PHYSICS-INFORMED MACHINE LEARNING AND GENERATIVE AI FOR SURROGATE MODELING IN SCIENCE AND INDUSTRY

MIKE O'KEEFFE, SENIOR SOLUTIONS ARCHITECT, NVIDIA

NEW YORK SCIENTIFIC DATA SUMMIT 2024: ADDRESSING DATA CHALLENGES IN DIGITAL TWINS

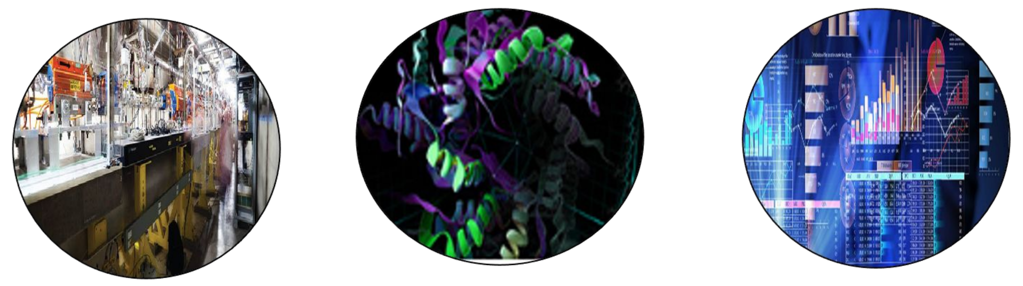
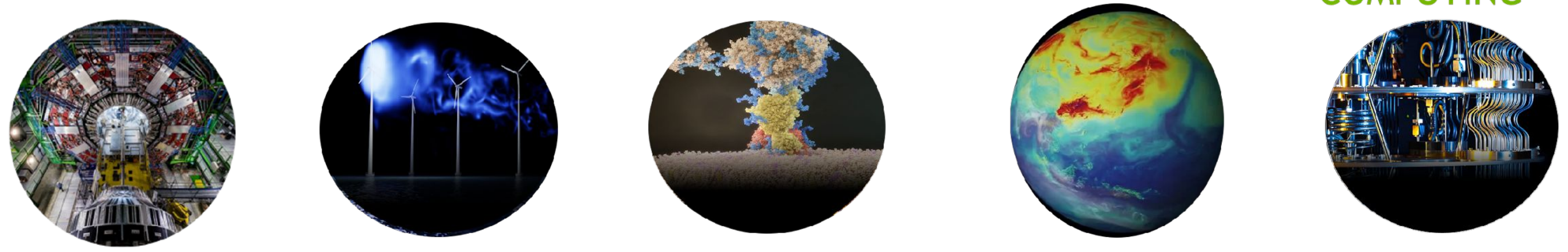
SCIENTIFIC COMPUTING IS EVOLVING

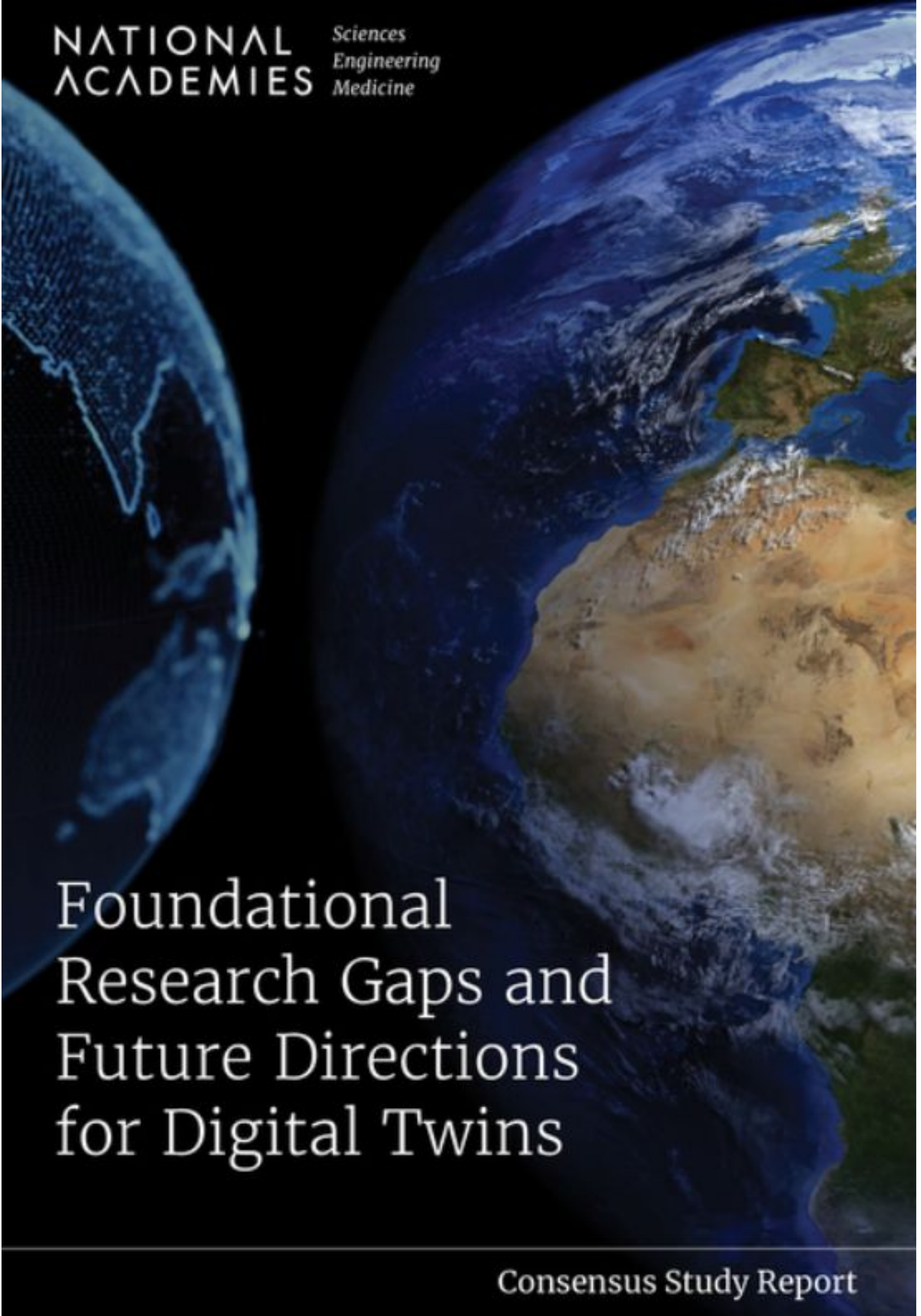
Thought Leaders Map Out the Opportunity and Constraints Given Current Technology and Market Reality

<u>Business-as-usual will not be adequate</u>

NVIDIA

TRANSITION TO POST EXASCALE ERA

FEATURE	EXPERIMENTS SIMULATION Viz  TERA THROUGH EXASCALE	EDGE HPC + AI SIMULATION DIGITAL TWIN QUANTUM COMPUTING  POST EXASCALE
USAGE	BATCH & MOSTLY LOCAL TO A SITE	INTERACTIVE & DISTRIBUTED WITH MULTIPLE SITES
WORKLOAD	SINGLE SIMULATION/ENSEMBLE	WORKFLOW COMPRISED OF SIMULATION ENSEMBLES, AI TRAINING AND INFERENCE, LIVE DATA ANALYTICS
EXPERIMENTS	OFFLINE DATA ANALYSIS FOR EXPERIMENTS	MIX OF REAL-TIME ANALYSIS TIGHTLY COUPLED WITH OFFLINE
DIGITAL TWINS	IN-SITU VISUALIZATION OFFLNE	INTERACTIVE_VISUAL MODEL COUPLED WITH PHYSICAL ASSET
QUANTUM COMPUTING	SIMULATION	SIMULATION PREPARING FOR A HYBRID MODEL
PROGRAMMING MODELS	FORTRAN, C++, MPI, OPENMP	STANDARD PARALLELISM SUPPORT IN FORTRAN, C++, MPI, OPENMP, OPENACC, PYTHON, JULIA, PYTORCH, TENSORFLOW
SYSTEM CONFIGURATION	MONOLITHIC	MODULAR
CLOUD	GRID	BURST CAPABILITIES, FASTER REFRESH CYCLE, ACCESS TO LATEST TECHNOLOGY AT SCALE



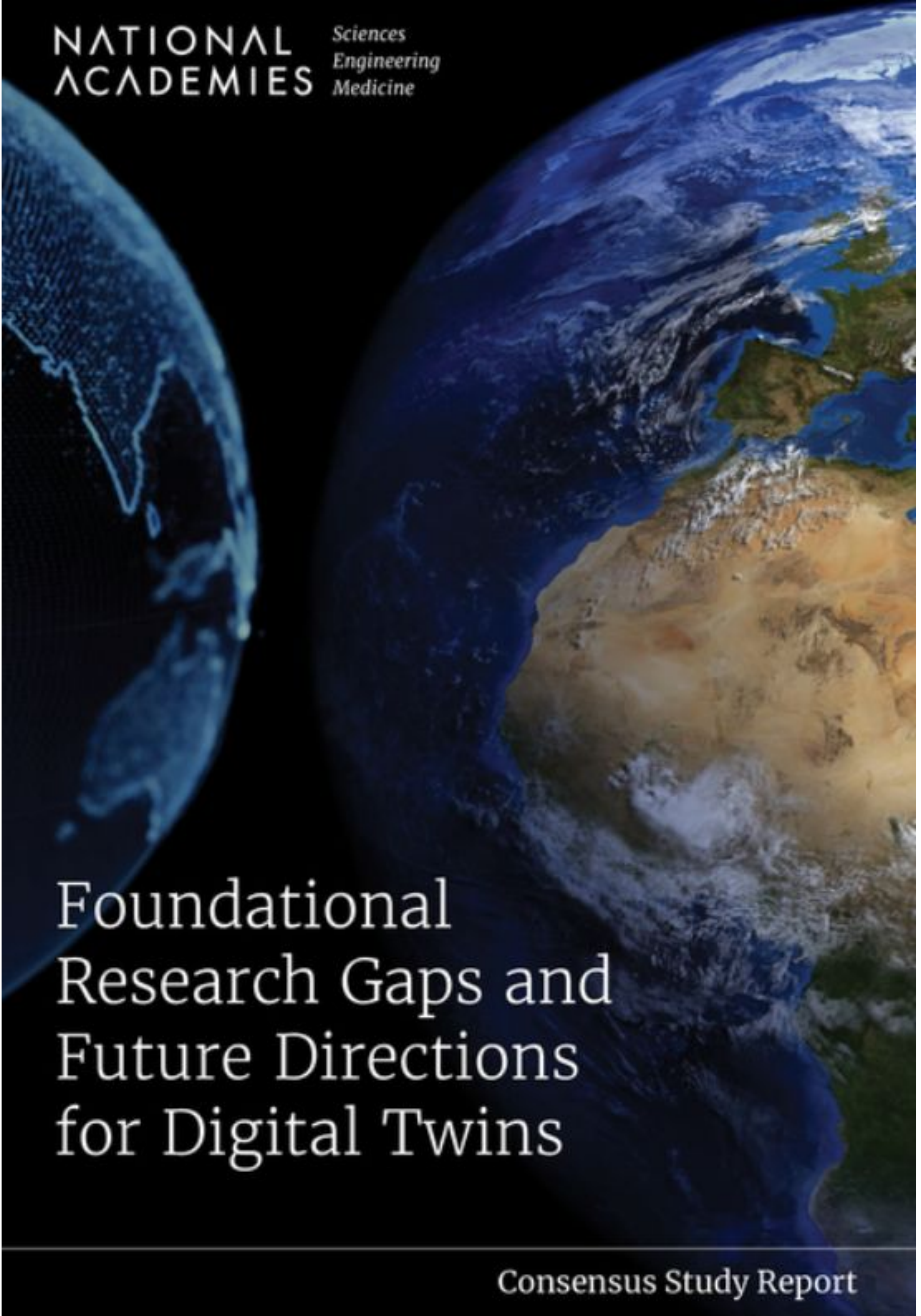
DIGITAL TWIN FOR SCIENCE

A Relatively New Modeling Concept That is Being Adopted
by the HPC Community in the Post Moore Era

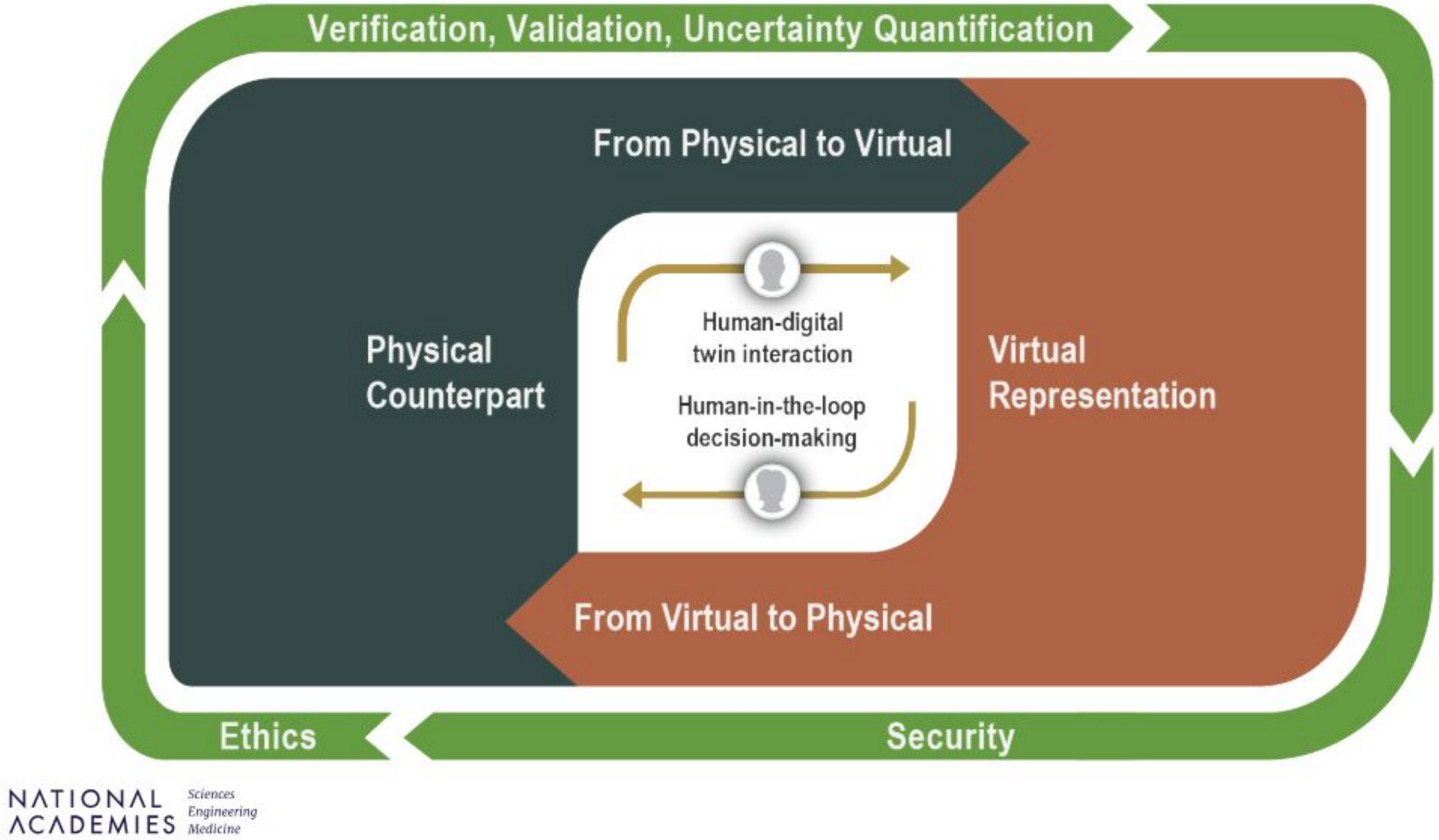
The concept was first publicly introduced in 2002 by Michael Grieves, at a Society of Manufacturing Engineers conference as the conceptual model underlying Product Life Cycle Management

A digital twin is a set of virtual information constructs that mimics the structure, context, and behavior of a natural, engineered, or social system (or system-of-systems), is dynamically updated with data from its physical twin, has a predictive capability, and informs decisions that realize value.

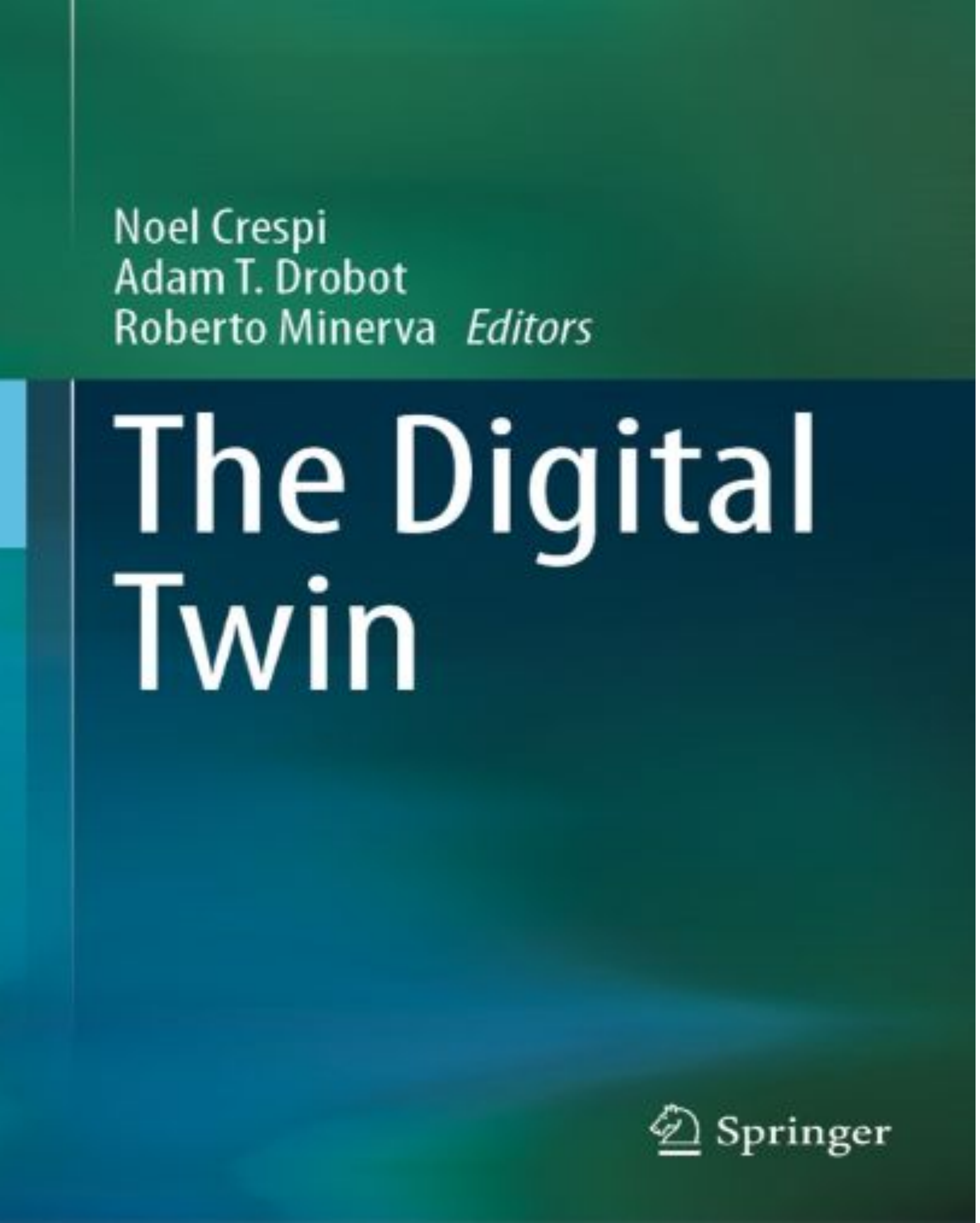
The bidirectional interaction between the virtual and the physical is central to the digital twin.



A Digital Twin is More Than Just Simulation and Modeling

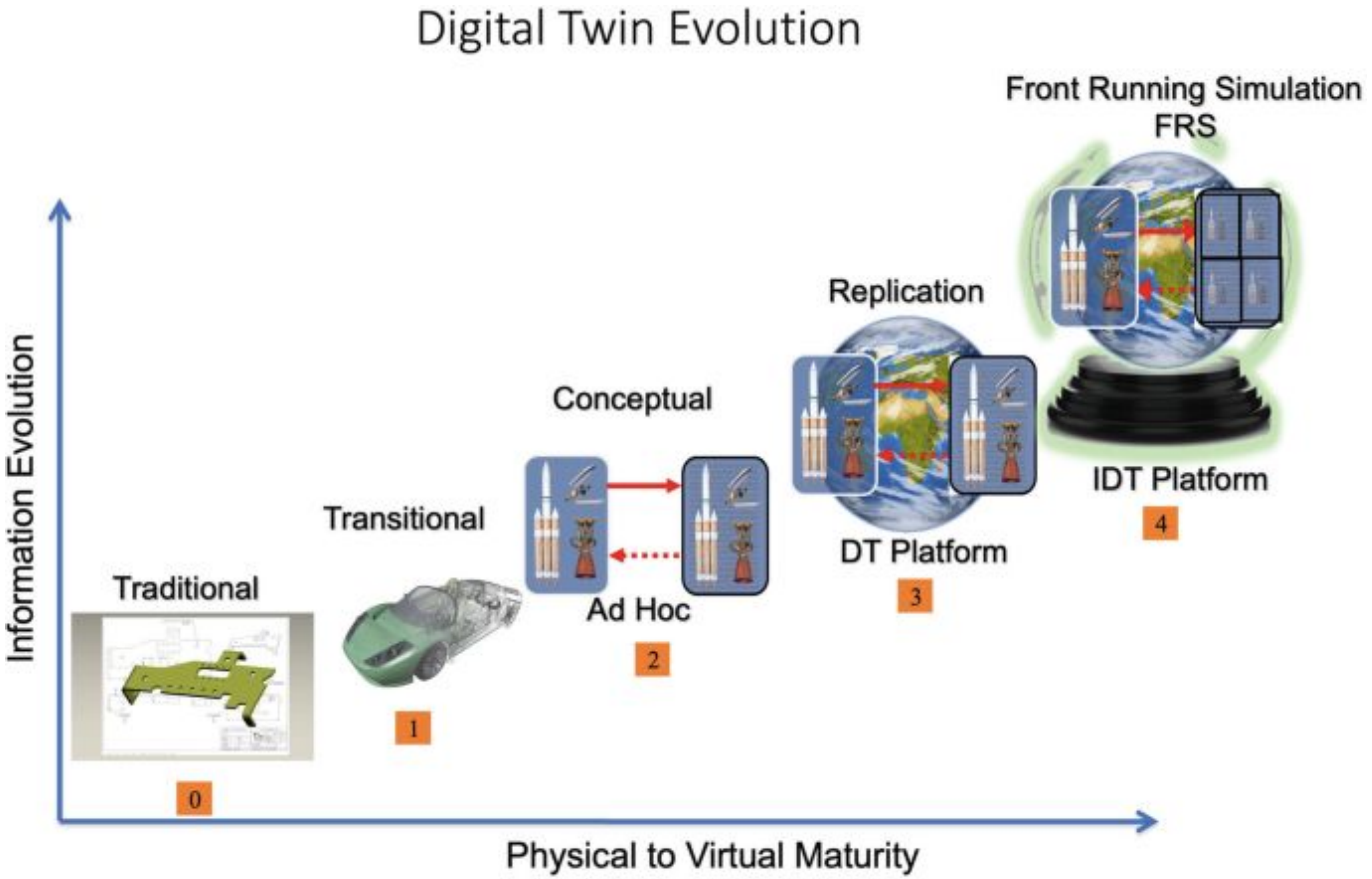


NVIDIA



CHAPTER: DIGITAL TWIN PAST, PRESENT AND FUTURE

Michael Grieves
Executive Director Chief Scientist Digital Twin Institute



https://www.brighttalk.com/webcast/18347/456987

AI ENABLES DIGITAL TWINS FOR SCIENCE

Quantum Accuracy at Cost for Physical Scale Models

NVIDIA

AI ENABLES DIGITAL TWINS FOR SCIENCE

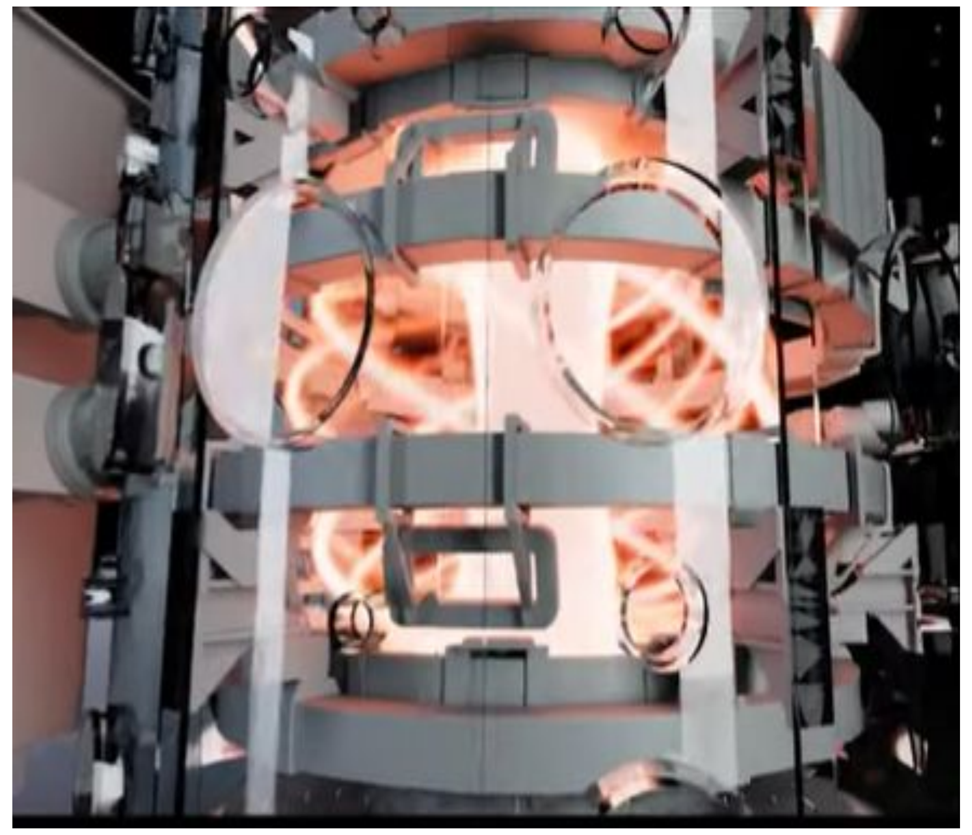
Quantum Accuracy at Cost for Physical Scale Models

AI INTRODUCES NEW USE CASES FOR SCIENCE AND ENGINEERING

AI Bridges the Gap Between Simulation and Real-Time

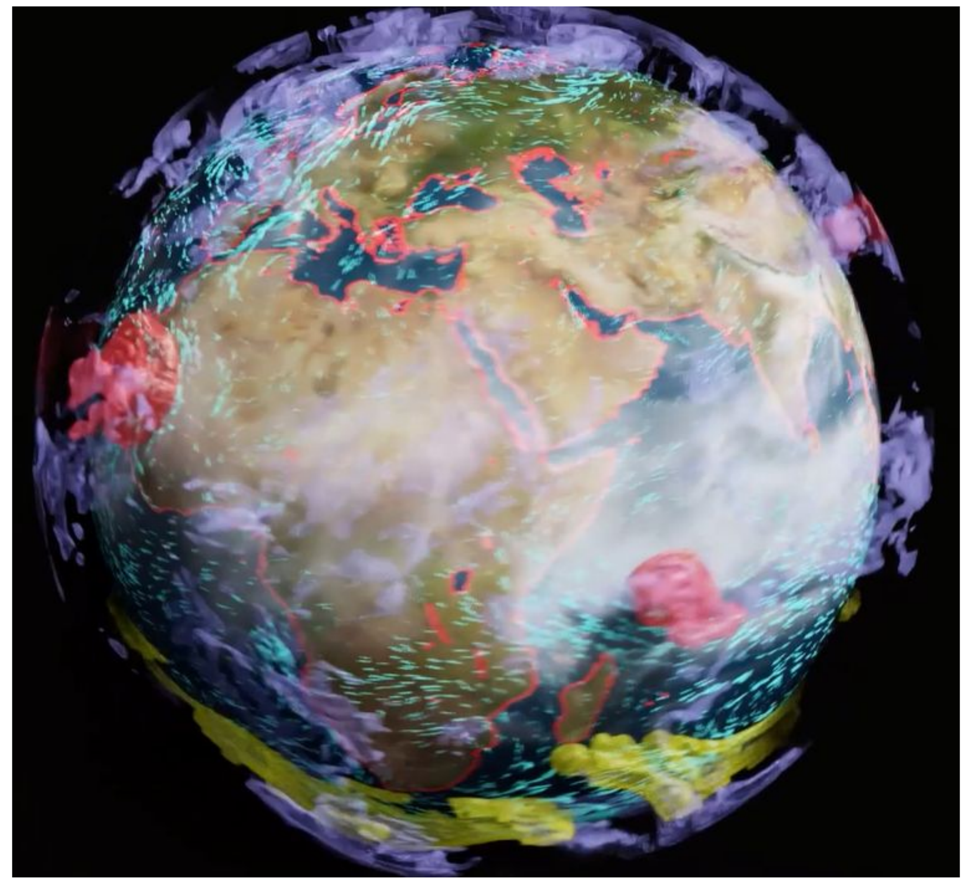
DIGITAL TWIN POC SCIENCE EXAMPLES

Collaborate with the Global Research Community to Pursue Science Discovery that Benefits Mankind



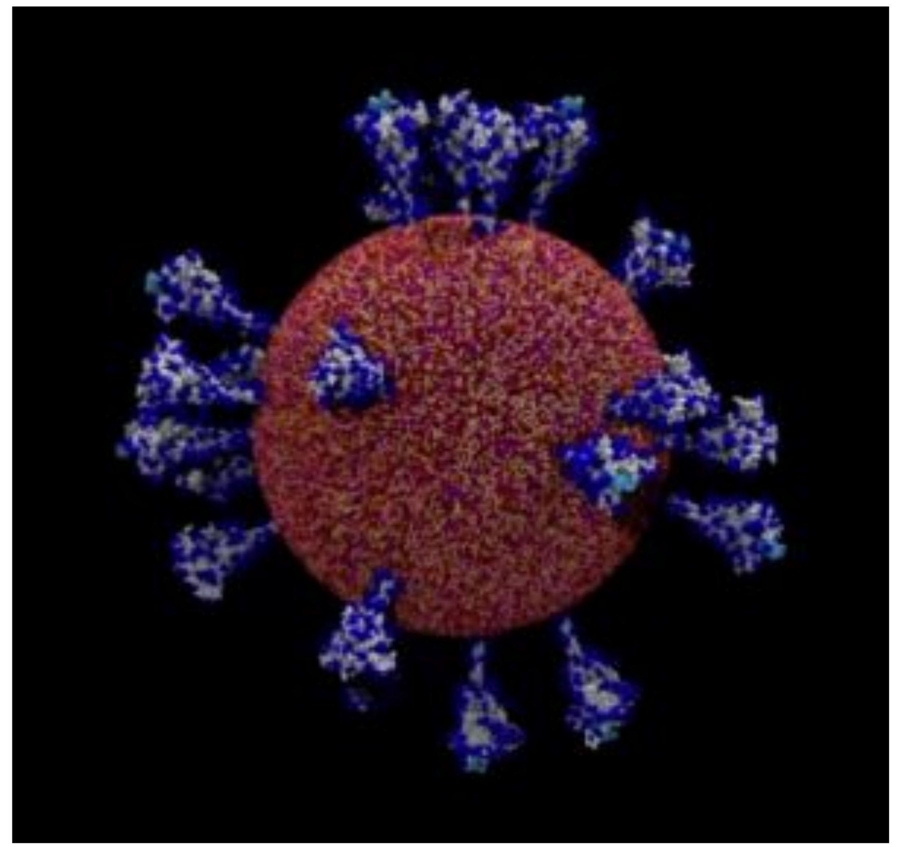
Towards Real time Fusion Reactor Design

Generative AI to Predict Disruption



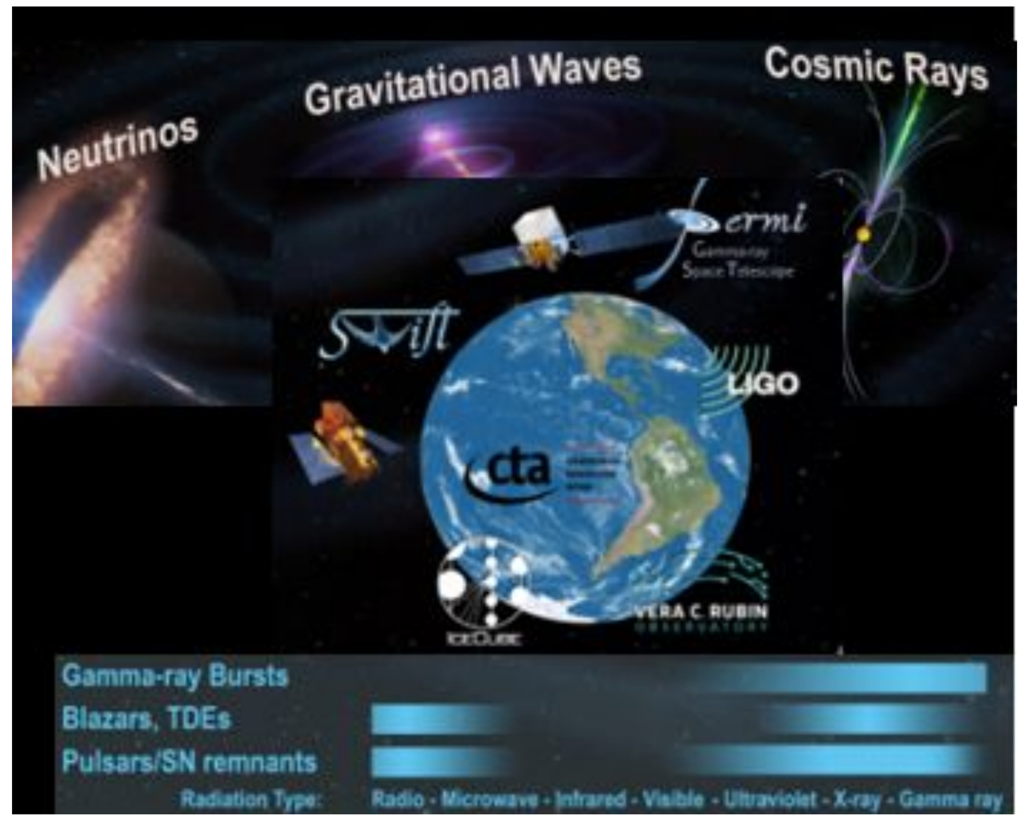
Earth 2

Destination Earth



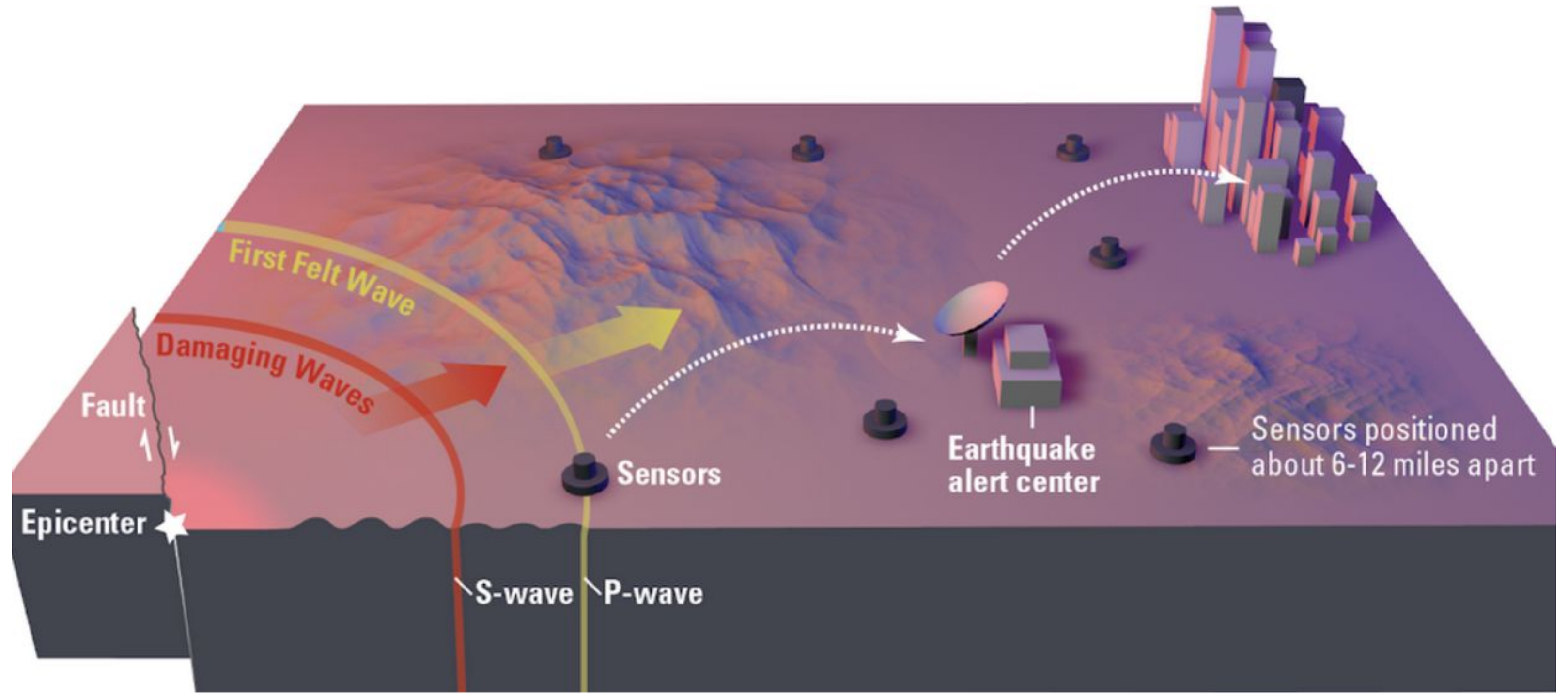
Genome Scale LLMs for Covid

Covid is Airborne



Real Time Multi-Messenger Astrophysics

Multi-Messenger Neutrino Detection



Earthquake Model with Machine Learning

Earthquake Early Warning SCEC

Kubota For Earth For Life

NVIDIA


NVIDIA

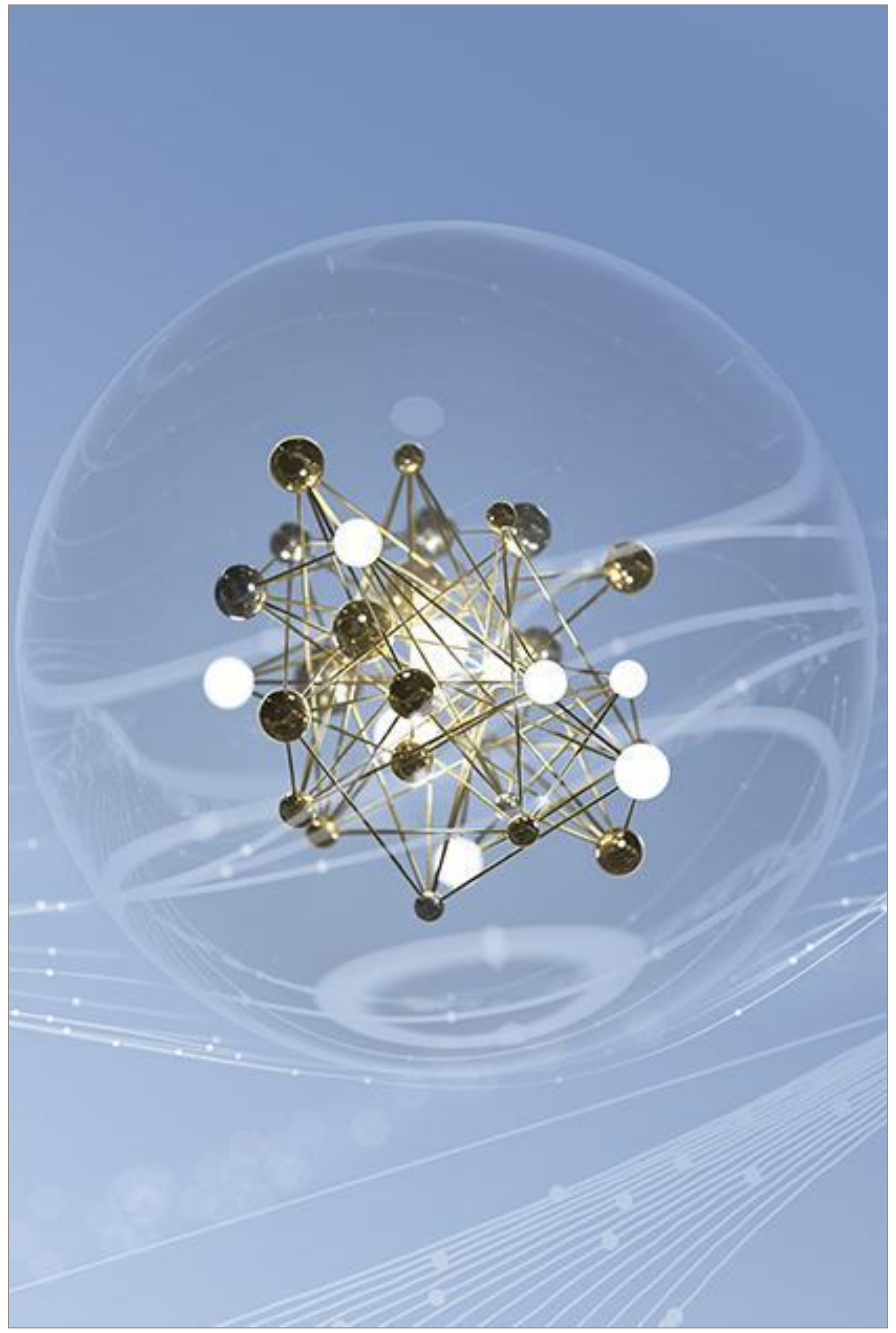
Earth-2 Program

Build the technology needed to create the digital twin of the earth's weather and climate systems

Accelerating NWP codes on GPU

AI research and collaboration with the science community

Interactive Visualization – Digital Twins



Operationalize using Cloud Services

NVIDIA

AI ALGORITHMS EVOLVING AT UNPRECEDENTED PACE

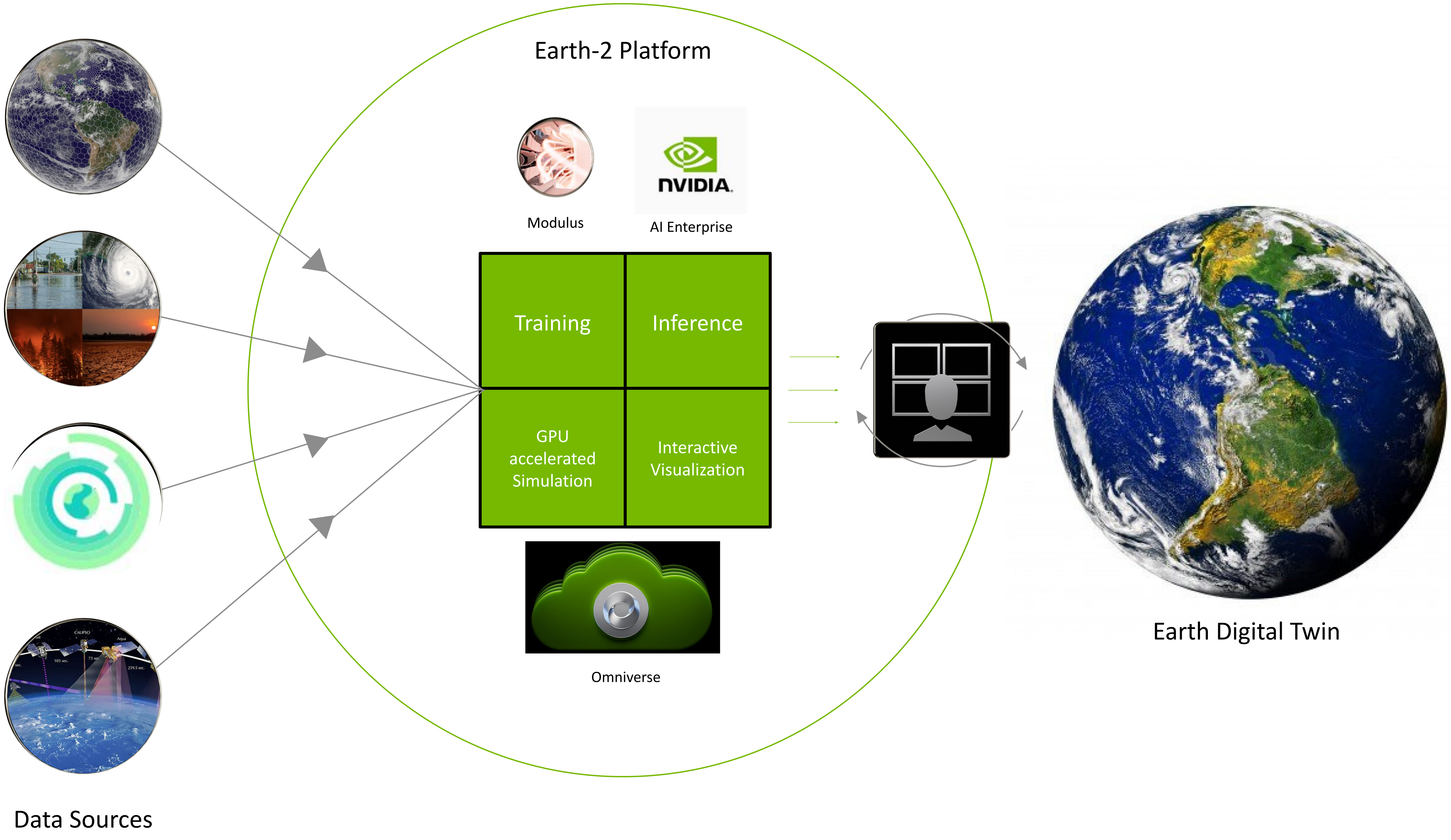
REGIONAL FORECASTING VIA KM-SCALE SUPER-RESOLUTION

Generative AI – Diffusion models

- Case Study:
- Super-resolve 25-km AI weather models (SFNO, GraphCast, Pangu Weather) 12.5x super-resolution & channel synthesis using CorrDiff over Taiwan (25 km --> 2 km)
- Sample diversity from Gen-AI of equivalently plausible fine-scale atmospheric conditions.
- 1000x Faster, 3000x more Energy Efficient, 200x Data Compression relative to WRF on CPU (Numerical Model)

EARTH-2

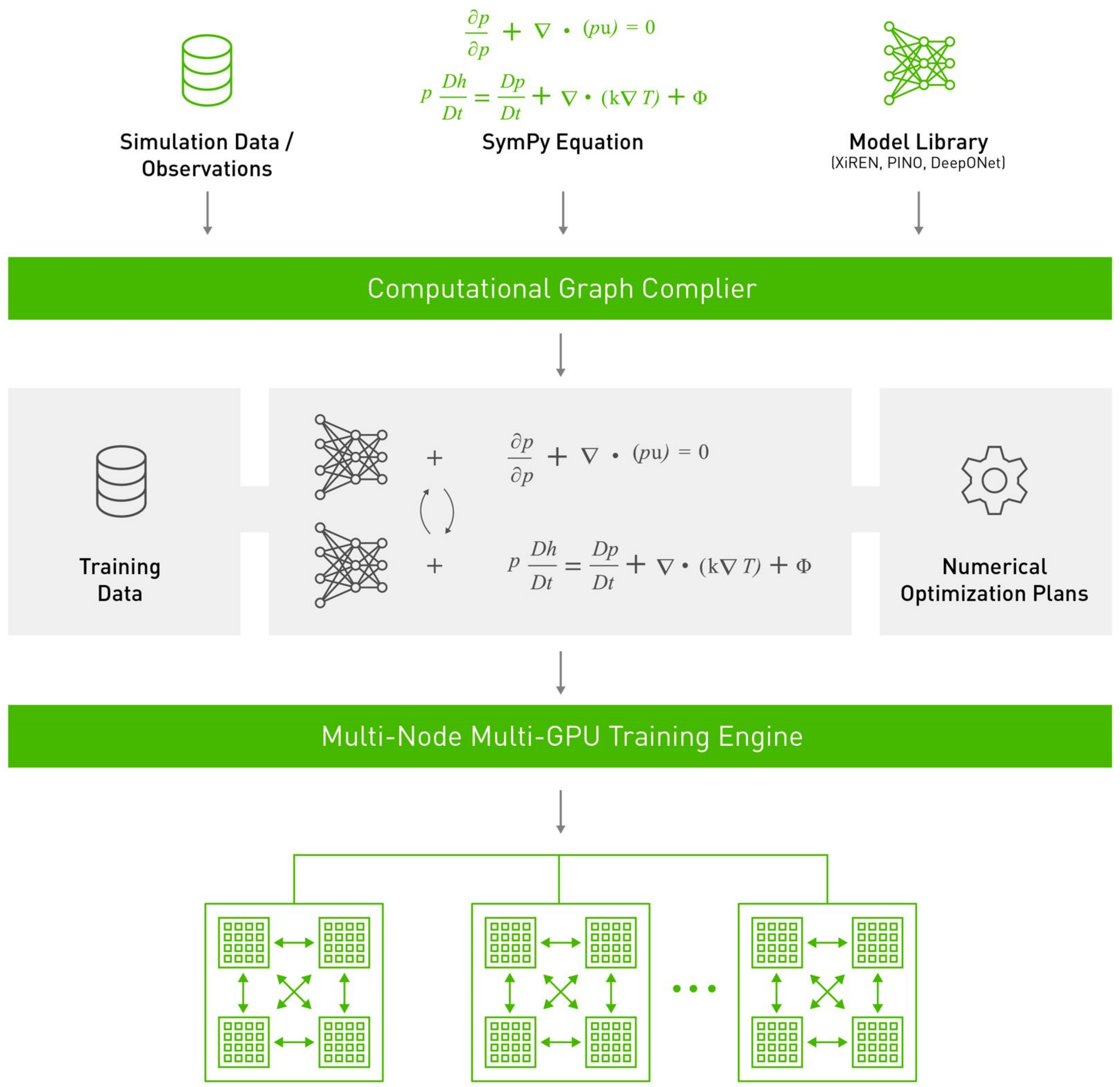
Connecting Complex Simulation, Data and AI Workflows



NVIDIA MODULUS

Open-Source Platform for Developing Physics-Based Machine Learning

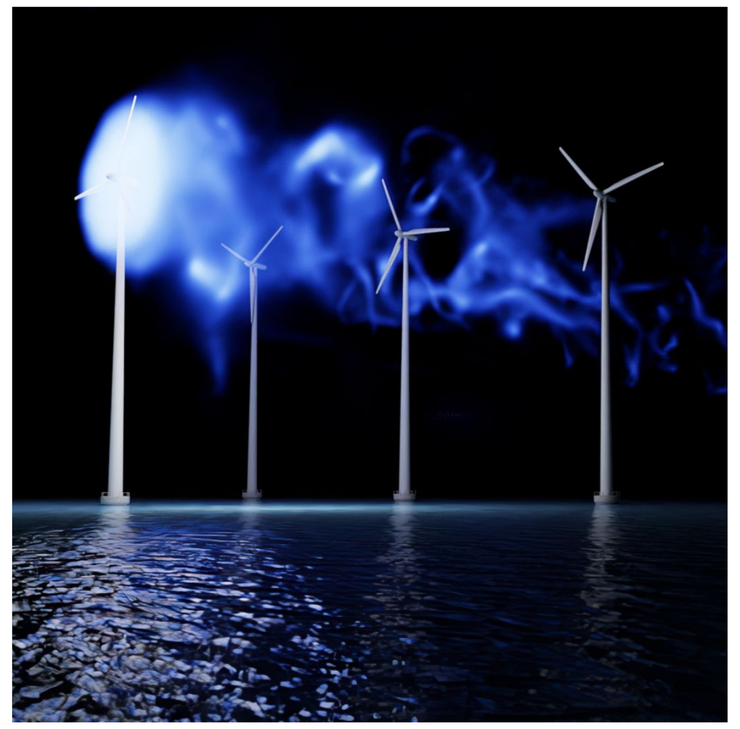
Training Neural Networks Using Both Data And The Governing Equations



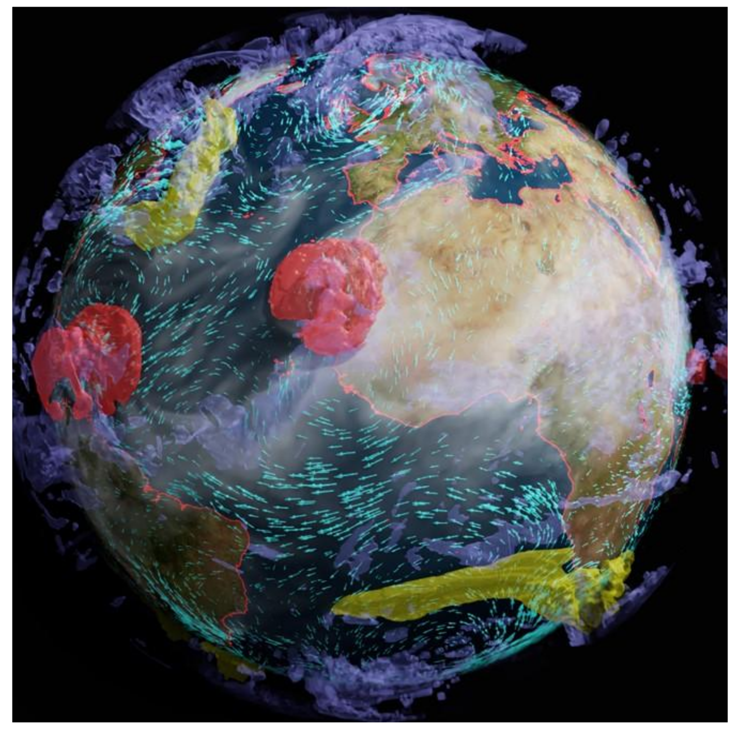
With generative AI using diffusion models, you can enhance engineering simulations and generate higher-fidelity data for scalable, responsive designs.

Advancing Scientific Discovery With Modulus

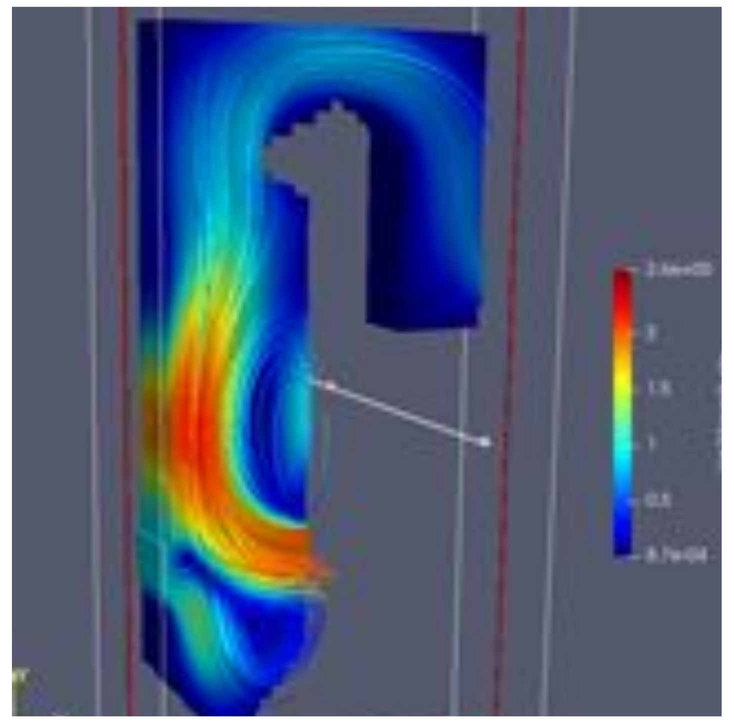
Renewable Energy
Siemens Gamesa: 4000X Faster wind turbine wake optimization



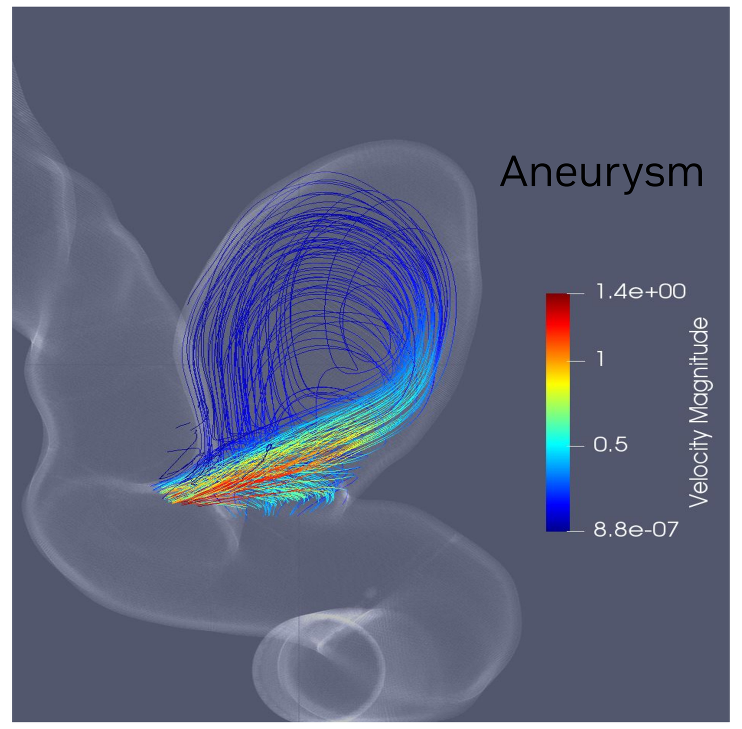
Climate Change
45,000X Faster extreme weather prediction with FourCastNet



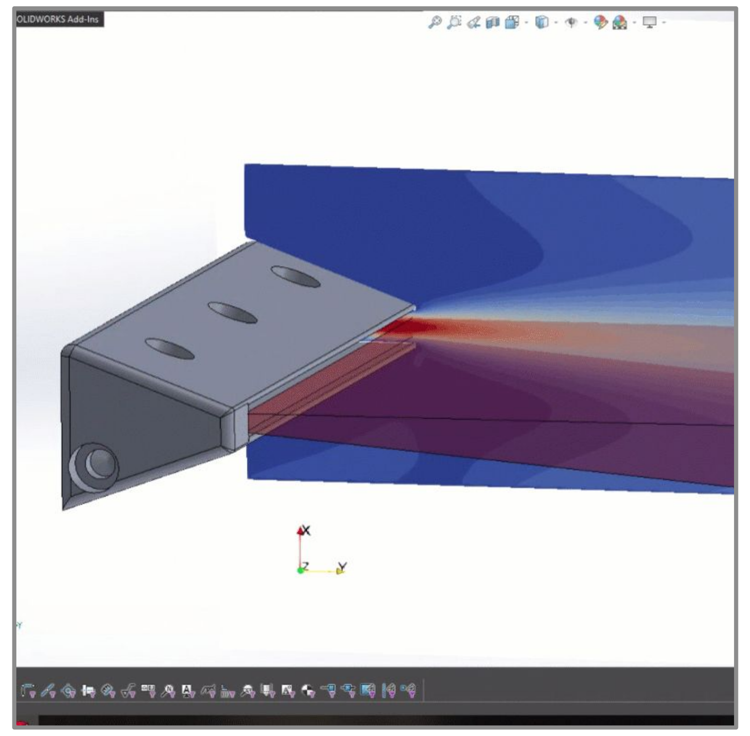
Industrial HPC
NETL: 10,000X Faster build of high-fidelity surrogate models



Healthcare
High-fidelity results faster for blood flow in inter-cranial aneurysm



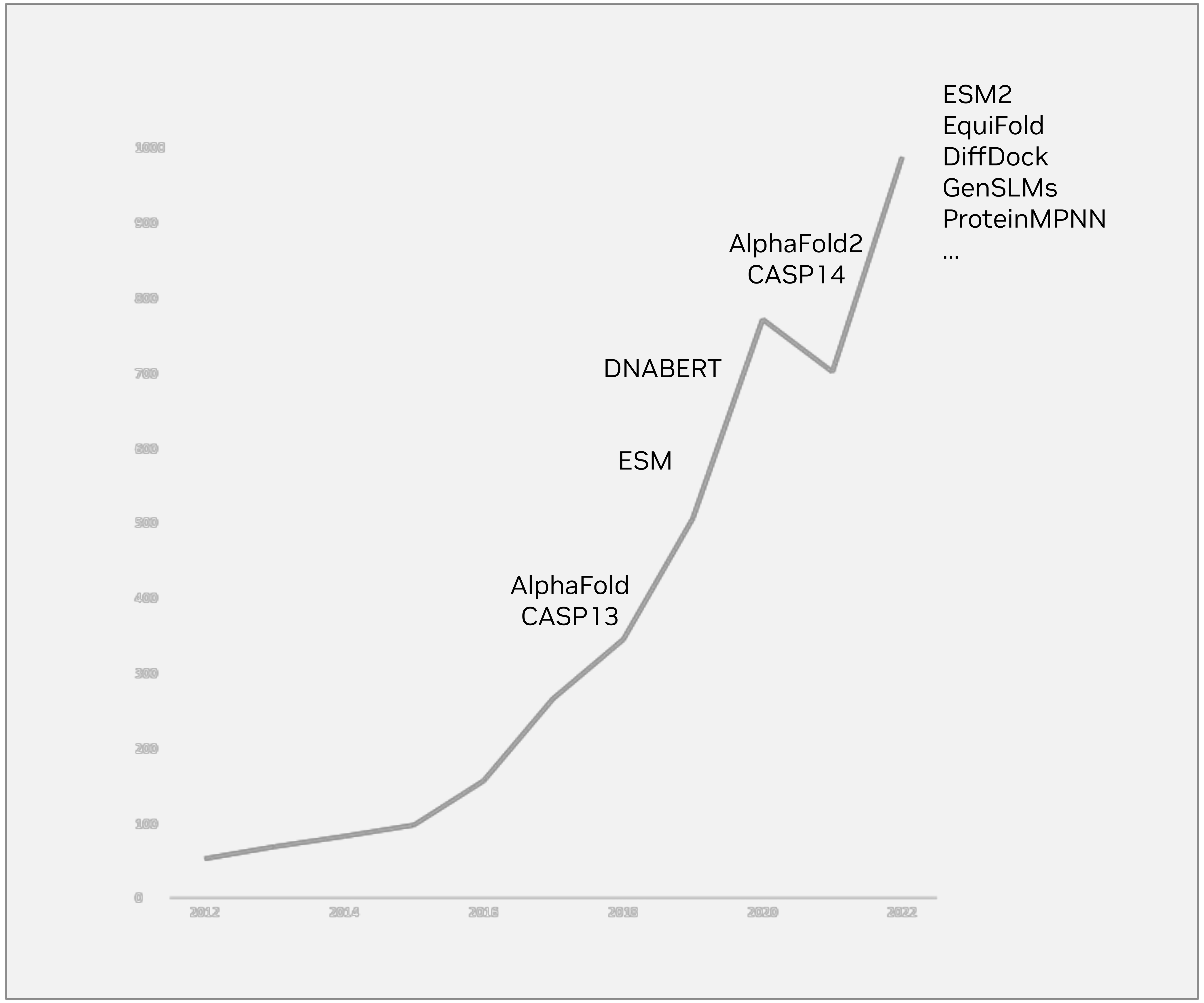
Digital Twins
Kinetic Vision: Design optimization using parameterized models



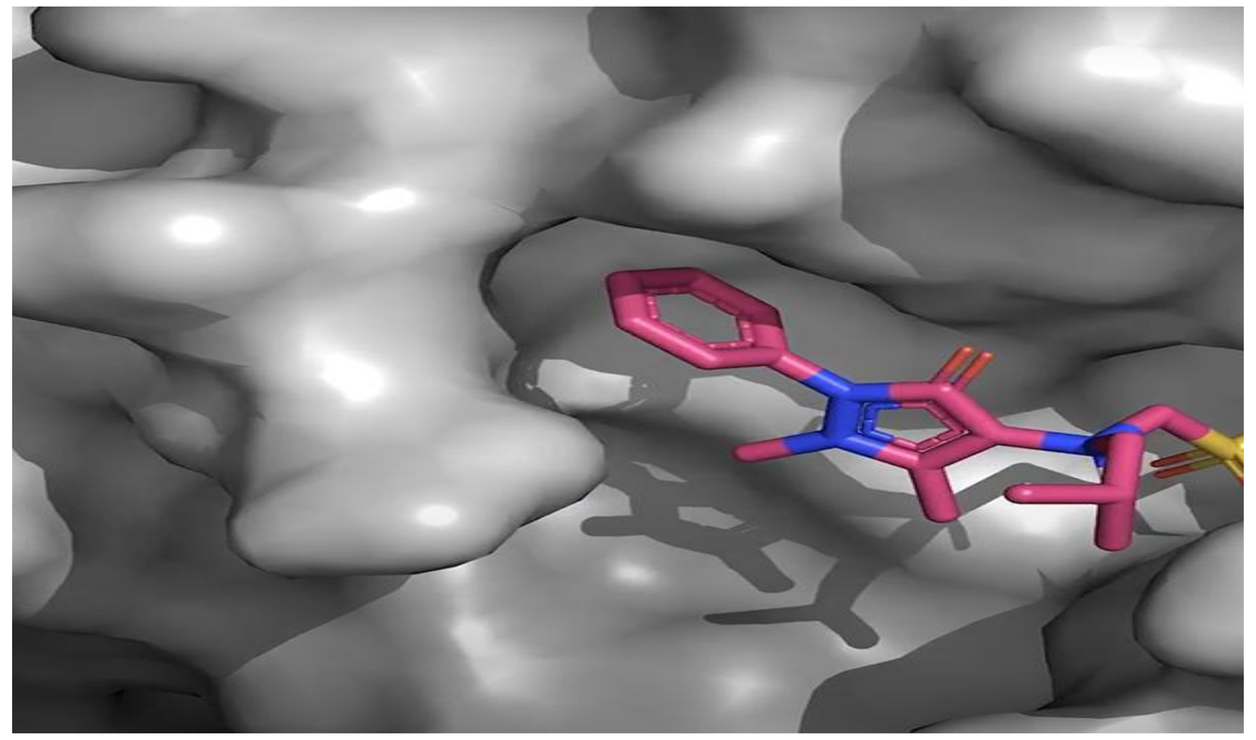
Science and Engineering Teaching Kit available now.

Generative AI making headway into Biology and Drug Discovery

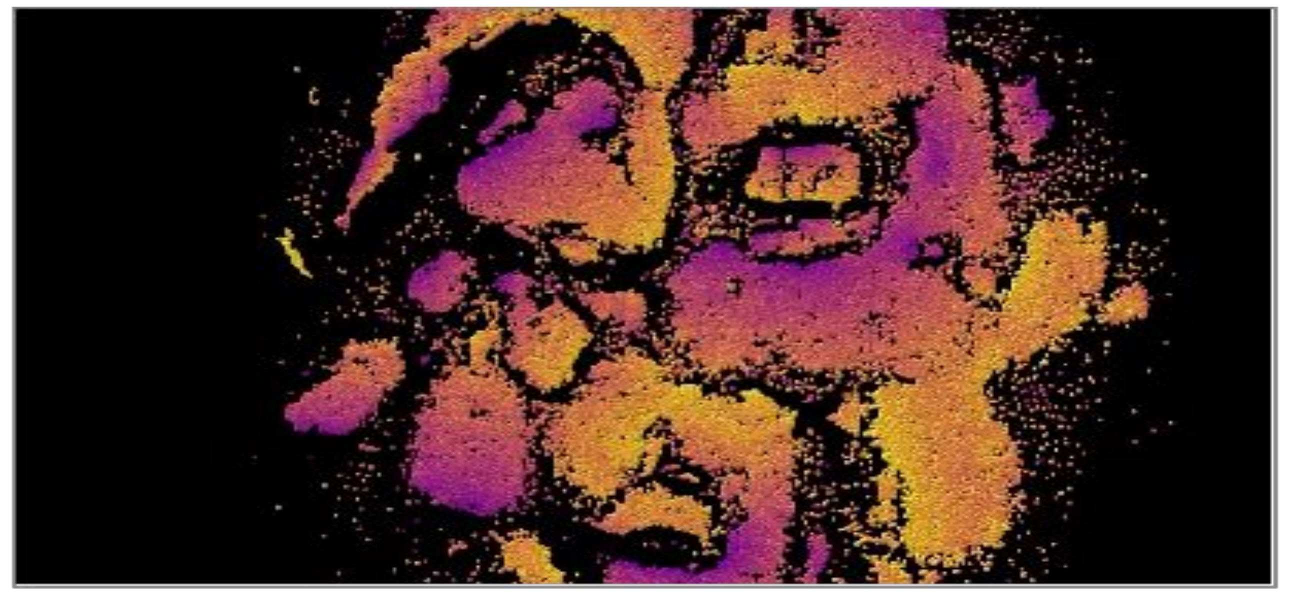
AI Published Papers



Lab Automation: Sensors & Robotics

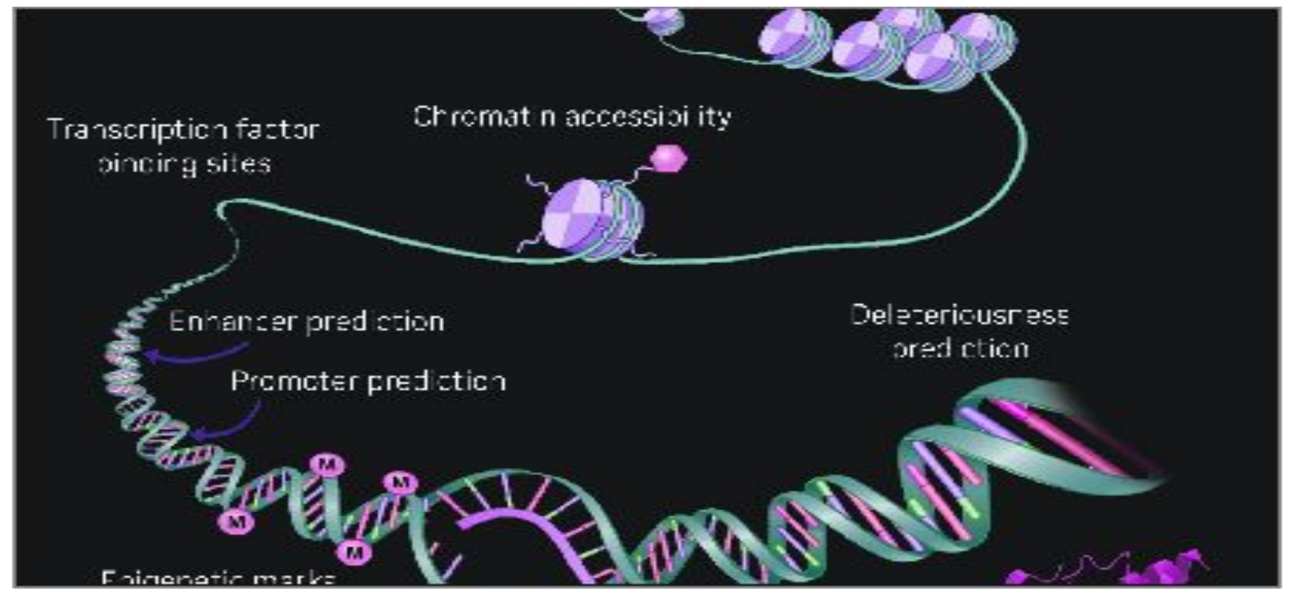


In Silico Drug Discovery: AI & Computing



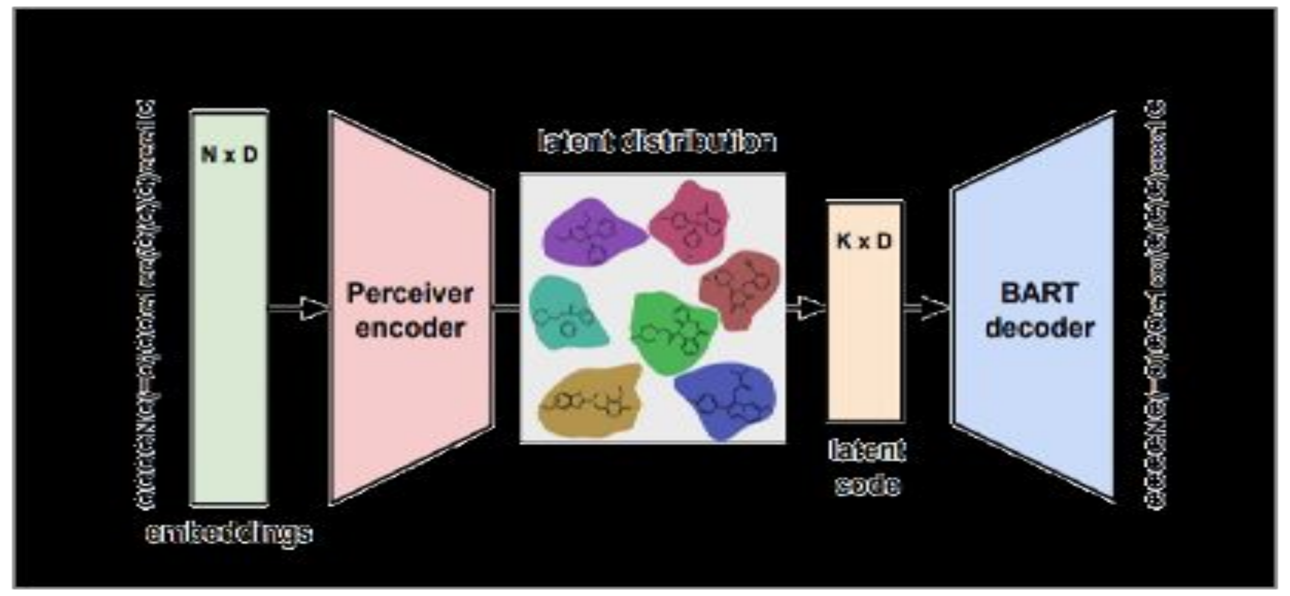
GensLMs

Genome-scale language models reveal SARS-CoV-2 Evolutionary Dynamics



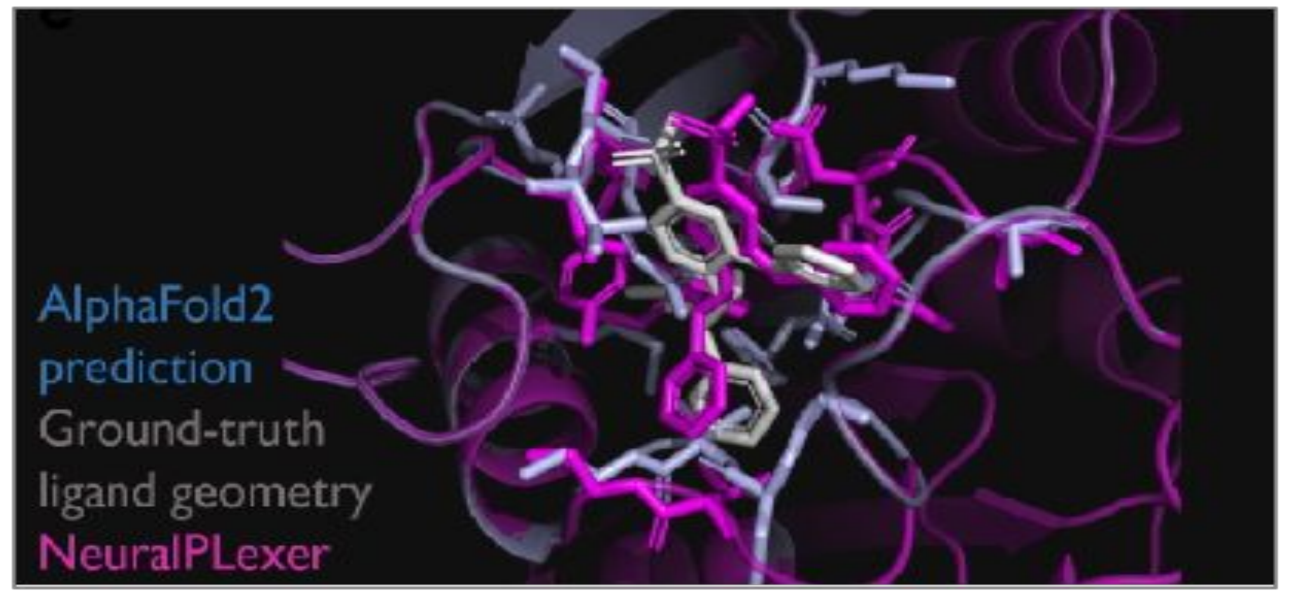
Nucleotide Transformer

Building and Evaluating Robust Foundation Models for Human Genomics



MolMIM

Improving Small Molecule Generation using Mutual Information Machine



NeuralPlexer

Dynamic-Backbone Protein-Ligand Structure Prediction with Multiscale Generative Diffusion Models

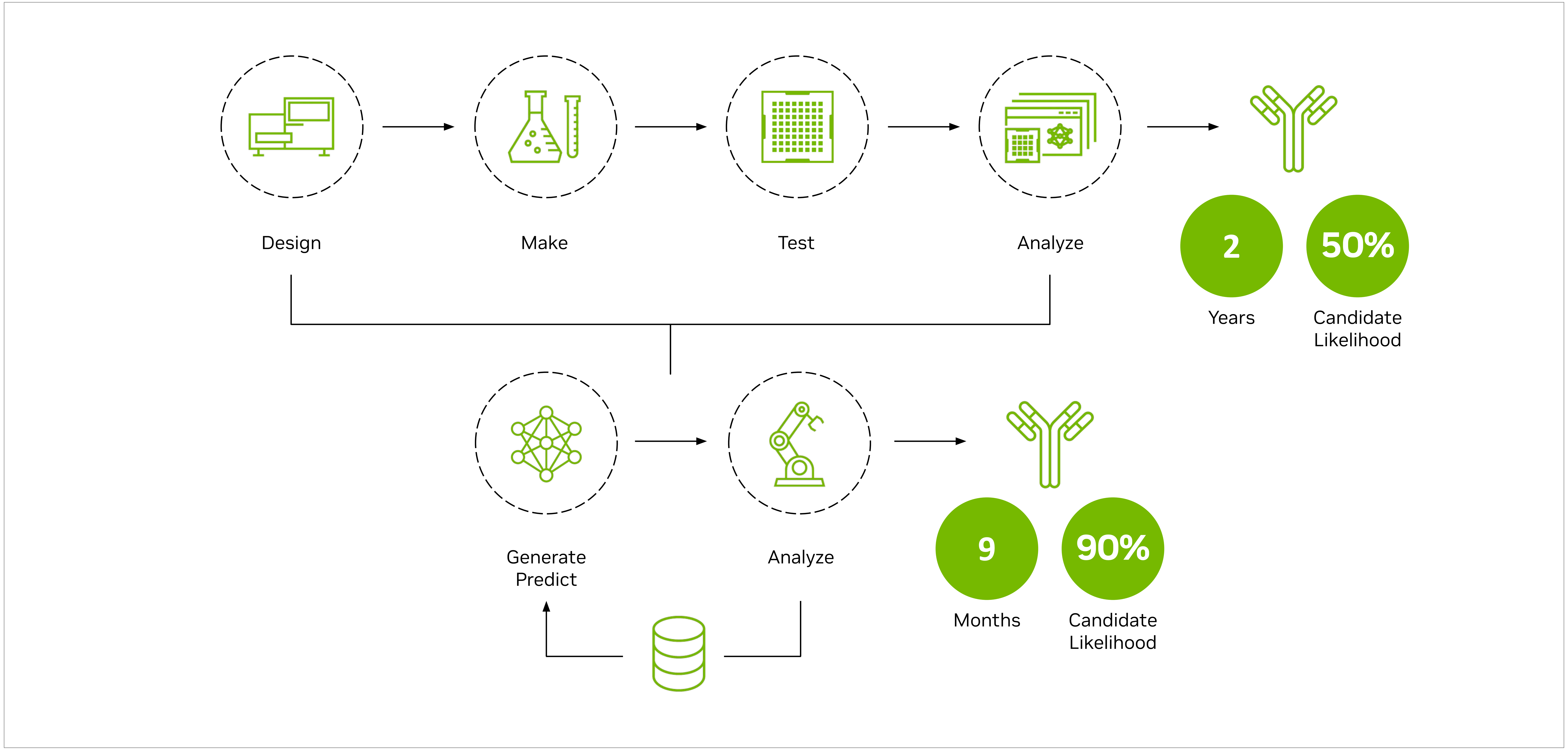
Source: arXiv.org Q-bio: AI, ML, DL, NN

DRUG DISCOVERY IS AT AN INFLECTION POINT

Computer Aided Drug Discovery is Expanding Exponentially

GENERATIVE AI DRY LABS ARE ACCELERATING DRUG DISCOVERY

3 Years Faster | 100s of Millions Cheaper

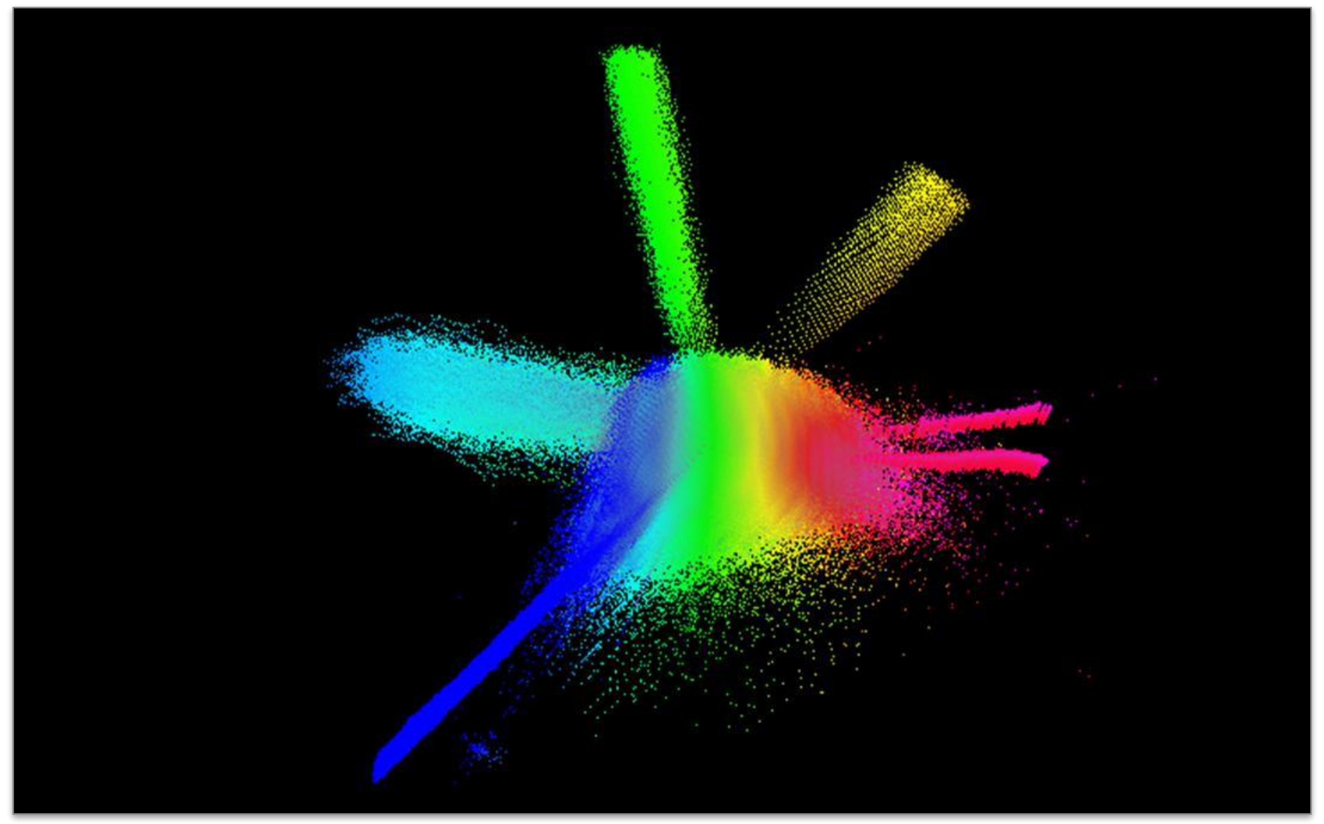


NVIDIA BioNeMo

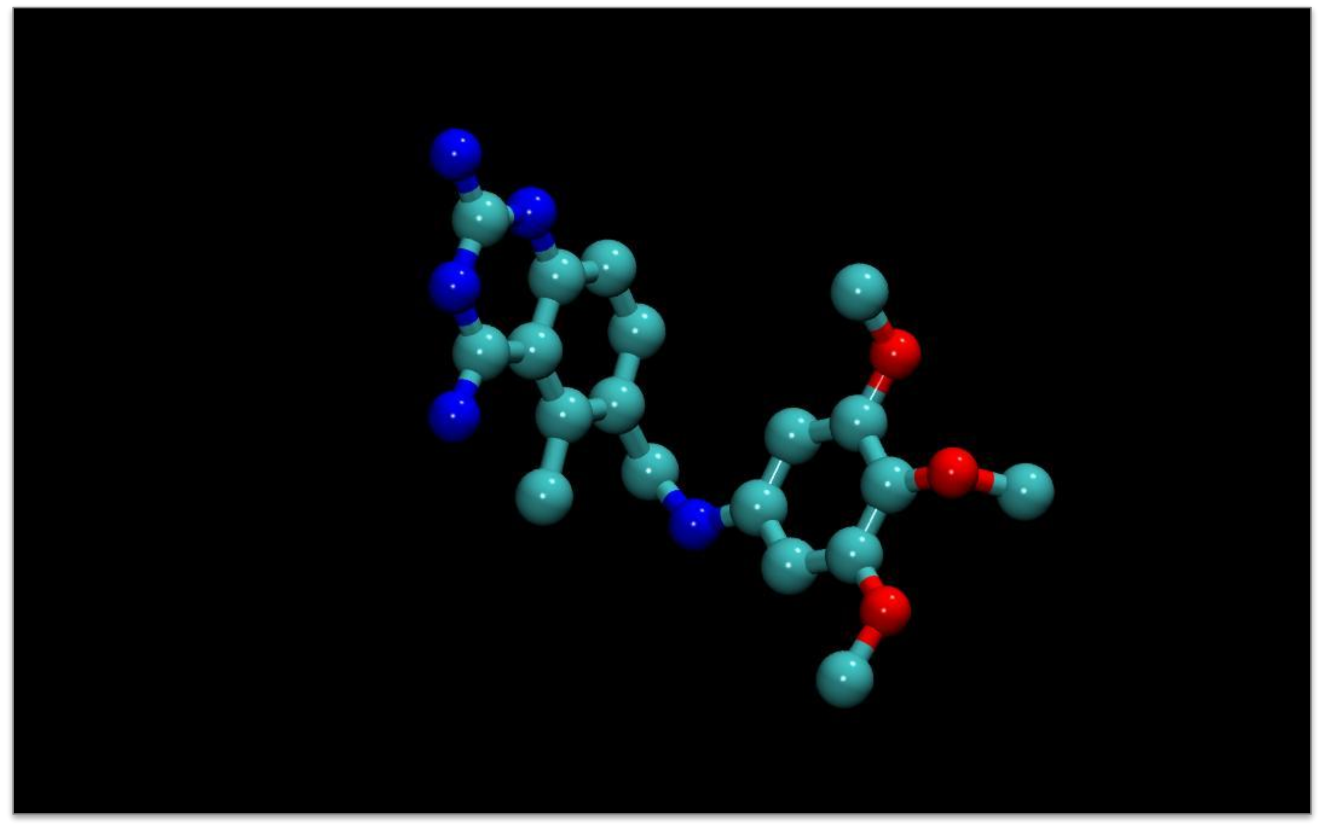
Build, Optimize and Deploy Foundation Models for Computer-Aided Drug Discovery

BioNeMo Framework Supports Optimized Biomolecular Models

Proteins | Small Molecules | Genomics

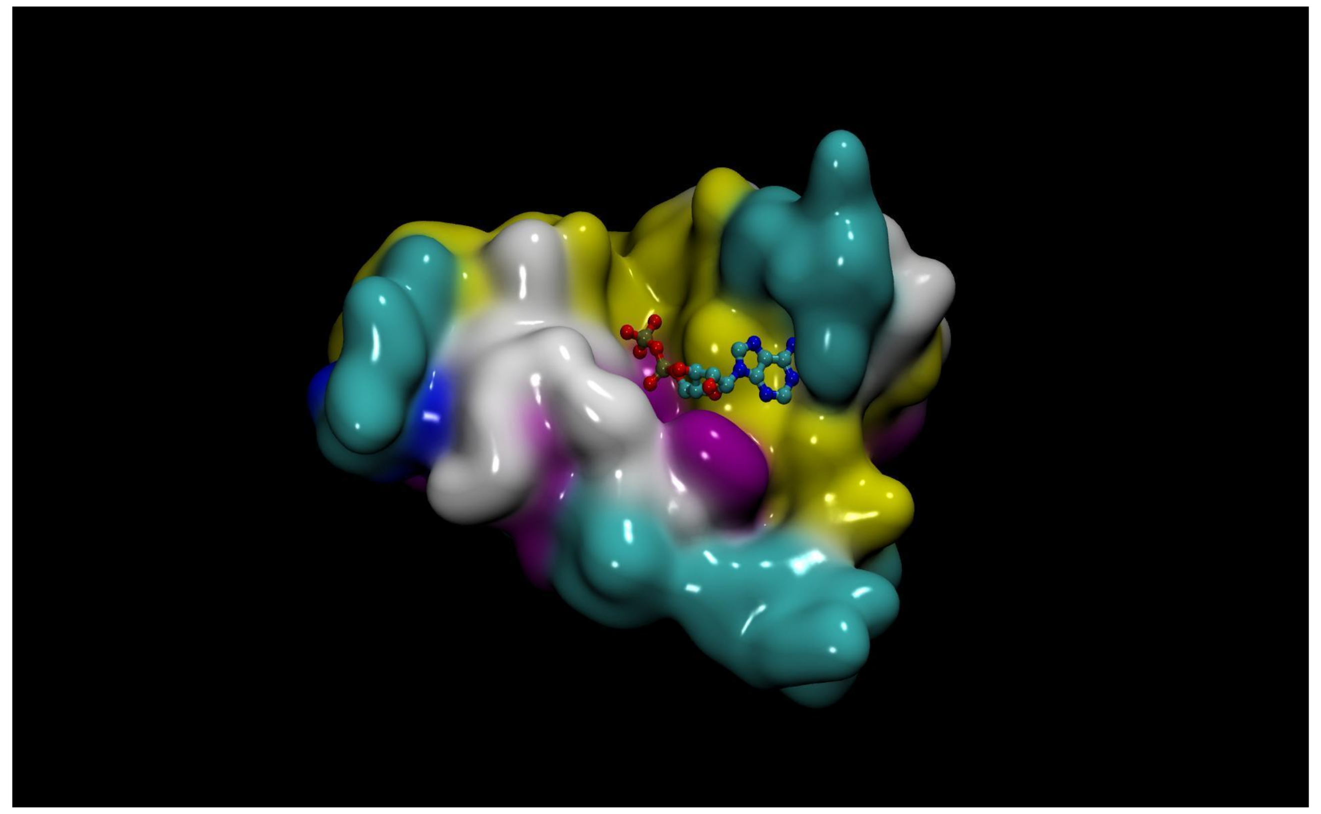


ESM-1 | ESM-2
Protein LLMs



MegaMolBART
Generative Chemistry Model

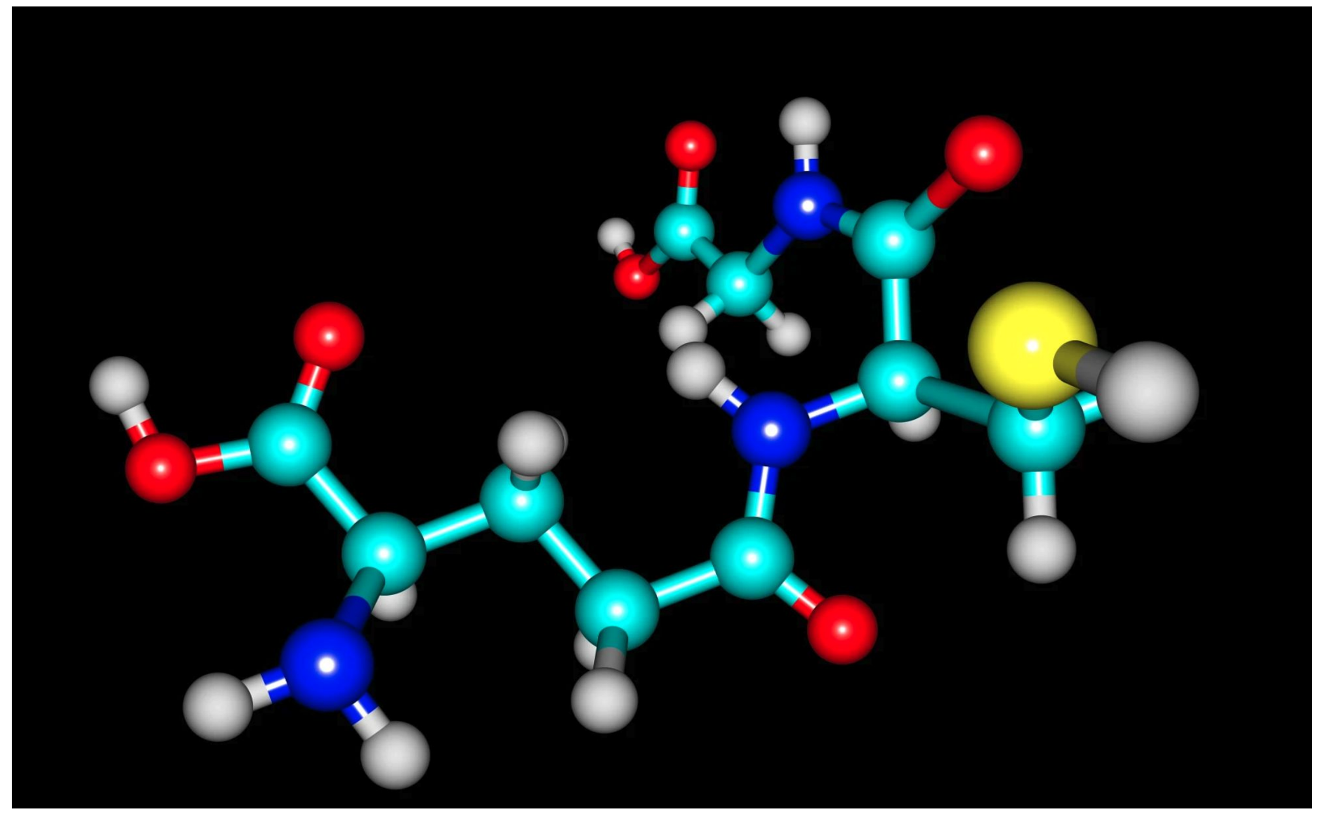
ProtT5
Protein Sequence Generation



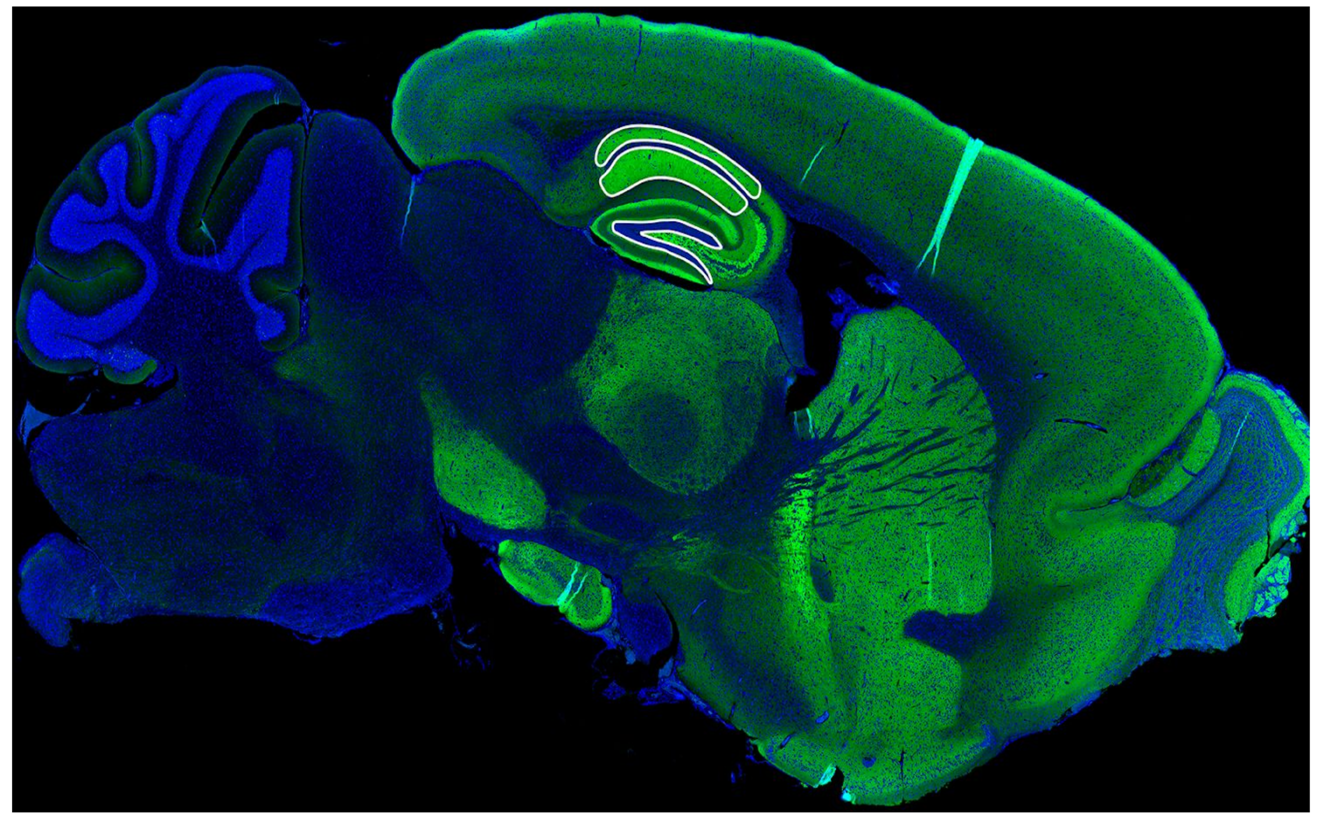
NEW: DiffDock | EquiDock
Docking Prediction

NEW: OpenFold
3D Protein Structure Prediction

NEW: DNABERT
DNA Sequence Model



COMING SOON: MolMIM
Molecular Generation

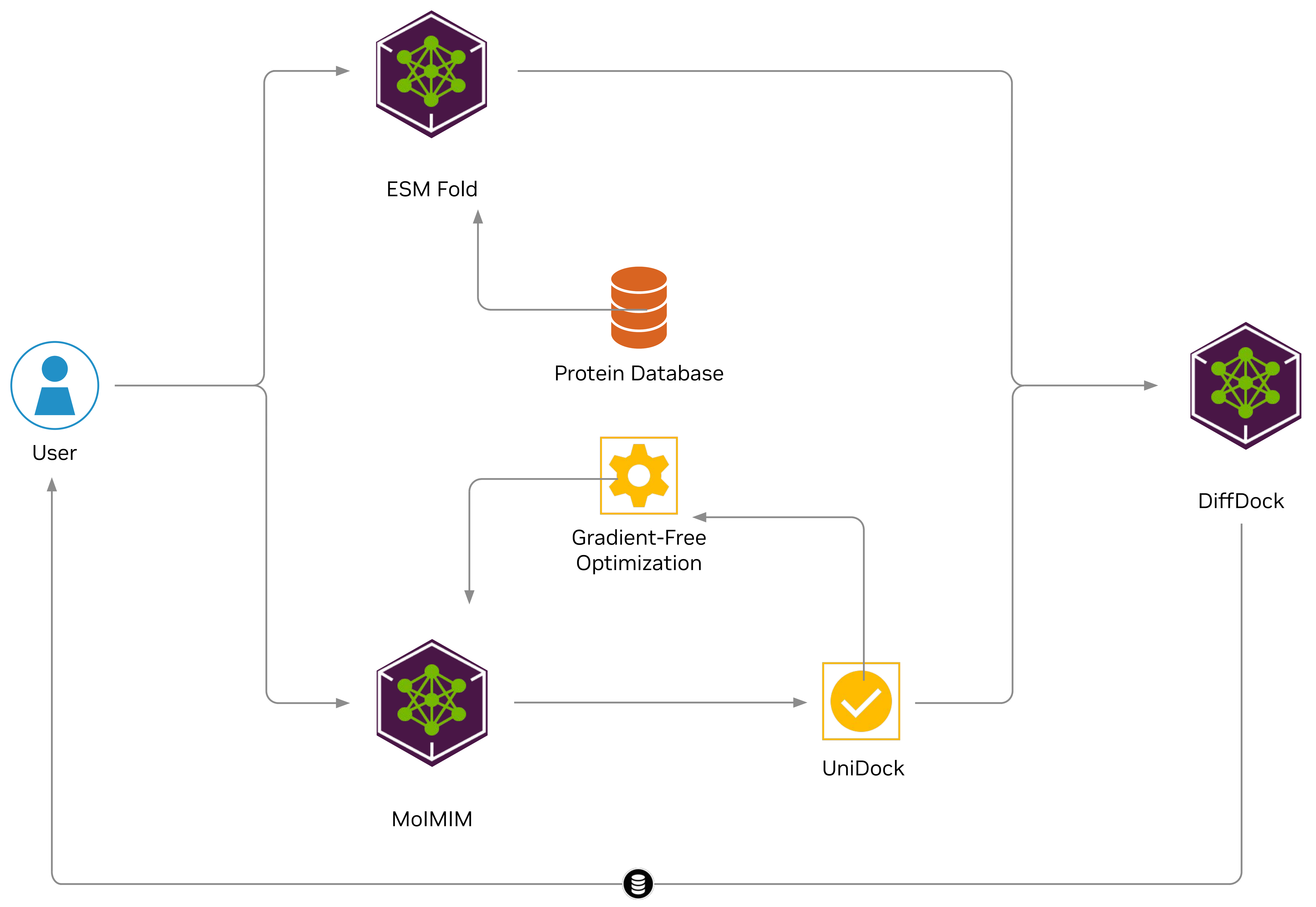


COMING SOON: Single Cell BERT
Single Cell Expression Model

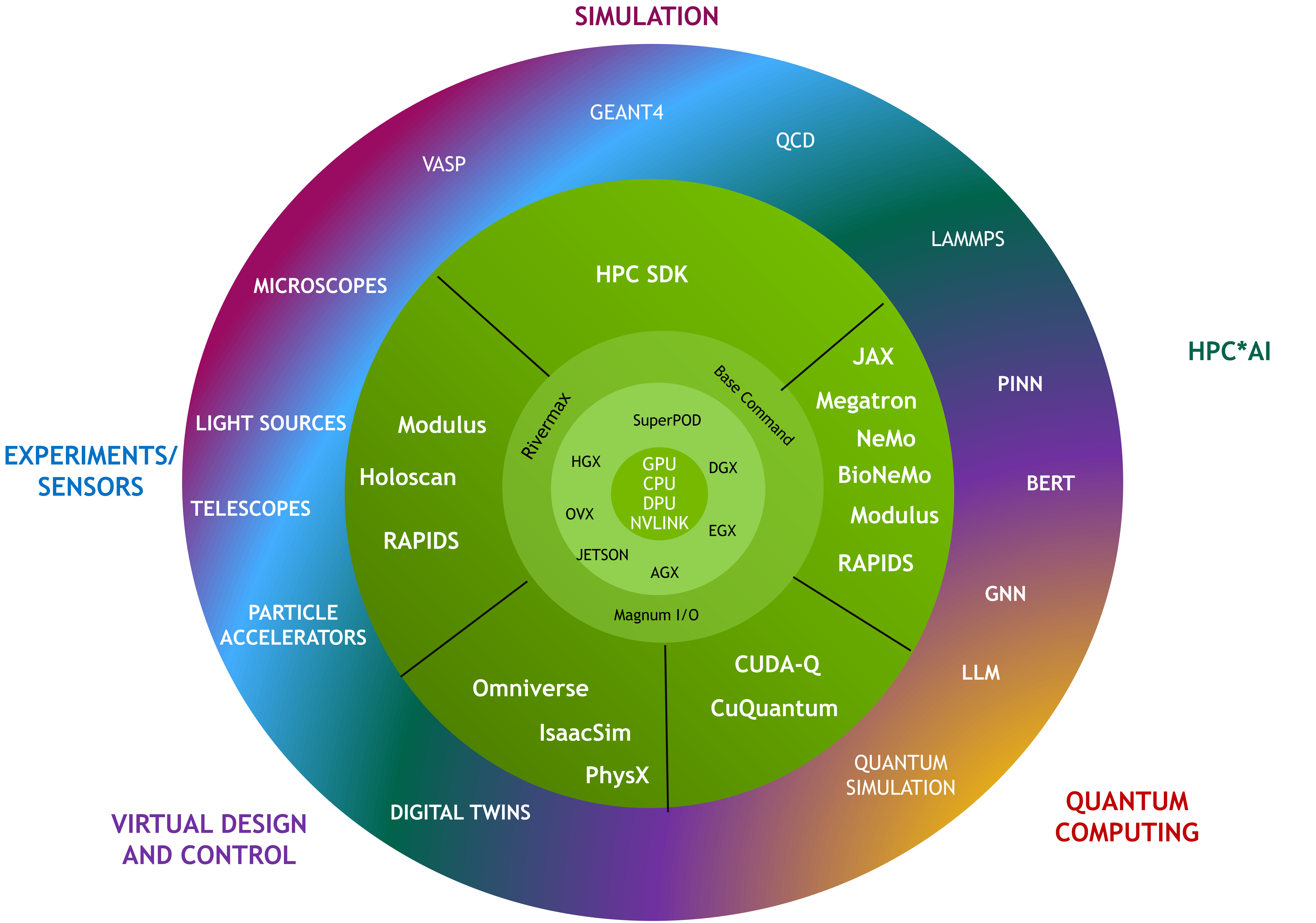
NVIDIA

Build Generative AI Virtual Screening Workflows with NVIDIA NIM

Use composable NVIDIA NIMS to build workflows for CADD applications



NVIDIA PLATFORM EVOLVING TO MEET THE CHALLENGE



NVIDIA

THANK YOU