Exascale Computing : The Coming Integration of Simulation, Data and Machine Learning

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Argonne National Laboratory
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Crescat scientia; vita excolatur

Rick Stevens

Position: Associate Laboratory Director for Computing, Environment and Life Sciences, Argonne National Laboratory and

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Research Background: Parallel Computing Software, Visualization, Automated Theorem Proving, Bioinformatics, Computer Architecture

Research Interests: Exascale Computing, Machine Learning for Medicine and Science, Neuroscience, Automation of Scientific Discovery

Personal Interests: Camping, Cooking, Drones, Politics, Philosophy, Natural History

THE UNIVERSITY OF CHICAGO

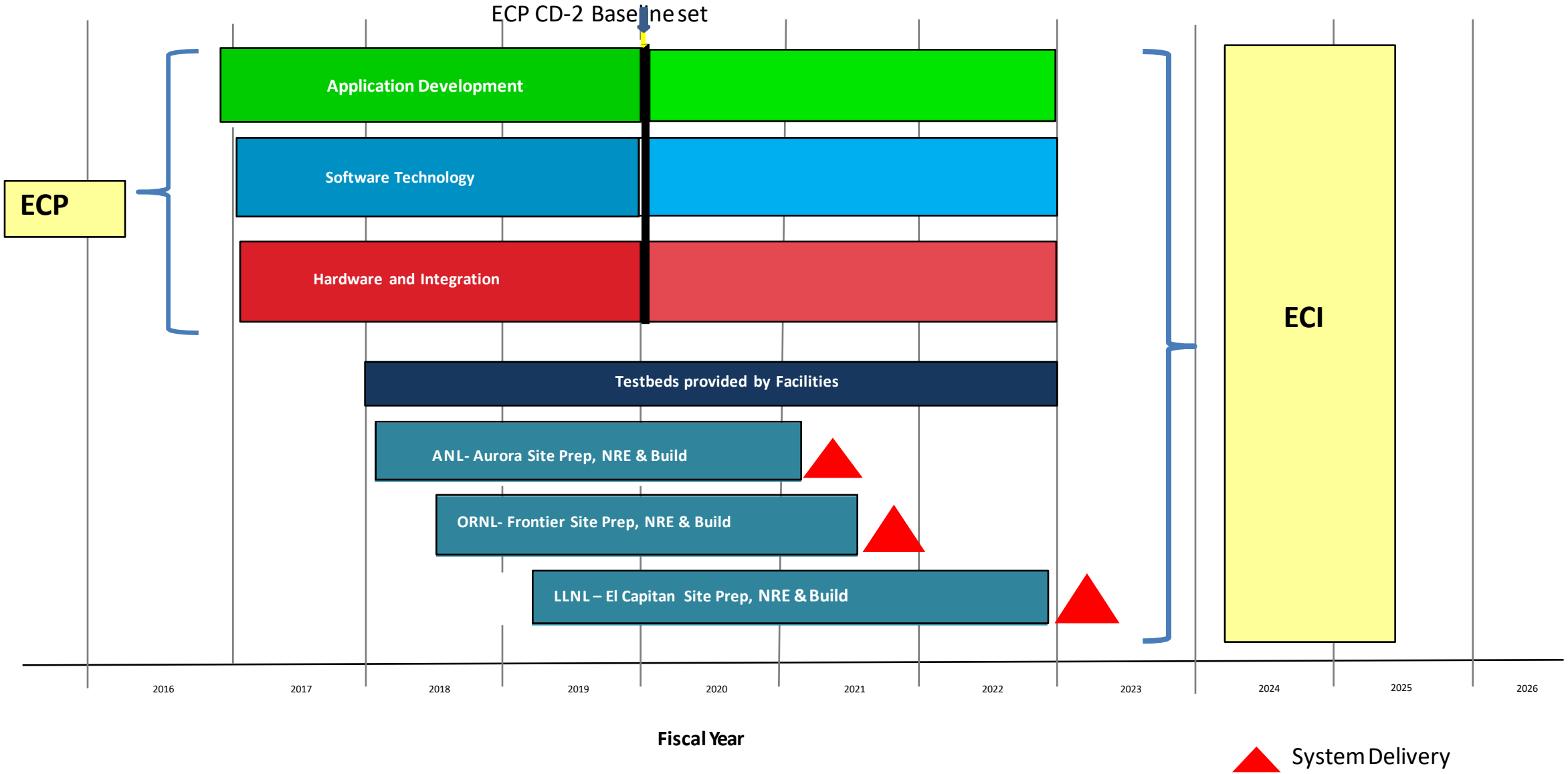
Argonne NATIONAL LABORATORY

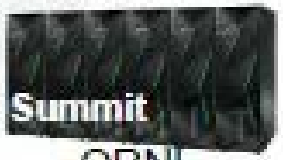
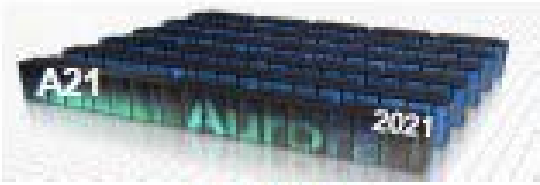
Aurora 2021 (A21) The first US Exascale System

Architecture supports three ways of computing

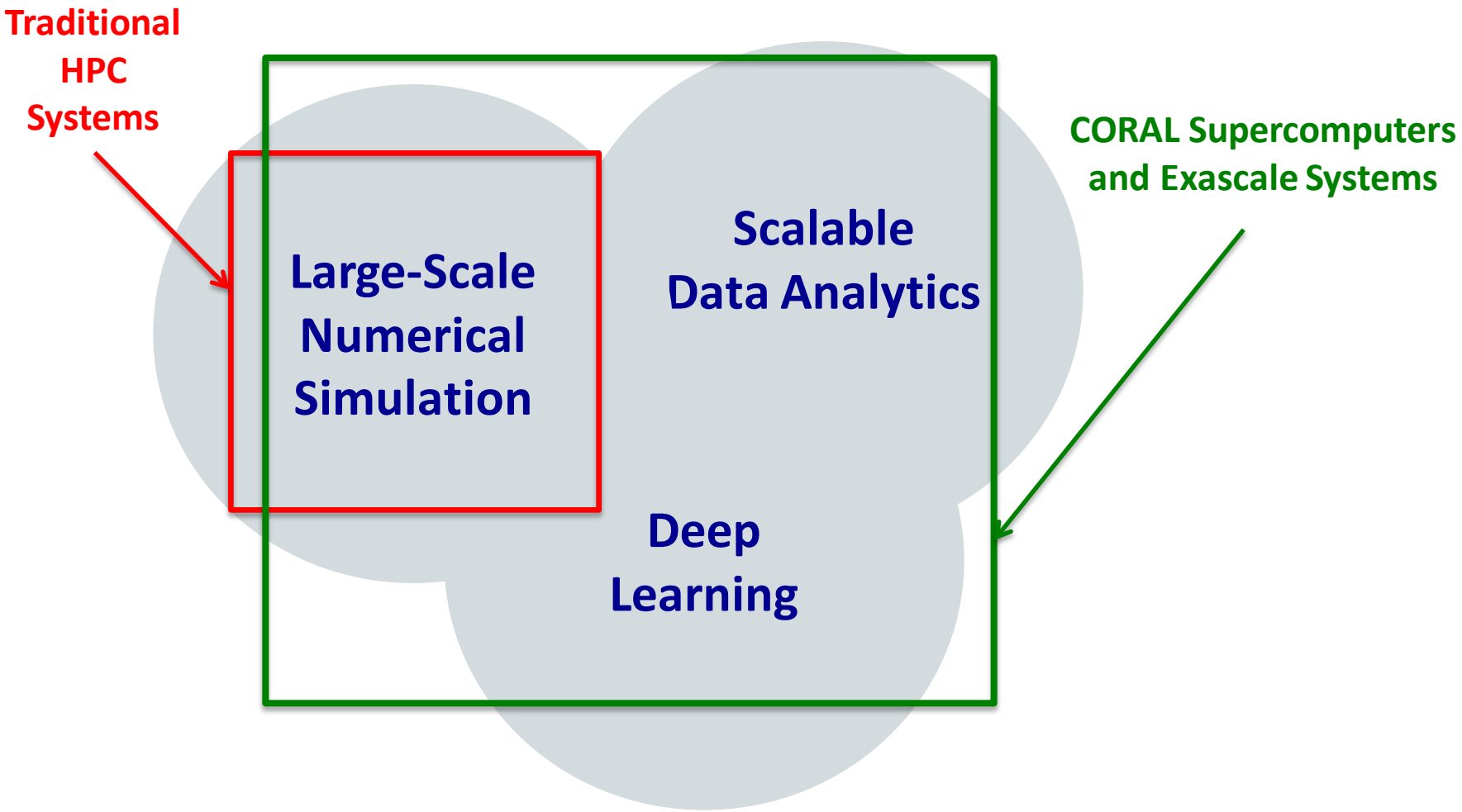
- **Large-scale Simulation (PDEs, traditional HPC)**
- **Data Intensive Applications (scalable science pipelines)**
- **Deep Learning and Emerging Science AI (training and inferencing)**

Current Exascale Timeline

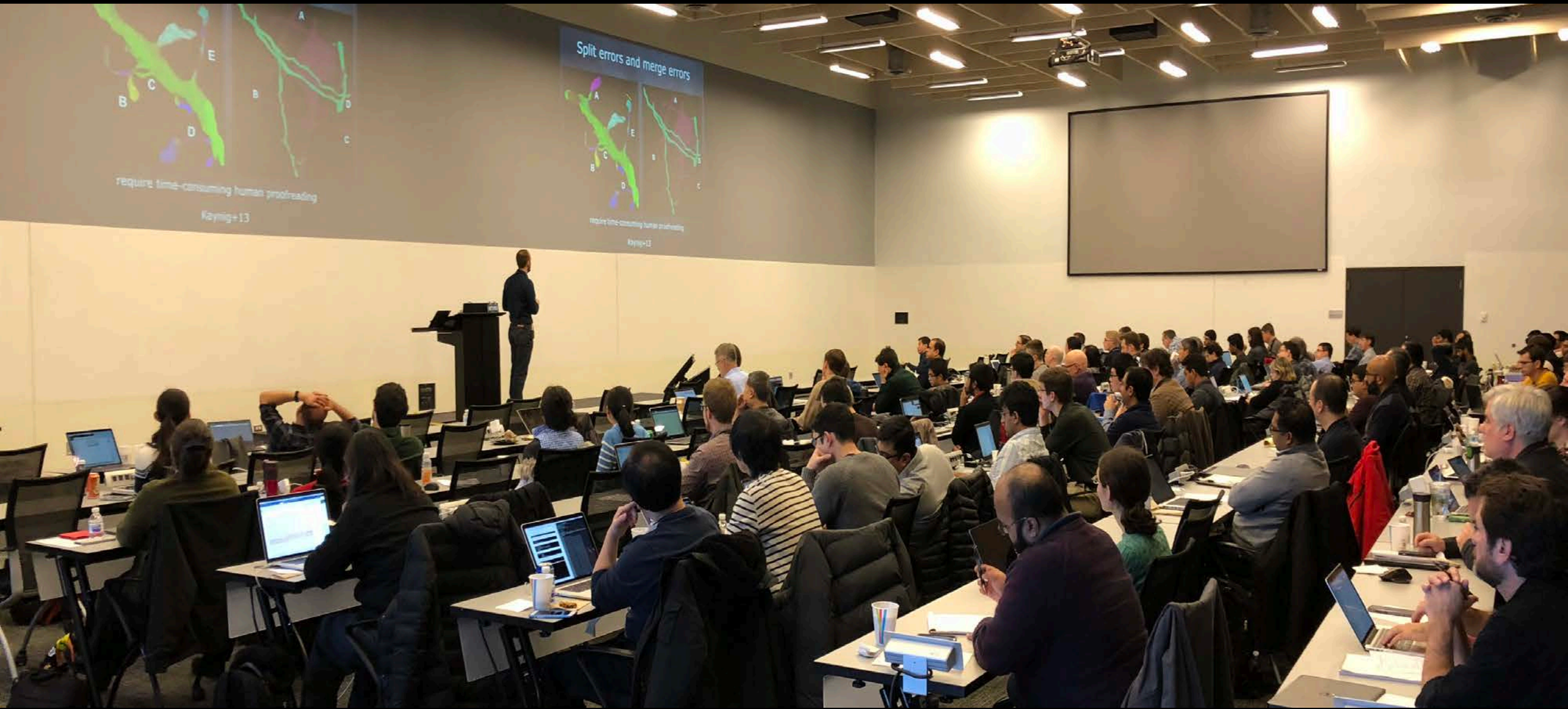


Pre-Exascale Systems				Exascale Systems
2013	2016	2018	2020	2021-2022
 Argonne IBM BG/Q Open	 Argonne Intel/Cray KNL Open	 ORNL IBM/NVidia P9/Volta Open	NERSC-9 LBNL TBD Open	 Argonne Intel/Cray TBD Open
 ORNL Cray/NVidia K20 Open	 LBNL Cray/Intel Xeon/KNL Unclassified			Frontier ORNL TBD Open
 LLNL IBM BG/Q Secure	 LANL/SNL Cray/Intel Xeon/KNL Secure	 LLNL IBM/NVidia P9/Volta Secure	Crossroads LANL/SNL TBD Secure	El Capitan LLNL TBD Secure

Simulation, Data Analytics and Machine Learning

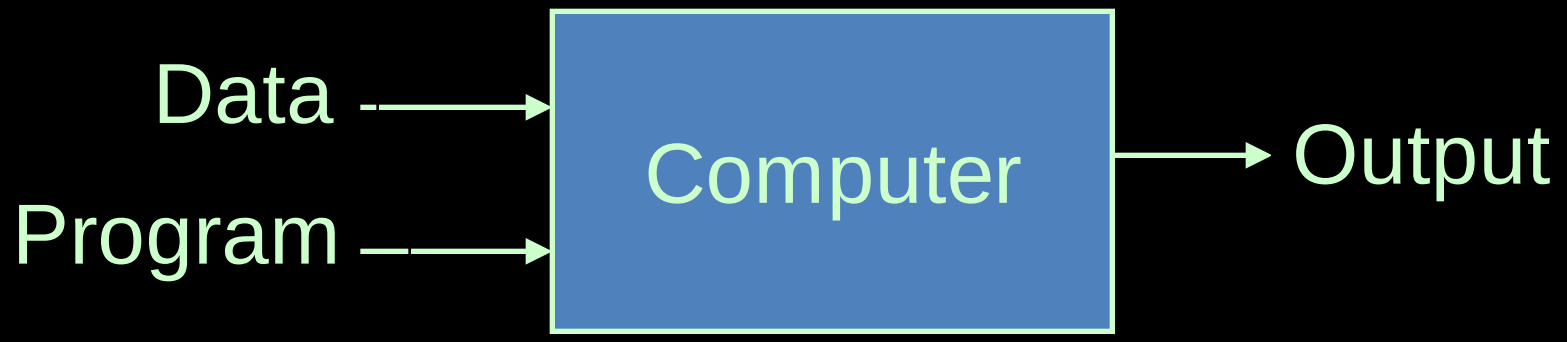


Machine Learning Interest is Exploding

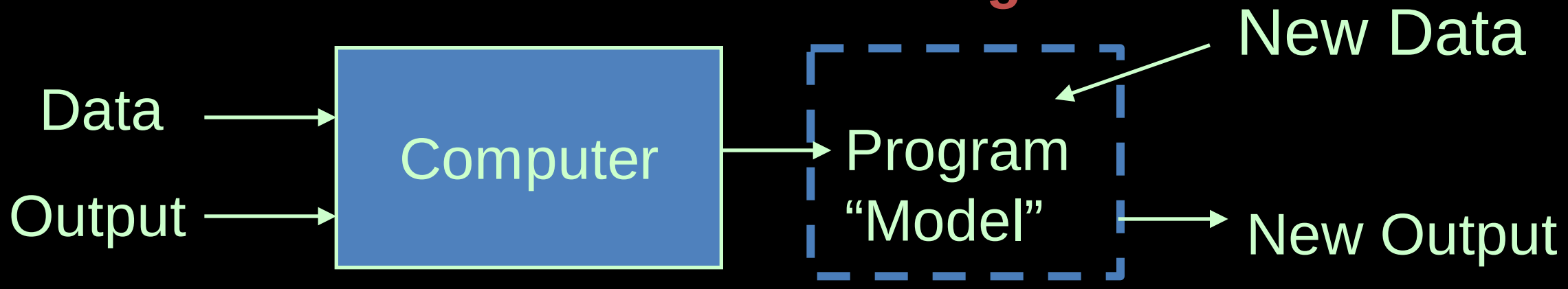


The Cartoon Form

Traditional Programming



Machine Learning

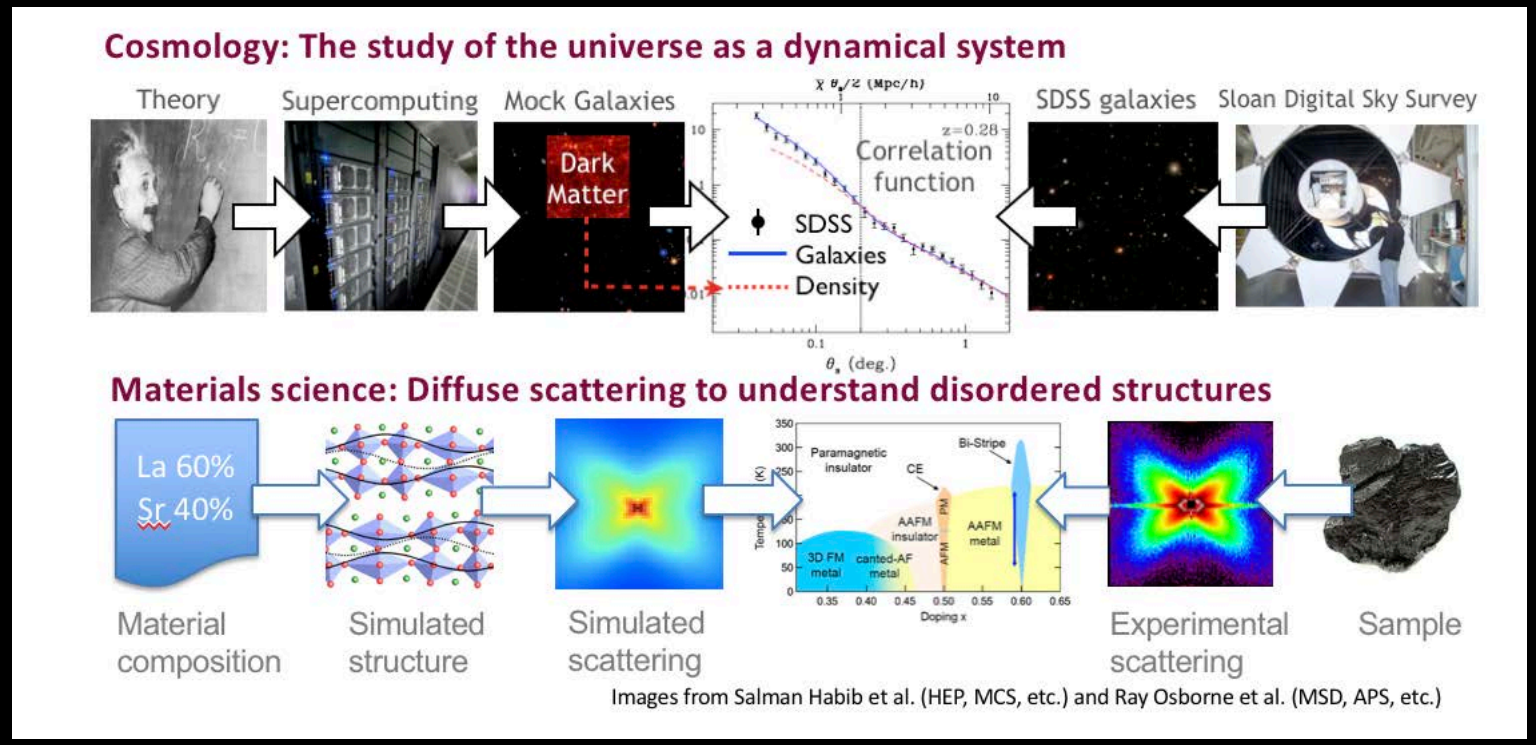


Training **Inferencing**

Machine Learning is becoming a major element of scientific computing applications

Across the DOE lab system hundreds of examples are emerging

- From fusion energy to precision medicine
- Materials design
- Fluid dynamics
- Synthetic Biology
- Structural engineering
- Intelligent sensing
- Etc.



Targets for Exascale Computers

Simulation Applications

- Materials Science
- Cosmology
- Molecular Dynamics
- Nuclear Reactor Modeling
- Combustion
- Quantum Computer Simulation
- Climate Modeling
- Power Grid
- Discrete Event Simulation
- Fusion Reactor Simulation
- Brain Simulation
- Transportation Networks

Big Data Applications

- APS Data Analysis
- HEP Data Analysis
- LSST Data Analysis
- SKA Data Analysis
- Metagenome Analysis
- Battery Design Search
- Graph Analysis
- Virtual Compound Library
- Neuroscience Data Analysis
- Genome Pipelines

Deep Learning Applications

- Drug Response Prediction
- Scientific Image Classification
- Scientific Text Understanding
- Materials Property Design
- Gravitational Lens Detection
- Feature Detection in 3D
- Street Scene Analysis
- Organism Design
- State Space Prediction
- Persistent Learning
- Hyperspectral Patterns

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A21 FOM Applications

	Application	Summary
Simulation	HACC	Particle/N-Body, FFT
	LAMMPS	Classical MD
	QMCPACK	Many-Body Theory
	Nekbone	Unstructured Grids, Spectral Element
Data	LSST-SVM	Multi-class classification or regression analysis using support vector machines. Datasets consistent with those expected from future cosmological surveys.
	Tomography Reconstruction	Fourier Time method. Used 1D and 2D FFTs, interpolation, and approximation functions. Dataset includes images.
	FCMA (SGEMM & SSYRK)	Interactions among brain regions in functional magnetic resonance imaging Data is a stream of 3D human brain data (volumes of voxel) over time, 4D data
Learning	Candle Pilot 1 (P1B2, P1B3)	Convolution Neural Nets (CNN), Multilayer Perceptrons (MLP) Datasets include gene sequences, drug responses, drug descriptors.
	Candle Pilot 3 (P3)	Hierarchical Attention Networks, Multi-task Learning Datasets include ontology reports
	Imaging (Inference)	Convolution Neural Nets, GANs, MLP. Datasets include images and potentially experimental settings

Simulation Targets and Needs

Performance Goal: >50x over 20PF systems

Typical Targets

- Materials and Physics
- Cosmology and Astronomy
- Climate and Energy
- Chemistry and Fluids
- Particles and Fields
- Flow in Networks

Newish Targets

- Quantum Computer Simulation
- Brain Simulation

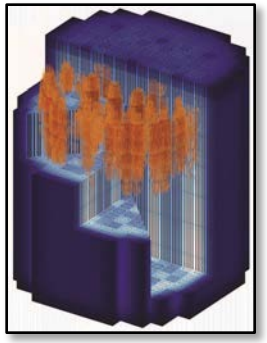
System Requirements

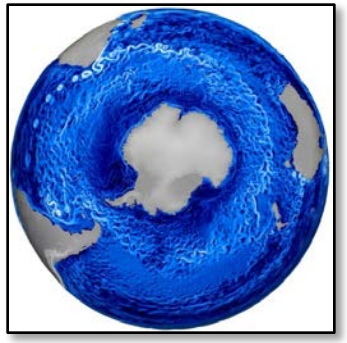
- Compute intensity (fp64)
- Memory Bandwidth (HBM2e)
- Memory Capacity (6-8PB)
- Large Coherency Domain (~TB)
- Unified Address Space CPU/Acc
- High Bisection Bandwidth (~PB/s)
- High Injection Bandwidth (~100's GB/s)
- Lowish Comm Latency (~us)
- Sustained IO Performance (~10's TB/s)

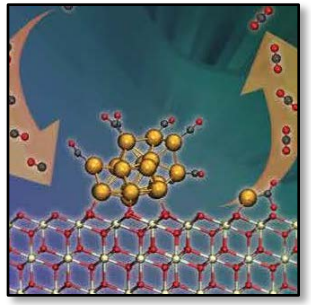
Exascale Applications Will Address National Challenges

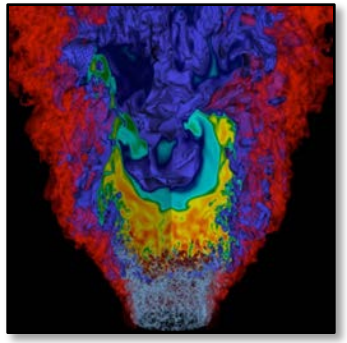
Summary of current DOE Science & Energy application development projects

Nuclear Energy (NE)	Climate (BER)	Chemical Science (BES, BER)	Wind Energy (EERE)	Combustion (BES)
Accelerate design and commercialization of next-generation small modular reactors* Climate Action Plan; SMR licensing support; GAIN	Accurate regional impact assessment of climate change* Climate Action Plan	Biofuel catalysts design; stress-resistant crops Climate Action Plan; MGI	Increase efficiency and reduce cost of turbine wind plants sited in complex terrains* Climate Action Plan	Design high-efficiency, low-emission combustion engines and gas turbines* 2020 greenhouse gas and 2030 carbon emission goals









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EXASCALE COMPUTING PROJECT

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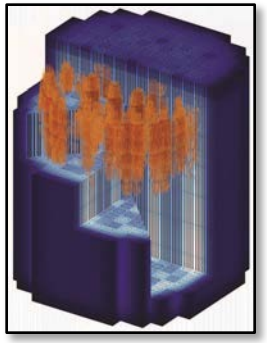
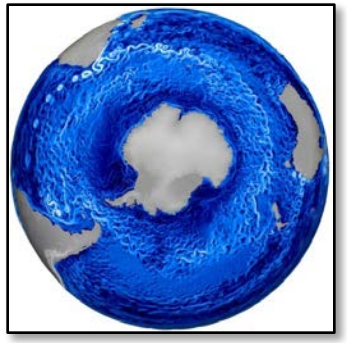


Climate (BER)

Accurate regional impact assessment of climate change*

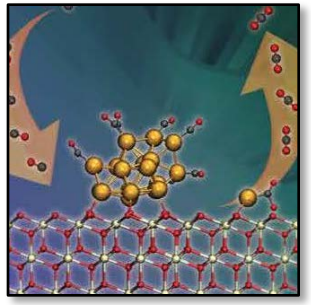
Climate Action Plan



Chemical Science (BES, BER)

Biofuel catalysts design; stress-resistant crops

Climate Action Plan; MGI



Wind Energy (EERE)

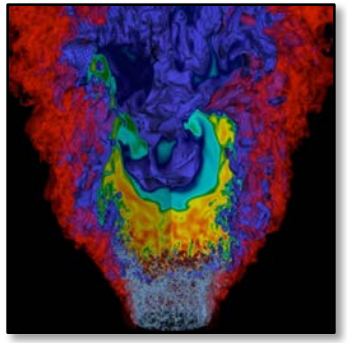
Increase efficiency and reduce cost of turbine wind plants sited in complex terrains*

Climate Action Plan

Combustion (BES)

Design high-efficiency, low-emission combustion engines and gas turbines*

2020 greenhouse gas and 2030 carbon emission goals



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Exascale Applications Will Address National Challenges

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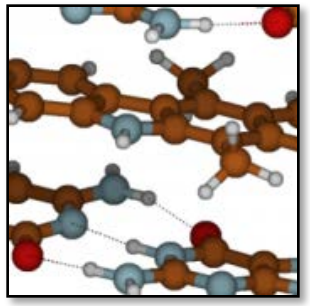
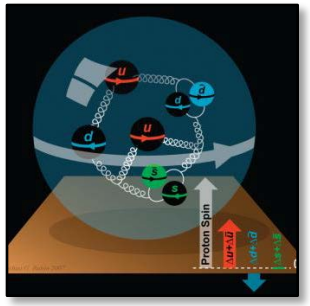
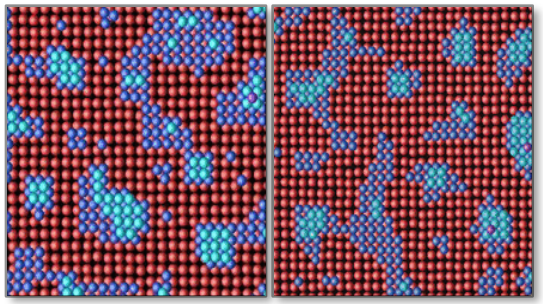
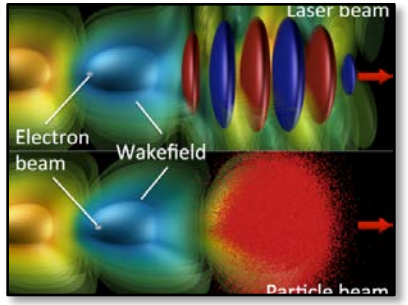
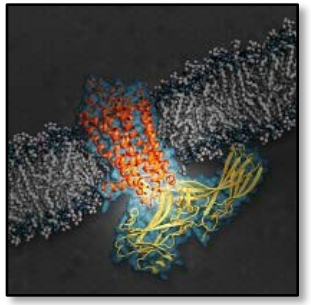
Materials Science (BES)	Nuclear Physics (NP)	Nuclear Materials (BES, NE, FES)	Accelerator Physics (HEP)	Materials Science (BES)
Find, predict, and control materials and properties: property change due to hetero-interfaces and complex structures MGI	QCD-based elucidation of fundamental laws of nature: SM validation and beyond SM discoveries 2015 Long Range Plan for Nuclear Science; RHIC, CEBAF, FRIB	Extend nuclear reactor fuel burnup and develop fusion reactor plasma-facing materials* Climate Action Plan; MGI; Light Water Reactor Sustainability; ITER; Stockpile Stewardship Program	Practical economic design of 1 TeV electron-positron high-energy collider with plasma wakefield acceleration* >30k accelerators today in industry, security, energy, environment, medicine	Protein structure and dynamics; 3D molecular structure design of engineering functional properties* MGI; LCLS-II 2025 Path Forward











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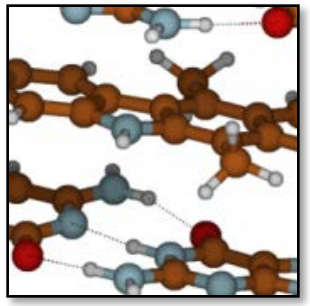
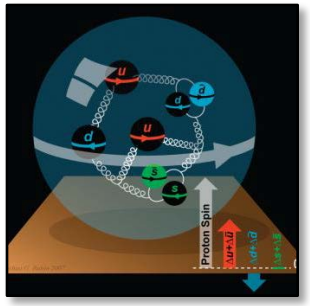


Nuclear Physics (NP)

QCD-based elucidation of fundamental laws of nature: SM validation and beyond SM discoveries

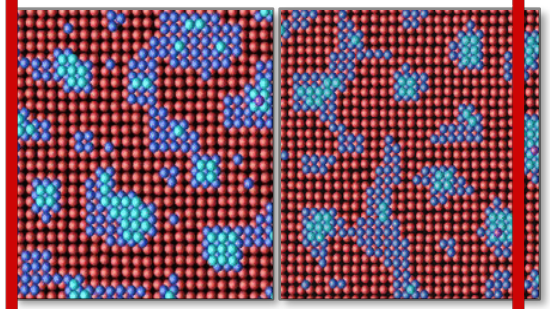
2015 Long Range Plan for Nuclear Science; RHIC, CEBAF, FRIB



Nuclear Materials (BES, NE, FES)

Extend nuclear reactor fuel burnup and develop fusion reactor plasma-facing materials*

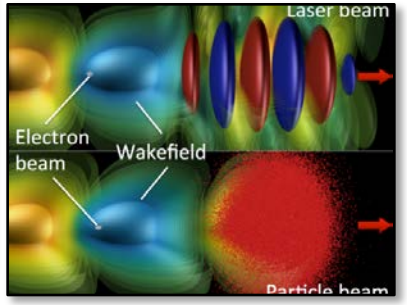
Climate Action Plan; MGI; Light Water Reactor Sustainability; ITER; Stockpile Stewardship Program



Accelerator Physics (HEP)

Practical economic design of 1 TeV electron-positron high-energy collider with plasma wakefield acceleration*

>30k accelerators today in industry, security, energy, environment, medicine



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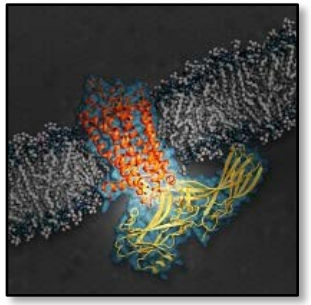

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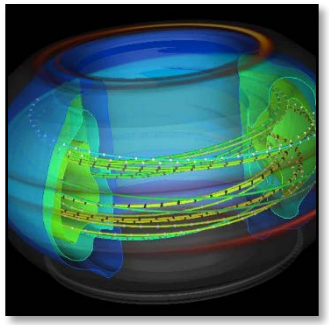
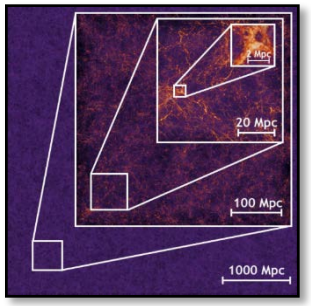
EXASCALE COMPUTING PROJECT

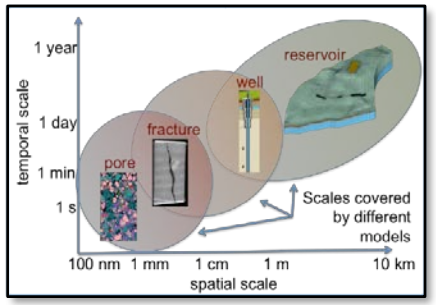
Exascale Applications Will Address National Challenges

Summary of current DOE Science & Energy and Other Agency application development projects

Magnetic Fusion Energy (FES)	Advanced Manufacturing (EERE)	Cosmology (HEP)	Geoscience (BES, BER, EERE, FE, NE)	Precision Medicine for Cancer (NIH)
Predict and guide stable ITER operational performance with an integrated whole device model*	Additive manufacturing process design for qualifiable metal components*	Cosmological probe of standard model (SM) of particle physics: Inflation, dark matter, dark energy*	Safe and efficient use of subsurface for carbon capture and storage, petroleum extraction, geothermal energy, nuclear waste*	Accelerate and translate cancer research in RAS pathways, drug responses, treatment strategies*
ITER; fusion experiments: NSTX, DIII-D, Alcator C-Mod	NNMIs; Clean Energy Manufacturing Initiative	Particle Physics Project Prioritization Panel (P5)	EERE Forge; FE NRAP; Energy-Water Nexus; SubTER Crosscut	Precision Medicine in Oncology; Cancer Moonshot







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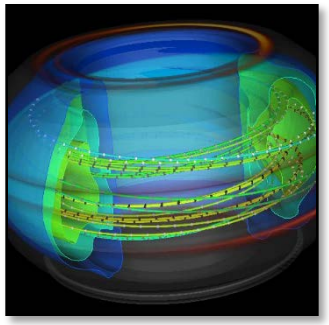


Advanced Manufacturing (EERE)

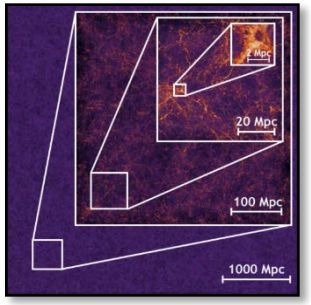
Additive manufacturing process design for qualifiable metal components*

NNMIs; Clean Energy Manufacturing Initiative

Cosmology (HEP)

Cosmological probe of standard model (SM) of particle physics: Inflation, dark matter, dark energy*

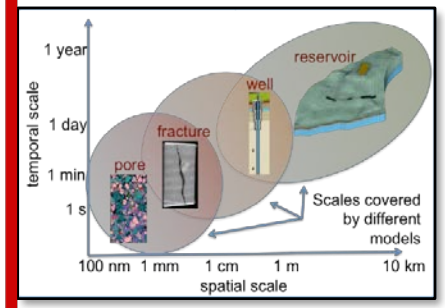
Particle Physics Project Prioritization Panel (P5)



Geoscience (BES, BER, EERE, FE, NE)

Safe and efficient use of subsurface for carbon capture and storage, petroleum extraction, geothermal energy, nuclear waste*

EERE Forge; FE NRAP; Energy-Water Nexus; SubTER Crosscut



Precision Medicine for Cancer (NIH)

Accelerate and translate cancer research in RAS pathways, drug responses, treatment strategies*

Precision Medicine in Oncology; Cancer Moonshot

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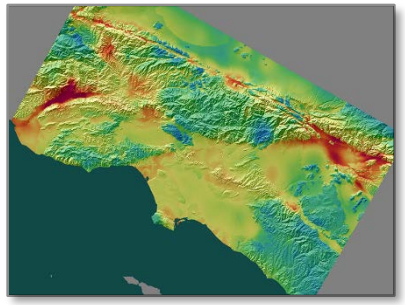
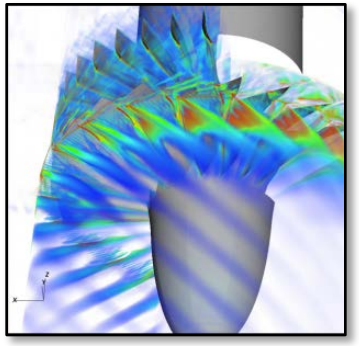
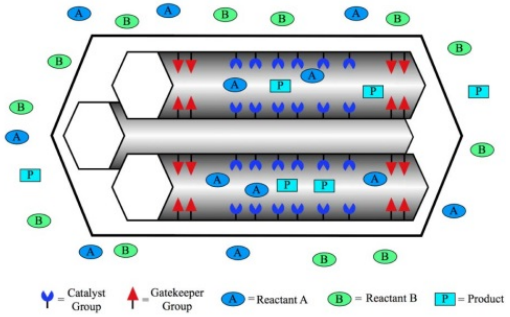
Summary of current DOE Science & Energy application development seed projects

Seismic (EERE, NE, NNSA)	Carbon Capture and Storage (FE)	Chemical Science (BES)	Urban Systems Science (EERE)
Reliable earthquake hazard and risk assessment in relevant frequency ranges*	Scaling carbon capture/storage laboratory designs of multiphase reactors to industrial size	Design catalysts for conversion of cellulosic-based chemicals into fuels, bioproducts	Retrofit and improve urban districts with new technologies, knowledge, and tools*
DOE Critical Facilities Risk Assessment; urban area risk assessment; treaty verification	Climate Action Plan; SunShot; 2020 greenhouse gas/2030 carbon emission goals	Climate Action Plan; SunShot Initiative; MGI	Energy-Water Nexus; Smart Cities Initiative







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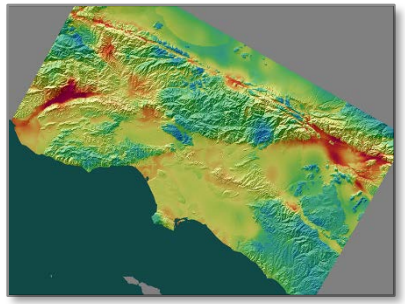
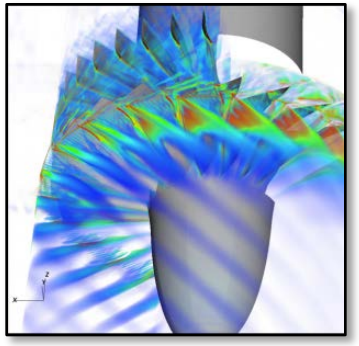
DOE Critical Facilities Risk Assessment; urban area risk assessment; treaty verification



Carbon Capture and Storage (FE)

Scaling carbon capture/storage laboratory designs of multiphase reactors to industrial size

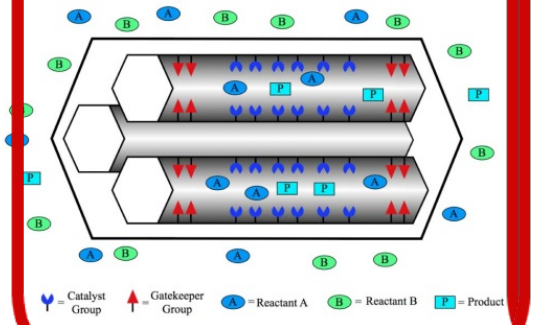
Climate Action Plan; SunShot; 2020 greenhouse gas/2030 carbon emission goals



Chemical Science (BES)

Design catalysts for conversion of cellulosic-based chemicals into fuels, bioproducts

Climate Action Plan; SunShot Initiative; MGI



Urban Systems Science (EERE)

Retrofit and improve urban districts with new technologies, knowledge, and tools*

Energy-Water Nexus; Smart Cities Initiative

* Scope includes a discernible data science component

EXASCALE COMPUTING PROJECT

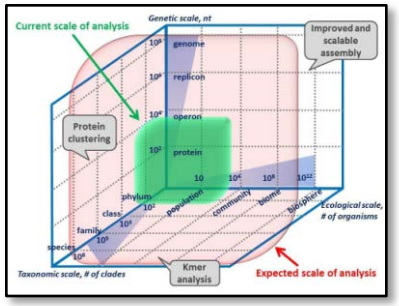
Exascale Applications Will Address National Challenges

Summary of current DOE Science & Energy application development seed projects

Metagenomics (BER)

Leveraging microbial diversity in metagenomic datasets for new products and life forms*

Climate Action Plan; Human Microbiome Project; Marine Microbiome Initiative



Astrophysics (NP)

Demystify origin of chemical elements (> Fe); confirm LIGO gravitational wave and DUNE neutrino signatures*

2015 Long Range Plan for Nuclear Science; origin of universe and nuclear matter in universe

Power Grid (EERE, OE)

Reliably and efficiently planning our nation's grid for societal drivers: rapidly increasing renewable energy penetration, more active consumers*

Grid Modernization Initiative; Climate Action Plan

* Scope includes a discernible data science component

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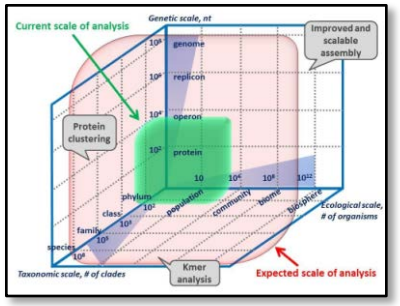

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EXASCALE COMPUTING PROJECT

Data Analysis Targets and Needs

Performance Goal: >50x over 20PF systems

Instrument data

- APS data streams
- Connectome Imaging
- LSST data streams
- ARM radar data streams
- HEP detector data streams

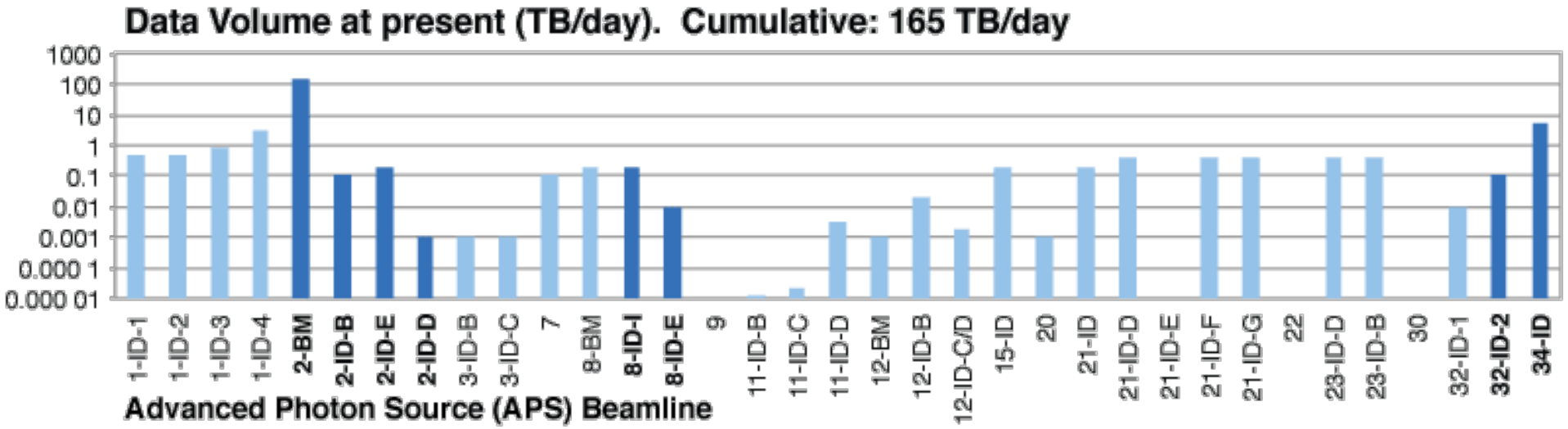
Simulation data

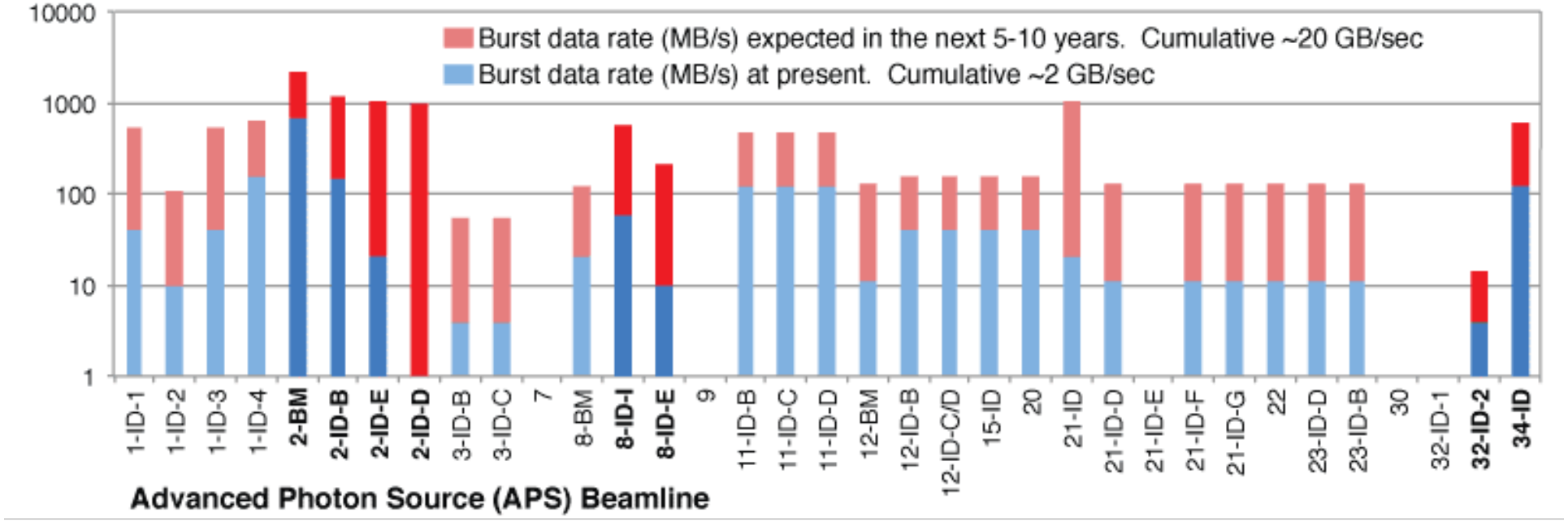
- Climate output analysis
- Cosmology output analysis
- Detector simulation output analysis

System Requirements

- Streaming IO bandwidth (~10's TB/s)
- Large RAM for in memory (~PBs)
- Large coherency domain (~TB)
- Flexible control flow (CPU+X)
- Flexible SW Stack (x86+ Containers)
- Workflow support (Spark, Swift)
- Scripting Language Support (Python)
- Accelerated xform libraries
- Embedded machine learning
- Embedded simulation

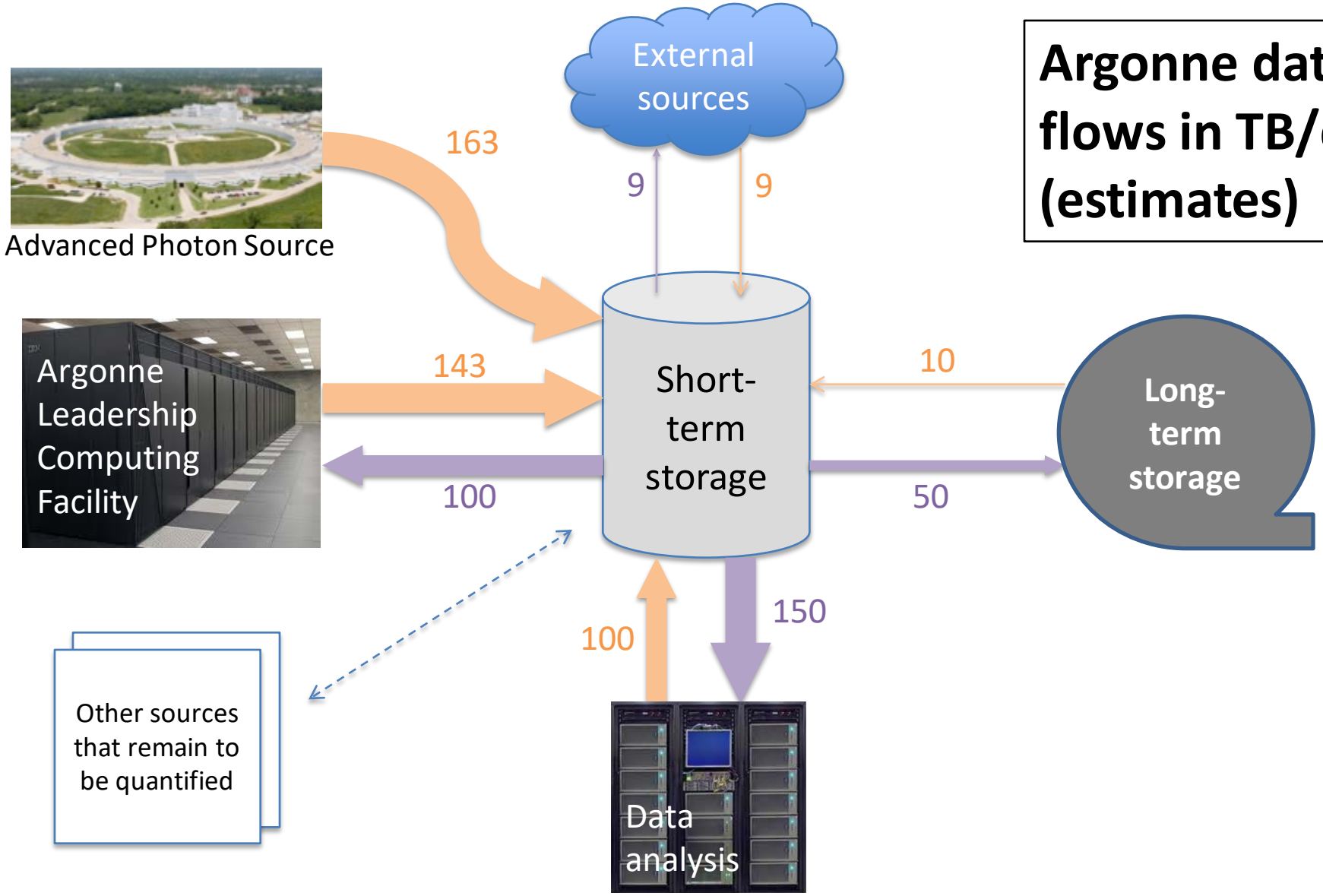
APS data volumes already equal those from LHC



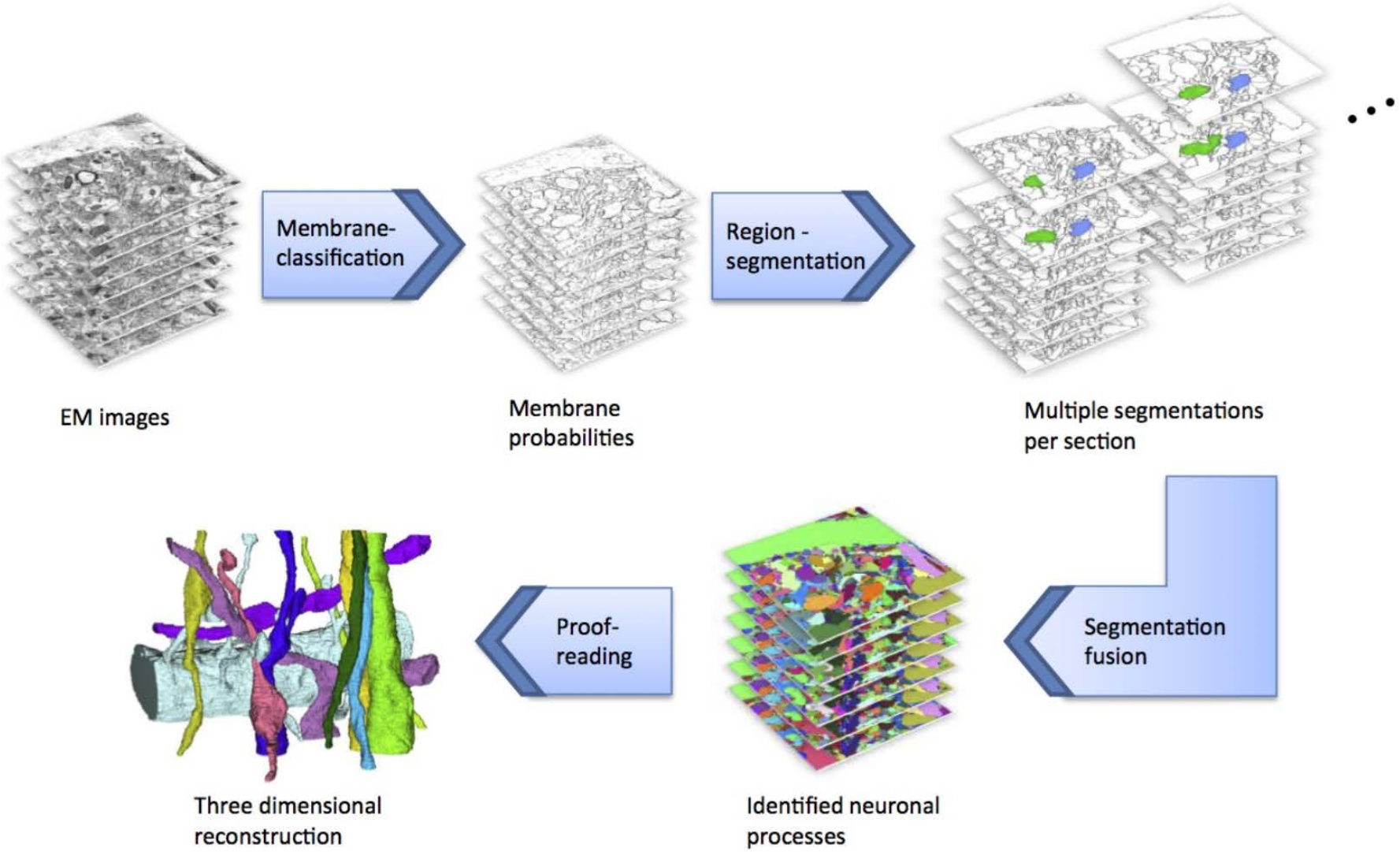


Source: Francesco de Carlo

Local flows already exceed those of LHC



Reconstructing Brain Connectivity from stacked EM images



Machine Learning Targets and Needs

Performance Goal: >50x over 20PF systems

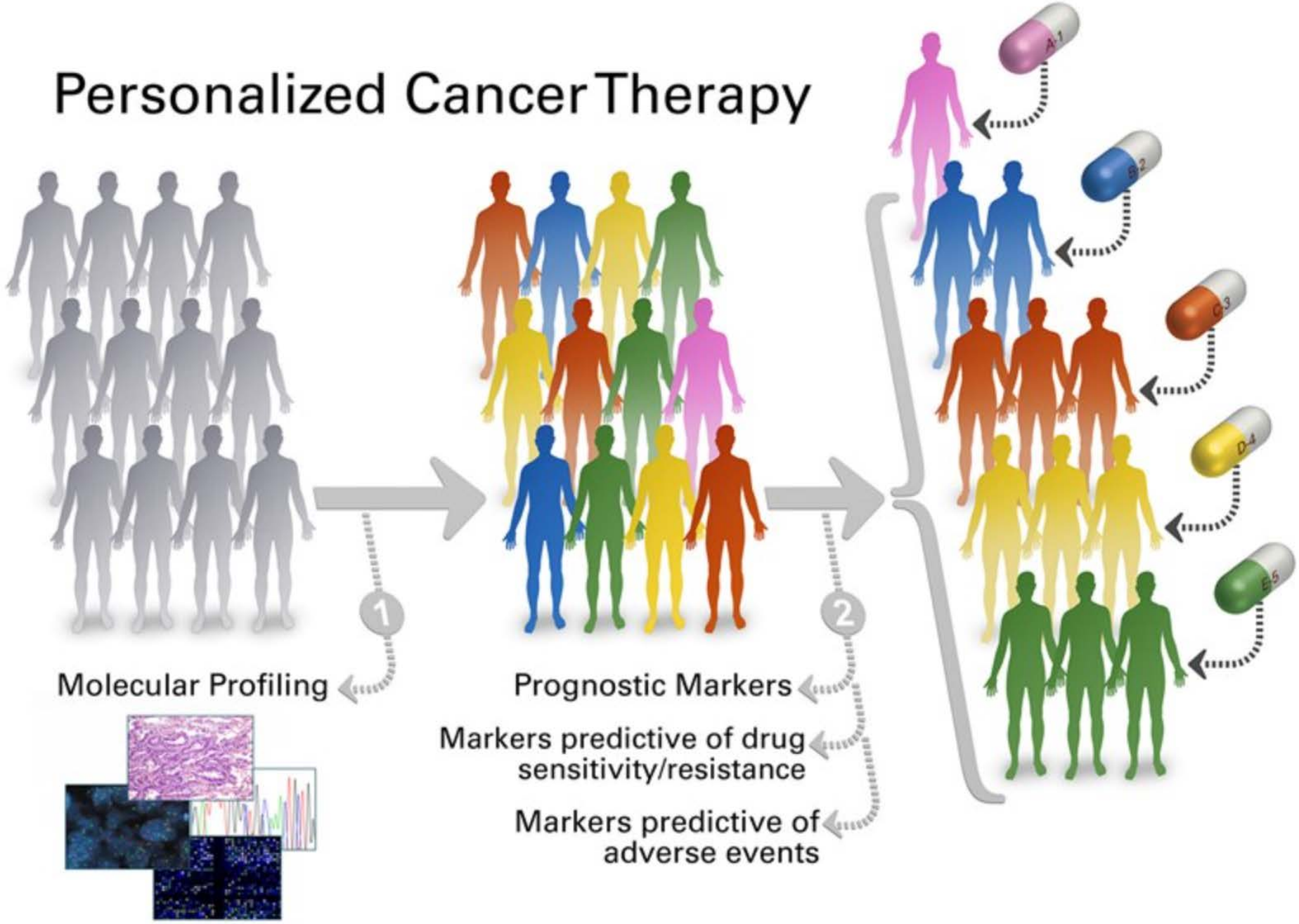
Targets

- Materials (Energy Storage)
- Dark Matter (Lensing)
- Organism Design
- Advanced Manufacturing
- Cancer Therapeutics (Drugs)
- Traumatic Brain Injury
- Genomics (AMR, CVD)
- Software Design/Improvement
- Theory Integration with ML

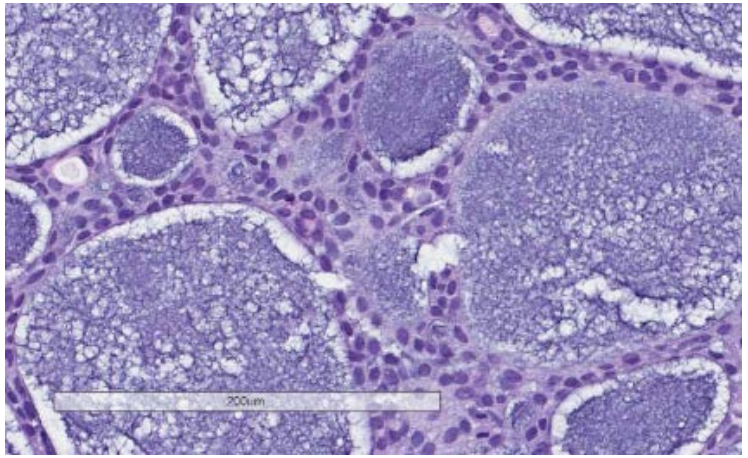
Systems Requirements

- Compute Intensity (fp32, bfp16)
- Large Coherency domain (~TB)
- Large Memory (~PB)
- Unified Address Space CPU/Acc
- Data Sparsity Support (S/G)
- Sustained IO Performance (~10's TB/s)
- High Injection Bandwidth (~100's GB/s)
- Flexible SW Stack (x86+ Containers)
- Workflow support (Spark, Swift)
- Scripting Language Support (Python)

Personalized Cancer Therapy

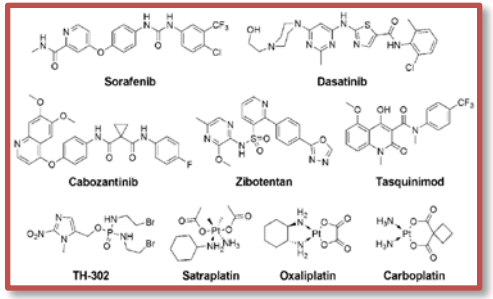


Modeling Cancer Drug Response

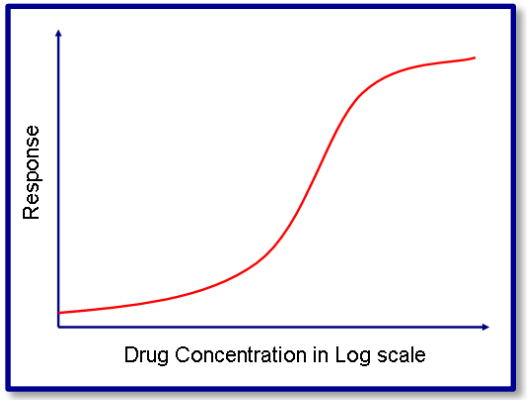


Drug (s)

- descriptors
- fingerprints
- structures
- SMILES
- dose



$$\mathcal{R} = f(\mathcal{T}, \mathcal{D}_1, \mathcal{D}_2)$$

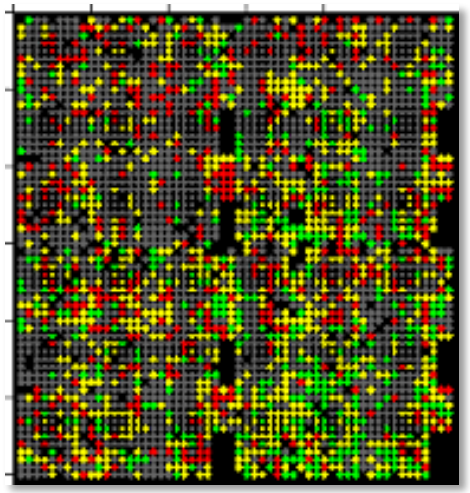


IC50
GI50
% growth
Z-score

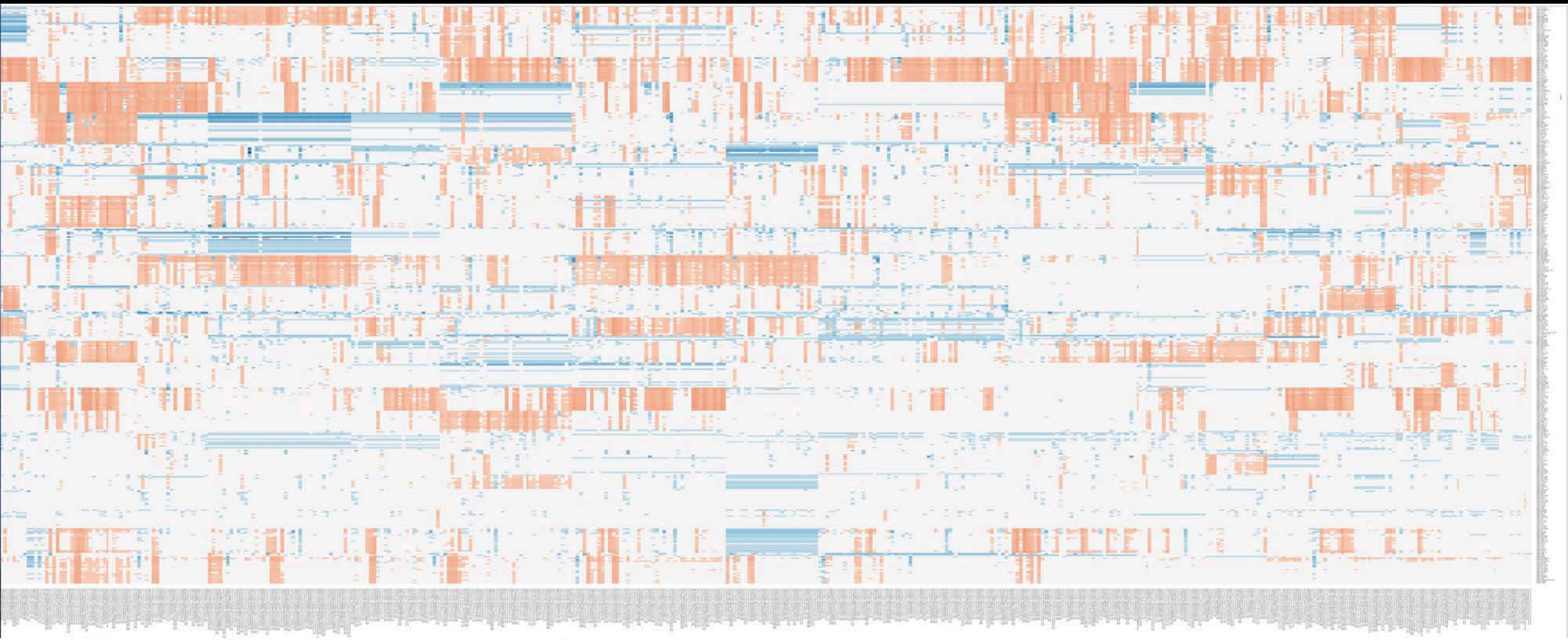
Response

gene expression levels
SNPs
protein abundance
microRNA
methylation

Tumor

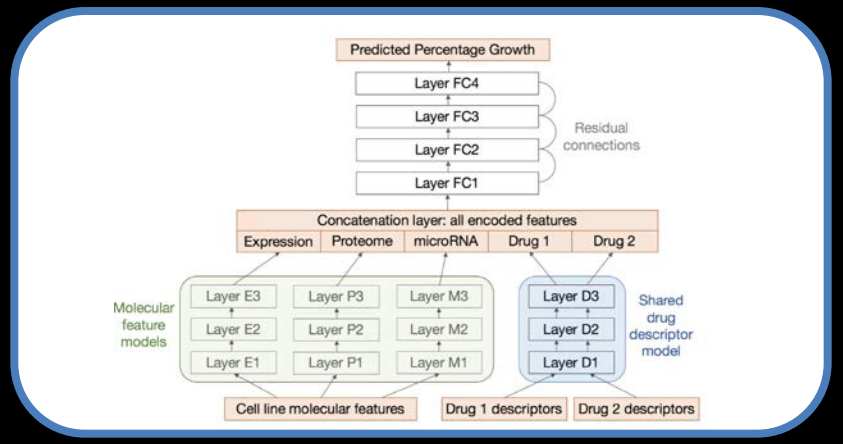


Combined Synergy and Uncertainty Map



Machine Learning Models with UQ

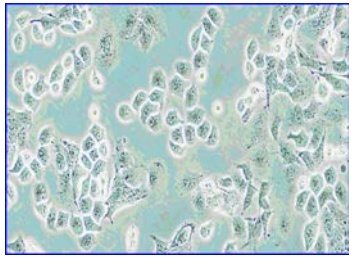
Training Data



Interesting Biology

Model Uncertainty

[High-]Throughput Experiments

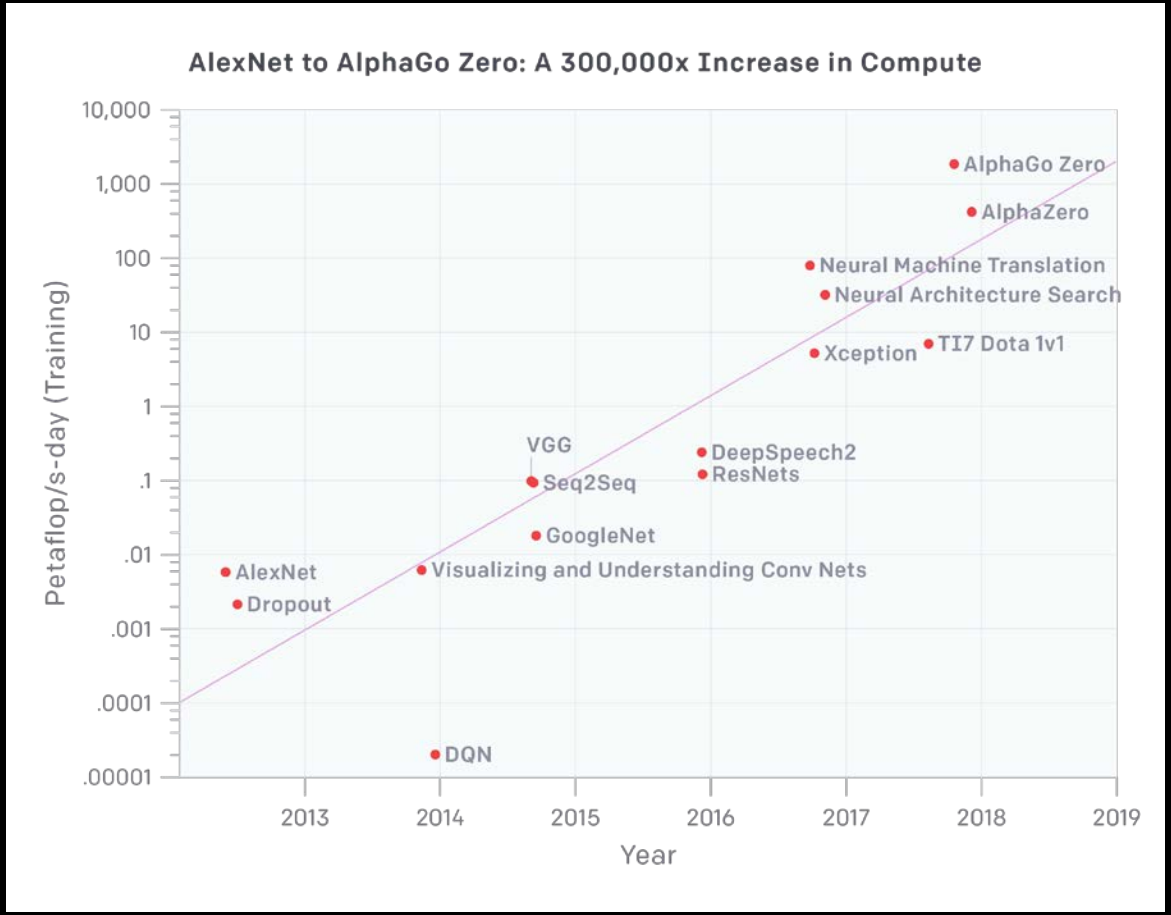


Additional Training Data

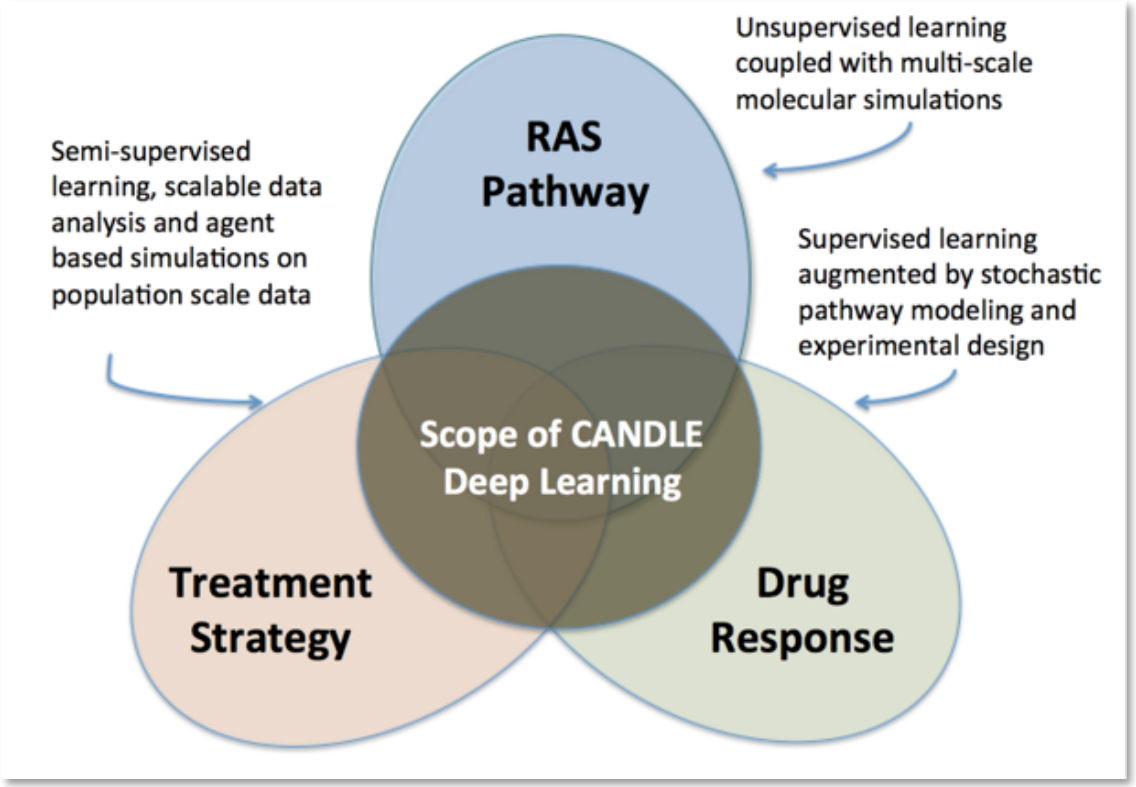
CANDLE: Deep Learning Meets HPC

Exascale Needs for Deep Learning

- Automated Model Discovery
- Hyper Parameter Optimization
- Uncertainty Quantification
- Flexible Ensembles
- Cross-Study Model Transfer
- Data Augmentation
- Synthetic Data Generation
- Reenforcement Learning



ECP-CANDLE: CANcer Distributed Learning Environment



CANDLE Goals

Develop an exscale deep learning environment for cancer and DOE mission applications

Build on open source deep learning frameworks

Optimize for CORAL and exascale platforms

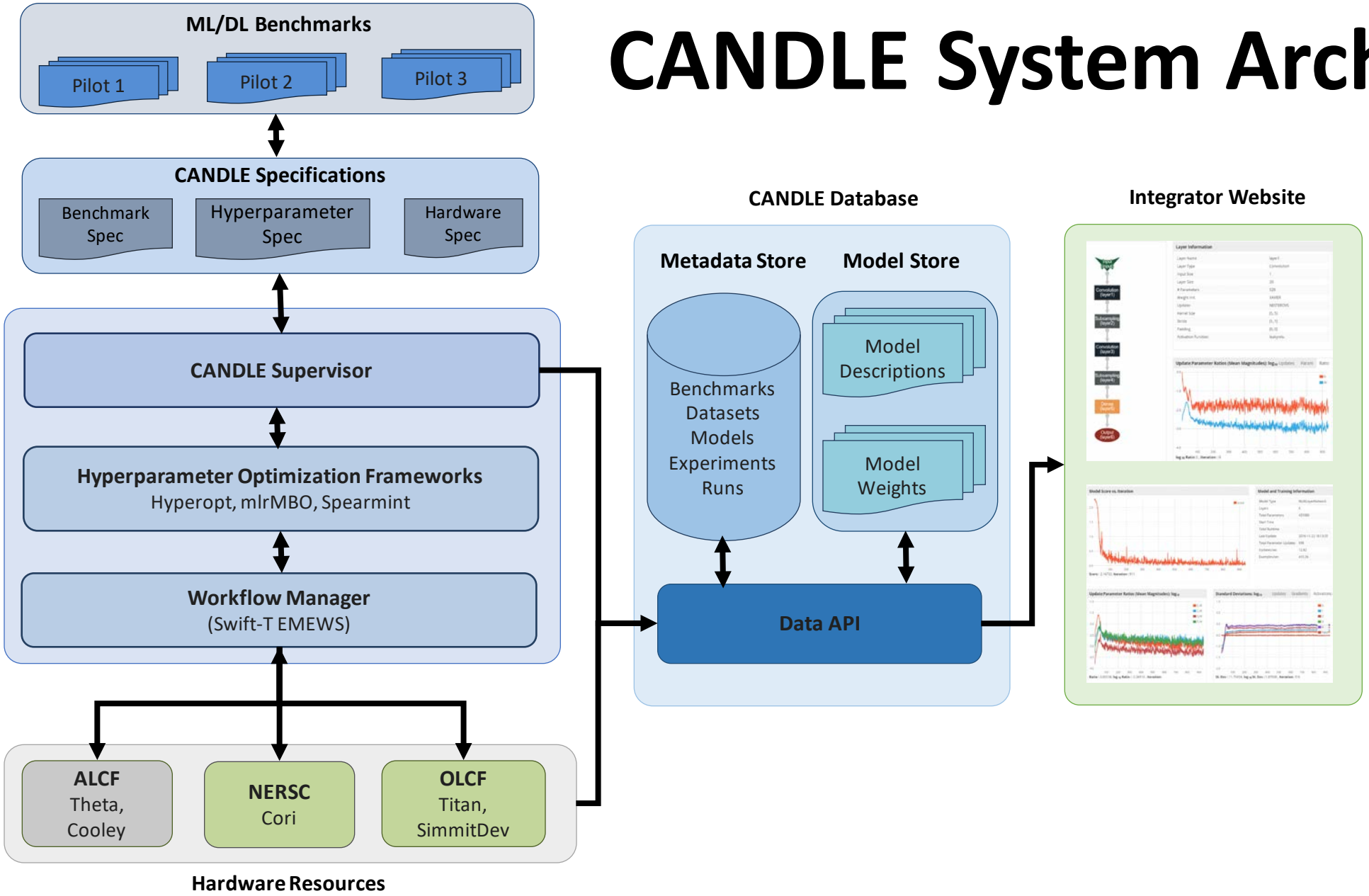
Support all three Cancer pilot project needs for deep dearning

Collaborate with DOE computing centers, HPC vendors and ECP co-design and software technology projects

CANDLE Software Stack

Hyperparameter Sweeps, Data Management (e.g. DIGITS, Swift, etc.)	**Workflow**
Network description, Execution scripting API (e.g. Keras, Mocha)	**Scripting**
Tensor/Graph Execution Engine (e.g. Theano, TensorFlow, LBANN-LL, etc.)	**Engine**
Architecture Specific Optimization Layer (e.g. cuDNN, MKL-DNN, etc.)	**Optimization**

CANDLE System Architecture



GitHub and FTP

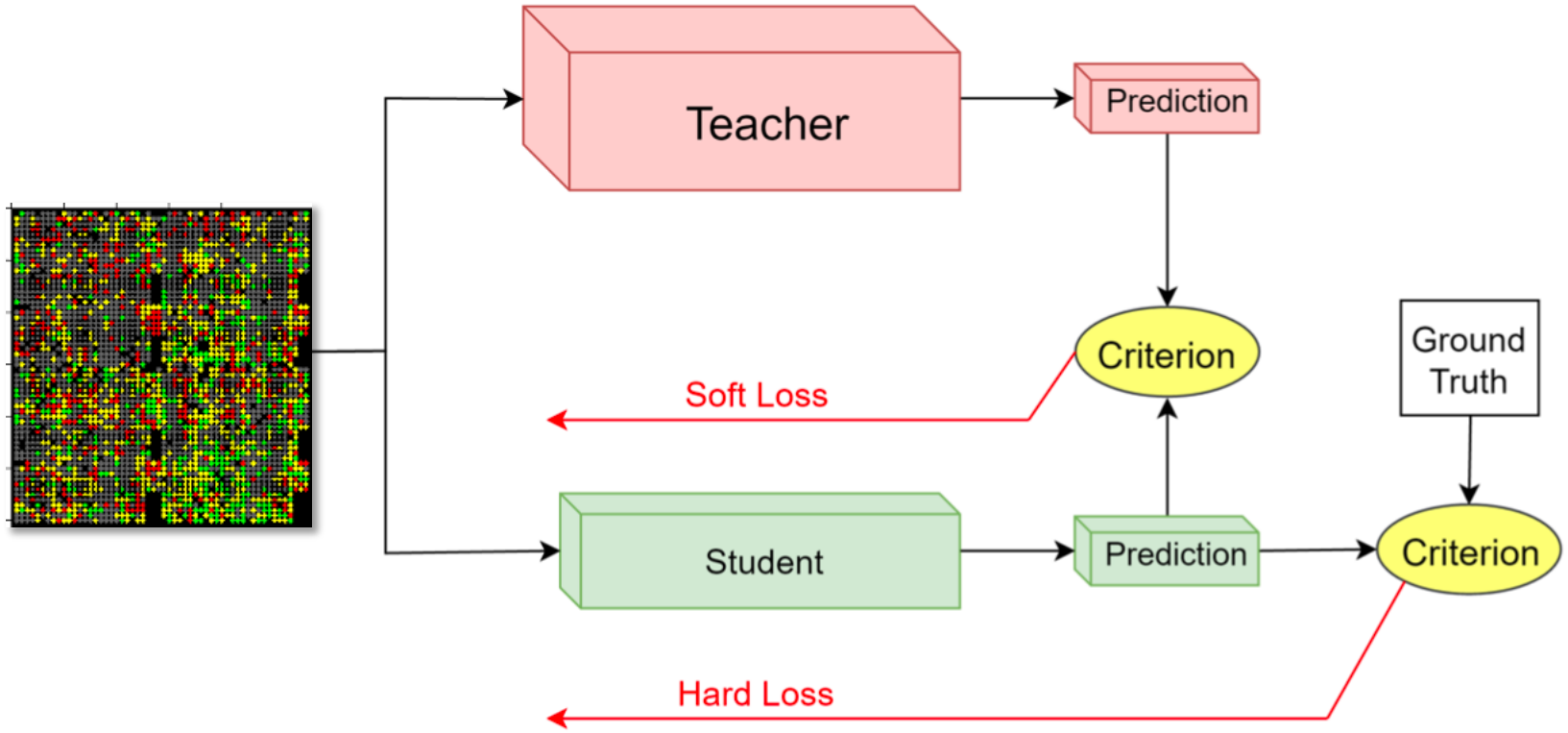
- **ECP-CANDLE GitHub Organization:**
- https://github.com/ECP-CANDLE

- **ECP-CANDLE FTP Site:**
- The FTP site hosts all the public datasets for the benchmarks from three pilots
- http://ftp.mcs.anl.gov/pub/candle/public/

Integration of Simulation and ML

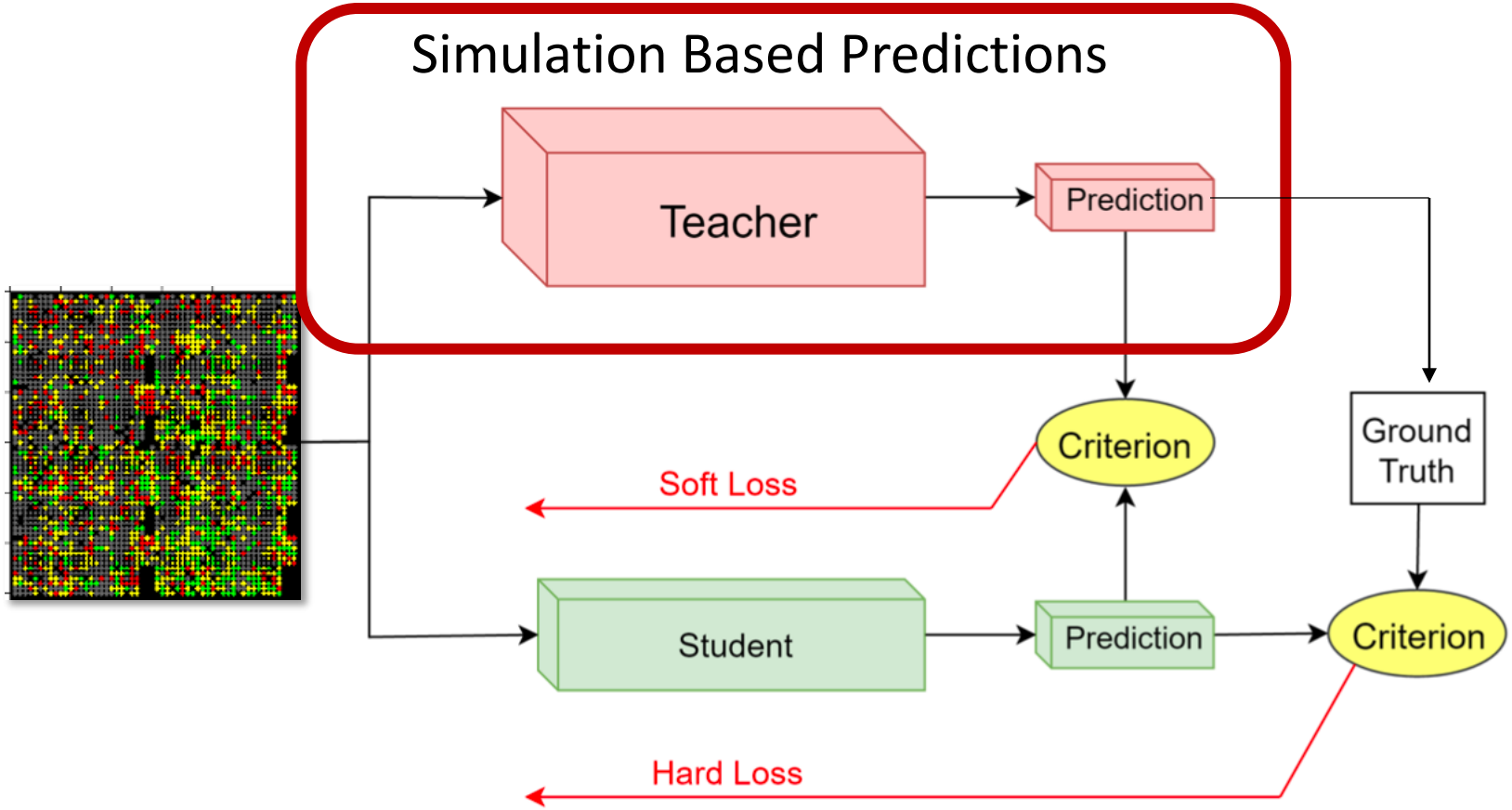
- Steering of simulations and Planning N moves ahead
  - ML/RL making decisions what to do next
- Embedding ML into Simulation
  - Replacing explicit functions/kernels with learned models
  - Trading accuracy for speed/power improvements ±7% for 2x ?
- Tuning or Customization of Kernels and Parameters
  - Customization of force fields in MD simulations (most accurate H_2O sim)
- Function/Property association
  - VAE to map latent representation to properties and generating candidates
- Student Teacher Model for Learning
  - Augment training data with simulation generated ground truth

Teacher-Student Network Model



(a) Standard: student network learns from teacher guidance (soft loss) and ground truth (hard loss).

Teacher-Student Sim/Network Model



Revised Model: Student Learns from data, from hints from simulation and from enhanced Ground Truth.

Integrating ML and Simulation

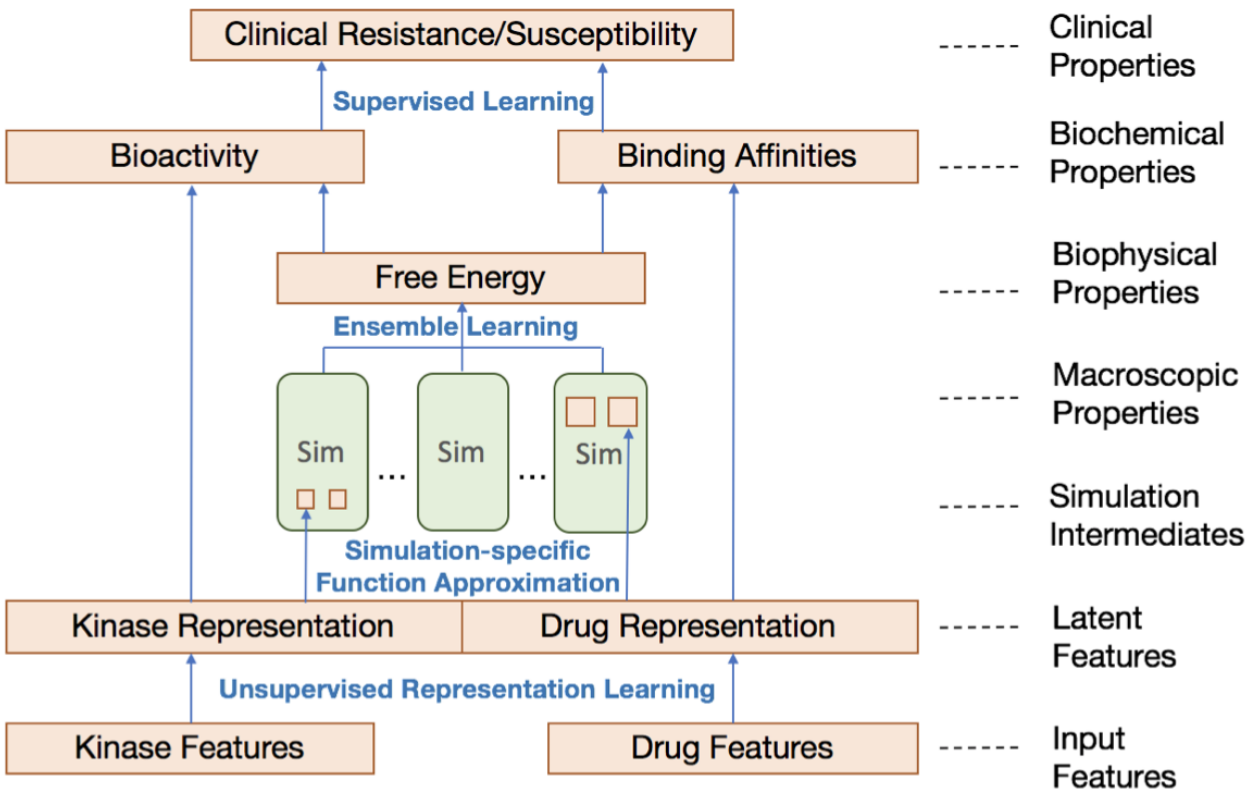
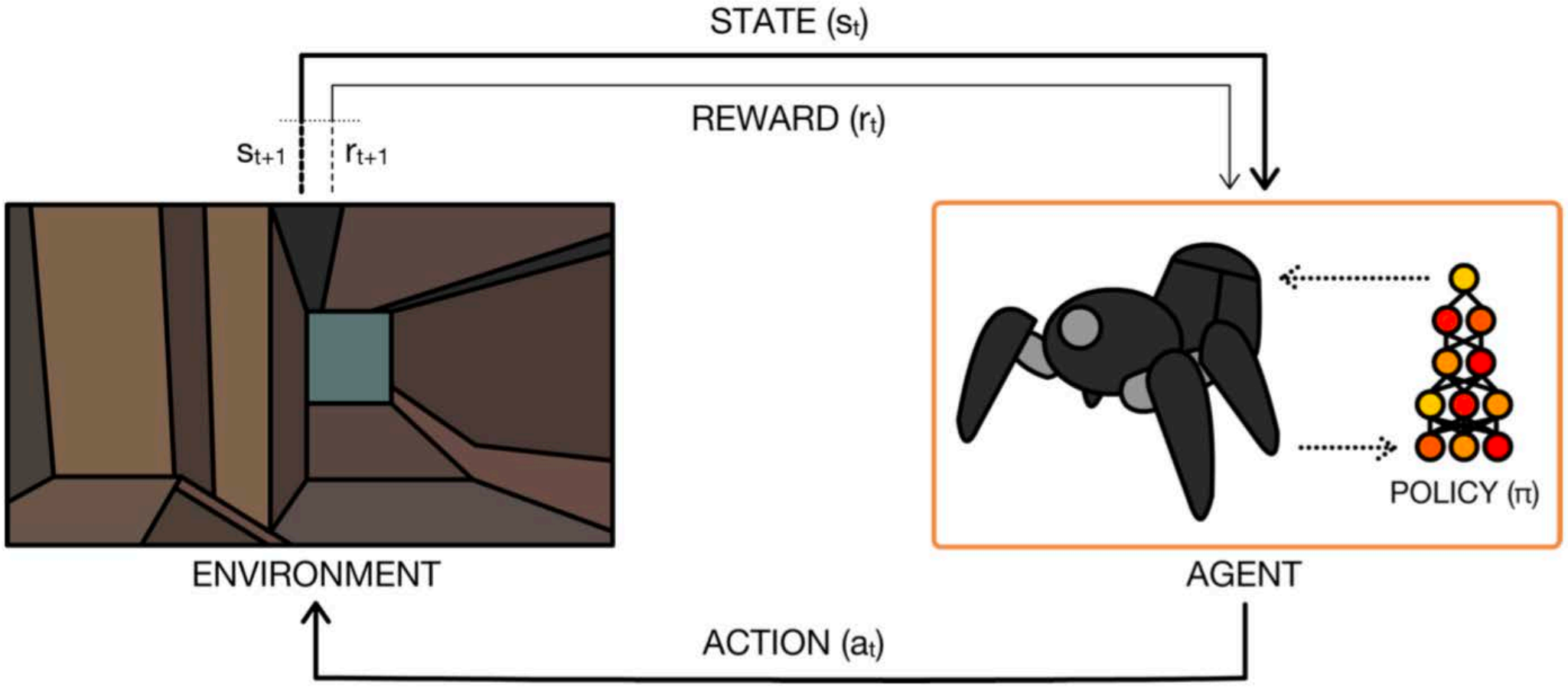


Figure 3: Overview of how data at all steps will be integrated using machine learning. The orange square boxes represent the three types of data in this project: kinases, drugs, and their interactions at various levels. The green rounded boxes denote the variety of MD simulations for free energy calculation. Each blue arrow represents an ML model; they combine in a joint predictive model that integrates all datasets.

Not just Deep Learning

- Last five years many problems have fallen to deep neural networks and “convolutional neural networks” (representational learning)
- AI is also advancing in “Re-enforcement Learning” where the reward is delayed
  - Game Playing, Stock Portfolios, Planning, Preference Systems, etc.
- Re-enforcement learning uses an intermediate entity called an ”agent” driven by a “policy” to evaluate “moves” in the “game”. Policy gets updated based on delayed feedback. Policy needs to give a good estimate of the value of alternative moves. Agent/Policy plays the game, machine learning improves the policy. Policies themselves might be machine learning based.


STATE (s_t)
REWARD (r_t)
s_{t+1}
r_{t+1}
ENVIRONMENT
AGENT
POLICY (π)
ACTION (a_t)

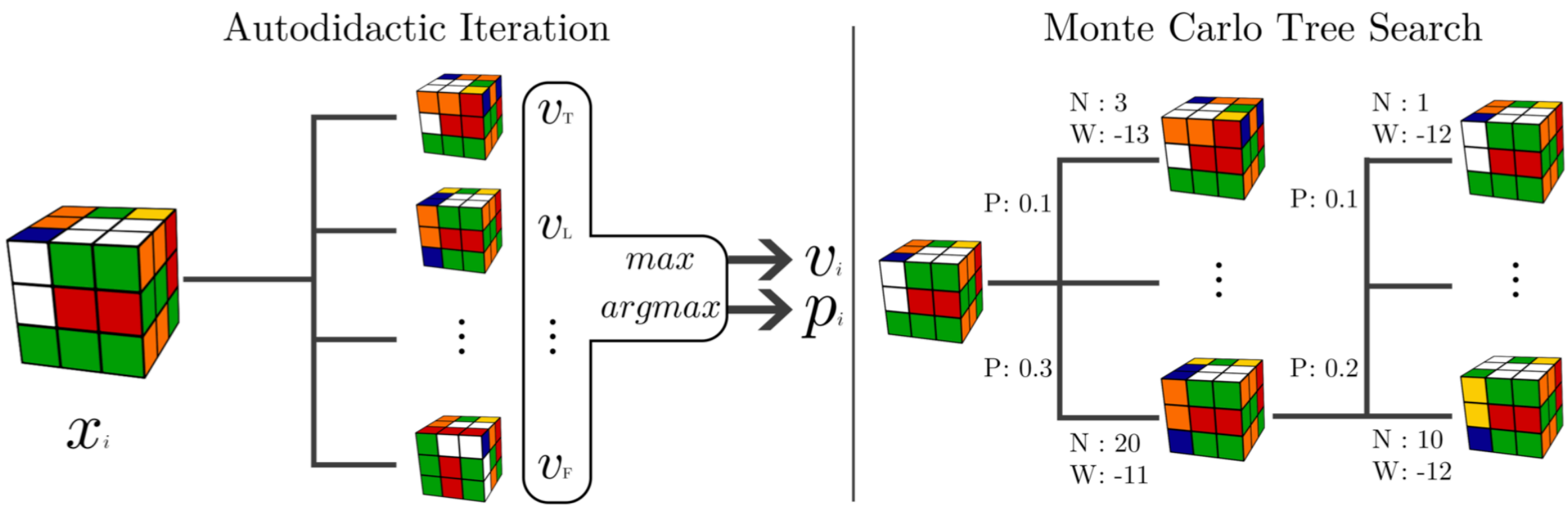
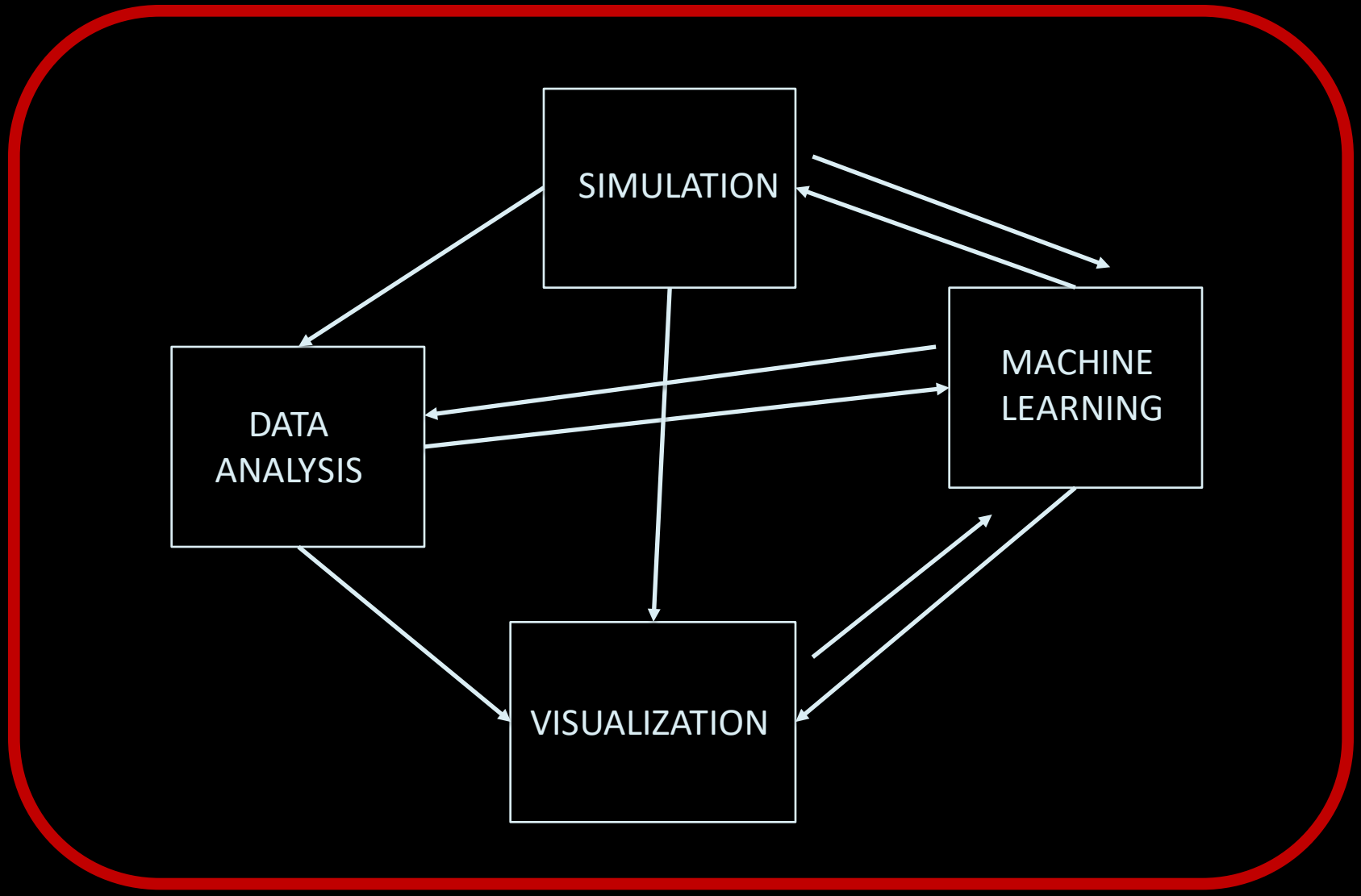


Figure 1: An illustration of DeepCube. The training and solving process is split up into ADI and MCTS. First, we iteratively train a DNN by estimating the true value of the input states using breadth-first search. Then, using the DNN to guide exploration, we solve cubes using Monte Carlo Tree Search. See methods section for more details.

The New HPC + AI "Paradigm"



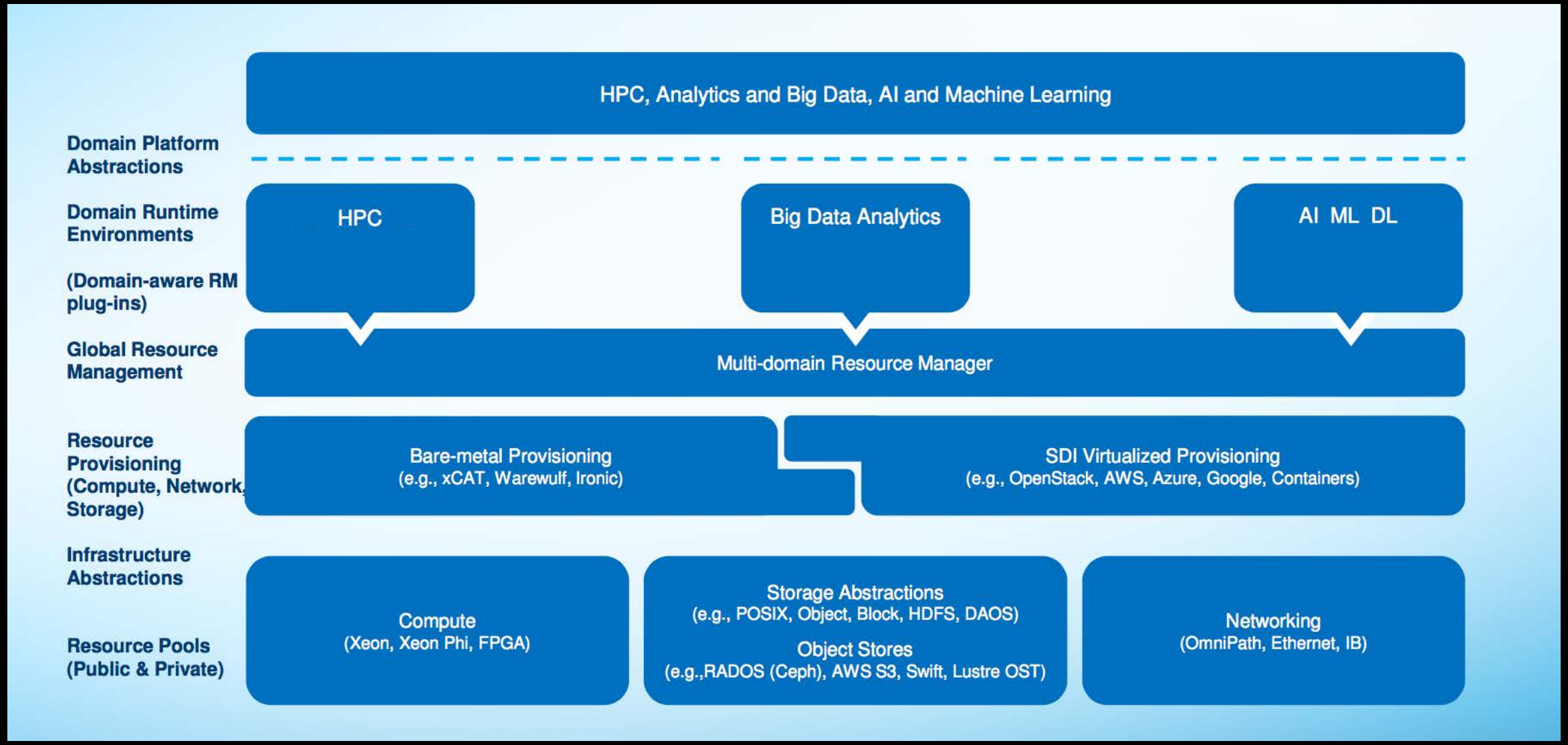
Exascale Programming

- MPI + X { where X could be OpenMP, CUDA, other (UPC) + libraries }
- C/C++ is likely ahead of Fortran for software support
- Think ~10K separate address spaces via message passing
- Think ~100 CPU threads per address space
- Think 4-16 accelerator contexts per node address space
- Some support for data objects + traditional filesystem I/O
- Manual checkpointing (system MTBF < ~4 days)
- In most cases > 90% of the flops are in the accelerator
- In most cases > 4x-8x of the memory bandwidth is in the accelerator

Exascale Software Stack

- Single Unified stack with resource allocation and scheduling across all pillars and ability for frameworks and libraries to seamlessly compose
- Minimize data movement: keep permanent data in the machine via distributed persistent memory while maintaining availability requirements
- Support standard file I/O and path to memory coupled model for Sim, Data and Learning
- Isolation and reliability for multi-tenancy and combining workflows

Towards an Integrated Sim, Data, Learn Stack



Goal 2025 Automate and Accelerate

High Throughput Laboratory Synthesis, Characterization, Imaging

- **Data Generation**
- ***In Vitro* and *In Vivo* Experiments**
- **Hypothesis Testing**

High Performance Computing and Accelerated Machine Learning

- **Data Analysis**
- **Simulation + Machine Learning**
- **Experimental Design + Uncertainty Quantification**

Acknowledgements

Many thanks to DOE, NSF, NIH, DOD, ANL, UC, Moore Foundation, Sloan Foundation, Apple, Microsoft, Cray, Intel and IBM for supporting my research group over the years