GTC UPDATE
- MODULUS & CUQUANTUM

JAY CHEN | DATA SCIENTIST, APRIL 2022.

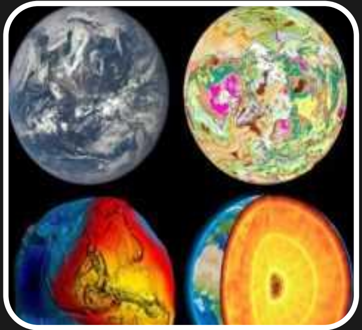
NVIDIA MODULUS

- An AI-Accelerated Multi-Physics Simulation Framework

COMPUTATIONAL DOMAINS

Computational Eng.

Solid & Fluid Mechanics,
Electromagnetics,
Thermal, Acoustics,
Optics, Electrical,
Multi-body Dynamics,
Design Materials



Earth Sciences

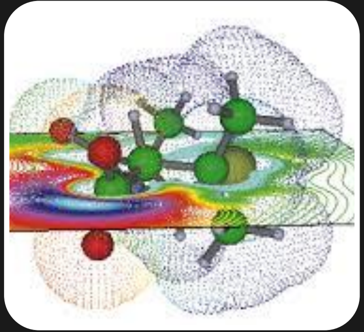
Climate Modeling,
Weather Modeling,
Ocean Modeling,
Seismic Interpretation

Life Sciences

Genomics,
Proteomics

Computational Physics

Particle Science,
Astrophysics

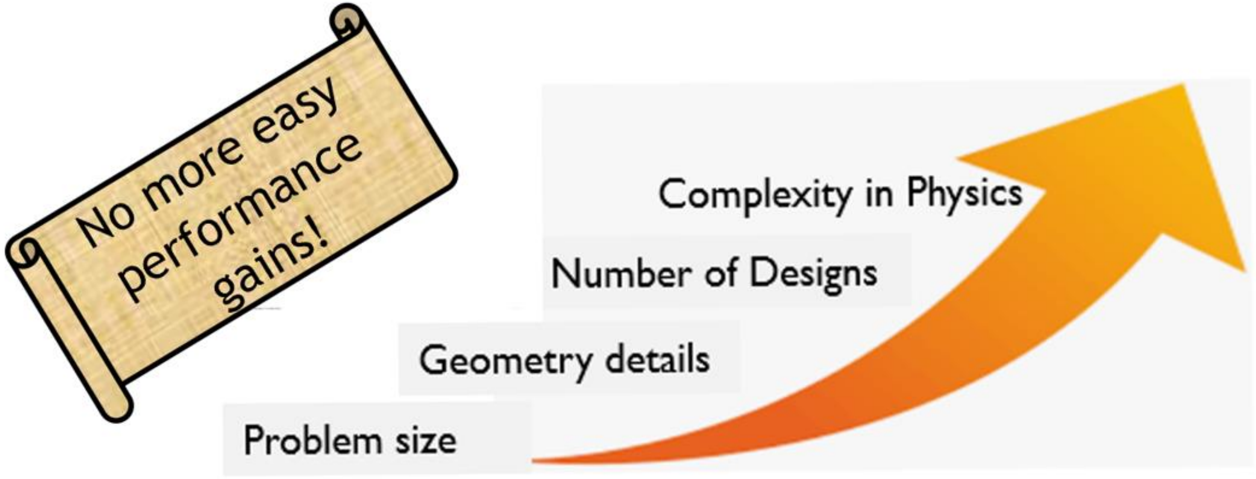


Computational Chemistry

Quantum Chemistry,
Molecular Dynamics

SATURATING PERFORMANCE IN TRADITIONAL HPC

Simulations are getting larger & more complex



Traditional simulation methods are:

- Computationally expensive
- Demand ever-increasing resolution
- Plagued by domain discretization techniques
- Not suitable for data-assimilation or inverse problems

MILLION-X CLIMATE SCIENCE

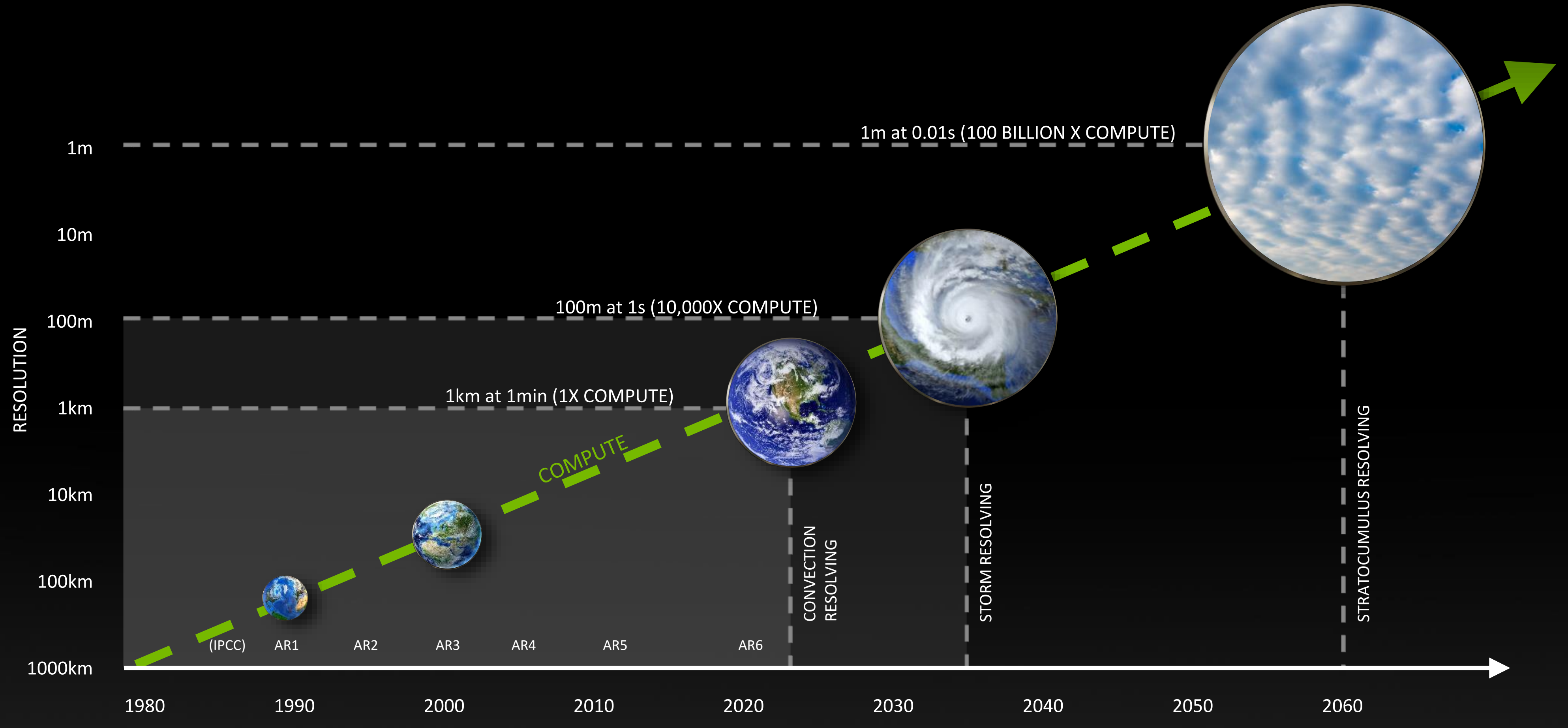
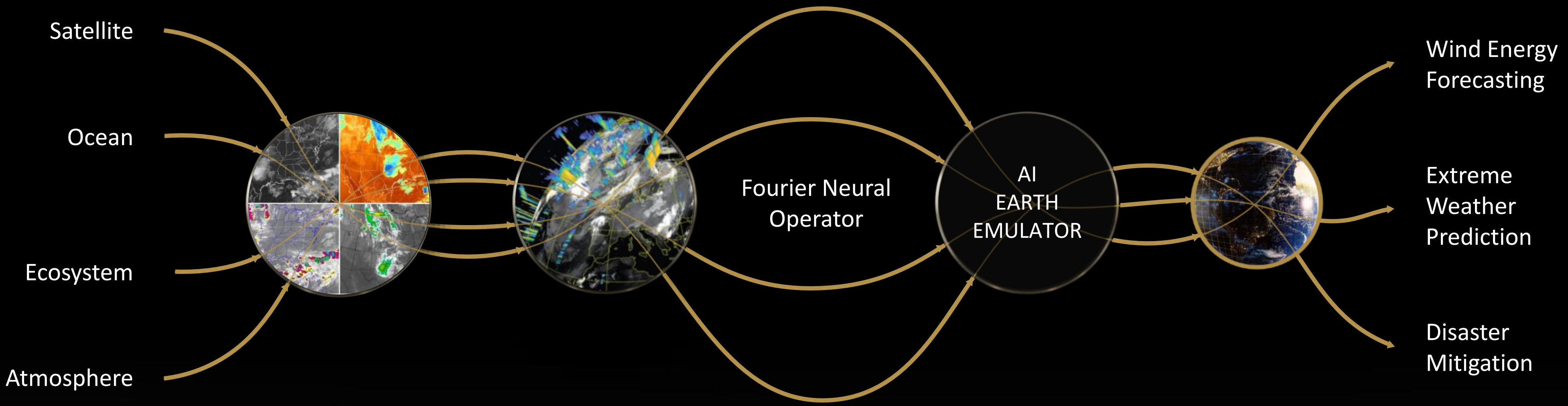


Figure adapted from: Schneider, T., Teixeira, J., Bretherton, C. *et al.* Climate goals and computing the future of clouds. *Nature Clim Change* **7**, 3–5 (2017). https://doi.org/10.1038/nclimate3190

ACCELERATING EXTREME WEATHER PREDICTION WITH FOURCASTNET

EARTH DIGITAL TWIN IN OMNIVERSE



ERA5 ECMWF
Atmospheric Winds & Geopotential
10 TB | 30km | 5 Atmos Layers

100,000X Speed-Up
2 Seconds for 7-Day Forecast
Training: 16 Hours on 64 A100 GPUs

Digital Twin
Interactivity & Verification

RAPIDS — Modulus — Omniverse

DATA PROCESSING — **AI-SIMULATION** — **VISUALIZATION**

AI IN COMPUTATIONAL SCIENCES

Primary Driver: Data vs. Physics

Physics ← No Physics

Forward Solution	Data Assimilation	Data Driven

No Data → Big Data

Traditional Numerical Solvers

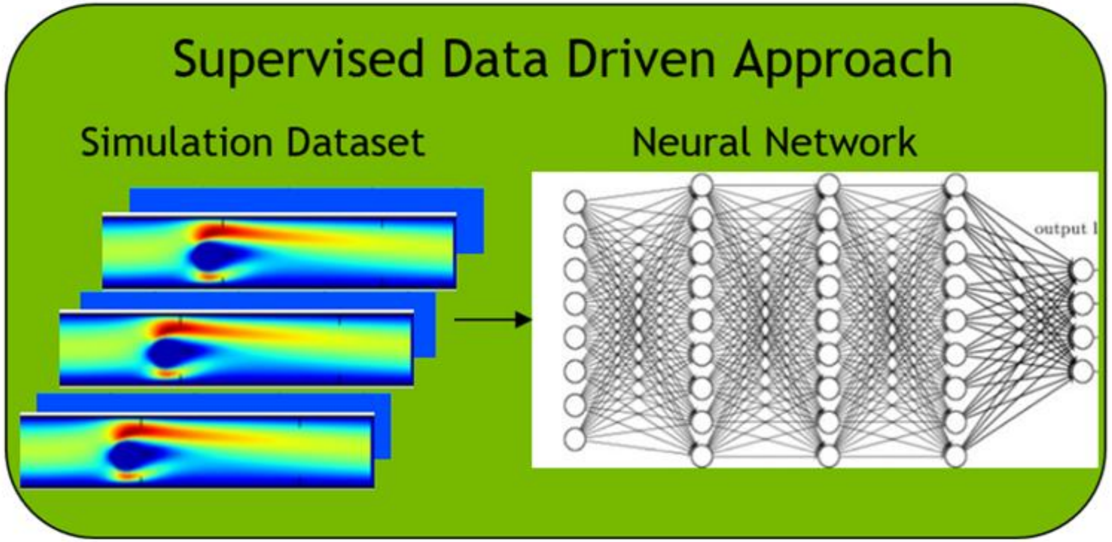
Modulus

NVIDIA Modulus

Solving PDEs with neural networks

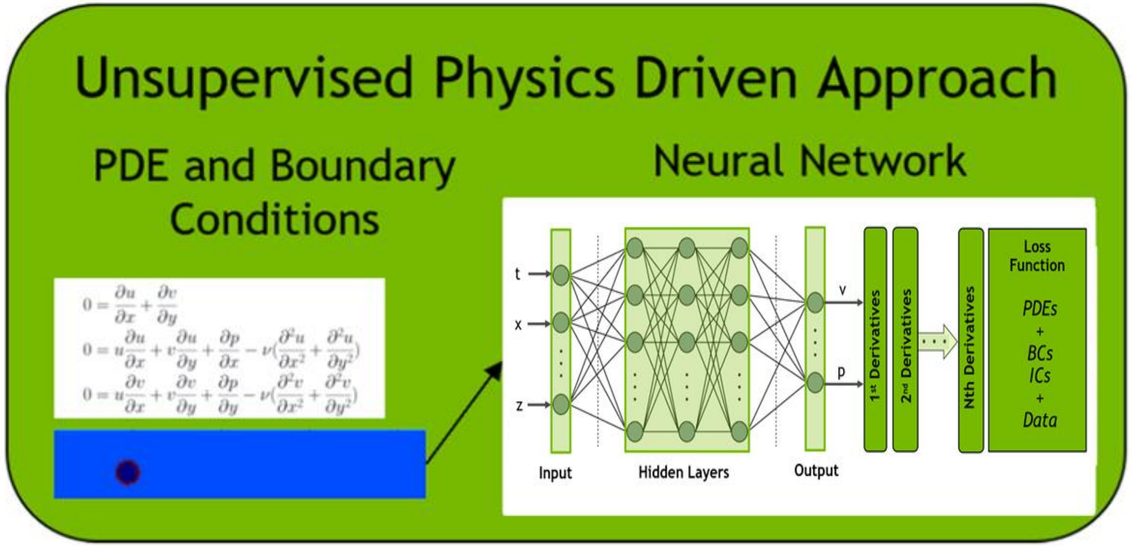
https://docs.nvidia.com/deeplearning/modulus/index.html

A **Data Driven Neural Network** requires training data



N layers

A **Physics Driven Neural Network** solver does **NOT** require training data

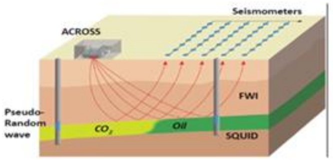


m*N layers (for m^th^ order PDE)

AI ENABLING NEXT GENERATION SIMULATION

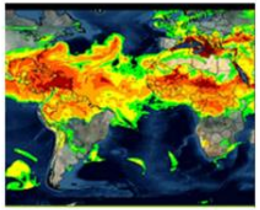
Single Simulation

Inverse & Data Assimilation Problems



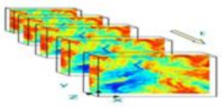
Oil & Gas

Medical Imaging

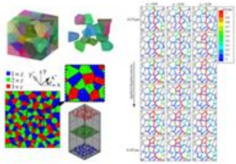


Climate

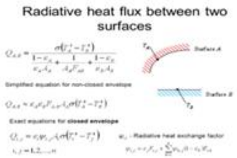
Improved Physics & Predictions



Turbulence



Micro-mechanical Material Model

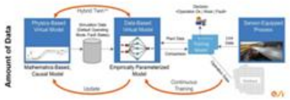


Radiation

Multiple Simulations

Real Time Simulations

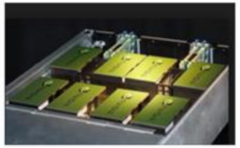
Robotics



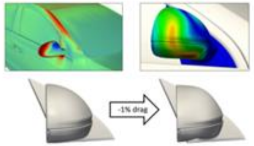
Digital Twin

Autonomous Ride & Handling

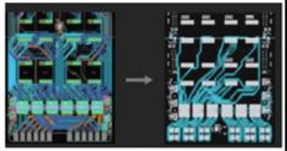
Digital Design & Manufacturing



Heat Sink



Aerodynamics



Vias on a PCB

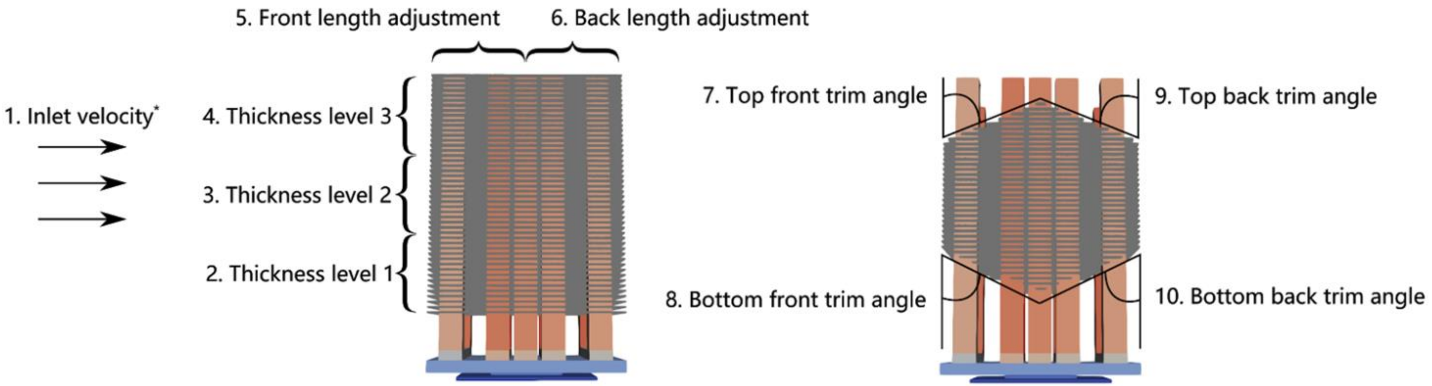
Physics & Data - No Traditional Solver

Physics - Traditional Solver (Speed is a limitation)

PARAMETERIZED A100 NVSWITCH HEAT SINK

Optimization with 10 Design Parameters

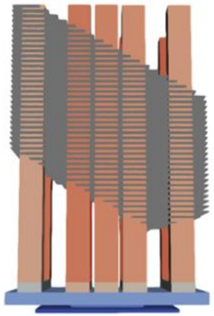
Limerock Design Variables



*Inlet velocity is not a design variable. It will be used for robust design optimization of Limerock in future.

Limerock Optimal Design

1. Inlet velocity: 5.7 m/s
2. Thickness level 1: 0.0031
3. Thickness level 2: 0.0044
4. Thickness level 3: 0.0030
5. Front length adjustment: -0.0124
6. Back length adjustment: 0.0025
7. Top front trim angle: 0.0223 rad
8. Bottom front trim angle: 0.5197 rad
9. Top back trim angle: 0.5147 rad
10. Bottom back trim angle: 0.2217 rad

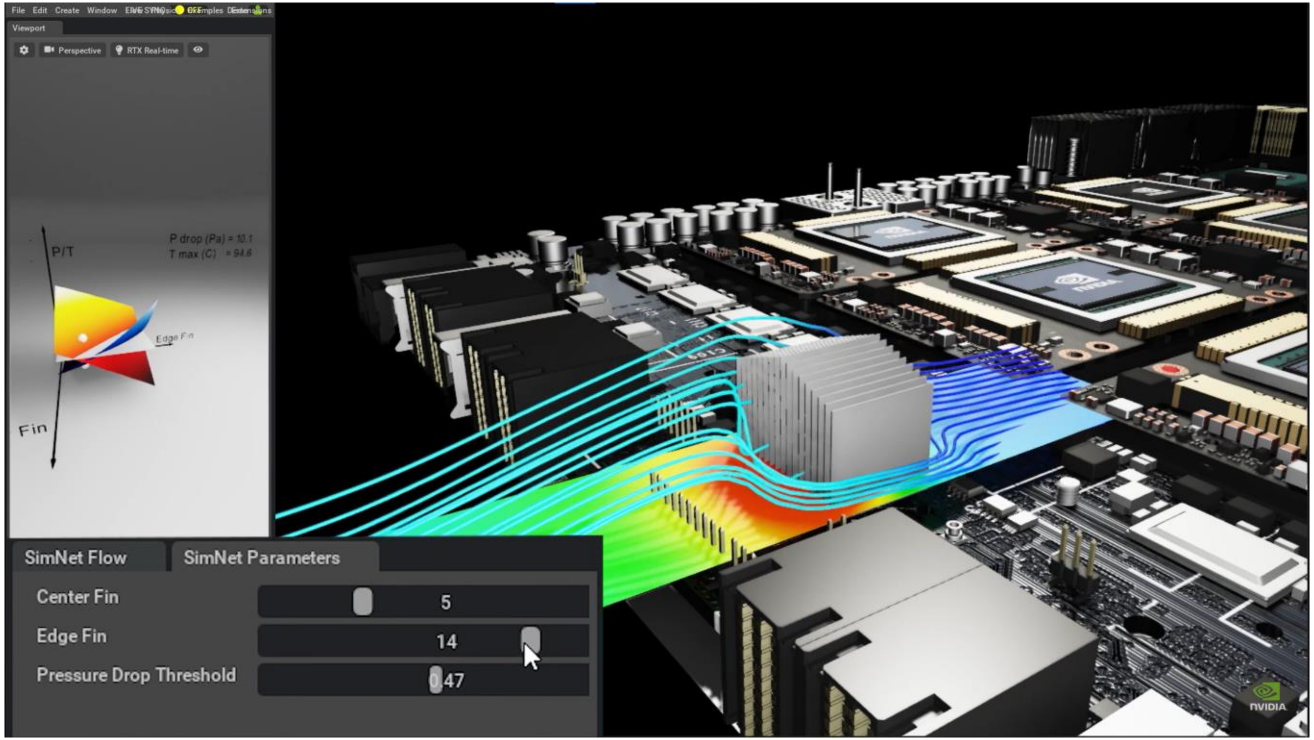


Max allowed pressure drop: 2.59
Number of random design evaluations: 4M

Peak temperature: 38.25 degC
Pressure drop: 2.5896

A100 NVSWITCH HEAT SINK

Multi-Physics Application: Fluids + Heat Transfer

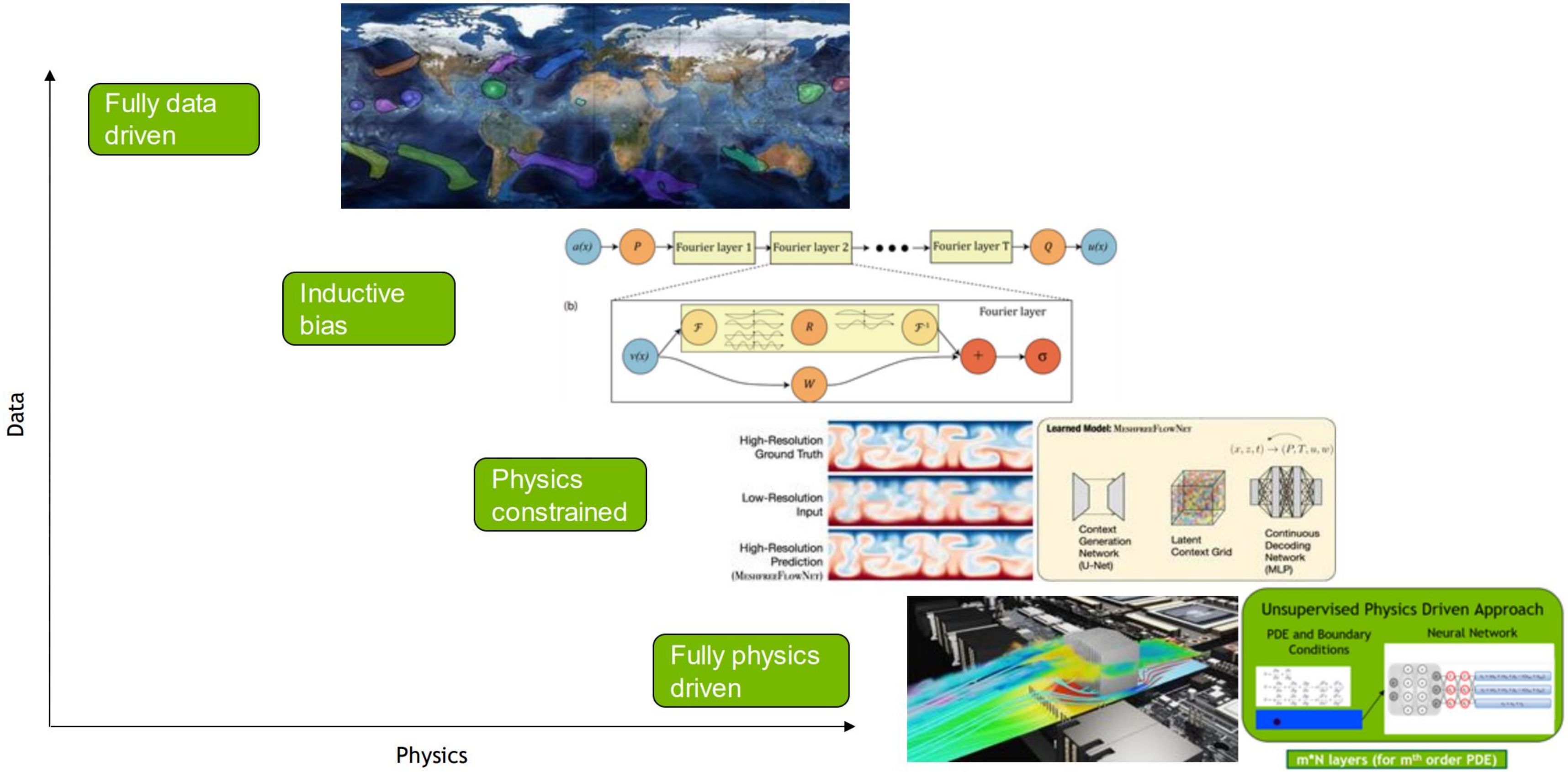


https://www.youtube.com/watch?v=Oq2Mpi5pF1w&ab_channel=NVIDIADeveloper

Turbulent Flow (Re=19,000)		
	Temperature	Pressure Drop
SimNet - Fourier Network	43.1 °C	4.05
OpenFOAM (method 1)	41.6 °C	3.56
OpenFOAM (method 2)	41.6 °C	4.58
Computational Times (10 parameters, 3 values per parameter)		
Modulus	1000 V100 GPU hrs.	
~=18000x speedup		
Traditional Solver (OpenFOAM) 59,049 separate runs (26 wall hours on 12 CPU cores)	18.4 Million CPU hrs.	

NVIDIA MODULUS TEAM @ GTC 22

https://www.nvidia.com/en-us/on-demand/session/gtcspring22-s41823/



NATIONAL ENERGY TECH LAB @ GTC 22

https://www.nvidia.com/en-us/on-demand/session/gtcspring22-s41325/

PINN for reacting flows

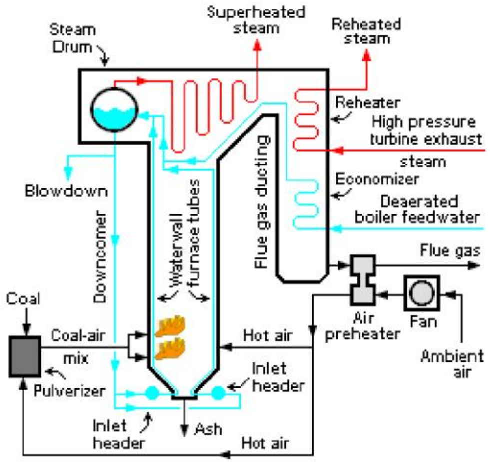
Formulation and PINN vs CFD

- **Aim:** Create a digital twin of an industrial scale boiler
- Simplified methane oxidation
- Implemented reacting flow transport equations for kinetics-controlled combustion
- No requirement for training data

★ Single PINN model for a range of input conditions

★ Fidelity and accuracy comparable to CFD

★ Trained PINN can provide near-instantaneous inference for any input condition



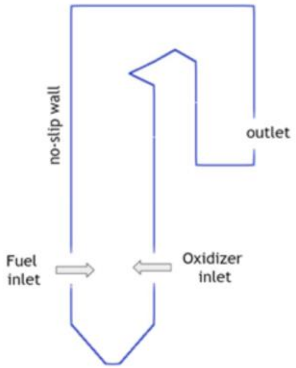
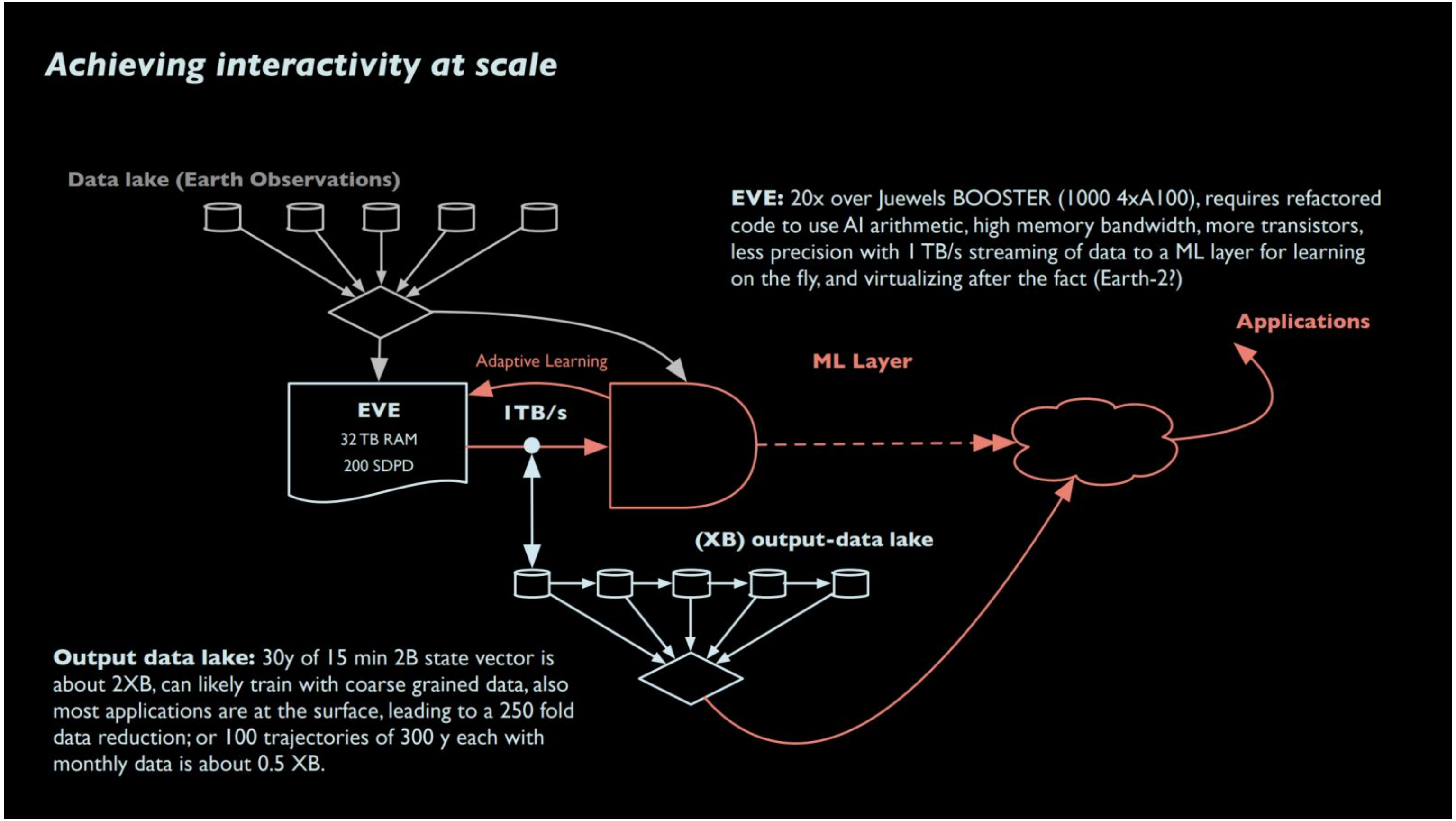


Figure source: https://commons.wikimedia.org/wiki/File:Steam_Generator.png

MAX PLANCK INSTITUTE FOR METEOROLOGY @ GTC 22

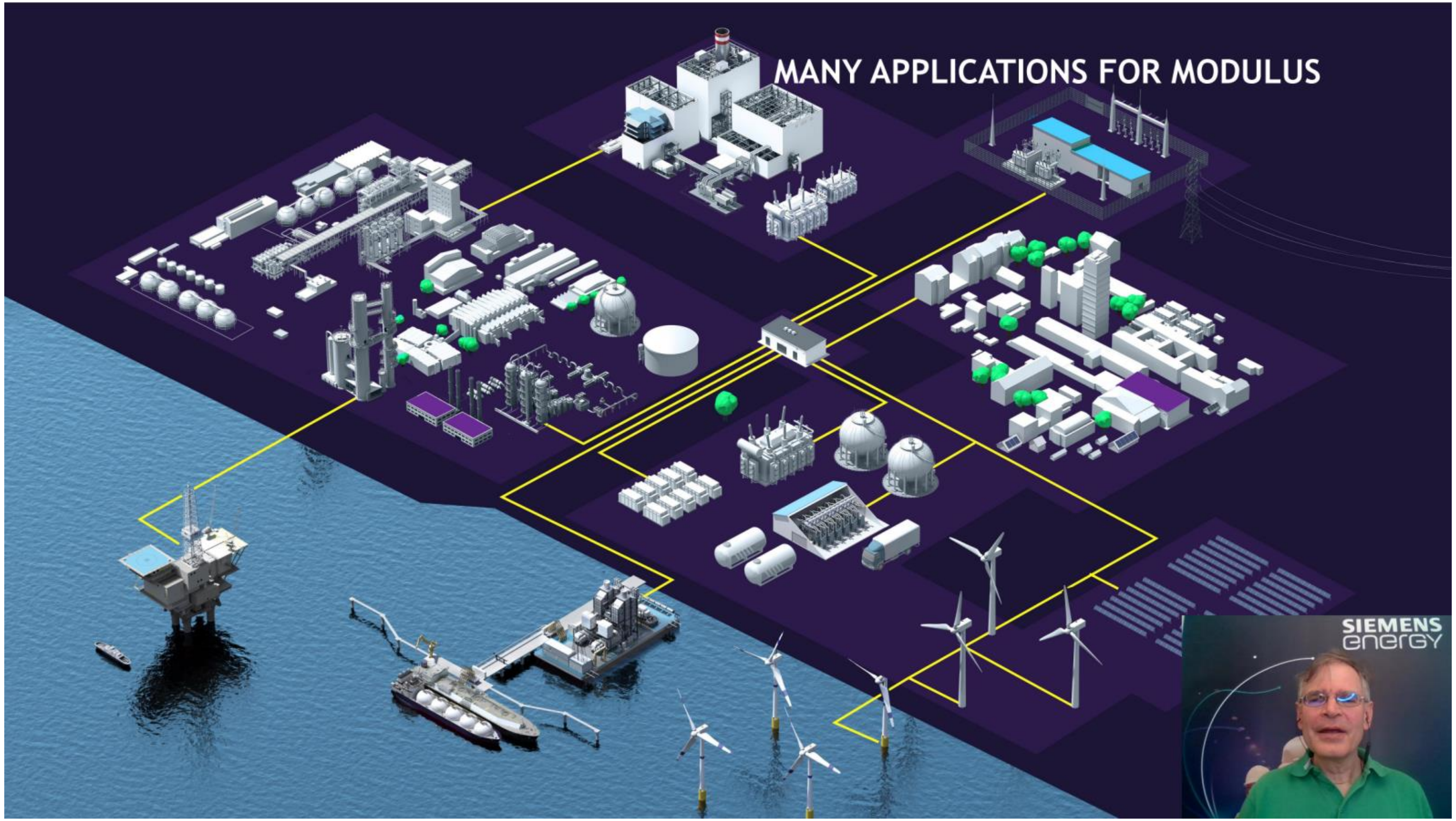
https://www.nvidia.com/en-us/on-demand/session/gtcspring22-s41950/

An Earth Virtualization Engine (EVE) - by Prof. Bjorn Stevens



SIEMENS ENERGY @ GTC 22

https://www.nvidia.com/en-us/on-demand/session/gtcspring22-s41671/
https://blogs.nvidia.com/blog/2021/11/15/siemens-energy-nvidia-industrial-digital-twin-power-plant-omniverse/

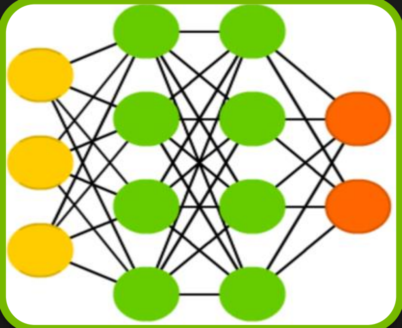


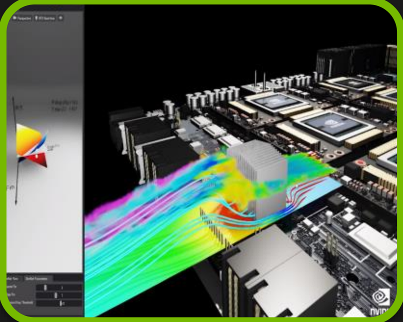
SIEMENS ENERGY HRSG DIGITAL TWIN SIMULATION USING NVIDIA MODULUS AND OMNIVERSE

MODULUS

AI-accelerated Physics Simulation Toolkit

https://docs.nvidia.com/deeplearning/modulus/index.html





Solve larger problems faster
XLA, AMP TF32
Multi-GPU
Multi-Node

Advanced Model
Multiple Physics
Forward
Inverse
Data Assimilation

Solve
multiple scenarios simultaneously

APIs for
Physics
Geometry
Domains

User Guide examples

NVIDIA CUQUANTUM

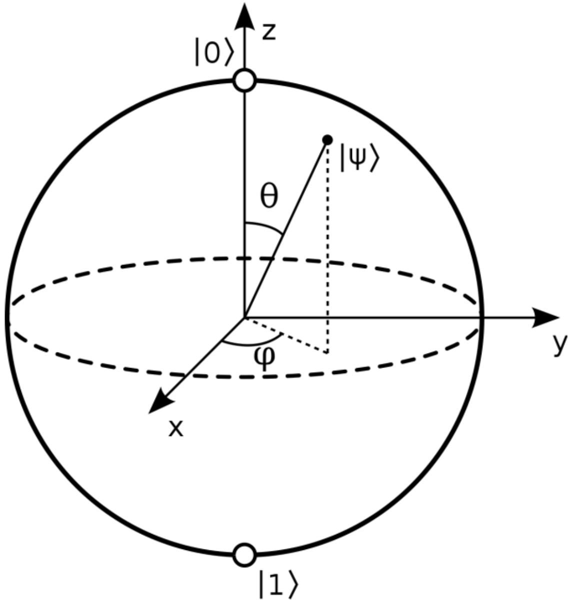
- A GPU-Accelerated Quantum Circuit Simulation Research Platform

QUANTUM COMPUTING BASICS OPERATIONS

Superposition and Measurement

Bit

Qubit



$$|\Psi\rangle = a|0\rangle + b|1\rangle = \begin{bmatrix} a \\ b \end{bmatrix}$$

Measurement: wavefunction collapse

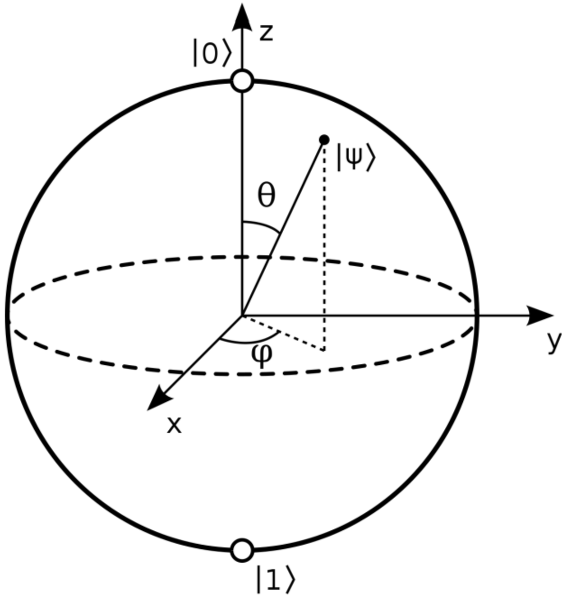
– measure only one state

$P_0 = |a|^2$

$P_1 = |b|^2$

QUANTUM COMPUTING BASICS OPERATIONS

Superposition and Measurement



0

0	1

1	0	1

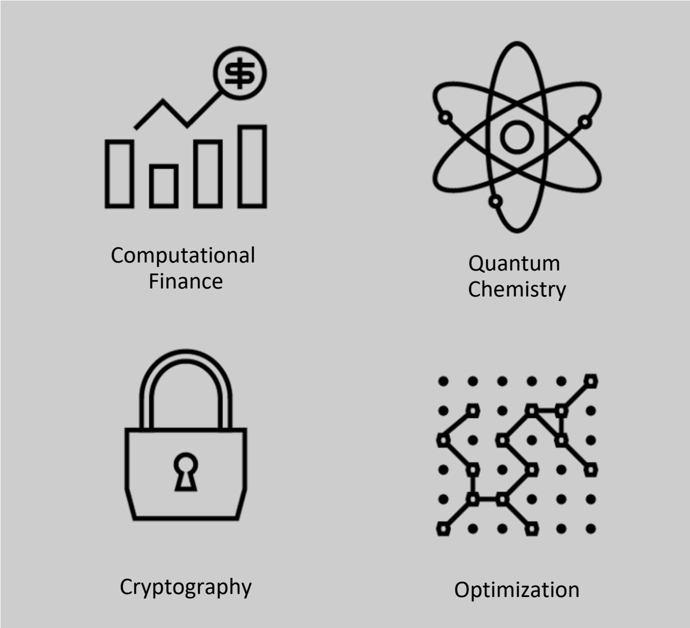
$$c_0|0\rangle + c_1|1\rangle = \begin{bmatrix} c_0 \\ c_1 \end{bmatrix}$$

$$c_{00}|00\rangle + c_{01}\,|01\rangle + c_{10}\,|10\rangle + c_{11}\,|11\rangle = \begin{bmatrix} c_{00} \\ c_{01} \\ c_{10} \\ c_{11} \end{bmatrix}$$

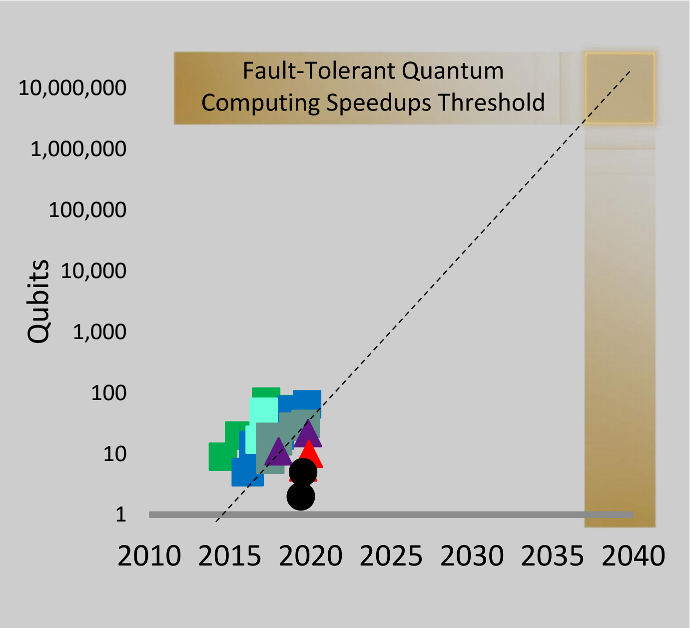
$$\begin{matrix} c_{000}|000\rangle + c_{001}\,|001\rangle + c_{010}\,|010\rangle + c_{011}\,|011\rangle \\ c_{100}|100\rangle + c_{101}\,|101\rangle + c_{110}\,|110\rangle + c_{111}\,|111\rangle \end{matrix} = \begin{bmatrix} c_{000} \\ c_{001} \\ c_{010} \\ c_{011} \\ c_{100} \\ c_{101} \\ c_{110} \\ c_{111} \end{bmatrix}$$

A NEW COMPUTING MODEL - QUANTUM

NEW COMPUTING MODEL



POTENTIAL USE CASES

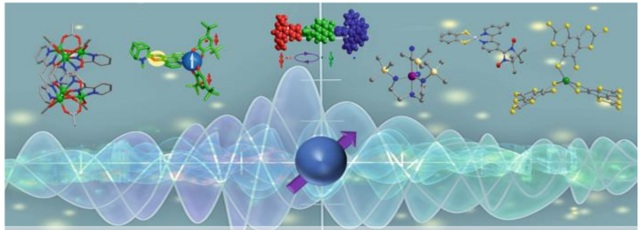


QUANTUM SYSTEMS SCALING EXPONENTIALLY

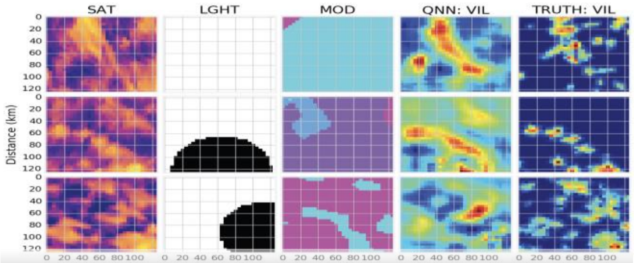
CUQUANTUM

Research the Computer of Tomorrow with the Most Powerful Computer Today

ENABLING SCIENTIFIC BREAKTHROUGHS



QC Ware: QChem Simulation on Perlmutter



Rigetti & NERSC: Quantum ML Climate Modeling on Perlmutter

ANNOUNCING NEW RELEASES & EXPANDING ECOSYSTEM

cuQuantum SDK
GA Release

cuQuantum DGX Appliance
Beta
Optimized Simulation Stack

Integrations w/ leading quantum computing frameworks

Quantum AI

IBM

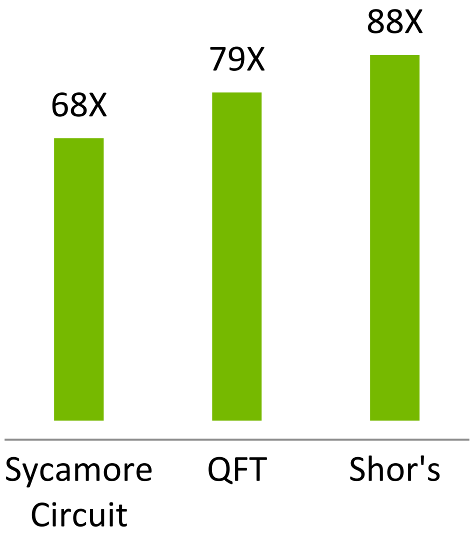
XANADU

OAK RIDGE National Laboratory

CLASSIQ

ZAPATA

70X SPEEDUP ON CUQUANTUM APPLIANCE

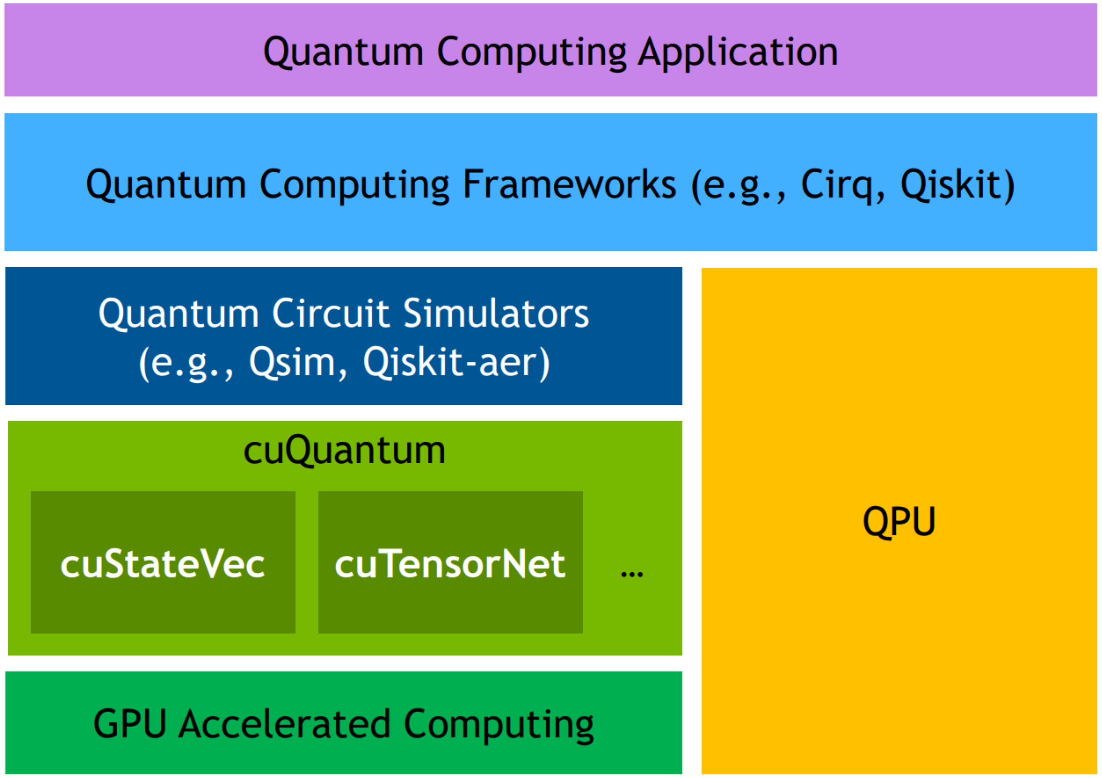


DGX Appliance gains over Dual Core CPU

Introducing cuQuantum

- cuQuantum is a platform for quantum computing research
  - Accelerate Quantum Circuit Simulators on GPUs
  - Simulate ideal or noisy qubits
  - Enable algorithms research with scale and performance not possible on quantum hardware, or on simulators today
- General Access available now, integrated
  - Google Cirq
  - IBM Qiskit
  - Xanadu PennyLane
- DGX Quantum Appliance now available on NGC

Cirq Qiskit Pennylane




NVIDIA