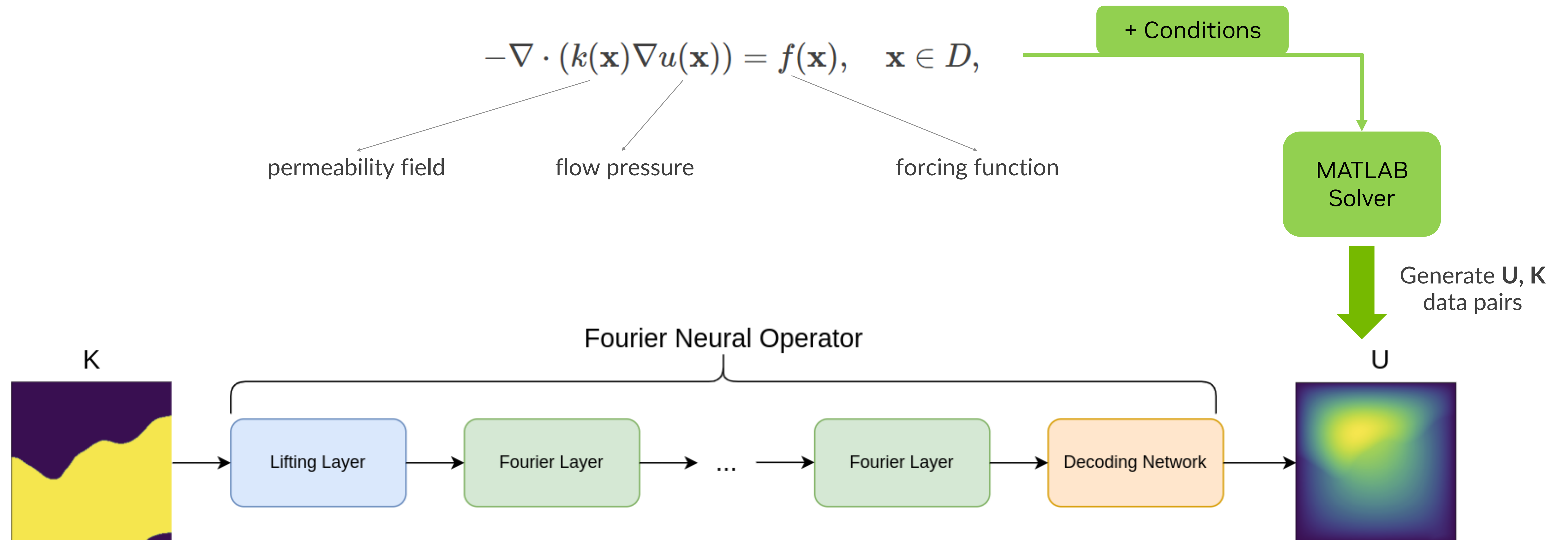




Data-driven approach

Darcy Flow Example

DATA: https://github.com/zongyi-li/fourier_neural_operator



This problem develops a surrogate model that learns the mapping between a permeability field and the pressure field, $K \rightarrow U$, for a distribution of permeability fields $K \sim p(K)$. This is a key distinction of this problem from other examples, you are *not* learning just a single solution but rather a distribution.

A NOTE: Math behind Neural Operator

Anima Anandkumar - Neural operator: A new paradigm for learning PDEs

Neural Operator: Learning Maps Between Function Spaces

Nickola K., Zongyi L. et. al., Caltech.

<https://zongyi-li.github.io/neural-operator/>

Green Function

$$\text{Goal : } Lu = f$$

$$\text{Def : } L^\dagger G = \delta(x - \xi)$$

$$\langle Lu, G \rangle = \langle f, G \rangle$$

$$\langle u, L^\dagger G \rangle = \langle f, G \rangle$$

$$\langle u, \delta(x - \xi) \rangle = \langle f, G \rangle$$

$$u(\xi) = \langle f, G \rangle$$

- Note

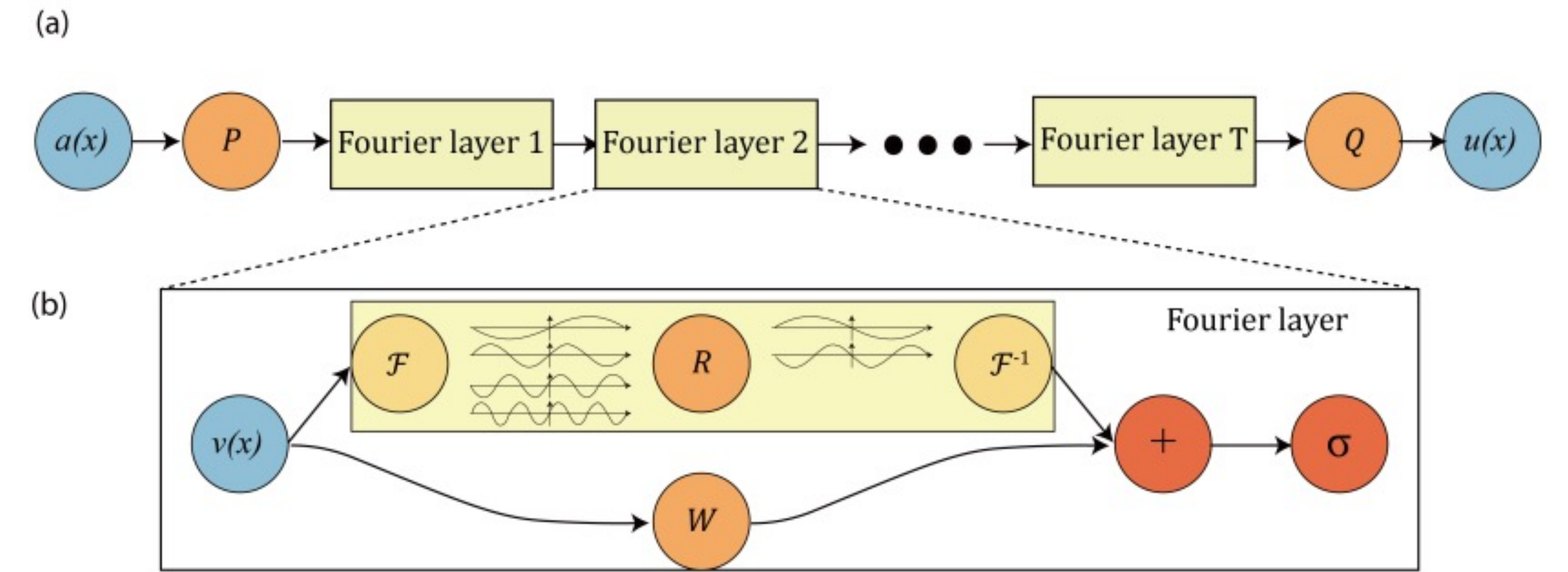
- $\langle, \rangle$: function space inner product, project one function to another, which is the integral of multiplying two functions.
- L : a linear operator.
- $L^\dagger$: a "adjoint" operator of L , if $L = L^\dagger$ then they should have the same boundary conditions, named "self-adjoint operator".
- δ : a `dirac function` use to `filter` function `u` at value ξ .
- u : target solution. and ξ is just a dummy variable, actually we could simply change it here $u(\xi) \rightarrow u(x)$, we get the final solution with proper form.

Fourier Neural Operator (FNO)

<https://arxiv.org/abs/2010.08895>, ICLR 2021.
FNO: FFT + NO, Zongyi L. et. al., Caltech+NVIDIA

- Contribution

- Learned an entire family of PDEs instead of solving only one instance such as FEM, FDM, PINN.
- Resolution-invariant, can do Zero-Shot super-resolution.
- Outperformed all existing DL methods with 30%+ lower error rate.
- Sped up more than 440x comparing to Spectral Method.



- Method

Definition 1 (Iterative updates) Define the update to the representation $v_t \mapsto v_{t+1}$ by

$$v_{t+1}(x) := \sigma \left(W v_t(x) + (\mathcal{K}(a; \phi) v_t)(x) \right), \quad \forall x \in D \quad (2)$$

Definition 2 (Kernel integral operator $\mathcal{K}$) Define the kernel integral operator mapping in (2) by

$$(\mathcal{K}(a; \phi) v_t)(x) := \int_D \kappa(x, y, a(x), a(y); \phi) v_t(y) dy, \quad \forall x \in D \quad (3)$$

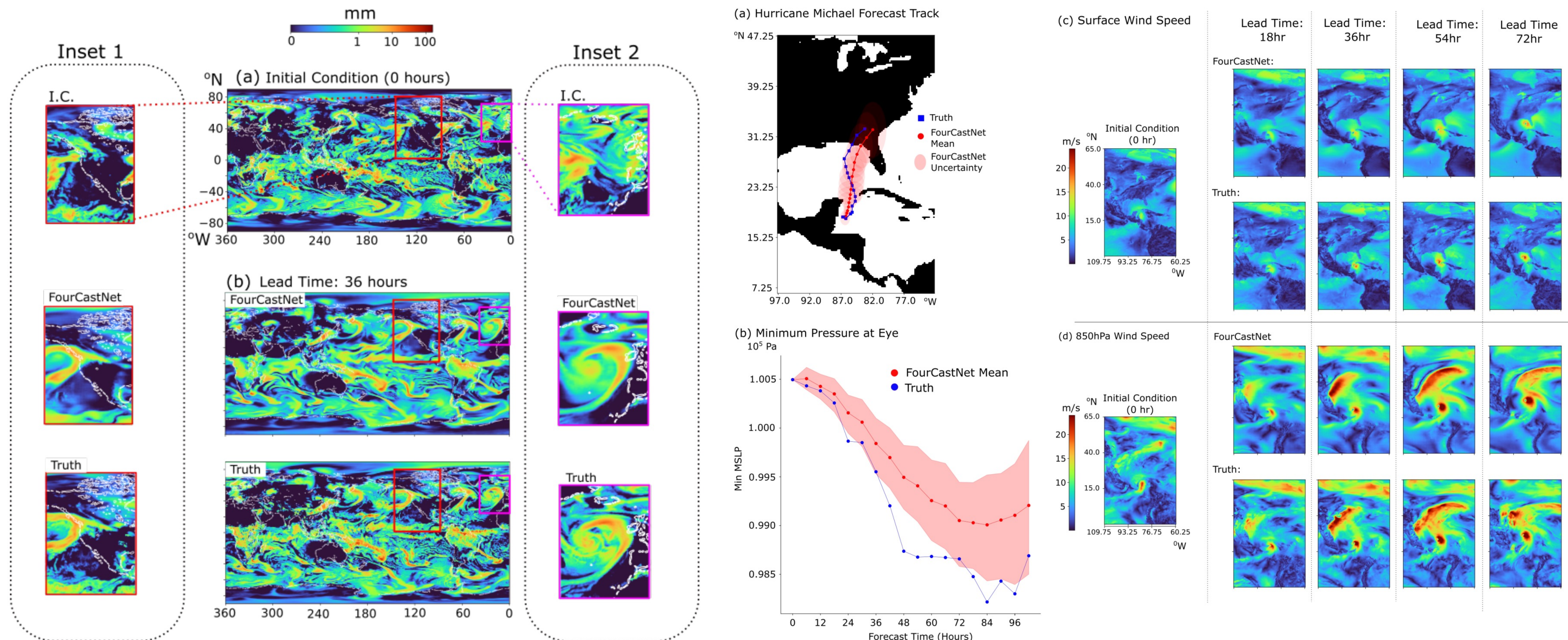
Definition 3 (Fourier integral operator $\mathcal{K}$) Define the Fourier integral operator

$$(\mathcal{K}(\phi) v_t)(x) = \mathcal{F}^{-1} \left(R_\phi \cdot (\mathcal{F} v_t) \right)(x) \quad \forall x \in D \quad (4)$$

FourCastNet: A Global Data-driven High-resolution Weather Model using Adaptive Fourier Neural Operators

<https://arxiv.org/abs/2202.11214>

NVIDIA, Lawrence Berkley National Lab, University of Michigan, Rice University, Caltech, Purdue University



FOURCASTNET: A GLOBAL DATA-DRIVEN HIGH-RESOLUTION WEATHER MODEL USING ADAPTIVE FOURIER NEURAL OPERATORS

■ Contribution

■ Super Accuracy

- Outperforming IFS for small-scale precipitation prediction within 48hr.
- FourCastNet resolves extreme events such as tropical cyclones and atmospheric rivers that prior DL models are failed owing to their coarser grids

■ Super Fast

- FourCastNet is about 45000 times faster than traditional NWP models on a node-hour basis.
- Enabling the generation of very large ensembles (1000+)
- FourCastNet generates a week-long forecast in less than 2 seconds, enabling rapid testing.

■ Super Efficient and Scalable

- Once trained FourCastNet uses about 12,000 times less energy to generate a forecast than the IFS model
- FourCastNet has 8 times greater resolution than the SOTA DL model.

■ Method

■ Training Time: 16 hours on a 64 NVIDIA A100 GPUs cluster.

■ Training Data: ERA5 Reanalysis dataset ([link](#))

- FourCastNet selects 20 variables at 5 vertical levels every 6 hours.
- Training 54020 samples; Validation 2920 samples; Testing ~1k samples;
- Resolution: 30km x 30km (720 x 1440 pixels x 20 variables), 8x8 patches

■ Comparison with NWP Model: ECMWF IFS

- has 150+ variables at 50+ vertical levels, 50 ensembles.

■ Model:

- Adaptive Fourier Neural Operator (AFNO) model with Fourier transform-based token-mixing scheme [Guibas et al., 2022]
- Vision transformer (ViT) backbone [Dosovitskiy et al., 2021].
 - convolutional architectures showed poor performance on capturing small scales over many time steps in auto-regressive inference

■ Note that Earth-2

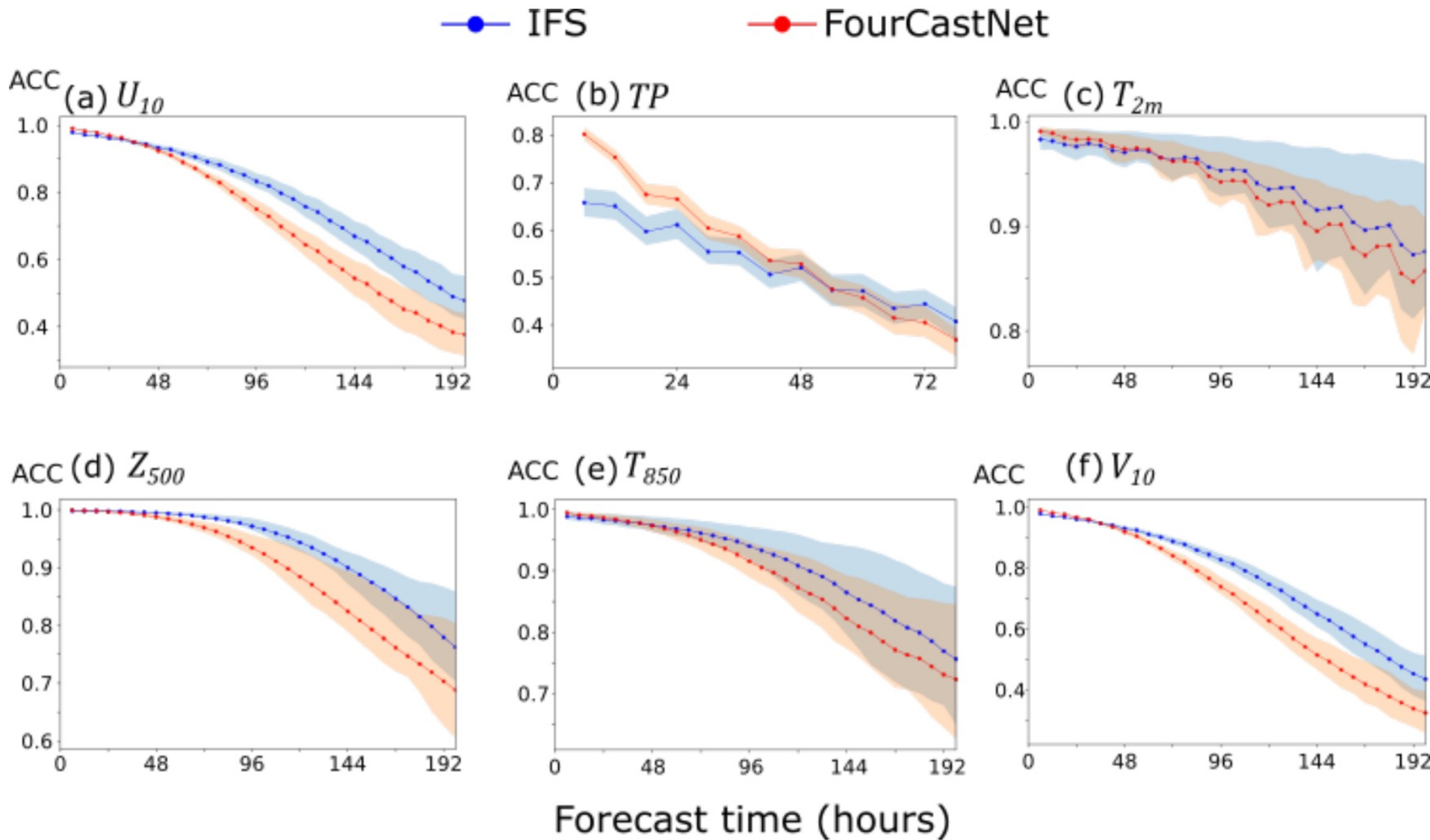
- Use to help NWP, and will not possible to replace NWP. (at least for now)
- has no Physics-Informed yet. (possible in future work)
- Build on top Pytorch, not Modulus and Omniverse yet. (possible in future work)

Vertical Level	Variables
Surface	$U_{10}, V_{10}, T_{2m}, sp, mslp$
1000hPa	U, V, Z
850hPa	T, U, V, Z, RH
500hPa	T, U, V, Z, RH
50hPa	Z
Integrated	$TCWV$

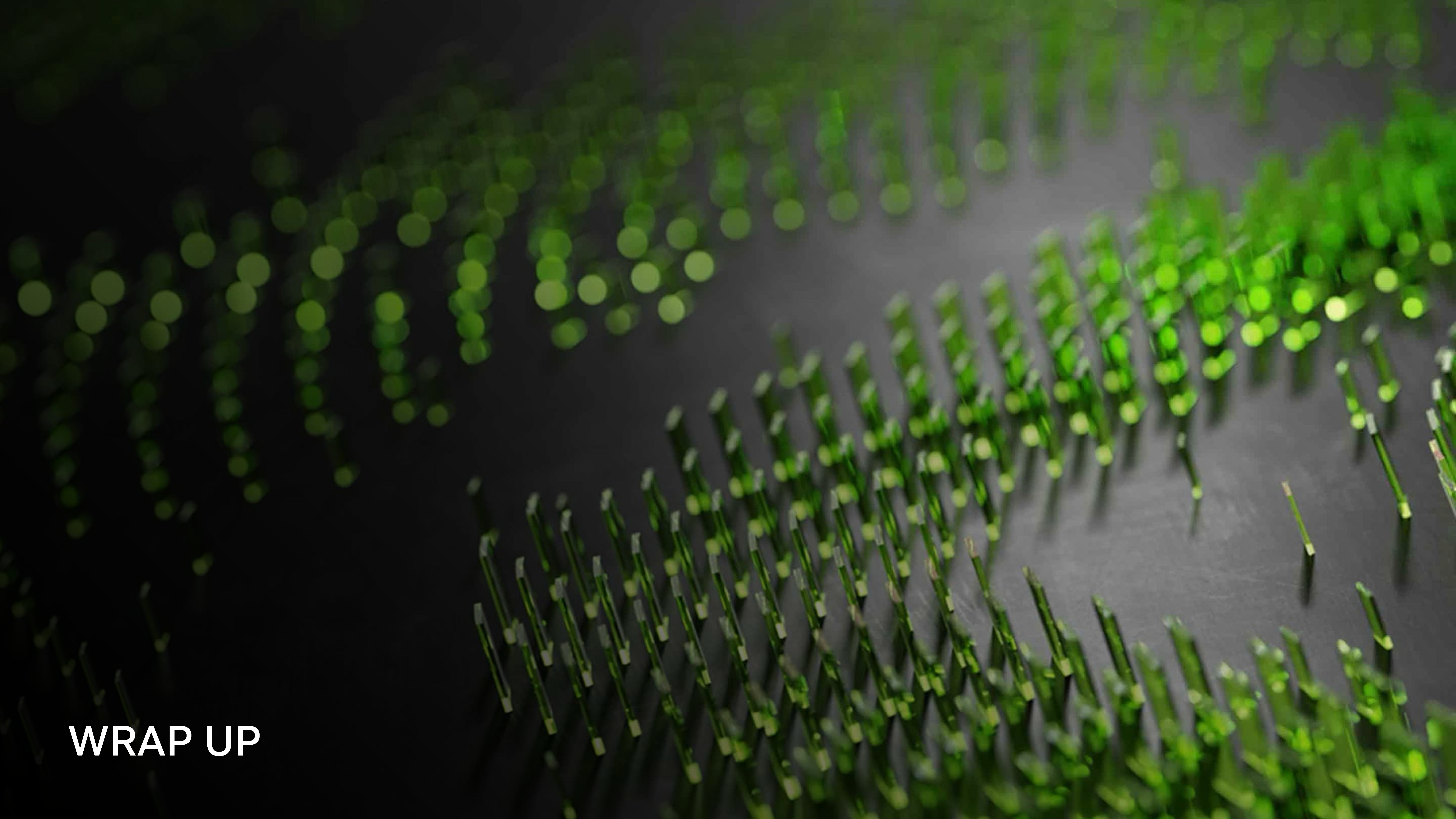
FourCastNet: A Global Data-driven High-resolution Weather Model using Adaptive Fourier Neural Operators

<https://arxiv.org/abs/2202.11214>

NVIDIA, Lawrence Berkley National Lab, University of Michigan, Rice University, Caltech, Purdue University



Latency and Energy consumption for a 24-hour 100-member ensemble forecast				
	IFS	FCN - 30km (actual)	FCN - 18km (extrapolated)	IFS / FCN(18km) Ratio
Nodes required	3060	1	2	1530
Latency (Node-seconds)	984000	7	22	44727
Energy Consumed (kJ)	271000	7	22	12318



WRAP UP

How does Modulus compliment PyTorch?

Features that can aid data and/or physics driven problems

Data & Physics oriented utils

- Performance Enhancements

CUDA graphs, kernel fusion, JIT compilation, data parallelism, model parallel, etc.

- Pre-built Network Architectures

Diffusion Models, Neural Hash Encoding, Neural Operators, Graph Networks, DCT-RNN, several variants of MLPs etc.

- Hydra Configuration

Hyper-parameter tuning and customization

- Data Pipeline

For very large data-driven problems using Zarr, NVComp, GDS

- Data and Inference Tools

Pre-defined datasets for common data formats (VTK, HDF5, ...). Model export functions to TensorRT and Triton

- Integration with Other Products

Omniverse, PySDF, NVFuser, Triton, Tensor RT, DALI, Warp, etc.

Physics oriented utils

- Geometry Module

Integrated, parameterized geometry module with point cloud/SDF

- Symbolic PDE Loss Construction

Automated PDE loss construction using SymPy API

- Automated Optimized Gradient Calculations

Automatic gradient calculations for physics-informed learning with optimizations such as FuncTorch, AMP16, mesh free derivatives etc.

- Convergence and Stabilization Methods

Mass balance control planes, loss balancing schemes, AdaHessian support, learning rate annealing, etc.

- Exact Boundary Enforcement

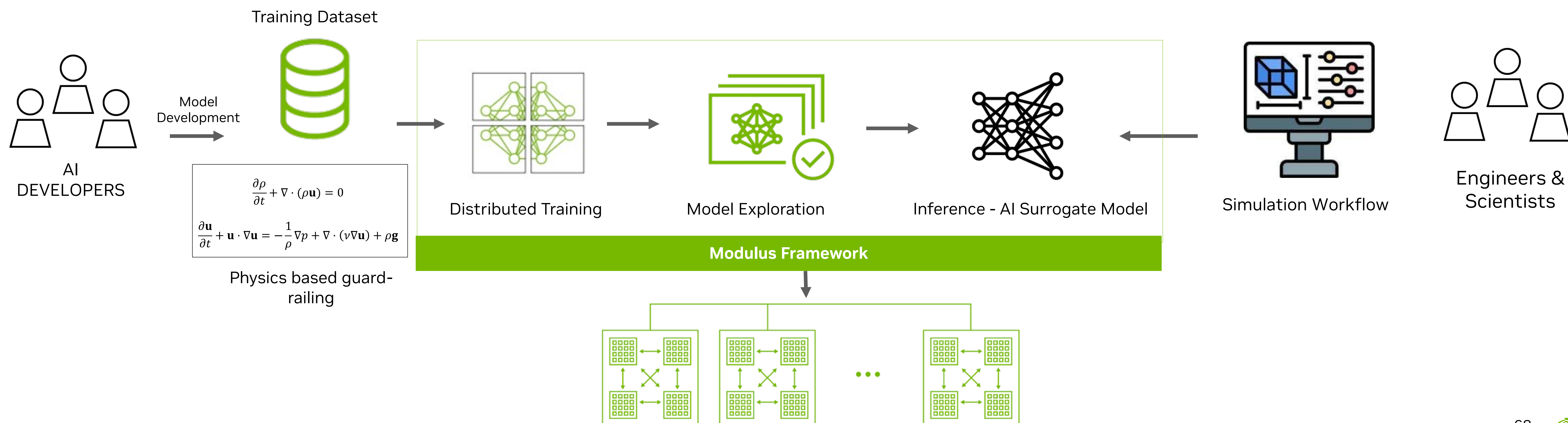
Exact enforcement of continuity or boundary conditions

- Variational Learning

Solving PDE systems using variational formulations

Summary: Modulus Framework

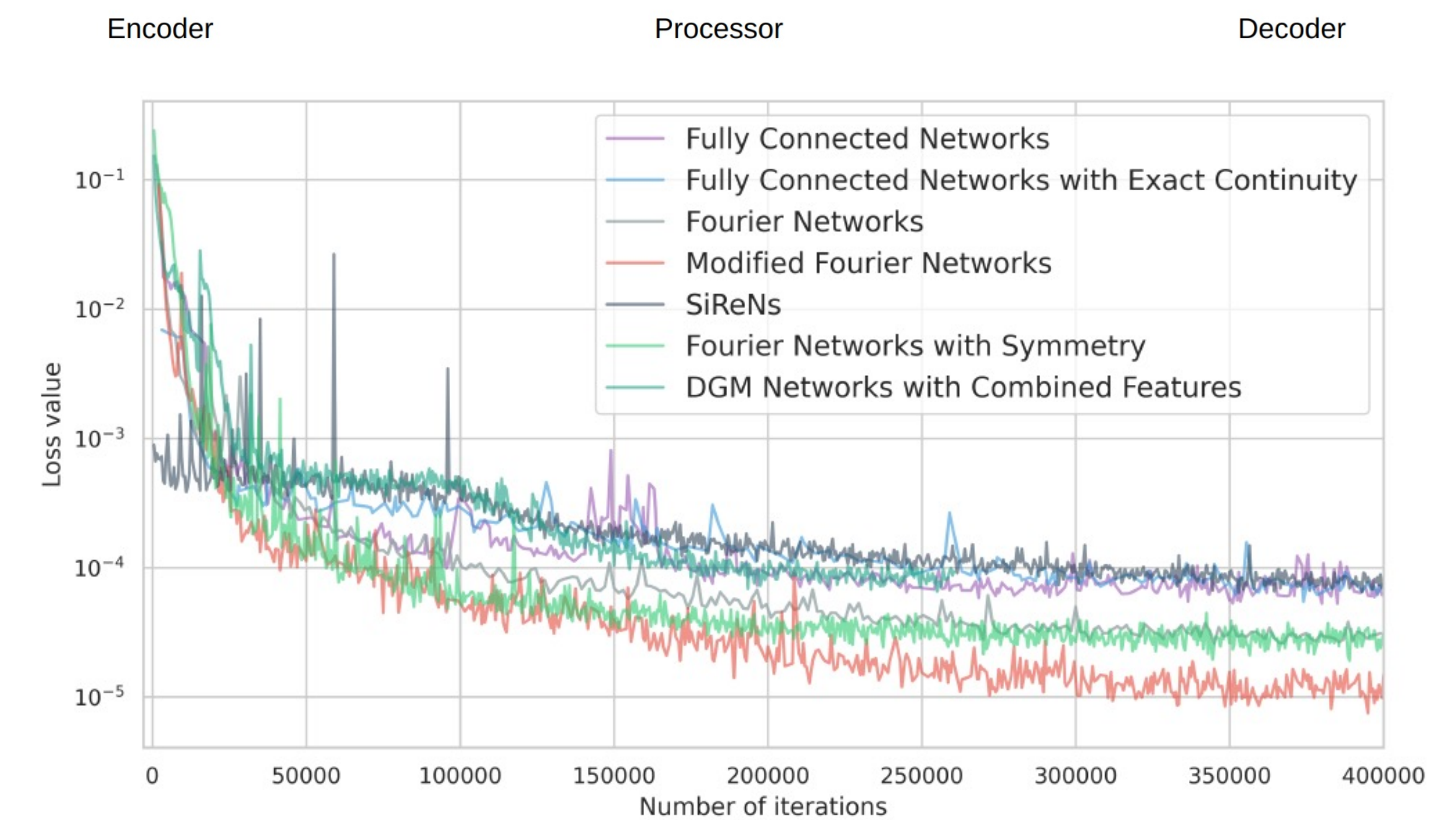
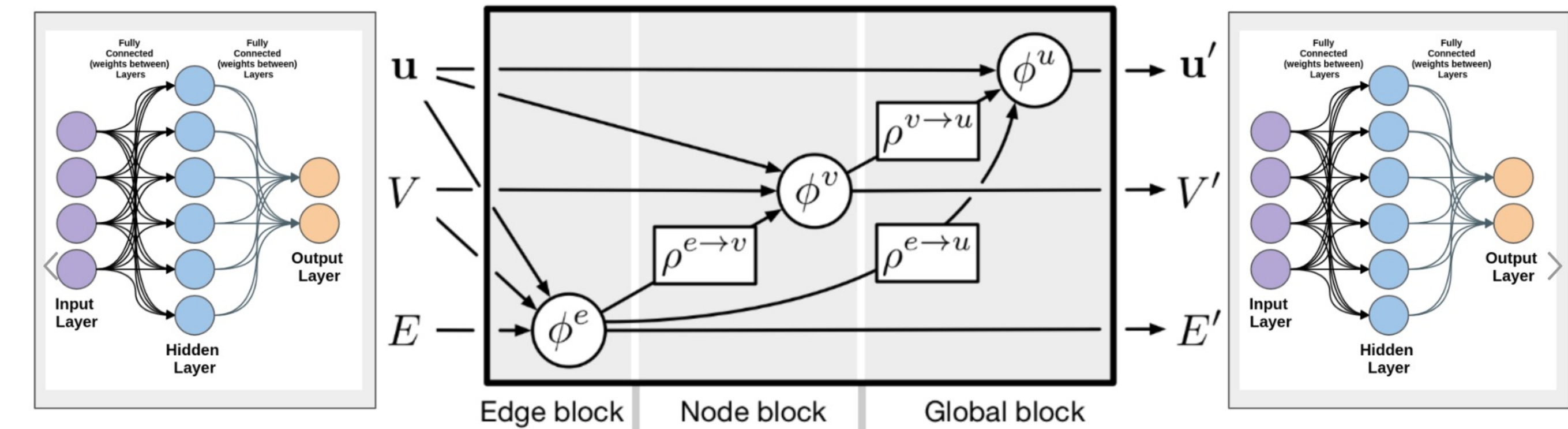
- Modulus is a framework to build and customize Physics-ML models and training workflows:
 - Built on top of PyTorch, interoperable with PyTorch
 - Utilities designed to enable DL researchers as well as Domain experts
 - A vast library of optimized models particularly suited for Physics-ML applications
 - Develop performant and scalable training pipelines with ease
 - Utilities to introduce Physics-based guard-railing
 - Several case studies across different domains to enable transition from POC to Industrial problems
 - Open Source and accessible via GitHub, NGC registry, PyPi



Summary: Modulus Framework

Variety of model architectures

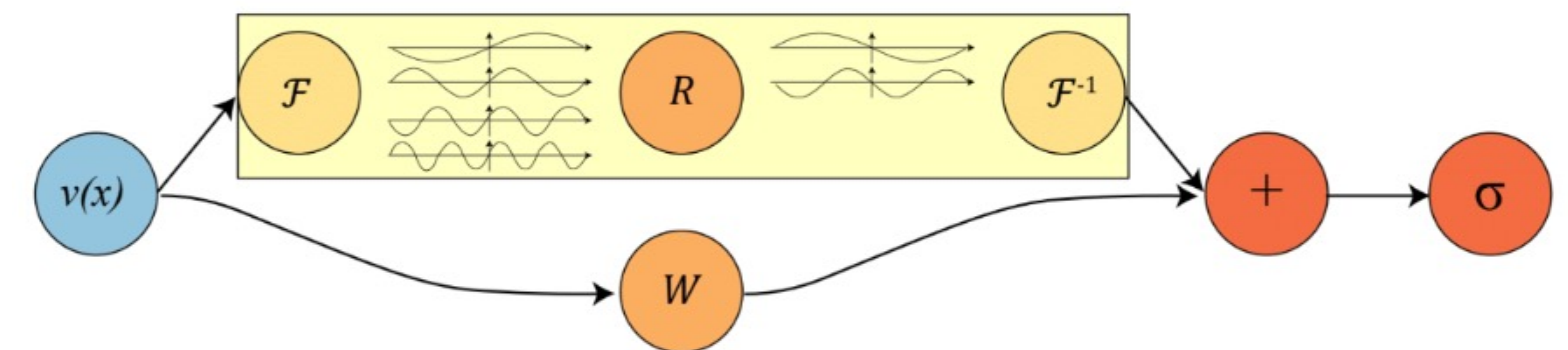
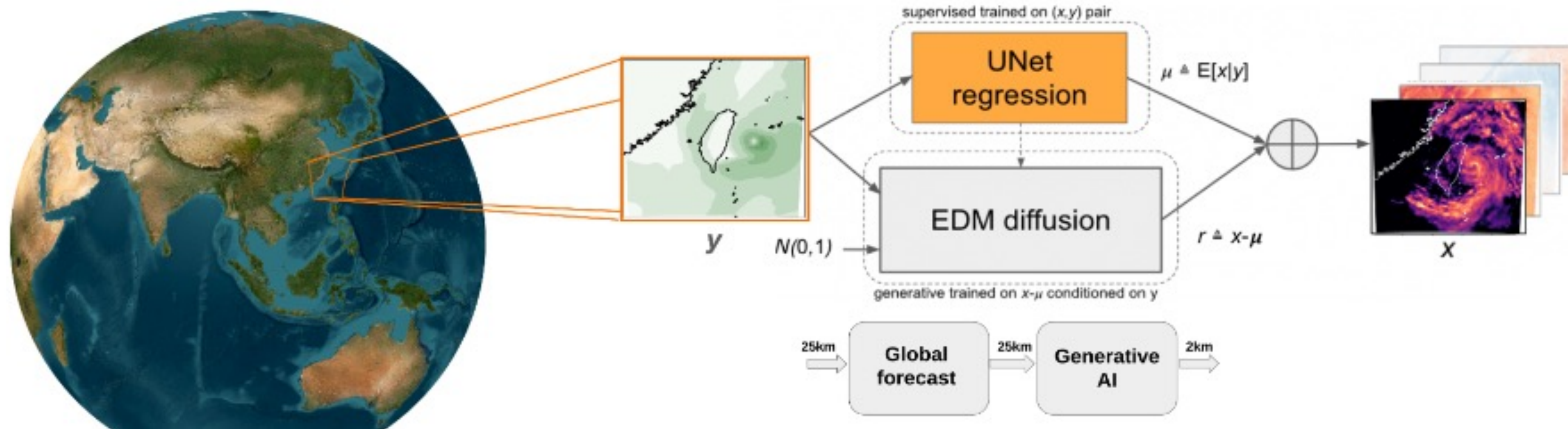
- Modulus Model Zoo - Diverse Physics-ML approaches:
 - Fully Physics driven AI models
 - Fully data driven AI models
 - Hybrid (data + Physics) AI models
- Models like GNNs, RNNs, Diffusion Models, Neural Operators (FNO, DeepONet, etc.), MLPs and its variants available to use out-of-the-box or use optimized layers and components in your custom models
- Modulus Model enable features like:
 - Argument-less checkpoint loading
 - Model registry
 - ...



12.5x super-resolution + radar channel synthesis

FEATURES:
ERA5:
36 x 36 (20-ch)

TARGETS:
Radar-assimilating WRF
448x448 (4-ch)

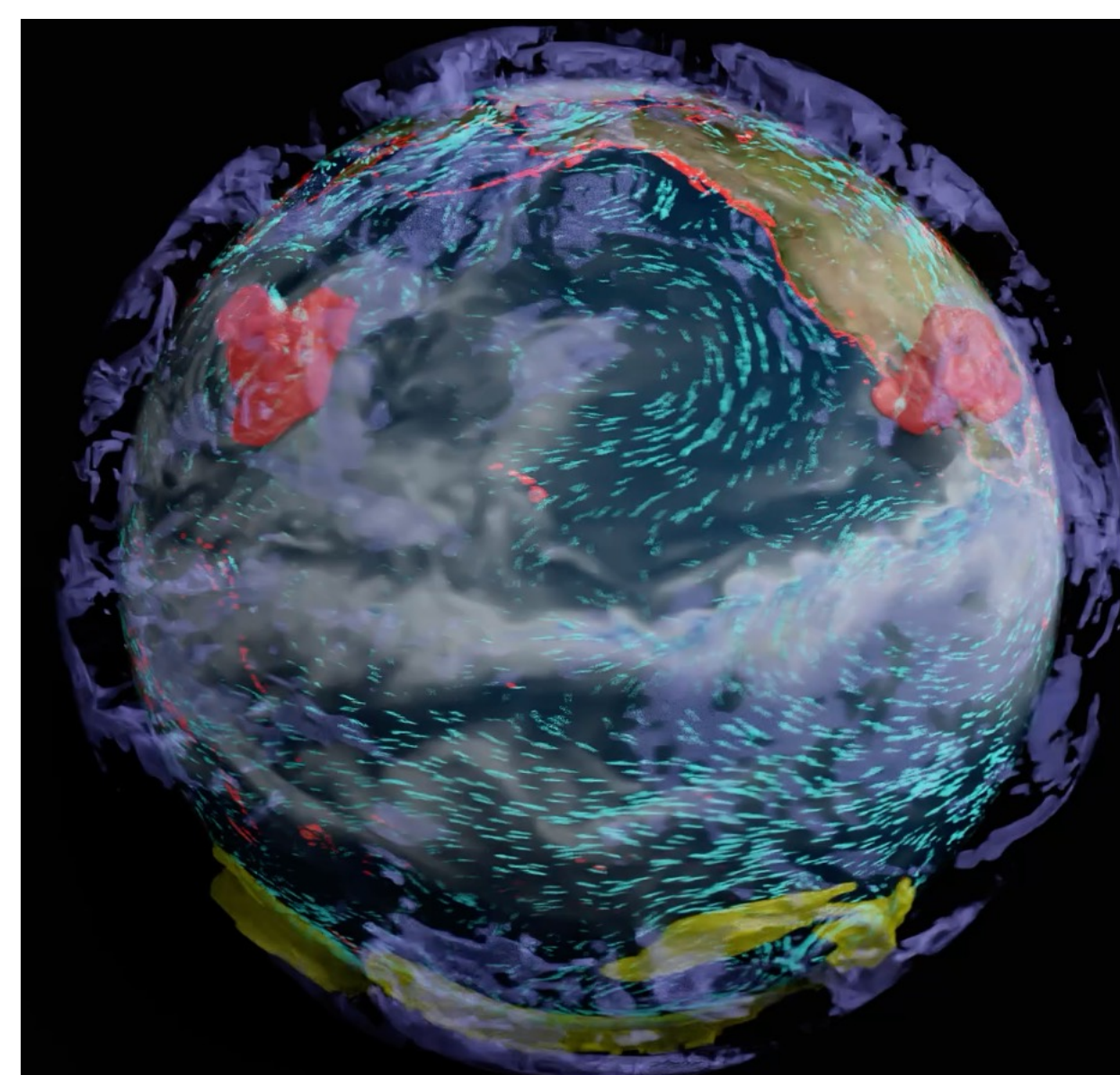


Summary: Modulus Framework

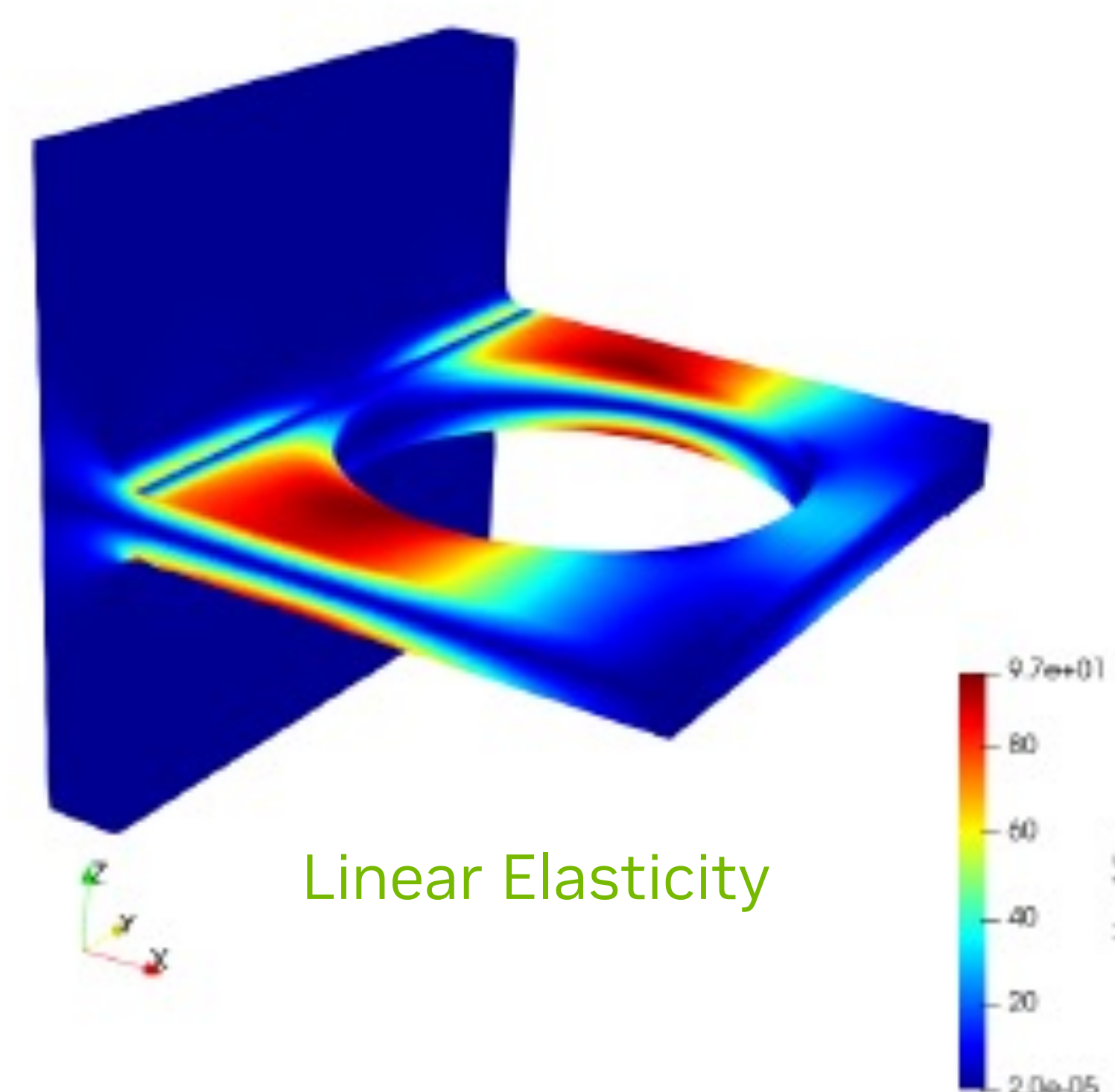
Variety of physics applications

- Sample case studies and use cases covering diverse physical domains like:

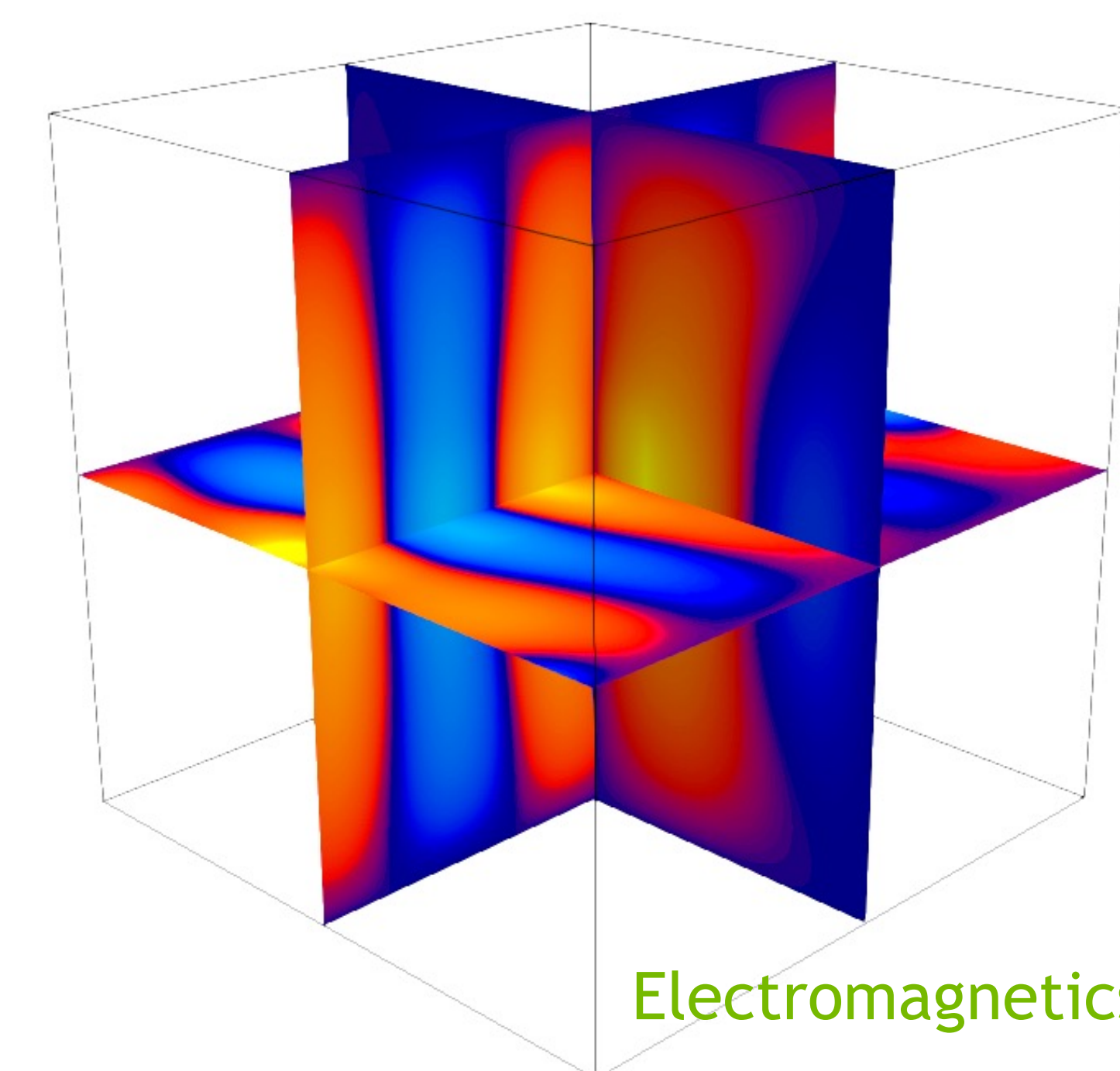
- Fluid dynamics
- Heat transfer
- Acoustics and waveform inversion
- Linear Elasticity
- Molecular Dynamics
- Electromagnetics
- Turbulence modeling
- Weather and climate modeling
- And more....



Weather/climate modeling

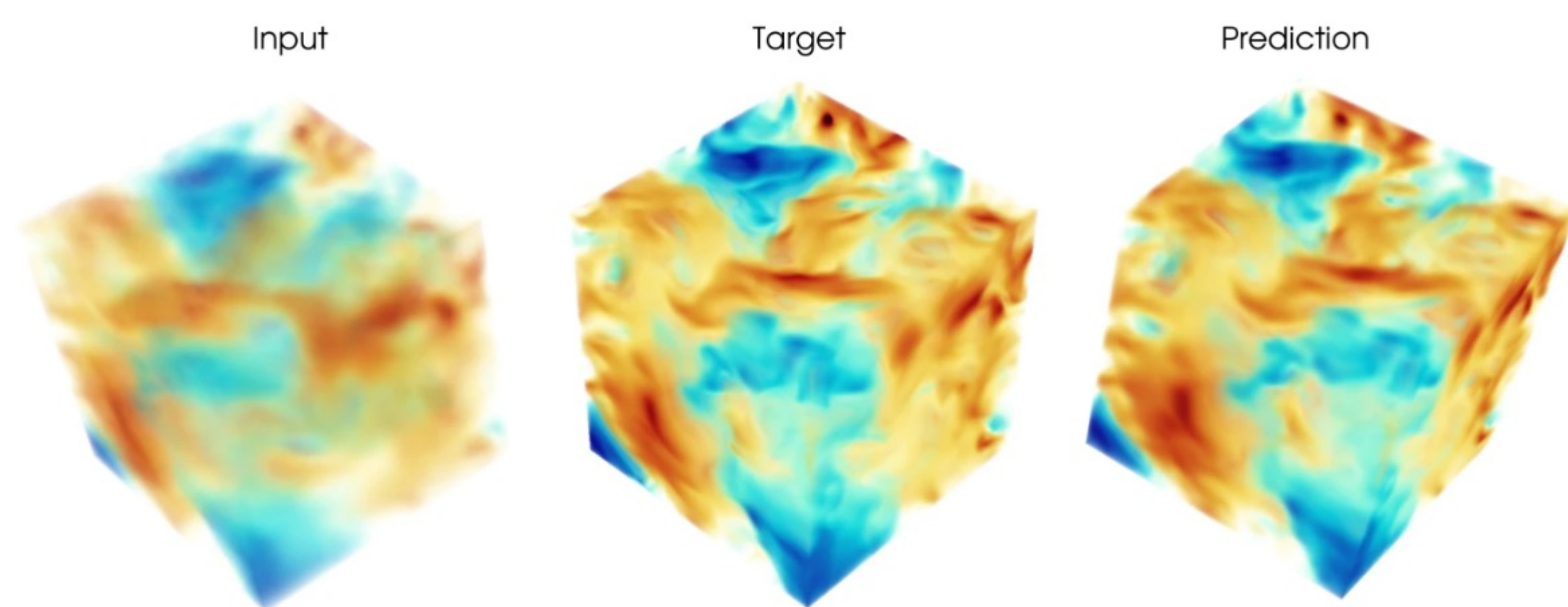


Linear Elasticity



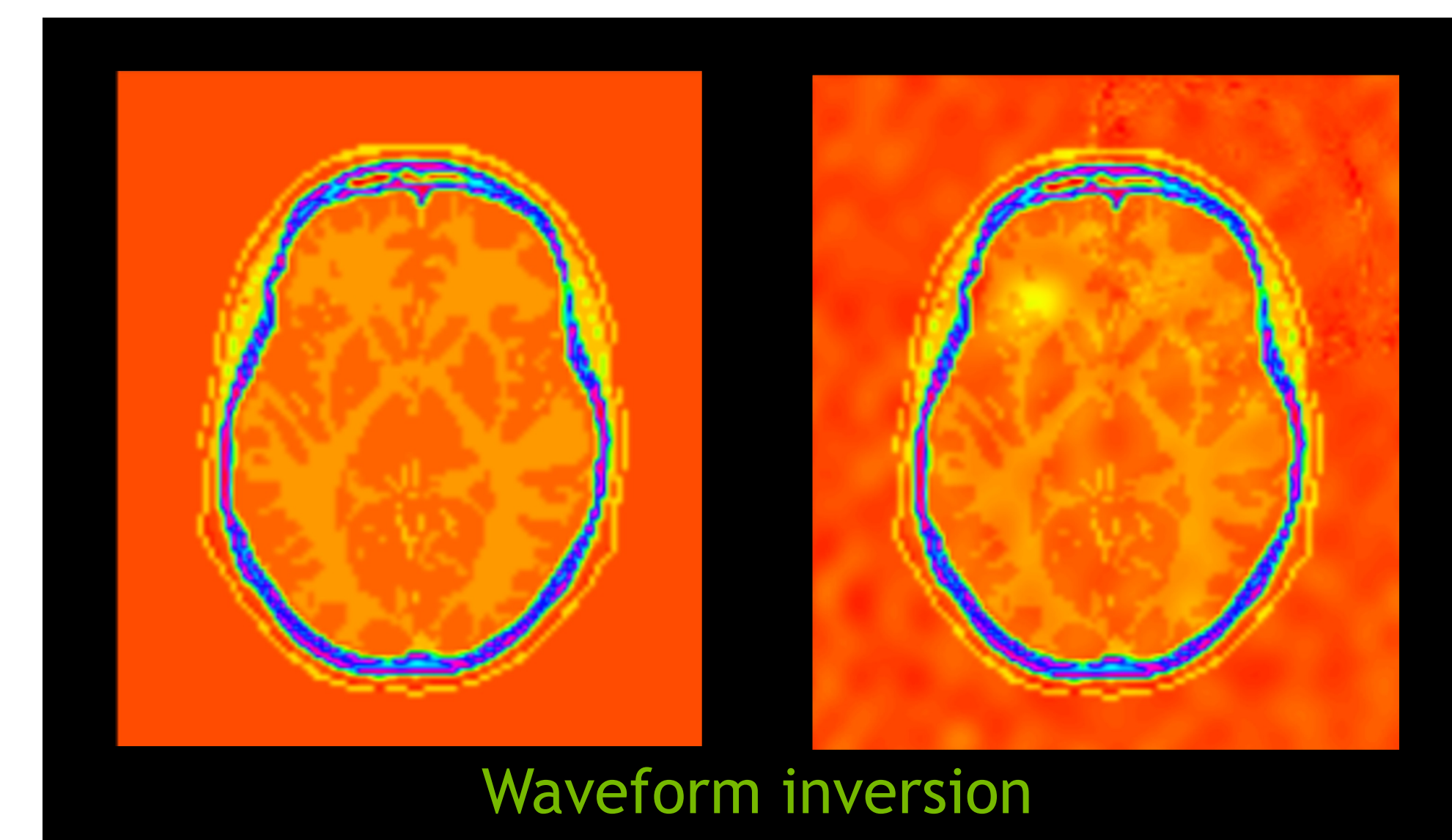
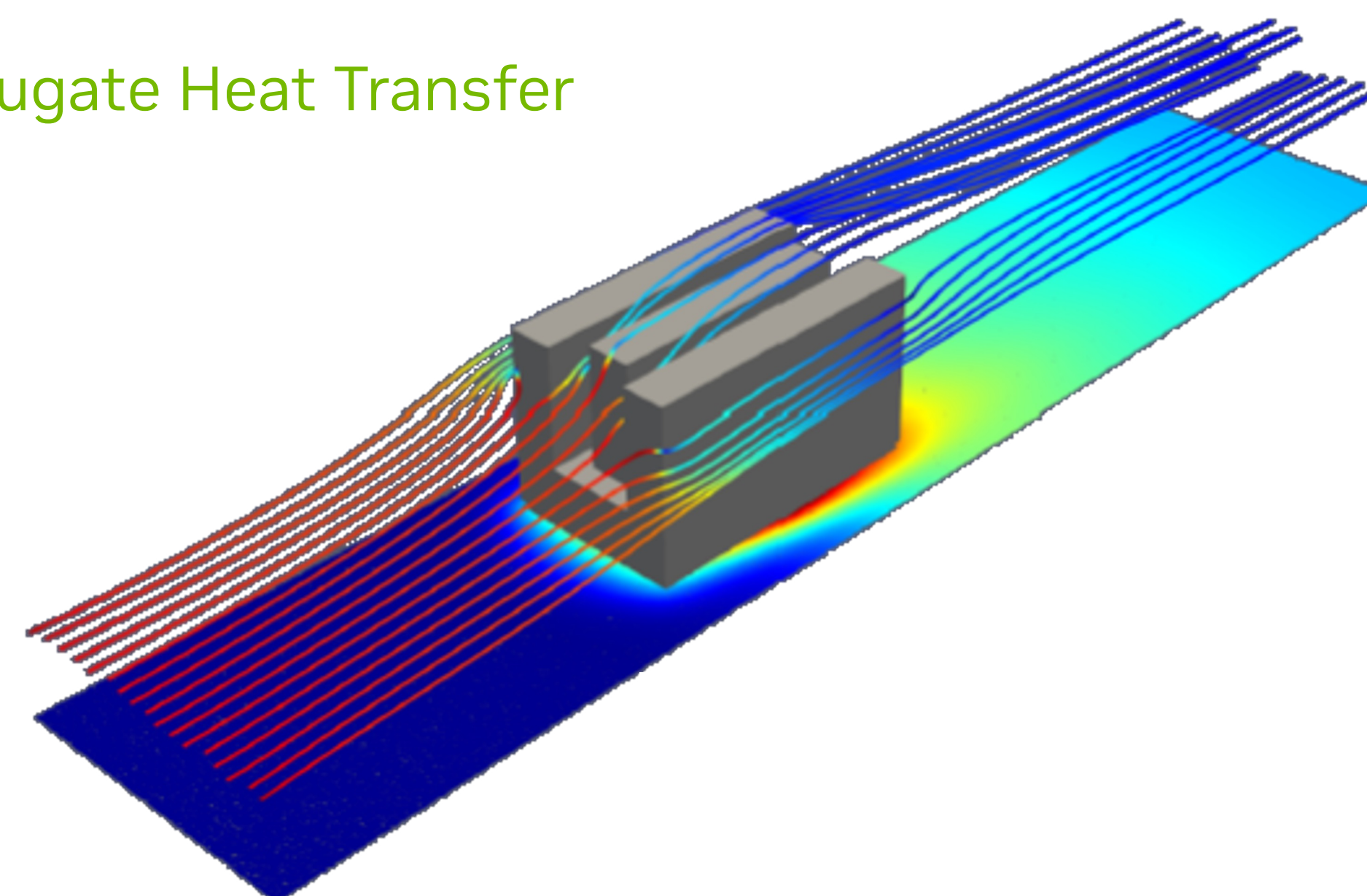
Electromagnetics

- Reference samples for [Modulus](#), and [Modulus-Sym](#)



Turbulence Super Resolution

Conjugate Heat Transfer

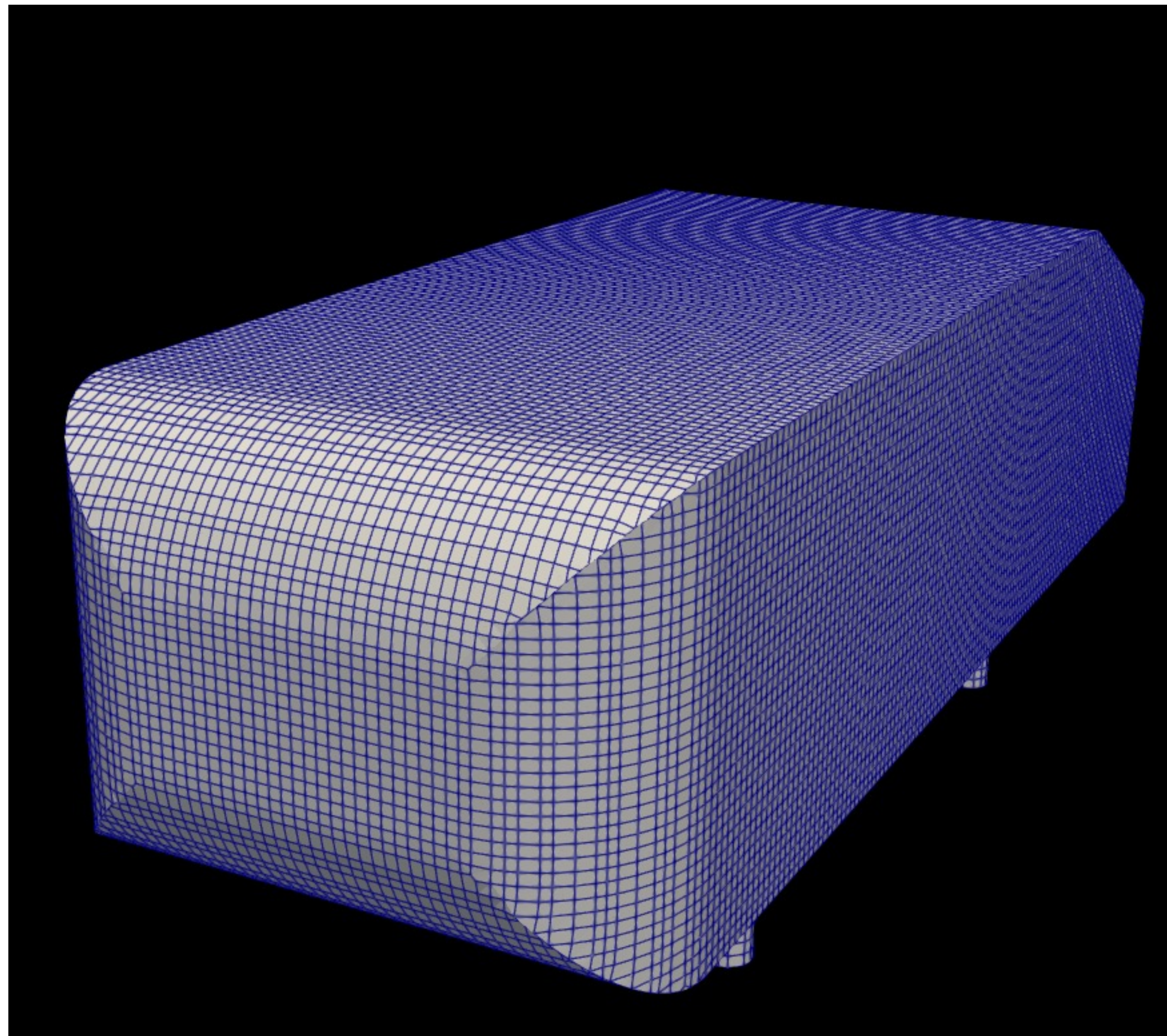


Waveform inversion

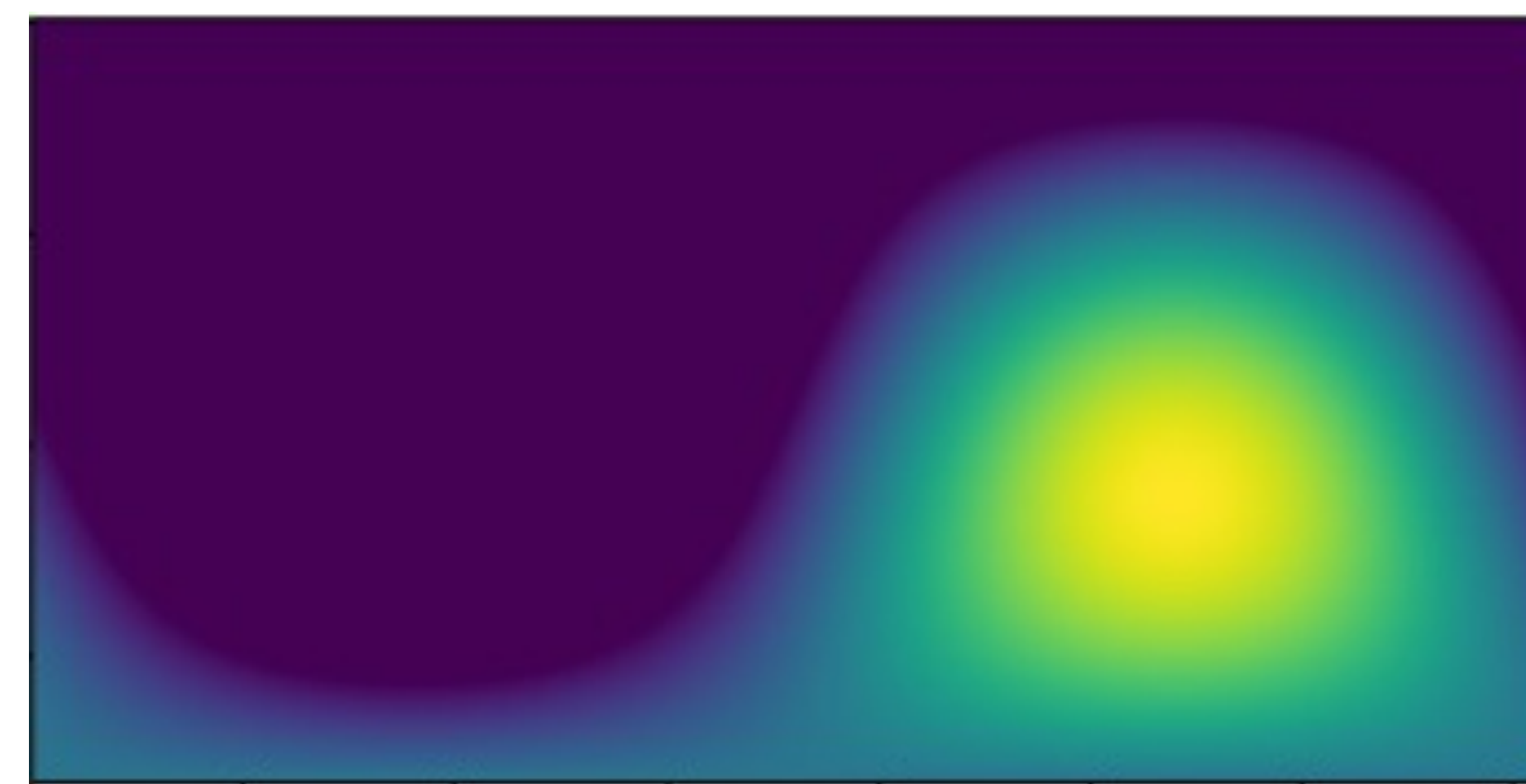
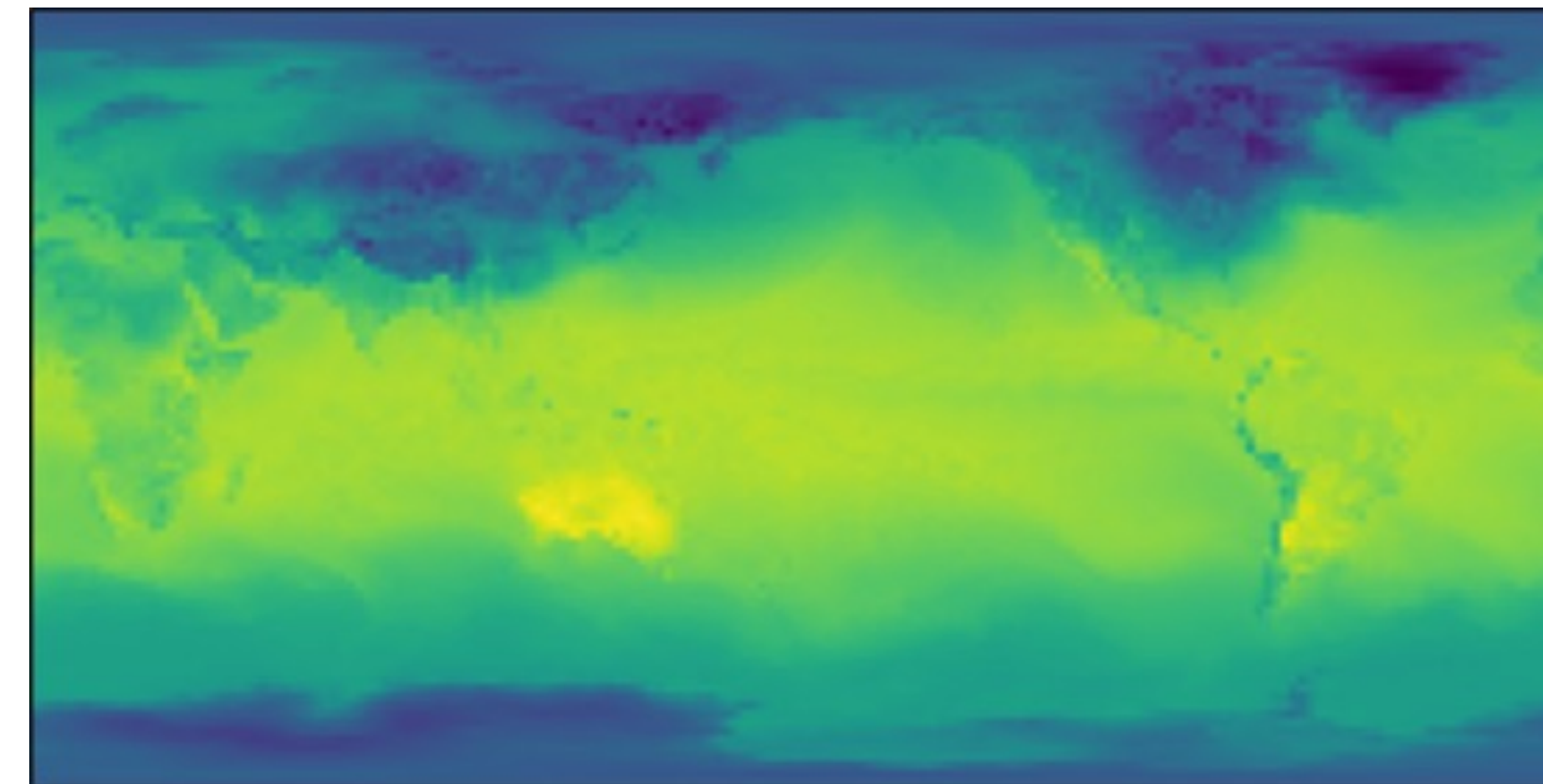
Summary: Modulus Framework

Variety of data handling

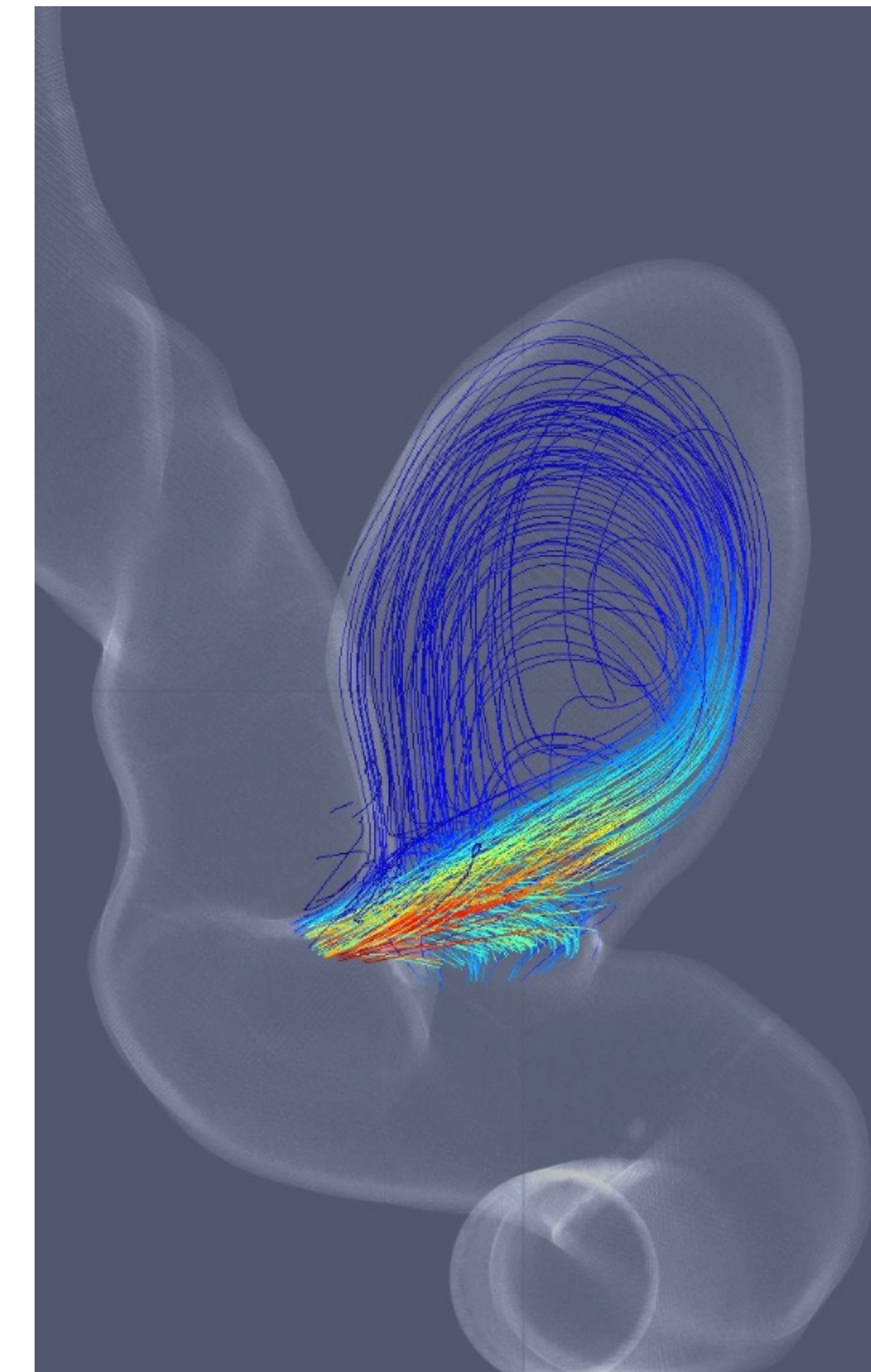
- Optimized datasets and data loaders to work with:
 - Point Clouds
 - Constructive Solid Geometry
 - STL
 - Grid Based
 - Graph/Mesh Based



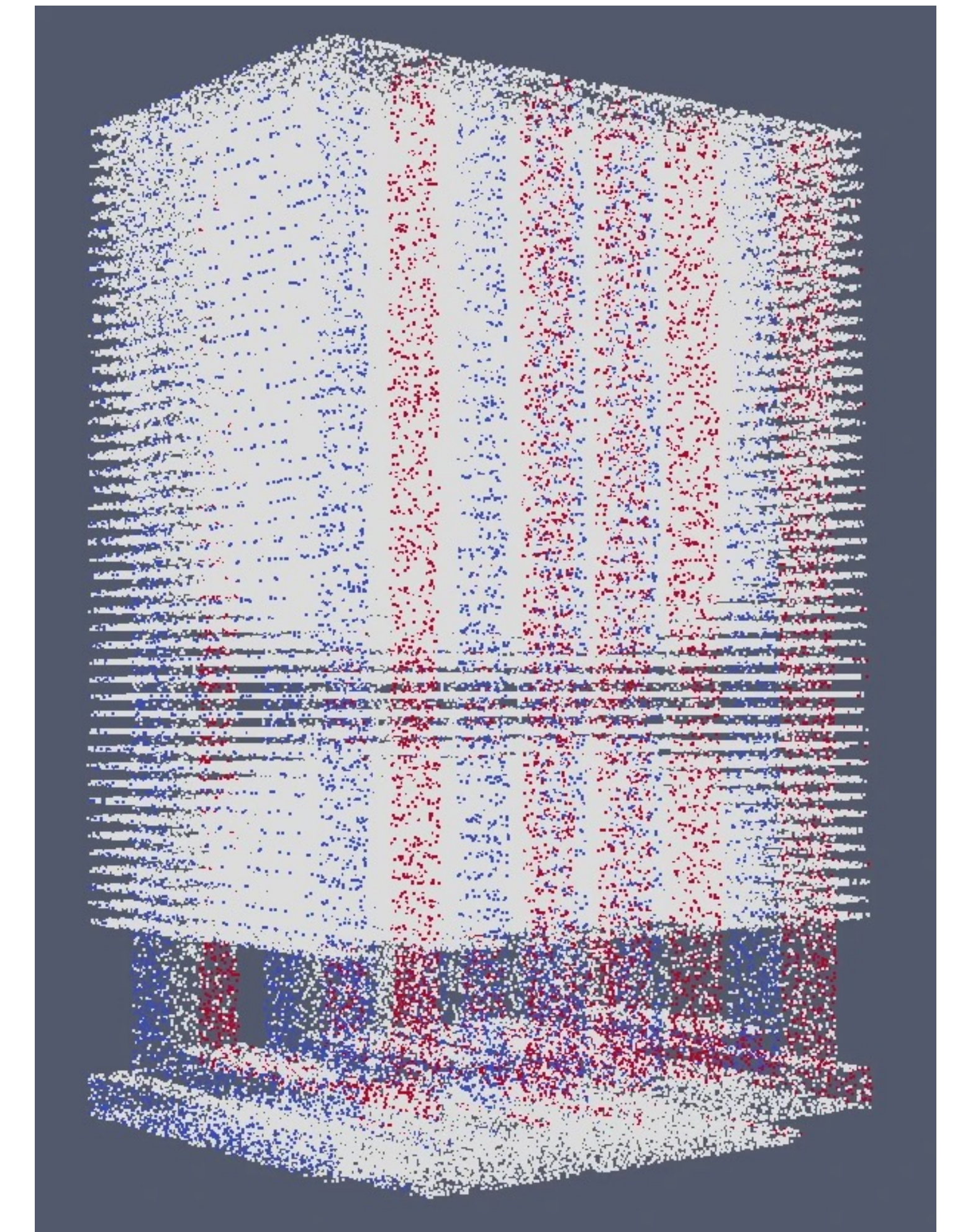
Ahmed body dataset and data loader
(graph)



Weather/climate data loaders (grid)



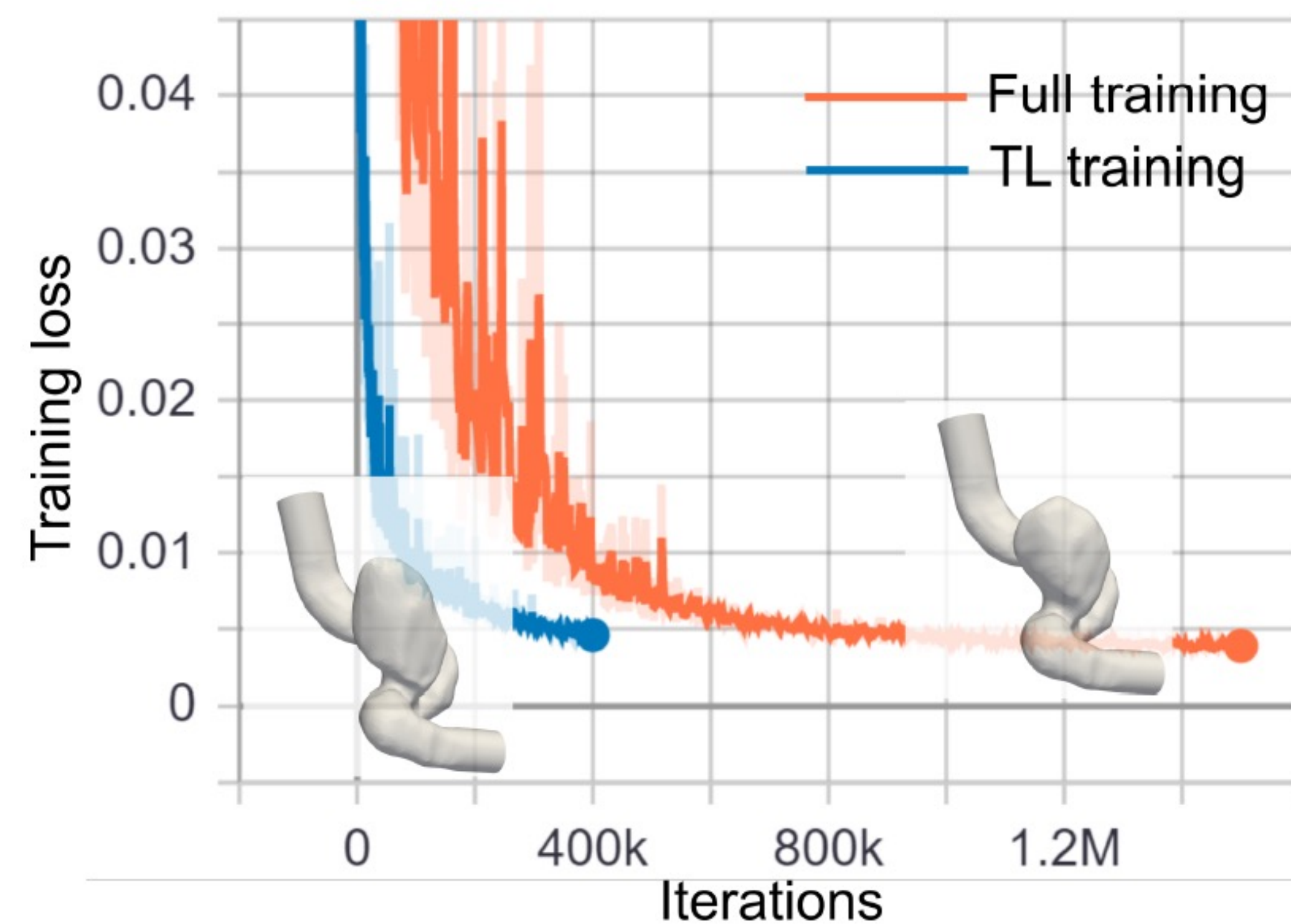
STL and Constructive Solid Geometry (point cloud)



Summary: Modulus Framework

Other miscellaneous features

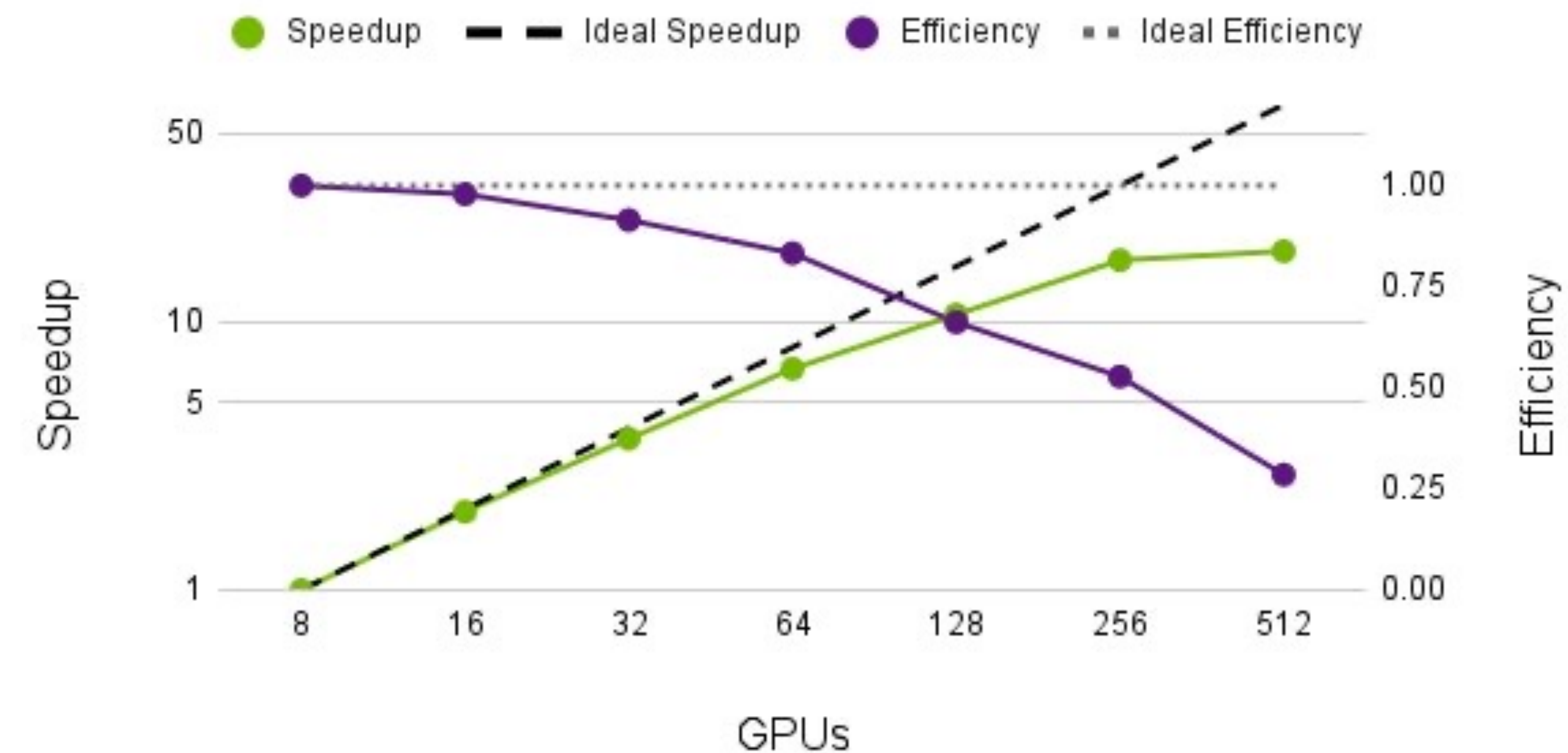
- Distributed utils
- Performance and scaling utils:
 - Abstractions for AMP, CUDA Graphs, JIT
 - Multi-GPU/Multi-Node scaling
 - Gradient aggregation
- Training features:
 - Support for several optimizers
 - Etc.



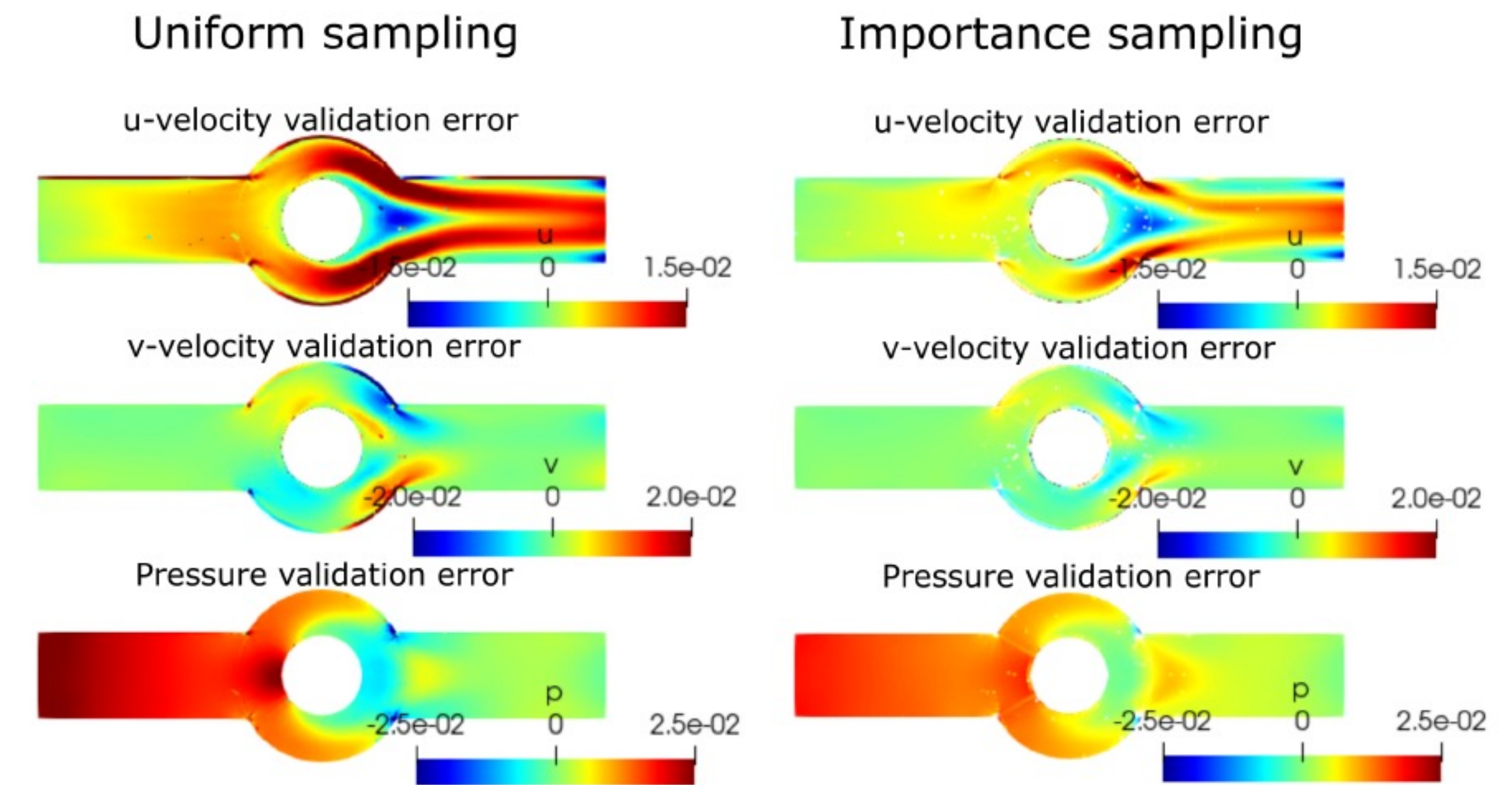
STL geometry and Transfer Learning

3D Taylor Green strong scaling

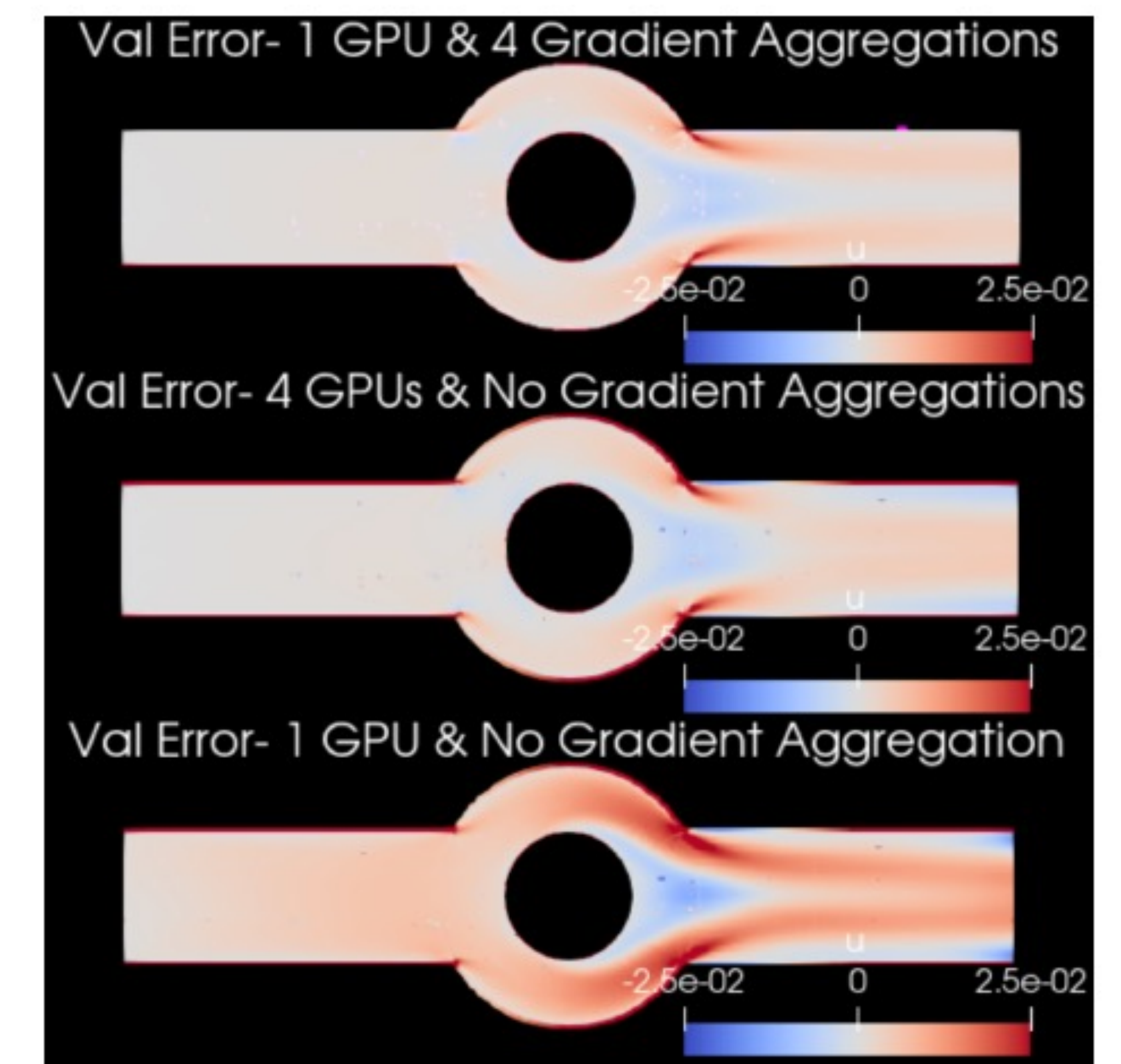
DGX A100 80G



Mult-GPU, Multi-Node scaling



Importance sampling



Gradient Aggregation

Modulus access

Availability via PyPi, NGC Container registry and GitHub

- Download [Modulus Docker Container](#)

```
docker run --gpus all -it nvidia/modulus/modulus:24.01 bash
```

- Download [Modulus via PyPi](#)

```
pip install nvidia-modulus nvidia-modulus.sym
```

- Develop using Modulus ([OSS on GitHub](#))

```
git clone https://github.com/NVIDIA/modulus.git
```


Modulus NGC resources

Pre-trained checkpoints, datasets and resources available via NGC to enable scientific exploration

Models

The NGC catalog offers 100s of pre-trained models for computer vision, speech, recommendation, and more. Bring AI faster to market by using these models as-is or quickly build proprietary models with a fraction of your custom data.

Modulus

Sort: Alphabetic (A-Z)

Use Case

- ☐ High Performance Computing 7
- ☐ Forecasting 4
- ☐ Simulation and Modeling 4
- ☐ Graph Neural Networks 2

NVIDIA AI Enterprise Support ⓘ N...

NVIDIA Platform

- ☐ Modulus 7
- ☐ PyTorch 1

NVIDIA AI Enterprise Exclusive No ...

Framework

Industry

Solution

Publisher

Language No results found

Other No results found

Displaying 8 models



Modulus Checkpoints: Ahmed Body Mes...
MeshGraphNet model package for external aerodynamics evaluation of Ahmed body-type geometries.

[View Labels](#) [Learn More](#)



Modulus Checkpoints: DLWP Cubesphere
DLWP Cubesphere model checkpoint package. DLWP is a light-weight deep learning model for weather prediction th...

[View Labels](#) [Learn More](#)



Modulus Checkpoints: Earth-2 MIP Diag...
Diagnostic model checkpoints for Earth-2 MIP.

[Learn More](#)



Modulus Checkpoints: FourCastNet
FourCastNet model checkpoint package. FourCastNet is a deep learning model for weather prediction that uses Adaptive...

[View Labels](#) [Learn More](#)



Modulus Checkpoints: FourCastNet V2 ...
FourCastNet V2 (small) model checkpoint package. FourCastNet V2 is a deep learning model for weather prediction th...

[View Labels](#) [Learn More](#)



Modulus CHT PINN MLP
Parameterized PINN that uses MLP layers and incorporates PDEs in the loss function. You can incorporate Fourier...

[View Labels](#) [Learn More](#)

[Modulus Models on NGC](#)
Pre-trained model packages

Resources

The NGC catalog offers step-by-step instructions and scripts through Jupyter Notebooks for various use cases, including machine learning, computer vision, and conversational AI. These resources help you examine, understand, customize, test, and build AI faster, while taking advantage of best practices.

Modulus

Sort: Alphabetic (A-Z)

Use Case

- ☐ Simulation and Modeling 6
- ☐ Graph Neural Networks 5
- ☐ High Performance Computing 4
- ☐ Forecasting 3

NVIDIA Platform

- ☐ Modulus 7
- ☐ PyTorch 2
- ☐ Deep Graph Library 1

NVIDIA AI Enterprise Support ⓘ

- ☐ Yes 1

NVIDIA AI Enterprise Exclusive No ...

Quick Deploy ⓘ No results found

Framework

Industry

Solution

Publisher

Type

Language

Other No results found

Displaying 7 resources



Modulus Datasets: Ahmed Body Aerody...
Preview dataset for the Ahmed body aerodynamics with parameterized shapes and variable Reynolds number

[View Labels](#) [Learn More](#)



Modulus Datasets: Cardiovascular Simu...
The dataset includes 310 simulations obtained on 8 patient-specific models with varying inflow and outflow boundar...

☆ NVIDIA AI Enterprise Supported

[View Labels](#) [Learn More](#)



Modulus Datasets: CWA
CWA dataset in Zarr format used in the CorrDiff model:
<https://arxiv.org/pdf/2309.15214.pdf>

[View Labels](#) [Learn More](#)



Modulus Datasets: Stokes Flow
Stokes flow dataset with parameterized domain

[View Labels](#) [Learn More](#)



NVIDIA Modulus Examples Supplement...
This contains all the supplemental data for Modulus examples. This includes files apart from the actual dataset required f...

[View Labels](#) [Learn More](#)



NVIDIA Modulus Reservoir Examples Su...
Supplemental material for reservoir simulation examples using Modulus.

[View Labels](#) [Learn More](#)

[Modulus Resources on NGC](#)
Datasets and supplemental materials

(FREE DLI SELF-PACED
COURSE)

INTRODUCTION TO PHYSICS- INFORMED MACHINE LEARNING WITH MODULUS

[https://learn.nvidia.com/courses/course-
detail?course_id=course-v1:DLI+S-OV-04+V1](https://learn.nvidia.com/courses/course-detail?course_id=course-v1:DLI+S-OV-04+V1)

Self-paced Course

Introduction to Physics-informed Machine Learning with Modulus

Learn how to use NVIDIA Modulus for physics-informed deep learning, and how the Modulus framework integrates with the overall NVIDIA Omniverse platform.

Continue Learning

About Course

Objectives

Topics Covered

Course Outline

Stay Informed

Contact Us

Continue Learning

About this Course

High-fidelity simulations in science and engineering are computationally expensive and time-prohibitive for quick iterative use cases, from design analysis to optimization. NVIDIA Modulus, the physics machine learning platform, turbocharges such use cases by building physics-based deep learning models that are 100,000x faster than traditional methods and offer high-fidelity simulation results.

Upon completion, you will have an understanding of the various building blocks of Modulus and the basics of physics-informed deep learning. You'll also have an understanding of how the

Course Details

Duration: 04:00

Price: Free

Level: Technical - Beginner

Subject: Deep Learning

Language: English

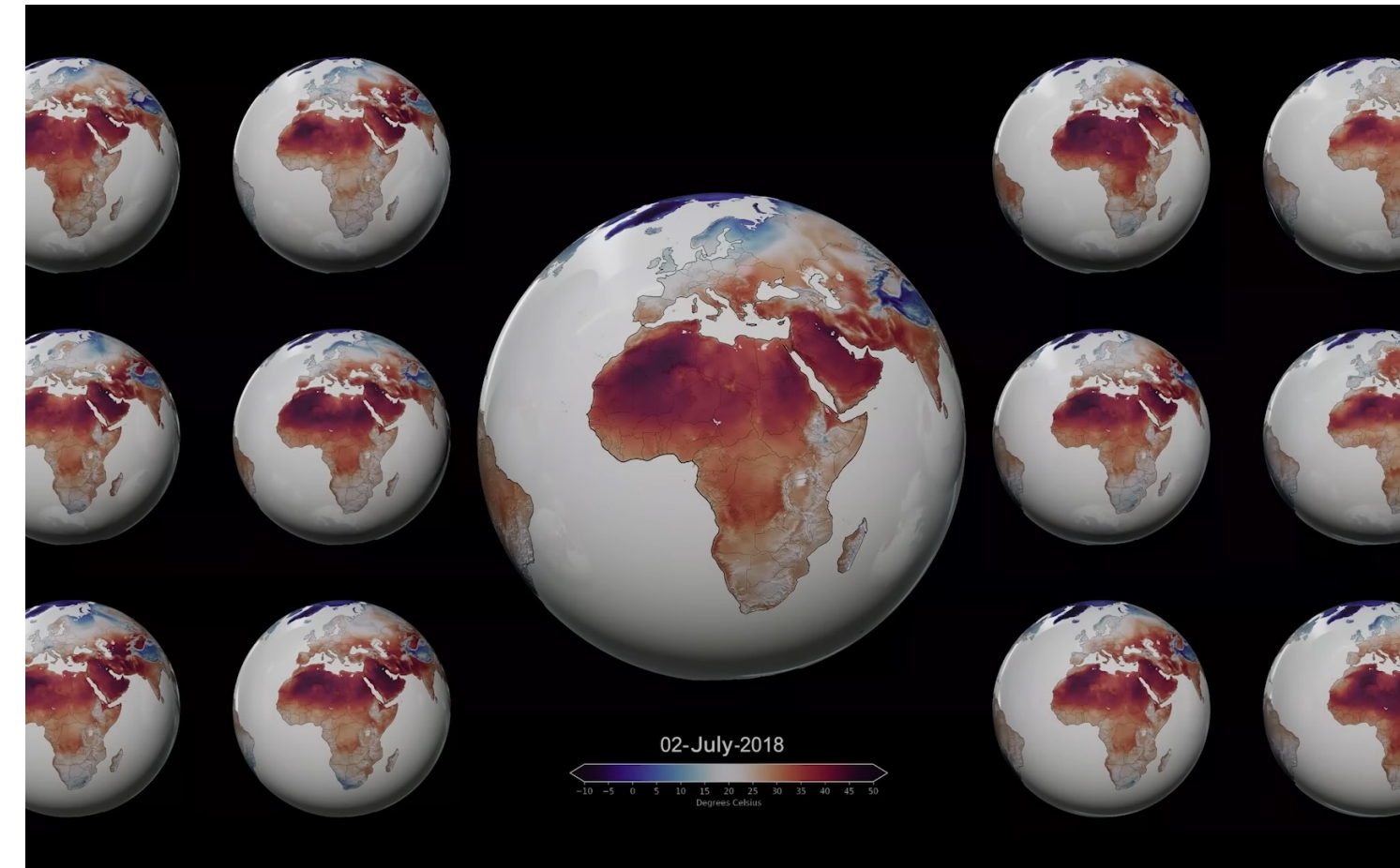
6/26 NCHC End-to-End AI for Science Feedback Survey

FEEDBACK SURVEY

<https://forms.office.com/r/ZJ6a4SjdWT>



Physics-ML Success stories - Modulus Case-Studies



Weather modeling

Demo: [Link 1](#), [Link 2](#), [Link 3](#)



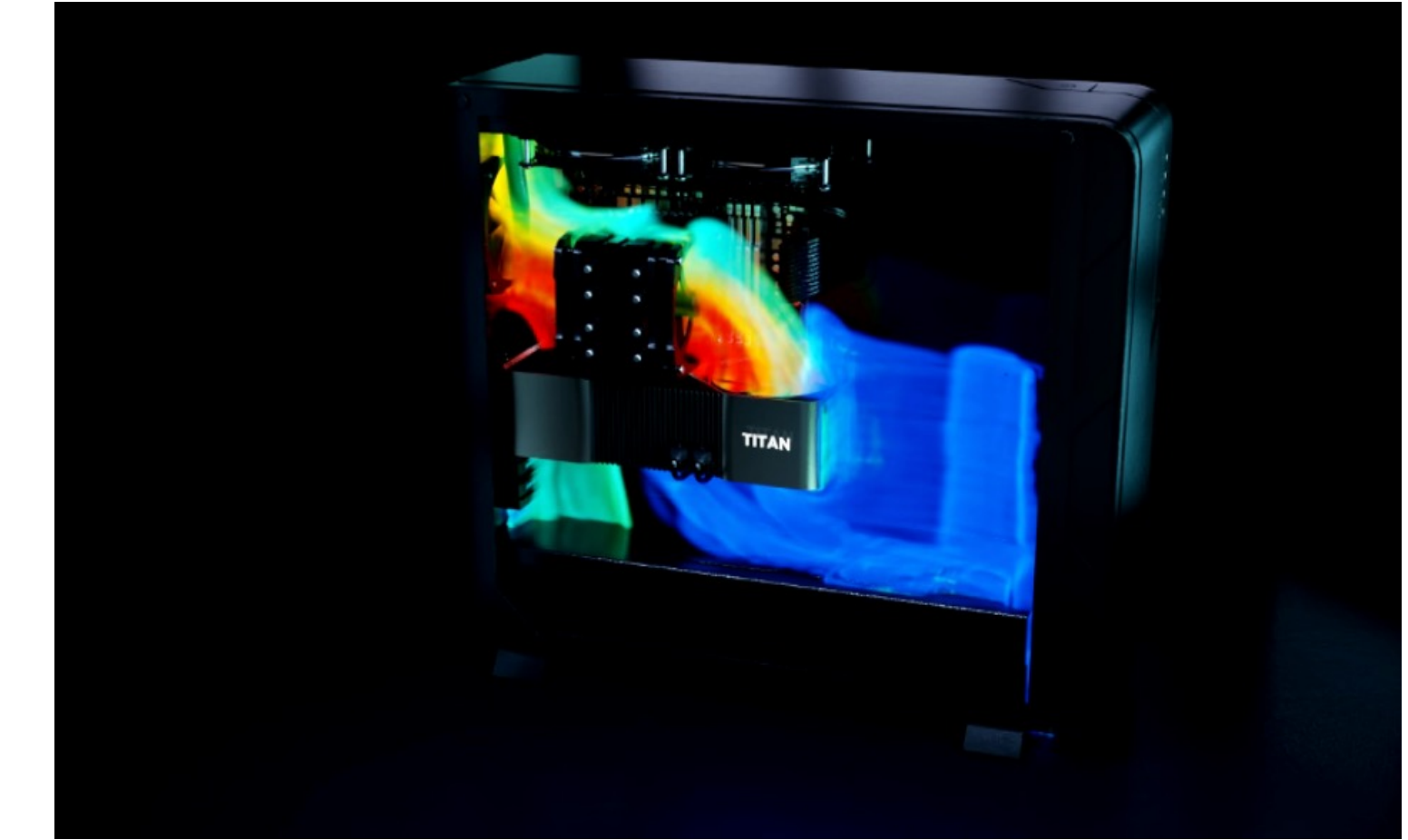
Wind farm Super Resolution

Demo: [Link](#), Blog: [Link](#)



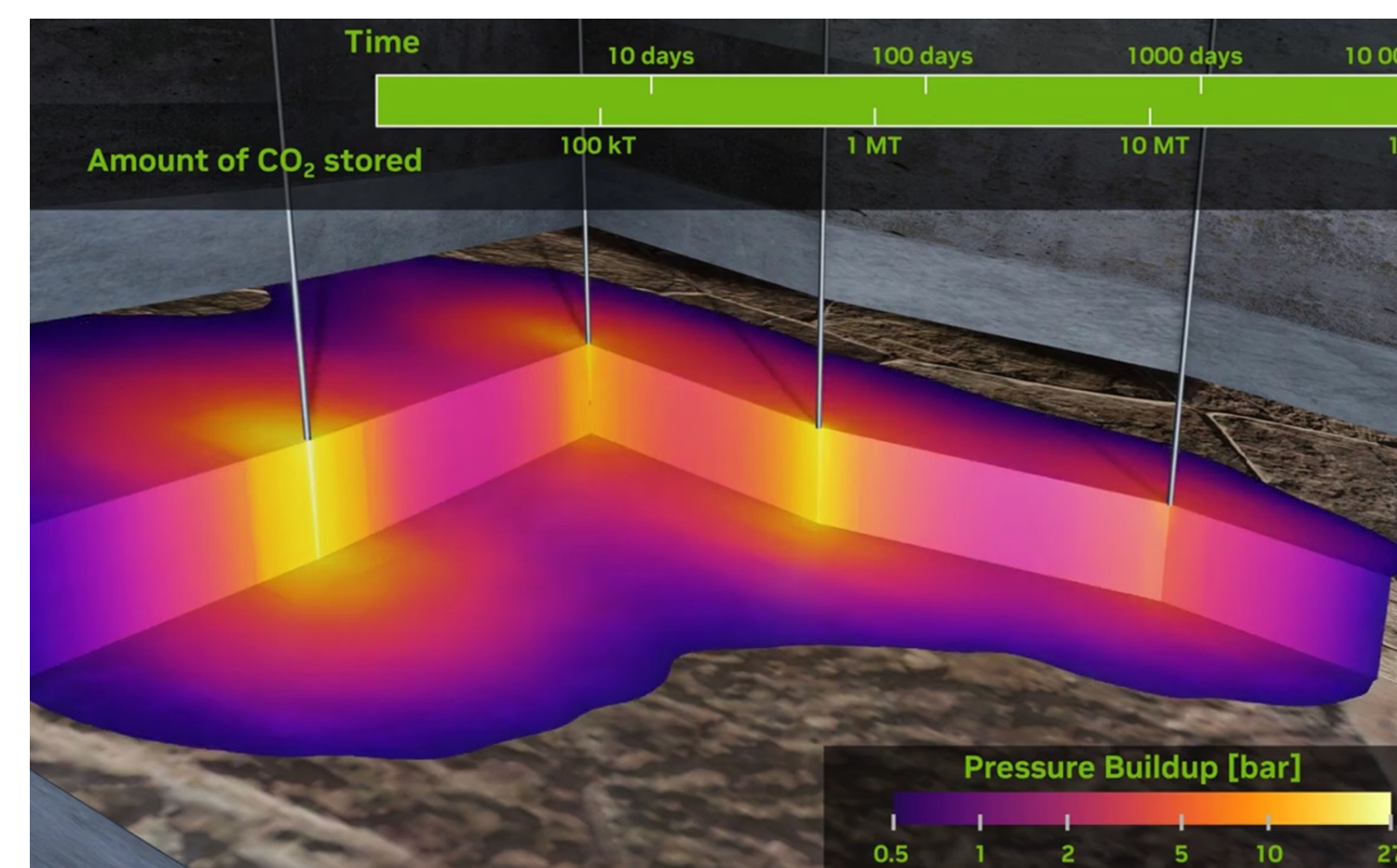
Automotive CFD

[GTC 2024 Keynote](#)



RTX 4090 heat sink design

Demo: [Link](#)



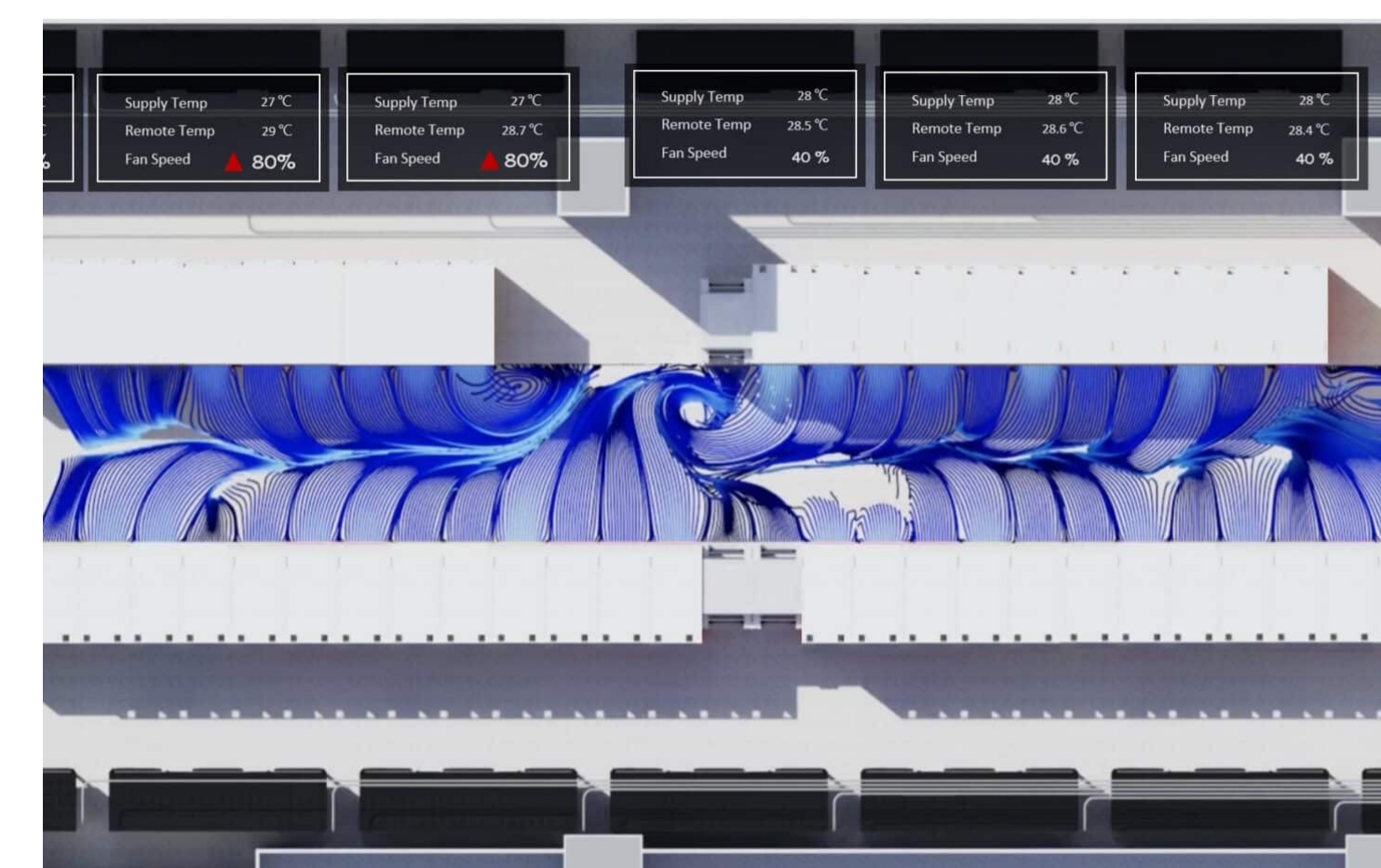
Carbon capture and storage

Demo: [Link](#), Blog: [Link](#)



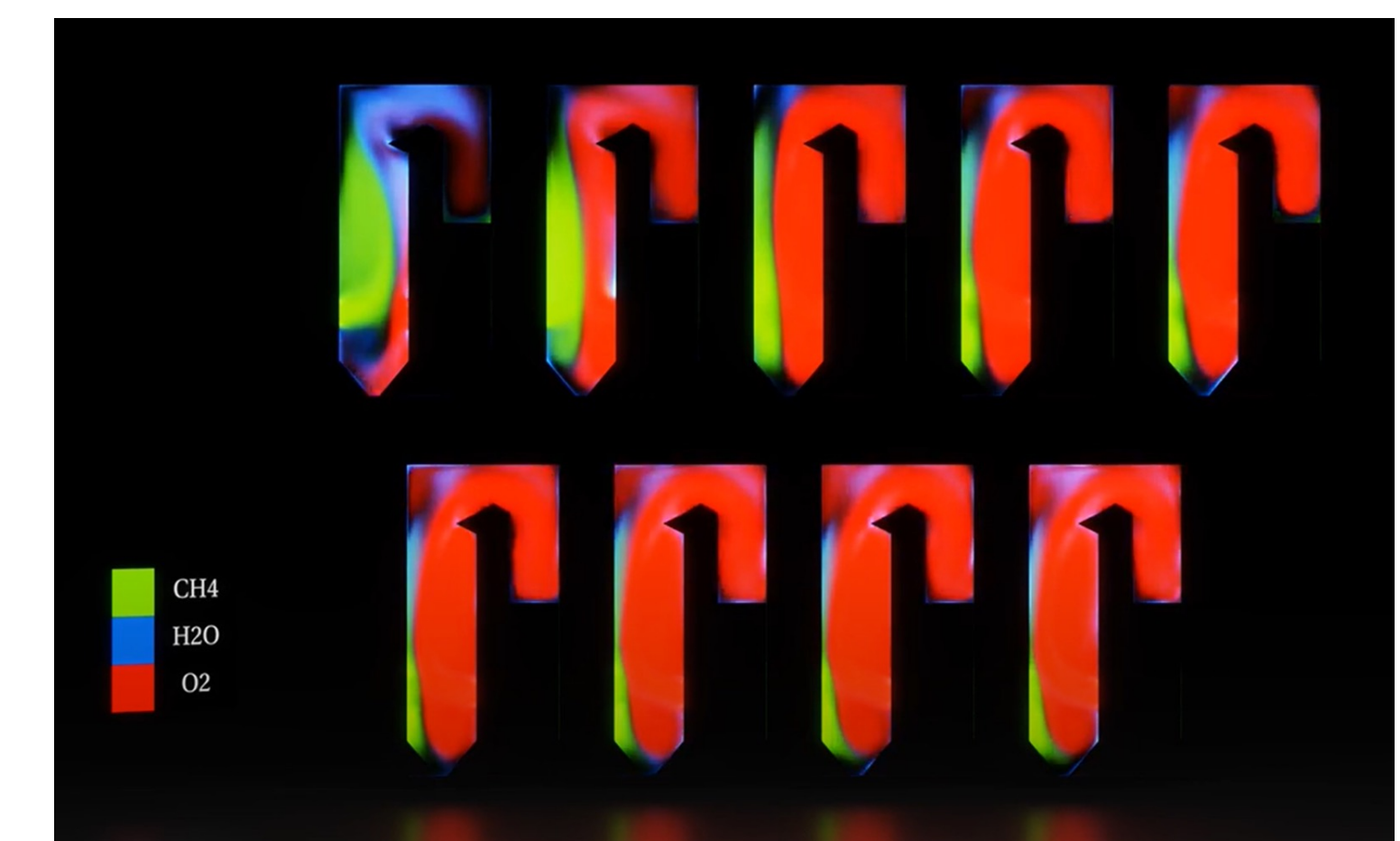
HRSG Digital Twin

Demo: [Link](#), GTC Session: [Link](#)



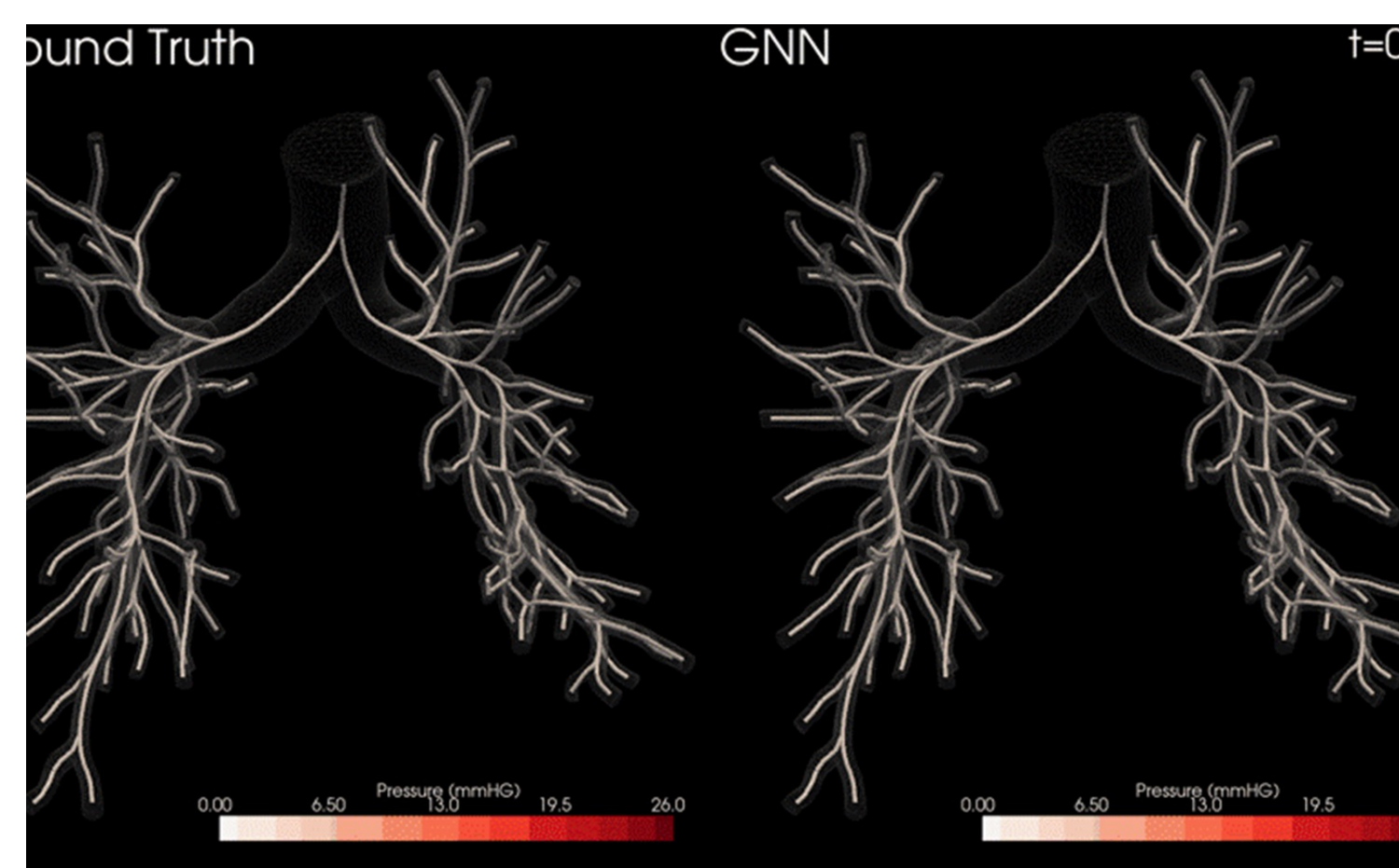
Data Center Digital Twin

Blog: [Link](#), GTC Session: [Link](#)



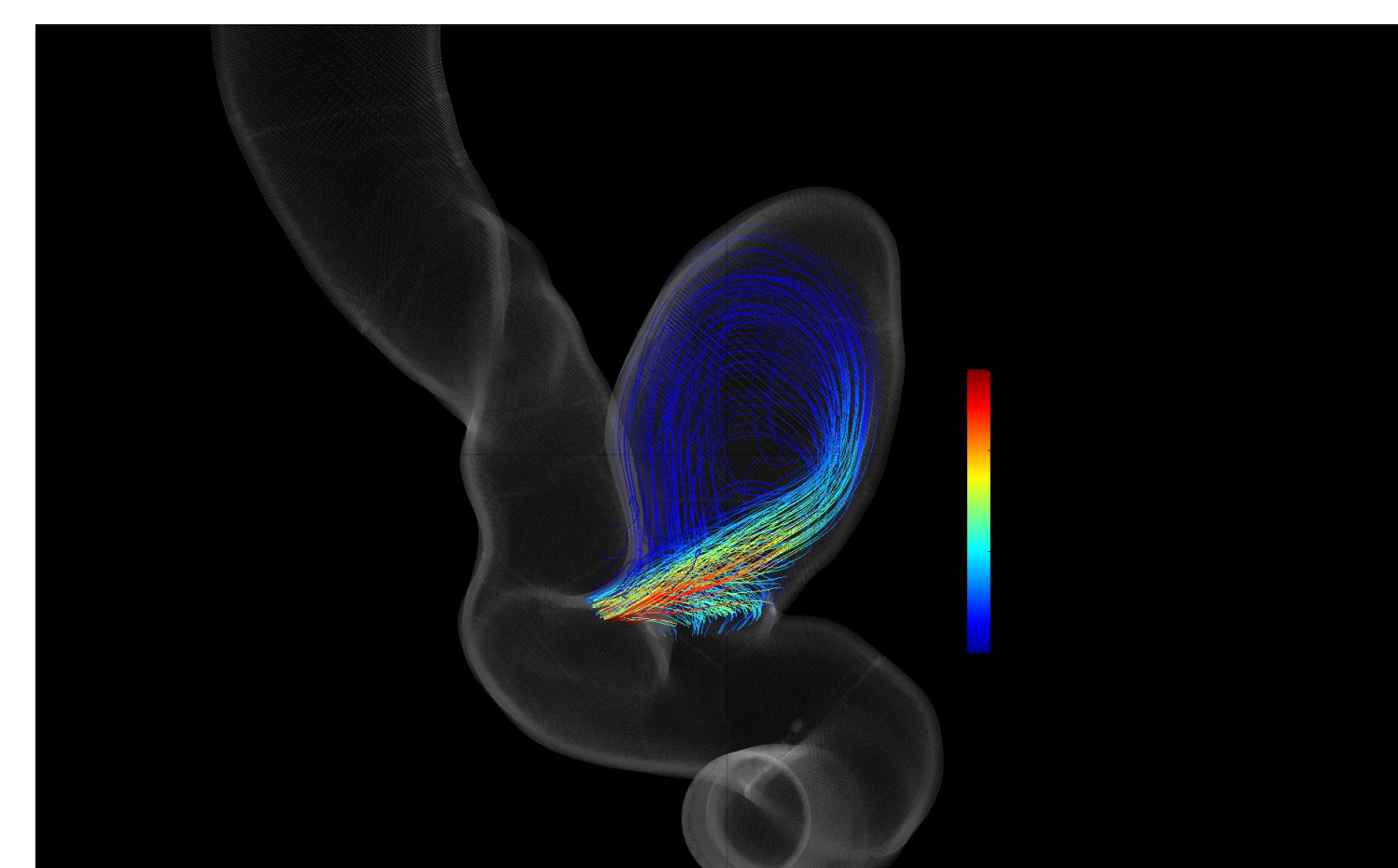
Thermal Boiler Digital Twin

Blog: [Link](#), GTC Session: [Link](#)



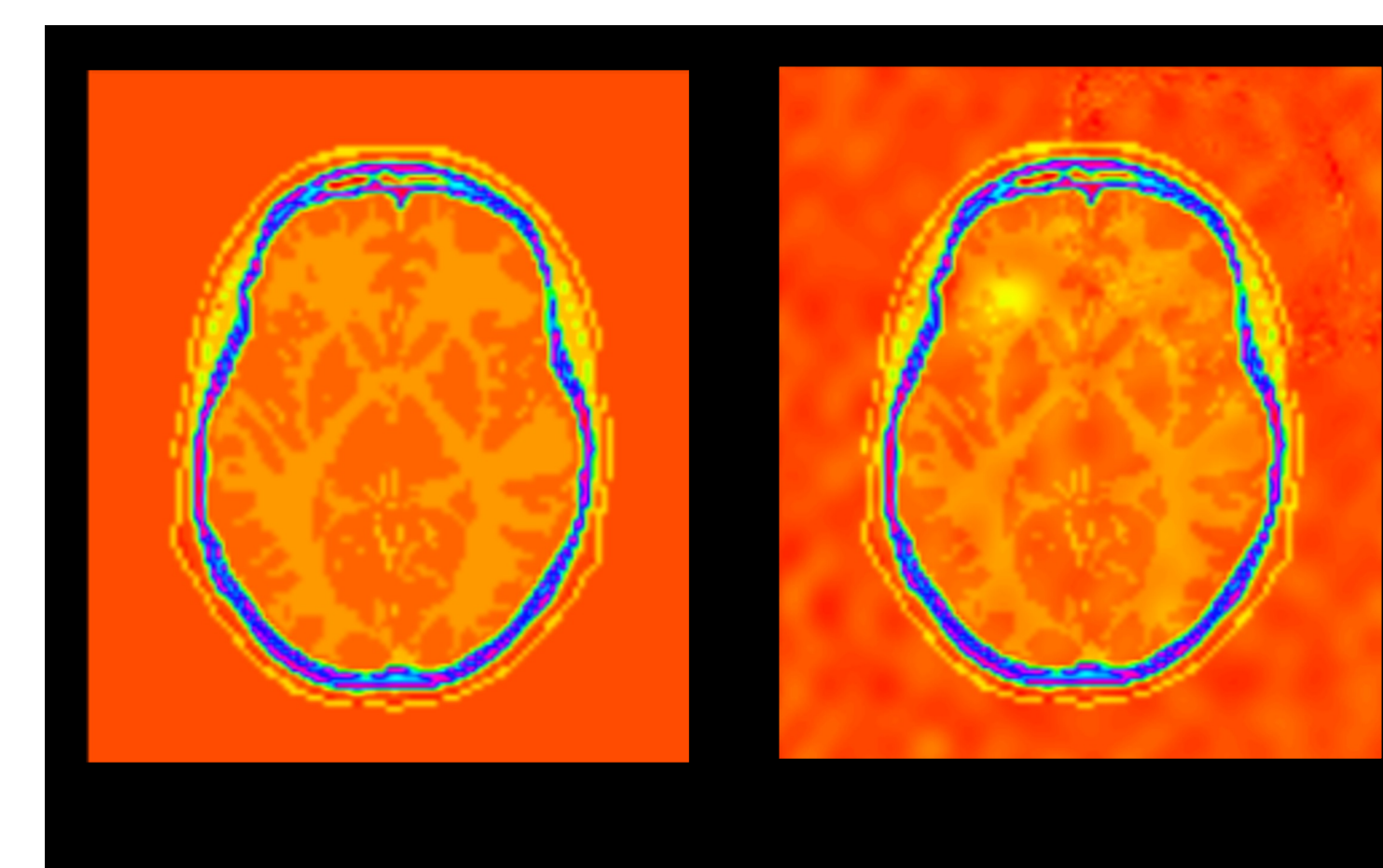
Cardiovascular Simulation

Blog: [Link](#)



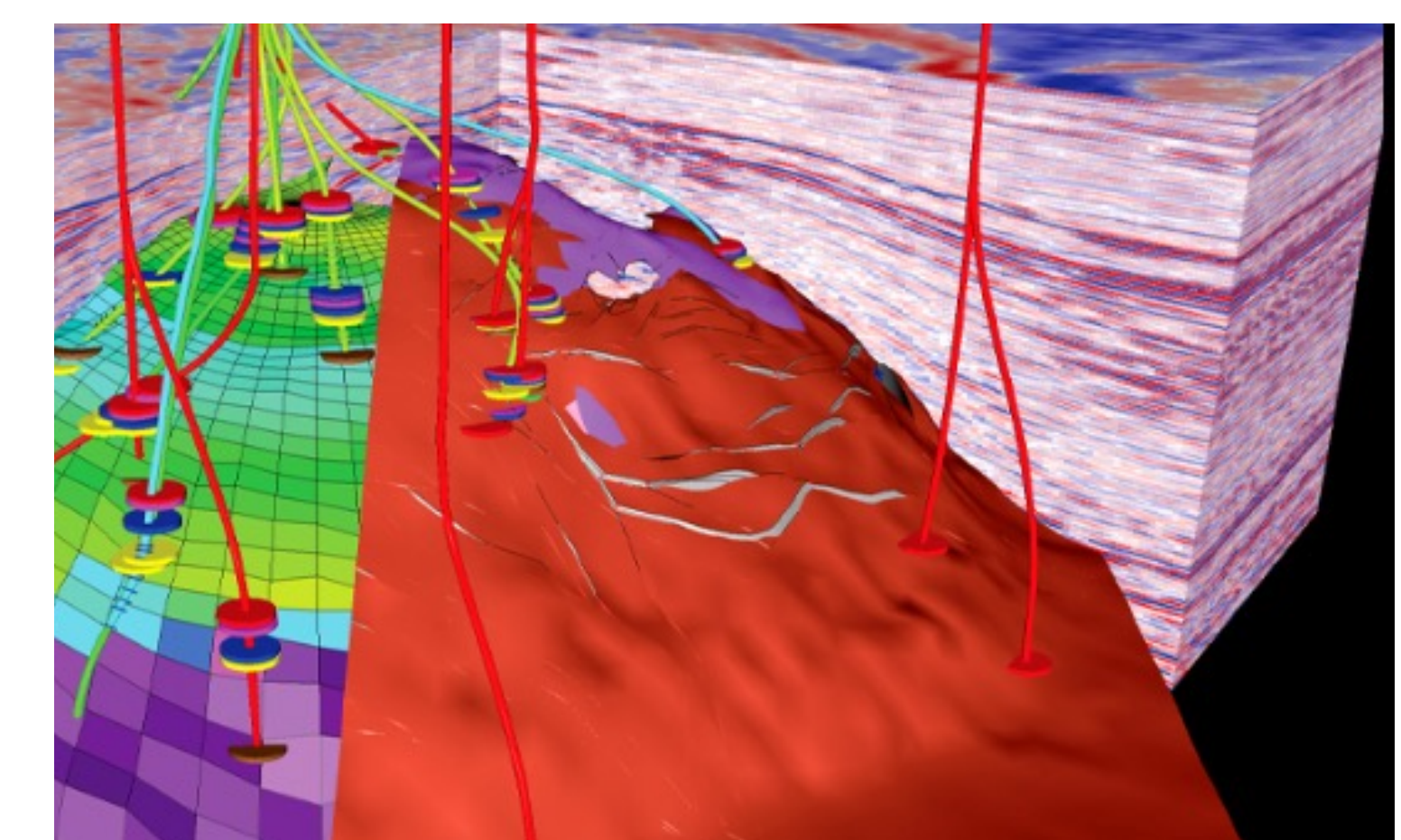
Brain Aneurysm Simulation

Demo: [Link](#)



Brain Anomaly Detection

Resource: [Link](#)



Sub surface simulations

Resource: [Link](#)



THANK YOU