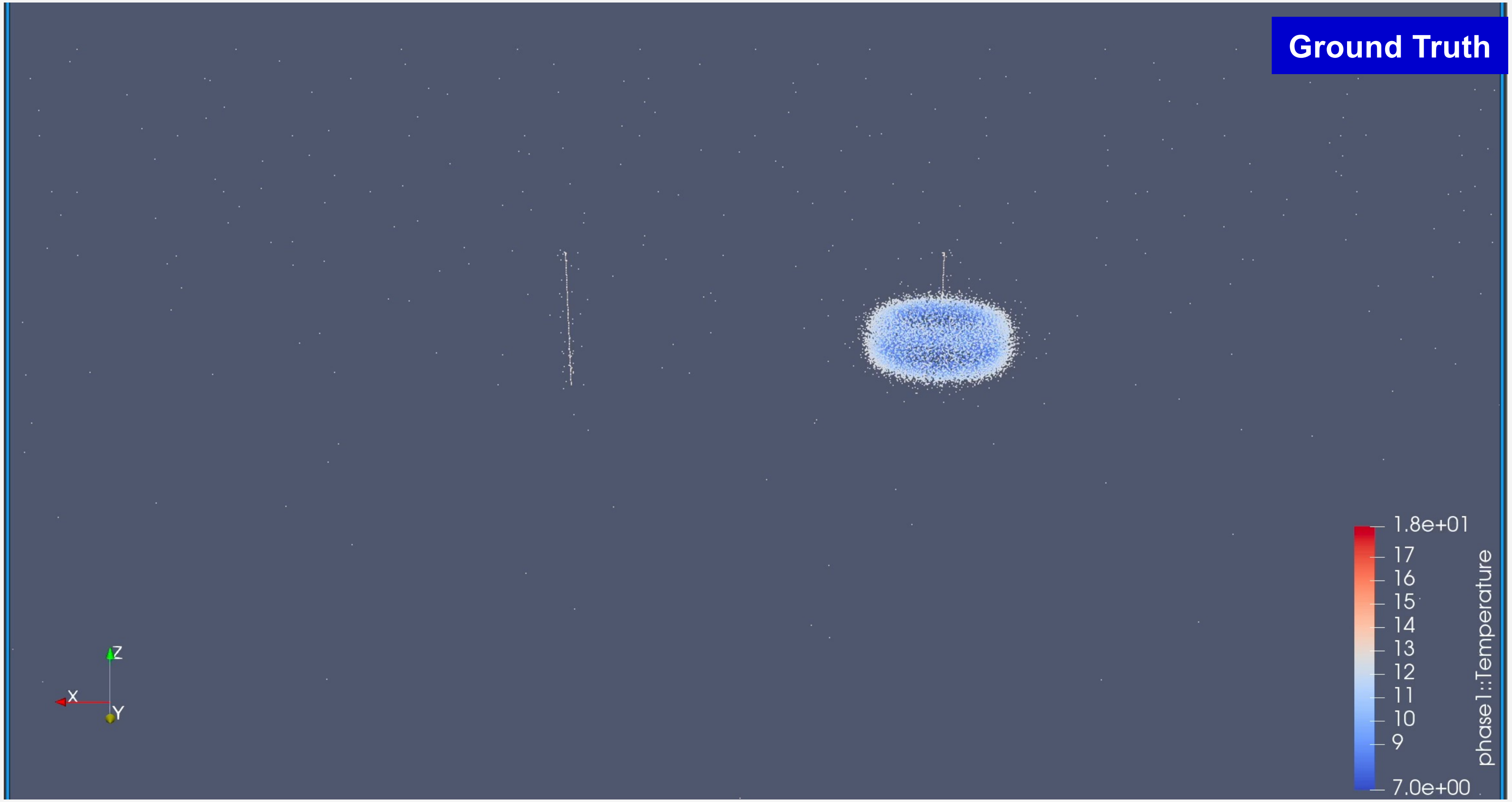
Model Performance | R2 score

	Train dataset		Test dataset	
	Temperature	Pressure	Temperature	Pressure
U-GCN (forward)	88.14%	92.54%	85.67%	91.52%
U-GCN (backward)	93.93%	93.44%	91.65%	90.58%
Hybrid U-GAT (forward)	89.94%	92.58%	86.87%	91.66%
Hybrid U-GAT (backward)	**93.93%**	**91.20%**	**92.20%**	**90.08%**
Multi-hop GCN (K = 2 | backward)	93.88%	92.10%	91.21%	89.92%
Multi-hop GCN (K = 3 | backward)	93.80%	90.81%	91.98%	89.66%

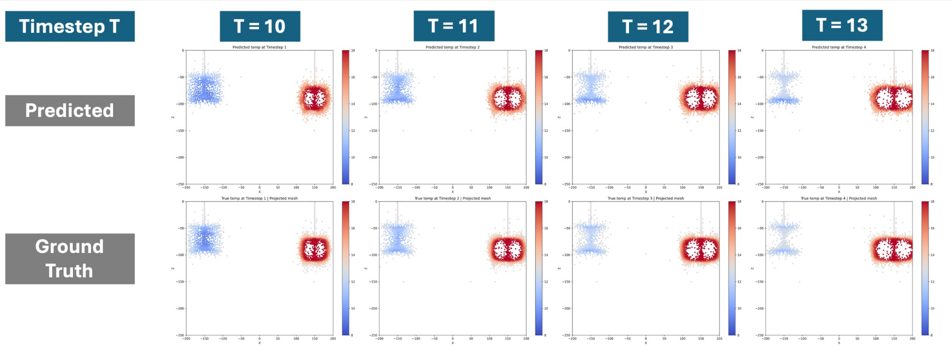
Model Visualization

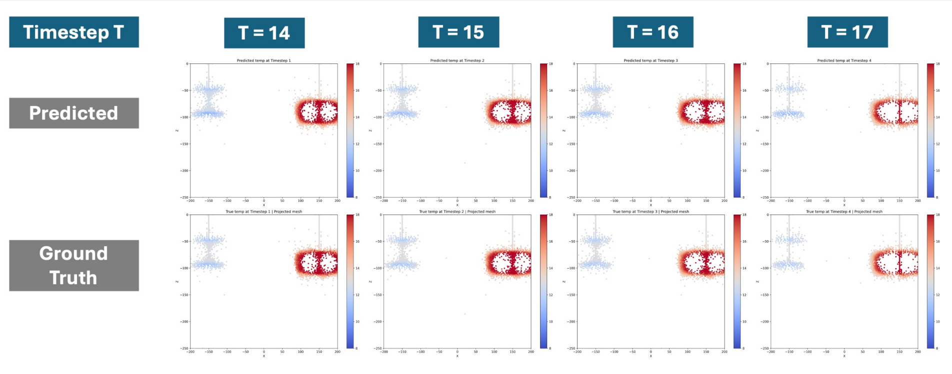


Model Visualization



Result visualization





Accurately capturing the plume diffusion

- Capture both value + shape accurately
- Grasp of general solution of plume diffusion
- Accurate gradient at the fringe of plume
- Steady-state diffusion (stable injection or pure diffusion)

◀ The evolution of phase 1 temperature in scenario 200.

Forward Projection | GCNConv | XZ Cross-section at vertical profile y = 0

Result visualization

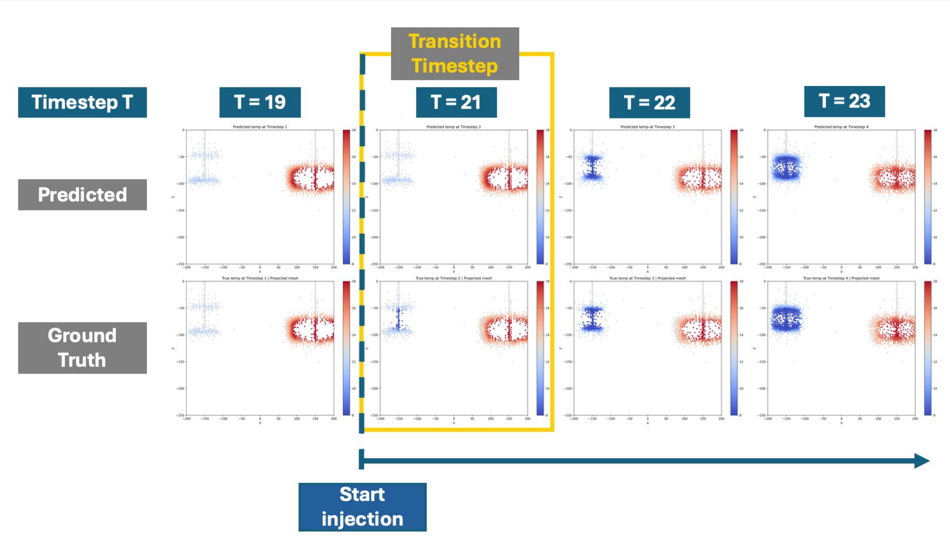
◀ The evolution of phase 1 temperature in scenario 200.

Backward Projection | GCNConv | XZ Cross-section at vertical profile y = 0

Higher R2 score in Backward Projection

- Back projection yields an overall higher R2 score in predictions across all model architecture
- Does NOT necessarily mean that backward projection is of better performance (not indicative)
- Backward projection offer less nodes on the high gradient area in the prediction (output state | timestep t+1)
- Restricted expressiveness in backward propagation
- Not directly comparable and indicative

Result visualization



The evolution of phase 1 temperature in scenario 200 during transition timestep

Forward Projection | GCNConv | XZ Cross-section at vertical profile y = 0

Limitations on injection phase transition

- The mode struggles to capture the start of injection from stationary phase
- Physical understanding : Transient solution vs Steady-state solution
- ML understanding : imbalance dataset (< 10 % of dataset)

Adaptive Meshing

Limitations on constant mesh for U-GNN

- Graph U-net architecture : constant input and output tensor
- The GNN model itself could not benefit from adaptive mesh refinement for variable resolution
- Constrained expressiveness on : (1) high-gradient area (2) fine-grained changes
- Representation of mesh topology on replicating actual fluid flow in porous medium

Reinforcement Learning (RL) for adaptive mesh refinement (AMR)

- Apply AMR with proposed auto-regressive ML approach
- (1) Refine the resolution at high-gradient area and injection well screen to capture finest details
- (2) Coarsen the resolution at steady region to increase computational efficiency
- (3) Restructure the mesh topology (node movement / edge connectivity)

Conclusion

Rapid modelling of ATES using ML

- Created a fast proxy of ATES simulation while retaining accuracy with over 92% of R2 score
- Can capture accurate shape of plume + temperature values
- Limitations on transition of injection phase

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End of slides

Thank you