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DEEP LEARNING APPLICATIONS FOR SCIENTIFIC VISUALIZATION

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Argonne National Laboratory is a
U.S. Department of Energy laboratory
managed by UChicago Argonne, LLC.



WHAT IS SCIENTIFIC VISUALIZATION

Converts *multidimensional scientific data* into *visual representations*

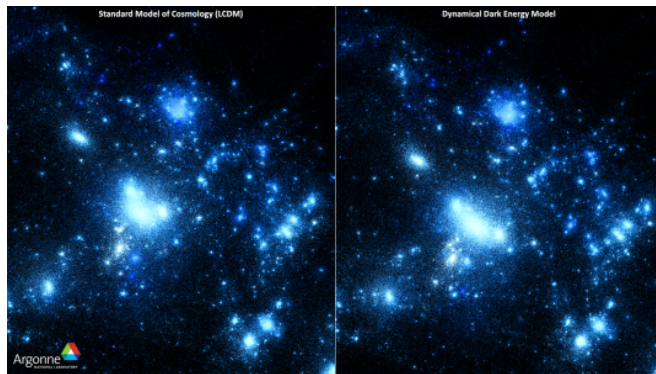
Techniques: isosurface extraction, volume rendering, flow visualization (pathlines, streamlines)

Typical workflow:

- Simulation → Data → Rendering → Analysis

Benefits of Scientific Visualization:

- **Insight:** reveals hidden patterns
- **Exploration:** test hypotheses interactively
- **Communication:** conveys results clearly
- **Decision support:** guide simulations and experiments



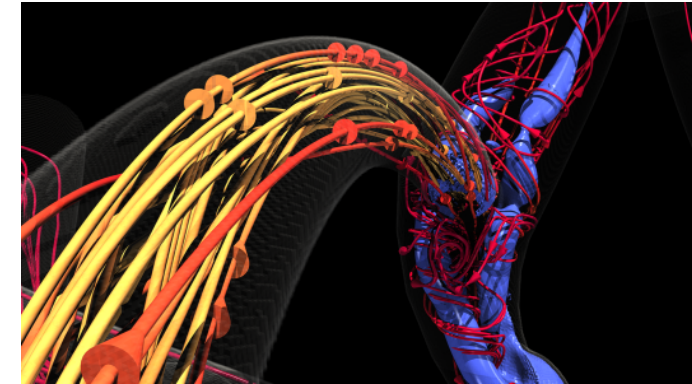
Dark Matter Model

(Image: ALCF Visualization and Data Analytics Team)



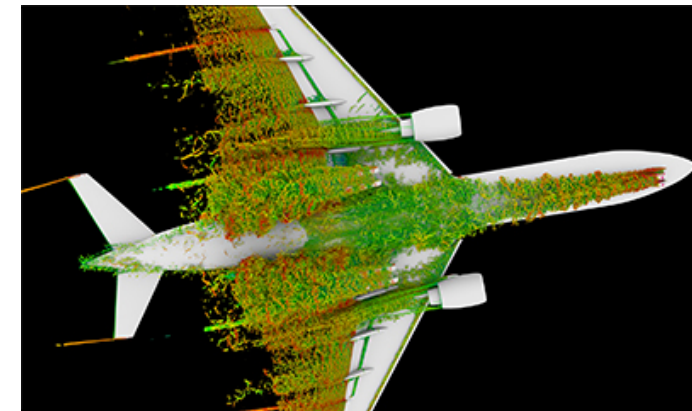
Earth Mantle Convection

(Image: ALCF Visualization and Data Analytics Team)



Tumor Cell Trajectories

(Image: ALCF Visualization and Data Analytics Team)



Airliner Landing Model

(Image: NASA)

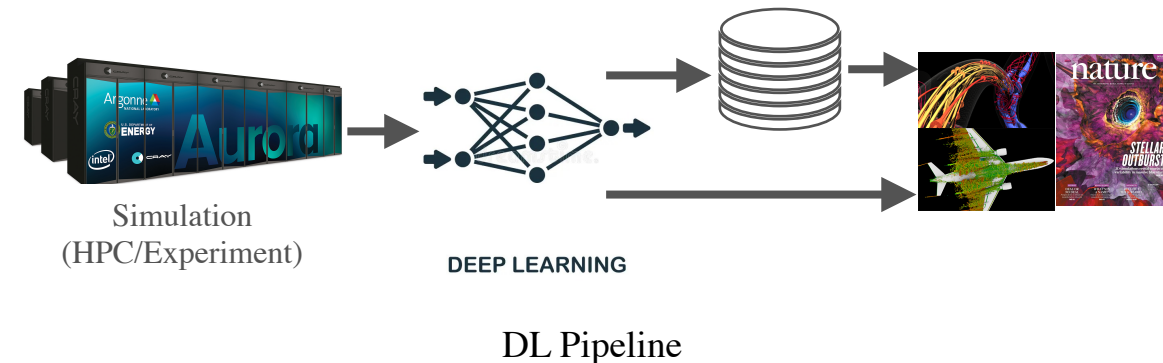
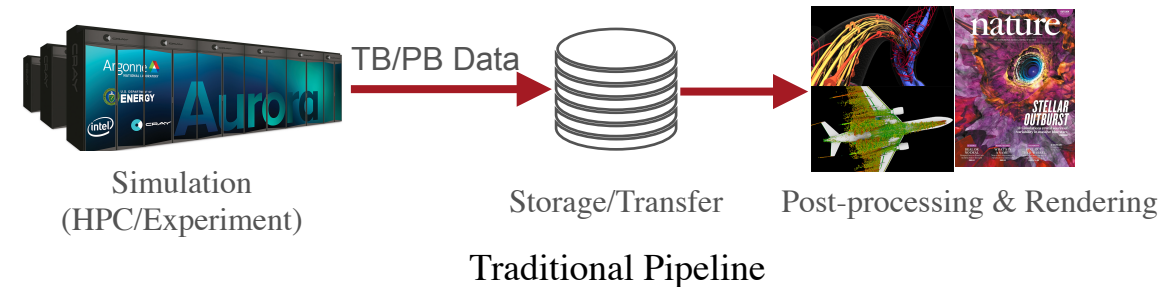
WHY DEEP LEARNING FOR VISUALIZATION

Pain Points of Traditional Visualization

- **Large-Scale Data:**
 - Storage & I/O bottlenecks
 - Long post-processing times
 - Limited interactivity with massive datasets
- **Complex Workflows:**
 - Requires specialized visualization expertise
 - Difficult for domain scientists to explore results directly

How Deep Learning Helps

- **Data Efficiency:** Learn compact neural representations → save storage & I/O
- **Function Approximation**
 - Learn continuous field representations: $f(x, y, z, t) \rightarrow \text{value}$
 - Learn *image formation*: parameters → image
 - Learn *feature detection*: flow → vortex labels
- **Neural Rendering:**
 - Replace traditional rendering with learned 3D reconstructions (e.g., 3D Gaussian Splatting, NeRF)
- **Accessibility:**
 - Large-language-model interfaces allow non-visualization experts to generate visualizations from natural-language prompts



APPLICATIONS IN SCIENTIFIC VISUALIZATION

1 Neural Field Representations

- Learn continuous fields → compact models: Implicit Neural Networks
- Replace large grids; enable instant rendering: NeRF, 3D Gaussian Splatting

2 Accelerated Rendering & Analysis

- Deep surrogates for ray-casting, isosurfaces, pathlines
- 10×–100× faster; real-time interaction

3 Uncertainty & Feature Learning

- Predict mean / variance fields
- Detect vortices, shocks, key structures

4 In-Situ & Interactive Visualization

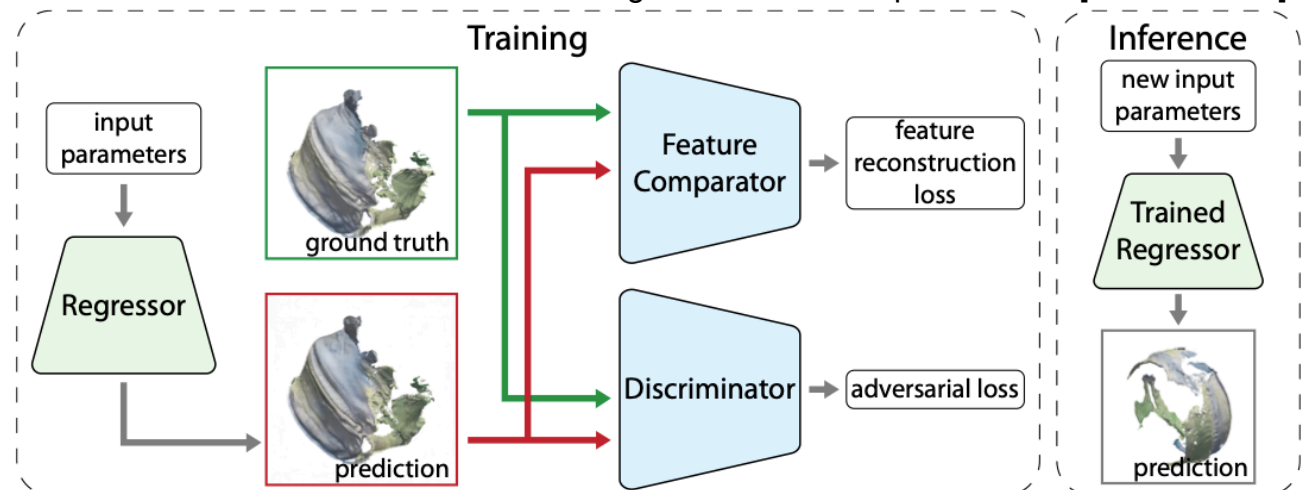
- Train during simulations; avoid data dumps
- Live previews; steer simulations in real time

5 AI-Assisted Interfaces

- Natural-language control via LLMs
- Let non-experts generate visualizations



Interactive Volume Visualization via Multi-Resolution Hash Encoding based Neural Representation [Qi et al. 2024]



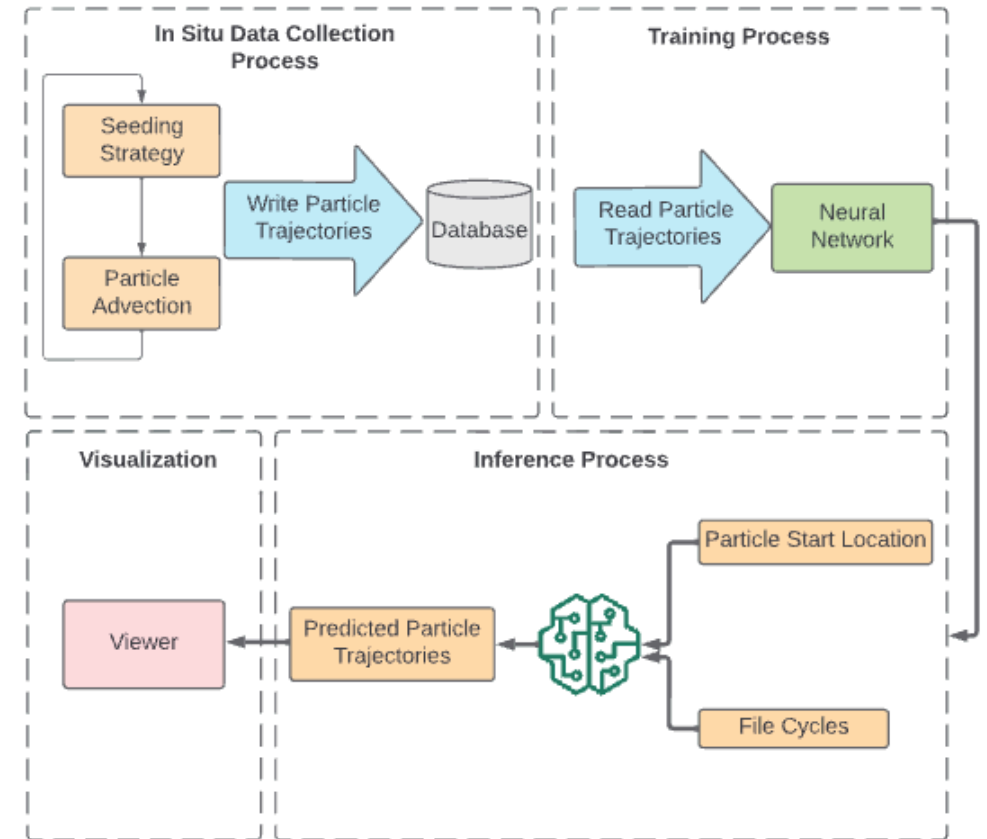
InsituNet Pipeline [He et al. 2019]

EXAMPLE CASE STUDIES

Interactive Visualization of Time-Varying Flow Field using Particle Tracing Neural Network

💡 Motivation

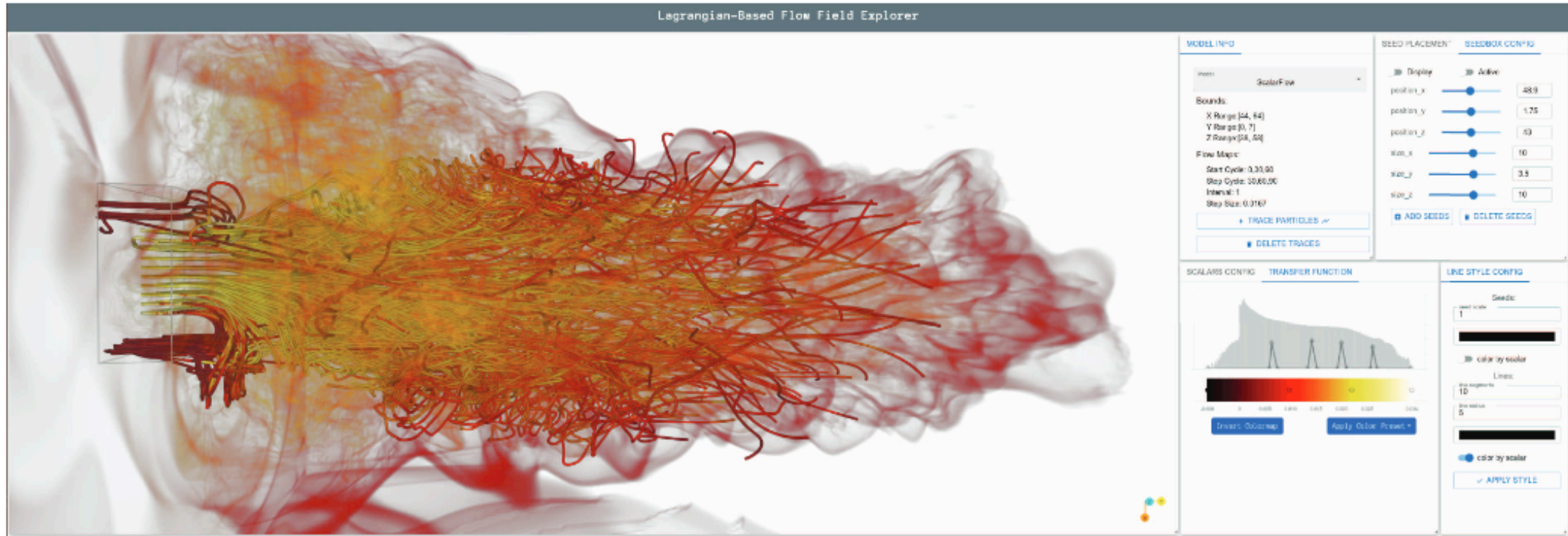
- Modern scientific simulations generate **massive, complex 3D flow data**
- Traditional visualization relies on **particle tracing**, which involves:
 - Placing seed points
 - Retrieving velocity fields
 - Advecting particles over time
- This process is **computationally expensive** due to:
 - Heavy storage and I/O demands
 - Costly advection and triangulation steps (especially for unstructured grids)
- Domain scientists often lack **intuitive and interactive tools** for exploring flow dynamics
- **Need:** scalable methods that **reduce data movement** and **lower the barrier** to effective visualization



The workflow of our deep learning-based particle tracing neural network

EXAMPLE CASE STUDIES

Interactive Visualization of Time-Varying Flow Field using Particle Tracing Neural Network



Our web-based visualization interface, integrated with our particle tracing neural networks, enables users to visualize and explore large 3D time-varying flow fields interactively. In this example, the model trained on the **Scalar Flow dataset** was used to display pathlines, with the FTLE of the dataset serving as the scalar field defining the background volume and pathlines' color mapping. The training dataset was generated using 100,000 seeds. It took one second to load the models and **2.7 seconds** to infer 300 pathlines displayed in the visualization.

EXAMPLE CASE STUDIES

Distributed 3D Gaussian Splatting for High-Resolution Isosurface Visualization

3D Gaussian Splatting (3D-GS) → real-time, photorealistic rendering using anisotropic Gaussians.

Originally for graphics; now adapted to scientific data.

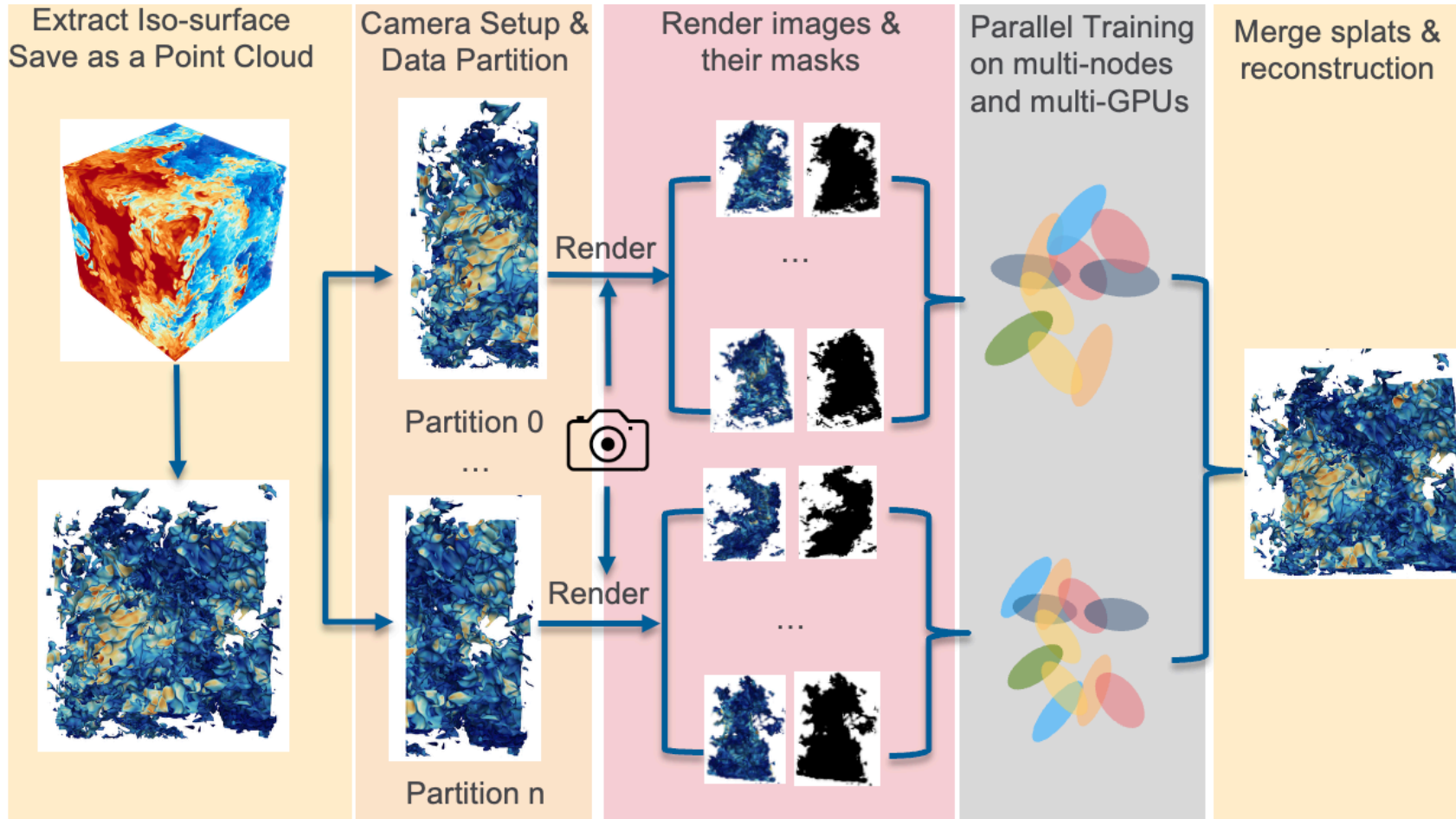
Challenge: prior SciVis 3D-GS limited to single GPU → not scalable for HPC data.

Our contribution: first *distributed multi-node 3D-GS* pipeline for large scientific datasets.



EXAMPLE CASE STUDIES

Distributed 3D Gaussian Splatting for High-Resolution Isosurface Visualization



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Distributed 3D Gaussian Splatting for High-Resolution Isosurface Visualization

Platform: Polaris @ Argonne (4× A100 GPUs / node).

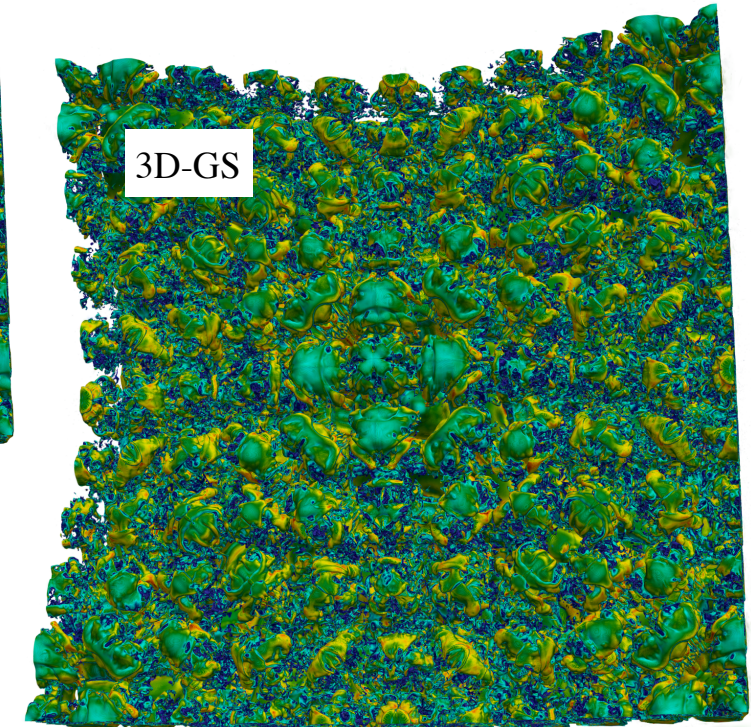
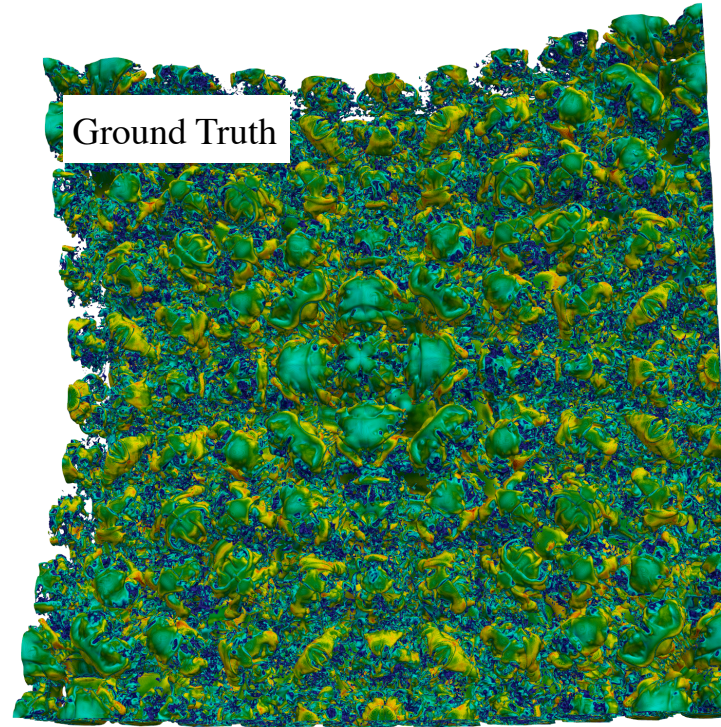
Performance:

- 3× speedup across 8 nodes (32 GPUs).

Quality: PSNR > 30, SSIM ≈ 0.99

- visually indistinguishable from ground truth.

Impact: Enables scalable, real-time, in-situ SciVis for multi-terabyte simulations.



BENEFITS AND LIMITATIONS

Benefits:

- ⚡ Speed & interactivity: real-time previews on GPUs/AI accelerators
- 🧩 Compactness: huge data → small models
- 🔄 Integration: works with HPC simulations (in situ or post hoc)

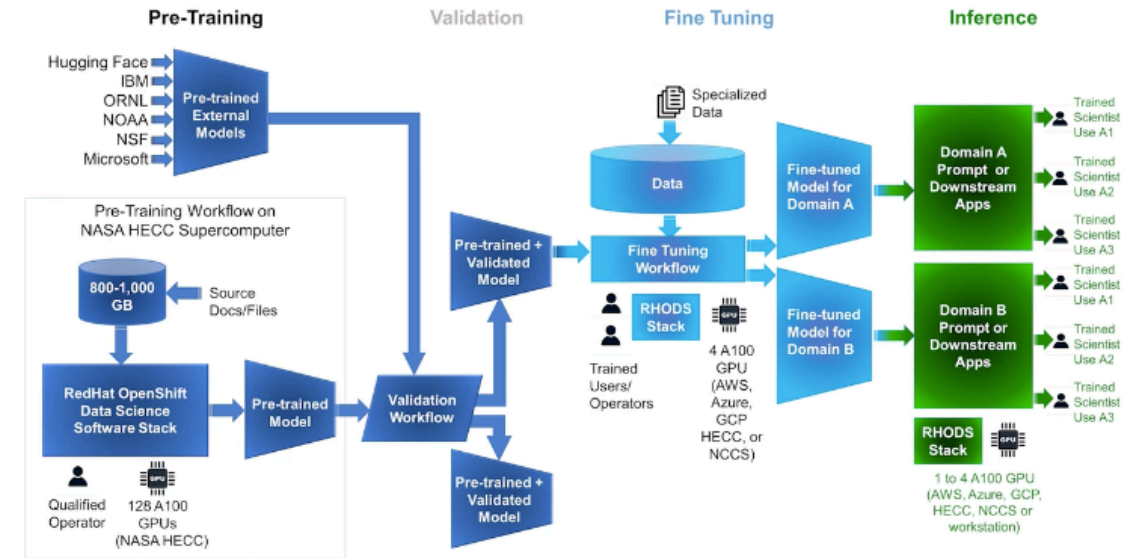
Limitations:

- 🧠 Training cost and data prep still non-trivial
- 🌀 Generalization across flow regimes not guaranteed
- 📄 Interpretability / uncertainty quantification open research topics

EMERGING DIRECTIONS

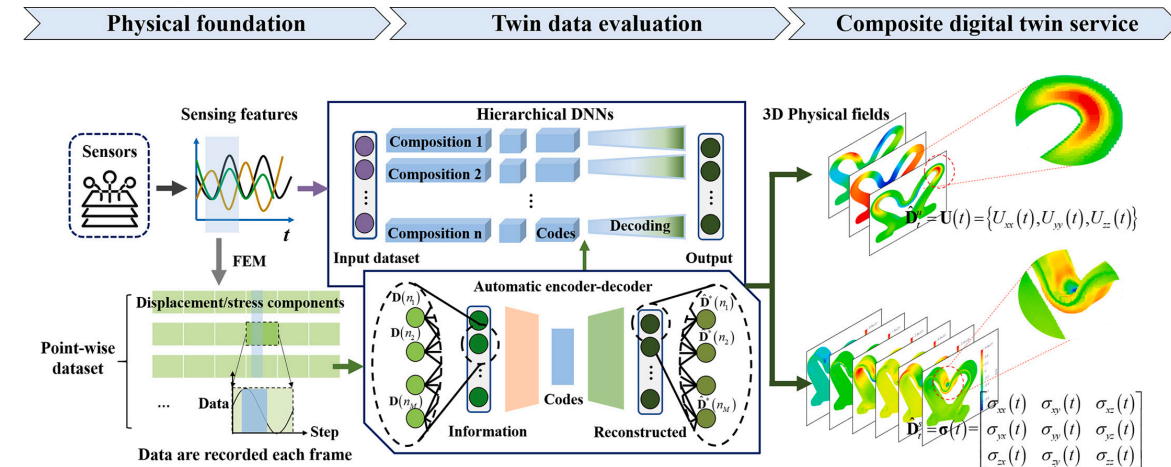
- **Hybrid Physics + DL:**
 - PINNs, FNOs combine governing equations with learning.
 - Fundamental model for science
- **Distributed & In-situ Training:**
 - leveraging HPC systems (Polaris, Aurora, etc)
- **Real-time Digital Twins:**
 - streaming sensors → neural visual models → control loops.
- **AI-assisted Visualization Design:**
 - automatic viewpoint selection, feature highlighting.

Concept of Operations for NASA Foundation Models



NASA Foundation Models

(<https://www.nas.nasa.gov/SC23/research/project34.html>)



Deep-learning-enhanced digital twinning of complex composite structures and real-time mechanical interaction [Xu et al. 2023]



QUESTIONS?



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