Accelerating Time-To-Science in Geophysical Simulations

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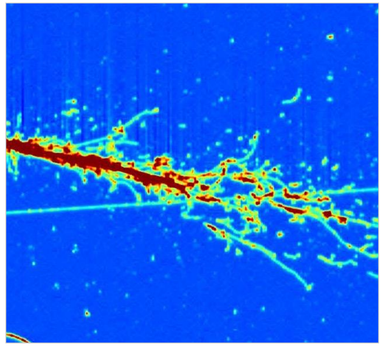
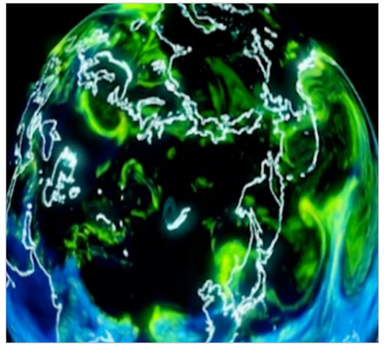
HPC Enabling Scientific and Industrial Achievements

PARTICLE PHYSICS
New Fundamental Particles

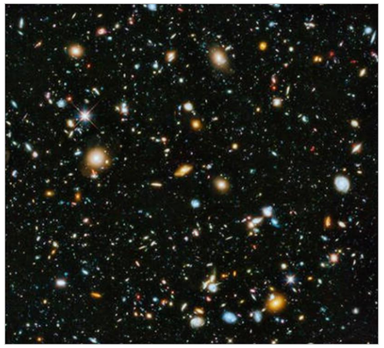


WEATHER & CLIMATE
FourCastNet

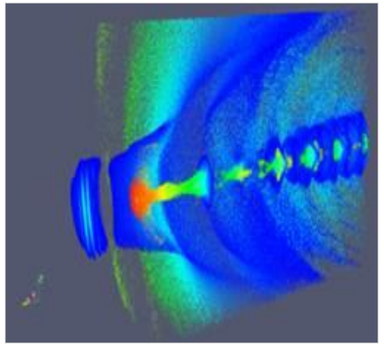


GENOMICS
Record DNA Sequencing

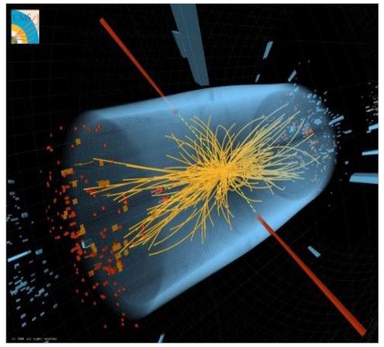
COSMOLOGY
ID Dark Matter



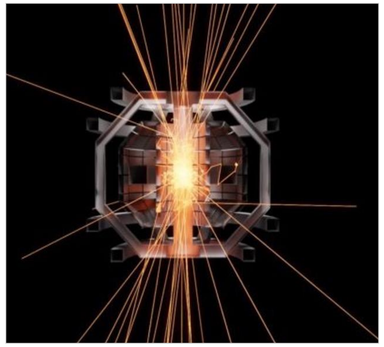
RADIOLOGY
GB: Laser Electron Accelerators



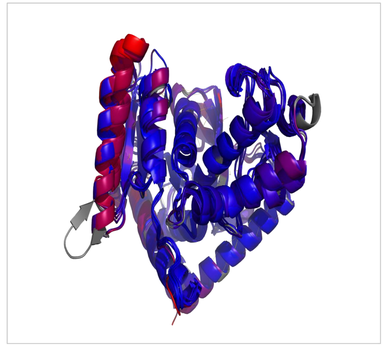
HIGH ENERGY PHYSICS
Collision Reconstruction



ENERGY
Plasma Modeling with FNO

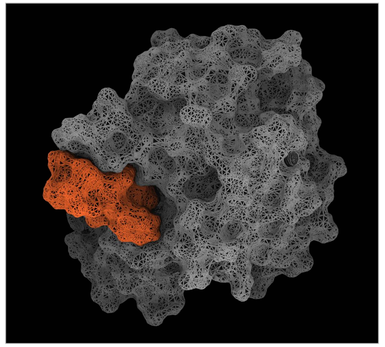


VIRUS PATHOLOGY
GB Finalist: CoVID variant classifier



ASTROPHYSICS
DL Classifies Distant Galaxies

LIFE SCIENCES
GB: Protein Similarity Search



2700+ GPU-Accelerated Applications

Plus many accelerated frameworks!

ARTIFICIAL INTELLIGENCE

- PyTorch
- TensorFlow
- JAX

...

CLIMATE & WEATHER

- Cosmos
- Gales
- WRF

...

COMPUTATIONAL FINANCE

- O-Quant Options Pricing
- MUREX
- MISYS

...

DATA SCIENCE & ANALYTICS

- Anaconda
- H20
- OmniSci

...

FEDERAL DEFENSE & OTHER

- ArcGIS Pro
- EVNI
- SocetGXP
- Cyllance
- FaceControl

...

LIFE SCIENCES

- Amber
- LAMMPS
- GROMACS
- NAMD
- Relion
- VASP

...

MANUFACTURING, CAD, & CAE

- Ansys Fluent
- Abaqus SIMULIA
- AutoCAD
- CST Studio Suite

...

MEDIA & ENTERTAINMENT

- DaVinci Resolve
- Premiere Pro CC
- Redshift Renderer

...

MEDICAL IMAGING

- aidoc
- PowerGrid
- RadiAnt

...

OIL & GAS

- Echelon
- RTM
- SPECFEM3D

...

RETAIL

- Everseen
- Deep North
- Third Eye Labs
- AWM
- Malong
- Clarifai
- Antuit

...

SUPERCOMPUTING & HER

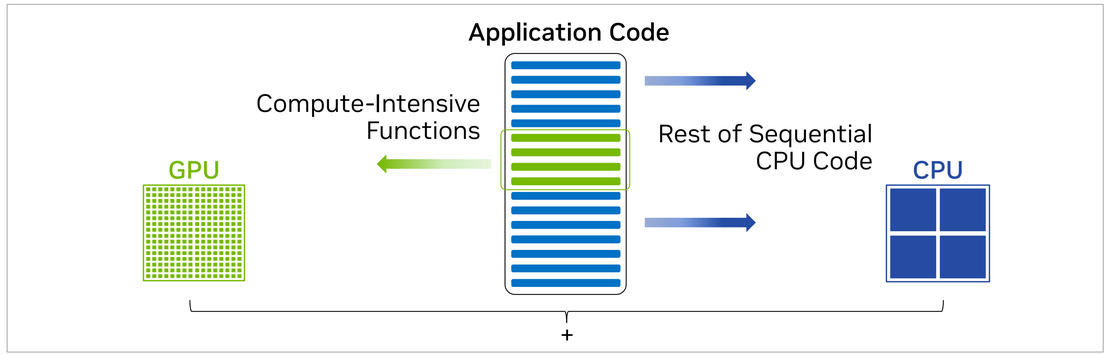
- Chroma
- GTC
- MILC
- QUDA
- XGC

...

For a comprehensive list of all apps, please refer to GPU application catalog: https://www.nvidia.com/content/dam/en-zz/Solutions/Data-Center/tesla-product-literature/gpu-applications-catalog.pdf

Why Accelerated Computing is Energy Efficient

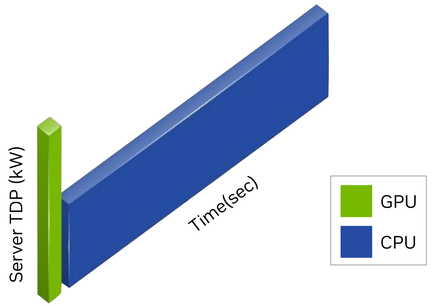
Hardware, Software, & Networking to Optimize Performance & Efficiency



Moving Compute Intense Sections to the GPU

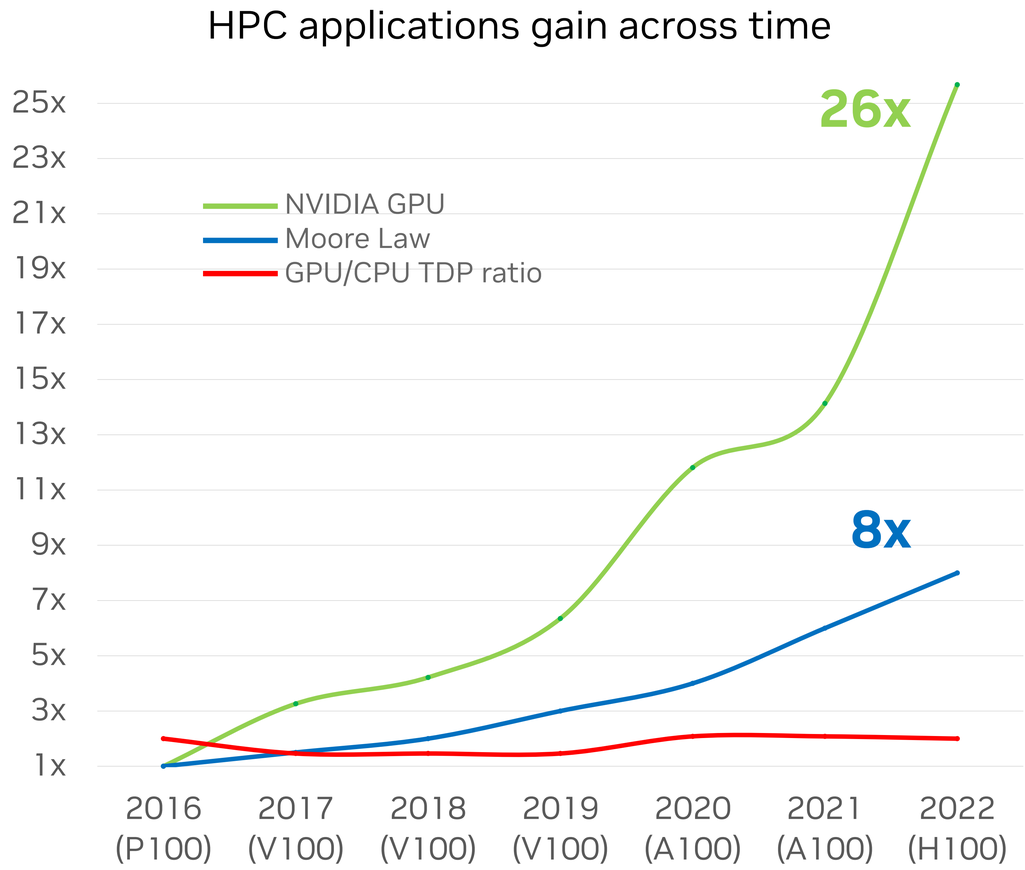
GPUs typically have **higher peak active power consumption** than CPUs

However, they complete workloads **significantly faster**



Energy Used in a Typical AI Inference Job

Consume Less Overall Energy



Center Panel: Geometric mean of application speedups vs. P100 | benchmark applications | Amber [PME-Cellulose_NVE], Chroma [HMC], GROMACS [ADH Dodec], MILC [Apex Medium], NAMD [stmv_nve_cuda], PyTorch (BERT Large Fine Tuner), Quantum Espresso [AUSURF112-jR]; TensorFlow [ResNet-50], VASP 6 [Si Huge], |GPU node: with dual-socket CPUs with 4x P100, V100, or A100 GPUs. H100 values shown for 2022 projected performance subject to change

NVIDIA H100

Unprecedented Performance, Scalability, and Security for Every Data Center

Highest AI and HPC Performance

4PF FP8 (6X)| 2PF FP16 (3X)| 1PF TF32 (3X)| 67TF FP64 (3.4X)
3.35TB/s (1.5X), 80GB HBM3 memory

Transformer Model Optimizations

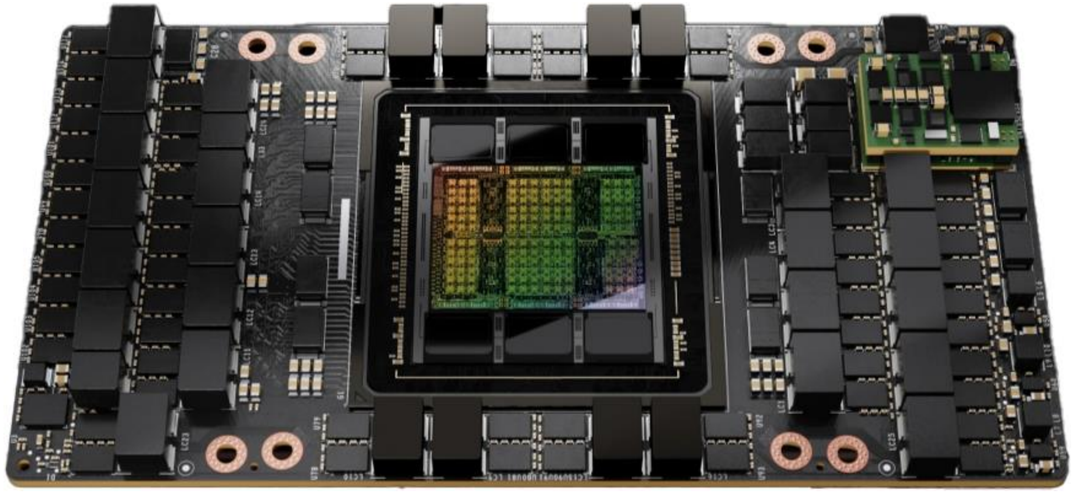
6X faster on largest transformer models

Highest Utilization Efficiency and Security

7 Fully isolated & secured instances, guaranteed QoS
2nd Gen MIG | Confidential Computing

Fastest, Scalable Interconnect

900 GB/s GPU-2-GPU connectivity (1.5X)
up to 256 GPUs with NVLink Switch | 128GB/s PCI Gen5



FP8, FP16, TF32 performance include sparsity. X-factor compared to A100

Programming the NVIDIA platform

CPU, GPU, and Network

ACCELERATED STANDARD LANGUAGES

ISO C++, ISO Fortran

```
std::transform(par, x, x+n, y, y,
    [=](float x, float y){ return y +
a*x; }
);
```

```
do concurrent (i = 1:n)
   y(i) = y(i) + a*x(i)
enddo
```

```
import cunumeric as np
…
def saxpy(a, x, y):
    y[:] += a*x
```

INCREMENTAL PORTABLE OPTIMIZATION

OpenACC, OpenMP

```
#pragma acc data copy(x,y) {
...
std::transform(par, x, x+n, y, y,
    [=](float x, float y){
        return y + a*x;
});
...
}
```

```
#pragma omp target data map(x,y) {
...
std::transform(par, x, x+n, y, y,
    [=](float x, float y){
        return y + a*x;
});
...
}
```

PLATFORM SPECIALIZATION

CUDA

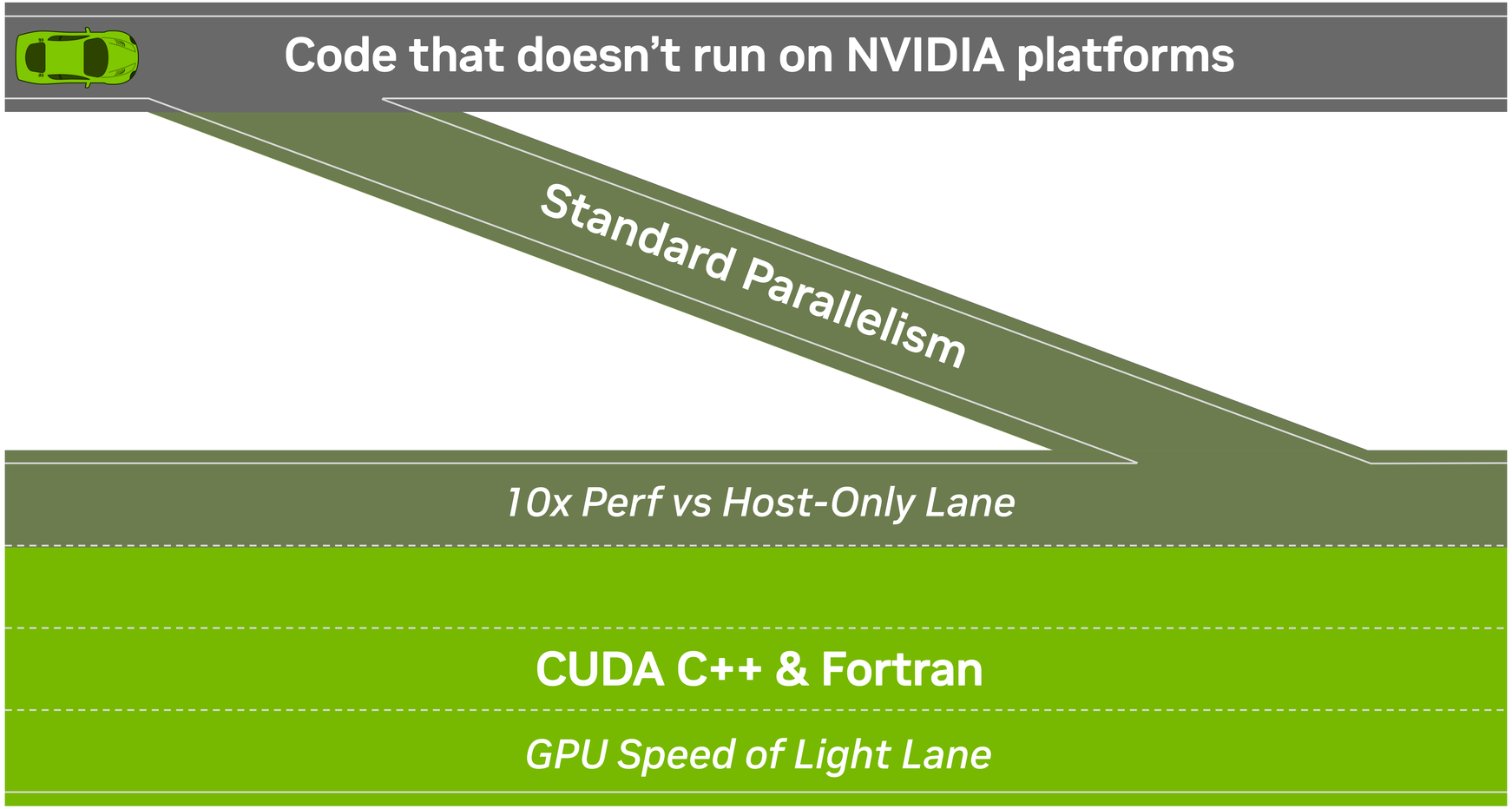
```
__global__
void saxpy(int n, float a,
            float *x, float *y) {
  int i = blockIdx.x*blockDim.x +
          threadIdx.x;
  if (i < n) y[i] += a*x[i];
}

int main(void) {
  ...
  cudaMemcpy(d_x, x, ...);
  cudaMemcpy(d_y, y, ...);

  saxpy<<<(N+255)/256,256>>>(...);

  cudaMemcpy(y, d_y, ...);
```

ACCELERATION LIBRARIES

Core	Math	Communication	Data Analytics	AI	Quantum

Scientists Need On-Ramps

Promote Parallelism, not Heterogeneity



Accelerated Standard Languages

Parallel performance for wherever your code runs

ISO C++

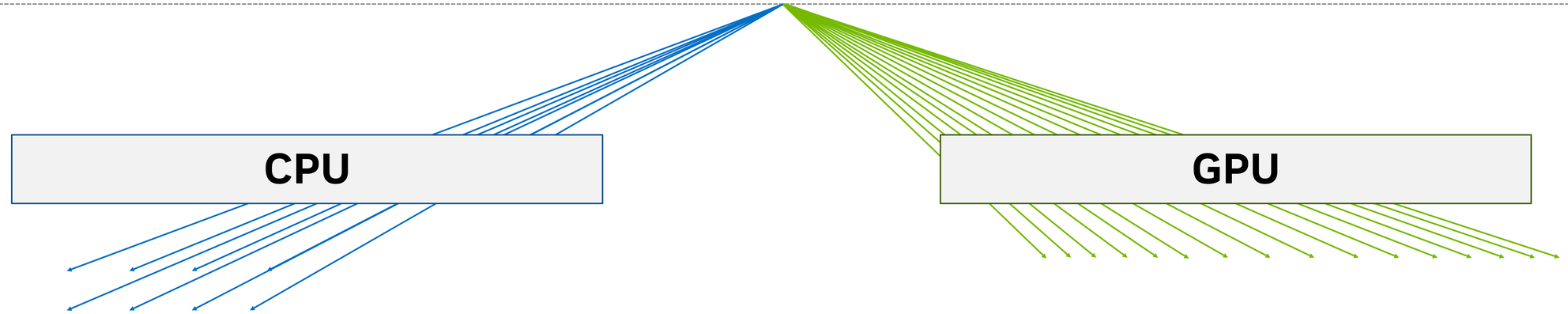
```
std::transform(par, x, x+n, y,
   y,[=](float x, float y){
      return y + a*x;
    }
);
```

ISO Fortran

```
do concurrent (i = 1:n)
   y(i) = y(i) + a*x(i)
enddo
```

Python

```
import cunumeric as np
…
def saxpy(a, x, y):
    y[:] += a*x
```

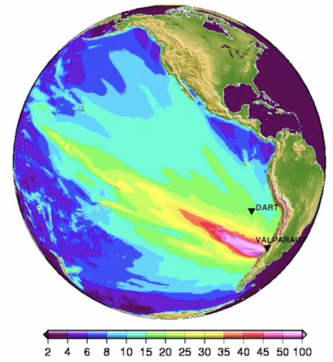


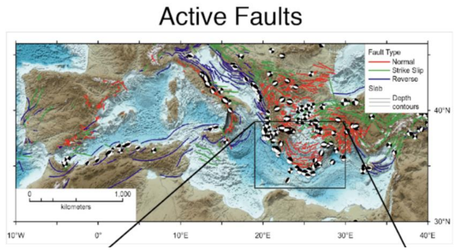

```
nvc++ -stdpar=multicore
nvfortran –stdpar=multicore
legate –cpus 16 saxpy.py
```

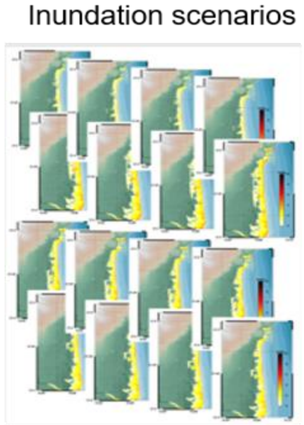
```
nvc++ -stdpar=gpu
nvfortran –stdpar=gpu
legate –gpus 1 saxpy.py
```

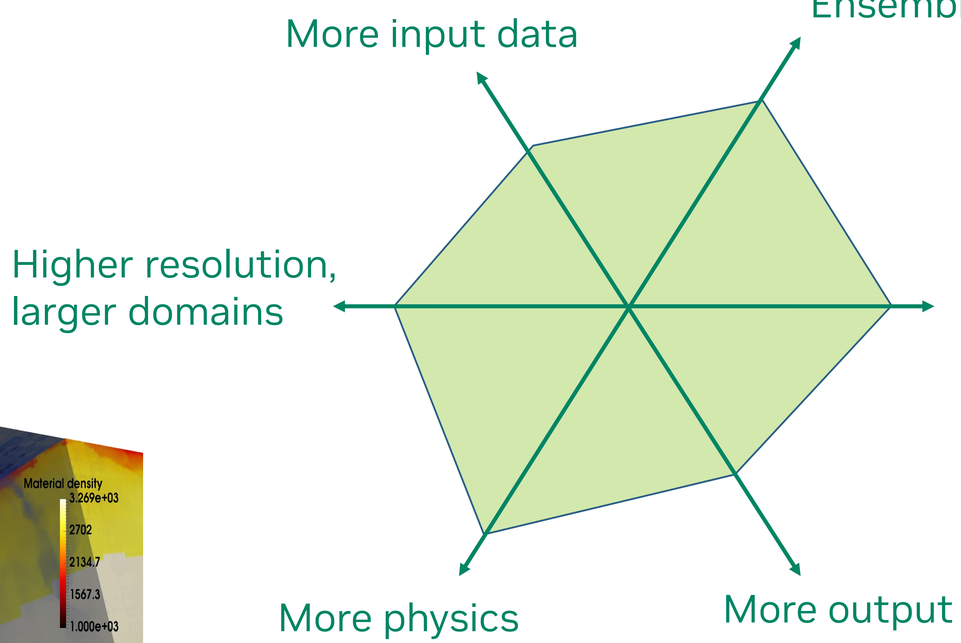
GPU Acceleration Enables Breakthrough New Science

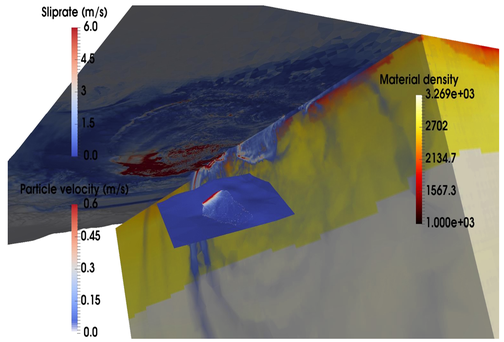
From **Petascale** (~10^4-10^5 CPU) to **Exascale** (×1000!)

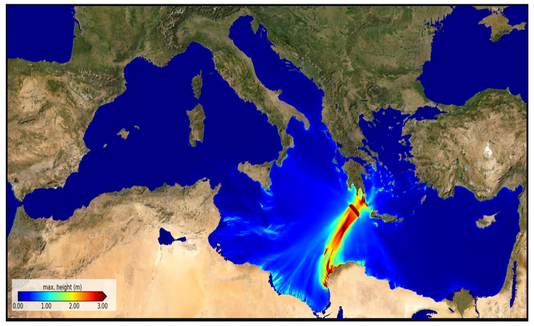










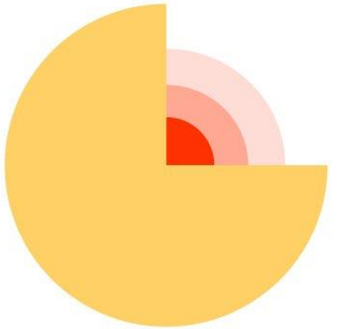


Data and visual assets courtesy of Stefano Lorito (INVG) and Manuela Volpe (INGV). Work supported by EU ChEESE Centre of Excellence in HPC Applications.

GPU-accelerated ChEESE applications

https://cheese-coe.eu/

Application	Programming Language	GPU	MPI+X
SeisSol	C/C++	Yes	CUDA
SPECFEM3D	Fortran	Yes	CUDA
ExaHyPE	C/C++	Partly	CUDA
xSHELLS	C/C++	Partly	CUDA
HySEA	C/C++	Yes	CUDA
FALL3D	Fortran	Yes	OpenACC



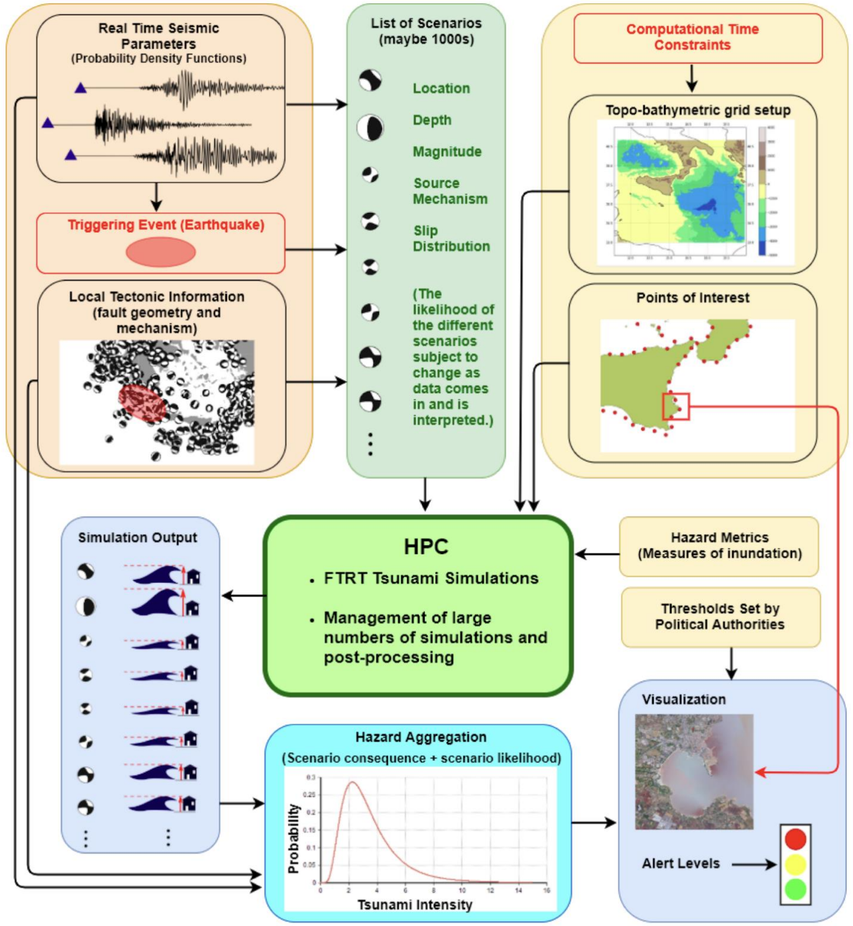
ChEESE

Center of Excellence for Exascale in Solid Earth

Data and visual assets courtesy of Piero Lanucara (CINECA) and Giorgio Amati (CINECA). Work supported by EU ChEESE Centre of Excellence in HPC Applications.

GPU-enabled ChEESE workflow

The ChEESE PD8: Probabilistic Tsunami Forecasting (PTF) for early warning and rapid post event assessment



Urgent computing workflow exercise on Marconi-100

Code: Tsunami-HySEA (TRL 6~7)

Scenario: On-the-fly simulations for POST-EVENT ASSESSMENT (tens of minutes) - NO Early Warning - the Samos Earthquake

- Simulation ensembles to be run from scratch on large enough HPC clusters in urgent computing mode.
- Provides exceedance probabilities for tsunami heights just off the coastline for almost equally spaced points of interest every 2 km in front of the coasts of the Mediterranean Sea

Outputs: ~38 000 scenario simulations

Resources: 805 nodes (3,220 V100 GPUs), ~25.7 PFlop/s

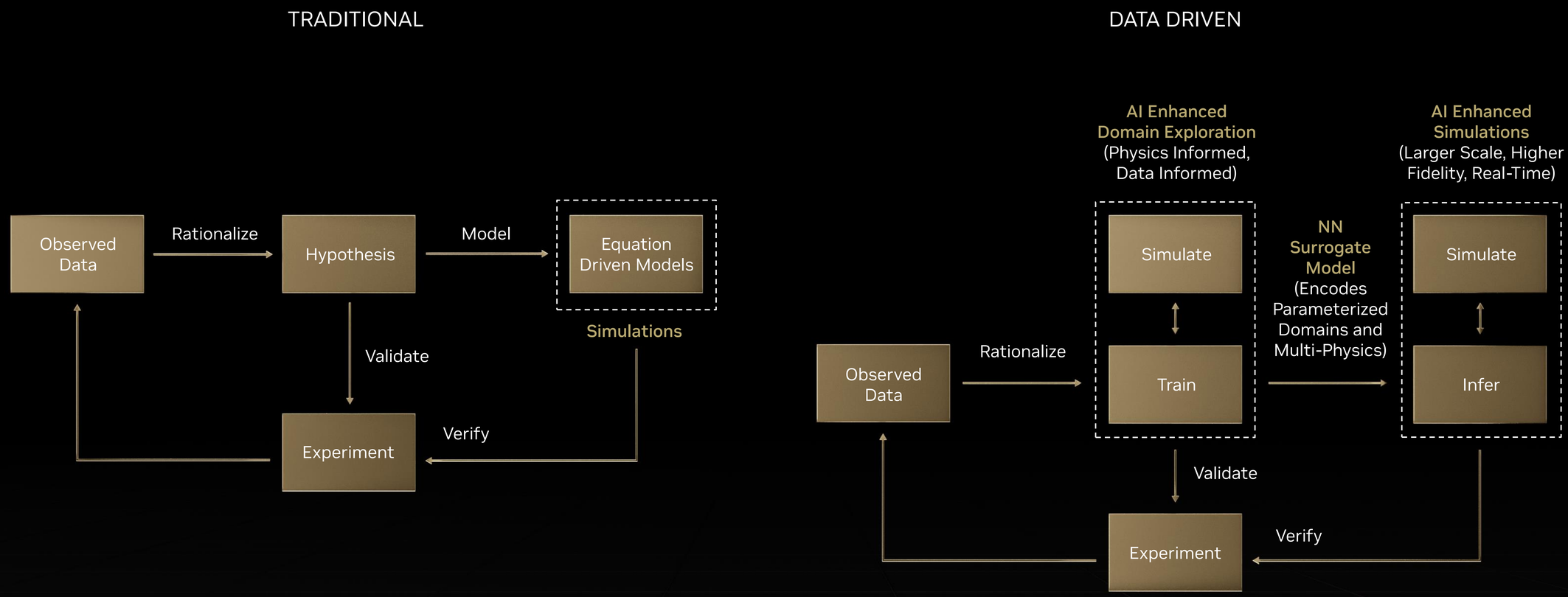
Data and visual assets courtesy of Stefano Lorito (INVG) and Manuela Volpe (INGV). Work supported by EU ChEESE Centre of Excellence in HPC Applications.

Beyond HPC

HPC+AI & Digital Twins

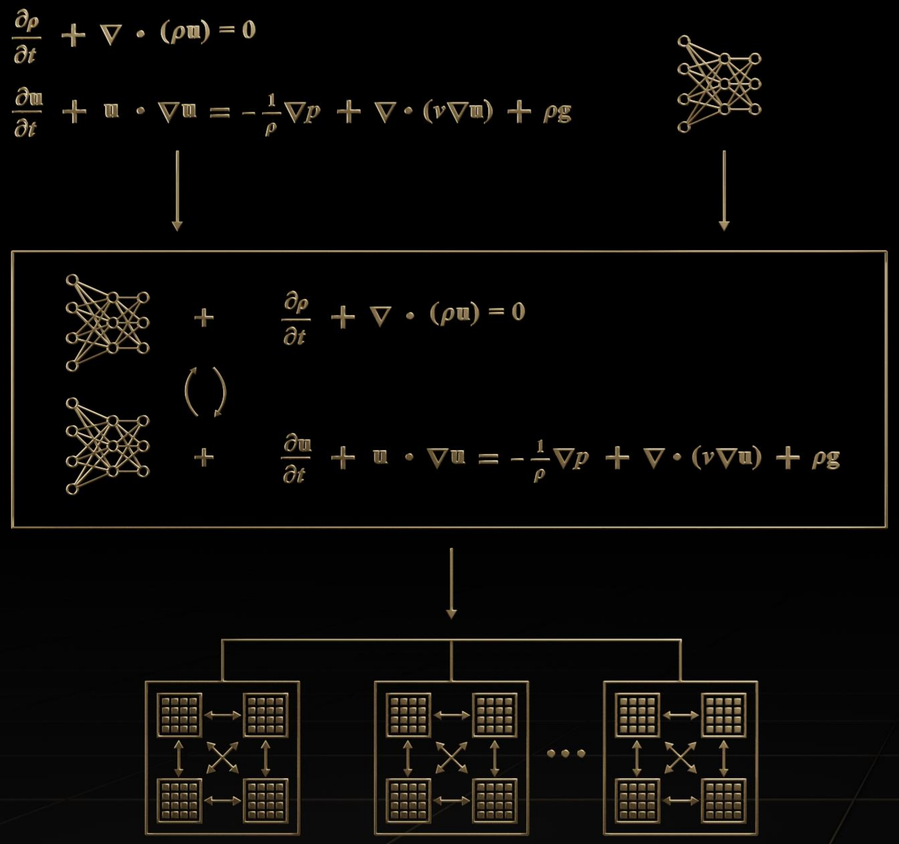
NVIDIA

AI IS THE 4TH PILLAR OF SCIENTIFIC DISCOVERY

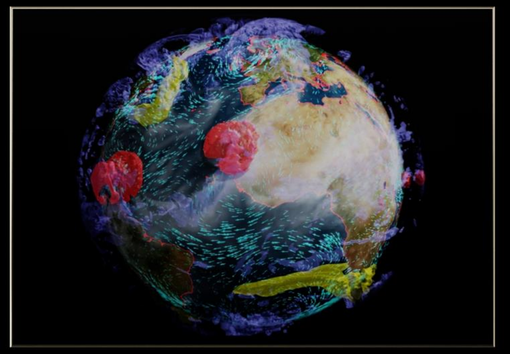


NVIDIA MODULUS

Shortcut to Surrogate Models for Interactive Simulation | Development Platform for AI Surrogate Models

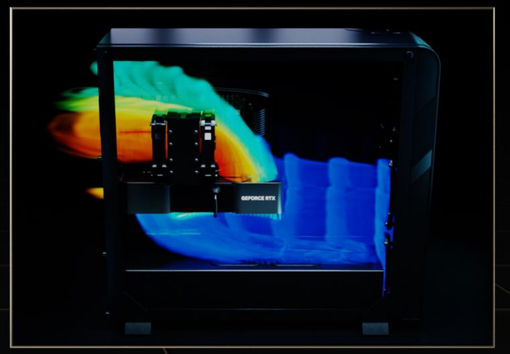


WEATHER & CLIMATE MODELING
FourCastNet



RENEWABLE ENERGY
Siemens Gamesa Wind Farm

PRODUCT DEVELOPMENT
Thermal Airflow Digital Twin

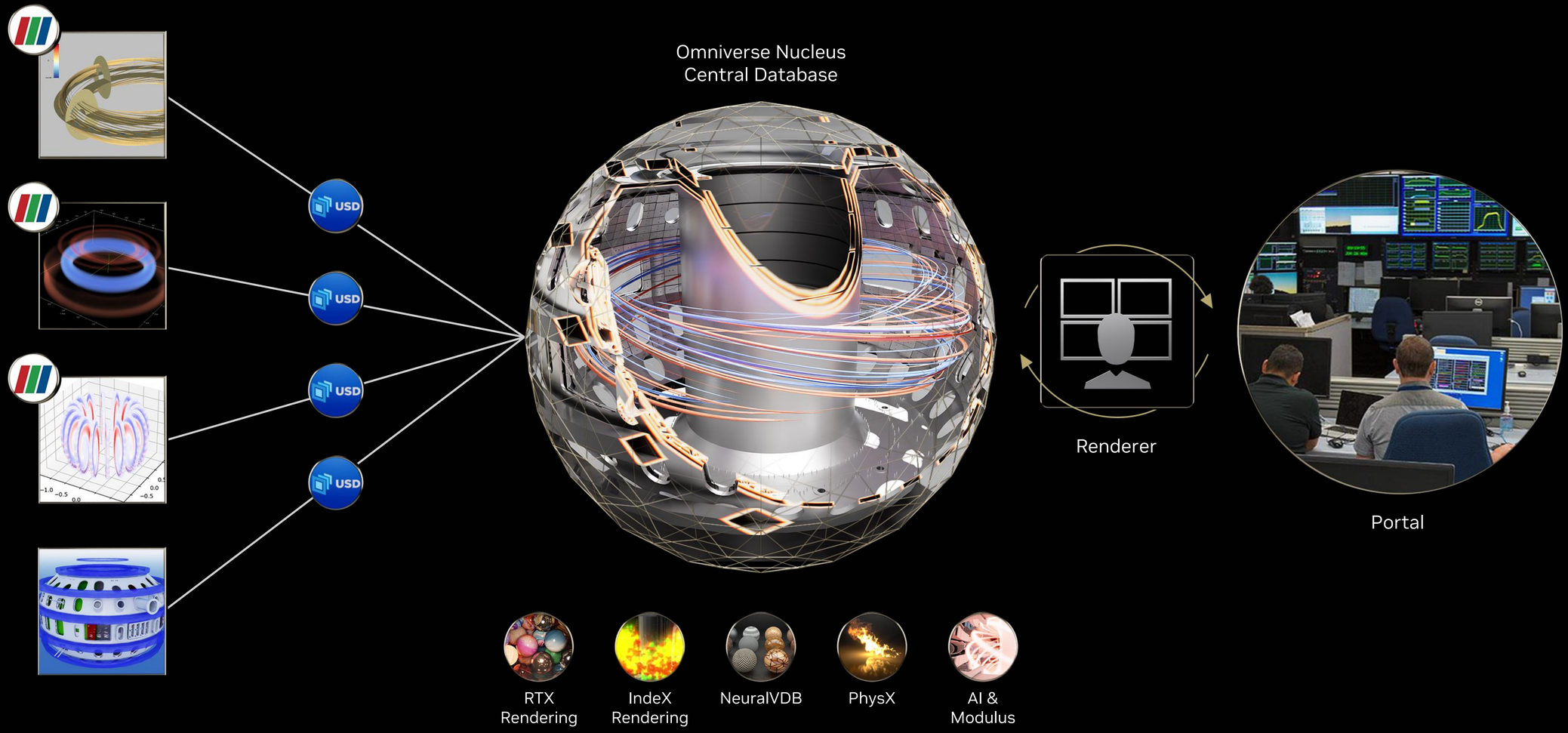


INDUSTRIAL DIGITAL TWIN
Data Center CFD Acceleration

Now Available on NVIDIA LaunchPad and Major CSPs

NVIDIA OMNIVERSE FOR SCIENTIFIC COMPUTING

Connecting Complex HPC 3D and Simulation Workflows

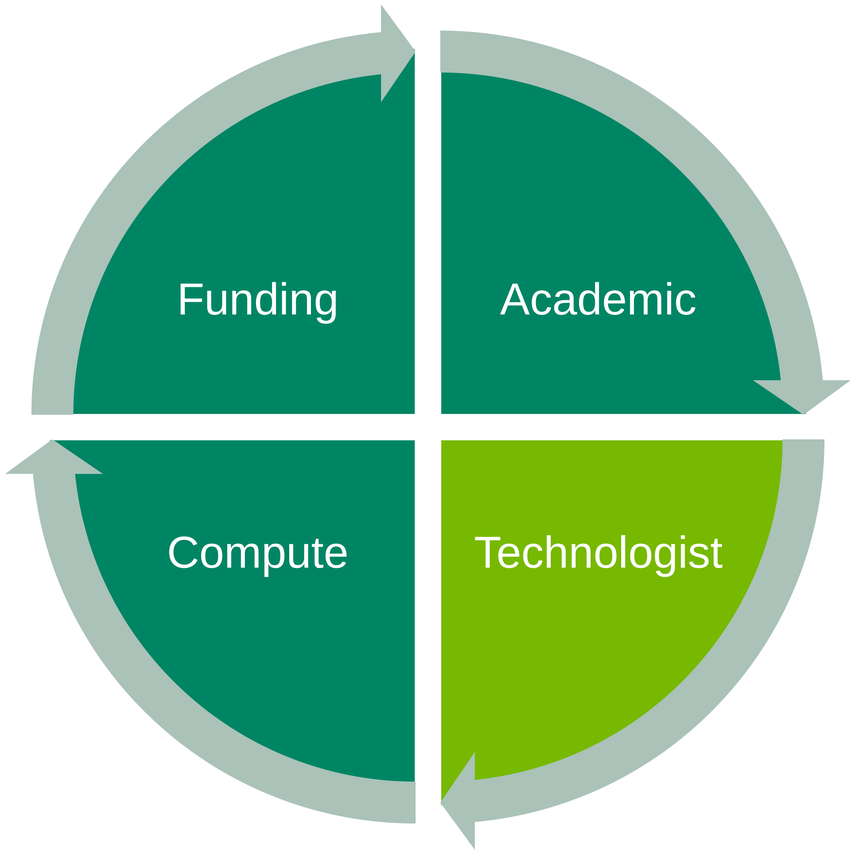


ABOUT NVAITC

RESEARCH COLLABORATIONS

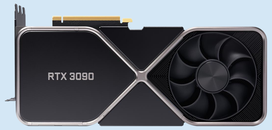
Enabling AI research through efficient GPU Computing

Industry Collaboration



Scientific Collaboration

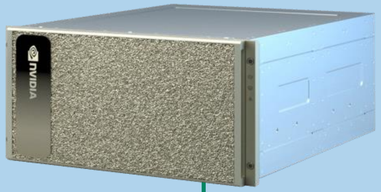
workstation

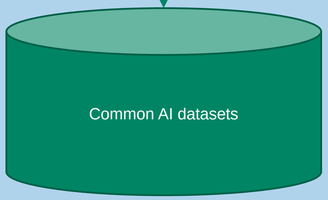


Each research has its own GPU for developing/debugging purposes.
They all use the same software stack and push developed code to a private *github* organization.

Local or Remote development

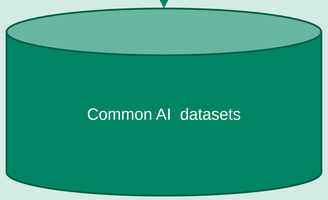
local cluster





~48 GPUs
Researchers access to resources through SLURM. According to priorities, seniority, SLURM partitions access policy may vary.
Senior researchers operate the local cluster.
Containers are pulled from NVIDIA NGC.

national facility



~5000 GPUs
Support for singularity, enroot.
DATASETS_AI is a fileset containing the most common datasets (imagenet, epic-kitchens, meccano, synlidar, etc).
Local conda channel (cineca-ai) to provide packages optimized for the local architecture.
Containers are pulled from NVIDIA NGC.


NVIDIA