

Application of Modified Meshgraphnets for Subsurface Prediction during CO₂ Sequestration

Chung Shih, Ph.D.



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National Climate Task Force Goals



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



50-52%

U.S. GREENHOUSE GAS EMISSIONS
REDUCTION BELOW 2005 LEVELS
I N 2 0 3 0



100%

CARBON POLLUTION-FREE
ELECTRICITY BY 2035



NET-ZERO

EMISSIONS ECONOMY BY 2050



40%

OF THE BENEFITS FROM FEDERAL
CLIMATE AND CLEAN ENERGY
INVESTMENTS TO DISADVANTAGED
C O M M U N I T I E S

The White House. (2021). President Biden's historic climate agenda. <https://www.whitehouse.gov/climate/>

The Science-informed Machine Learning for Accelerating Real-Time Decisions in Subsurface Applications (SMART) Initiative

- Ten-year, multi-organizational effort
- Transforming interactions within the subsurface and significantly improving efficiency and effectiveness of field-scale carbon storage operations.



Rapid Prediction
Virtual Learning



Real-Time Visualization
"CT" for the Subsurface



Real-Time Forecasting
"Advanced Control Room"

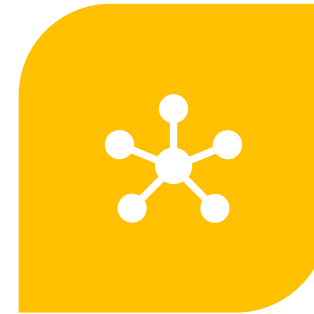
Modulus Graph Neural Network (MeshGraphNets) provides a flexible and generalizable AI/ML approach to address unique needs



**BE ABLE TO HANDLE
STRUCTURE AND
UNSTRUCTURED
DATA**



**LEARNING FROM
LIMITED DATA**



**CAPTURE GLOBAL
PROPERTIES FROM
LOCAL
NEIGHBORHOODS
VIA MESSAGE
PASSING AND
NODES/EDGES**

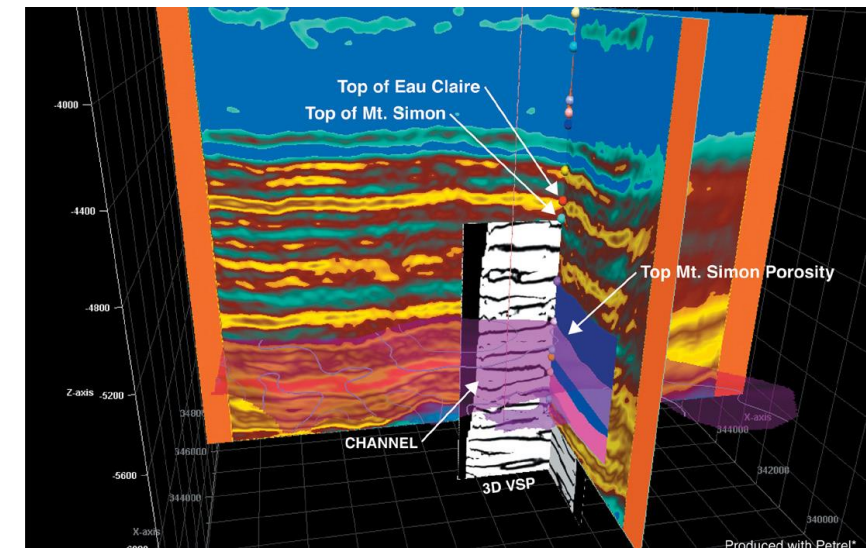
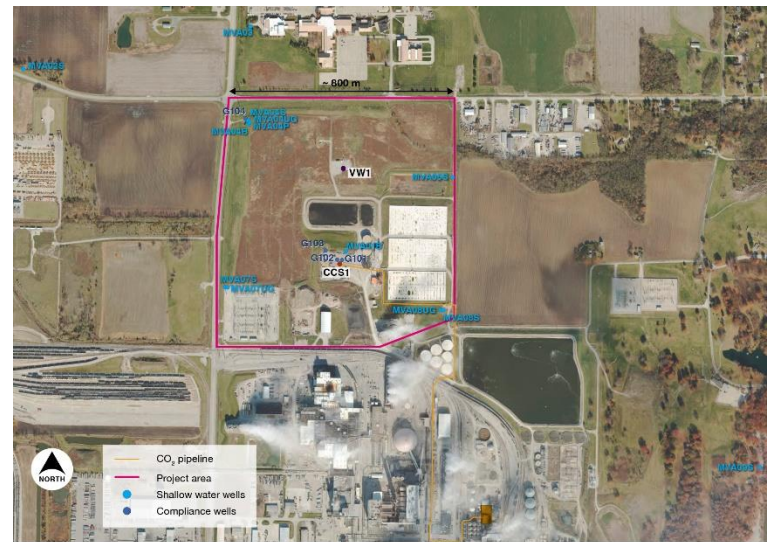


**SCALING AND
TRANSFER FROM
ONE SITE TO
ANOTHER FIELD**

The Illinois Basin Decatur Project (IBDP)

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

- The goal was to safely and effectively demonstrate the full carbon capture, utilization, and storage (CCUS) value chain in a saline reservoir
- The 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.
- The IBDP developed and implemented a rigorous and extensive monitoring, verification, and accounting (MVA) program
- 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).



<https://www.netl.doe.gov/sites/default/files/2018-11/Illinois-Basin-Decatur-Project.pdf>

IBDP Dataset for Training

Name	IBDP Model
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
Realization	100

IBDP GRID (X-Y)

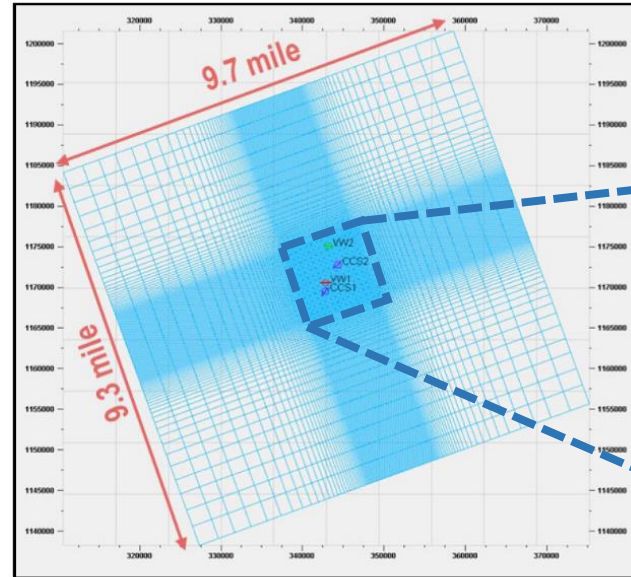
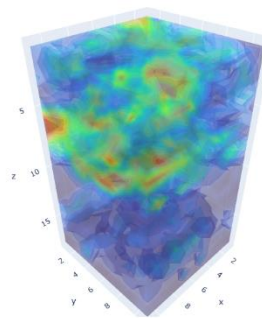
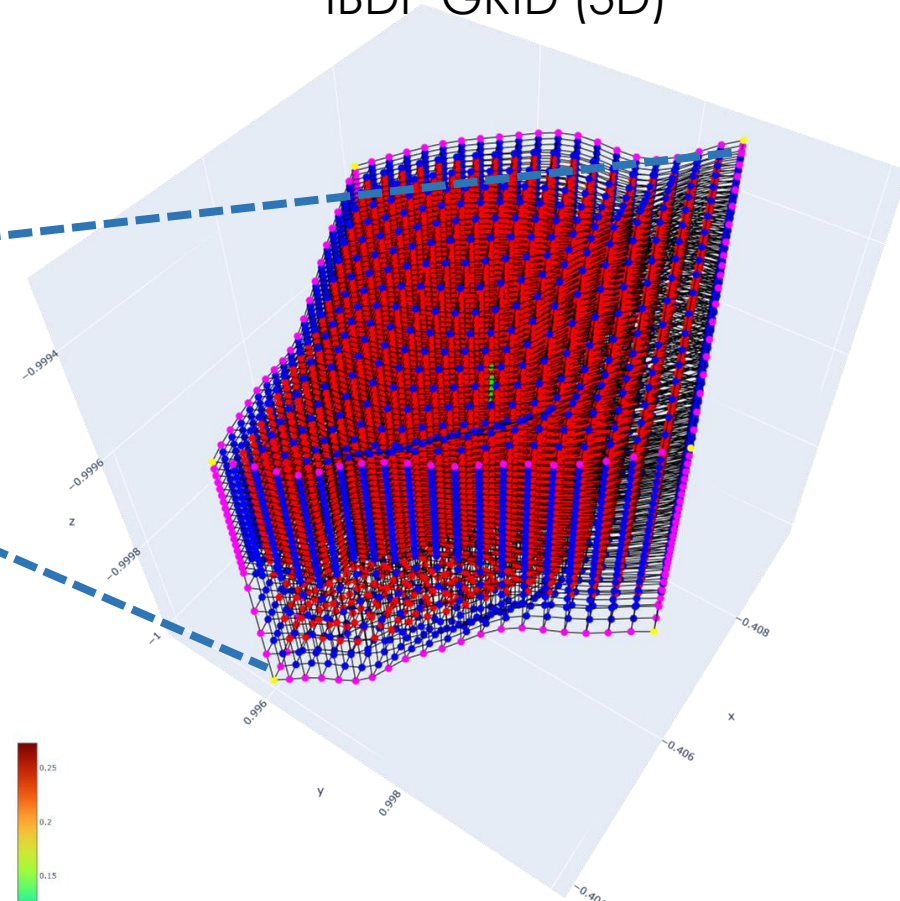
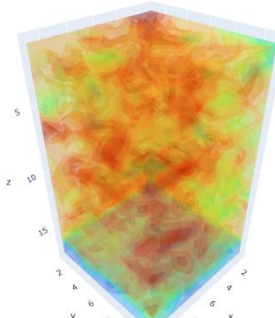


Figure 67. Dynamic model domain and tartan grid.

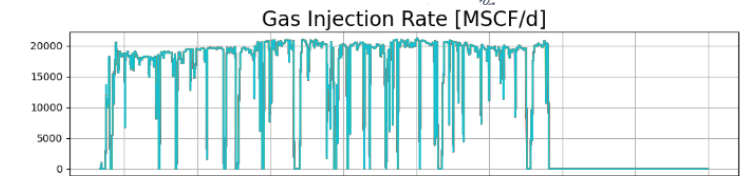
IBDP GRID (3D)



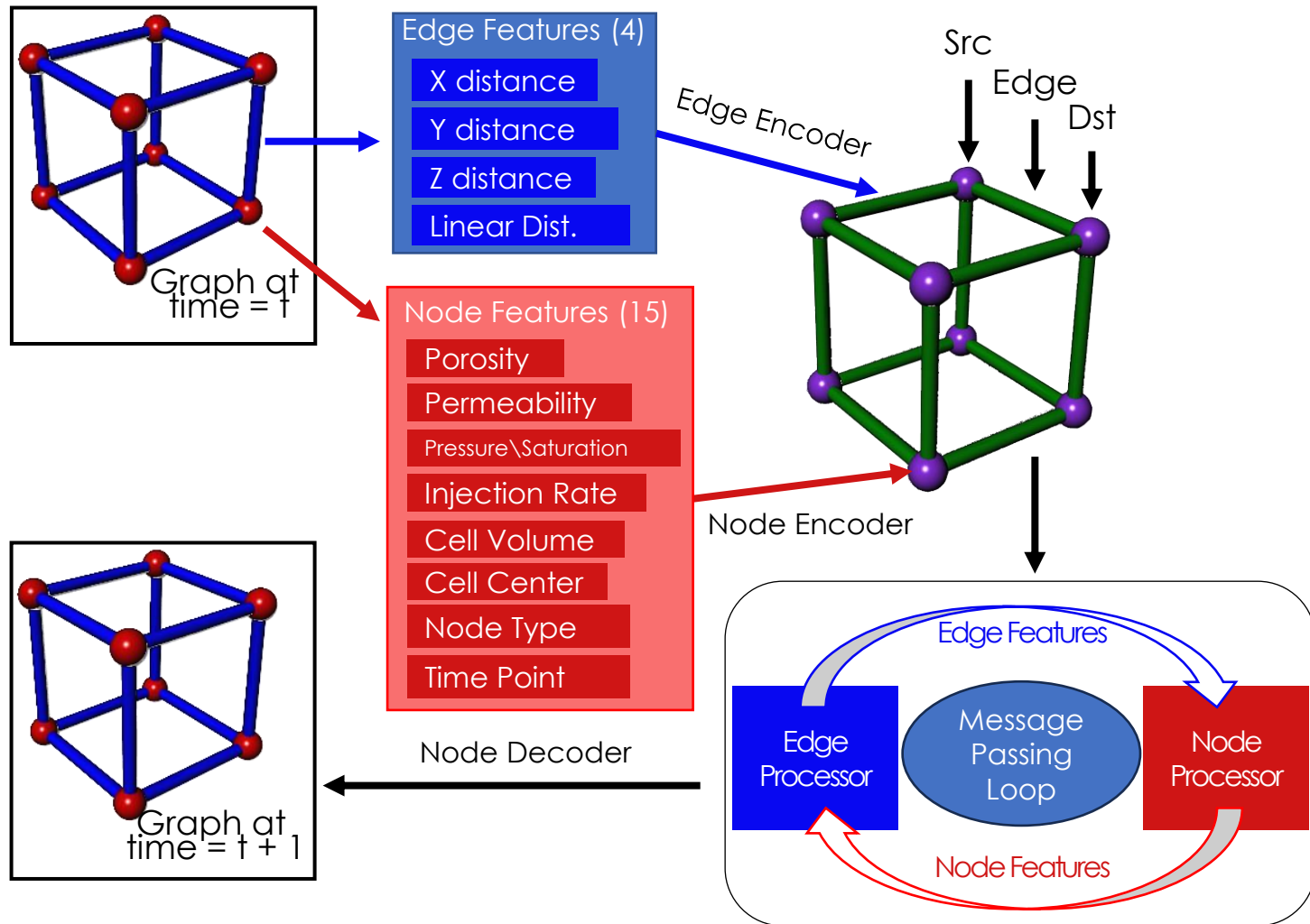
Avg. Permeability



Avg. Porosity



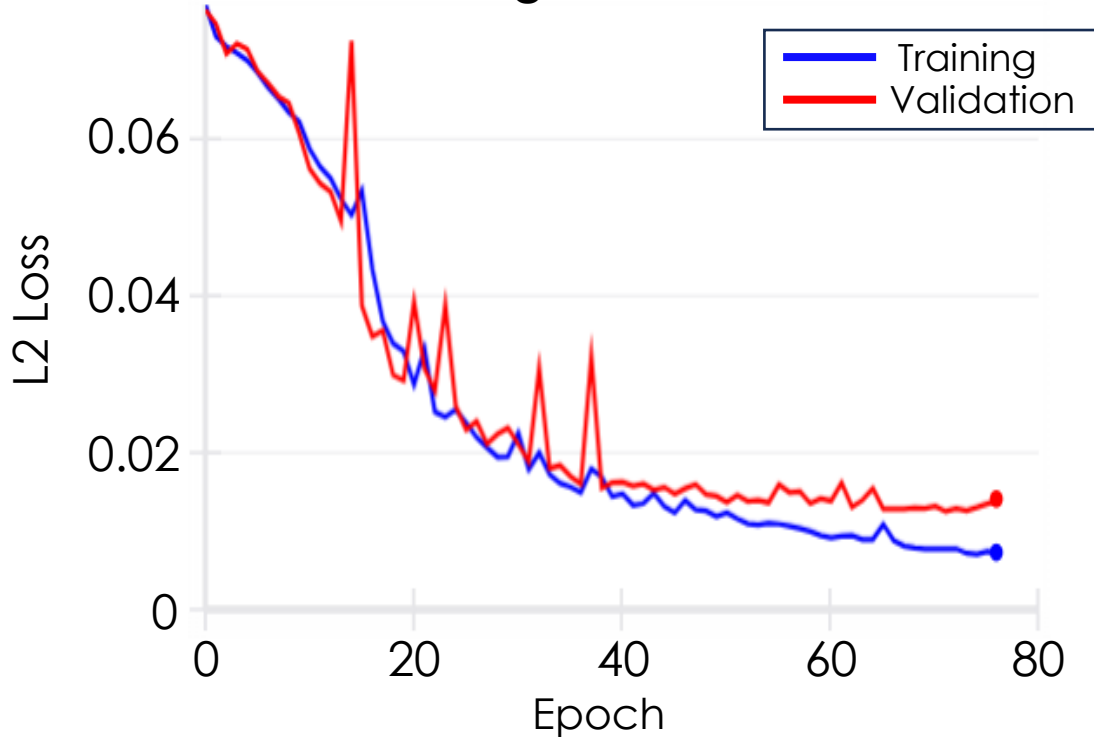
MeshGraphNets (MGN)



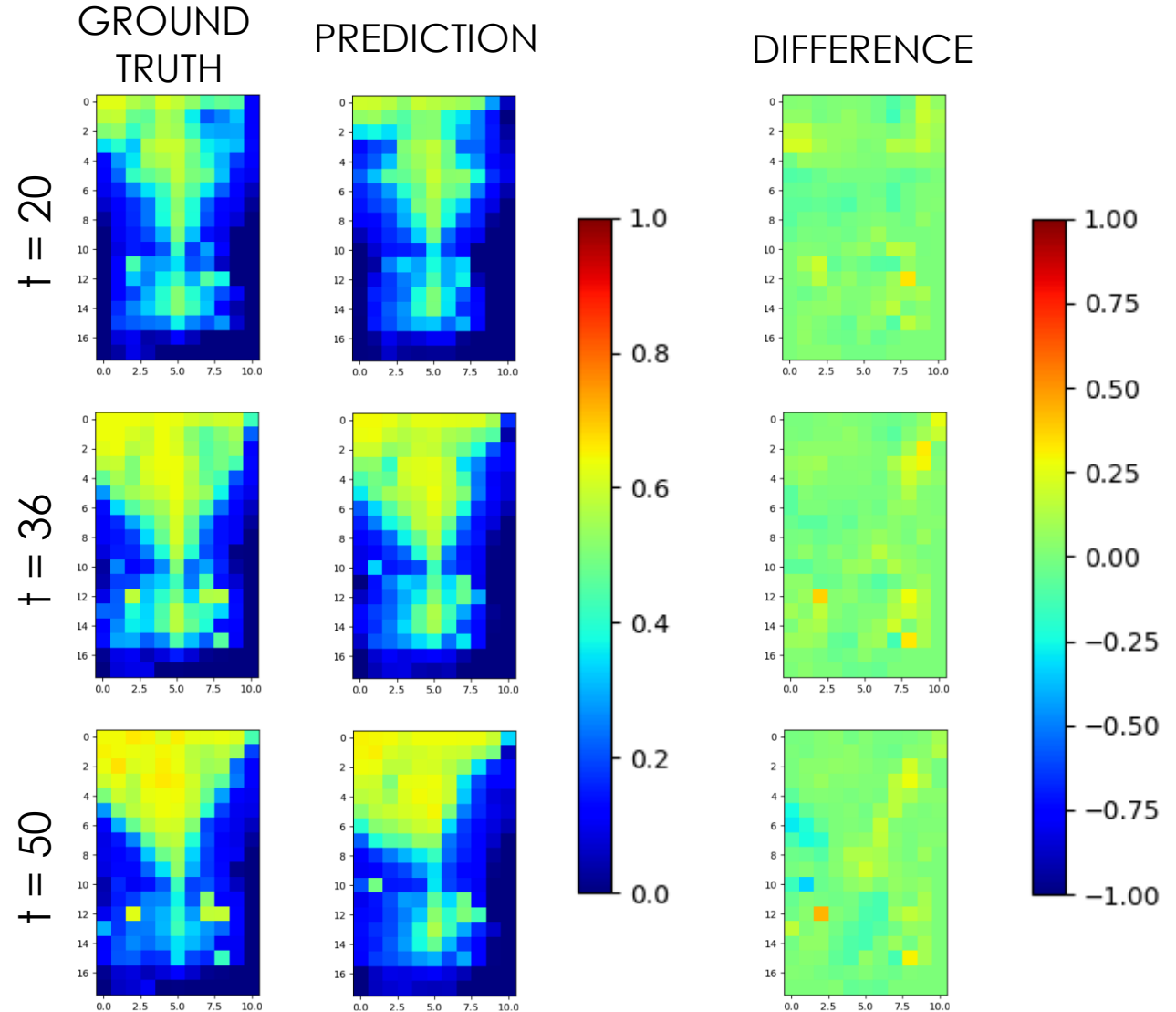
- Nodes contain cell-specific data
- Edges contain information on how information flows
- Message passing (MP) allows nodes to “see” neighbors by passing information through edges
- The distance a node can “see” is determined by the number of MP loops – “hops”

Saturation Prediction (MGN) – 50 Time Points

MGN Training and Validation Loss

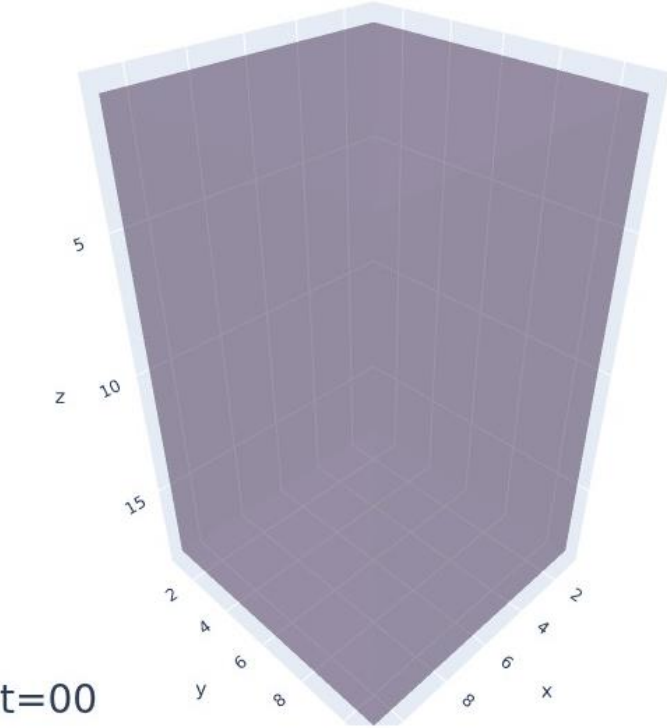


Root Mean-Squared Error (RMSE): 0.0735
Only Zeros RMSE: 0.0169
Nonzero RMSE: 0.0914

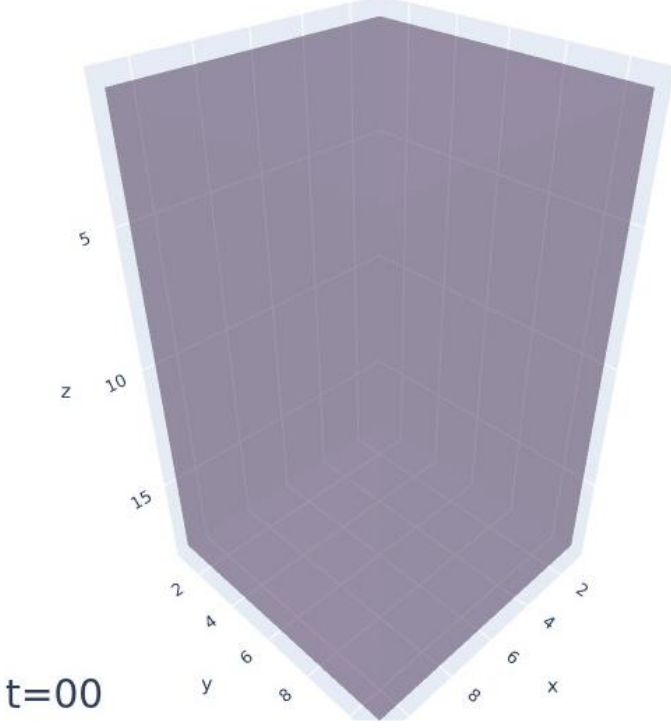


Saturation Prediction (MGN)

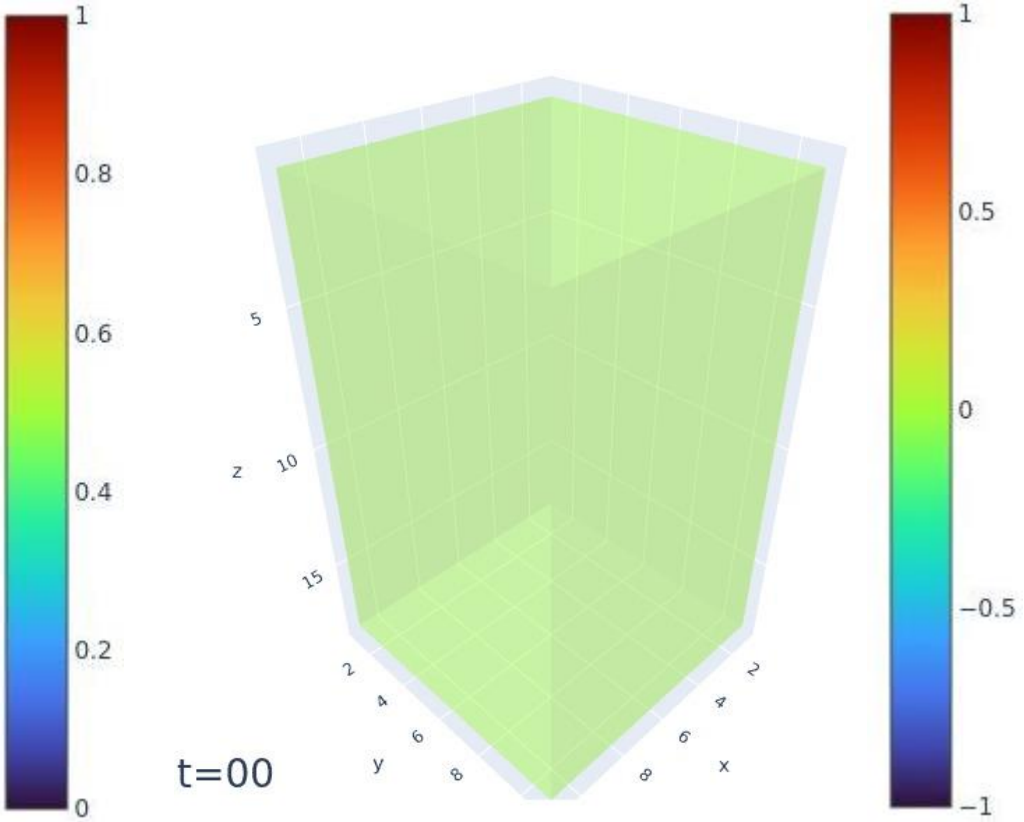
GROUND TRUTH



PREDICTION

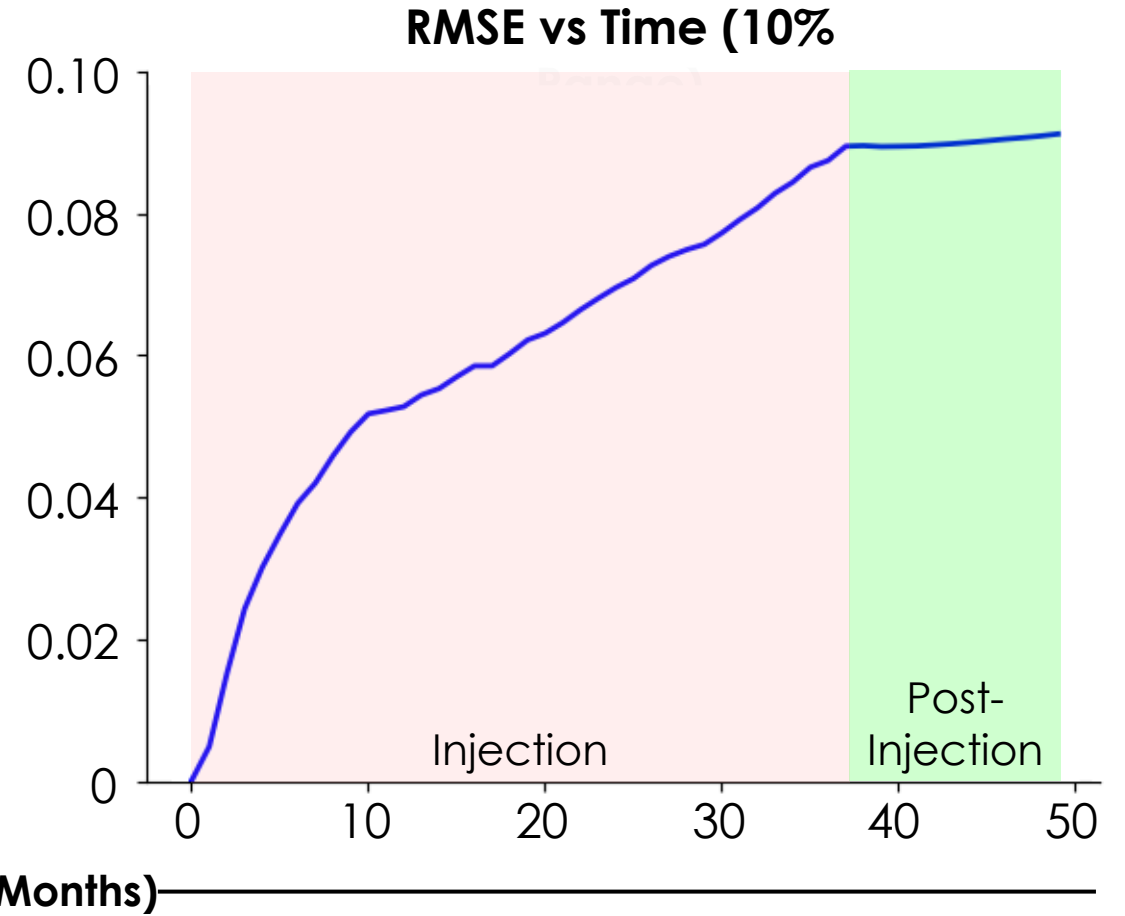
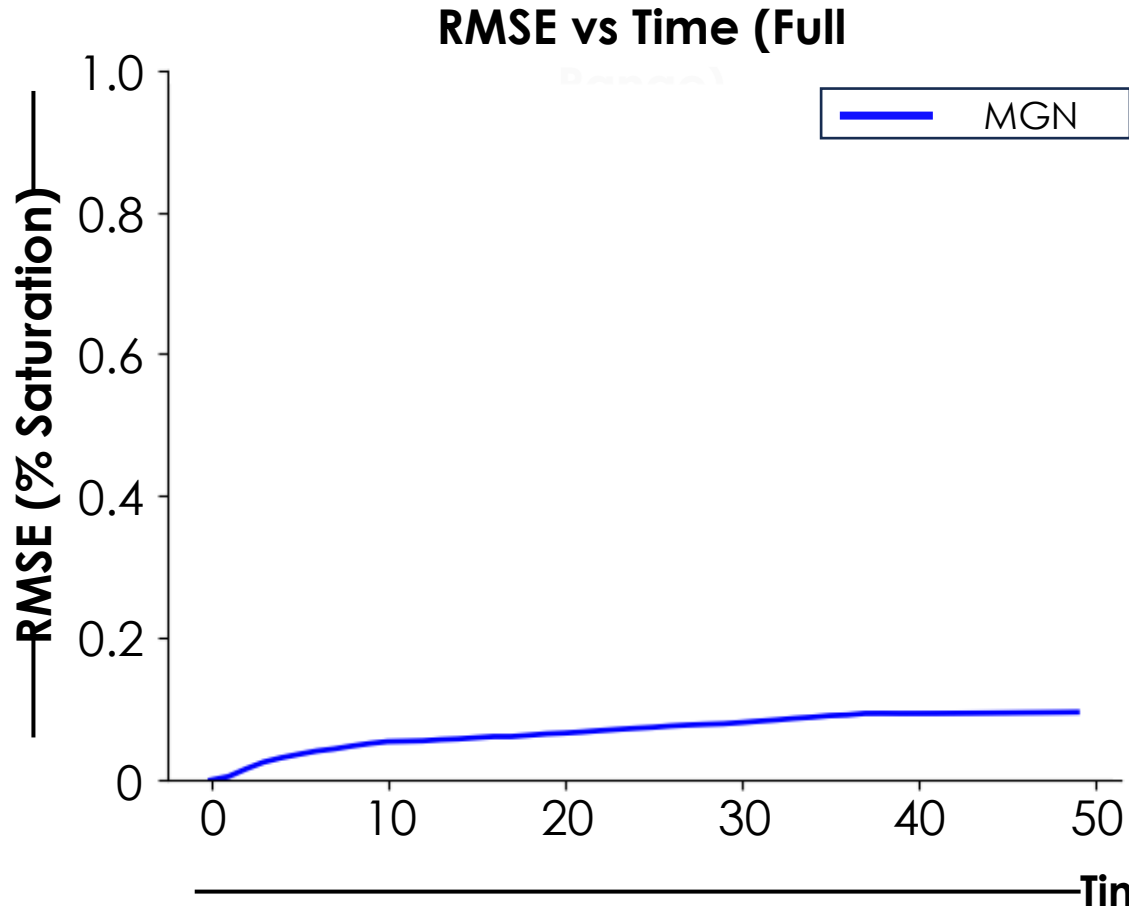


DIFFERENCE

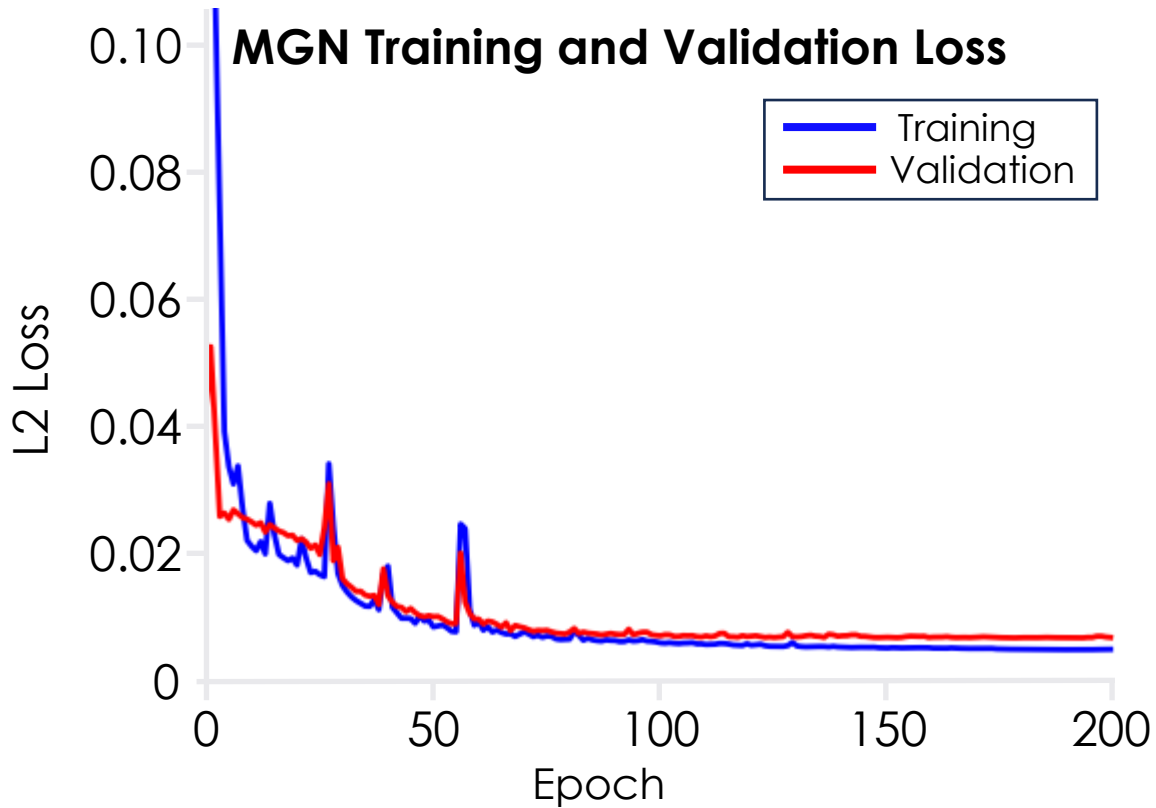


Saturation Results (MGN)

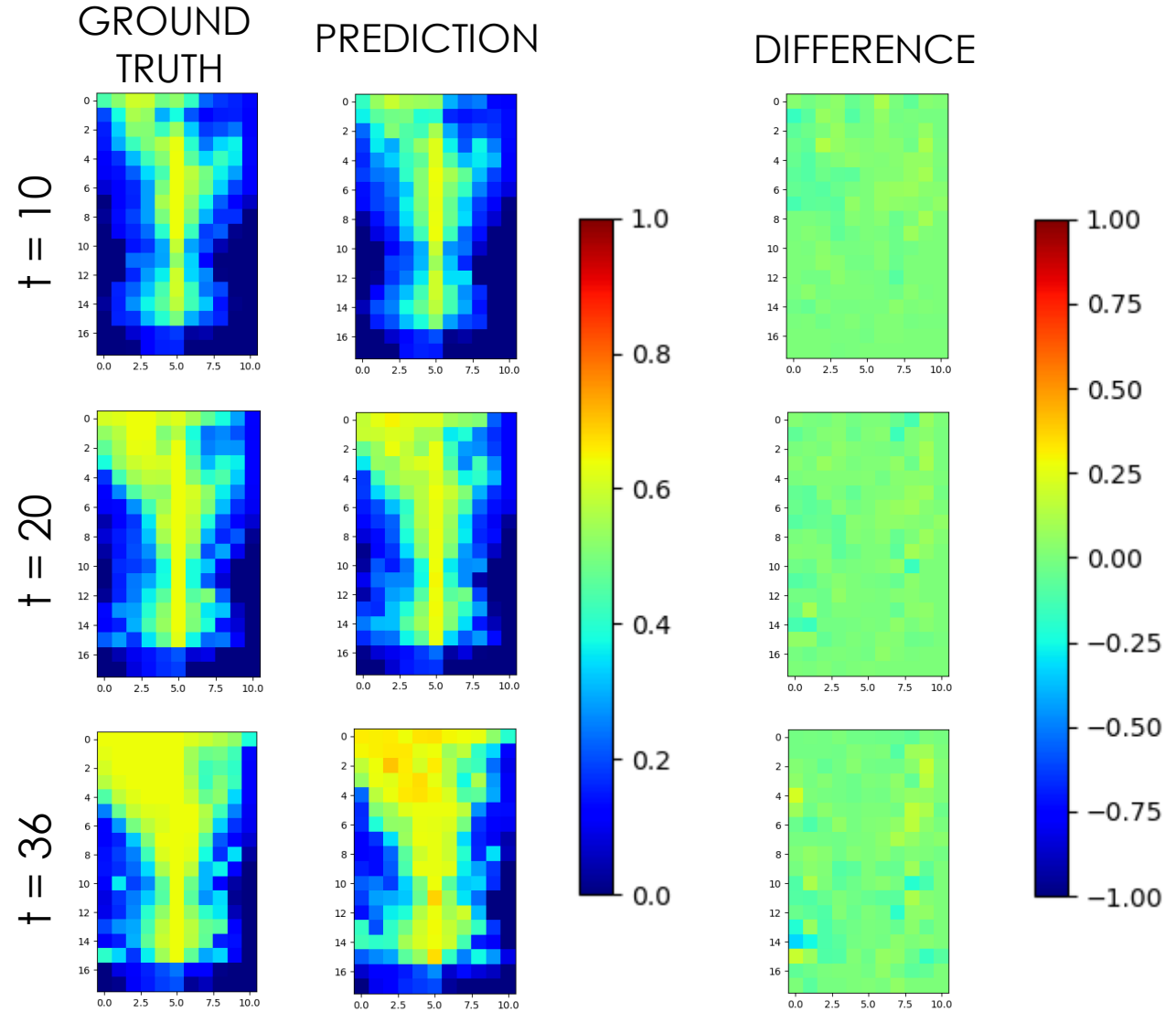
Autoregression and Temporal Instability



Saturation Prediction (MGN) – 36 Time Points



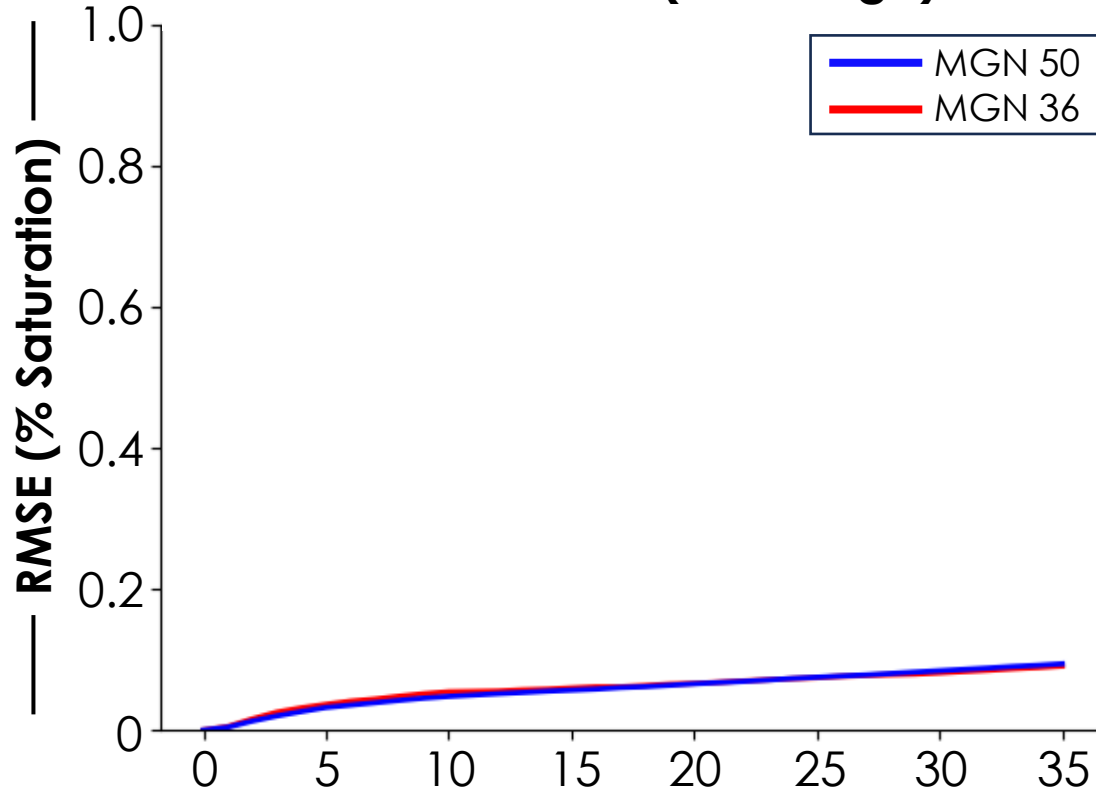
Root Mean-Squared Error (RMSE): 0.0630
Only Zeros RMSE: 0.0290
Nonzero RMSE: 0.0787



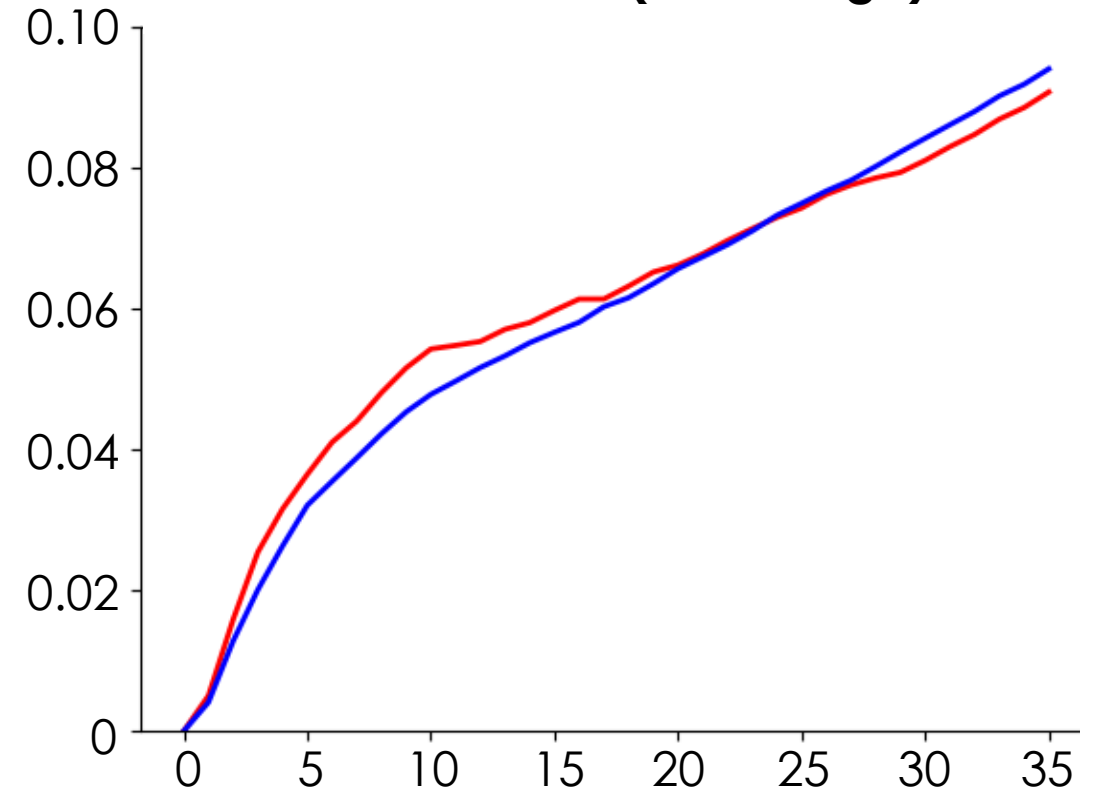
Saturation Results (MGN $t=50$ vs MGN $t=36$)

Autoregression and Temporal Instability

RMSE vs Time (Full Range)



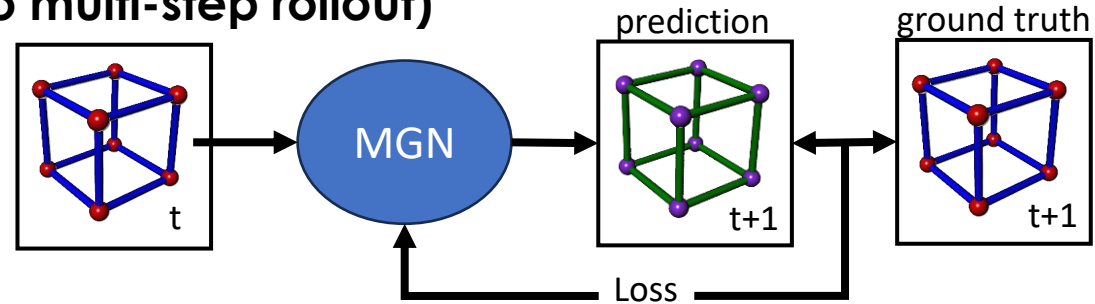
RMSE vs Time (10% Range)



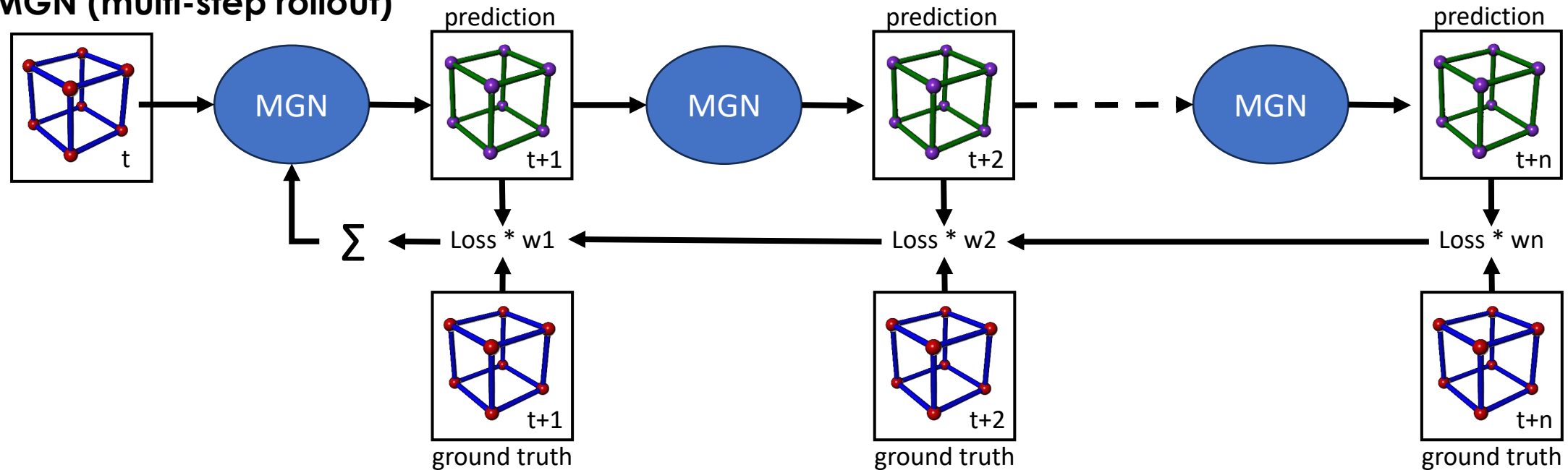
Time (Months)

MeshGraphNets with Multi-step Rollout (MGN-MR)

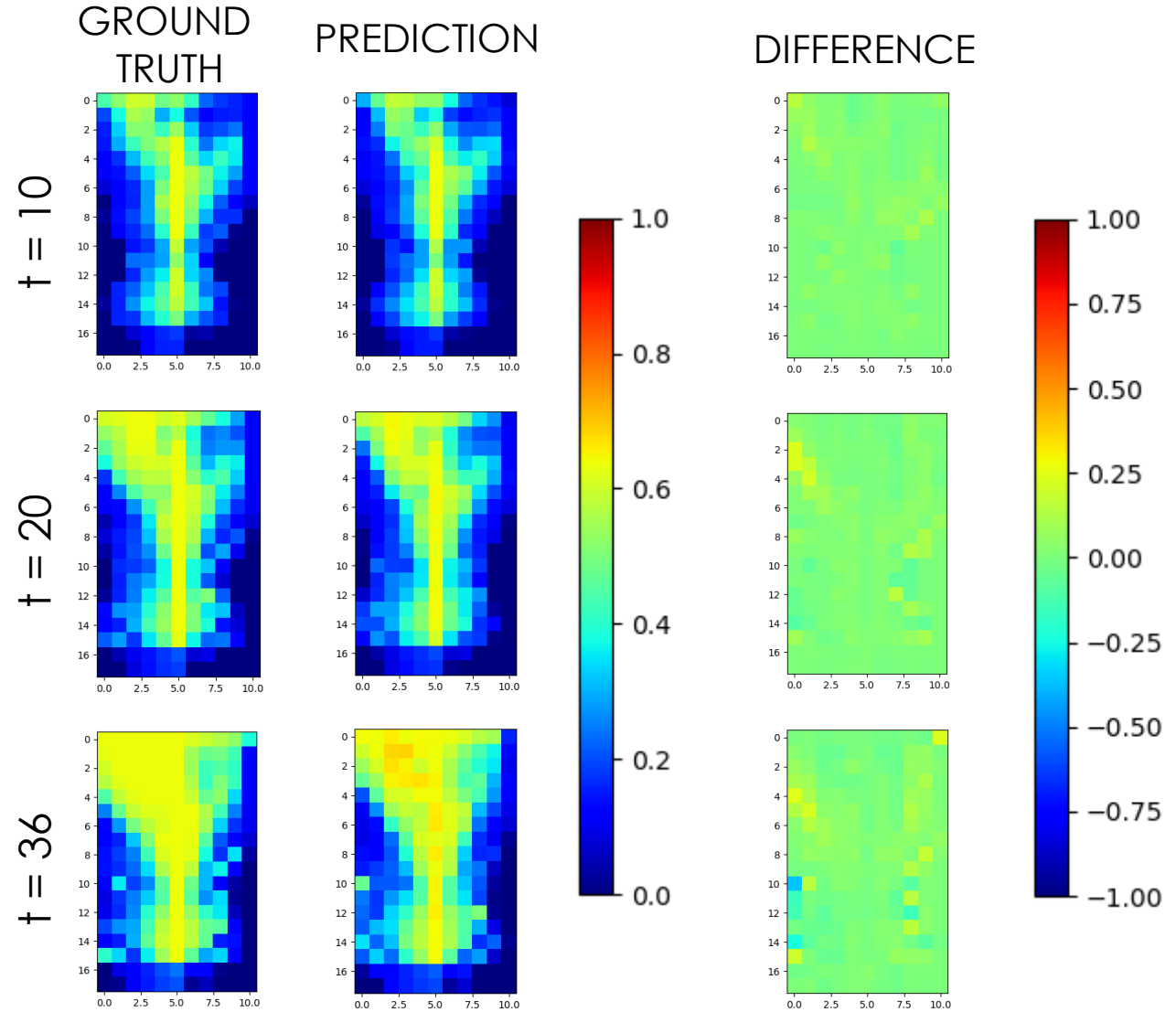
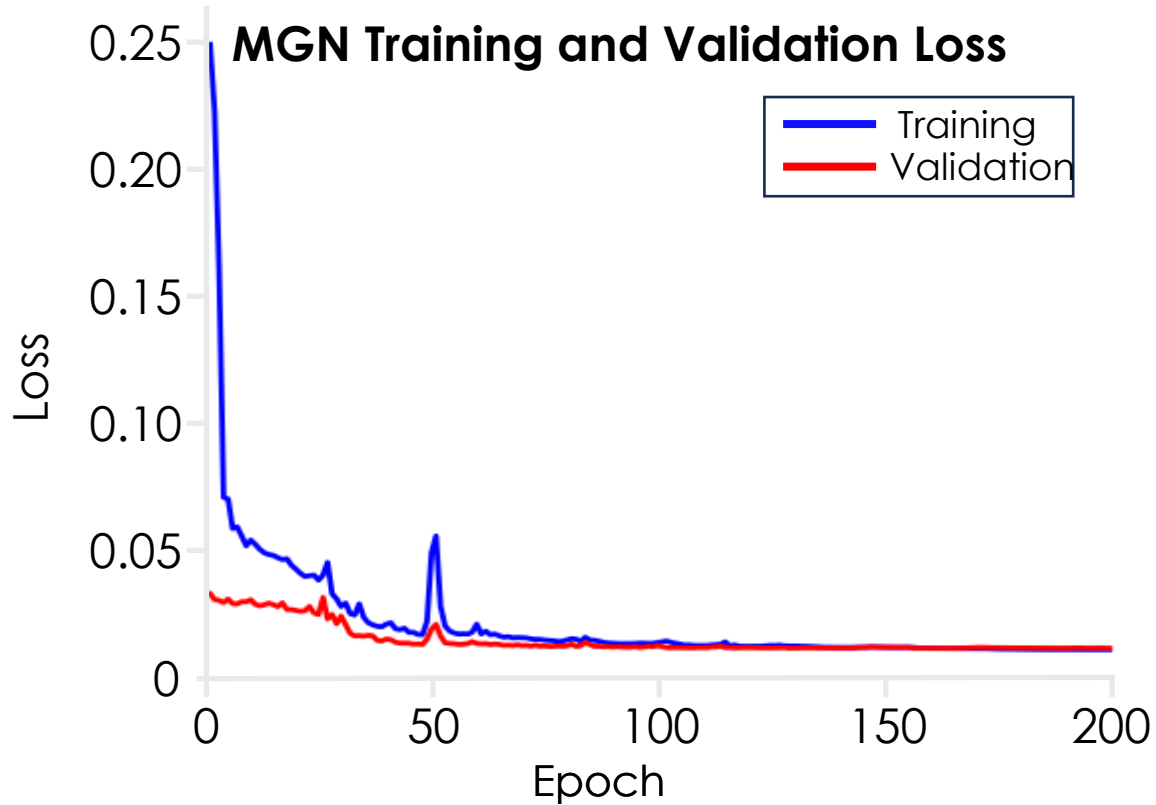
MGN (no multi-step rollout)



MGN (multi-step rollout)

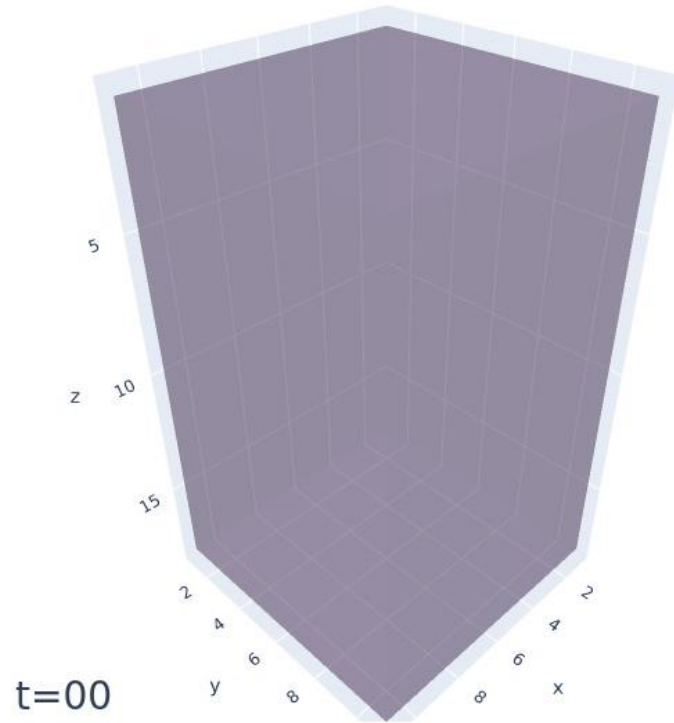


Saturation Prediction (MGN-MR)

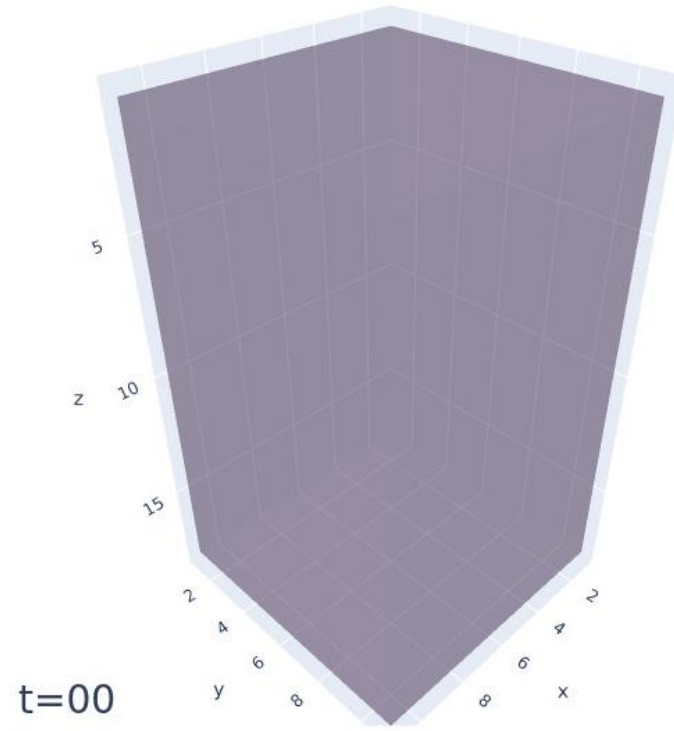


Saturation Prediction (MGN-MR)

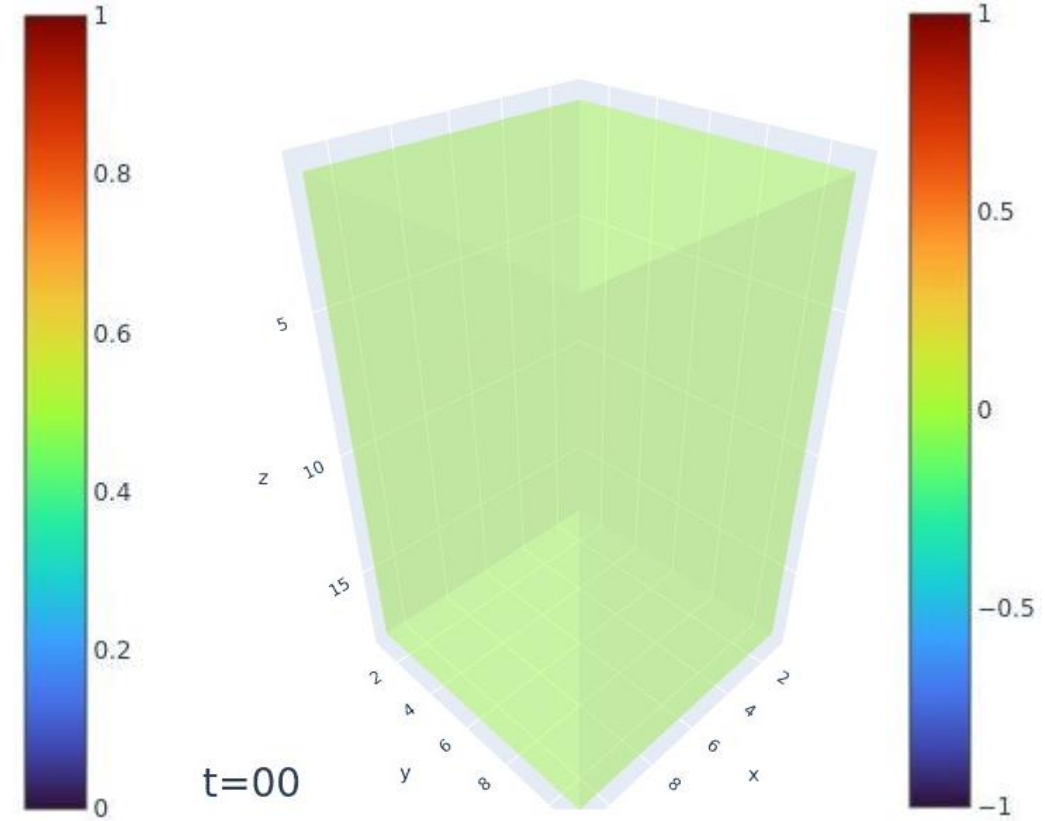
GROUND TRUTH



PREDICTION

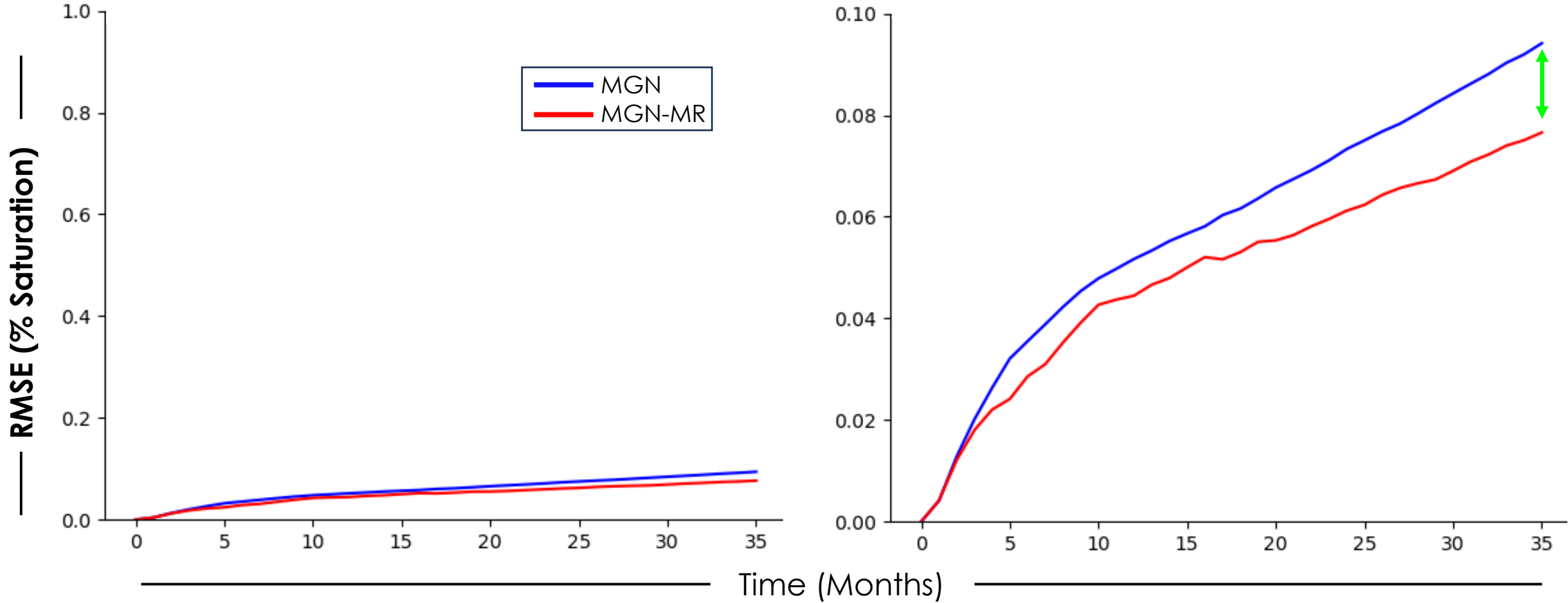


DIFFERENCE



Saturation Results (MGN VS MGN-MR)

Autoregression and Temporal Instability



Conclusion and Future Directions



- We established a 3D spatiotemporal MeshGraphNets with heterogeneous geological properties
- The initial results showed that GNN is capable of capturing patterns with a relatively small datasets (80 simulations)
- Temporal “drift” was found to be an issue using autoregression, but only in the injection regime
- Application of multi-step rollout improves stability when doing forward prediction

Thank you

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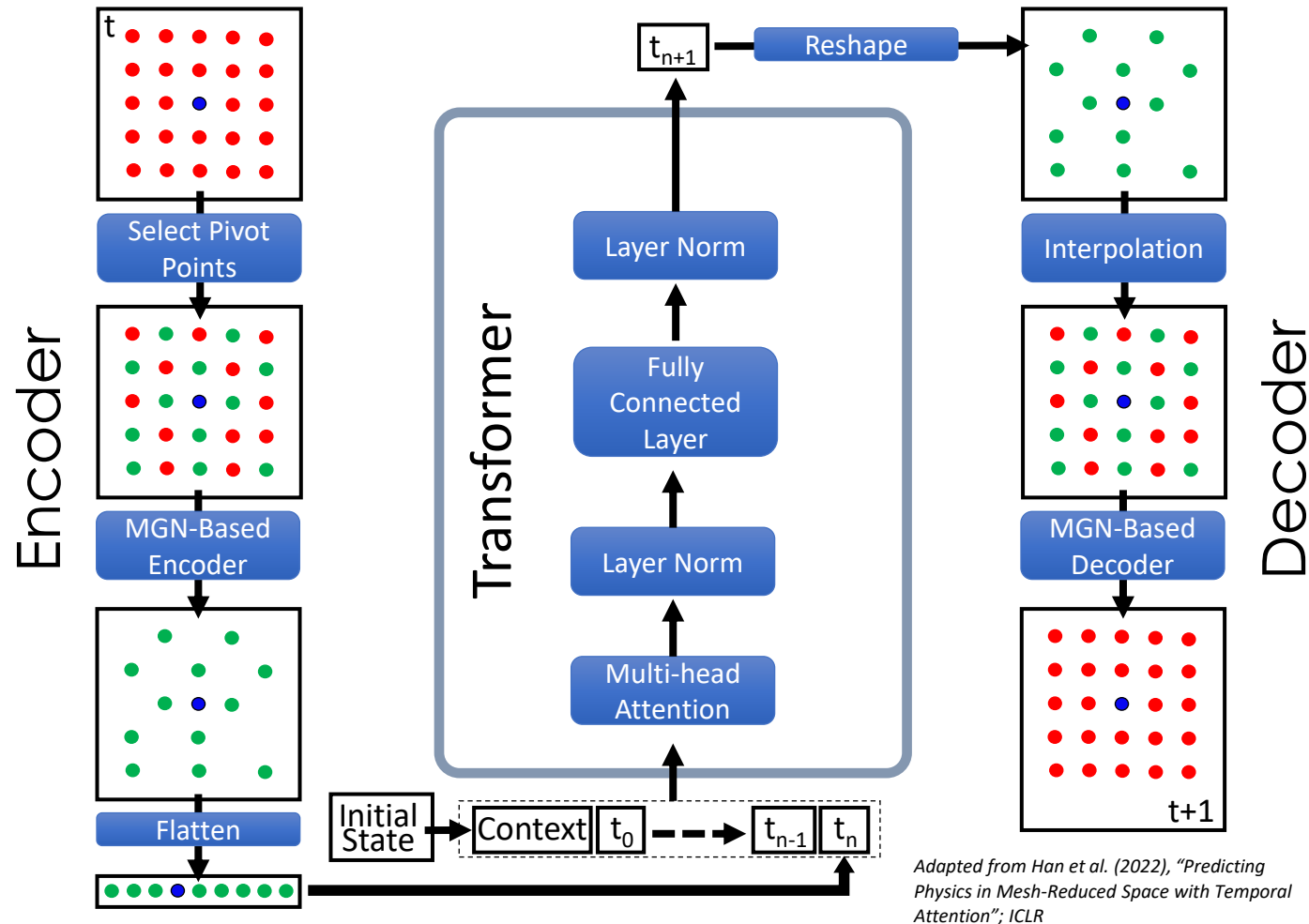
 @NationalEnergyTechnologyLaboratory

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MeshGraphNets with Transformer (MGN-T)



- Encoder/Decoder use MP to compress data into latent space
- Transformer uses each time point as a "token" to learn context – similar to LLM
- Model can "see" all previous time points

Saturation Prediction (MGN-T)



Saturation Prediction (MGN-T)



GROUND TRUTH

PREDICTION

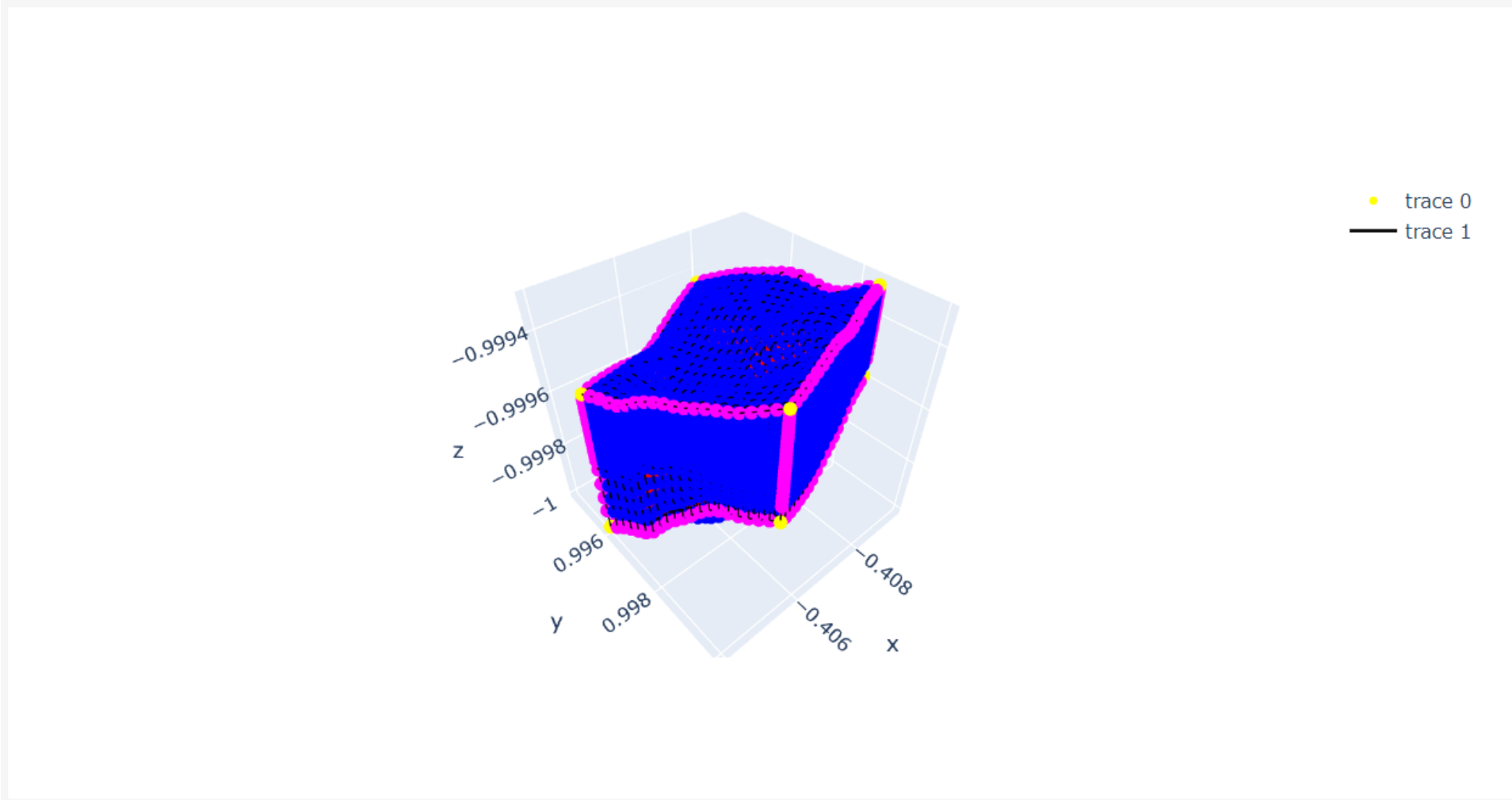
DIFFERENCE

Saturation Results (MGN-T)

Autoregression and Temporal Instability



IBDP Graph (11 x 11 x 18)

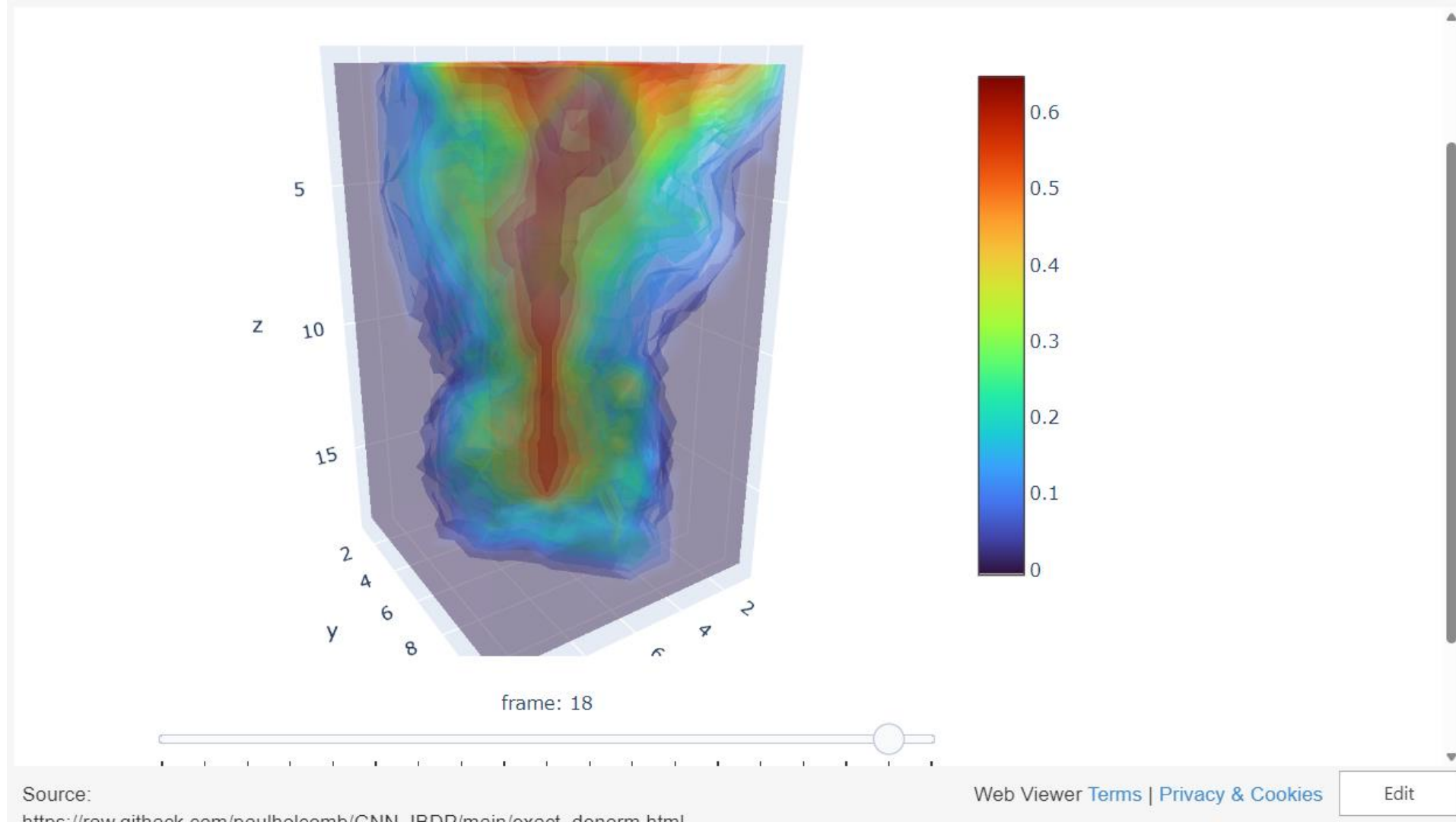


Source:
https://raw.githubusercontent.com/paulholcomb/CNN-IBDP/main/graph_3D.html

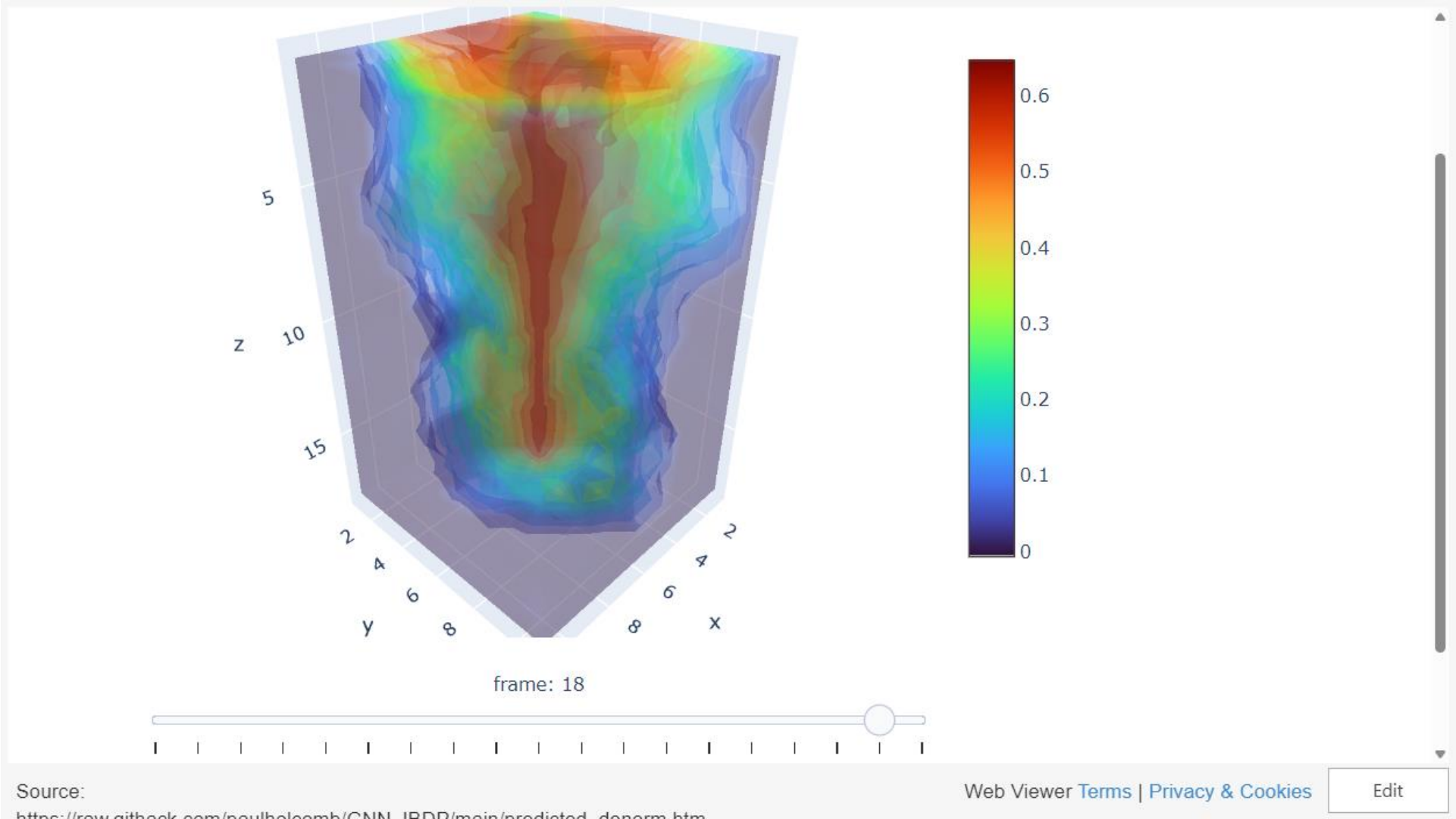
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IBDP Saturation (Ground Truth)



IBDP Saturation (Ground Truth)



IBDP Saturation (Ground Truth)

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