



NVIDIA and AI For Science

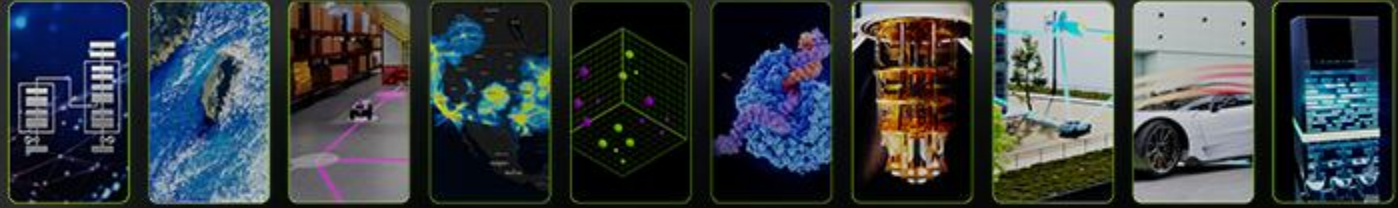
CUCAI 2026 | University of Toronto | 2026 Mar 7 | Jonathan Dursi

NVIDIA AI & HPC Platform

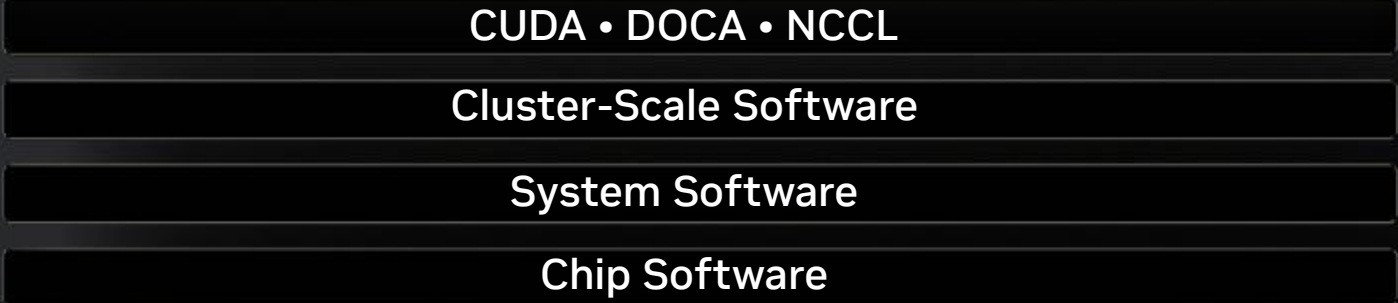
NIM
CUDA-Accelerated
Agentic AI Libraries



Omniverse
CUDA-Accelerated
Physical AI Libraries

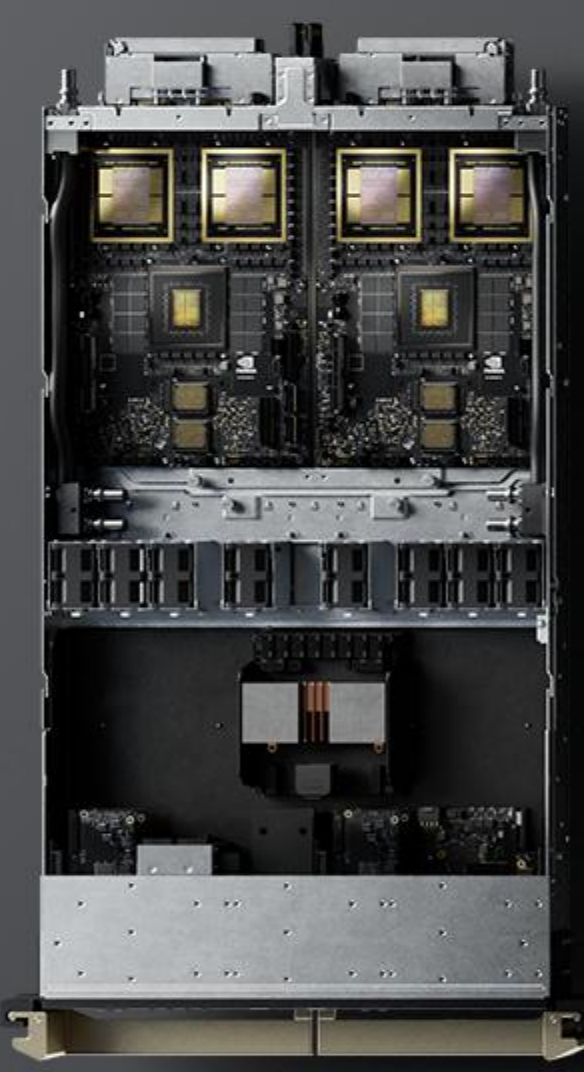


CUDA-X Libraries



Accelerated
Software Stack

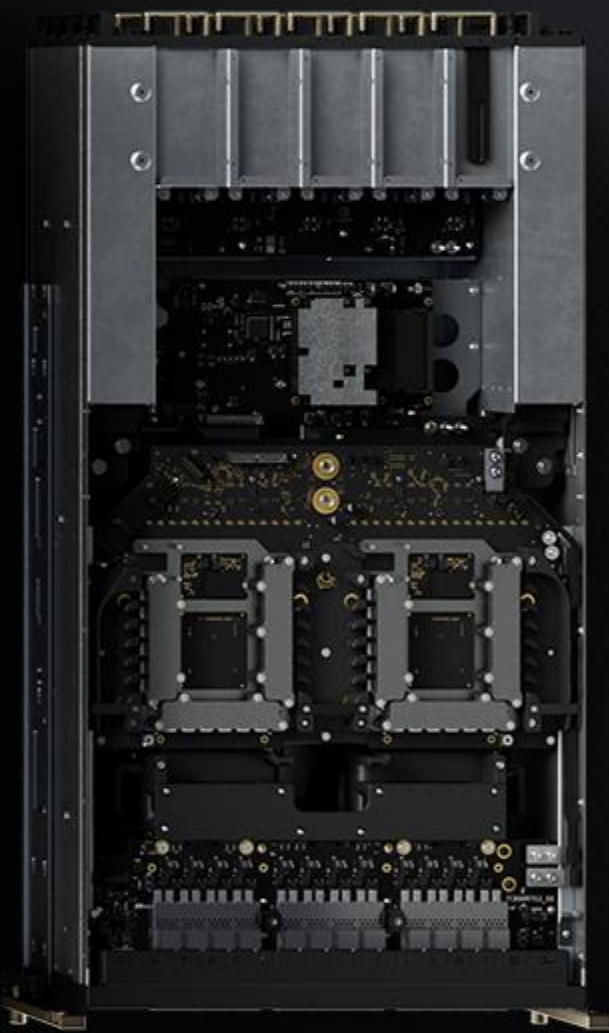
GB200 NVL72 SuperPOD



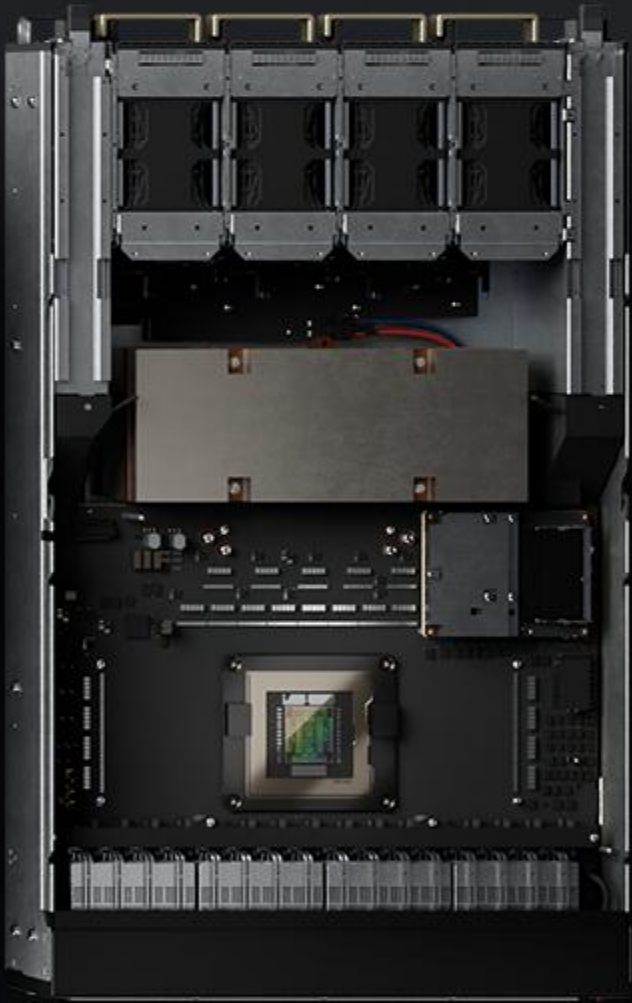
Grace Blackwell
MGX Node



NVLink Switch



Quantum Switch



Spectrum-X Switch

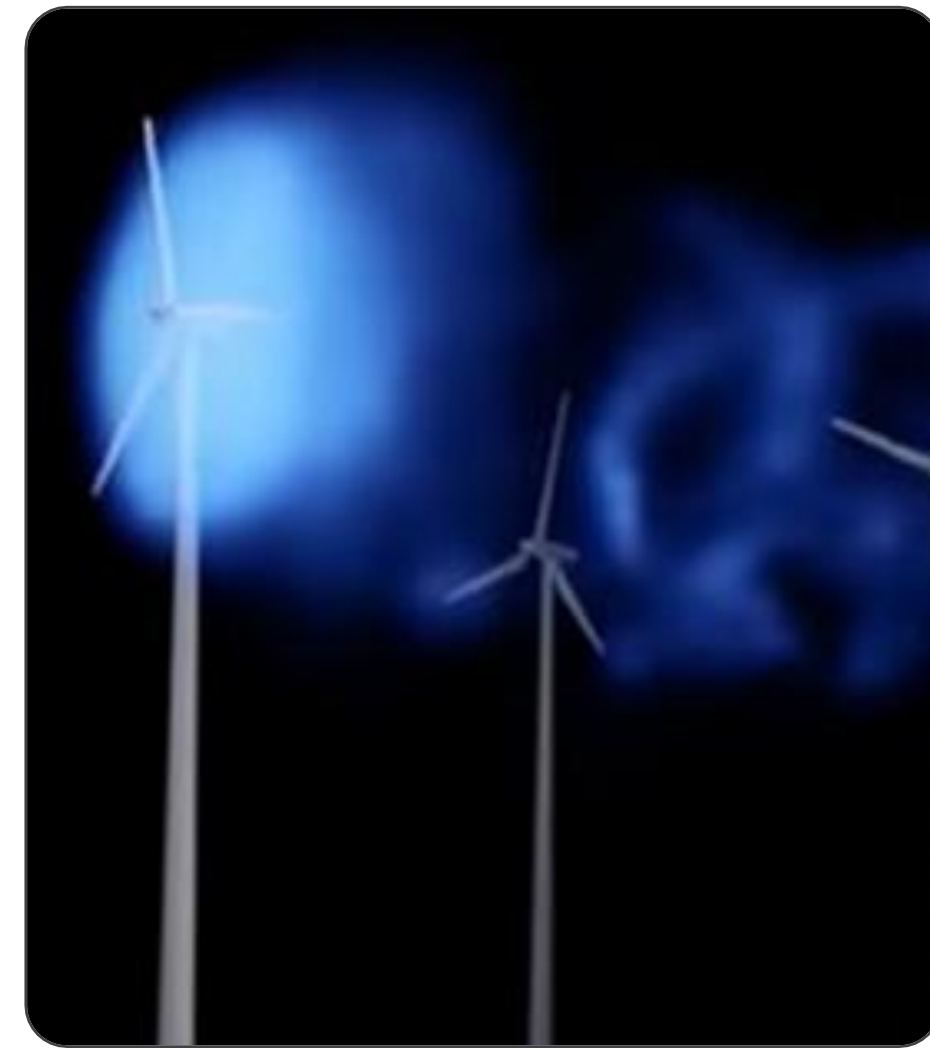


Chips Purpose-Built for AI Supercomputing
GPU | CPU | DPU | NIC | NVLink Switch | IB Switch | Enet Switch

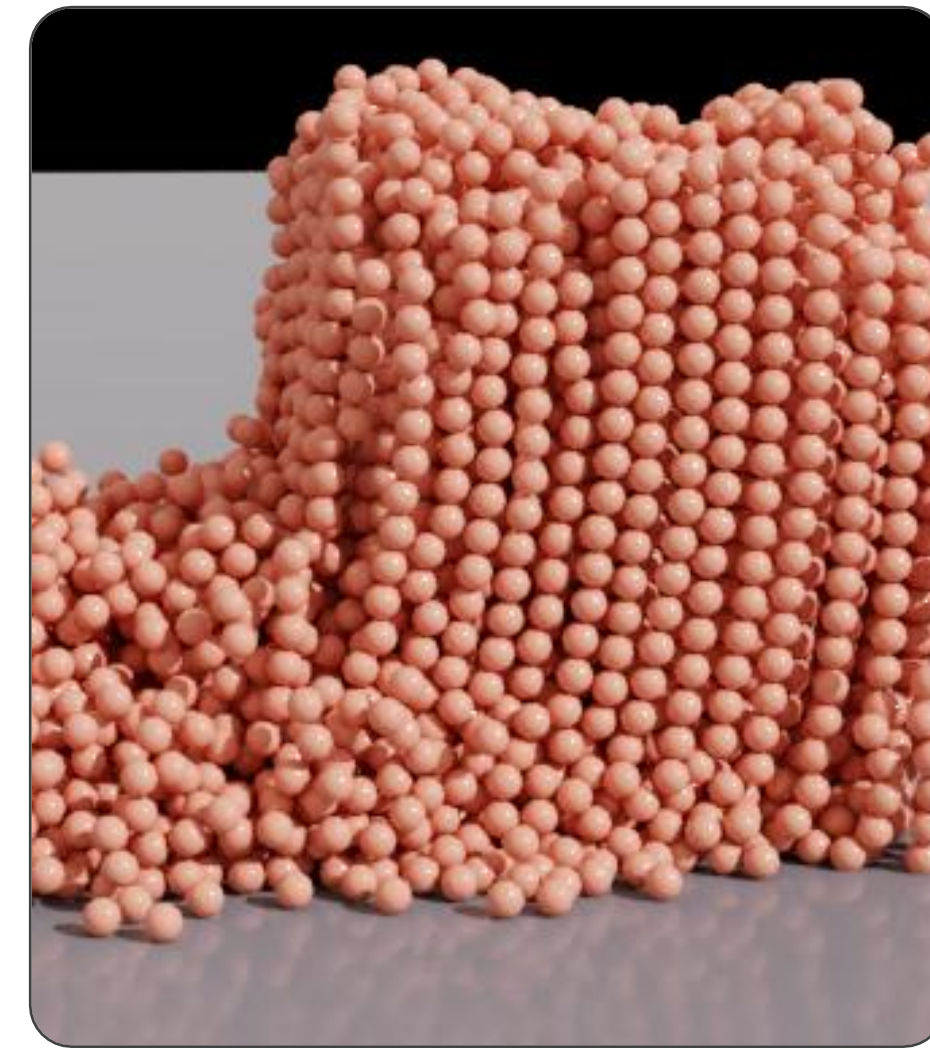
AI for Science(s)



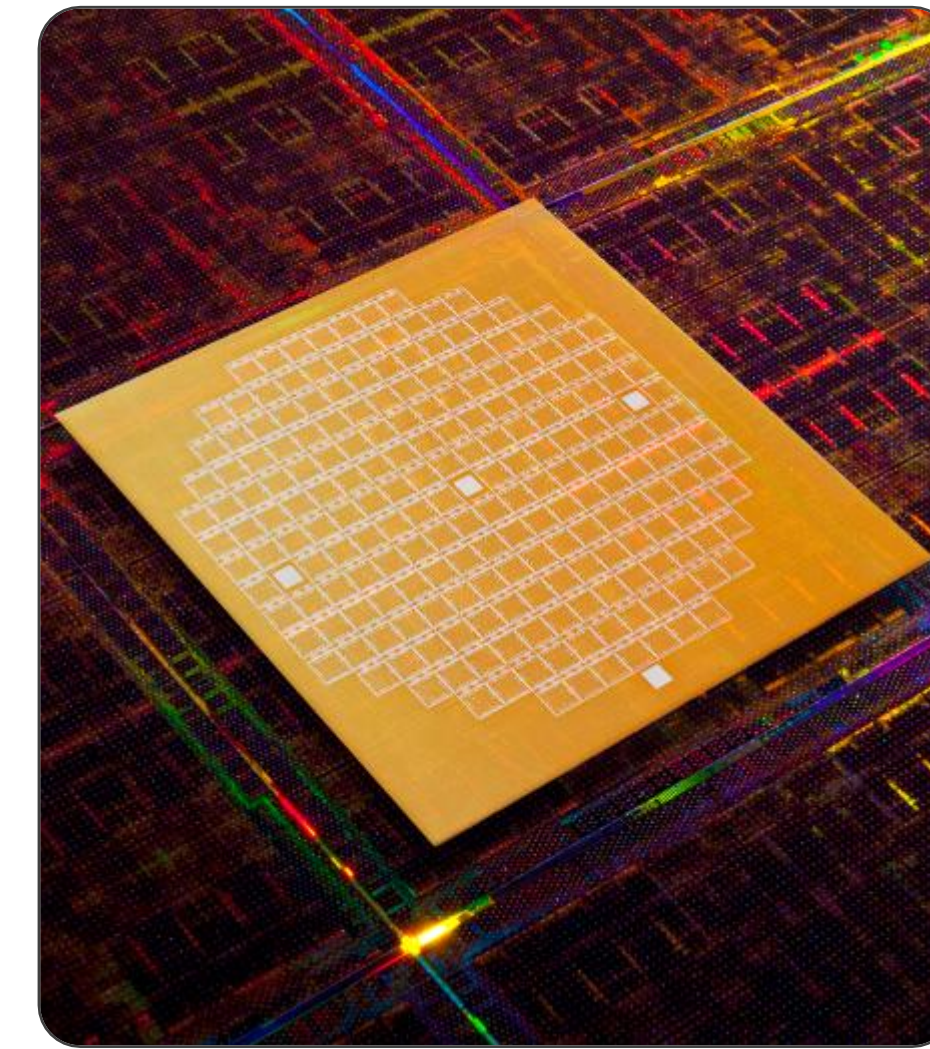
cuDSS
CAE



PhysicsNeMo
AI Physics



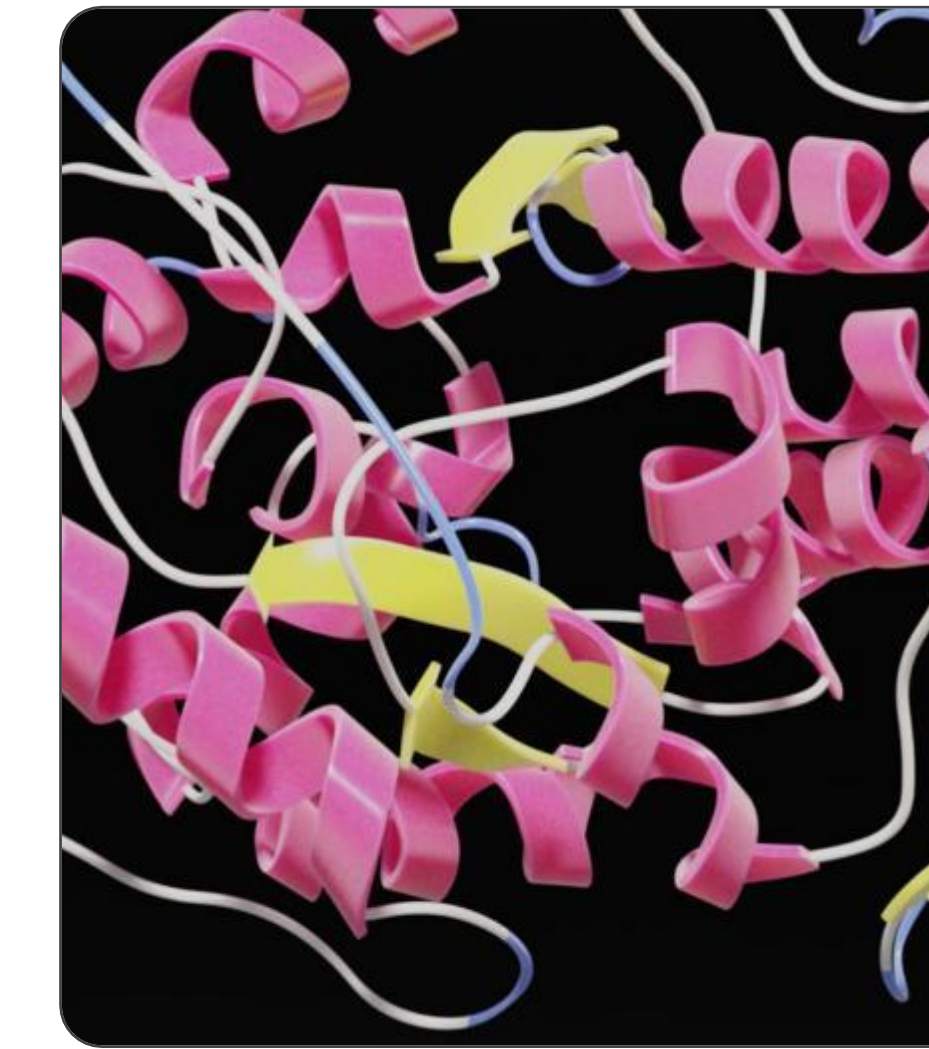
Warp
Physical Simulation



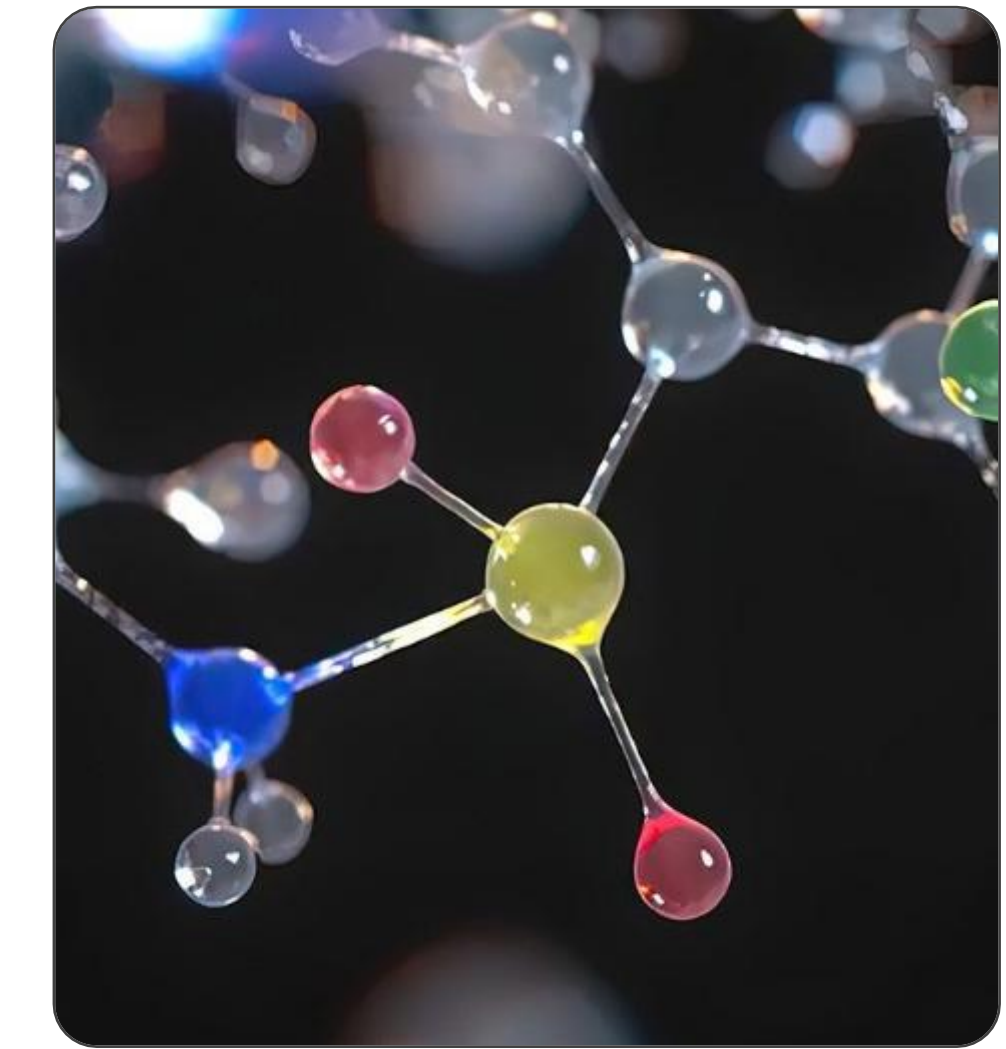
cuLitho
Computational
Lithography



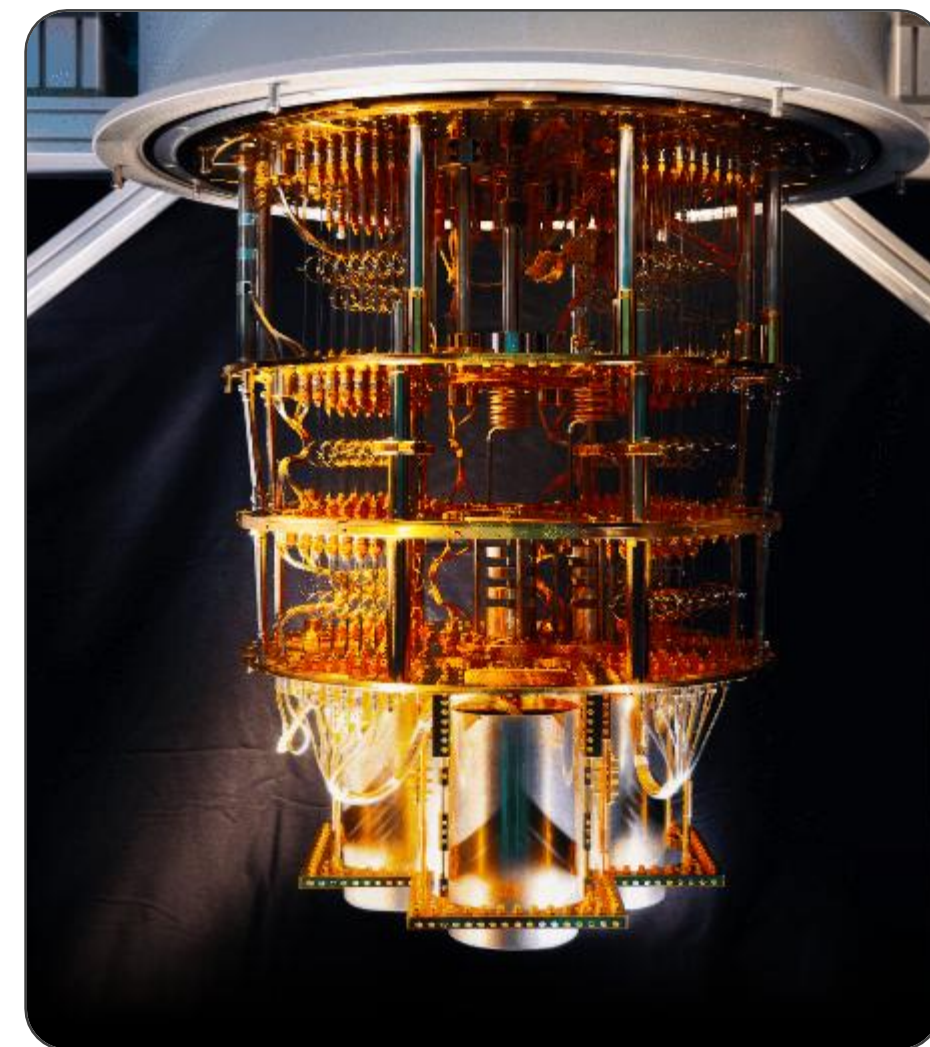
ALCHEMI
AI Materials Science



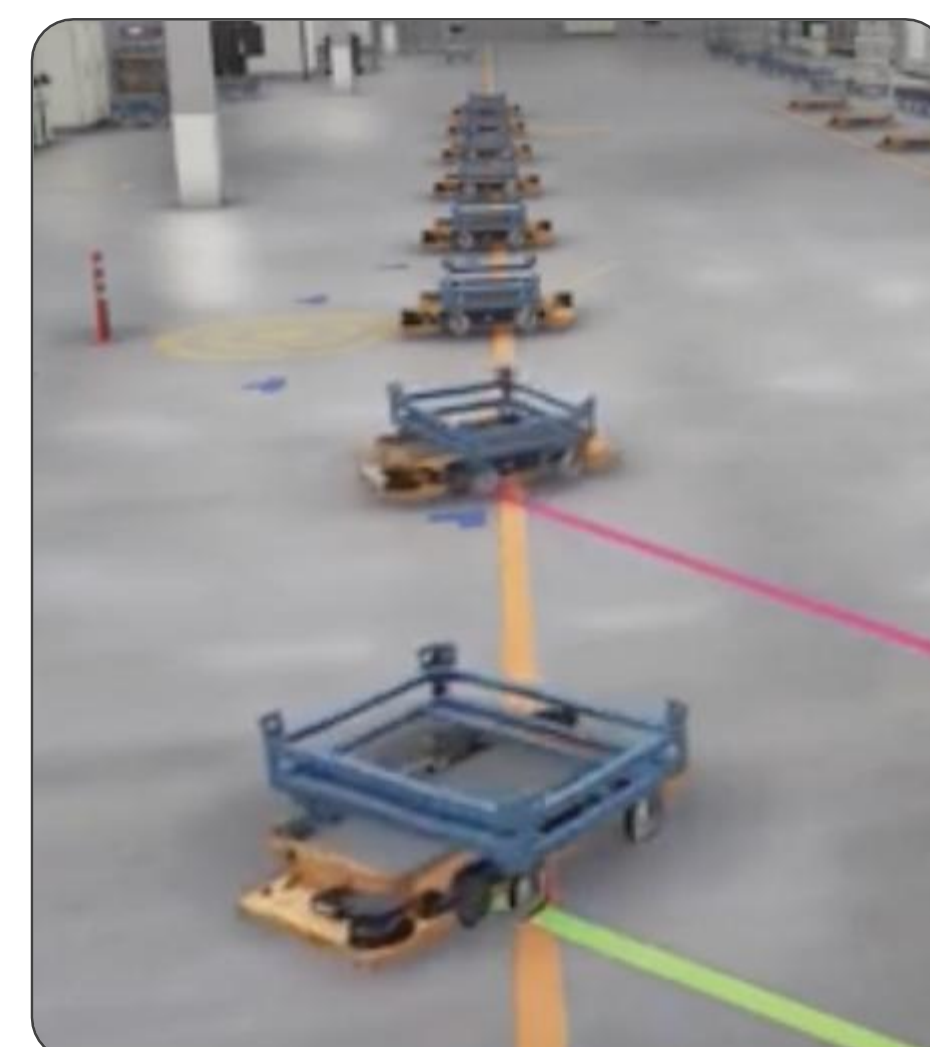
cuEquivariance
Drug & Materials
Discovery



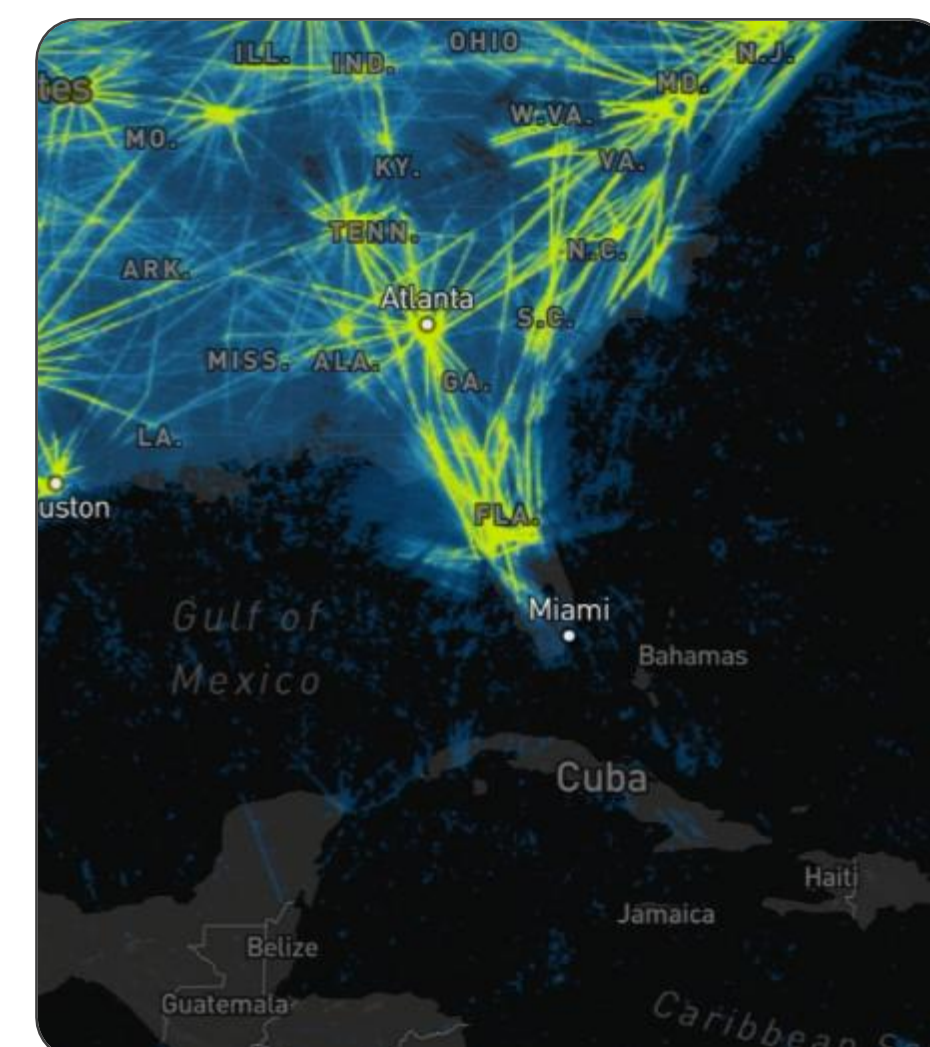
Parabricks
Gene Sequencing



CUDA-Q
Quantum Computing



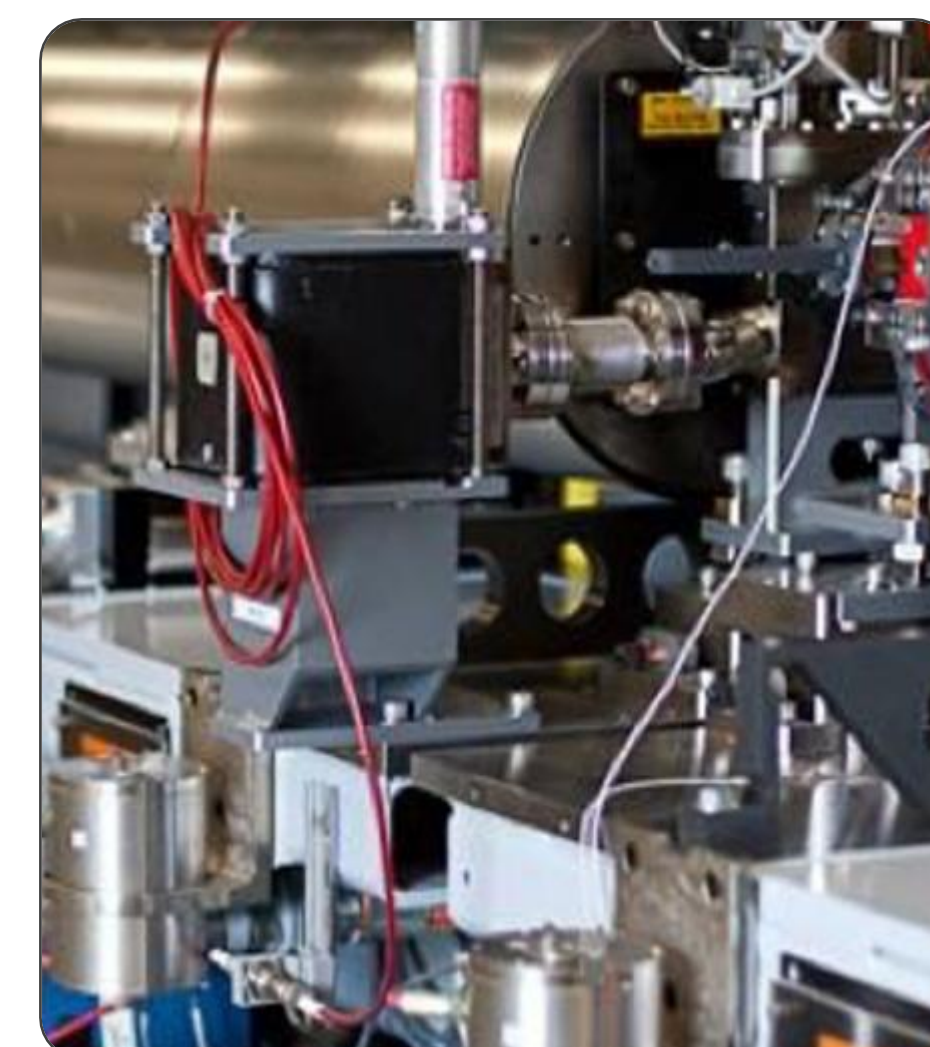
cuOpt
Decision Optimization



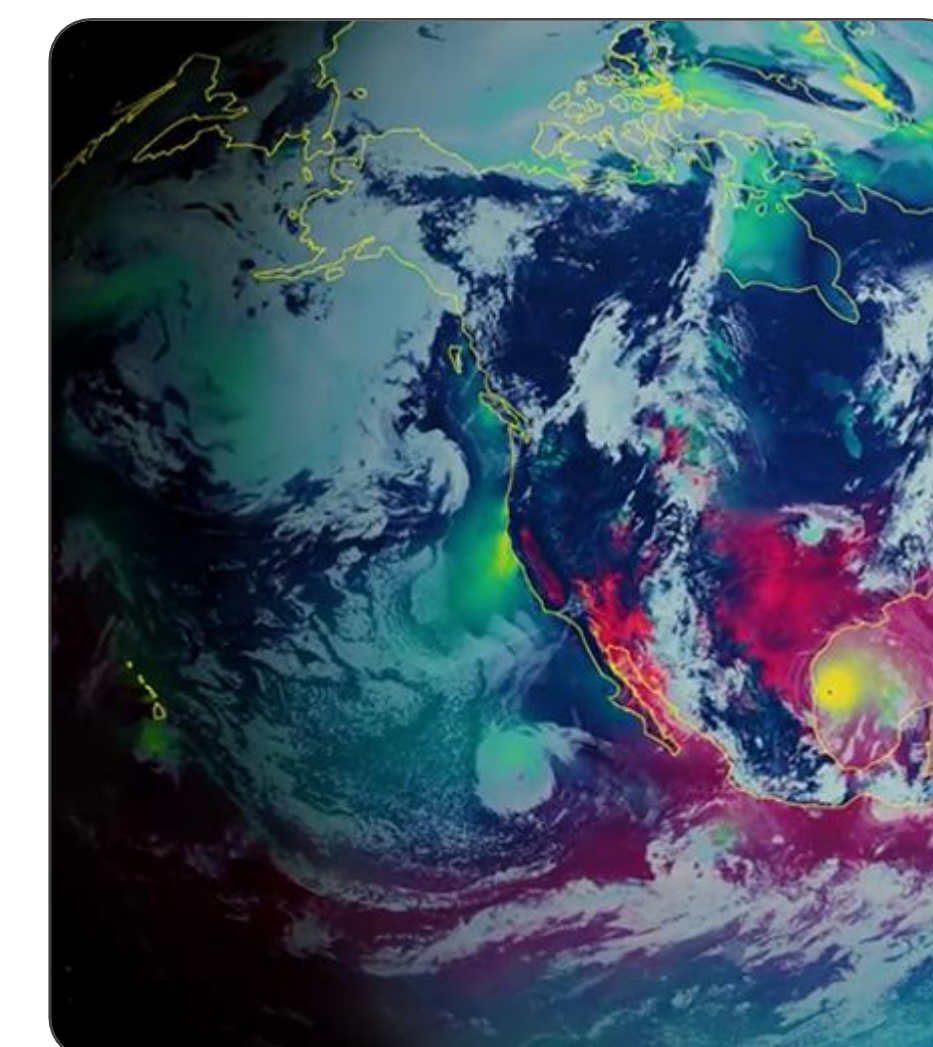
cuDF
Data Processing



cuPyNumeric
Numerical Computing



Holoscan
Edge HPC



Earth-2
Weather Analytics

“

One of the most amazing things that anyone has ever said to me came from a quantum chemist - ‘because of NVIDIA’s work, I can do my life’s work *in my lifetime*’

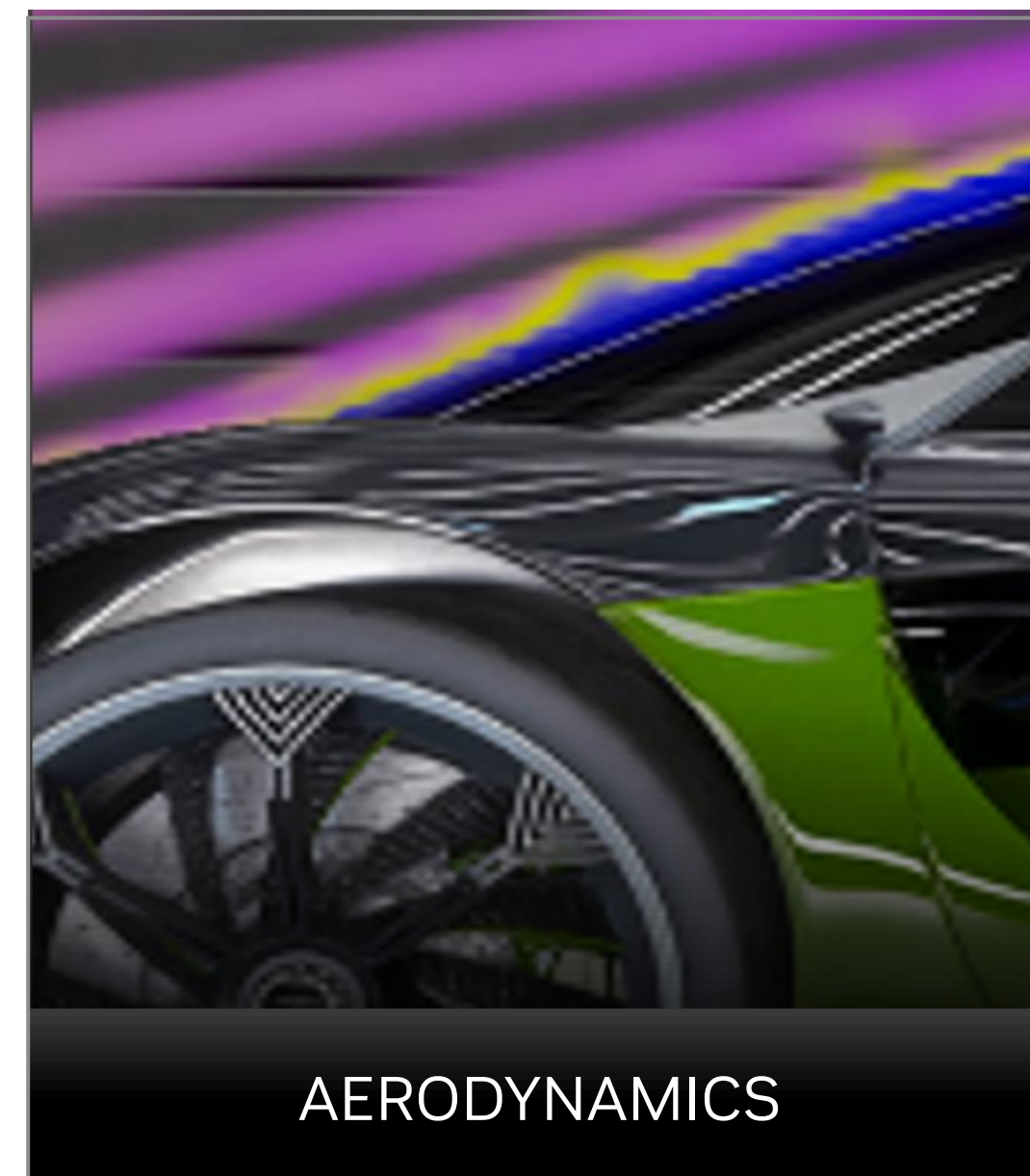
NVIDIA founder and CEO, Jensen Huang

”

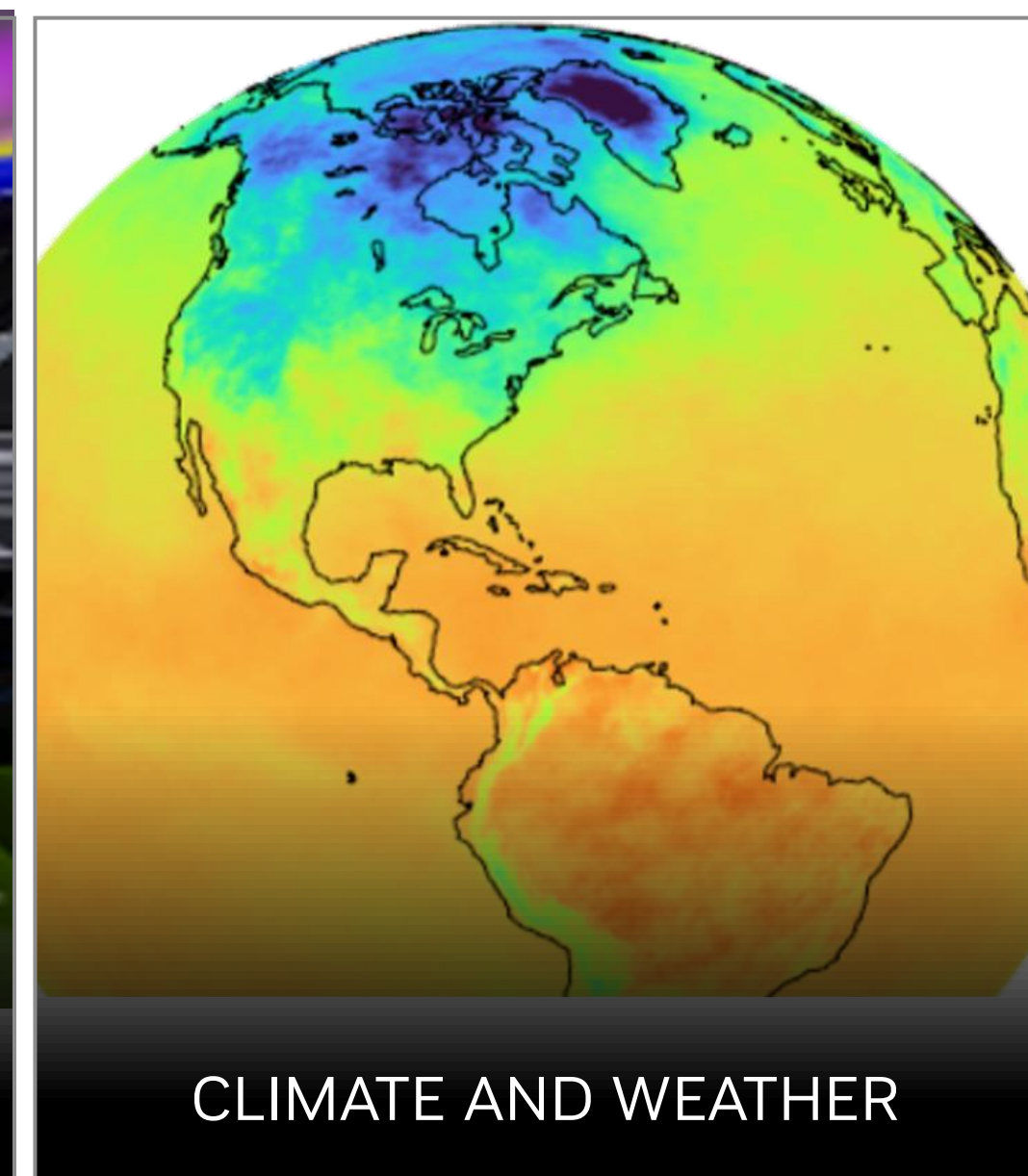
AI Accelerates Scientific Discovery



With Traditional Science, Discovery Takes Years



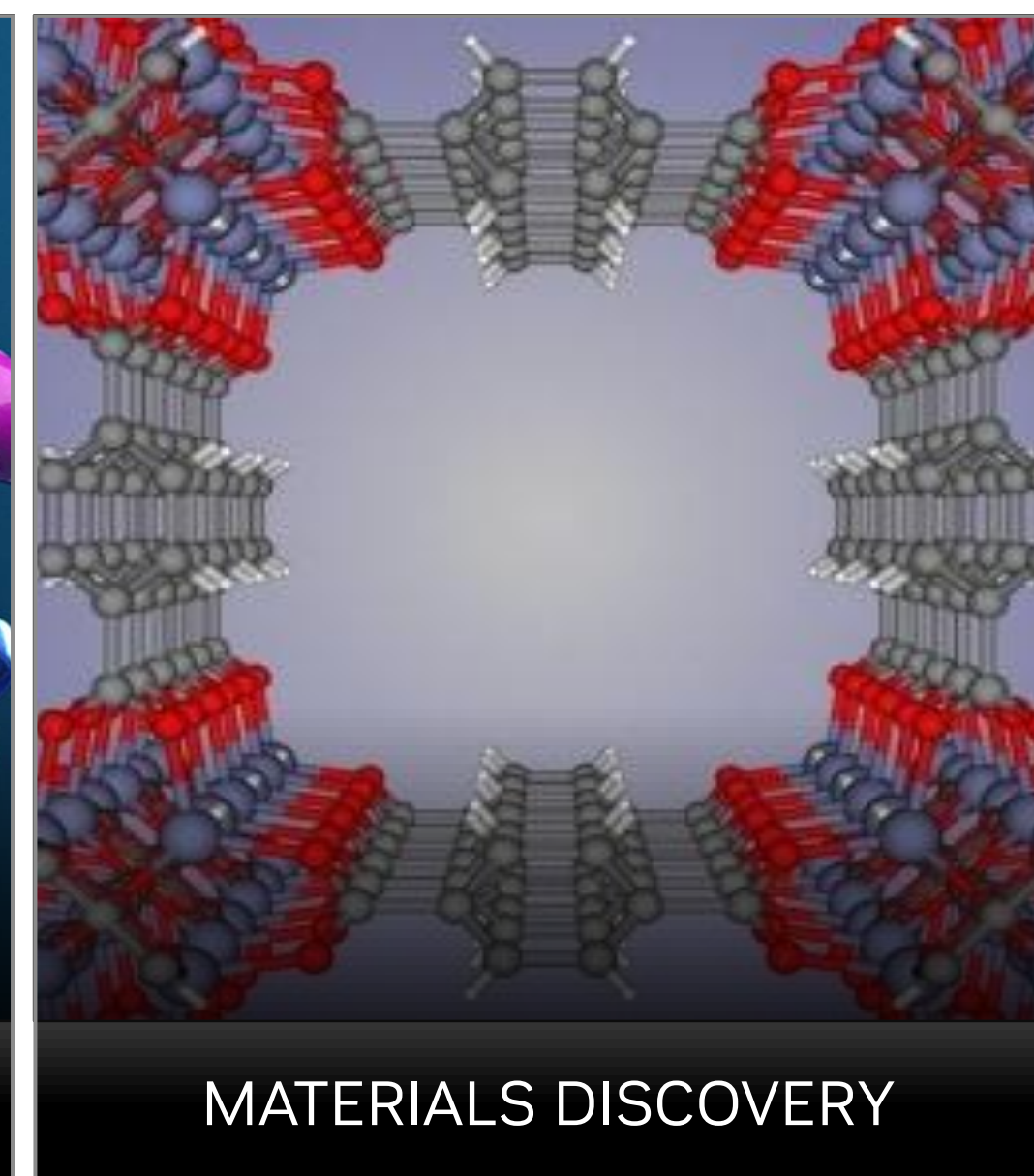
AERODYNAMICS



CLIMATE AND WEATHER



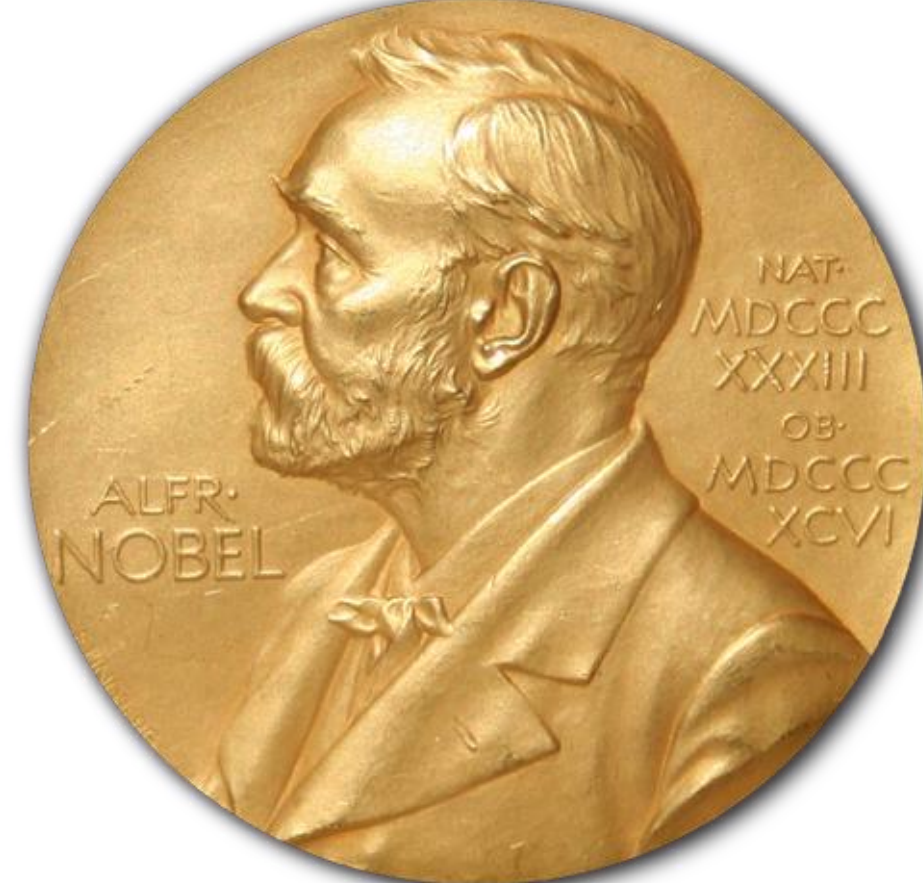
DRUG DISCOVERY



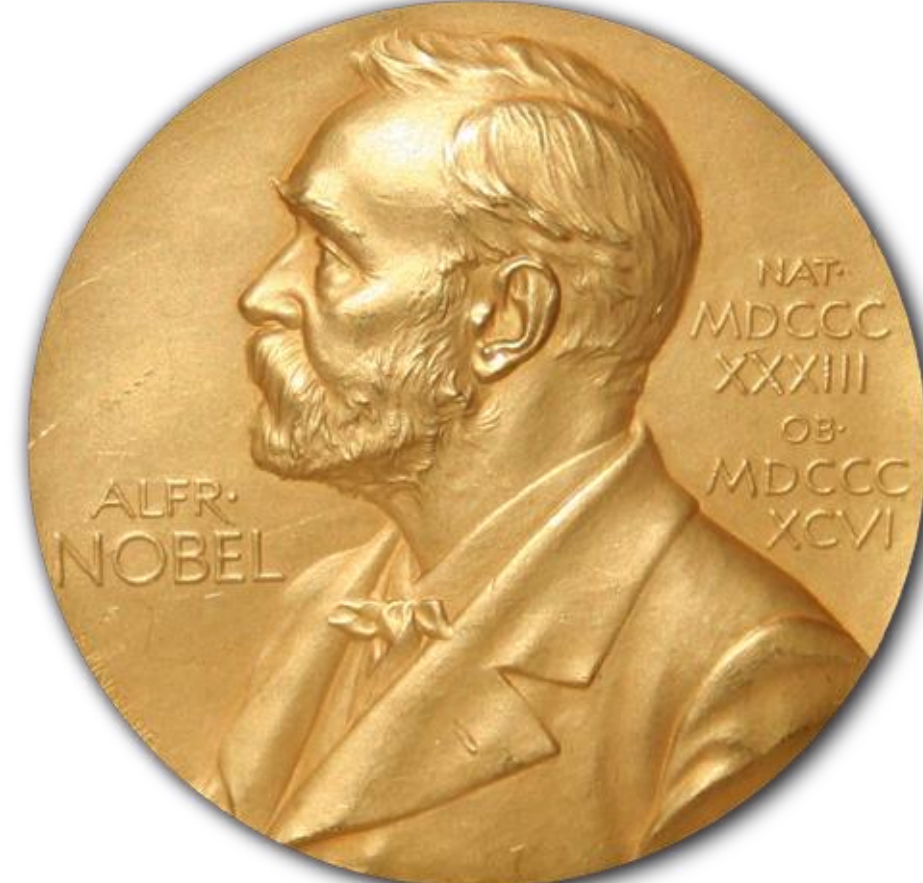
MATERIALS DISCOVERY

Across Domains, AI Shrinks Time-to-Science

Chemistry
Demis Hassabis, John Jumper for AlphaFold
David Baker for Rosetta (protein design)



Physics
Geoff Hinton and John Hopfield
for artificial neural networks



Groundbreaking Achievements with NVIDIA

Challenges - Saturating performance in traditional HPC

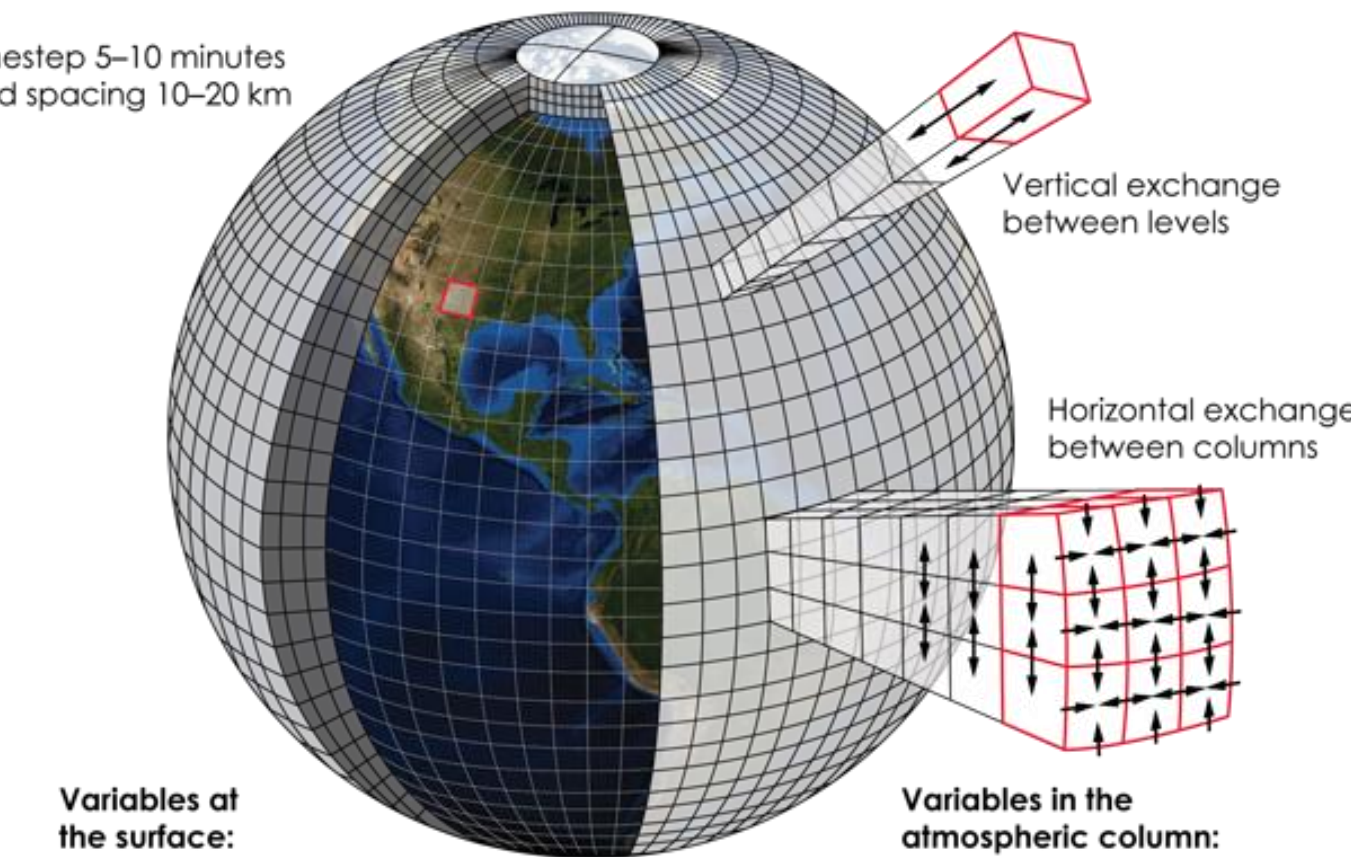
Simulations are getting larger and more complex

Traditional solution methods are:

- Computationally Expensive
- Plagued by Domain Discretization Techniques
- Not suitable for Data-assimilation or Inverse problems

Weather forecast modeling

Timestep 5-10 minutes
Grid spacing 10-20 km

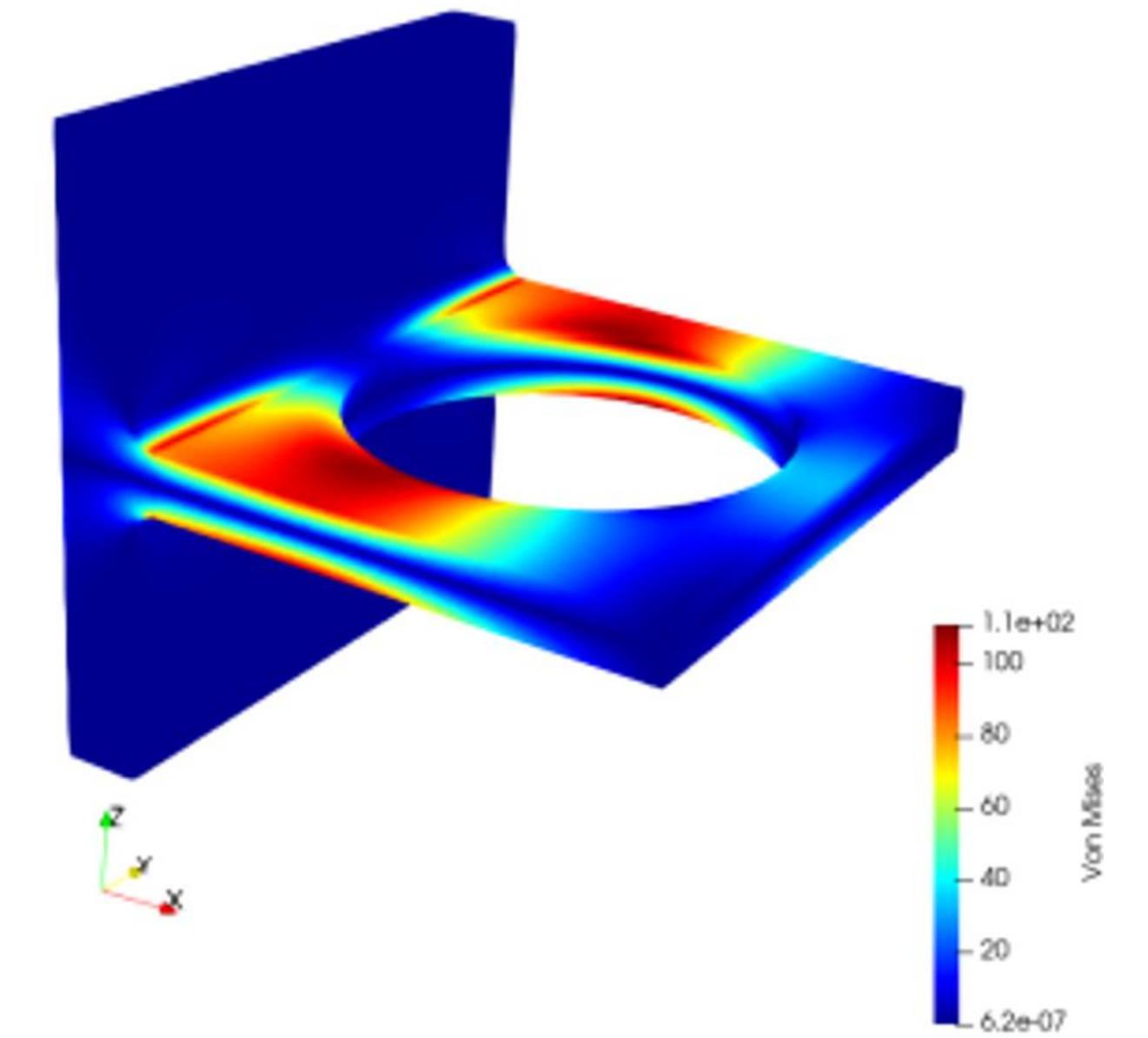


Variables at the surface:
Temperature
Humidity
Pressure
Moisture fluxes
Heat fluxes
Radiation fluxes

Variables in the atmospheric column:
Wind vectors
Humidity
Clouds
Temperature
Height
Precipitation
Aerosols

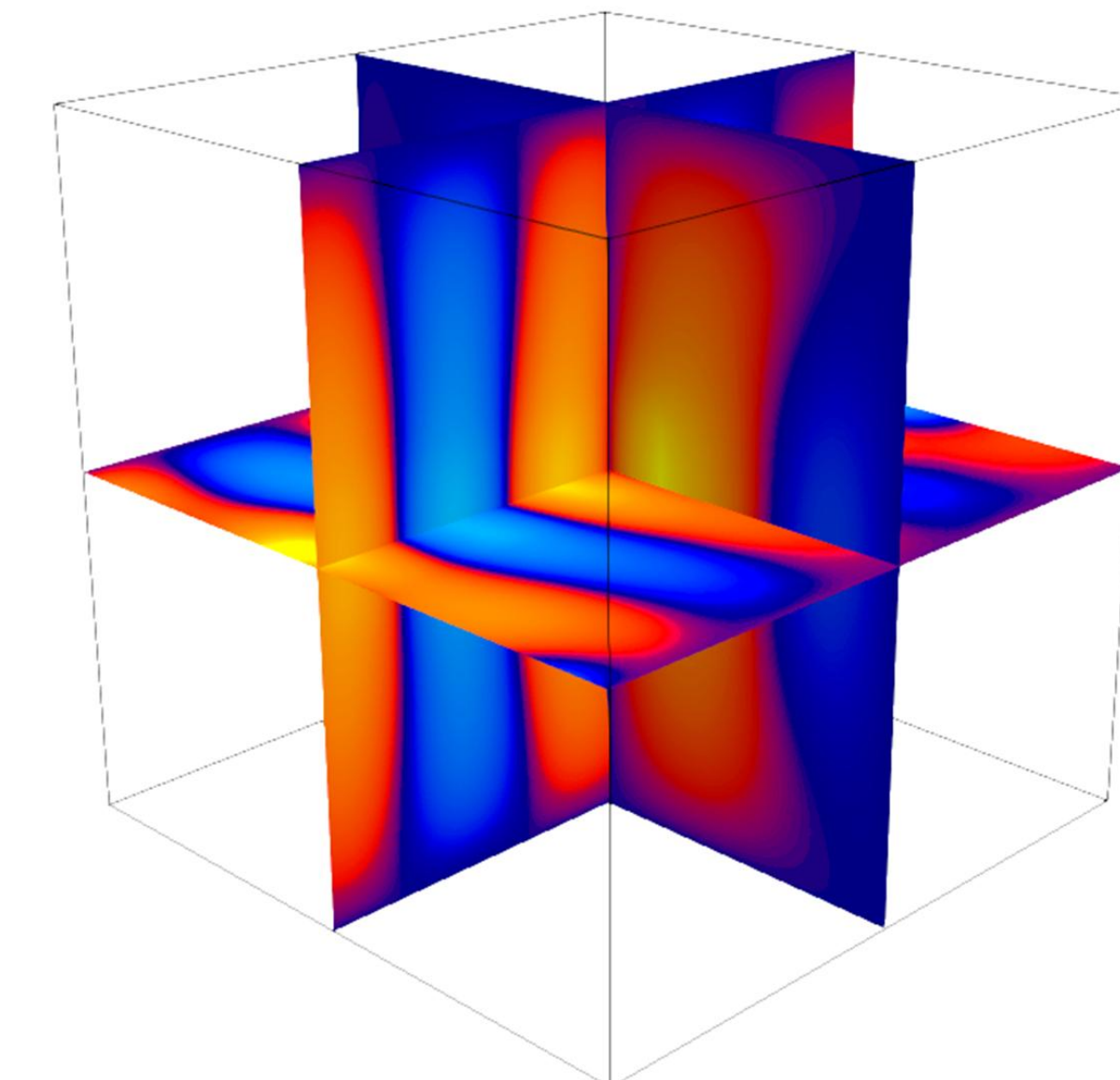
Atmospheric flows

Finite Volume Methods, Sub-grid scale modeling



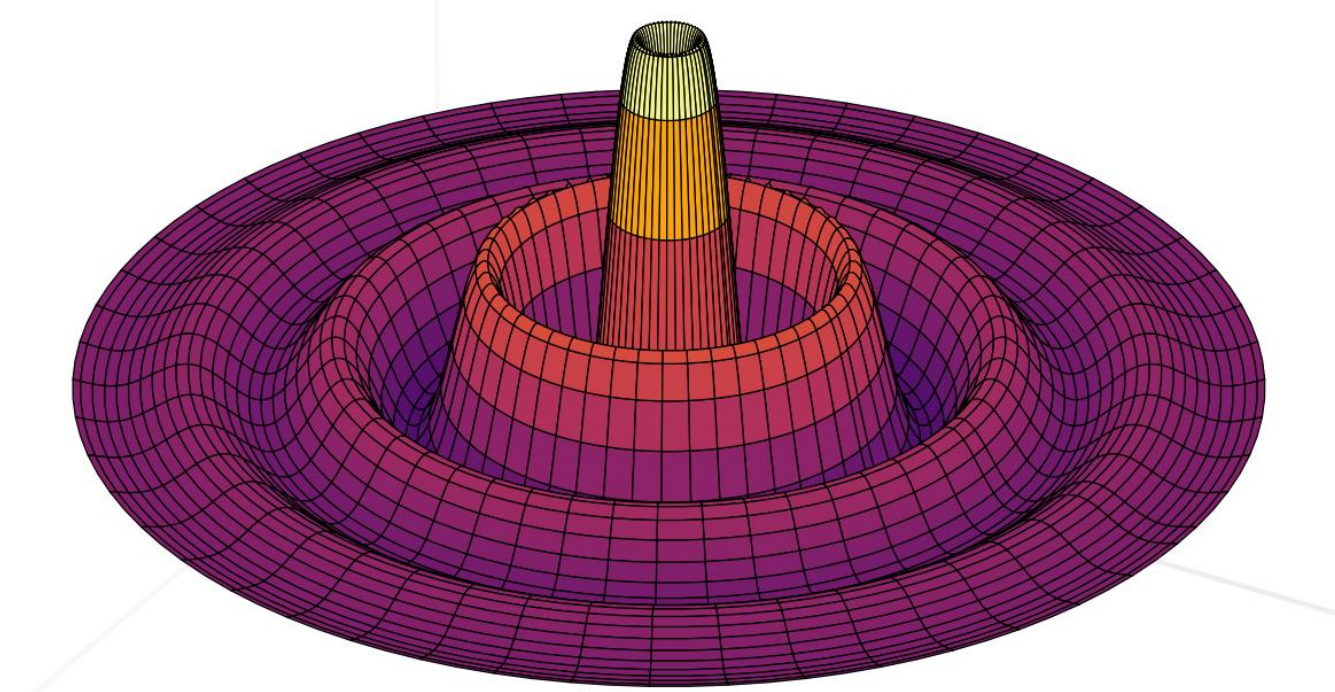
Structural Mechanics

Finite Element Methods



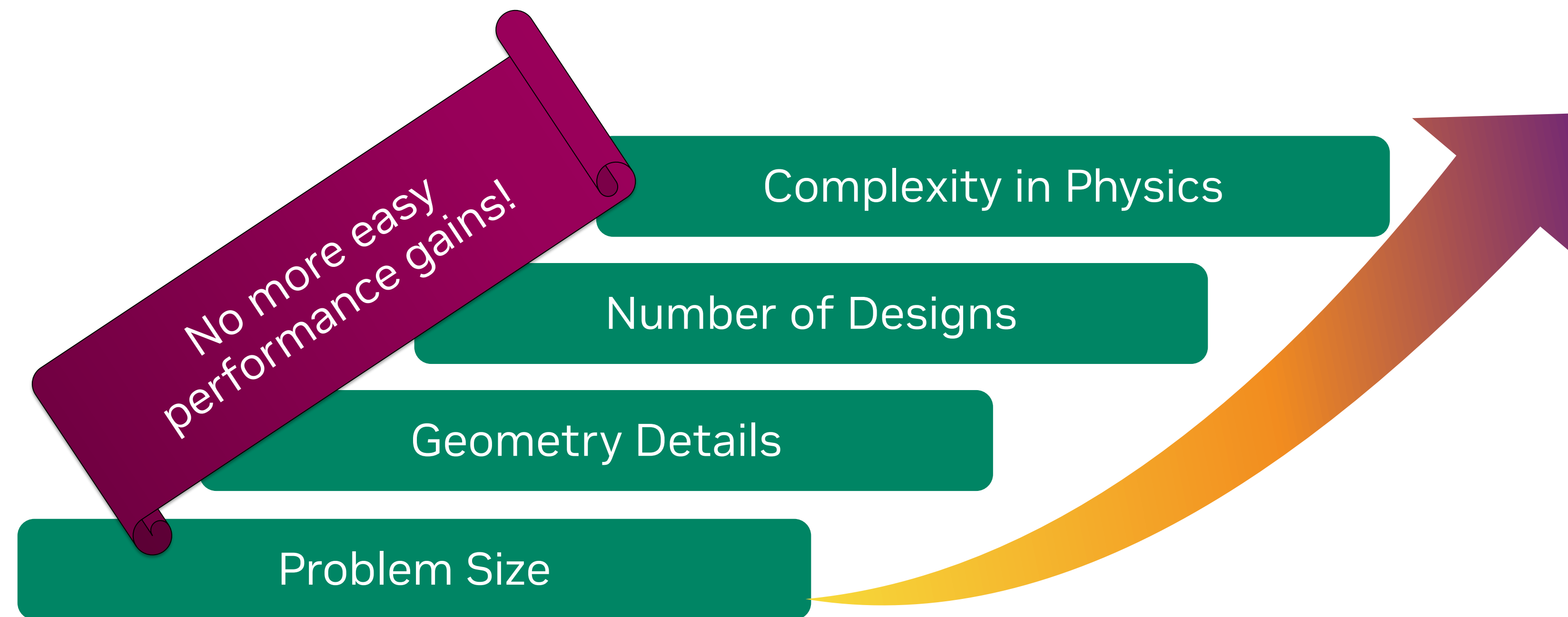
Electromagnetics

Finite Element and Frequency domain methods



Vibrations / Acoustics

Finite Difference Methods

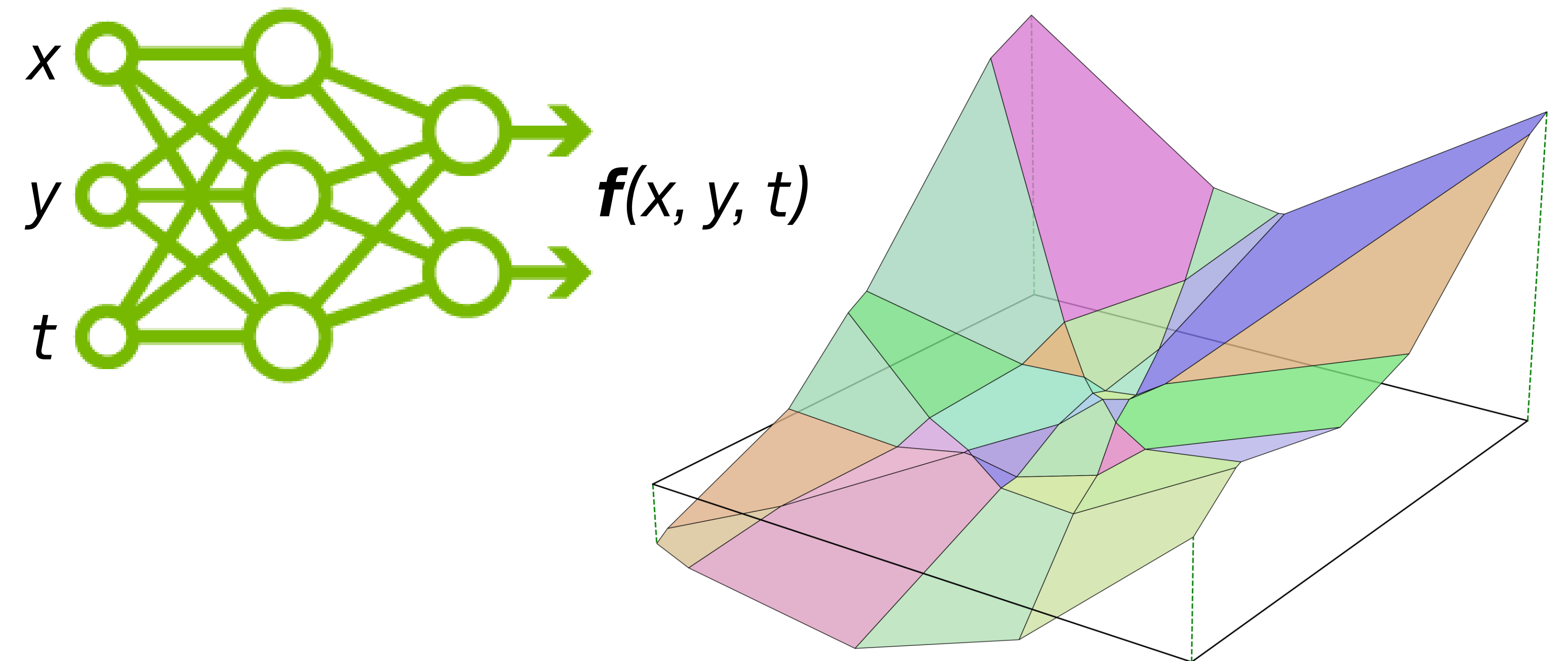
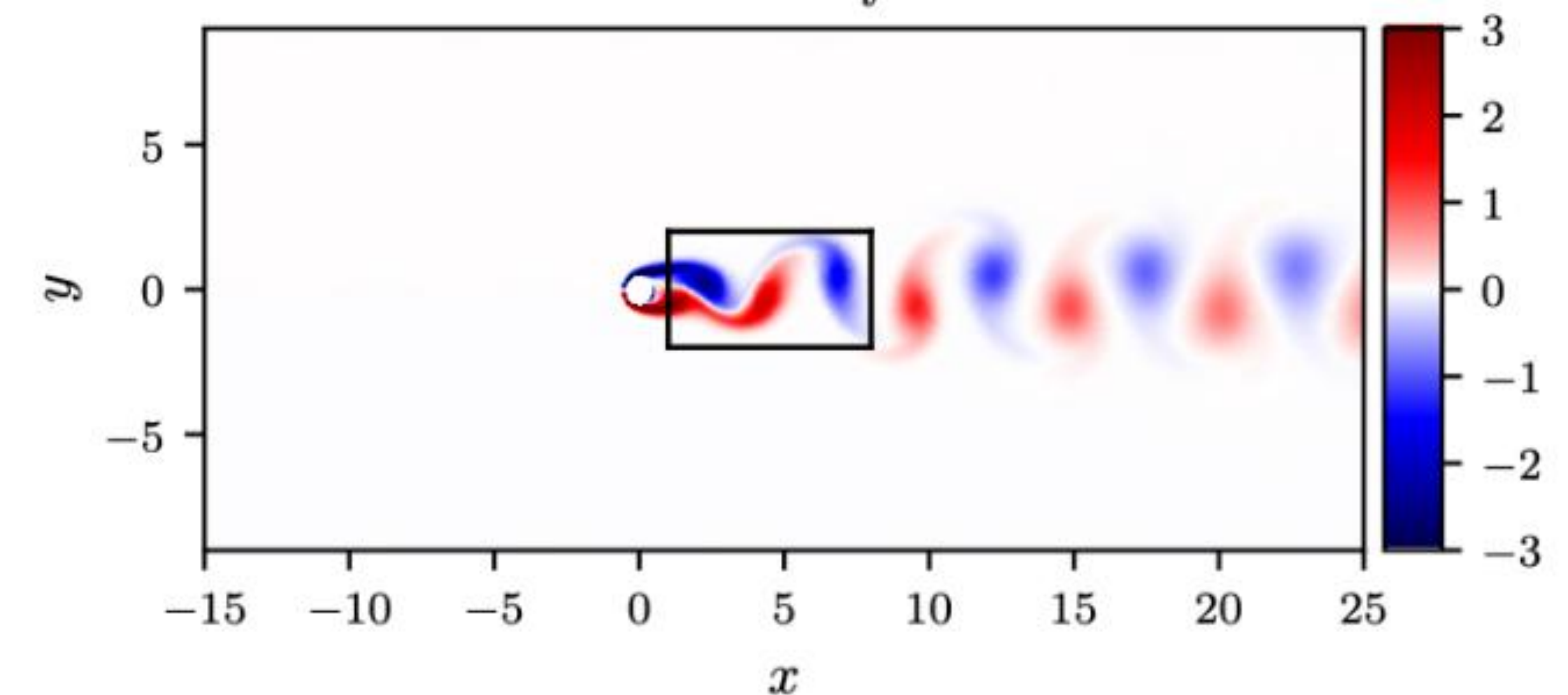


Universal Function Approximation

Use a NN as an approximation function

- When we're solving a PDE, we're looking for a function
- But multi-layer perceptrons can approximate arbitrary functions, given "enough" (surprisingly few) nodes, under various constraints given the details of the function, activations, *etc.*
- If this is new to you, looking into [Universal Approximation Theorem\(s\)](#) is a good starting point for the mathematics minded, or for the computational physics crowd (like me), I like a [post on Jane Street's blog using ReLU activations to model arbitrary piecewise-linear functions](#)
- Other kinds of networks can do this too! e.g. [Kolmogorov-Arnold Networks](#) This is part of the broad research efforts around PINN-type methods

Raissi, Perdikaris, & Karniadakis (2019)

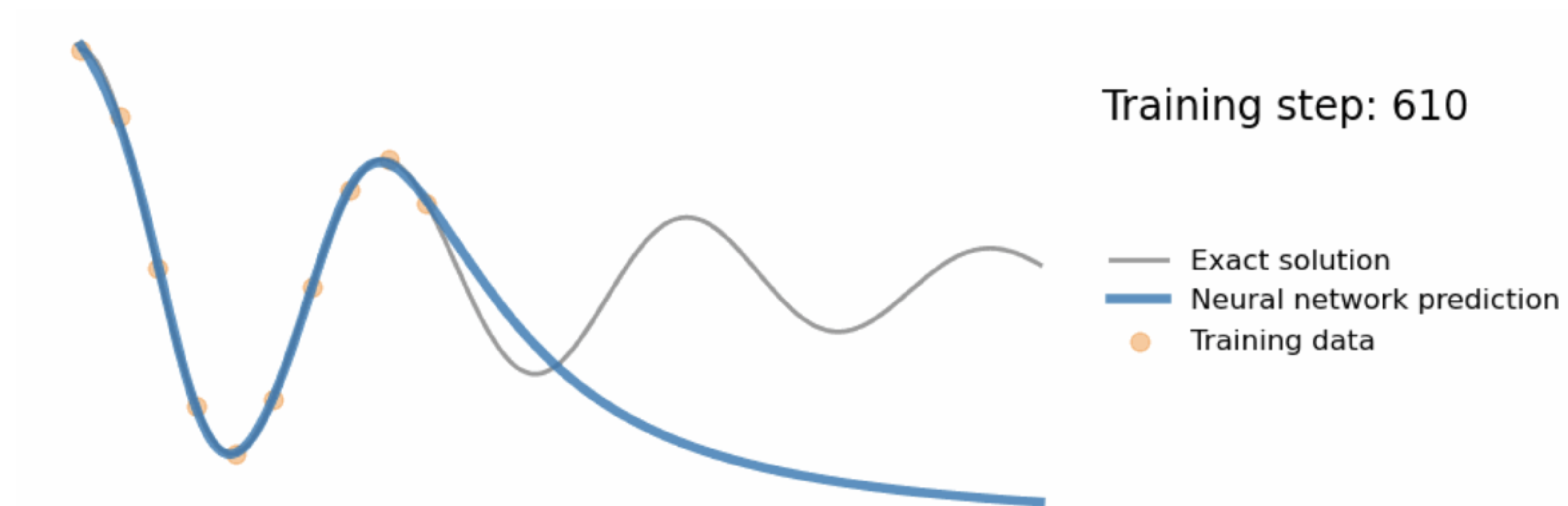


<https://blog.janestreet.com/visualizing-piecewise-linear-neural-networks/>

A Machine Learning Accelerator for Science

Naively using Deep Learning for scientific problems has its own challenges:

- Lack of interpretability
- Poor generalization – accurately models the process within vicinity of training data, but not away from this data.
- Lack of training data

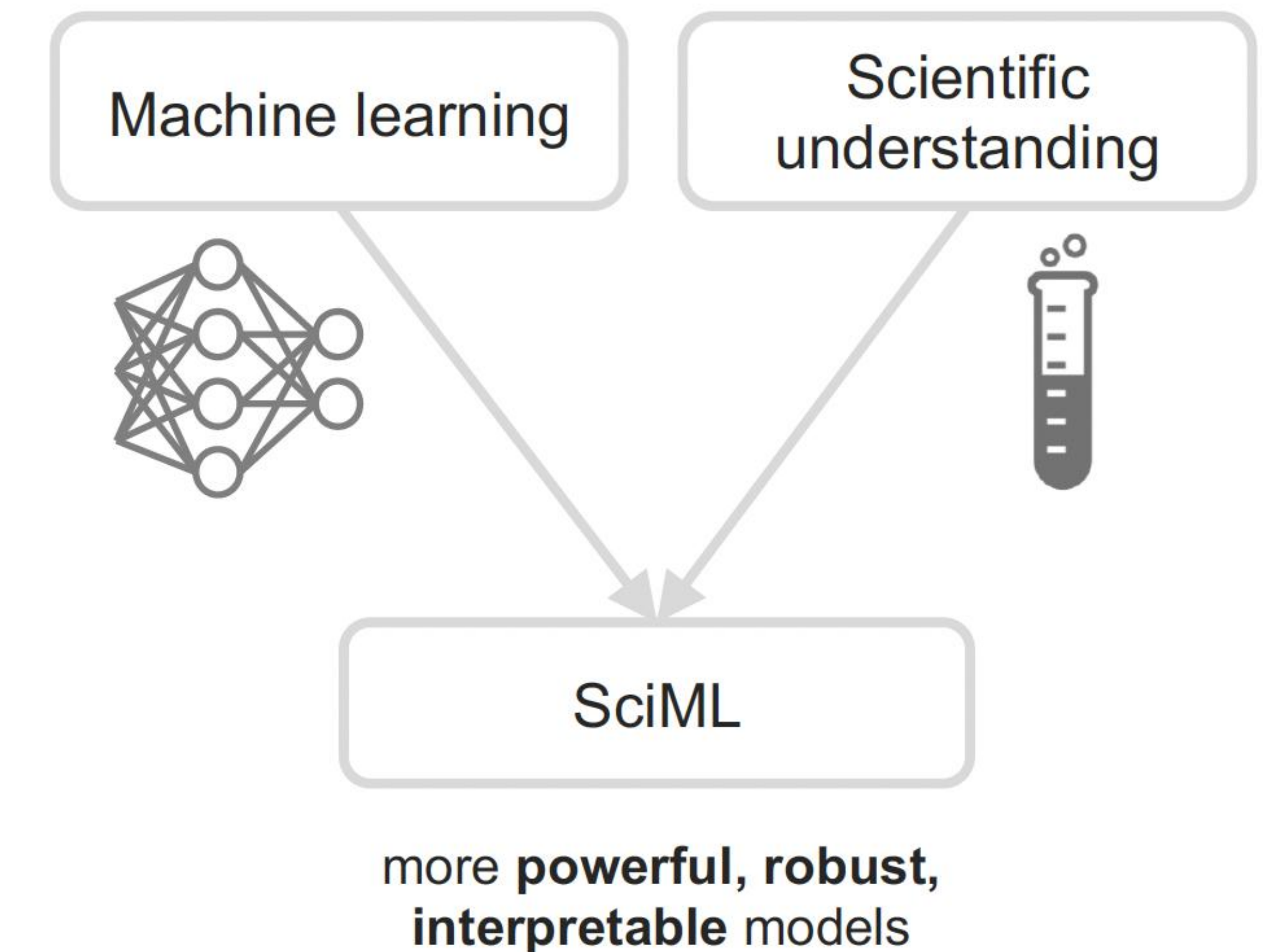


Source: <https://benmoseley.blog/my-research/so-what-is-a-physics-informed-neural-network/>
ETH Zürich 2024 AI in the Sciences and Engineering Master's course

Scientific Machine Learning

- What if we can somehow add the underlying physics to our ML workflows?
- This way we can take advantage of both the power of Neural Networks + our prior scientific knowledge.
- Advantages:
 - More accurate predictions even if we have sparse or no data, as we can leverage the physical laws.
 - Better generalization as the workflow is not confined to the training data only.
 - Useful in scenarios where data collection is challenging or expensive.

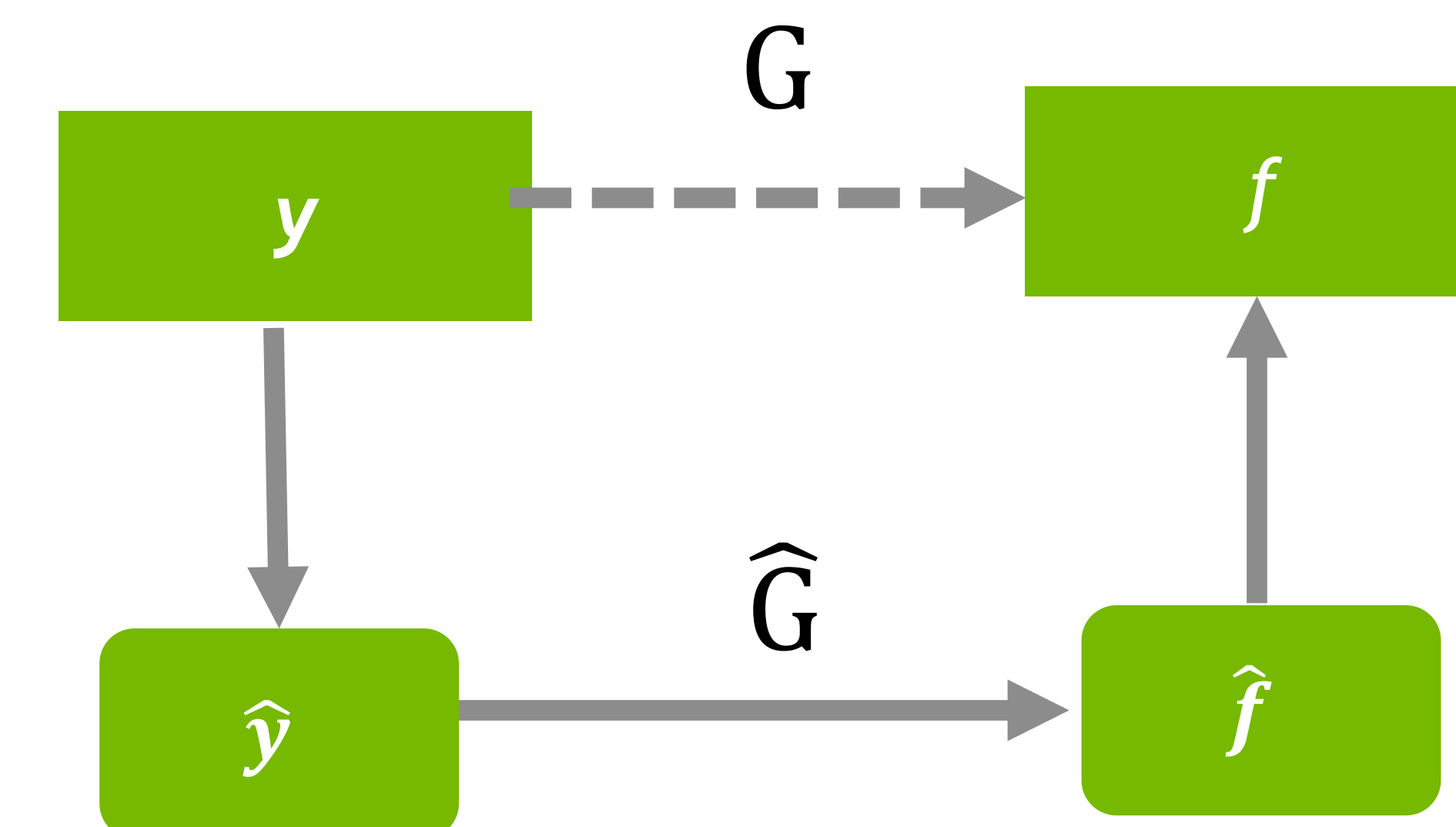
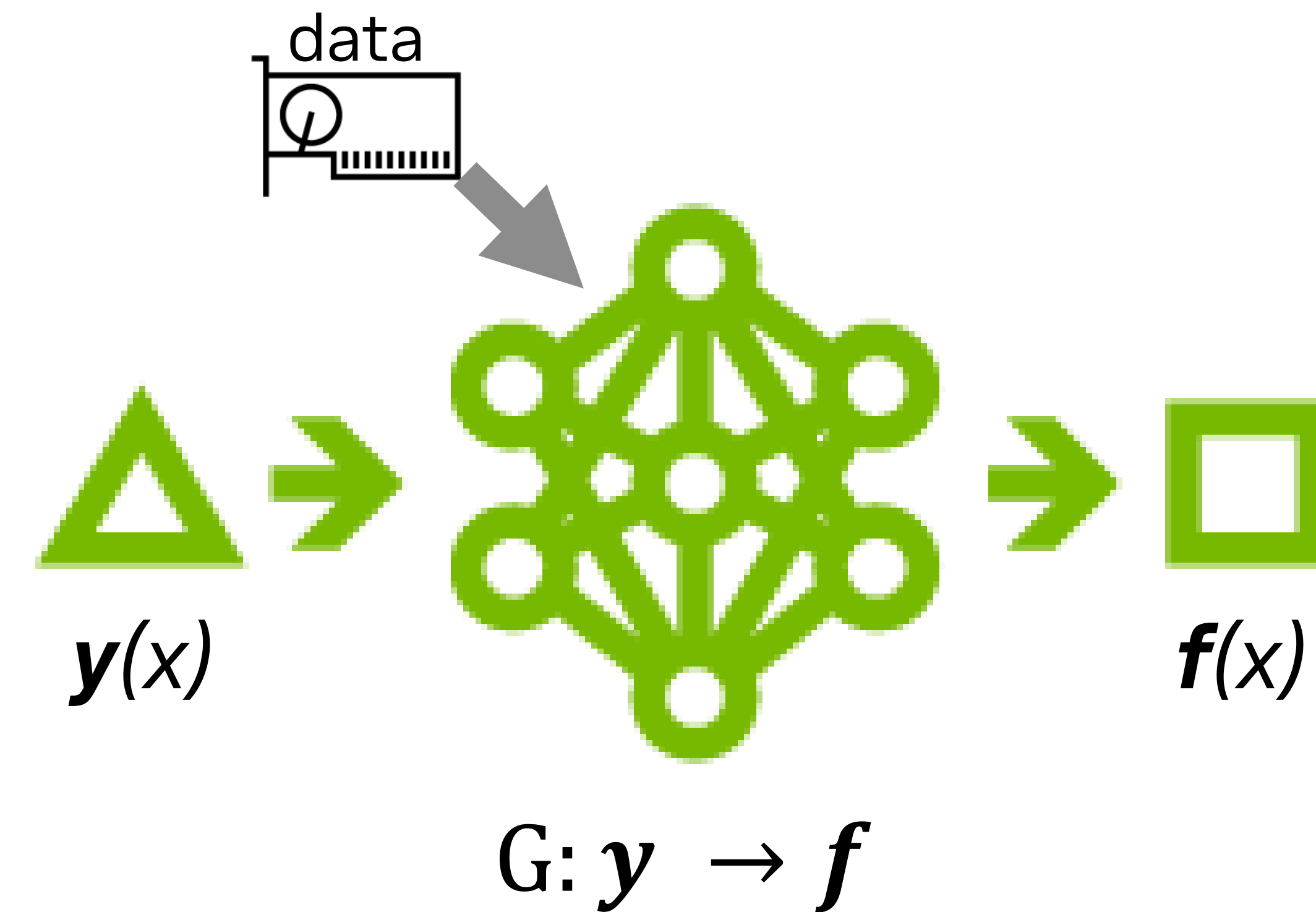
Solution



How Would Learning An Operator Even Work?

Handling mappings between infinite-dimensional objects

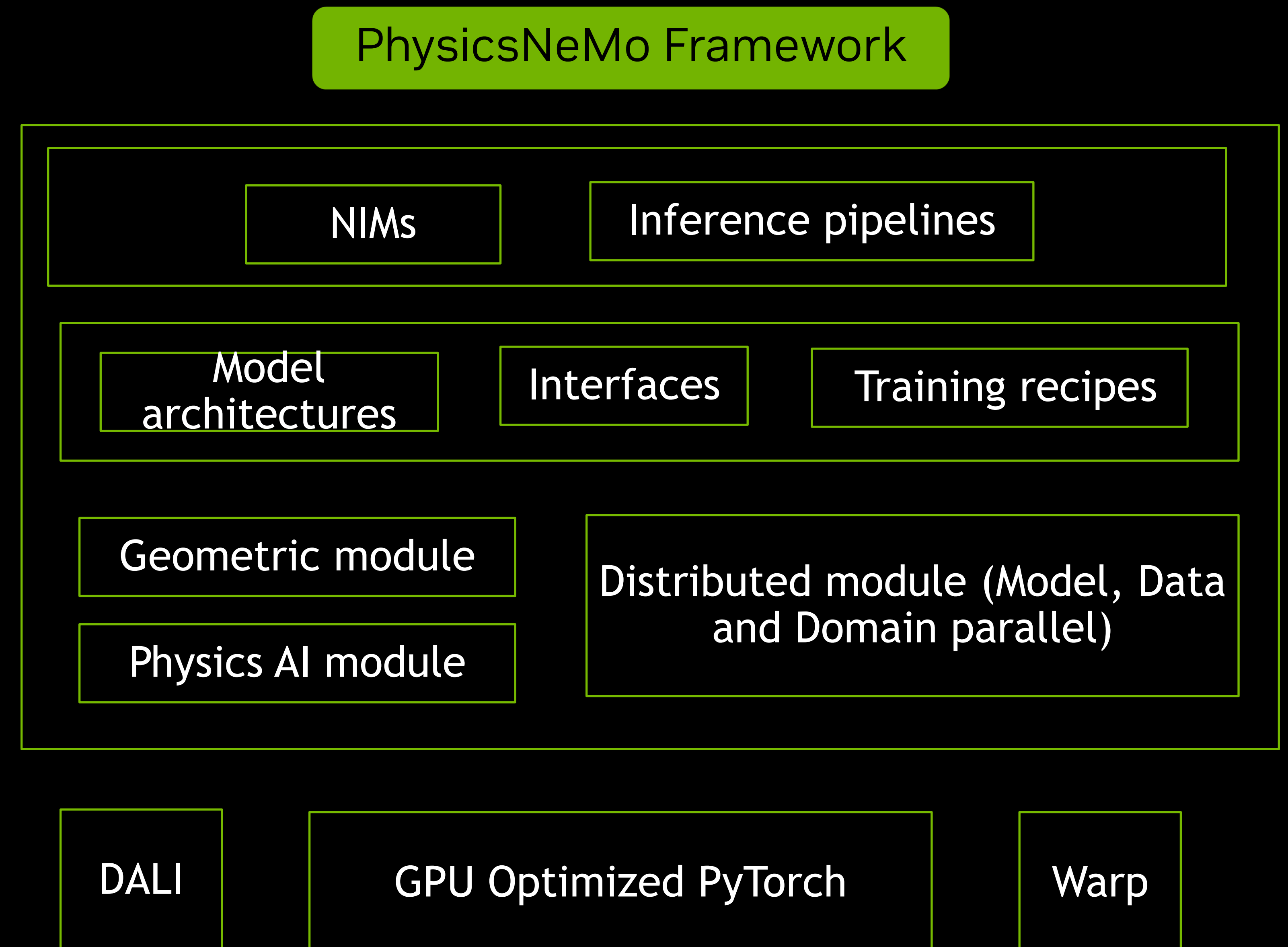
- It turns out there are universal approximation to nonlinear operator theorems, too (e.g. [Chen & Chen \(1995\) IEEE Tran. Neur. Net.](#))
- How do you handle an infinite dimensional input?
- Very traditional numerical approach – we don't
 - Project into some reduced-dimensionality space in some way
 - Work in that reduced space
 - Extrapolate back into the full space
- In contrast to PINNs, which needed no real training data, operator learning requires lots of training samples of input and output functions
 - Experimental data
 - Surrogate data such as simulations
- Training is very expensive, but can then inference very quickly with different ICs (and maybe BCs)



What is PhysicsNeMo?

Open-Source Framework for developing Physics AI algorithms

- Enterprise grade framework/toolkit for building physics AI models
 - Built-in physics AI training pipelines for CAE
 - Model architectures tuned for Physics AI
 - GPU accelerated data pipelines for engineering data formats and data structures
 - Utilities for injecting Physics – PDEs, BCs, Geometry constraints
 - Optimal and Scalable training pipelines
 - Memory optimized training pipelines and model architectures/layers
 - Scale to multi-node systems out of the box – data and model parallel
 - Reference AI enhanced sample applications



<https://github.com/NVIDIA/PhysicsNeMo>

What can Physics AI enable?

- Near-real time emulation
- High fidelity sim
- Representative of the high dimensional geometry and parameter design space



Built On Top Of 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

PhysicsNeMo Resources

[PhysicsNeMo Product page](#)

[Get an Overview – webinar](#)

[Download PhysicsNeMo Framework](#)

[PhysicsNeMo Documentation](#)

[Getting started guide](#)

[Reference samples 1](#)

[Reference samples 2](#)

[Reference blogs](#)

[Self paced DLI Course](#)

CFD

| Use case | Model |
|--|------------------------------|
| Vortex Shedding | MeshGraphNet |
| Ahmed Body Drag prediction | MeshGraphNet |
| Navier-Stokes Flow | RNN |
| Gray-Scott System | RNN |
| Darcy Flow | FNO |
| Darcy Flow using Nested-FNOs | Nested-FNO |
| Darcy Flow (Data + Physics Driven) using DeepONet approach | FNO (branch) and MLP (trunk) |
| Darcy Flow (Data + Physics Driven) using PINO approach (Numerical gradients) | FNO |
| Stokes Flow (Physics Informed Fine-Tuning) | MeshGraphNet and MLP |

Weather

| Use case | Model | AMP | CUDA Graphs | Multi-GP |
|---|-----------|-----|-------------|----------|
| Medium-range global weather forecast using FCN-SFNO | FCN-SFNO | YES | NO | YES |
| Medium-range global weather forecast using GraphCast | GraphCast | YES | NO | YES |
| Medium-range global weather forecast using FCN-AFNO | FCN-AFNO | YES | YES | YES |
| Medium-range and S2S global weather forecast using DLWP | DLWP | YES | YES | YES |

Healthcare

| Use case | Model | Transient |
|--|--------------|-----------|
| Cardiovascular Simulations | MeshGraphNet | YES |
| Brain Anomaly Detection | FNO | YES |

Molecular Dynamics

| Use case | Model | Transient |
|---|--------------|-----------|
| Force Prediction for Lennard Jones system | MeshGraphNet | NO |

Generative

| Use case | Model | Multi-GPU | Multi- |
|--|----------|-----------|--------|
| Generative Correction Diffusion Model for Km-scale Atmospheric Downscaling | CorrDiff | YES | YES |

Additional examples

In addition to the examples in this repo, more Physics-ML usecases and examples can be referenced from the ModuL

Introductory

| Use case | Model |
|--|------------------------------------|
| Lid Driven Cavity Flow | Fully Connected MLP PINN |
| Anti-derivative | Data and Physics informed DeepONet |
| Darcy Flow | FNO, AFNO, PINO |
| Spring-mass system ODE | Fully Connected MLP PINN |
| Surface PDE | Fully Connected MLP PINN |

Turbulence

| Use case | Model |
|--|-----------------------------------|
| Taylor-Green | Fully Connected MLP PINN |
| Turbulent channel | Fourier Feature MLP PINN |
| Turbulent super-resolution | Super Resolution Network, Pix2Pix |

Electromagnetics

| Use case | Model | Level | St |
|---------------------------|--------------------------|--------------|----|
| Waveguide | Fourier Feature MLP PINN | Intermediate | St |

Solid Mechanics

| Use case | Model | Level | In |
|------------------------------------|---------------------------------|--------------|----|
| Plane displacement | Fully Connected MLP PINN, VPINN | Intermediate | In |

Design Optimization

| Use case | Model |
|--|---------------------------------------|
| 2D Chip | Fully Connected MLP PINN |
| 3D Three fin Heatsink | Fully Connected MLP PINN |
| FPGA Heatsink | Multiple Models (including Four etc.) |
| Limerock Industrial Heatsink | Fourier Feature MLP PINN |

Geophysics

| Use case | Model | Level |
|--------------------------------------|--------------------------|----------|
| Reservoir simulation | FNO, PINO | Advance |
| Seismic wave | Fully Connected MLP PINN | Intermec |
| Wave equation | Fully Connected MLP PINN | Intermec |

Healthcare

Reference sample catalogue

<https://github.com/NVIDIA/PhysicsNeMo/tree/main/examples>

<https://github.com/NVIDIA/PhysicsNeMo-sym/tree/main/examples>

CFD

| Use case | Model | Transient |
|--|------------------------------|-----------|
| Vortex Shedding | MeshGraphNet | YES |
| Ahmed Body Drag prediction | MeshGraphNet | NO |
| Navier-Stokes Flow | RNN | YES |
| Gray-Scott System | RNN | YES |
| Darcy Flow | FNO | NO |
| Darcy Flow using Nested-FNOs | Nested-FNO | NO |
| Darcy Flow (Data + Physics Driven) using DeepONet approach | FNO (branch) and MLP (trunk) | NO |
| Darcy Flow (Data + Physics Driven) using PINO approach (Numerical gradients) | FNO | NO |
| Stokes Flow (Physics Informed Fine-Tuning) | MeshGraphNet and MLP | NO |

Weather

| Use case | Model | AMP | CUDA Graphs | Multi-GPU | Multi-Node |
|---|-----------|-----|-------------|-----------|------------|
| Medium-range global weather forecast using FCN-SFNO | FCN-SFNO | YES | NO | YES | YES |
| Medium-range global weather forecast using GraphCast | GraphCast | YES | NO | YES | YES |
| Medium-range global weather forecast using FCN-AFNO | FCN-AFNO | YES | YES | YES | YES |
| Medium-range and S2S global weather forecast using DLWP | DLWP | YES | YES | YES | YES |

Healthcare

| Use case | Model | Transient |
|--|--------------|-----------|
| Cardiovascular Simulations | MeshGraphNet | YES |
| Brain Anomaly Detection | FNO | YES |

Molecular Dynamics

| Use case | Model | Transient |
|---|--------------|-----------|
| Force Prediction for Lennard Jones system | MeshGraphNet | NO |

Generative

| Use case | Model | Multi-GPU | Multi-Node |
|--|----------|-----------|------------|
| Generative Correction Diffusion Model for Km-scale Atmospheric Downscaling | CorrDiff | YES | YES |

Additional examples

In addition to the examples in this repo, more Physics-ML usecases and examples can be referenced from the [Modulus-Sym examples](#).

Introductory

| Use case | Model | Level | Attributes |
|--|------------------------------------|--------------|-------------------------|
| Lid Driven Cavity Flow | Fully Connected MLP PINN | Introductory | Steady state, Multi-GPU |
| Anti-derivative | Data and Physics informed DeepONet | Introductory | Steady state, Multi-GPU |
| Darcy Flow | FNO, AFNO, PINO | Introductory | Steady state, Multi-GPU |
| Spring-mass system ODE | Fully Connected MLP PINN | Introductory | Steady state, Multi-GPU |
| Surface PDE | Fully Connected MLP PINN | Introductory | Steady state, Multi-GPU |

Turbulence

| Use case | Model | Level | Attributes |
|--|-----------------------------------|--------------|-------------------------|
| Taylor-Green | Fully Connected MLP PINN | Intermediate | Steady state, Multi-GPU |
| Turbulent channel | Fourier Feature MLP PINN | Intermediate | Steady state, Multi-GPU |
| Turbulent super-resolution | Super Resolution Network, Pix2Pix | Intermediate | Steady state, Multi-GPU |

Electromagnetics

| Use case | Model | Level | Attributes |
|---------------------------|--------------------------|--------------|-------------------------|
| Waveguide | Fourier Feature MLP PINN | Intermediate | Steady state, Multi-GPU |

Solid Mechanics

| Use case | Model | Level | Attributes |
|------------------------------------|---------------------------------|--------------|-------------------------|
| Plane displacement | Fully Connected MLP PINN, VPINN | Intermediate | Steady state, Multi-GPU |

Design Optimization

| Use case | Model | Level | Attributes |
|--|--|----------|--------------------------|
| 2D Chip | Fully Connected MLP PINN | Advanced | Steady state, Multi-GPU |
| 3D Three fin Heatsink | Fully Connected MLP PINN | Advanced | Steady state, Multi-Node |
| FPGA Heatsink | Multiple Models (including Fourier Feature MLP PINN, SIRENS, etc.) | Advanced | Steady state, Multi-Node |
| Limerock Industrial Heatsink | Fourier Feature MLP PINN | Advanced | Steady state, Multi-Node |

Geophysics

| Use case | Model | Level | Attributes |
|--------------------------------------|--------------------------|--------------|--------------------------|
| Reservoir simulation | FNO, PINO | Advanced | Steady state, Multi-Node |
| Seismic wave | Fully Connected MLP PINN | Intermediate | Steady state, Multi-Node |
| Wave equation | Fully Connected MLP PINN | Intermediate | Steady state, Multi-Node |

Healthcare

| Use case | Model | Level | Attributes |
|--|--------------------------|--------------|--------------------------|
| Aneurysm modeling using STL geometry | Fully Connected MLP PINN | Intermediate | Steady state, Multi-Node |

The background features a series of parallel, wavy lines in various shades of green, creating a sense of depth and movement. A solid green vertical bar is positioned on the far left side of the image.

Atmospheric Science

High-Resolution Climate Prediction is a Computational Challenge

Today's climate models are too low in resolution. Brute force numerical solvers are decades away from what is needed.

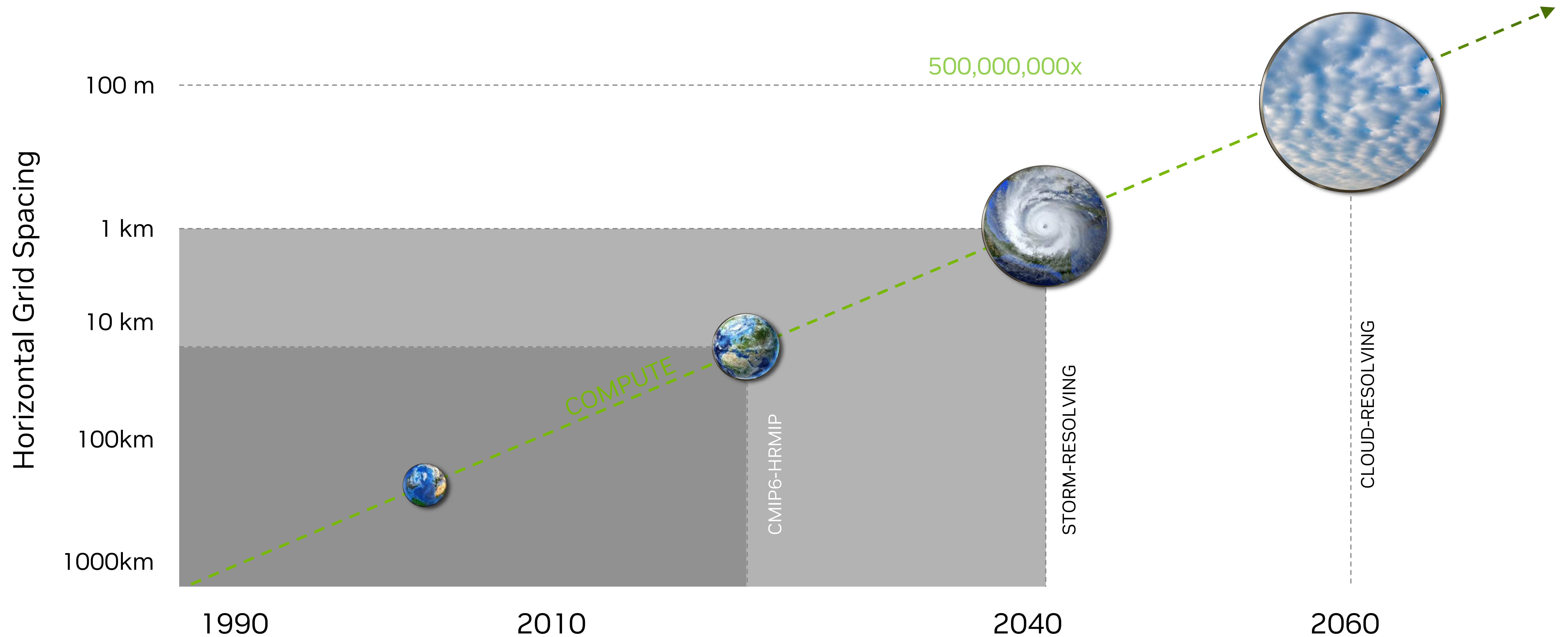


Figure adapted from: Schneider, T., Teixeira, J., Bretherton, C. et al. "Climate goals and computing the future of clouds". *Nature Climate Change* 7, 3-5 (2017)

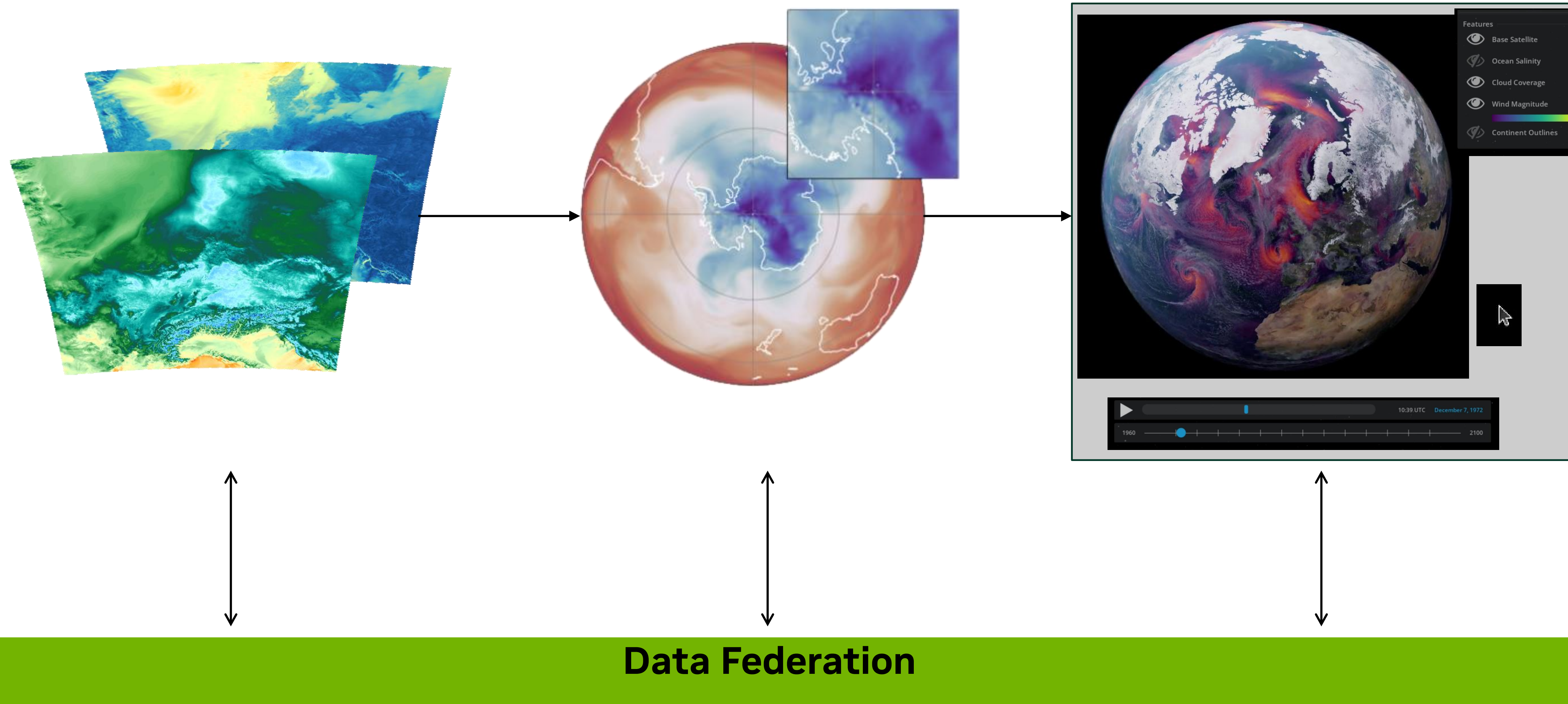
NVIDIA Earth-2

Platform for Accelerated Weather and Climate Modelling

Simulation

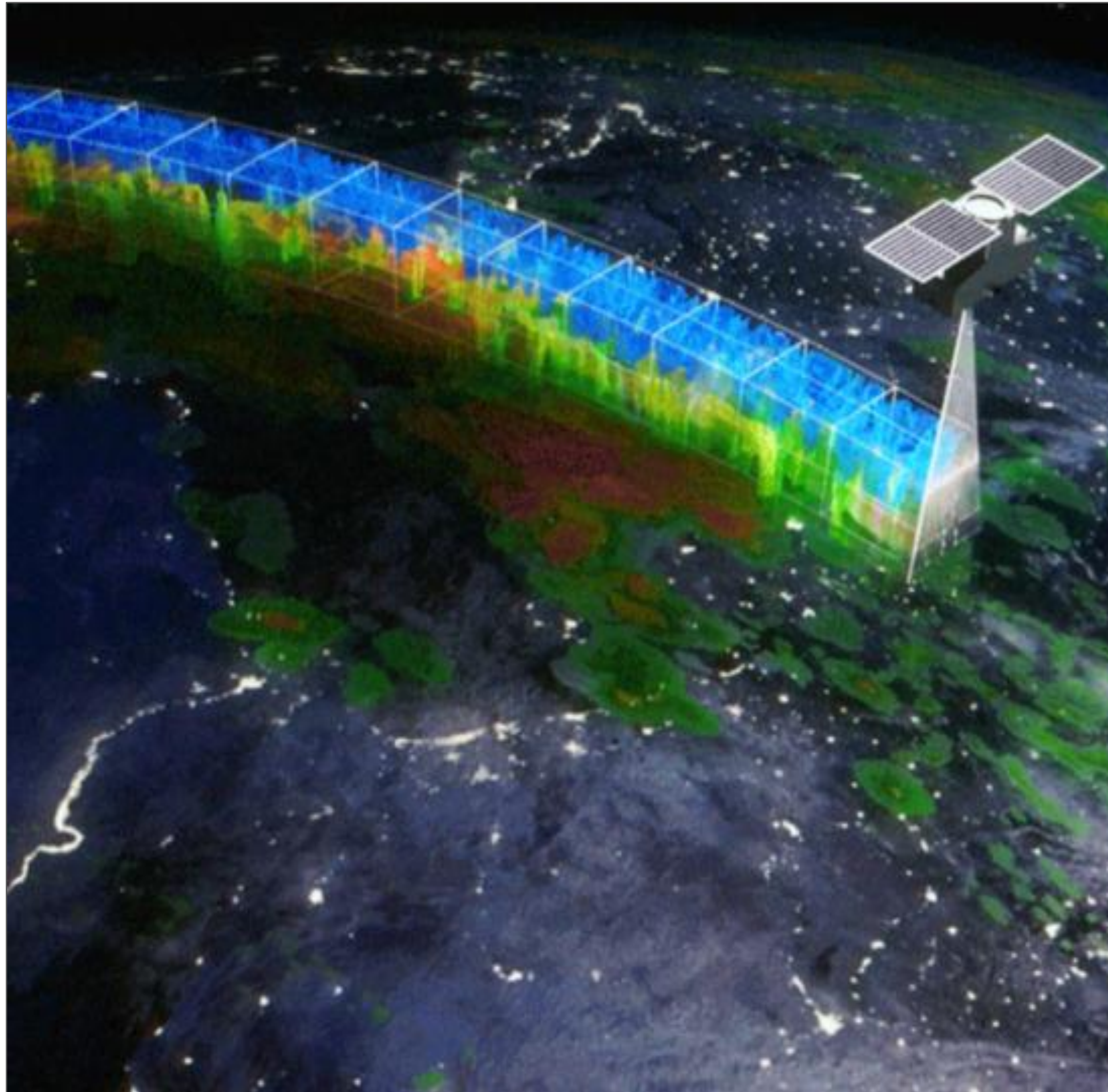
AI Training and Inference

Visualization



Enabling Accelerated Weather Intelligence for Accurate, Hyperlocal Forecasts

NVIDIA Earth-2 accelerates Tomorrow.io's computation from hours to minutes



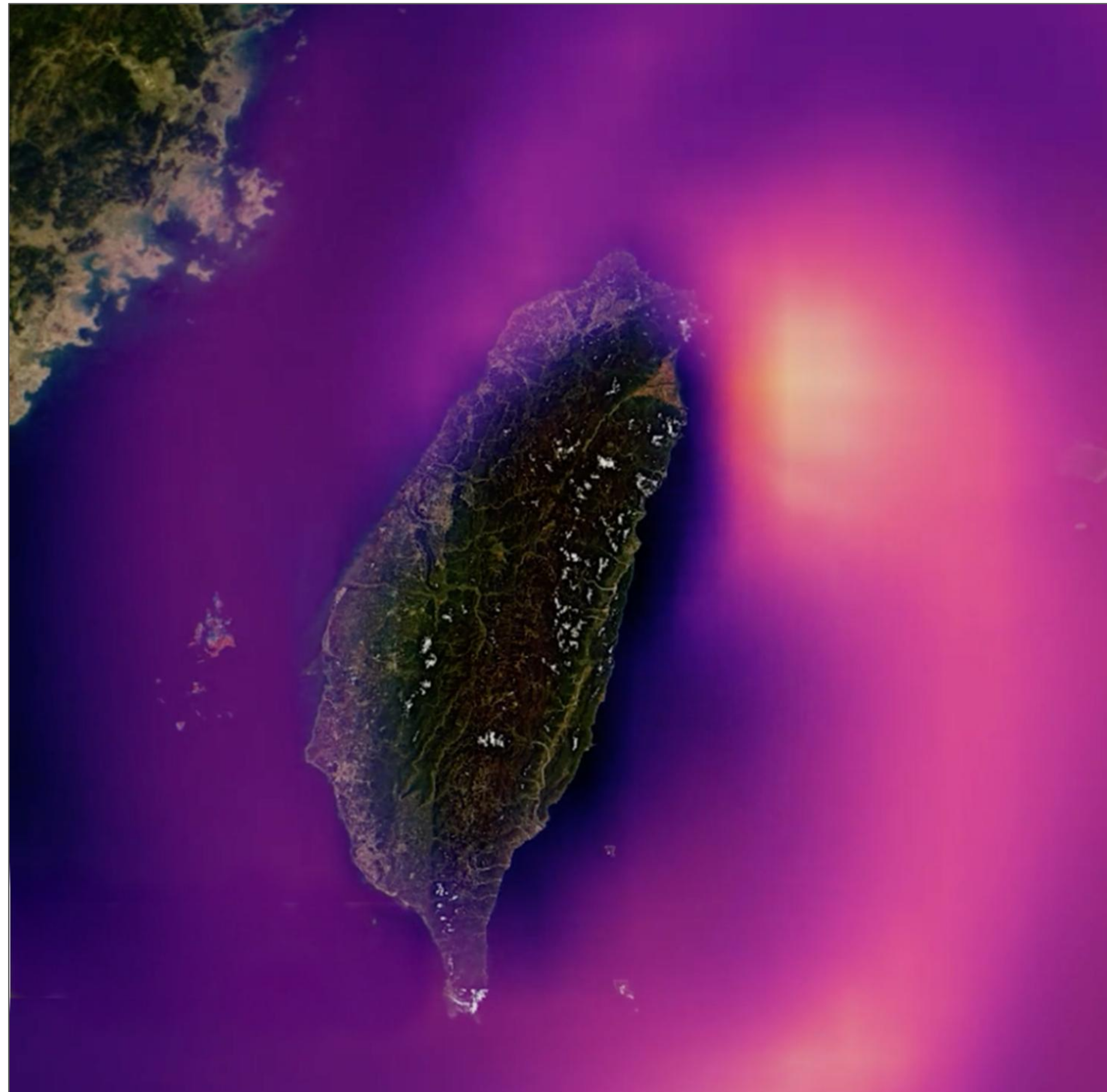
Satellite Imagery



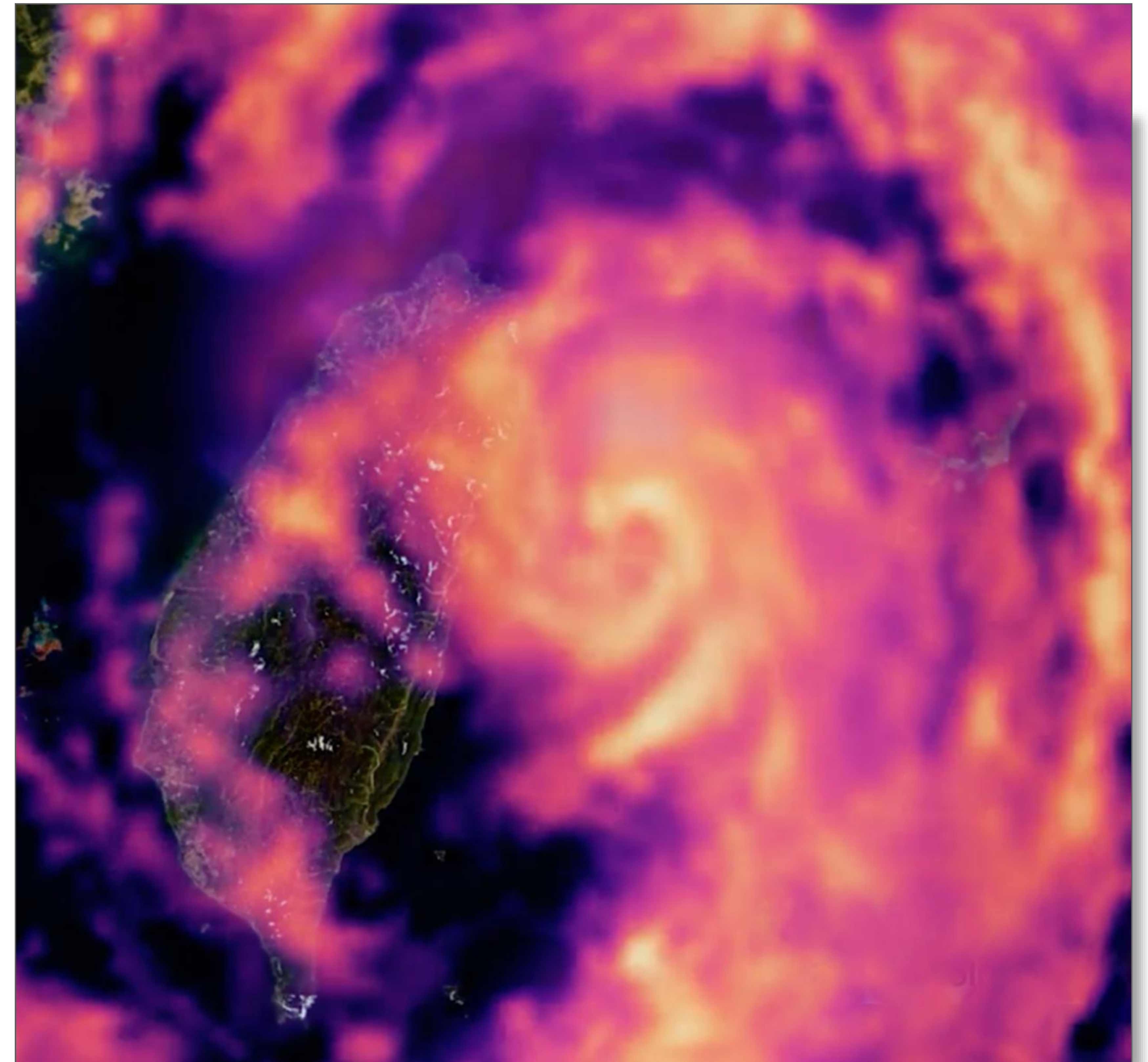
Map-based Weather View in Tomorrow.io Platform

Collaborated with Taiwan CWA to Predict Super Typhoons

1,000x faster and 3,000x more energy efficient than numerical modeling, 13x finer resolution



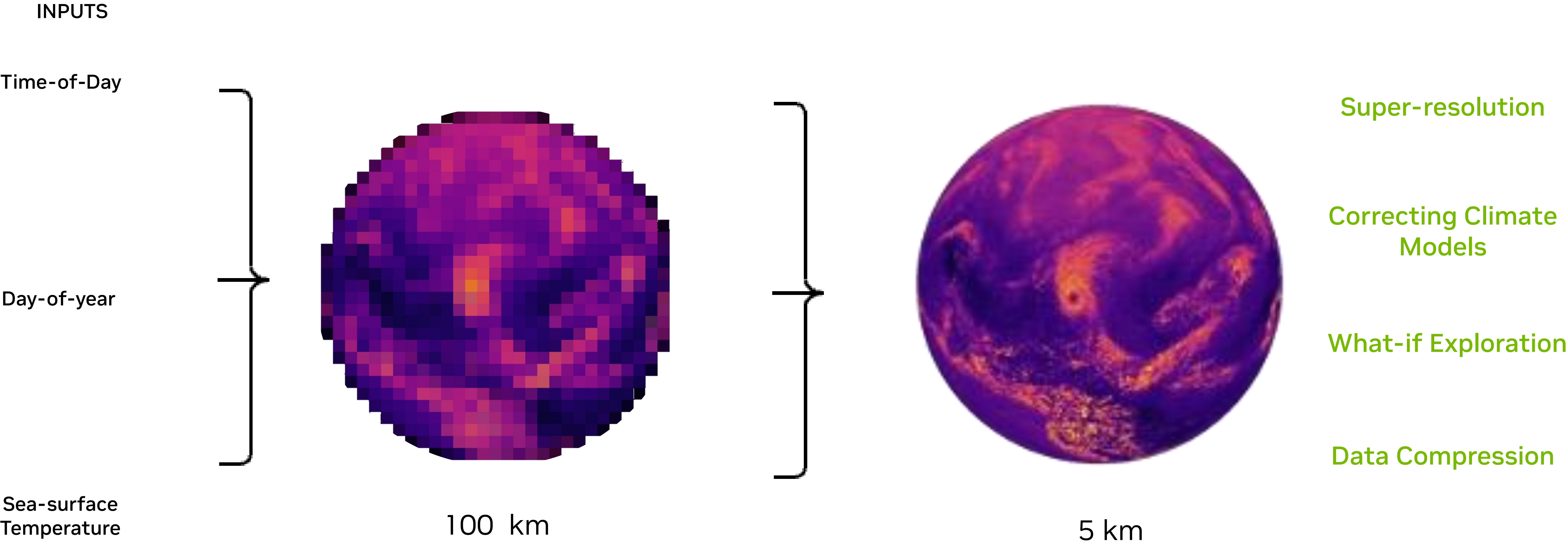
Global AI Forecast at 25km Resolution



CorrDiff at 2km Resolution

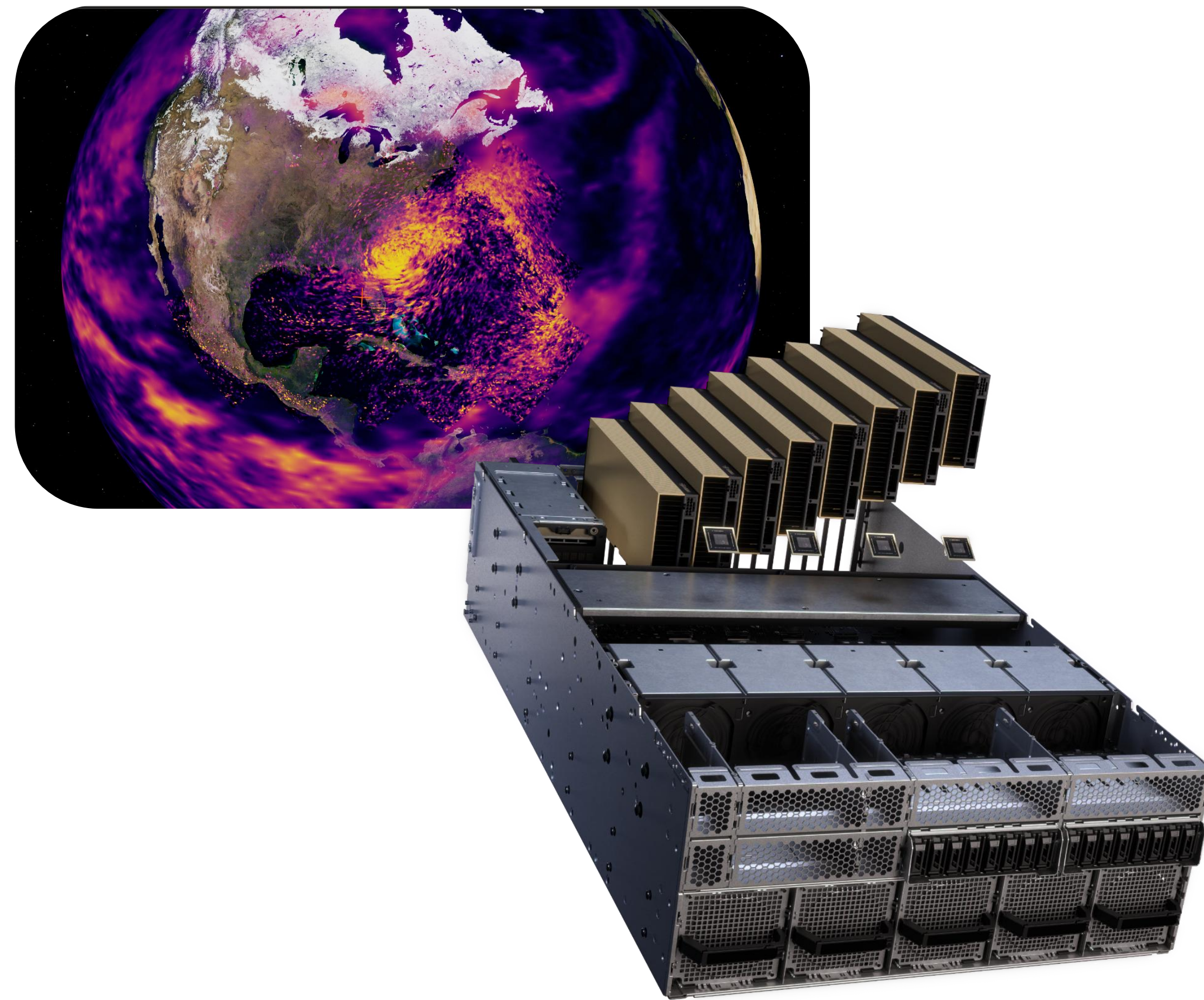
Earth-2 “Climate In A Bottle” Foundation AI Model

World’s First Generative AI Climate Model at Km-Scale Resolution



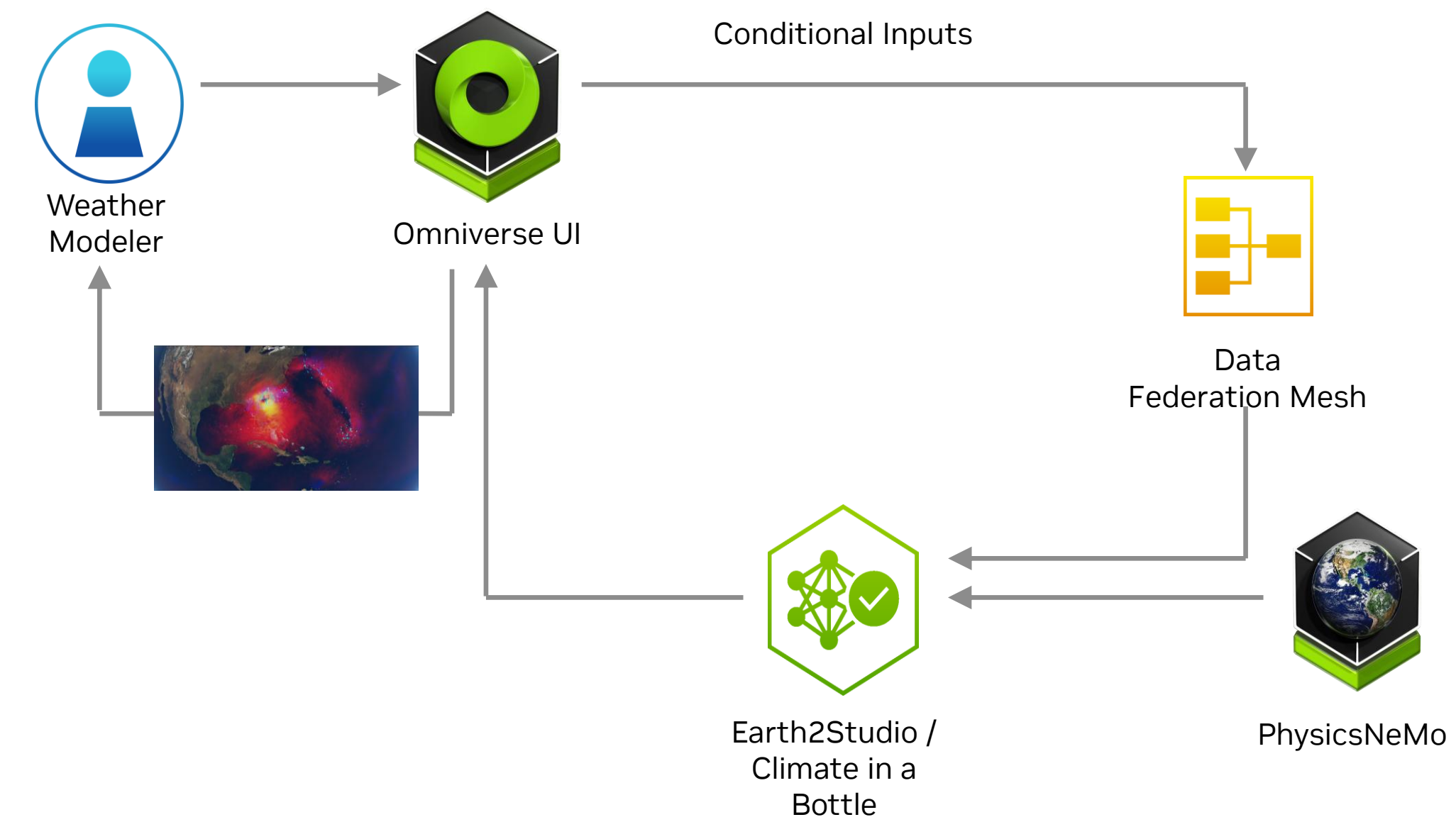
Earth-2 Powering Next-Gen Extreme Weather Simulation

AI Weather Generation

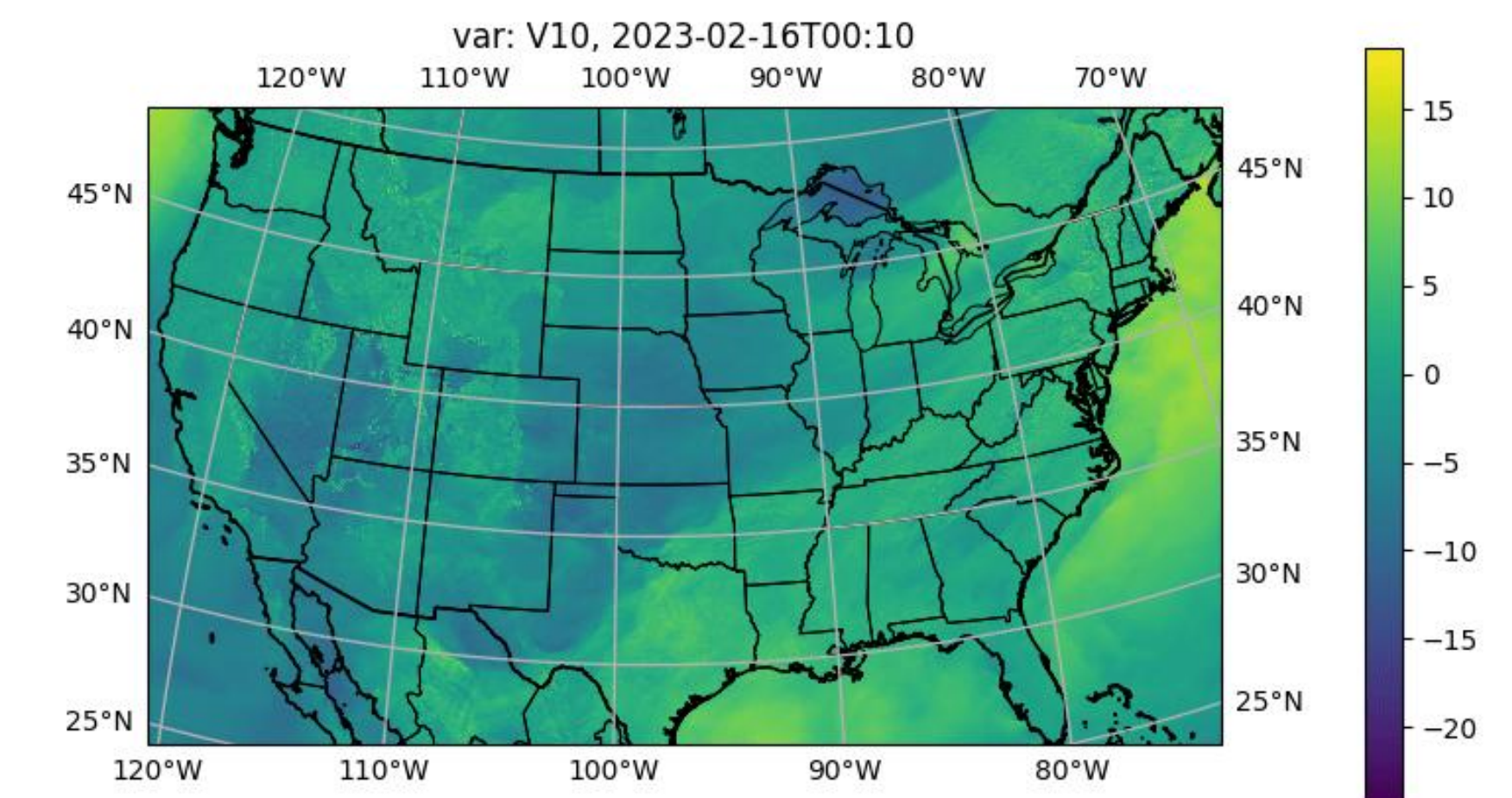


RTX PRO SERVER

Workflow for Conditional Weather Generation



Score-Based Data Assimilation

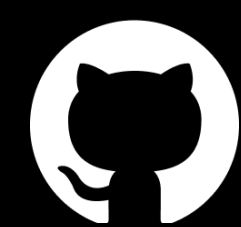


Earth-2 | PhysicsNeMo | Omniverse

Earth2Studio

Library for rapid exploration and validation of pretrained models

- Python library built on PhysicsNeMo for **AI weather model inference**
- Building blocks and recipes for specific tasks
 - medium range, seasonal forecasts with diagnostics
 - Ensemble forecasting
 - Generative downscaling
 - Validation case studies and examples
- Built-in data pipelines e.g., CDS, ARCO, GFS, HRRR, and local/custom
- Select from **NIMs, pretrained models or bring your own**
- Train your custom models in PhysicsNeMo
- Open-source library and enterprise support available through NVIDIA AI Enterprise (NVAIE)



OSS: <https://github.com/NVIDIA/earth2studio>

Examples: <https://nvidia.github.io/earth2studio/examples/>

Medium-range forecasting

- FourCastNet (AFNO/SFNO) [Publication](#)
- PhysicsNeMo-GraphCast (GNN) [Publication](#)
- AIFS [Publication](#)
- Aurora [Publication](#)
- FengWu (Transformer) [Publication](#)
- FuXi (Transformer) [Publication](#)
- PanguWeather (Transformer) [Publication](#)
- StormCast (Diffusion) [Publication](#)

Subseasonal-to-seasonal forecasting

- DLWP (CNN) [Publication](#)
- DLWP HEALPix (CNN) [Publication](#)

Generative downscaling

- CorrDiff (Diffusion) [Publication](#)
- Climate in a Bottle [Publication](#)

AI-on-top

- Precipitation (AFNO)
- Tropical cyclones (CNN) [Publication](#)
- Atmospheric rivers (CNN) [Publication](#)
- Temporal interpolation (AFNO) [Publication](#)

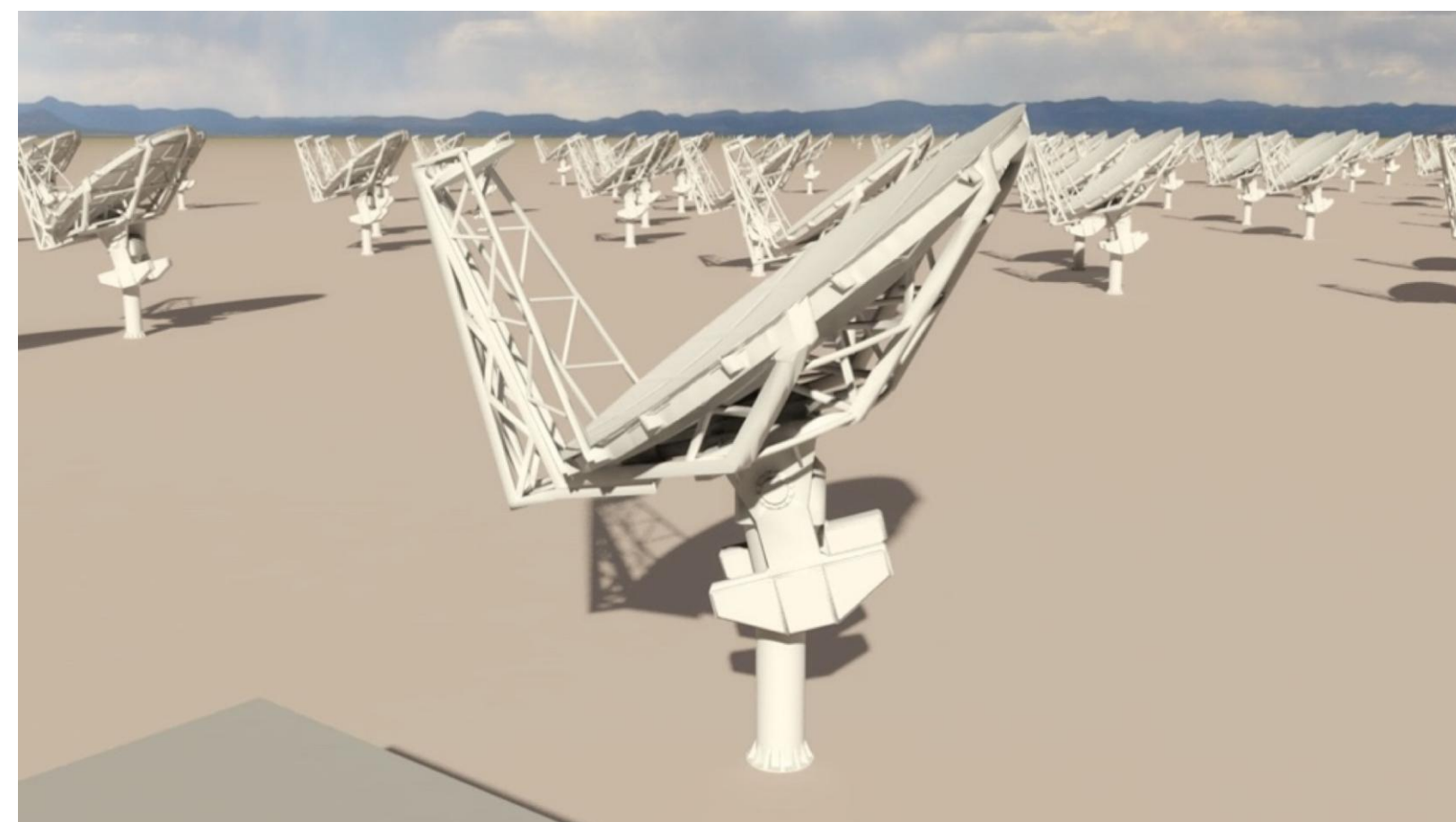
Edge Supercomputing

Next Generation Instruments are Producing Increasing Amounts of Data

Complexity of Experiments is Booming and Human Insight is Now the Bottleneck

Radio Astronomy

ngVLA – 244 Dishes
100 Petabytes per Year

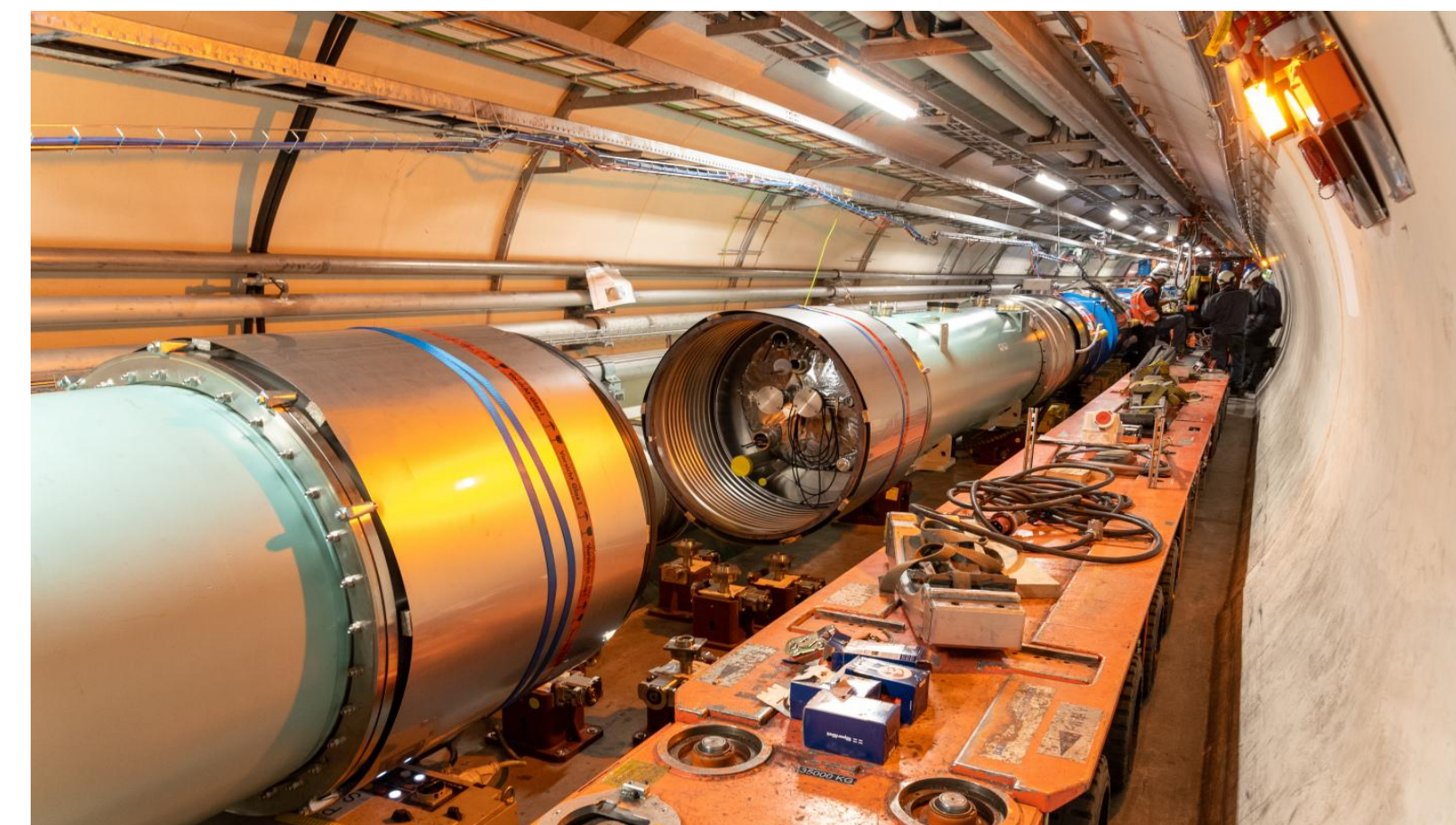


SKA – 200 Dishes
1 Exabyte per Year

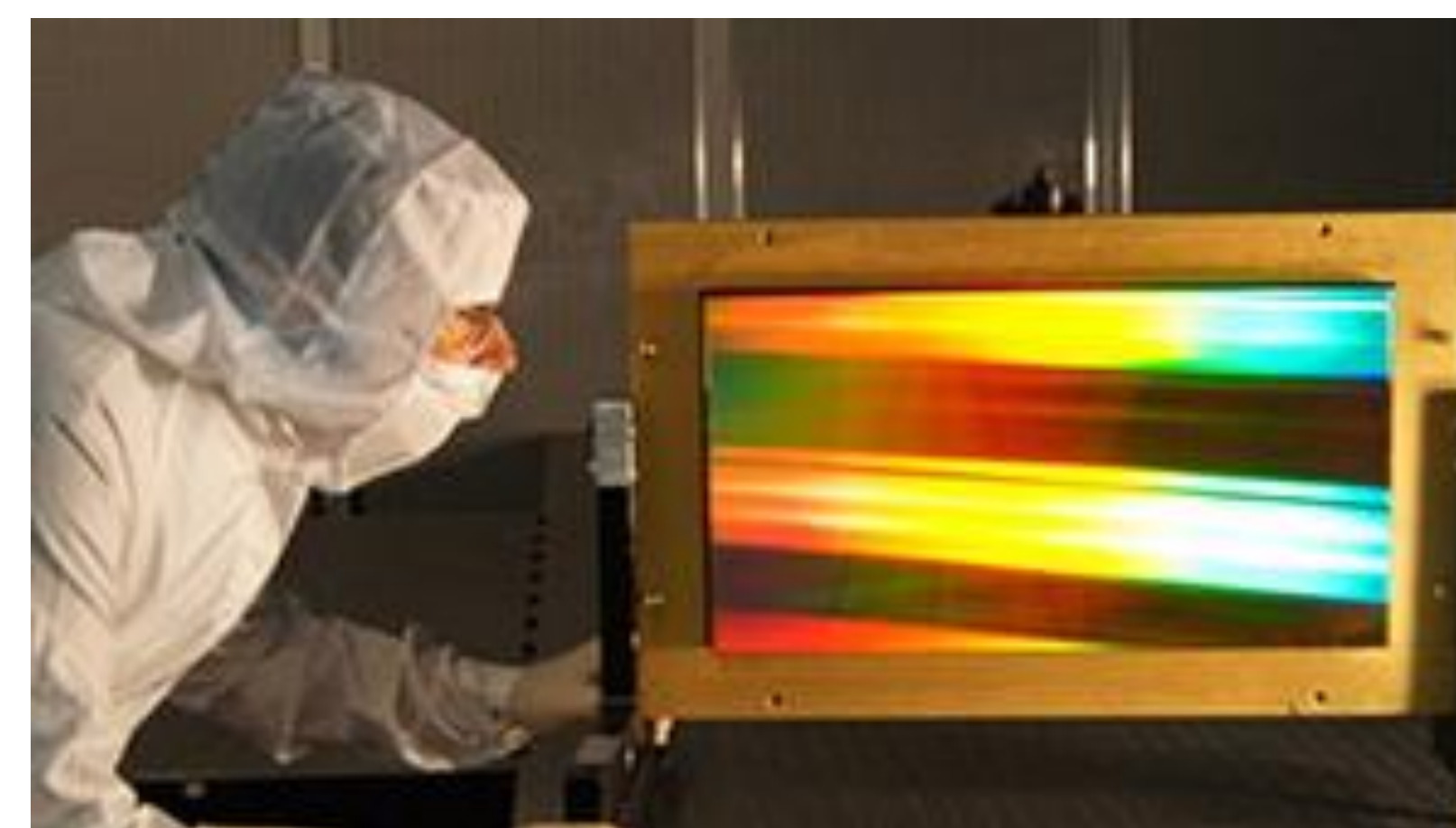


Particle Physics

High Luminosity LHC
100x Data than Higgs Boson Discovery



Advanced Laser Systems
100x Increase in Repetition Rate



Light Sources

APS-U – >60 beamlines
100-200 Petabytes per Year

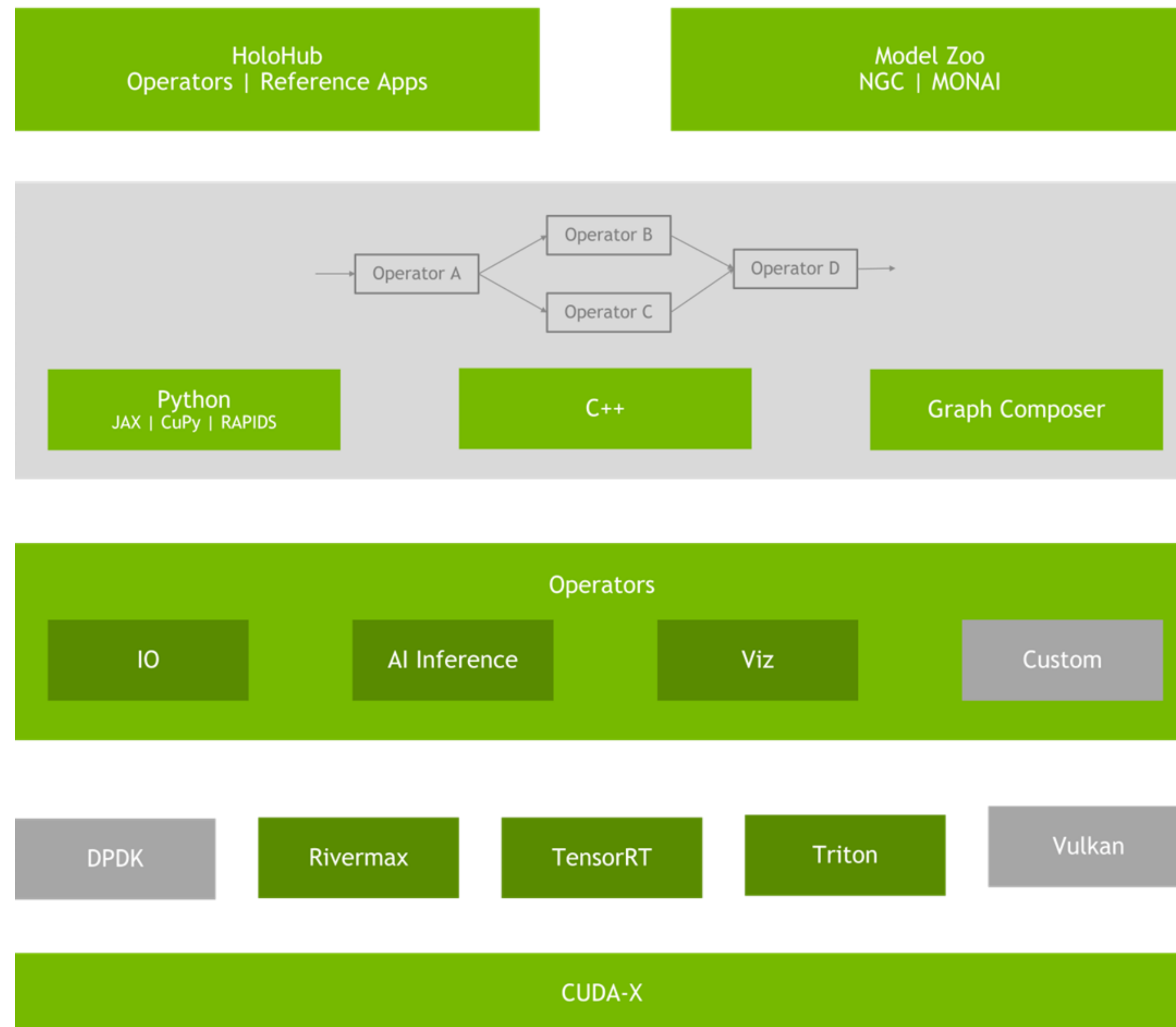


Free Electron Laser LCLS-II
1 MHz Rep-Rate Upgrade



NVIDIA Holoscan

SDK for Building AI-Enabled Sensor Processing Applications



Features

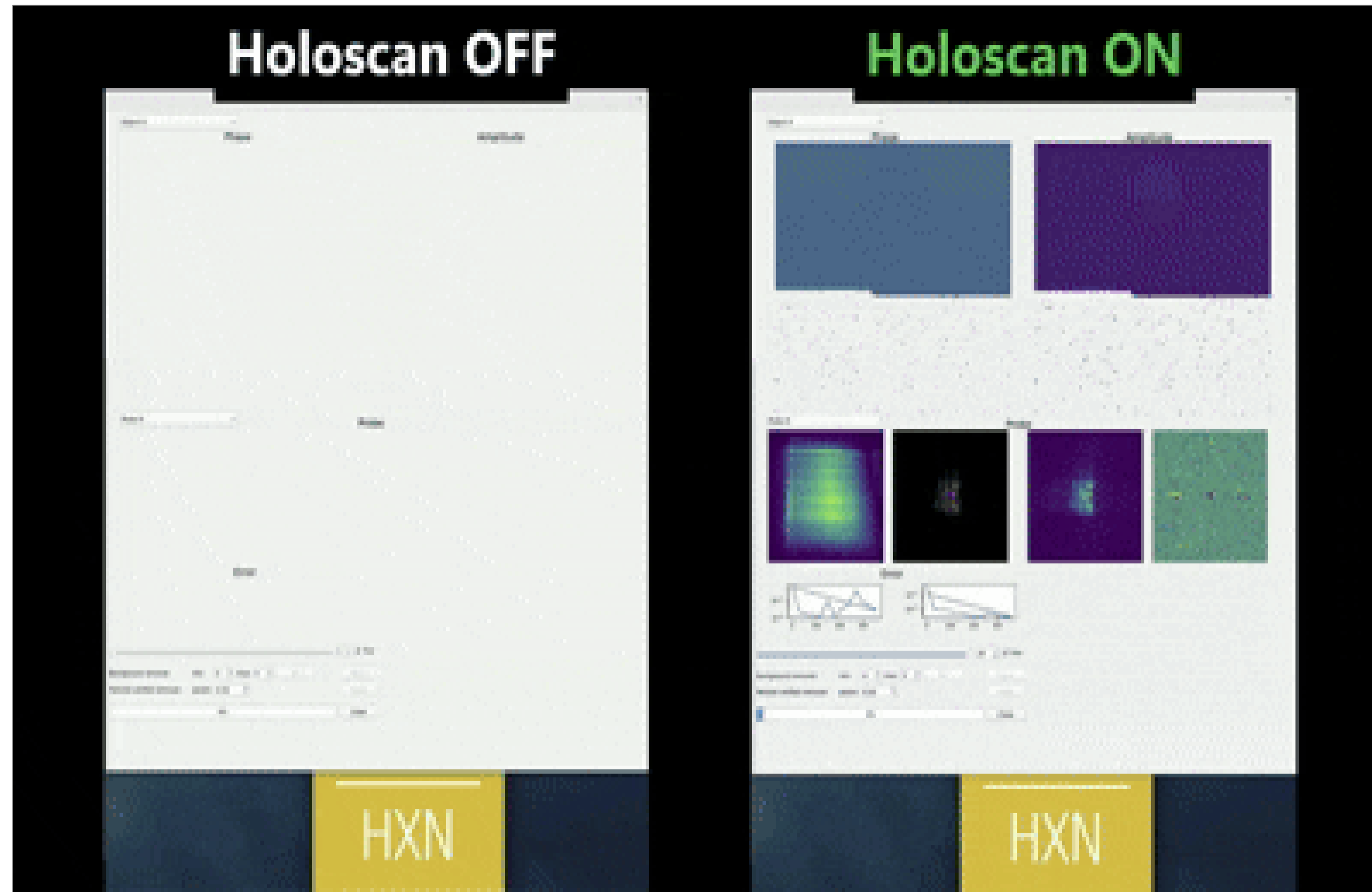
- C++ and Python APIs for **domain agnostic** sensor data processing workflows
- Scalable from IGX (ARM + GPU) to DGX (x86 + A100)
- Sample applications to jump-start ML/AI-enabled and Accelerated Computing sensor pipelines with [HoloHub](#)
- AI Inference with pluggable backends such as TensorRT
- Apache 2 Licensed and Available on [GitHub](#)

Benefits

- Simplifies sensor I/O to GPU
- Simplifies the deployment of an AI model in a streaming pipeline
- Provides customizable, reusable, and flexible components to build and deploy GPU-accelerated algorithms
- Scale workloads with Holoscan Cloud Native

Real Time Nanoscale Imaging with NVIDIA Holoscan

Brookhaven National Laboratory NSLS-II, DECTRIS



Demonstration of Offline versus Online Ptychographic Imaging

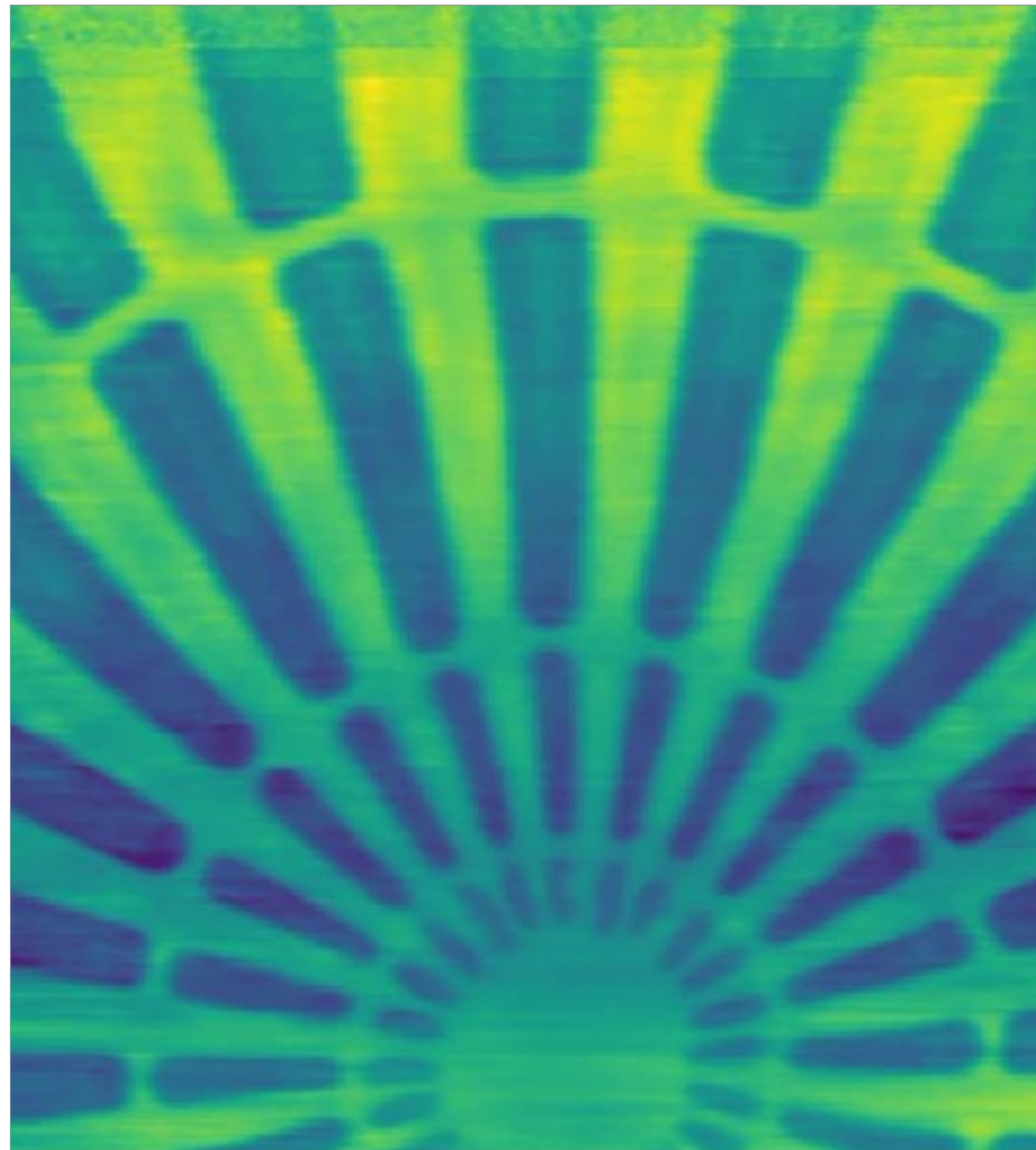
Self-assembly from nanoparticles, potentially useful as optical and mechanical metamaterials

For visualization purposes, both offline and online videos have been sped up by 2x

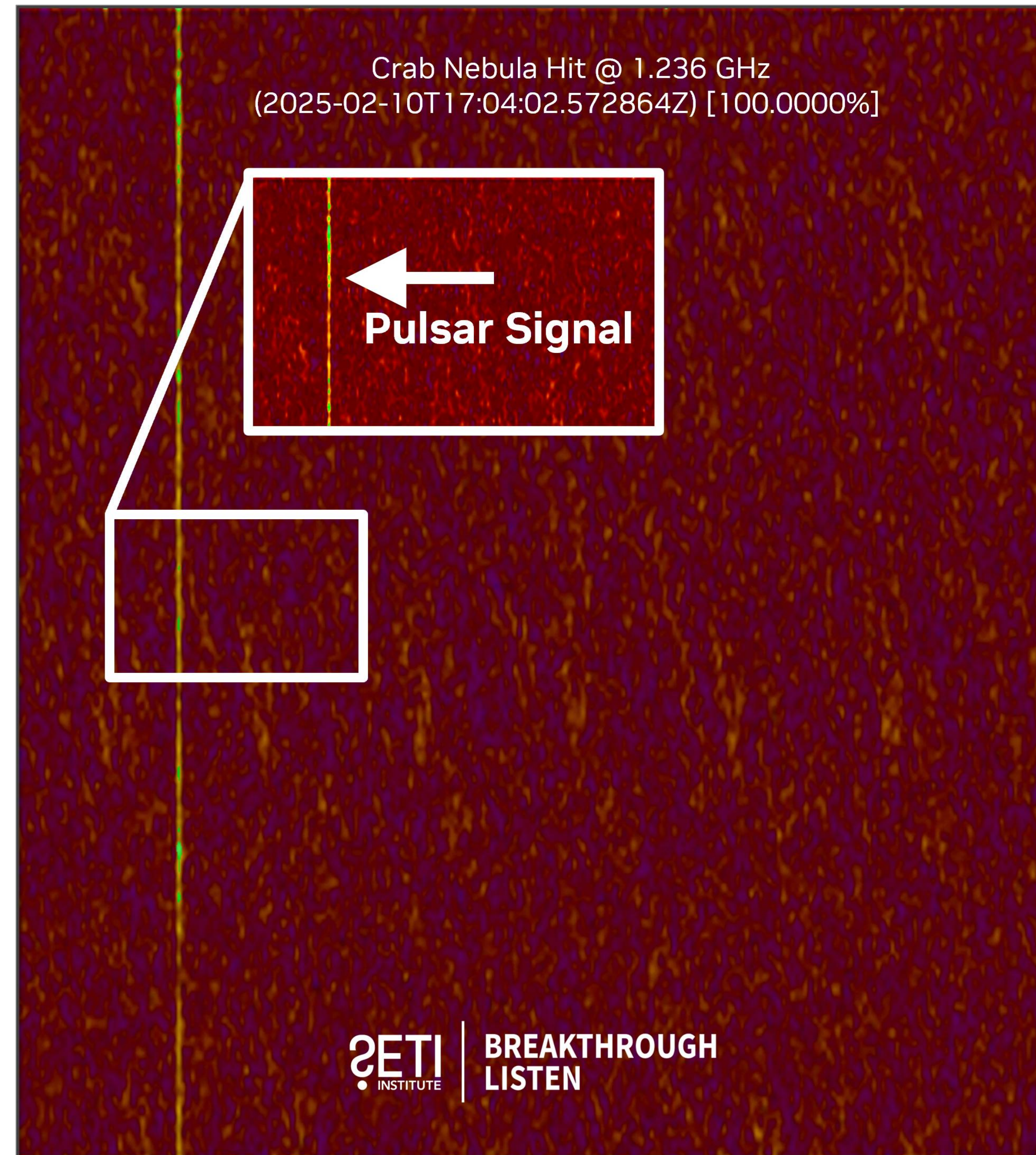
- **Current beamline scan takes about 8 seconds, with reconstruction taking 1-2 minutes**
 - Requires full dataset from x-ray detector and disk storage prior to reconstruction
- **Impact of Edge HPC and Holoscan for real time imaging**
 - Real time reconstruction provides instantaneous user feedback on experiment results
 - Ability to handle higher data rates yields higher resolution experiments and improved science products
 - Laying foundation for AI-driven agents and autonomous experimentation, including AI based scan patterns, leading to the **discovery of new materials at unprecedented rates**

HPC and AI at the Edge

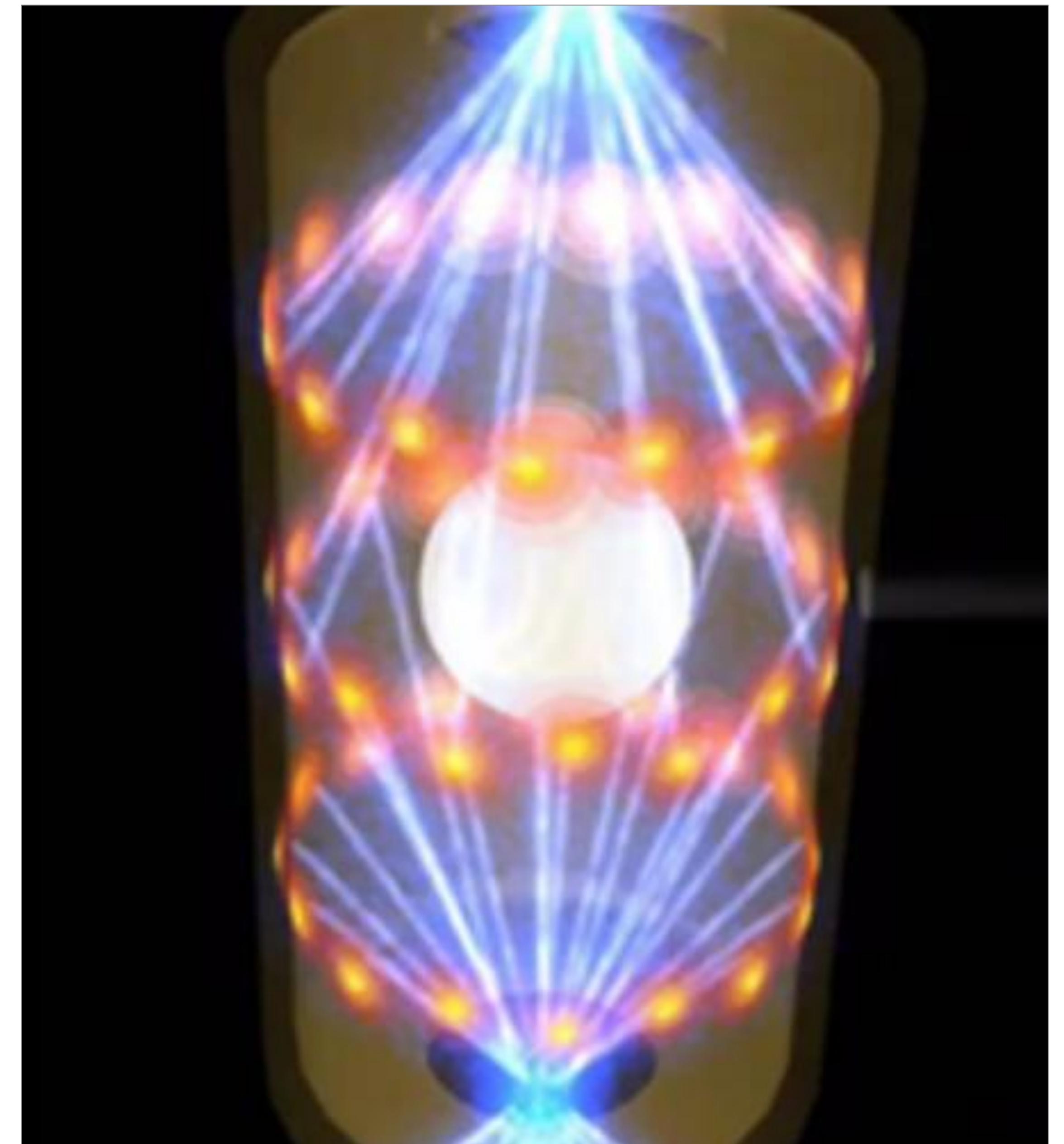
AI, Combined with, Streaming Data and Unprecedented Rates Welcomes New Scientific Discoveries



Nanoscale Imaging of Materials
Real Time Ptychography with NSLS-II and DECTRIS



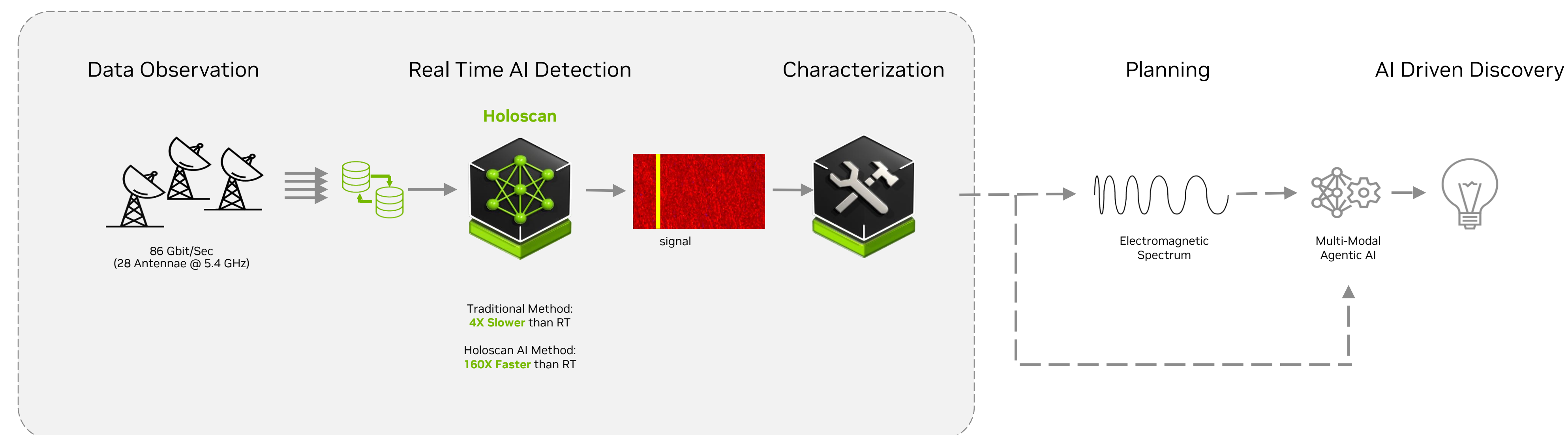
AI Search for Pulsars and Technosignatures
AI as a Detector with the SETI Institute and the Allen Telescope Array



Self Driving Experiments
AI Guided Fusion Research with Lawrence Livermore National Laboratory

NVIDIA Holoscan Enables Real-Time Signal Detection with AI

AI Enabled Real Time Signal Detection



Holoscan | CUDA-X | TensorRT | DOCA

The background features a series of parallel, wavy lines in various shades of green, creating a sense of depth and movement. A solid green vertical bar is positioned on the far left side of the image.

Computational Engineering



For illustration purposes only

The background features a series of parallel, slightly curved diagonal lines in various shades of green, creating a sense of depth and movement. A solid green vertical bar is positioned on the far left edge of the frame.

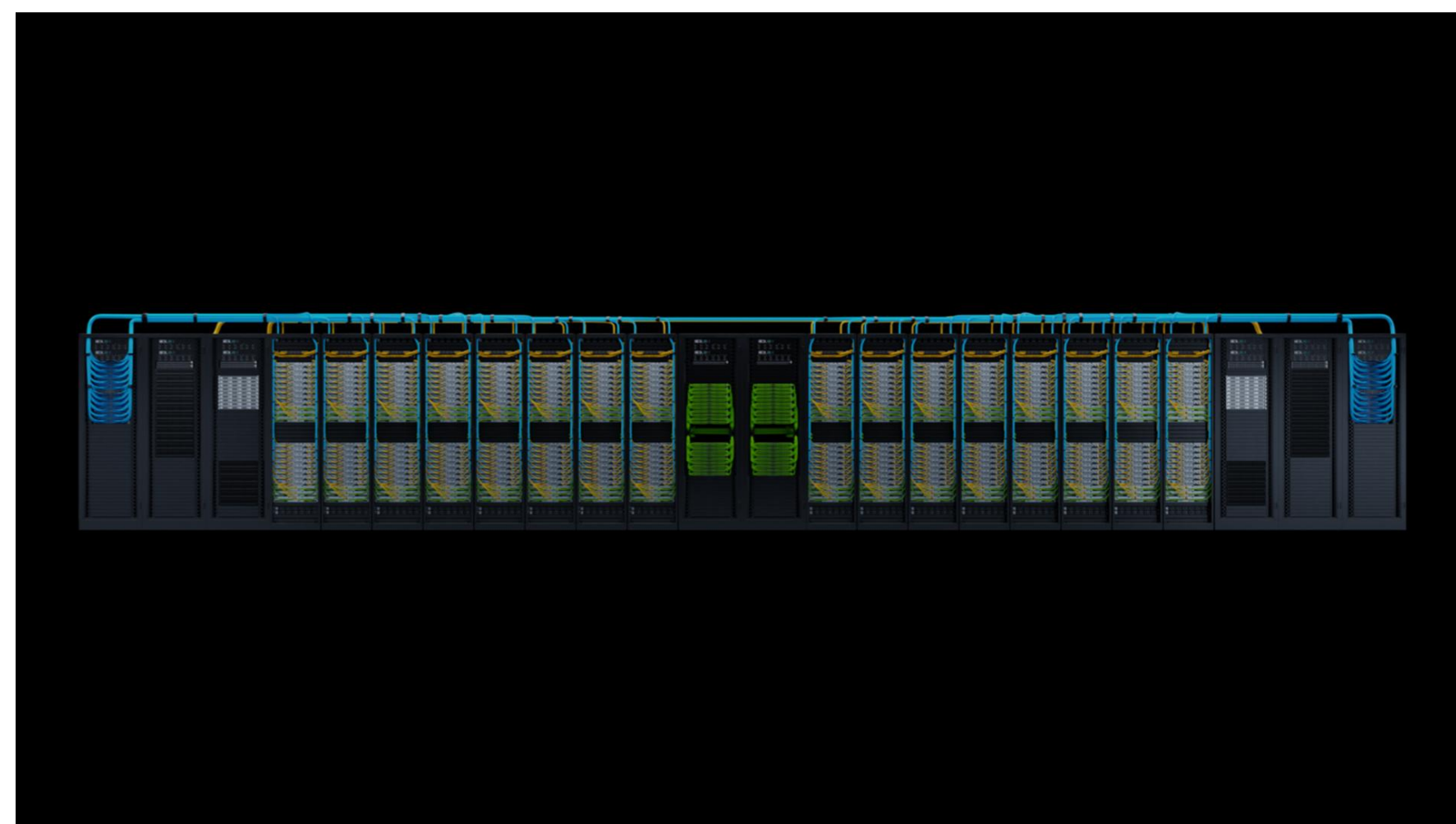
Quantum

Quantum-Accelerated Supercomputing

Supercomputers are the foundation of Quantum R&D

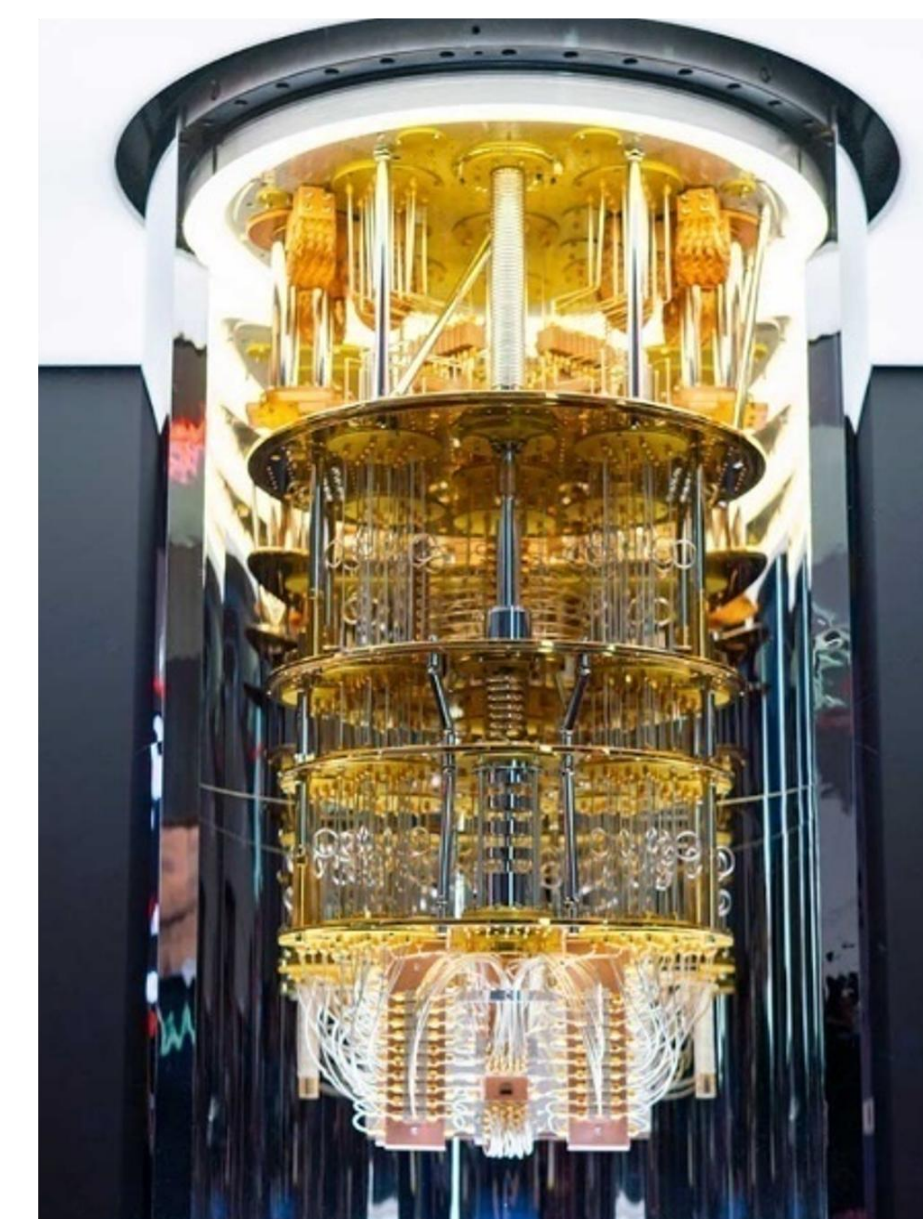
Simulation

- Quantum computers are small and error-prone -> simulation is an essential tool
- **Today:** Powerful simulators enable algorithm and application R&D - new approaches (e.g. tensor networks)
- **Future:** Digital twins of quantum computers for design and architecture optimization



HPC Quantum Integration

- Useful quantum computing will be hybrid
- **Today:** Enable domain scientists to start developing for QPUs, enable quantum researchers to use accelerated computing
- **Future:** quantum computers will integrate tightly with supercomputers as accelerators and be co-programmed



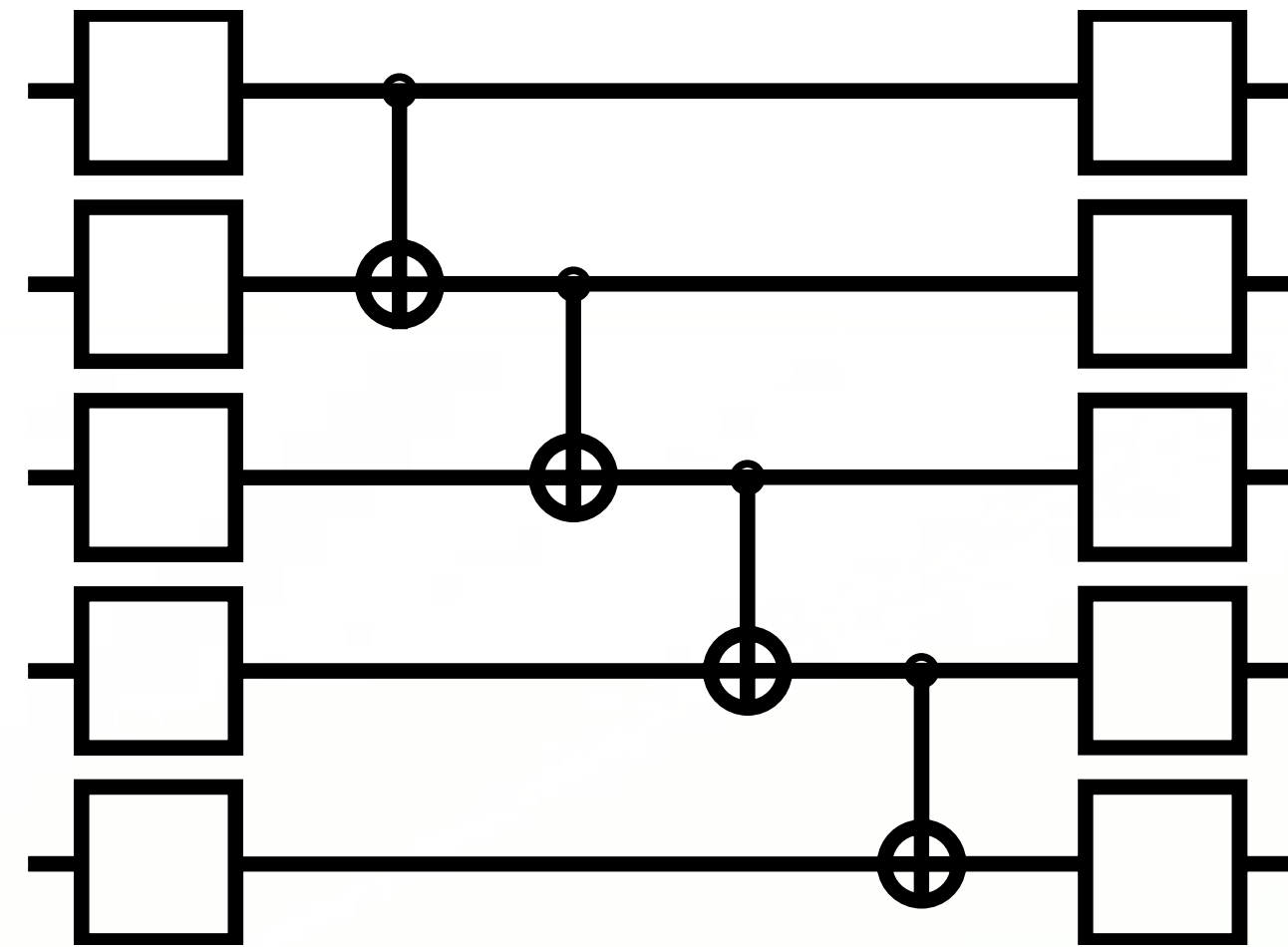
AI for Quantum

- Error correction, calibration, control, compilation are challenging computationally, real-time compute often needed
- Accelerated computing and AI can solve these problems
- **Today:** Enable AI research for all of the above
- **Future:** Hybrid Quantum+AI supercomputer with low-latency link



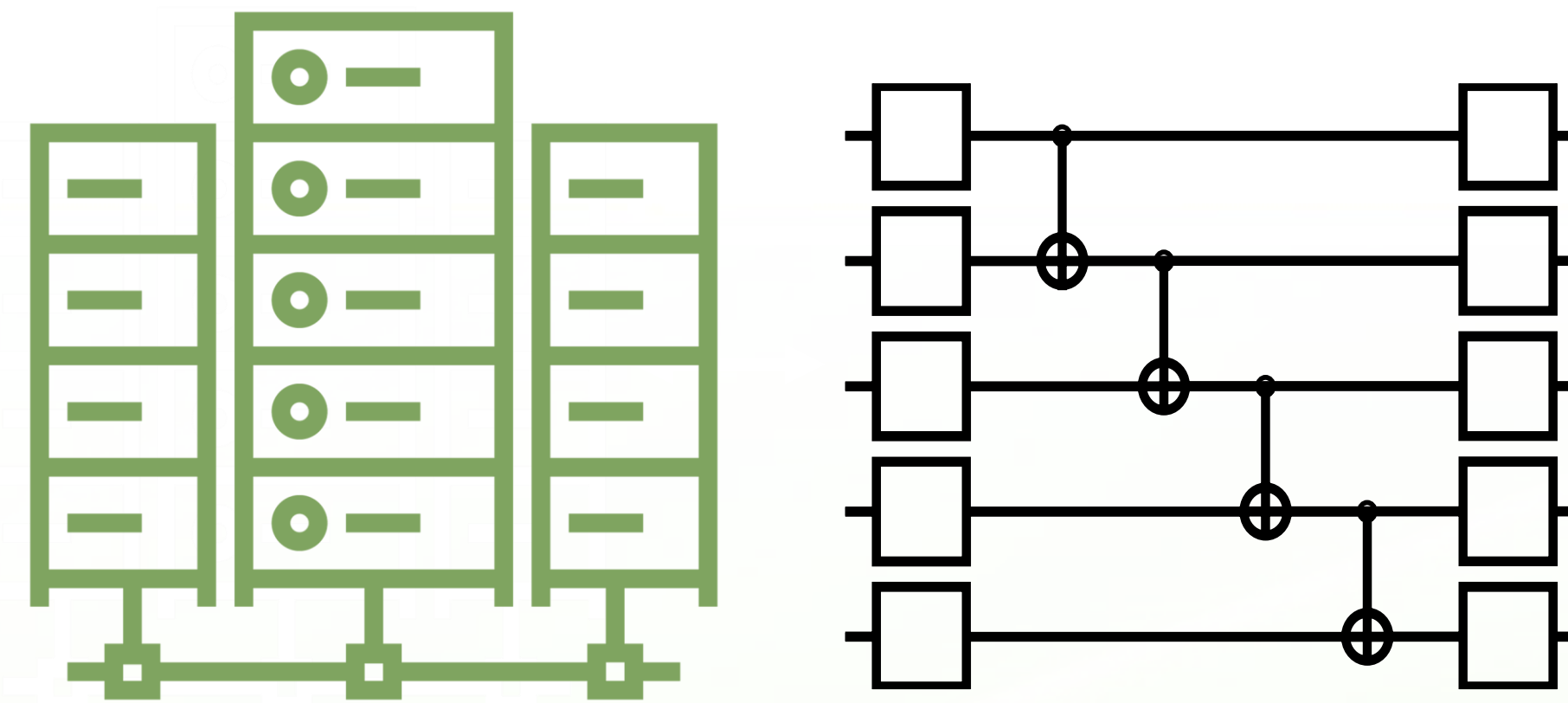
NVIDIA Quantum

Powering the Global Quantum Computing Community

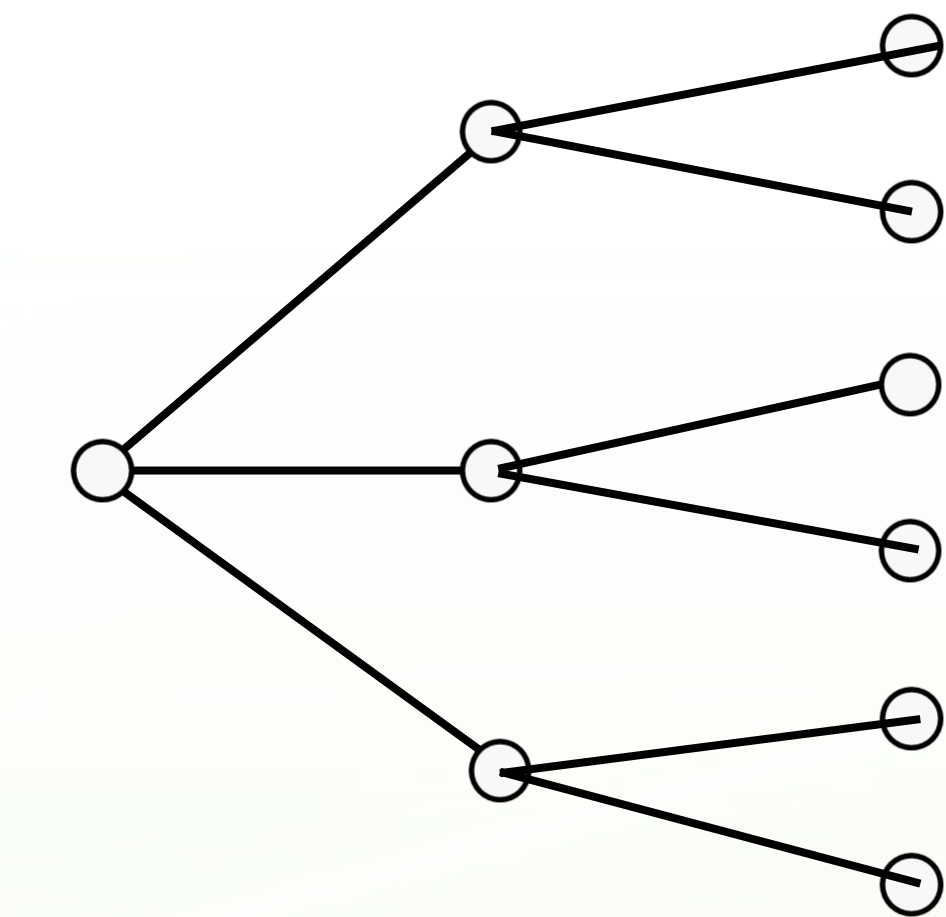


Simulation

Algorithm Design, Resource Estimation, QPU Design

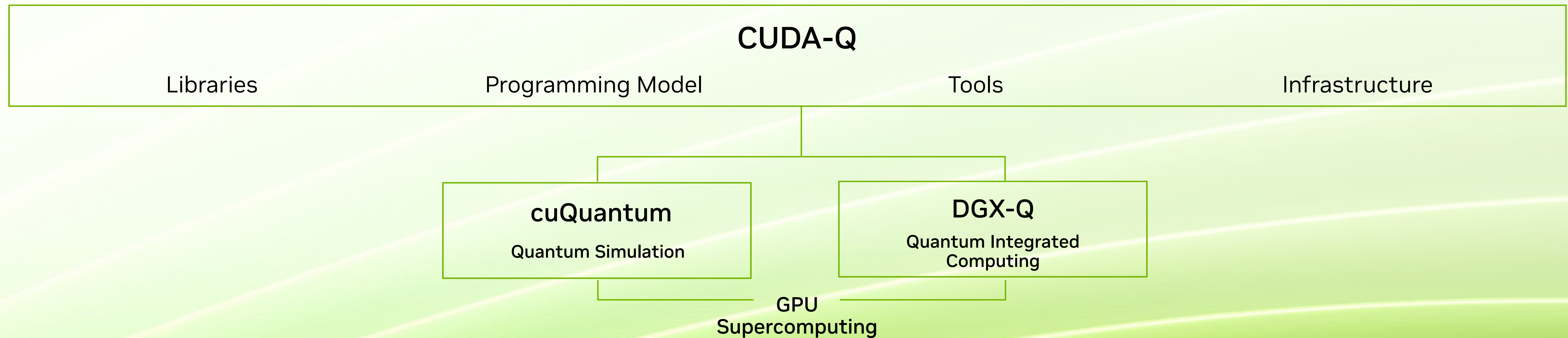


HPC Quantum Integration



AI for Quantum

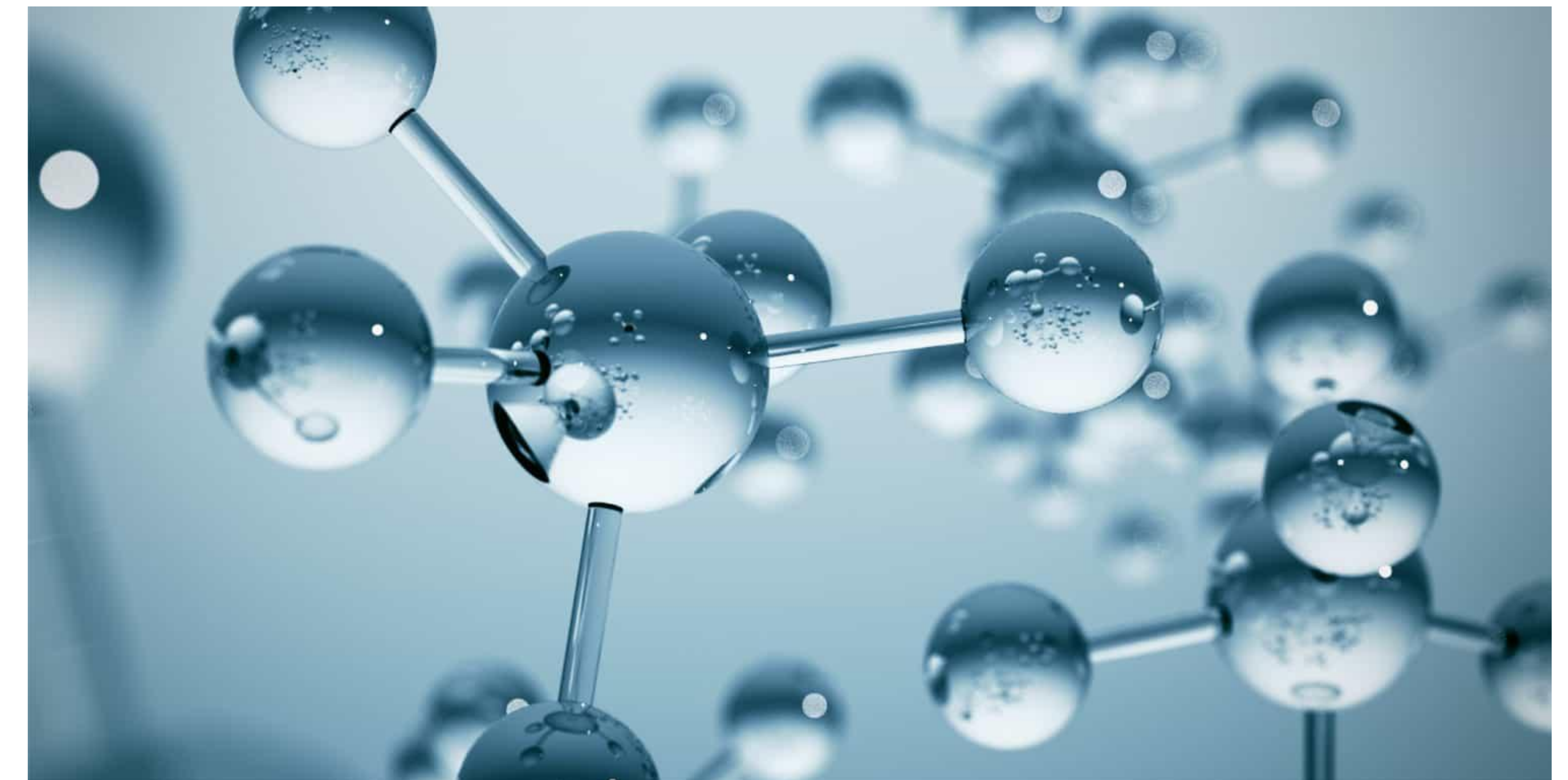
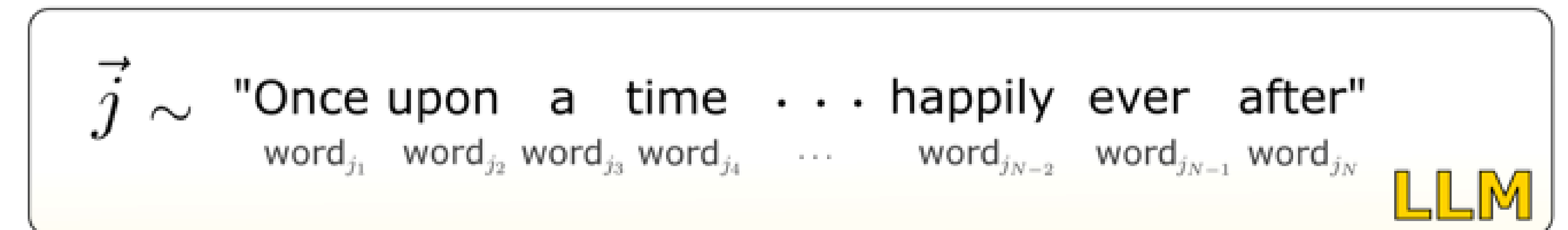
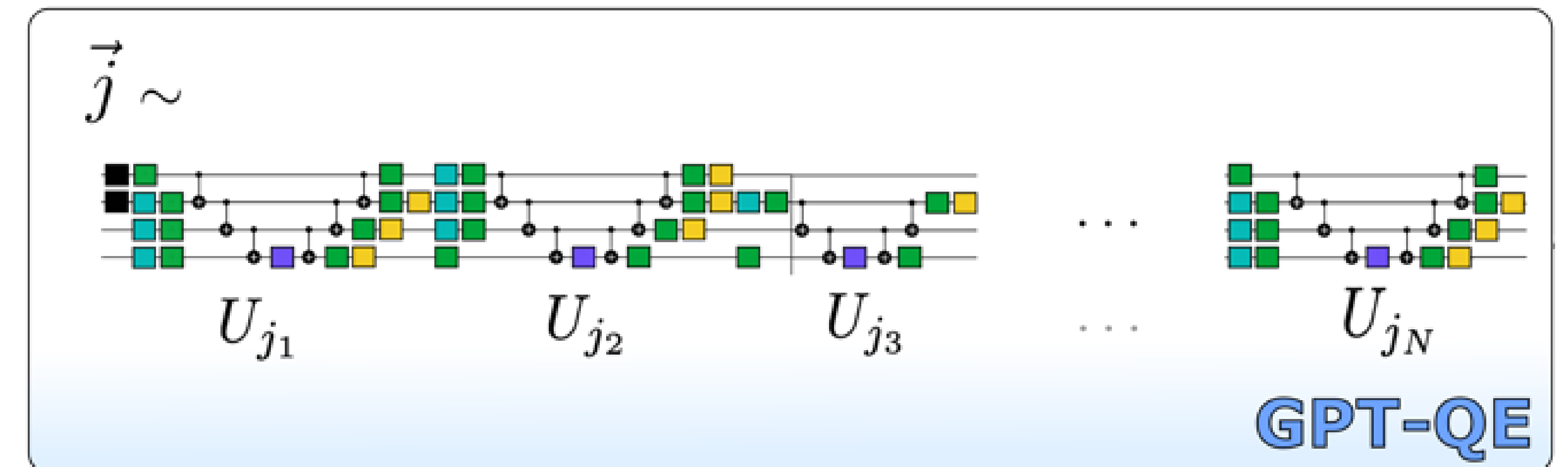
QEC, Calibration, Algorithms



The GPT Quantum Eigensolver

The University of Toronto, St. Jude Children's Research Hospital, and NVIDIA

- Developed a novel Generative Pre-Trained Transformer-based (GPT) method for computing the ground-state energy of molecules of interest
- The first demonstration of a GPT-generated quantum workload
- A powerful example of leveraging AI to accelerate quantum computing
- Executed using CUDA-Q on A100 GPUs on Perlmutter
- Opens the door to a wide variety of novel Generative Quantum Algorithms (GQAs) for drug discovery, materials science, and environmental challenges



<https://arxiv.org/pdf/2401.09253.pdf>



Announcing CUDA-Q Academic

Quantum Curriculum and Workforce Development Partnerships



- Coursework designed in partnership with academic institutions
- Access workshops from anywhere with GPU-acceleration in the cloud
- Active learning in distributed, quantum-accelerated computing and CUDA-Q
- Interactive Jupyter notebooks feature lectures, explanations, exercises, and assessments

ASU Arizona State University

Carnegie Mellon University

DARTMOUTH ENGINEERING

QUANTUM CENTER

FORDHAM UNIVERSITY

Mälardalen University

Northwestern

PITTSBURGH SUPERCOMPUTING CENTER

UNIVERSITAT POLITÈCNICA DE VALÈNCIA

PRINCETON UNIVERSITY

PURDUE UNIVERSITY

RMU ROBERT MORRIS

TUM Chair for Design Automation

Technion Israel Institute of Technology

UC DAVIS

10 Physical Computation Laboratory

THE UNIVERSITY OF CHICAGO

UF UNIVERSITY OF FLORIDA

UNIVERSITY OF ILLINOIS URBANA-CHAMPAIGN

University of Pittsburgh

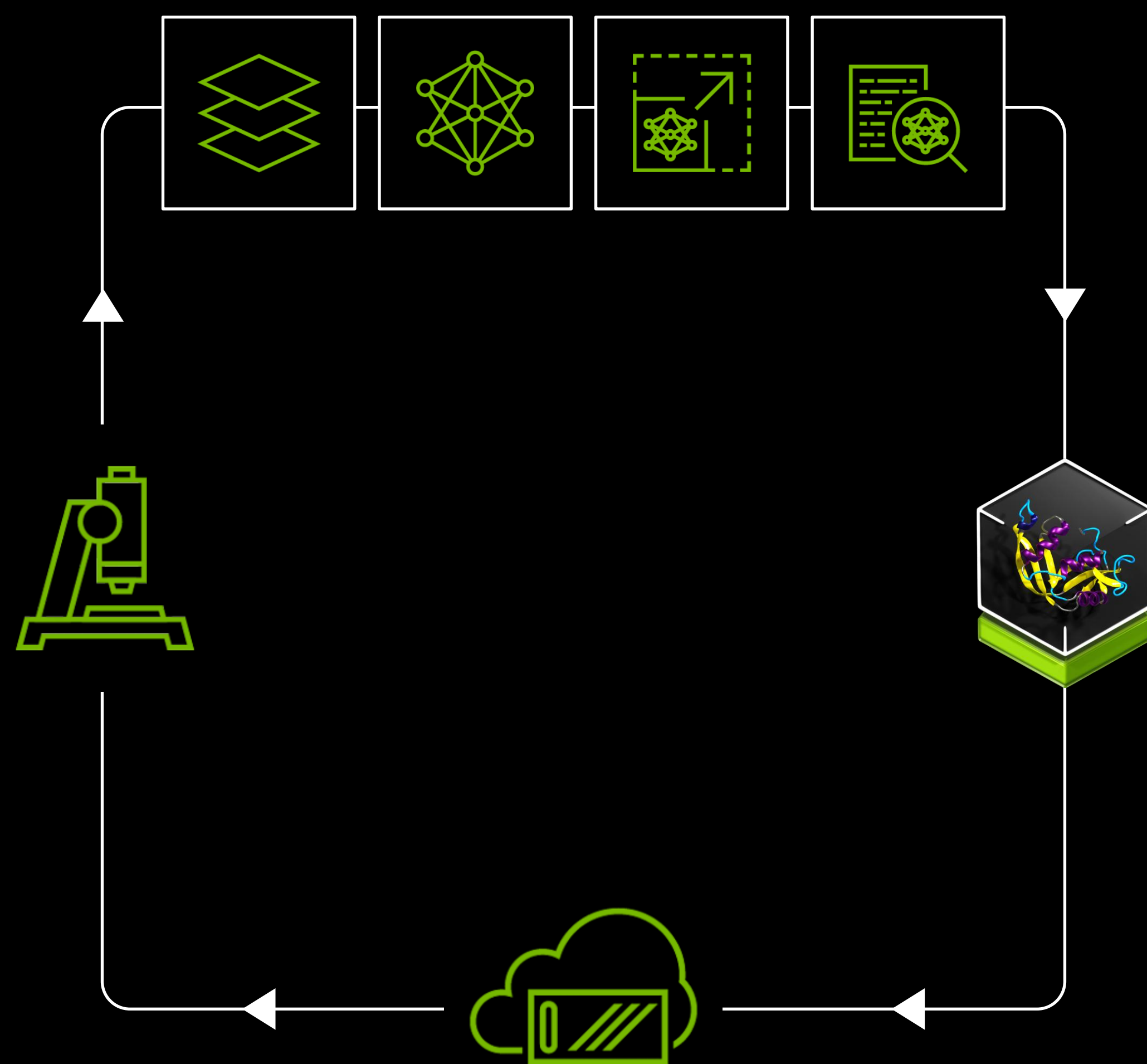
UNIVERSITAT POLITÈCNICA DE CATALUNYA BARCELONATECH



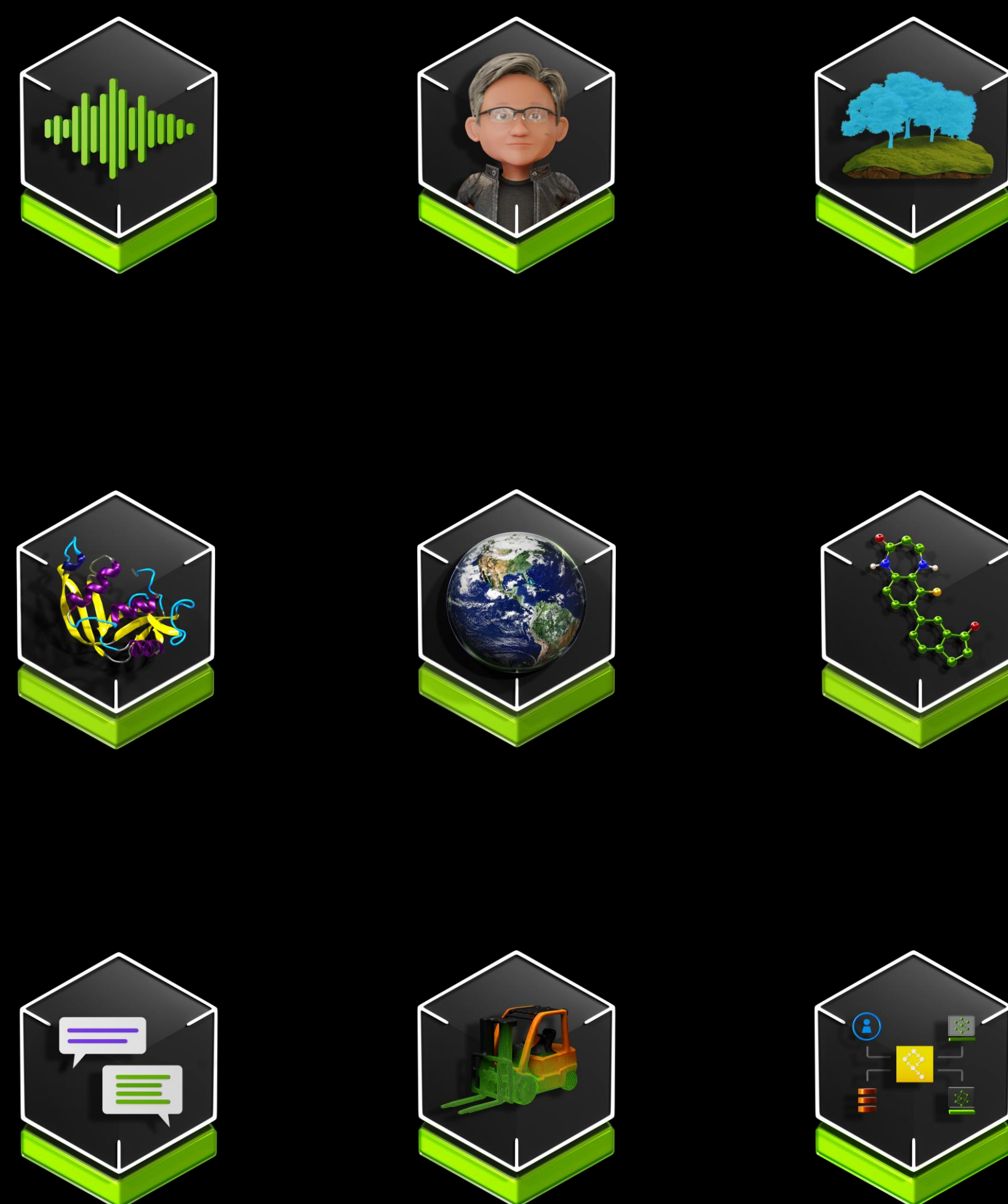
Drug Discovery

NVIDIA BioNeMo Platform

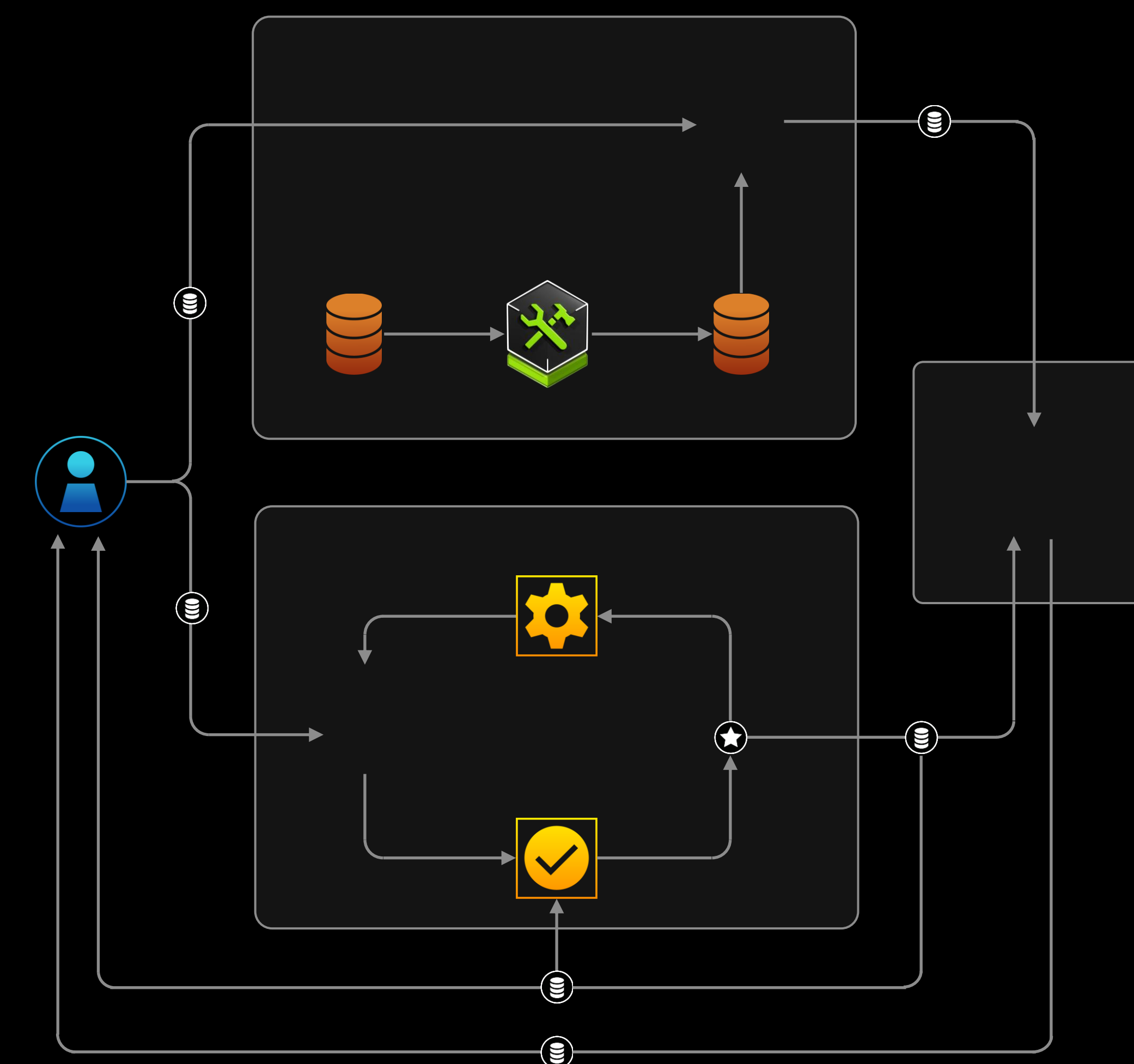
BioNeMo Training



BioNeMo NIMs



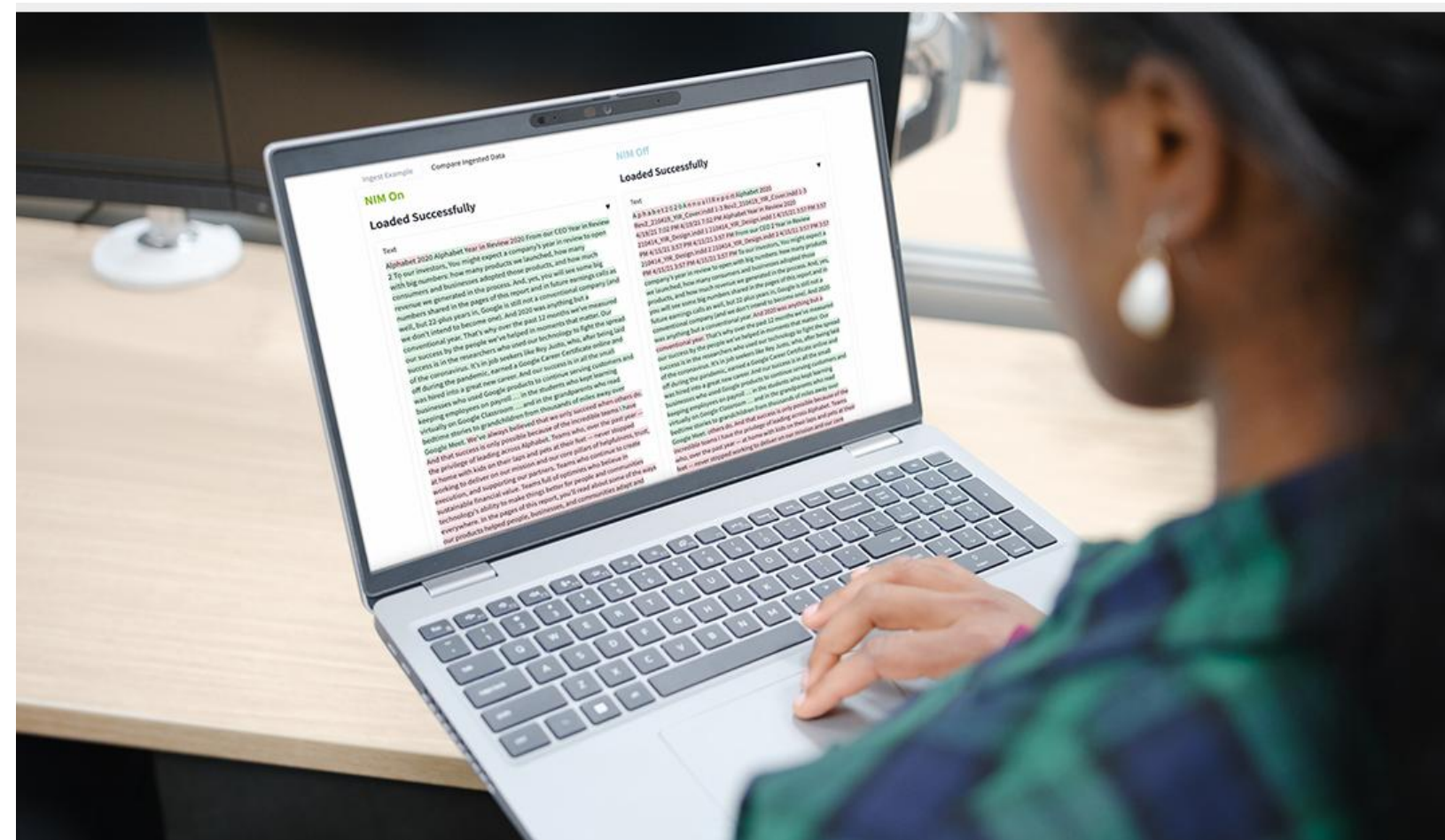
BioNeMo Blueprints



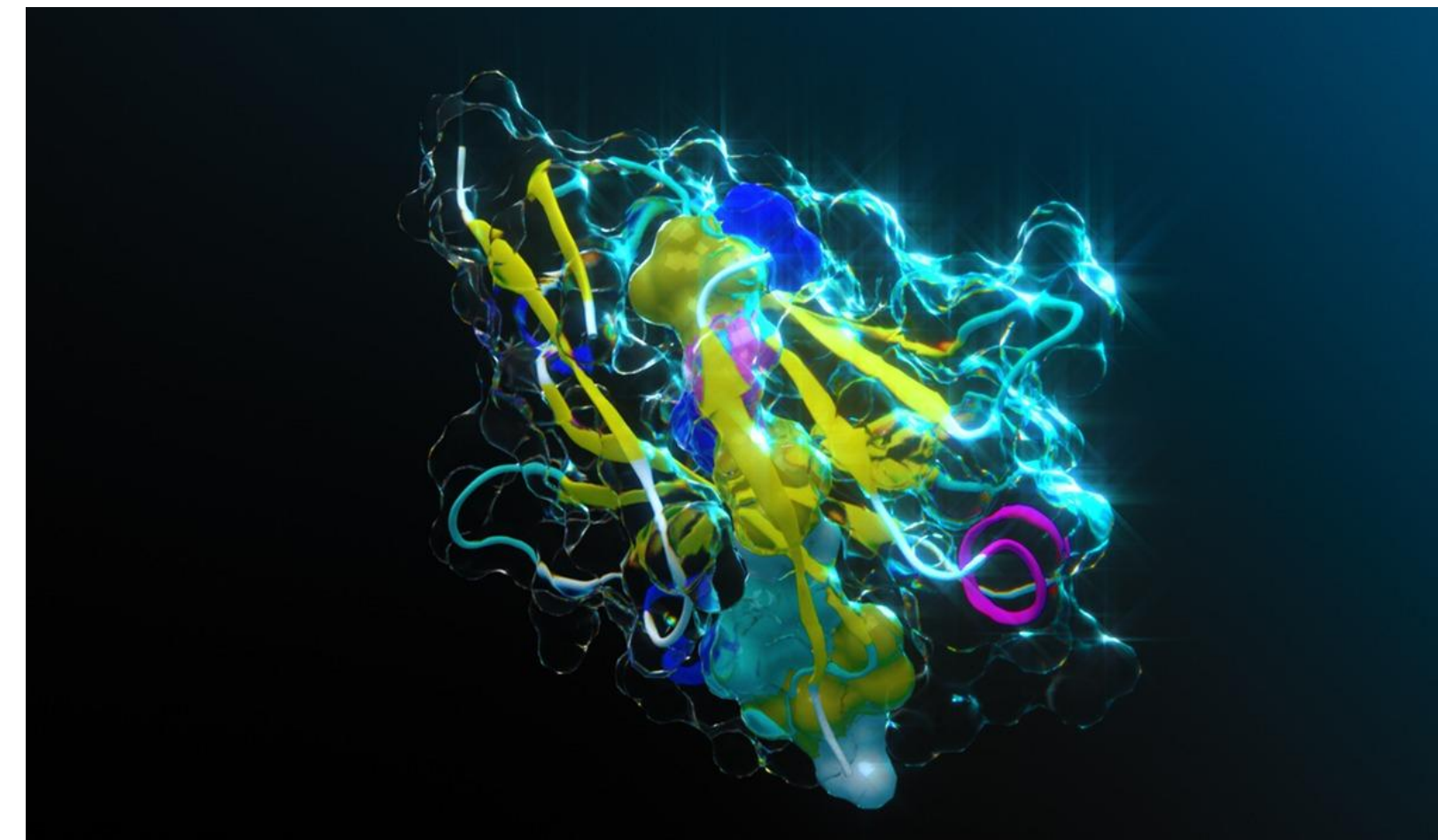
NVIDIA BioNeMo Blueprints Are Reference Workflows for Drug Discovery

Available on build.nvidia.com

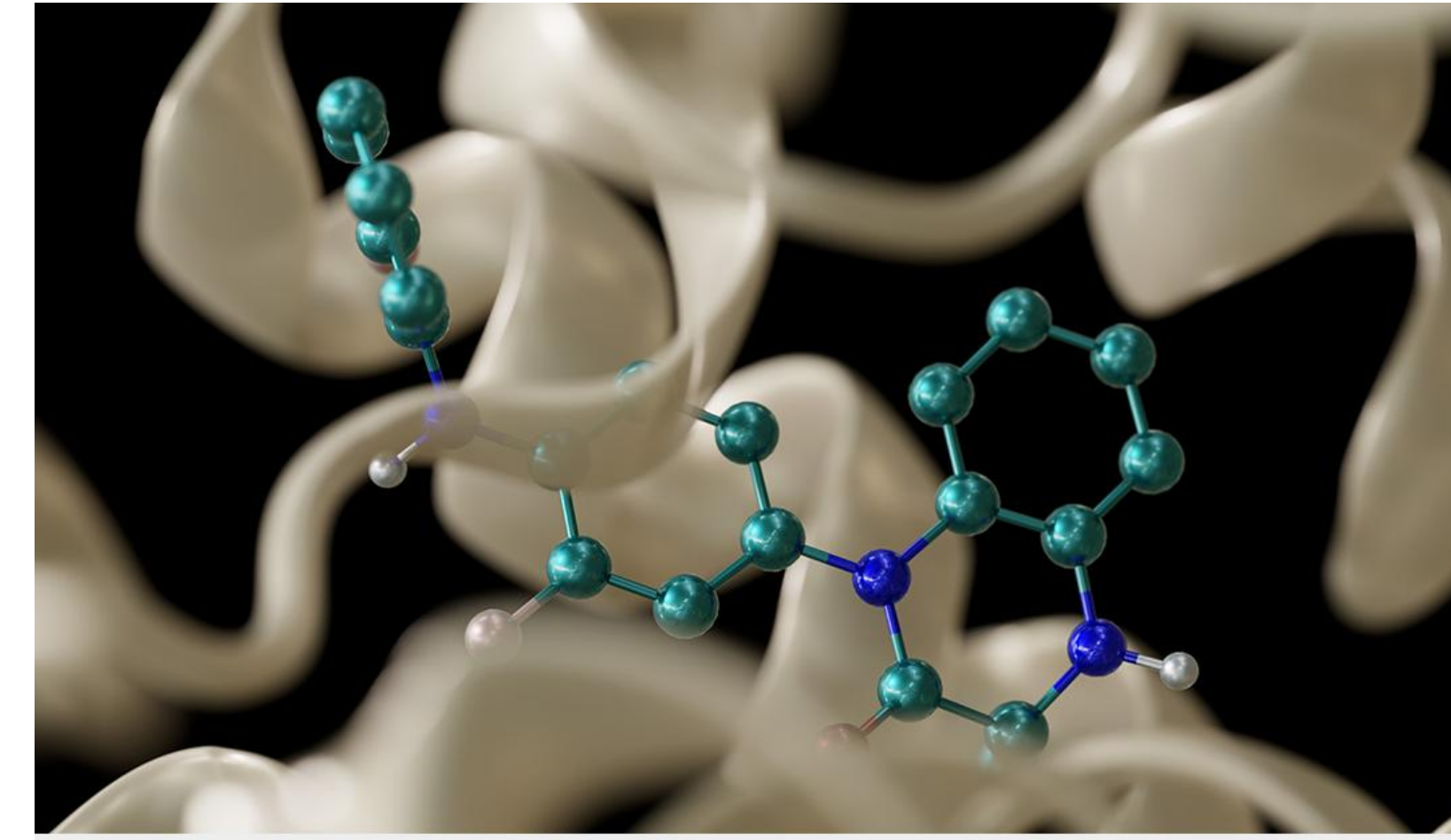
Multimodal PDF Data Extraction
for Enterprise RAG



Generative Protein Binder Design
for Drug Discovery



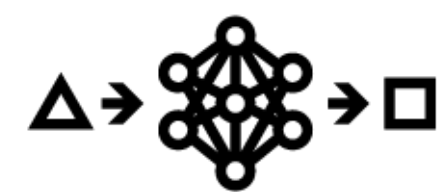
Generative Virtual Screening
for Drug Discovery



■ ■ ■
monthly release

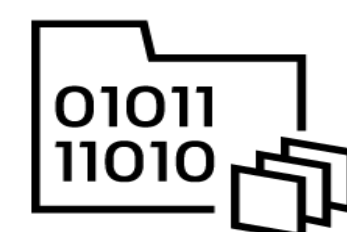
NVIDIA NIM Agent Blueprint

Example Application



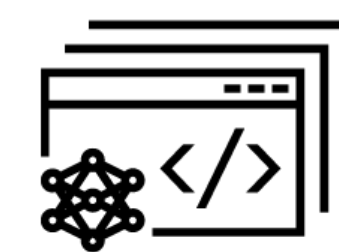
Interactive experience that
can be easily replicated

Sample Data



Public data for workflow
testing

Reference Code



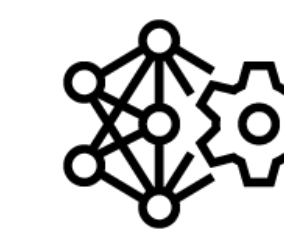
Reference code for
constructing workflows

Architecture



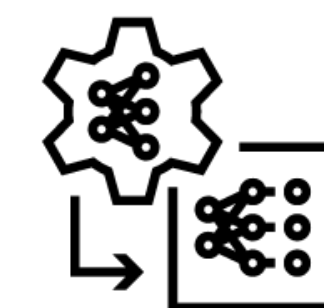
Reference architecture including
API definitions, NIM, and more

Customization Tools



Customize and evaluate models

Orchestration Tools



Deploy and manage workflow
microservices

Generative Protein Binder Design

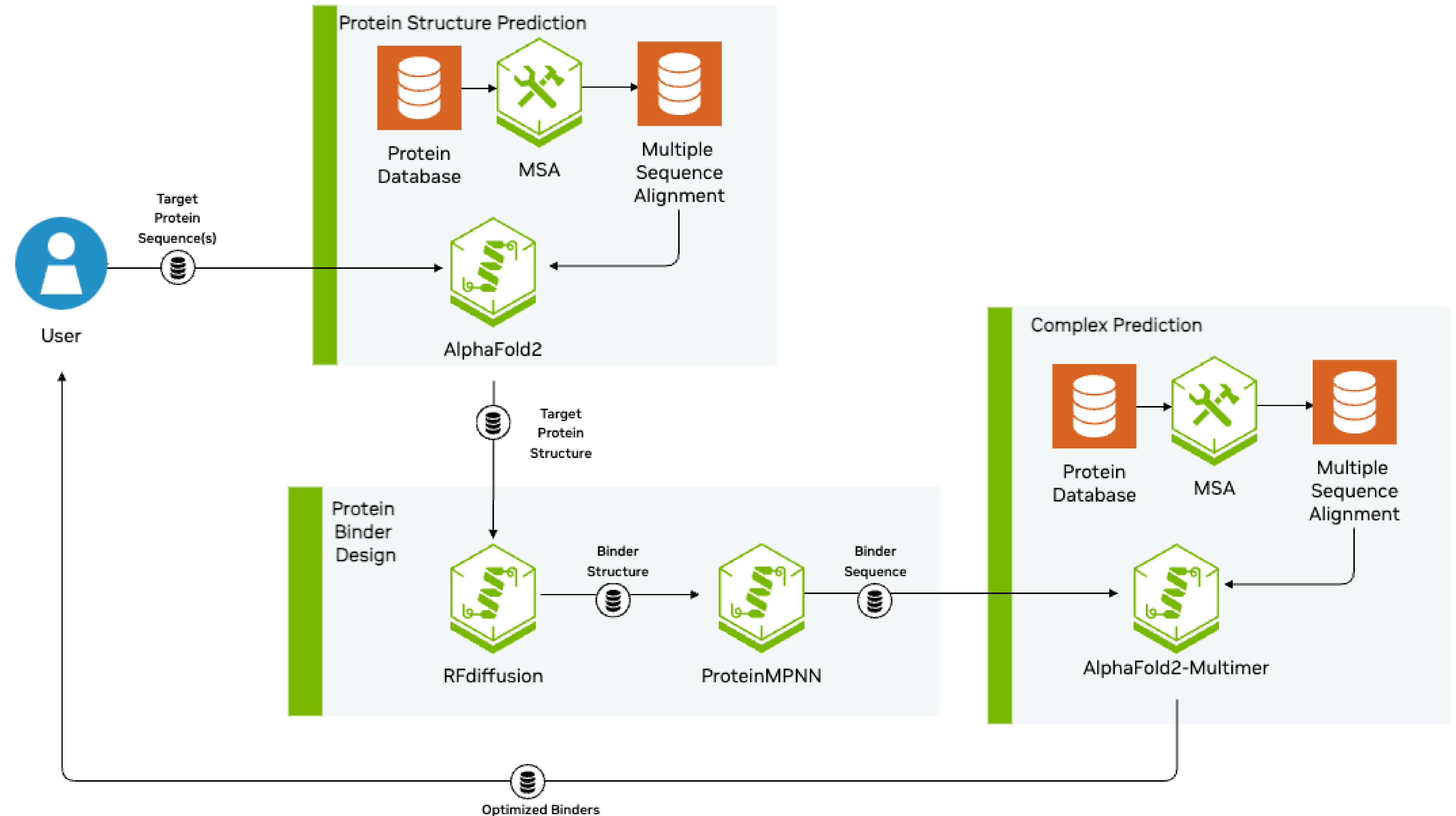
Models: MSA, AlphaFold2, Rfdiffusion, ProteinMPNN, Alphafold2-Multimer

Use Cases

- Design novel proteins to bind to a target of interest and/or perform a desired function.

Value Prop:

- Efficiently explore vast protein design space for structures with precise functional features
- SOTA speed and scalability over other approaches
- Identify high-affinity binders from a smaller set of designs



Working @ NVIDIA

Your Future Starts Here

NVIDIA is hiring! Our work in AI and the metaverse is transforming the world's largest industries and profoundly impacting society. Help shape what comes next.

- For internships and new college graduate roles www.nvidia.com/university
- General hiring areas <https://nvda.ws/nvur-jd>
- In the meantime, follow us on [LinkedIn](#), [Instagram](#) and [NVIDIA Blog](#) to stay connected!



Employee Benefits— Setting Us Apart (Canada)

Interns

- Health Benefits (six months or longer)
- Emergency PTO
- Housing Stipend (in-office)
- Ergonomic & Internet Stipend (remote)
- Holiday Pay & Free Days
- Equity (ESPP)
- Guidance Resources EAP
- Discounts & Services
- Intern Events

New College Graduate

- Health Benefits
- PTO & Emergency PTO
- Holiday Pay & Free Days
- Equity (RSUs & ESPP)
- Ergonomic & Internet Stipend (remote)
- Parental Leave
- Guidance Resources EAP
- Tuition Reimbursement
- RRSP Matching
- Discounts & Services



Find Your Perfect Fit

Search for your area of interest at [nvida.ws/nvur-jd](https://nvidia.ws/nvur-jd) and apply at www.nvidia.com/university

Hardware

- ASIC Design
- Verification
- Physical Design/VLSI
- Mixed Signal Design
- Digital Circuit Design

Architecture

- Computer Architecture
- Deep Learning Computer Architecture

Systems Software

- System Software
- Graphics Systems Software
- Compiler
- Firmware & Embedded Software
- Software Security

Software

- Development Tools
- Cloud
- Tools Infrastructure
- Machine Learning Operations

Autonomous Vehicles and Robotics

- Autonomous Vehicles
- Robotics

Deep Learning

- Deep Learning Applications & Algorithms
- Deep Learning Frameworks & Libraries

Research

- Research (PhD)
- Applied Research (BS, MS, PhD)

Business Operations

- Business Operations (MBA)

