DIGITAL TWINS FOR SCIENCE

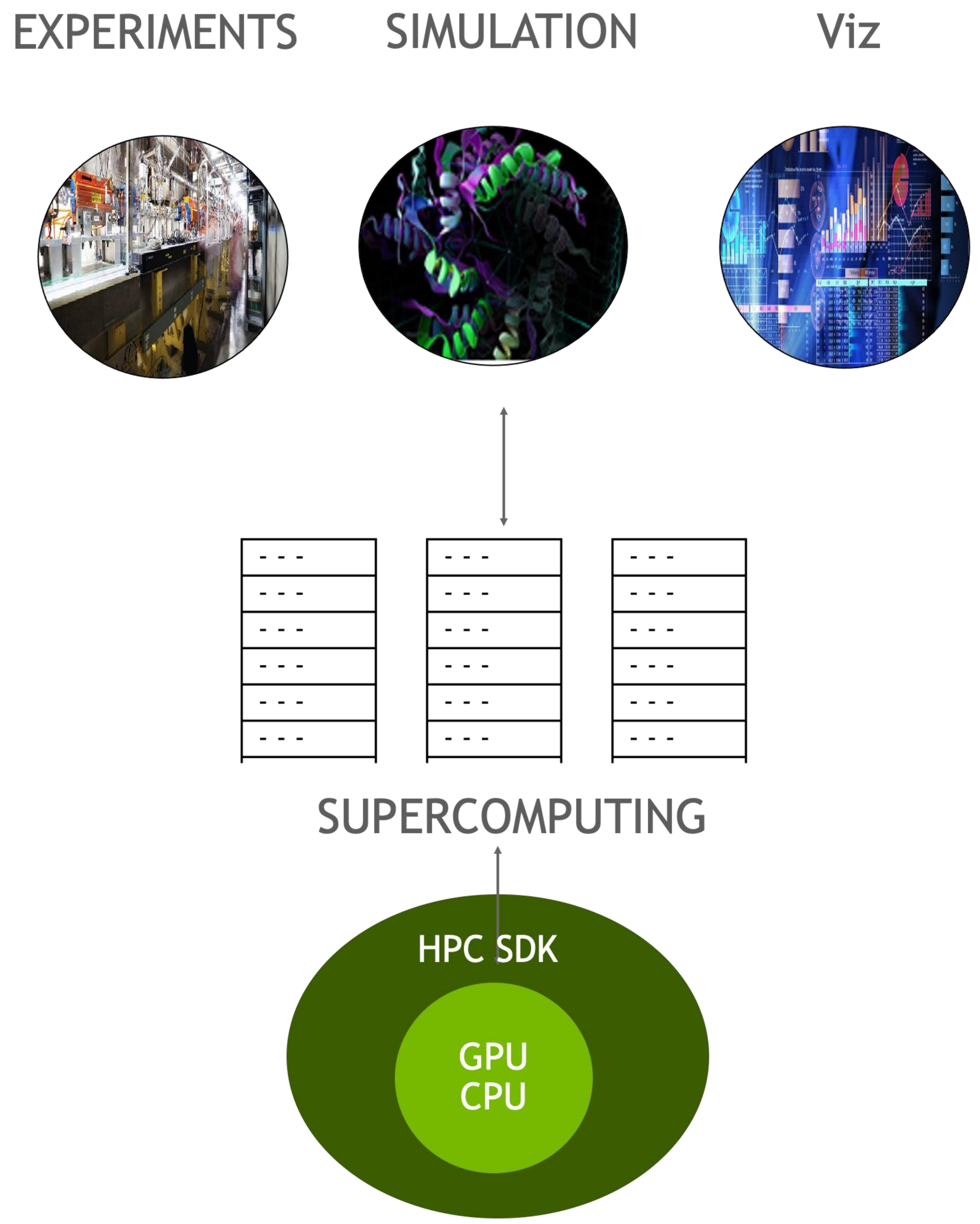
SCIENTIFIC COMPUTING IS EVOLVING

Thought Leaders Mapping Out the Opportunity and Constraints Given Current Market Reality

NVIDIA

A DEEPER LOOK AT THE NEW HPC

ADAPTING TO THE CONSTRAINTS, MARKET REALITIES AND EXPANDING OPPORTUNITY



ACM HPC Forecast
Reed and Dongarra

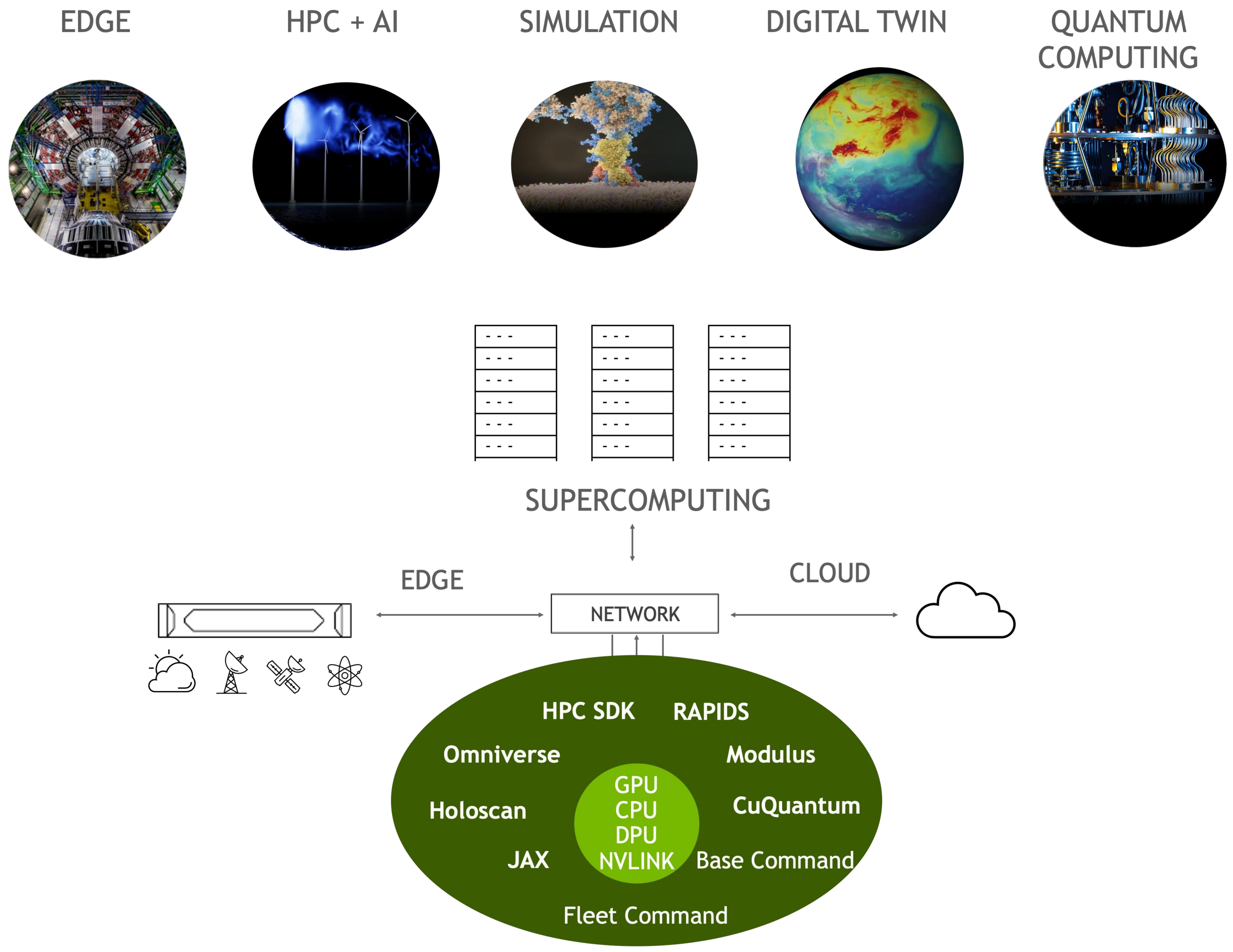
Semiconductor Constraints limit the potential increase in scale for legacy algorithms

New Algorithms offer potential for dramatic increase in model scale and reduction in latency

Cloud Economics have changed the supply chain ecosystem

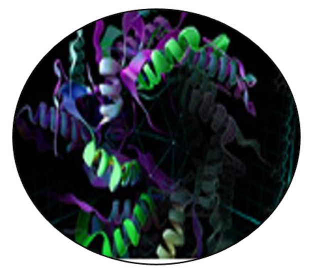
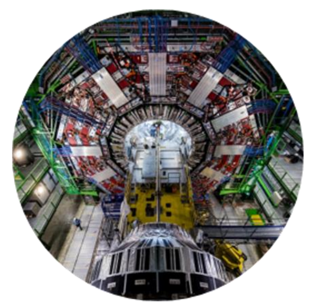
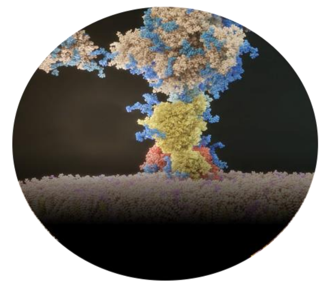
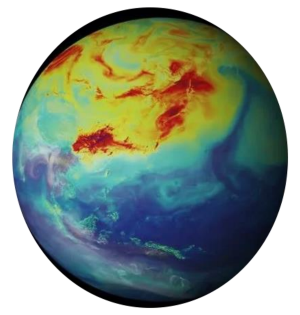
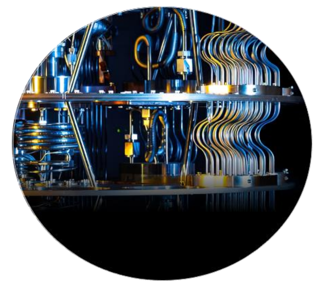
Charting a New Path Post
Exascale Computing NNSA

OVERARCHING FINDING: The combination of increasing demands for computing with the technology and market challenges in HPC requires an intentional and thorough reevaluation of …. algorithms, software development, system design, computing platform acquisition, and workforce development.



NVIDIA

TRANSITION TO POST EXASCALE ERA

FEATURE	TERA THROUGH EXASCALE	POST EXASCALE
	EXPERIMENTS  SIMULATION  Viz 	EDGE  HPC + AI  SIMULATION  DIGITAL TWIN  QUANTUM COMPUTING 
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, STEERING AND OFFLINE**
DIGITAL TWINS	**IN-SITU VISUALIZATION OFFLNE**	**INTERACTIVE_COMBINATION OF SIMULATION AND OBSERVATIONAL DATA**
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 Just Emerging for Science

Digital Twin Definition from Wikipedia

Digital model of an intended or actual real-world physical product, system, or process (a physical twin) that serves as the effectively indistinguishable digital counterpart of it for practical purposes.

The concept and model of the digital twin 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

National Academy of Science Report: Foundational Research Gaps and Future Directions:

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 for Science

A digital model with sufficient scale and accuracy to be indistinguishable from the real-world physical object, system or process that is dynamically updated with data from it’s physical twin, where the model has sufficient fidelity to meet the requisite accuracy with time to solution to inform decisions that improve the operation of the asset or process being modeled

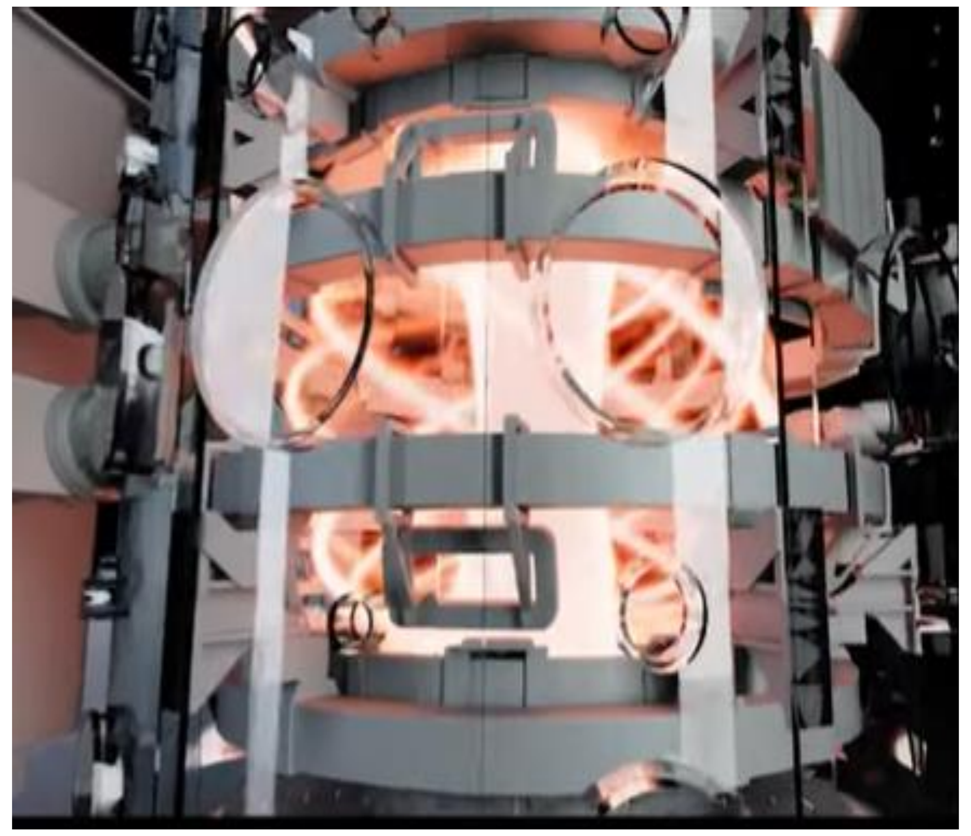
ML ENABLES REQUISITE ACCURACY/TIME TO SOLUTION

Allows the Model to be Indistinguishable and Interactive

ML POTENTIAL TO BRIDGE MODELS WITH CONTROL

EXAMPLES OF DIGITAL TWINS FOR SCIENCE

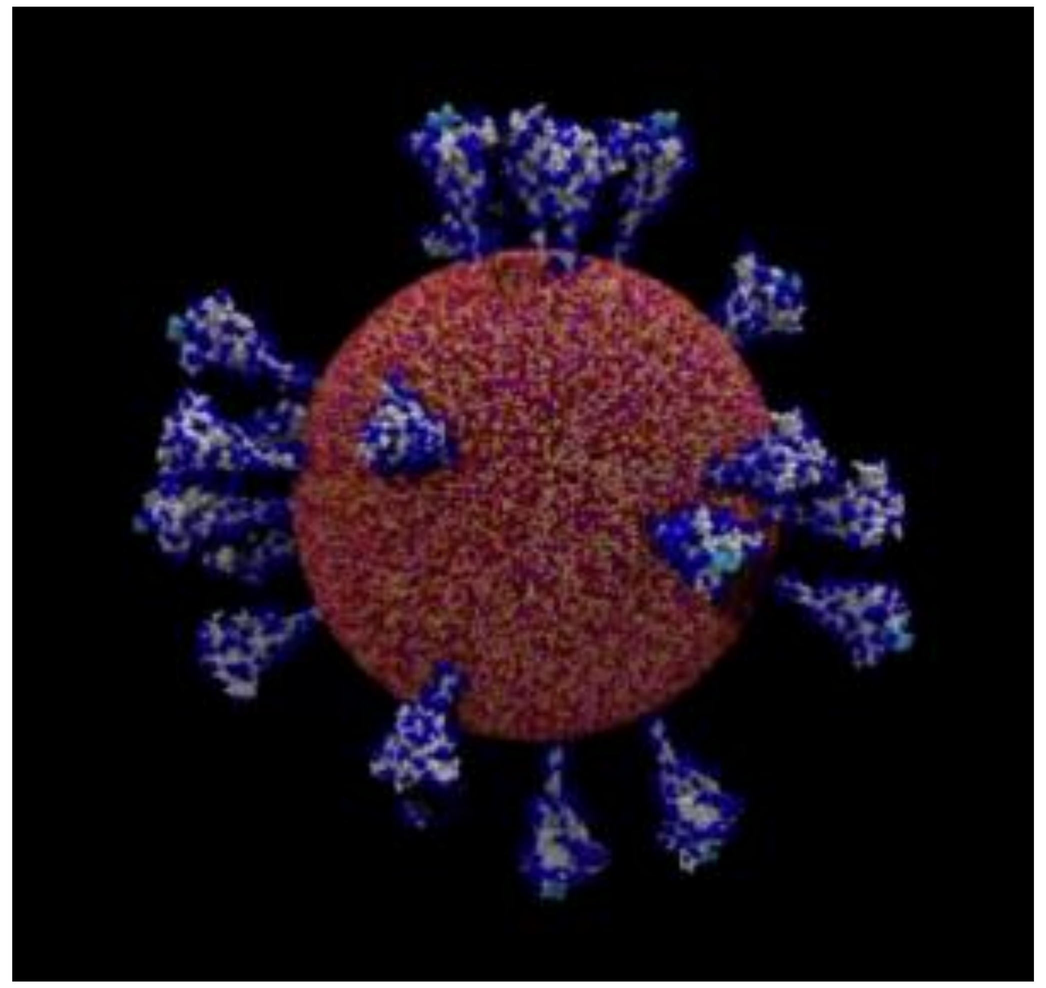
Collaborate with the Global Research Community to Pursue Science Discovery that Benefits Mankind



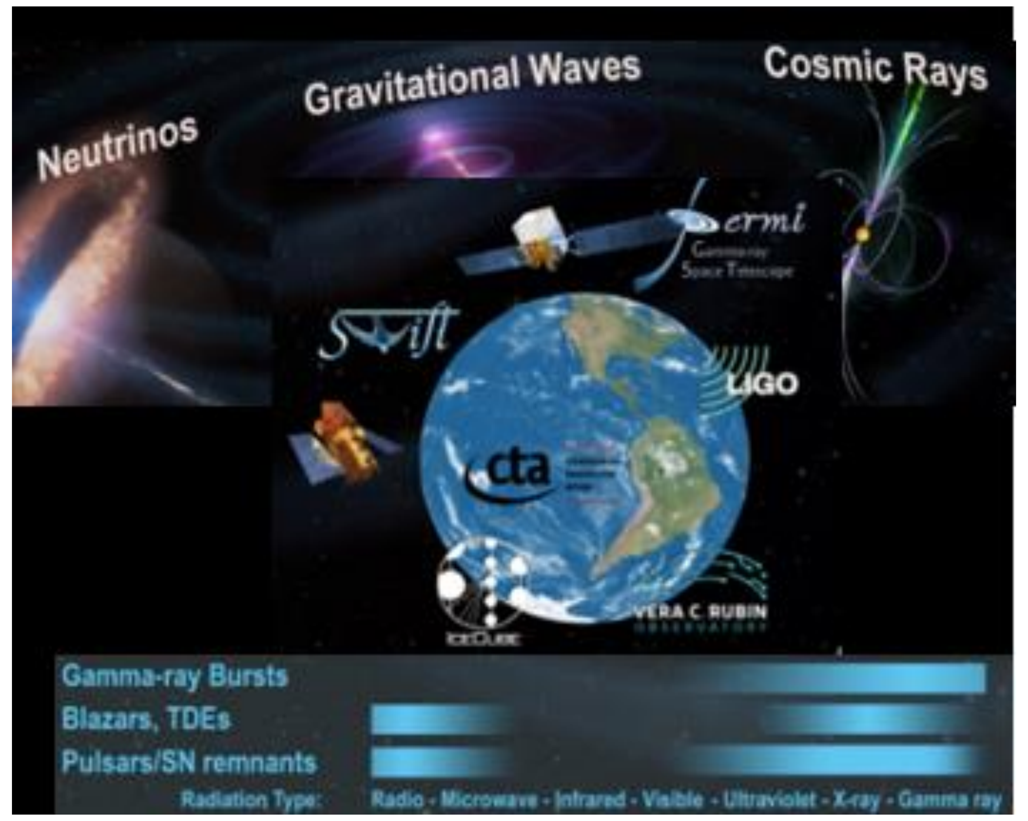
Towards Real time Fusion Reactor Design

Generative AI to Predict Disruption

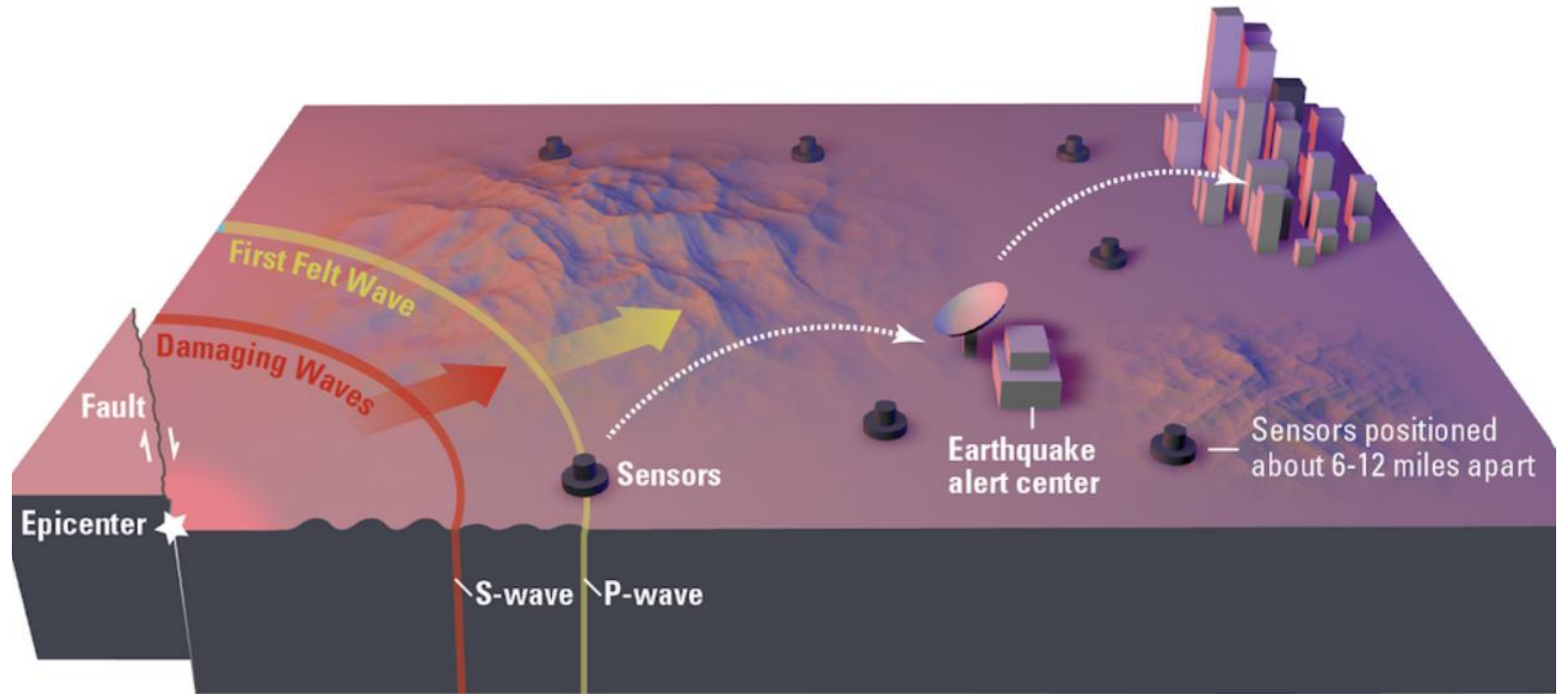
Large Hardon Collider



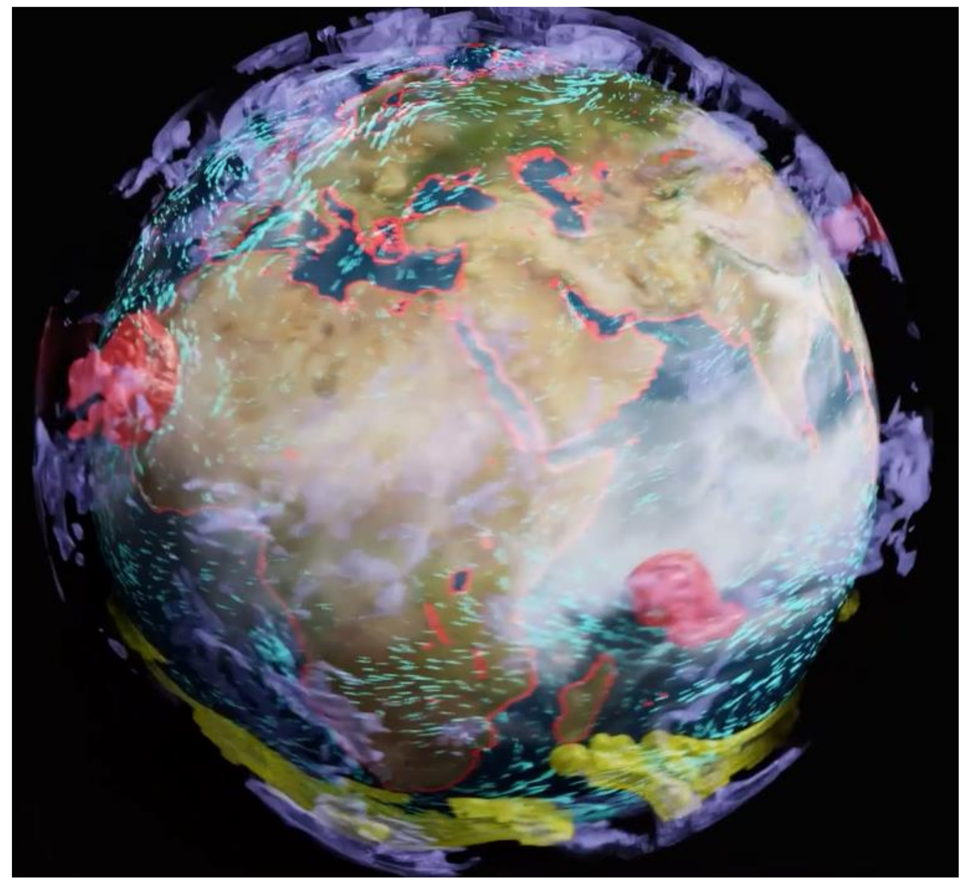
Genome Scale LLMs for Covid



Real Time Multi-Messenger Astrophysics



Earthquake Model with Machine Learning

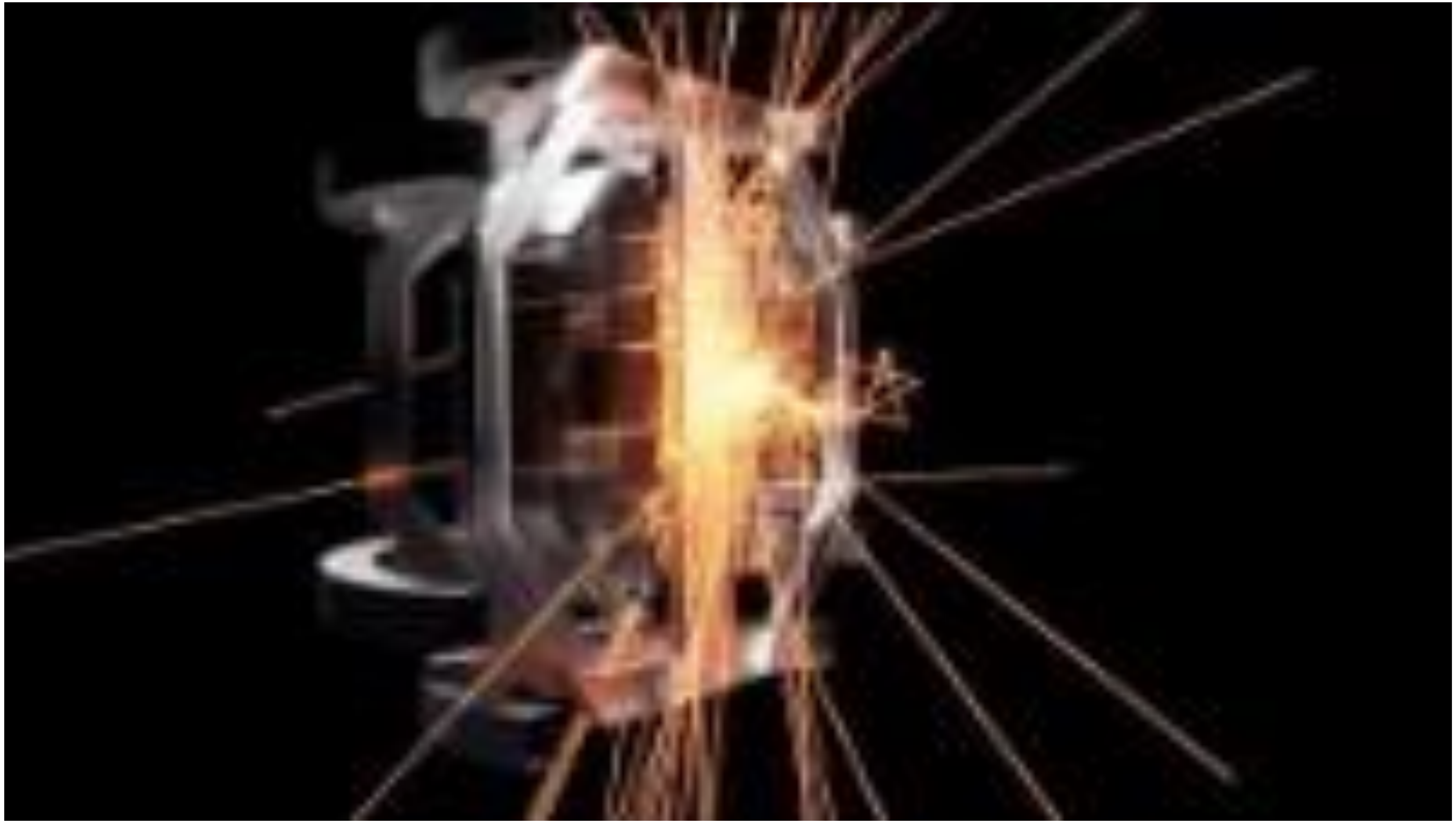


Destination Earth

NVIDIA

FUSION DIGITAL TWIN WITH CONVENTIONAL SIMULATION

https://www.youtube.com/watch?v=tJgR1TSBD0k

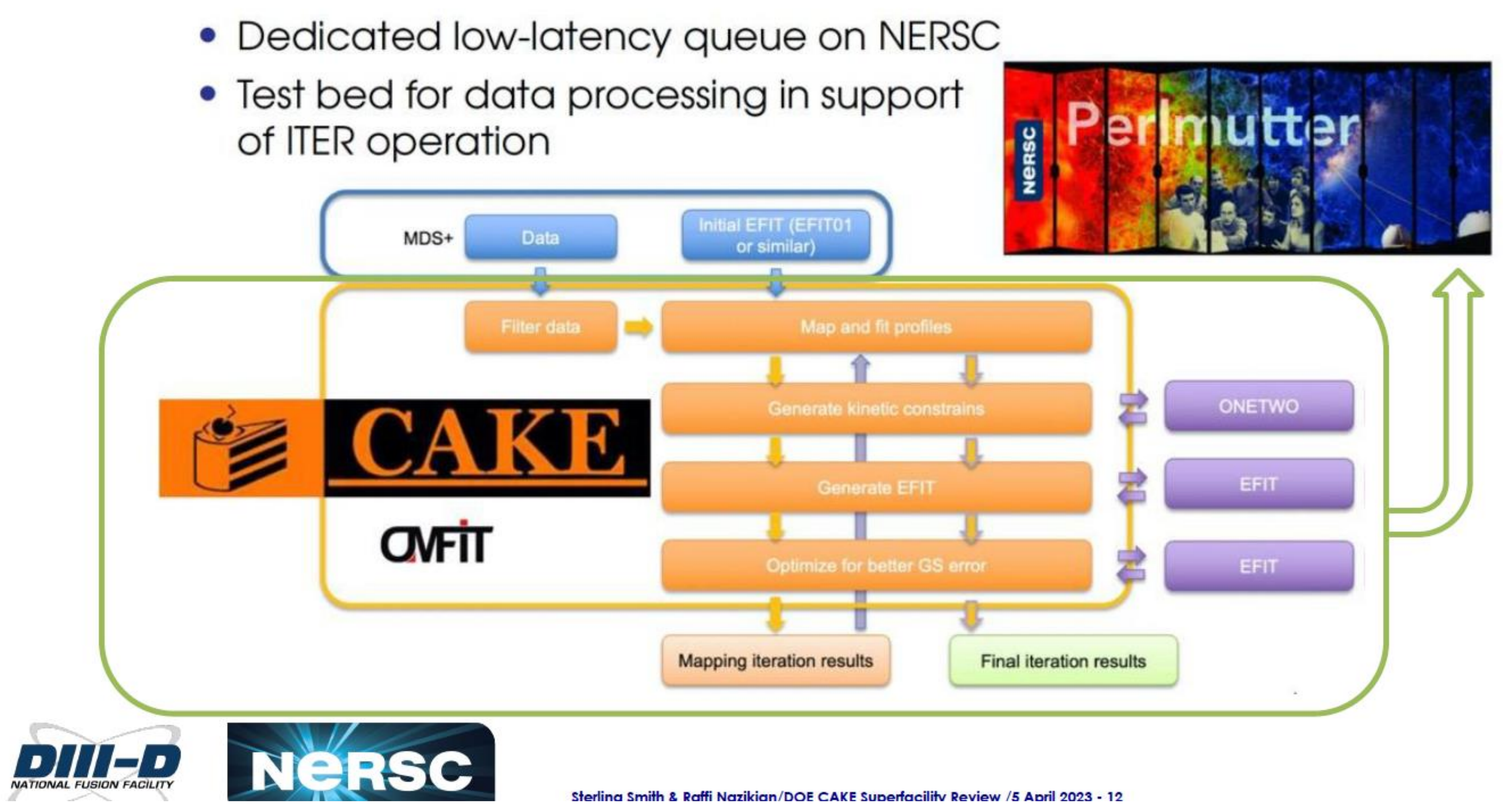


FUSION DIGITAL TWIN WORKFLOW WITH SGTC SURROGATE

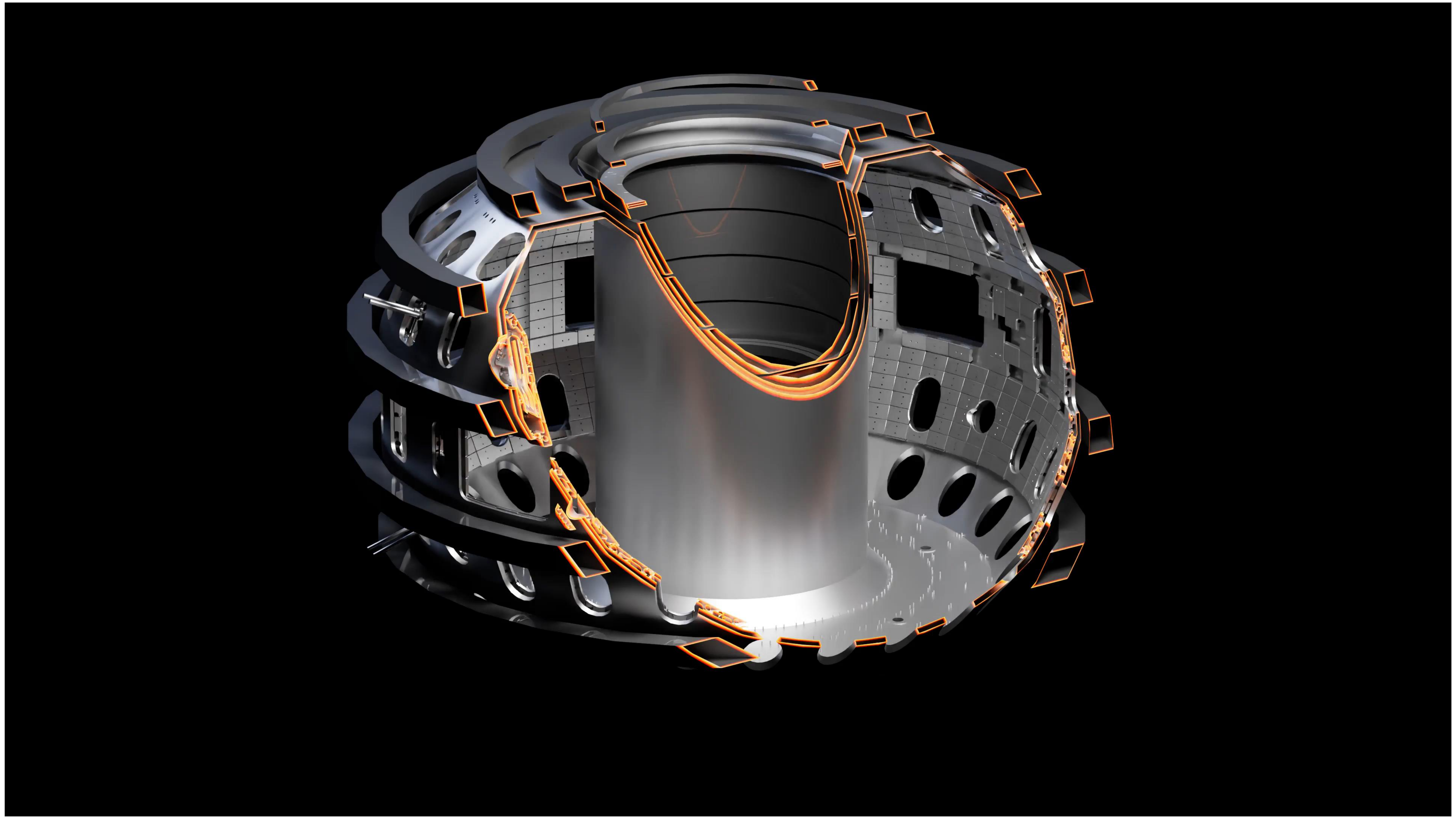
File-Based Prototype

SUPERFACILITY WITH NERSC AND GA DIII-D FUSION REACTOR

Couple EFIT Simulation with Experiment operation

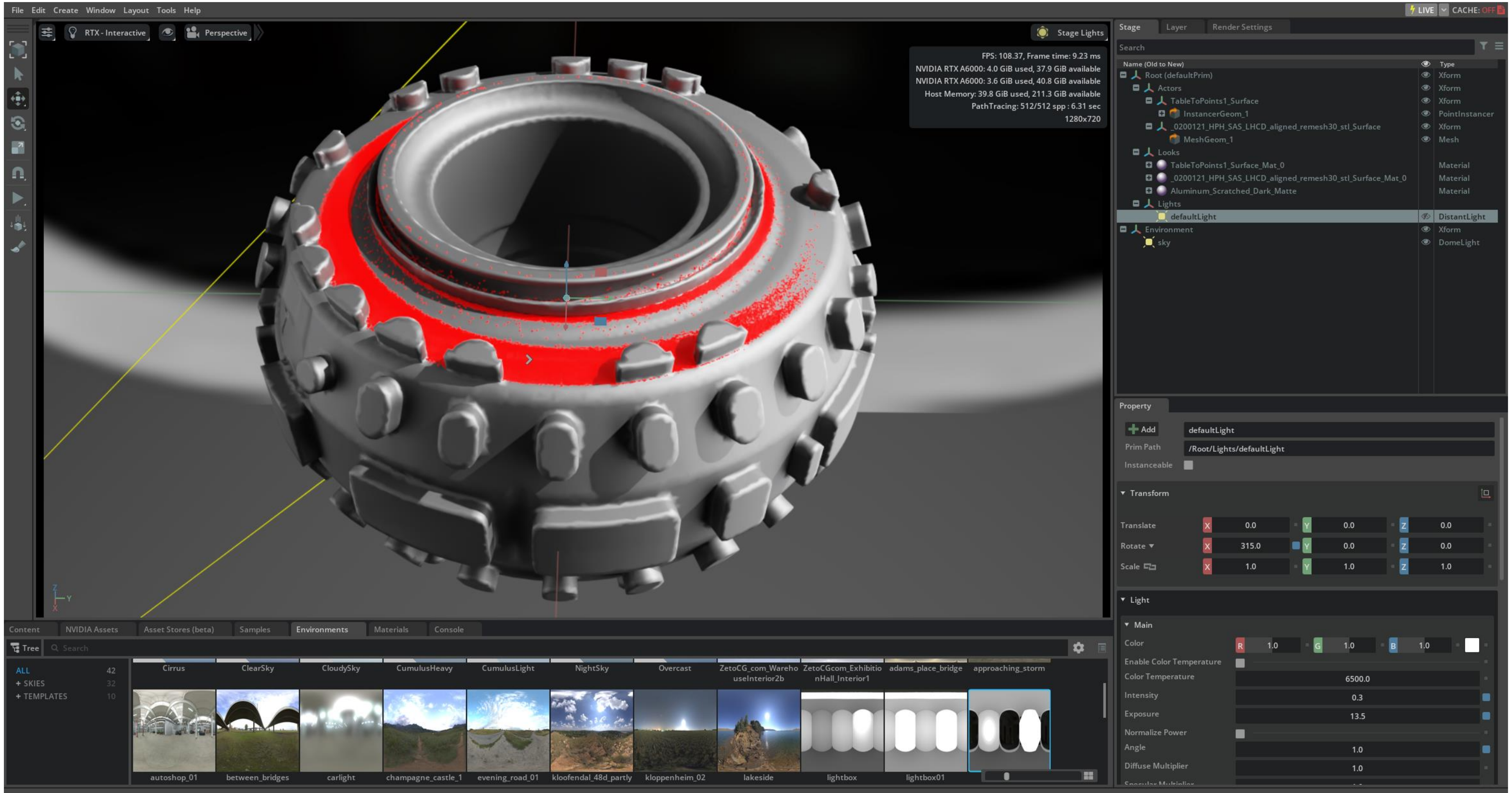


Current Conventional Model with the Twin



GA Ion Orbiter DIII-D Vacuum Vessel Impacts Postprocessing/Reprojection pipeline -> ParaView

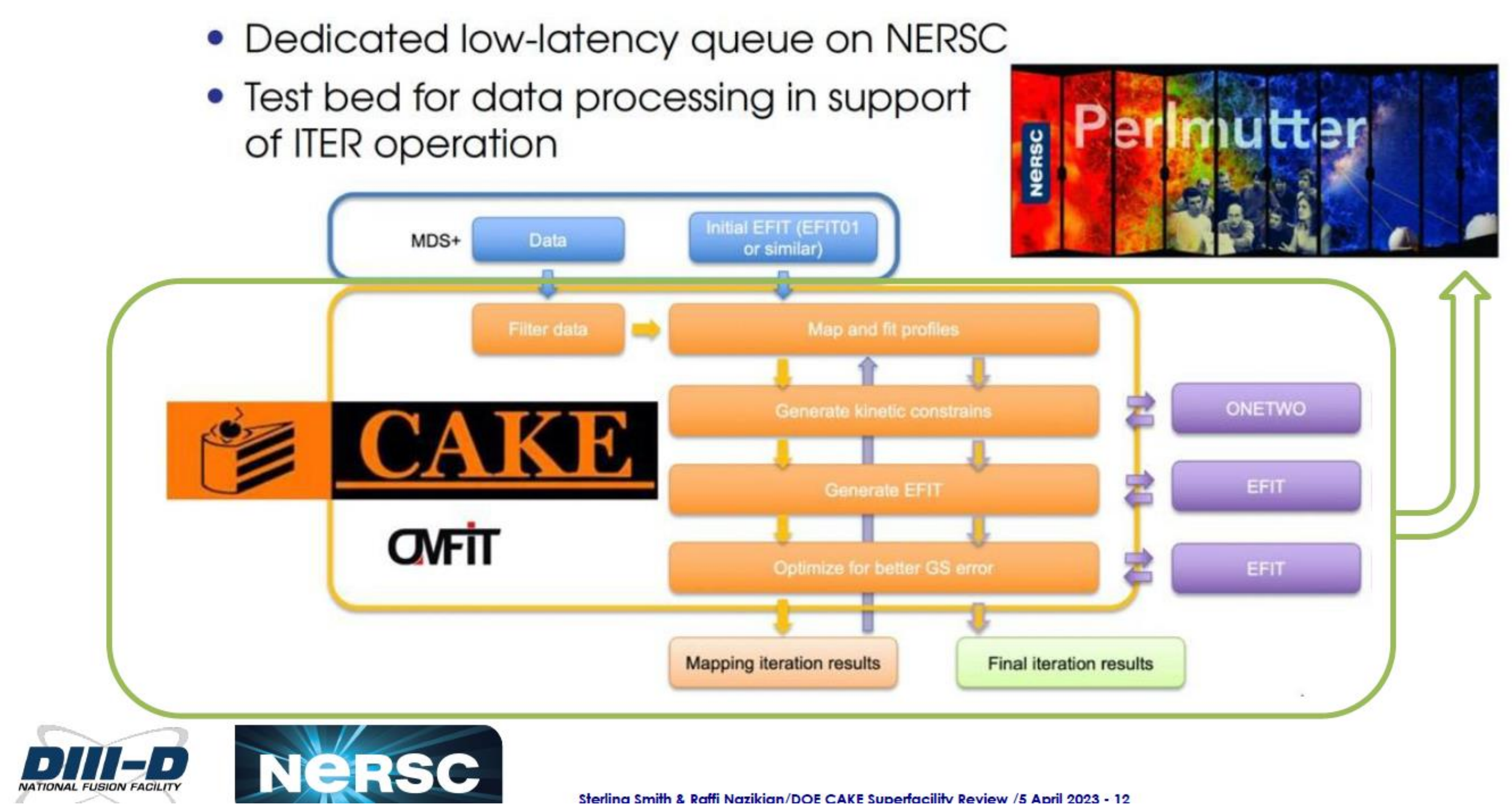
GA Ion Orbiter DIII-D Vacuum Vessel Impacts
Postprocessing pipeline -> ParaView -> Omniverse

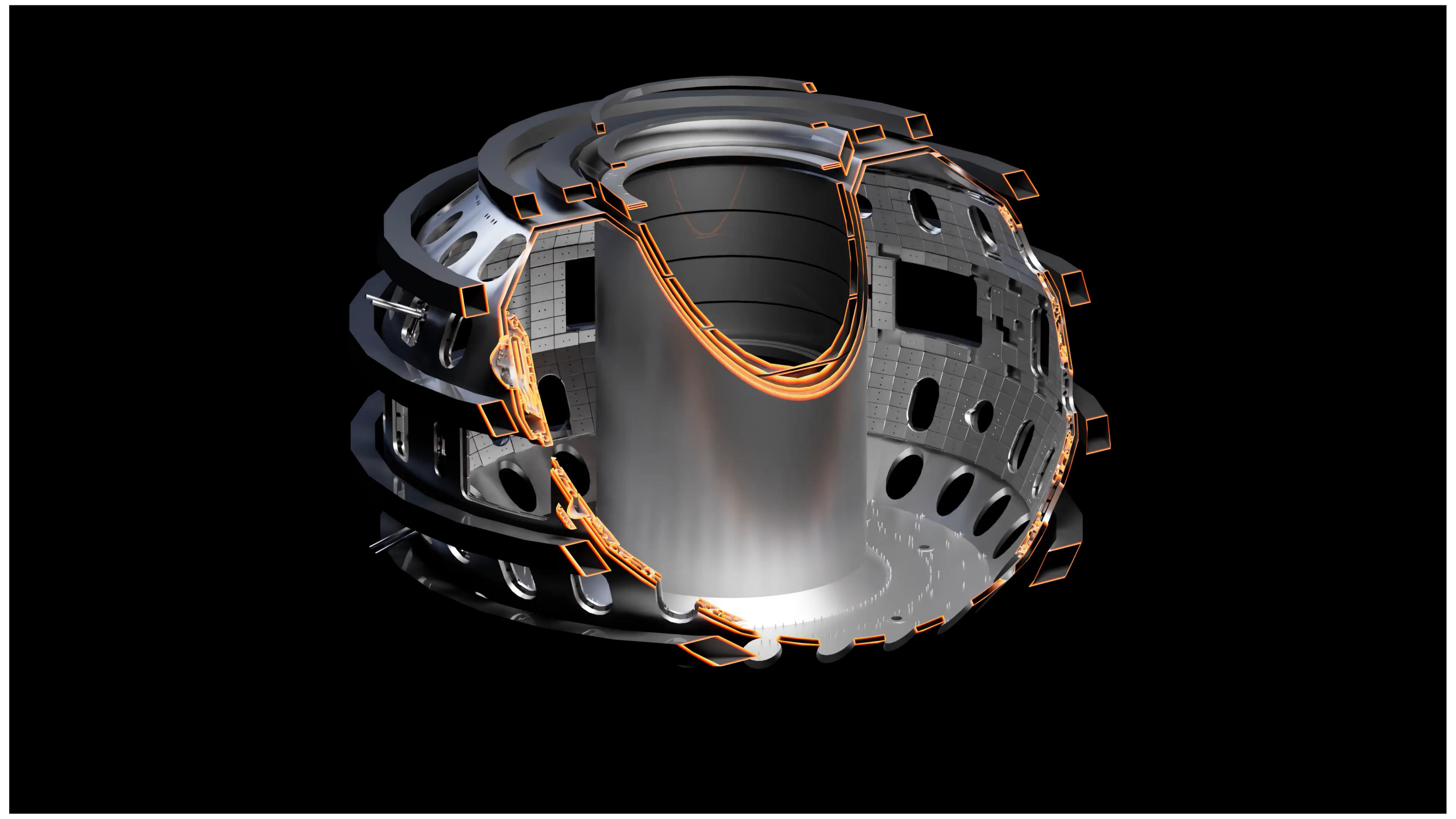


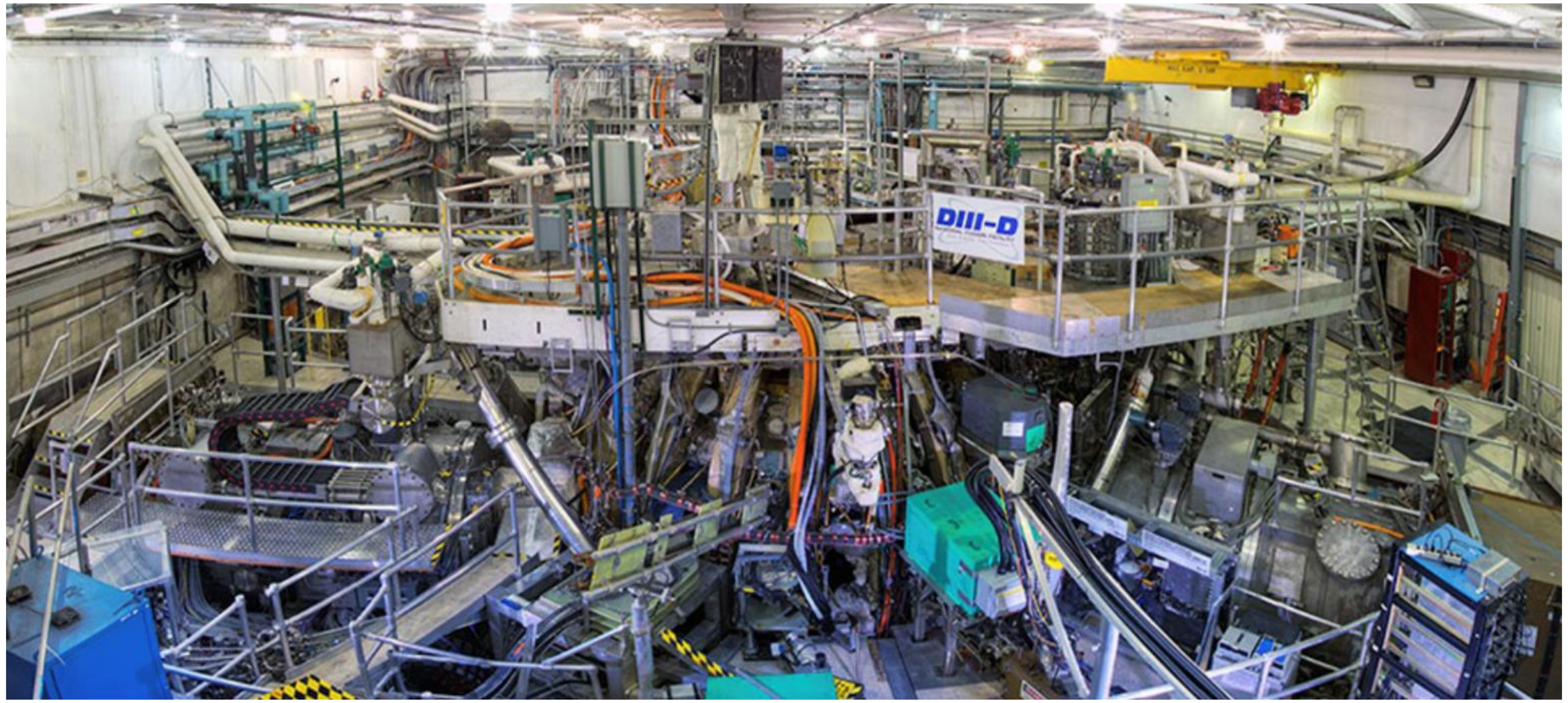
GA Ion Orbiter DIII-D Vacuum Vessel Impacts

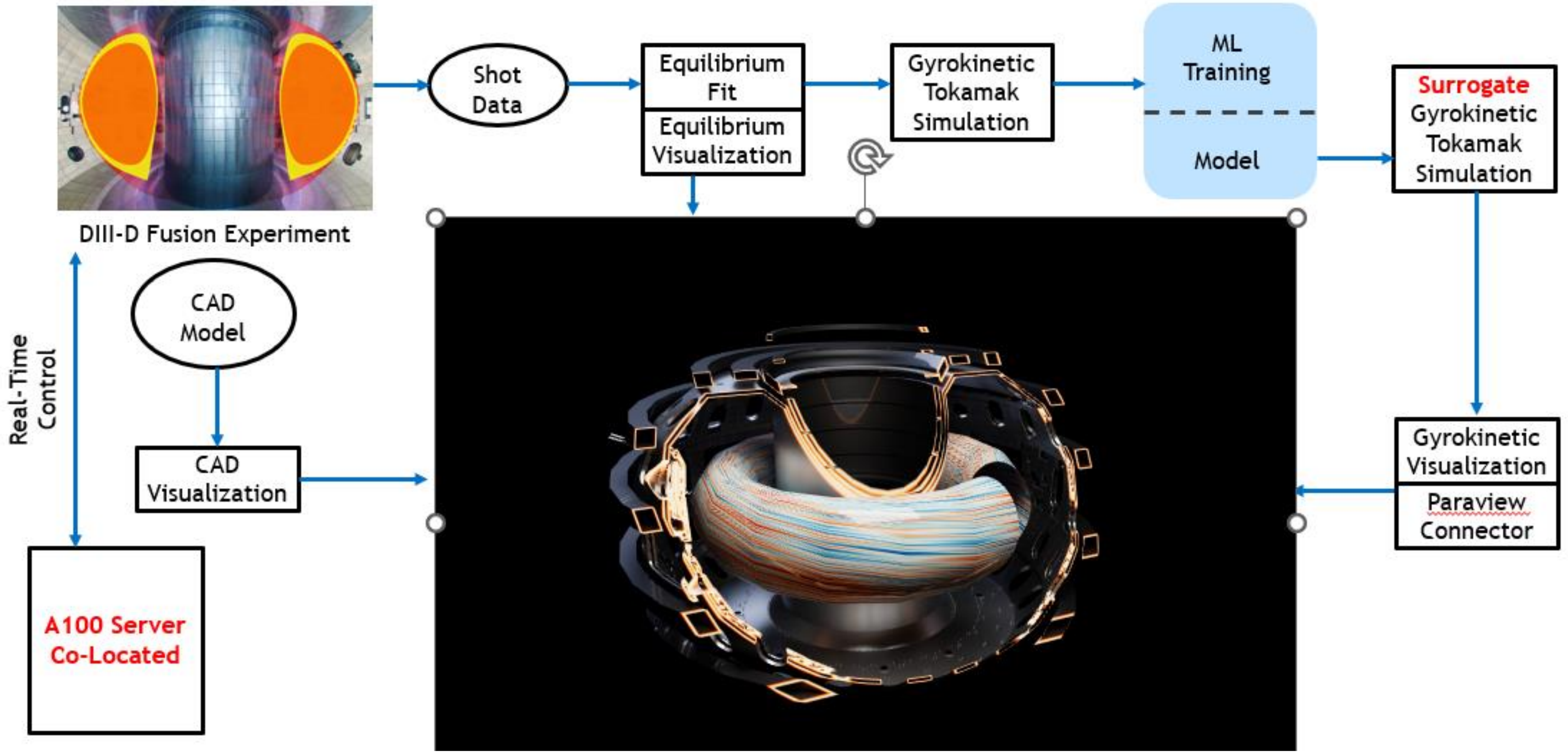
GA Ion Orbiter DIII-D Vacuum Vessel Impacts

GA PLAN:
DIGITAL TWIN ENABLED CONTROL ROOM



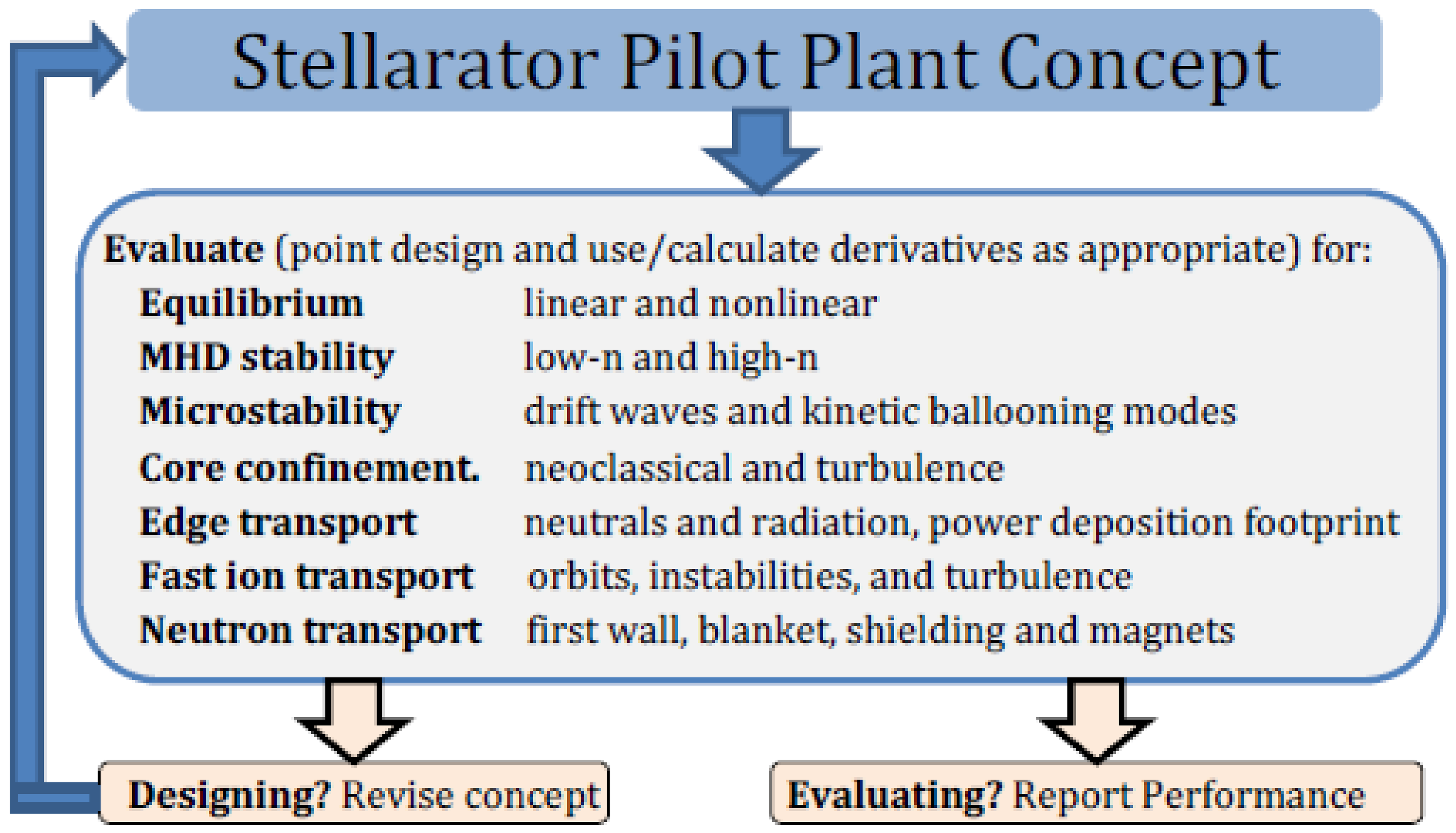






CONVERGED WORKFLOW FOR GYROKINETIC FUSION

Current StellFoundary Project Funded by DOE SCIDAC 2924 in 2023



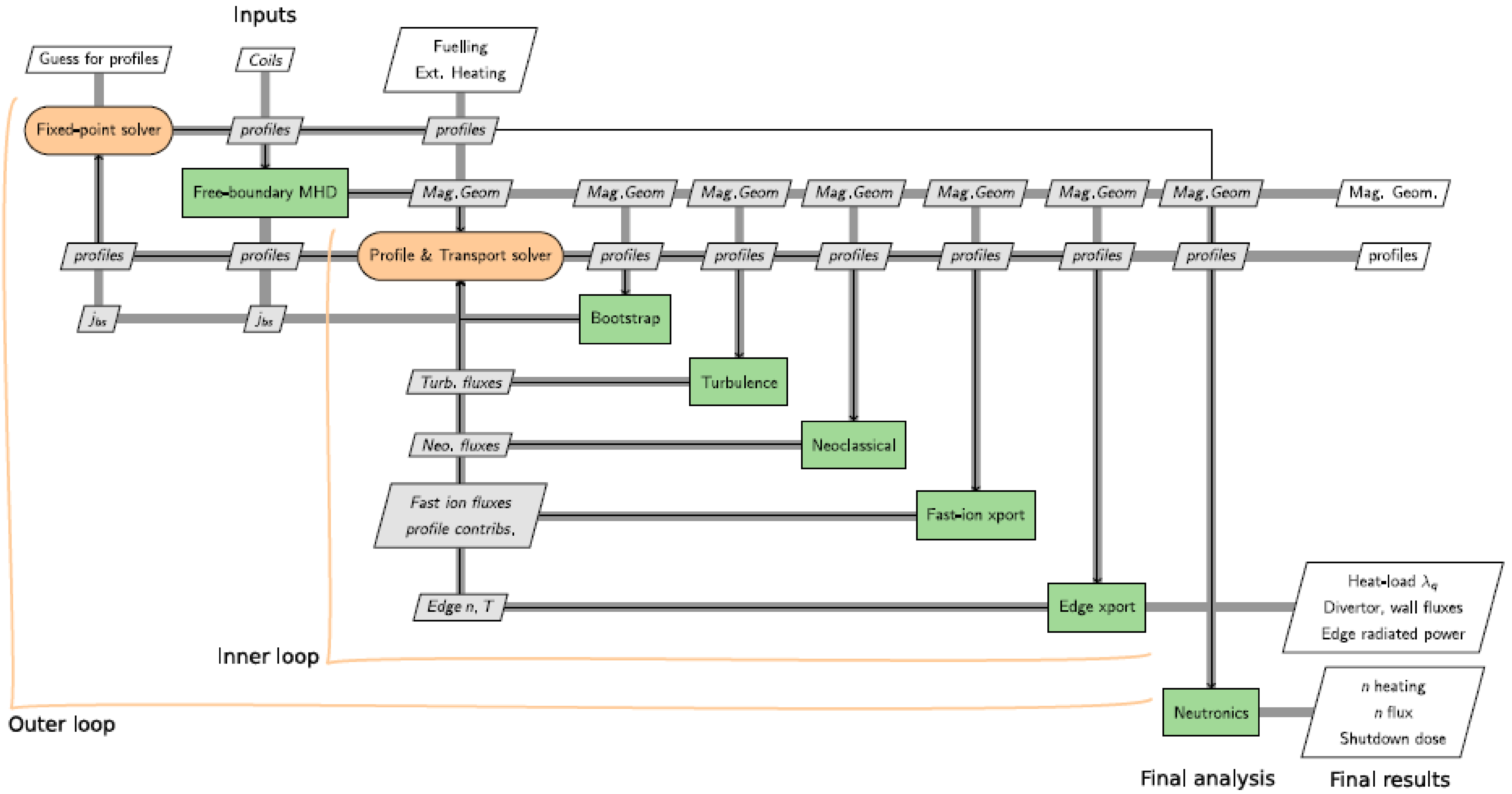
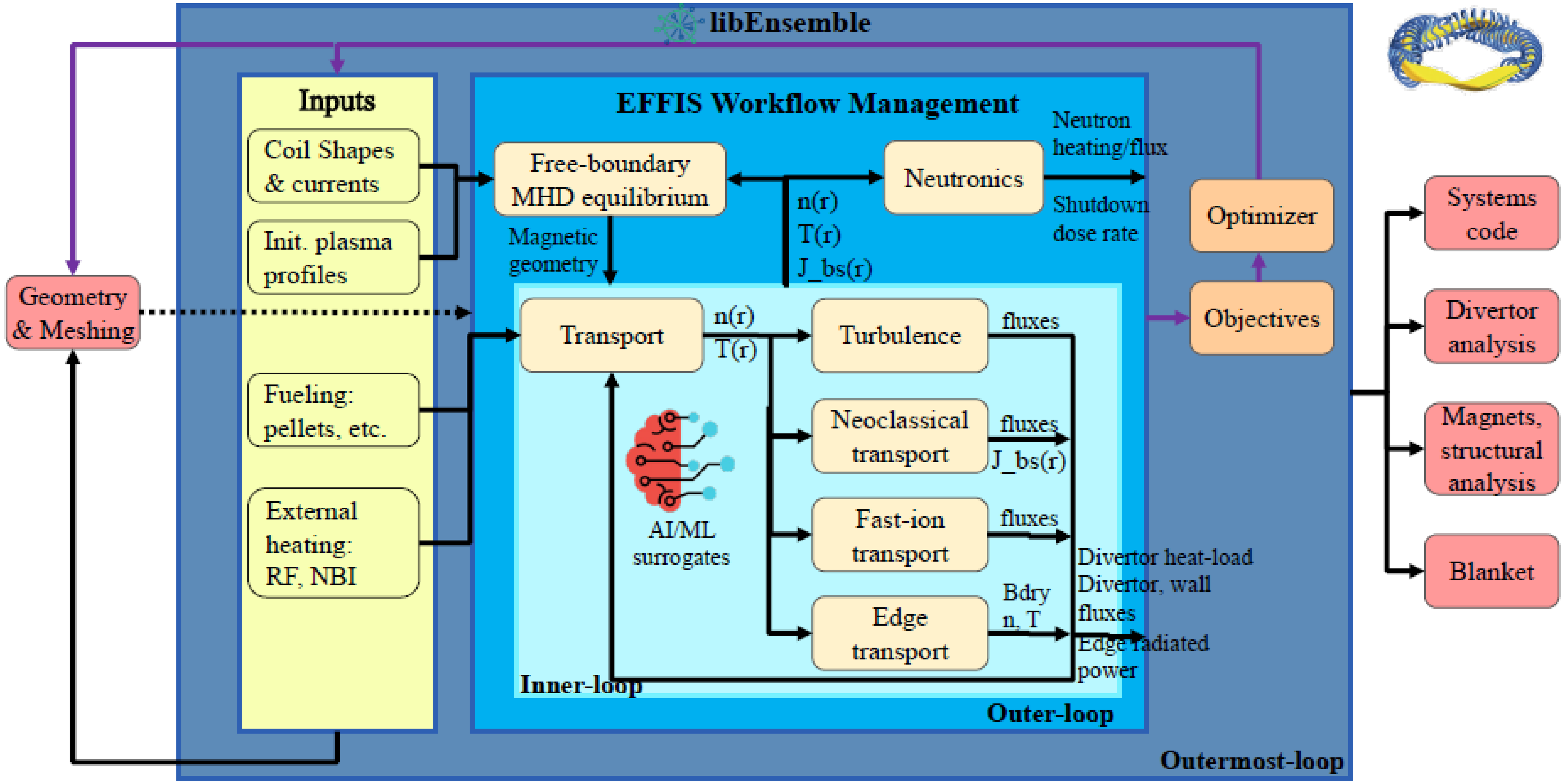
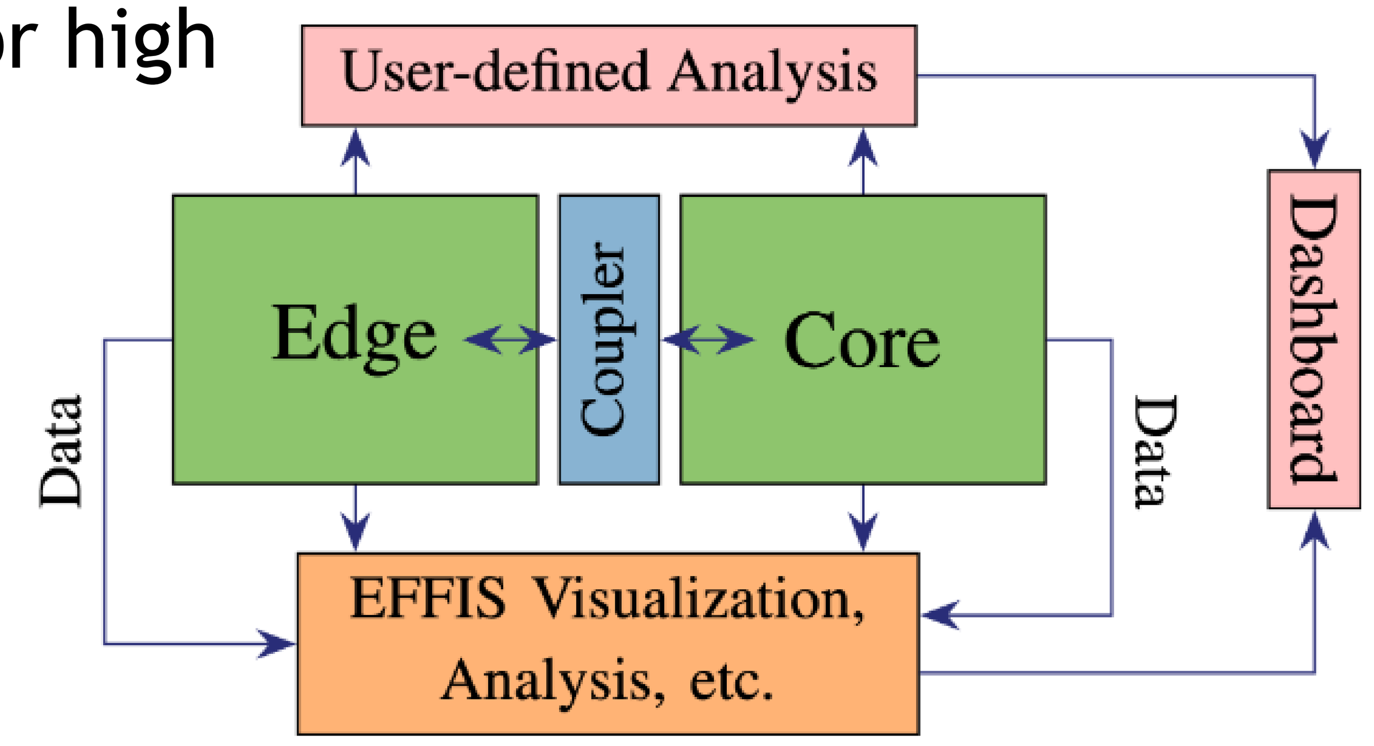


Figure 3: Example workflow for computing self-consistent plasma state. Green rectangles on the diagonal indicate the physics calculations, while the off-diagonal parallelograms show the data passed between codes.



Exascale Framework for high Fidelity Simulation



ALGORITHMS EVOLVING AT UNPRECEDENTED PACE

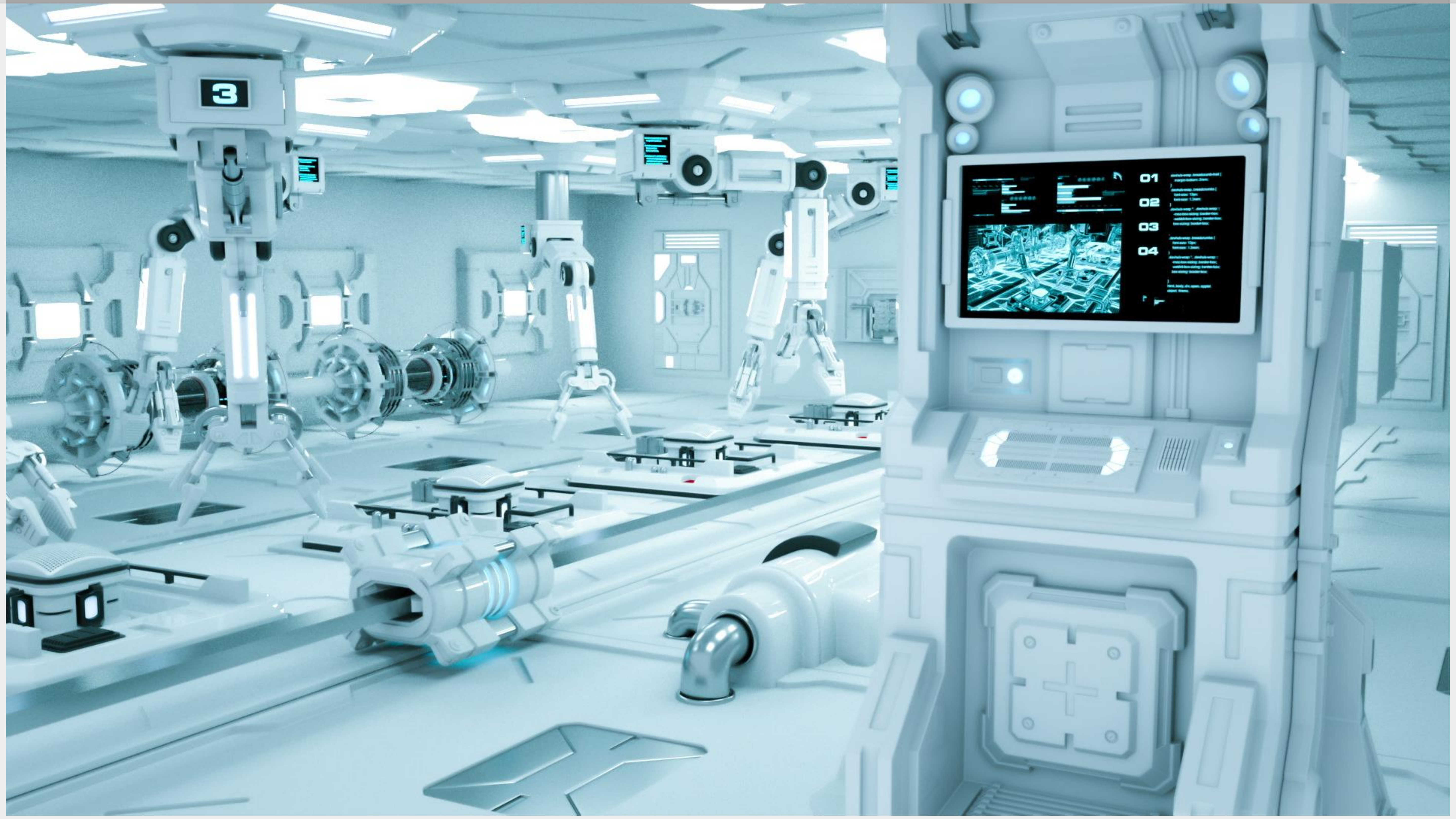
DIGITAL TWIN WITH EARTH2

https://www.youtube.com/watch?v=8cQoYcbUG_M

Our Vision: Smart “Factory” for Probing & Designing Complex Biological Systems

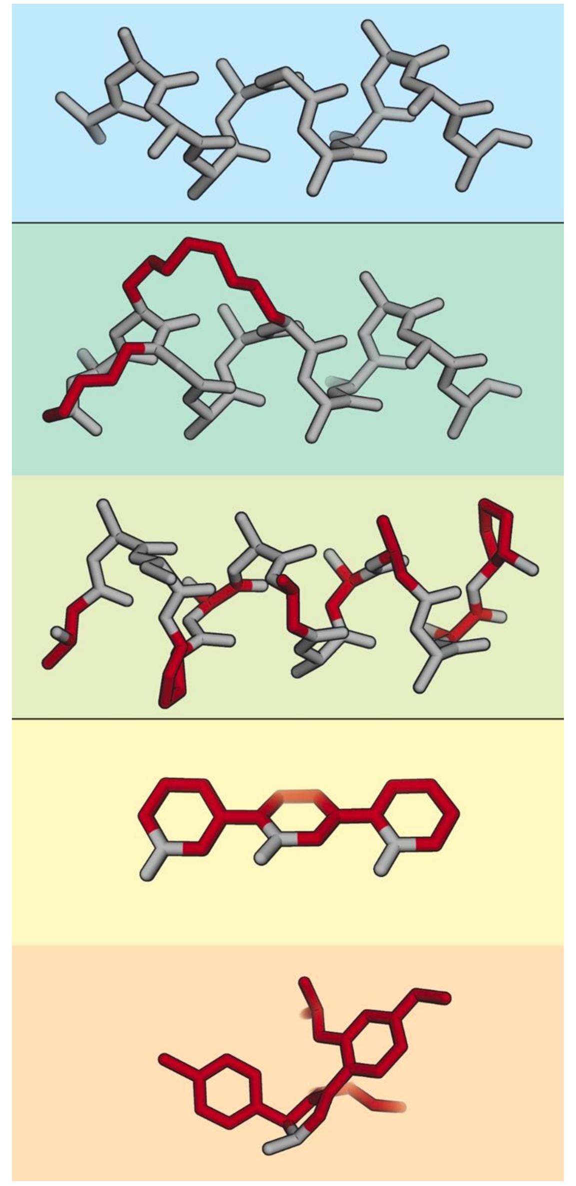
- Accelerate the discovery process
- Elevate human creativity to higher level goals
- Democratize biological systems design approaches
- Unbiased data collection and evaluation

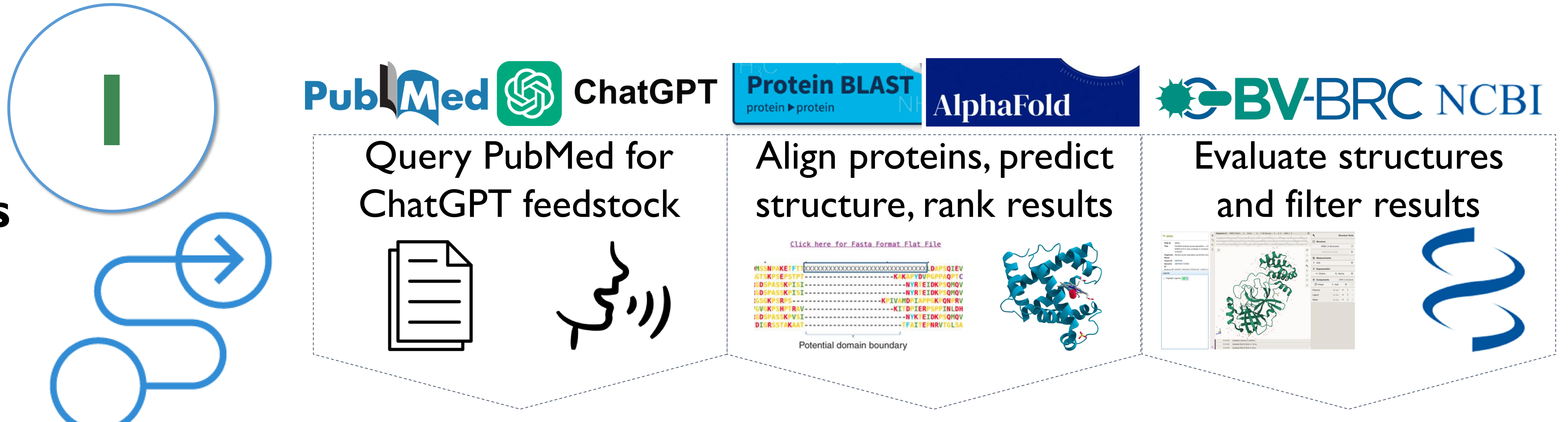
ARTIFICIAL INTELLIGENCE
GUIDED, ROBOTICALLY EXECUTED EXPERIMENTS



Link AI driven workflow with self-driving laboratory

Set of peptides as input

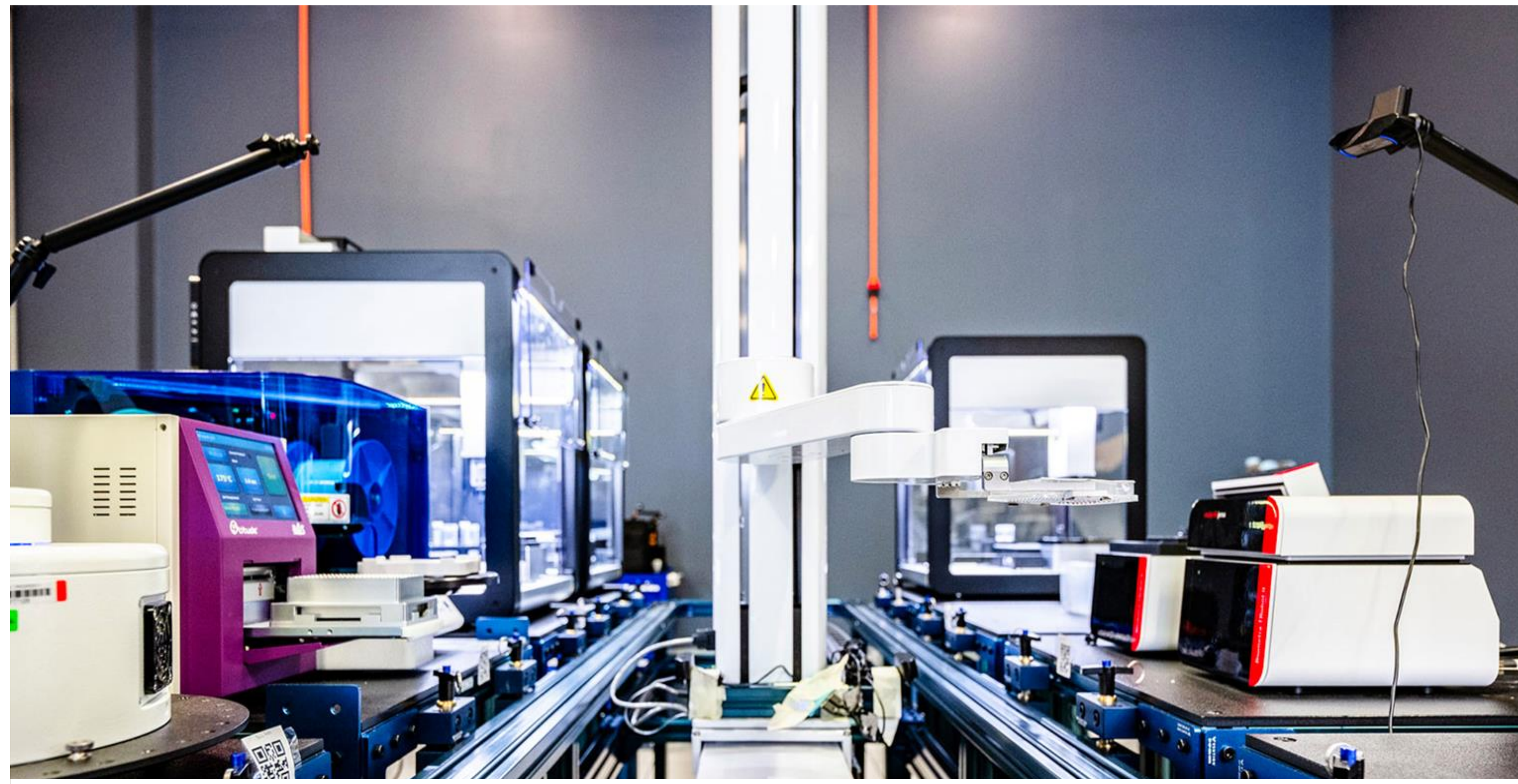




Agents run on HPC/AI resources

Candidates for experimental evaluation

2



3

Self-driving lab performs experiments

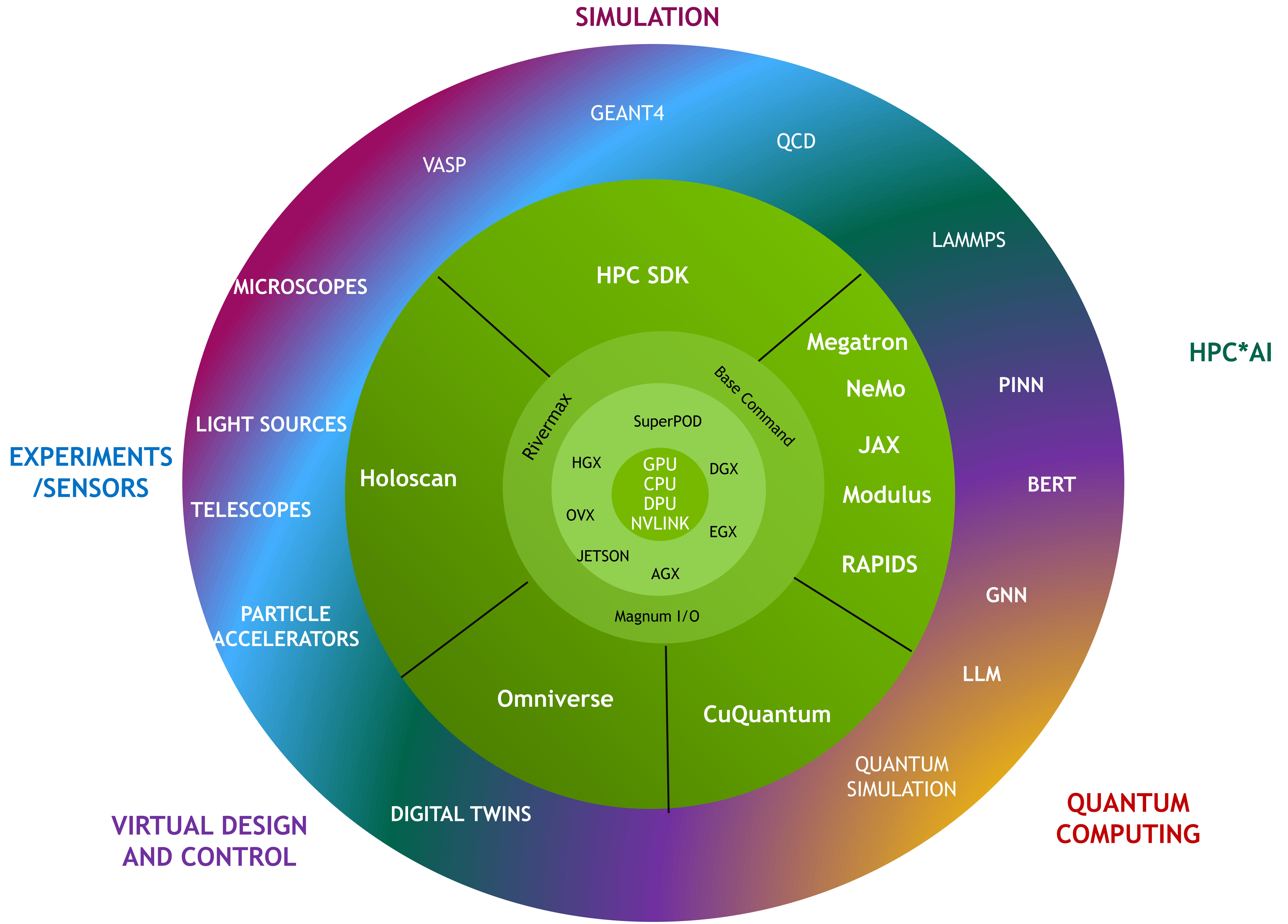
Courtesy: Ian Foster, ANL/ UChicago

Embodied Agent for Automated Lab Code Generation

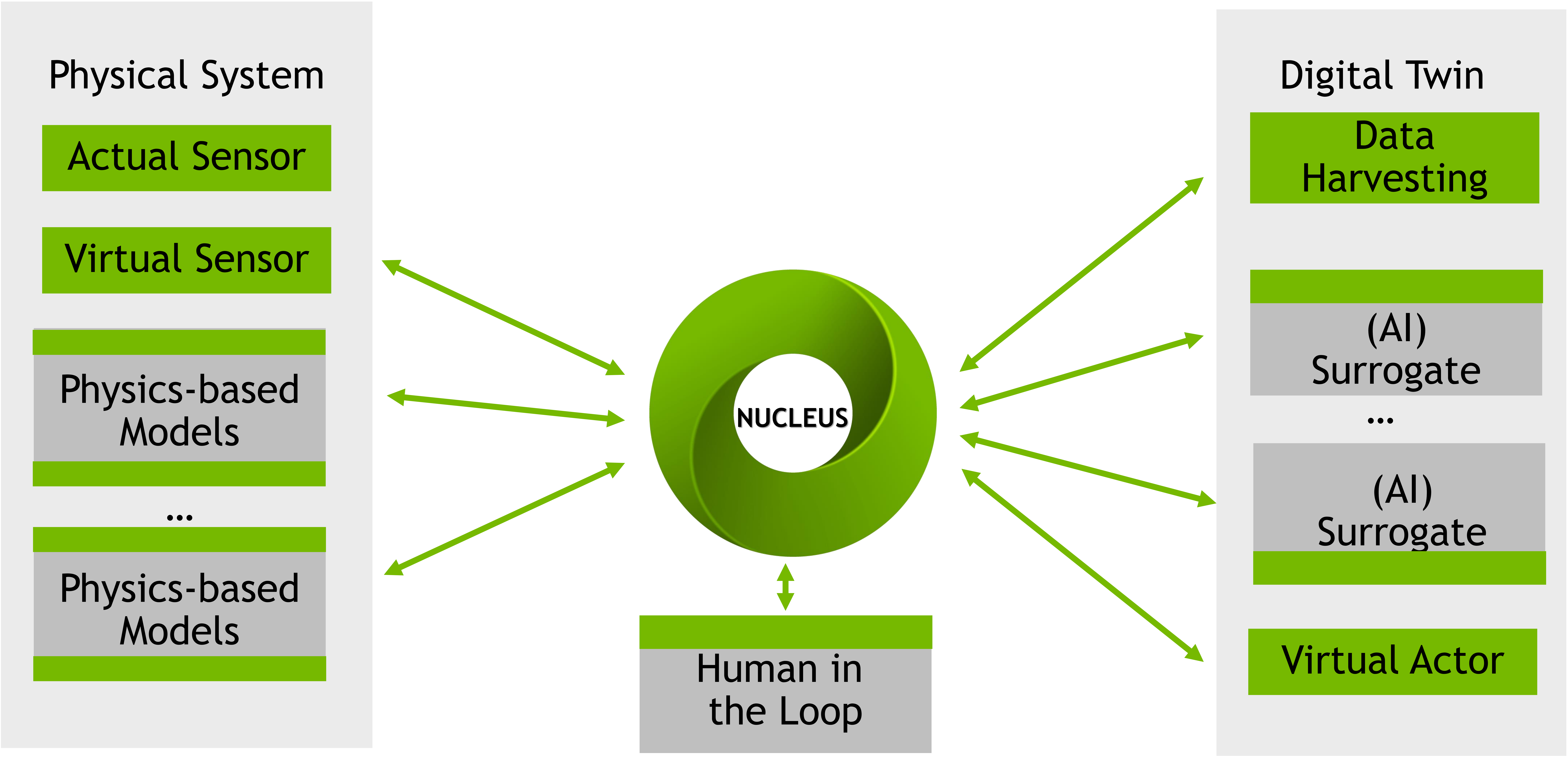
Feedback to define additional experiments


Omniverse: WebRTC Livestream Player
File Edit Create Window Tools Replicator Isaac Examples Isaac Utils Profiler Streaming Layout Help
LIVE
CACHE: ON
Viewport
RTX - Real-Time
Perspective
Stage Lights
Content
Console
Samples
Flow
Isaac Assets (Beta)
Materials
Finished initializing
Stop

NVIDIA PLATFORM EVOLVING TO MEET THE CHALLENGE



OMNIVERSE: PLATFORM FOR BUILDING DIGITAL TWINS



ADVANCED TOOLS AND TECHNOLOGIES

Foundational Platform Components

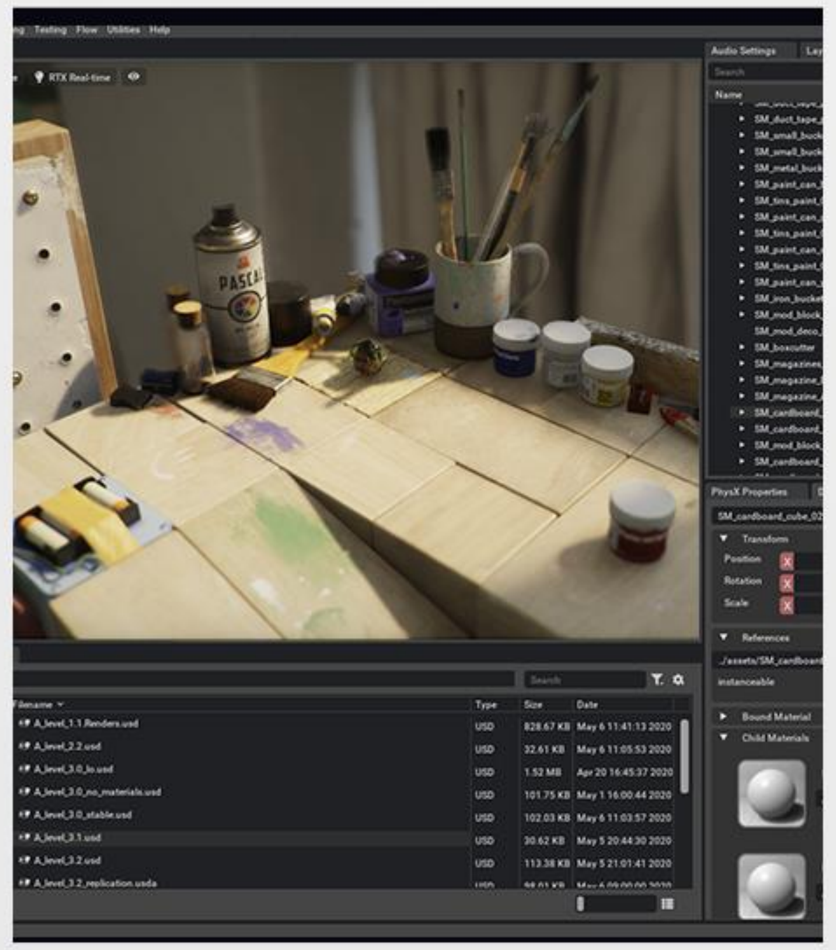
NUCLEUS

Source of truth

CONNECT

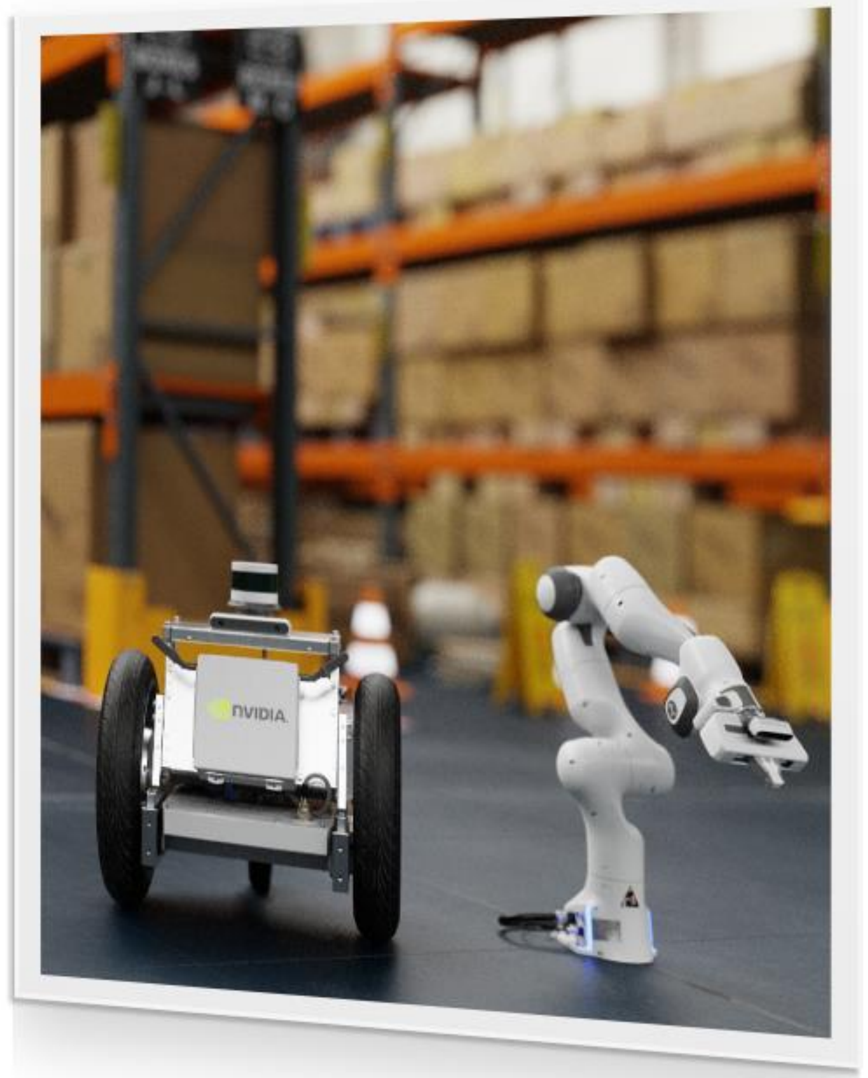
Coupling

KIT



Application API
User experience

SIMULATION



Virtual Actor

RTX RENDERER

Virtual Sensor

USD

NVIDIA

DATA AGGREGATION AND COORDINATION VIA USD

NVIDIA OMNIVERSE™

USD

UNIVERSAL SCENE DESCRIPTION

The “HTML” of 3D Virtual Worlds

- Developed by Pixar
- Foundation for NVIDIA Omniverse
- Open-sourced API and file framework for complex scene graphs
- Easily extensible, simplifies interchange of assets between industry software
- Introduces novel concept of layering
- Enables simultaneous collaboration for large teams in different department working on the same scene
- Originated in M&E, now becoming a standard across industries including AEC, Manufacturing, Product Design, Robotics

BACKUP

EXAMPLE OF DIGITAL TWIN FOR ASTROPHYSICS

Moonwalker Digital Twin of the South Pole of The Moon

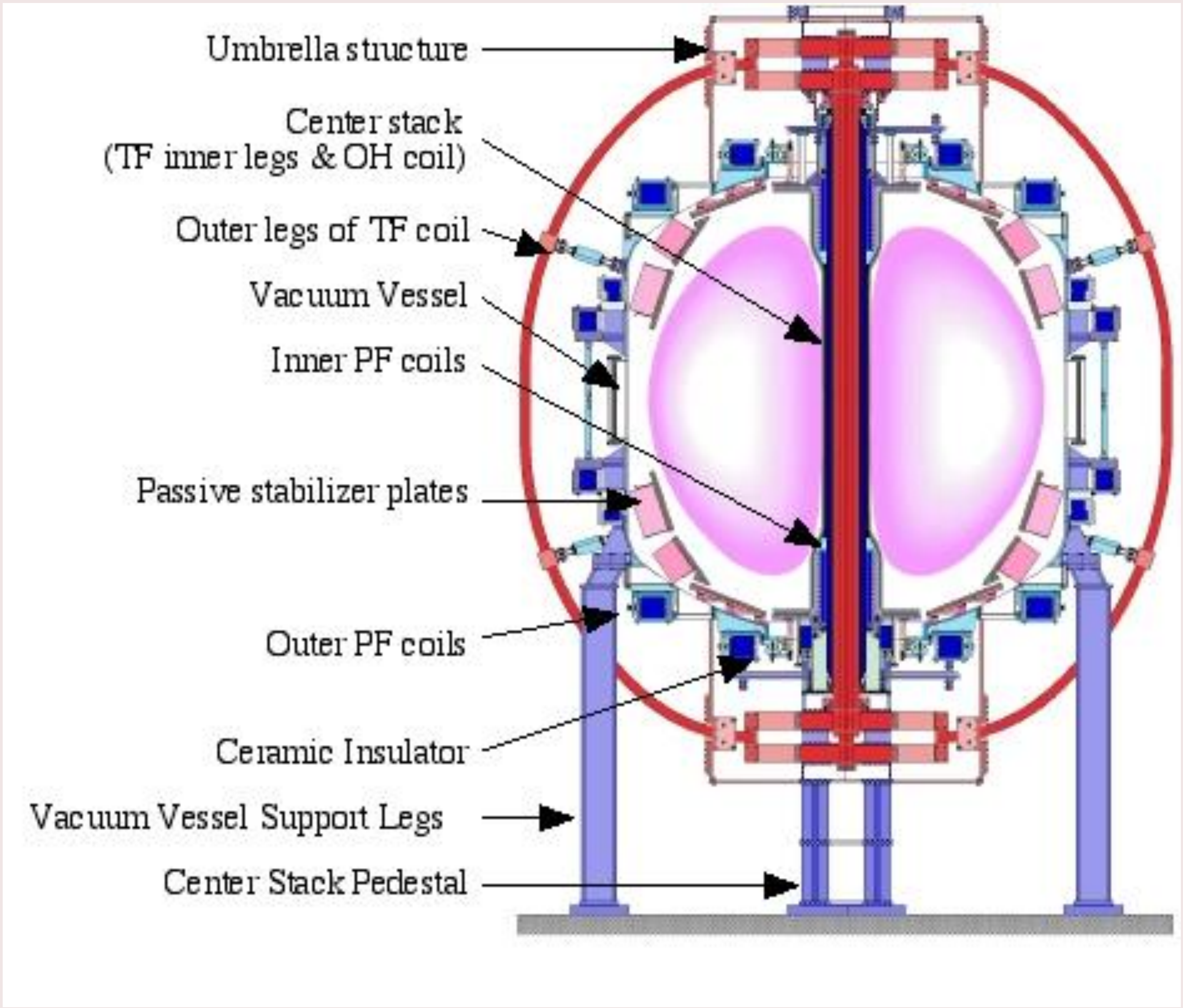
https://www.youtube.com/watch?v=E0Rz0ZbwhJY

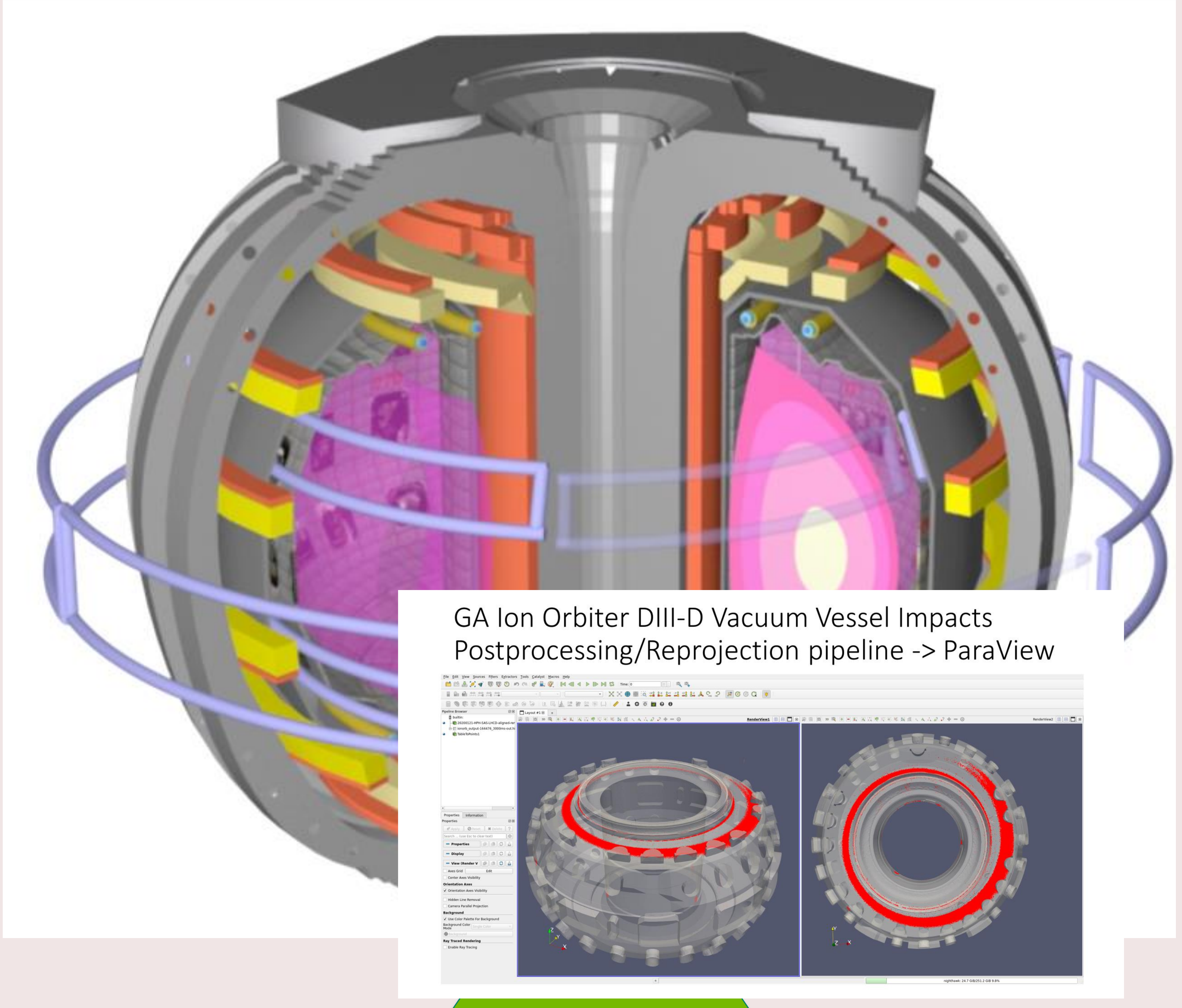
SUPERFACILITY WITH GA AND NERSC/ANL: VISION FOR FUTURE

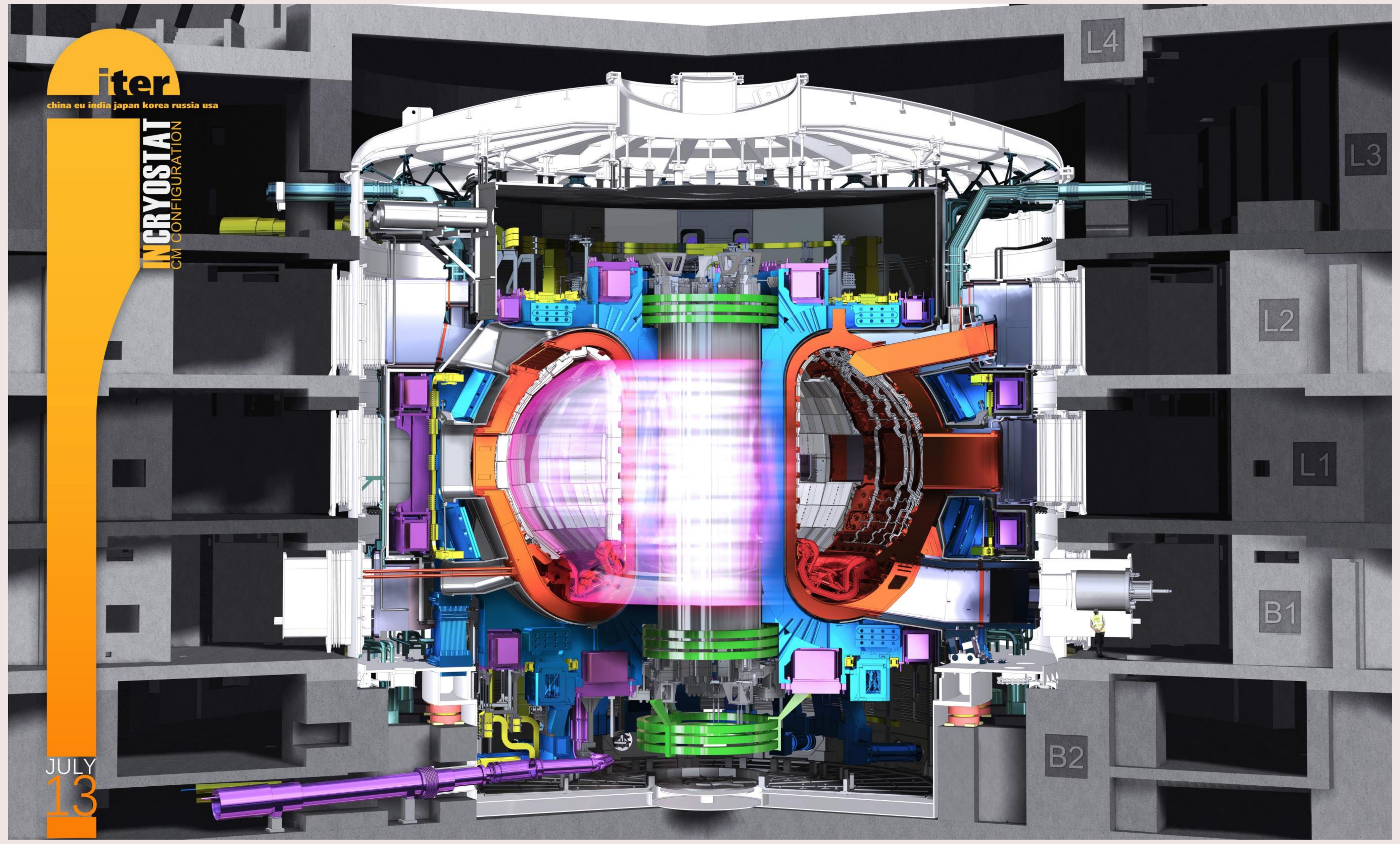
NSTX-U

DIII-D National Fusion Facility

ITER





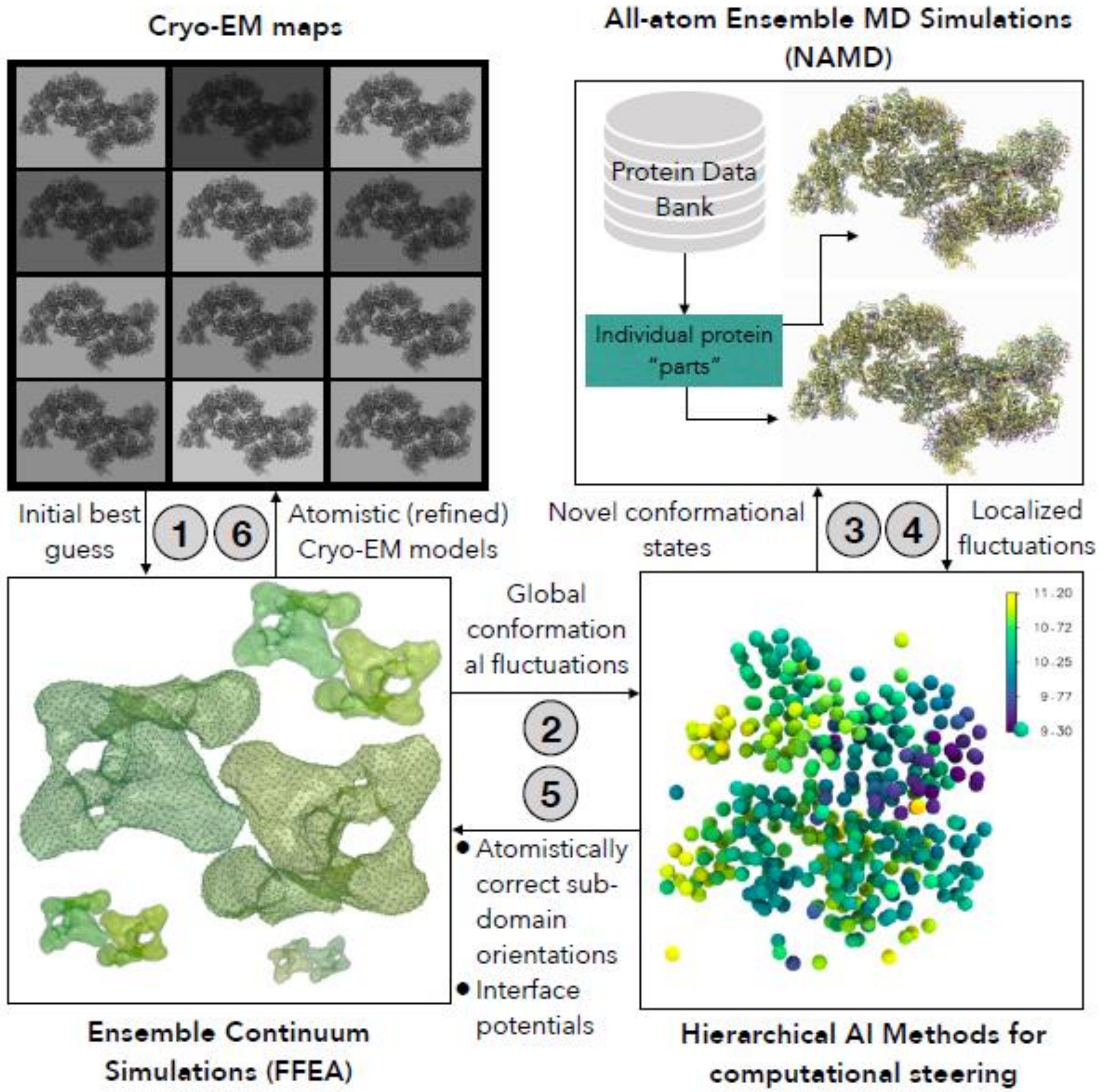


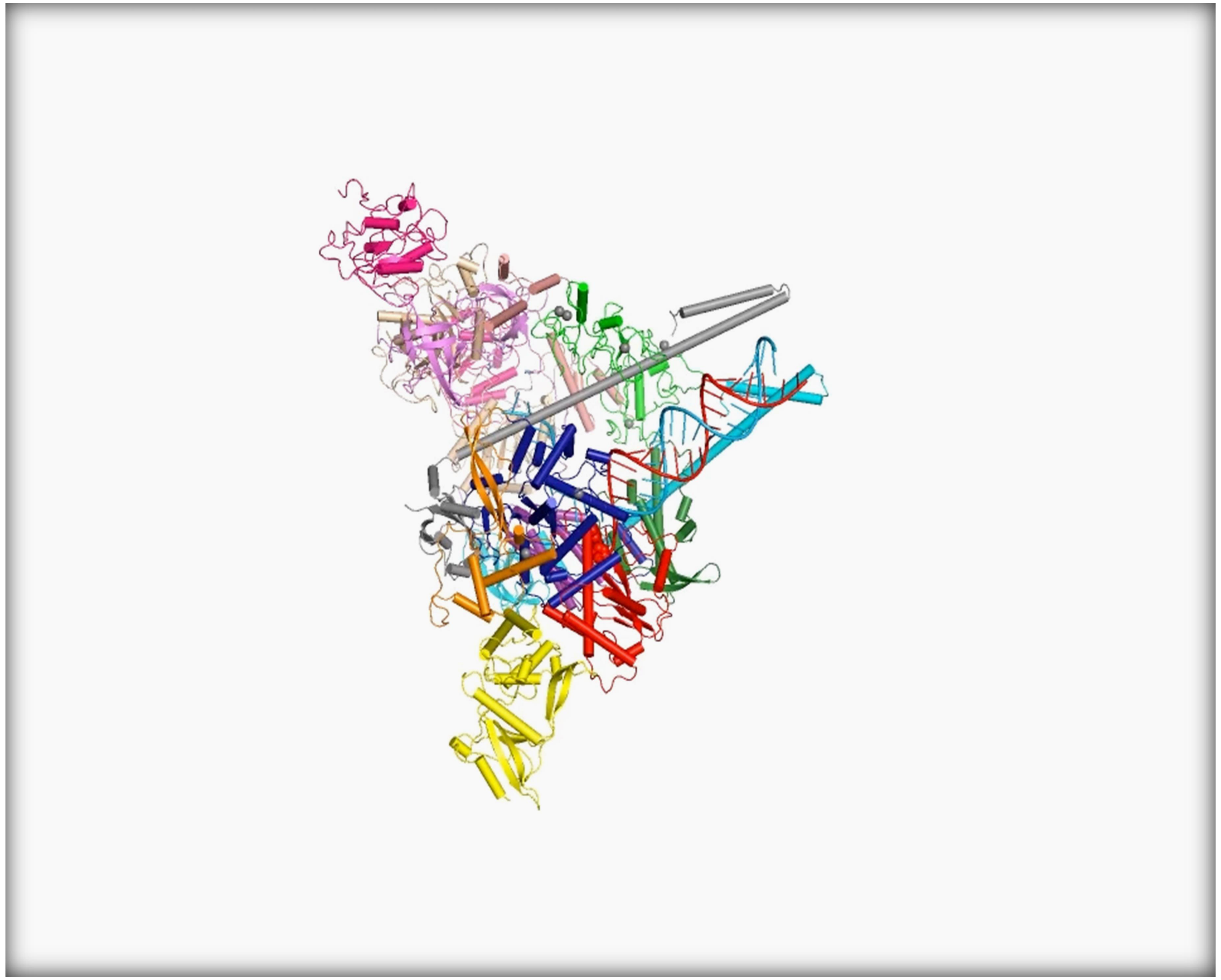
FUTURE POST Exascale

Using foundation models to predict SARS-CoV-2 evolution

- Periodically retrain on new variants sequenced across specific time window
- Performance: CS-2, Selene, Polaris

Science goal: Understand how to "trap" the SARS-CoV-2 replication-transcription complex (RTC) using Low Res CryoEM





GenSLMs finetuned on SARS-CoV-2 genomes can distinguish variants