Advancing Scientific Research with AI: Collaborative Efforts in Training Large Foundation Models on the Frontier Supercomputer

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Sajal Dash, Isaac Lyngus, Junqi Yin, Xiao Wang, Romain Egele, Austin Elis, Guojing Cong, Aristeidis Tsaris, Dan Lu, Feiyi Wang Massimiliano Lupo Pasini, Jong Choi, Xiao Wang, Pei Zhang, John Gounley, and Paul Laiu

U.S. DEPARTMENT OF ENERGY

ORNL has a rich history leveraging AI for science

Oak Ridge
Applied Artificial Intelligence
Project
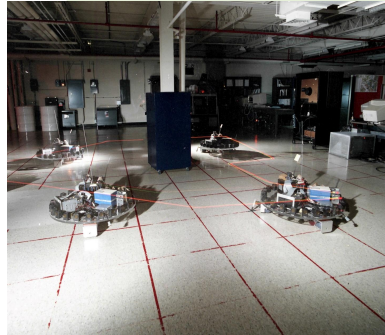
Automated
machines

- #1 HPL-MxP @10 exaflops for AI
- #2 on GREEN500
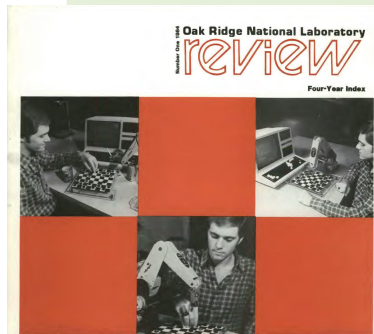- Scaled to 1T+ parameter AI model training

1940–1970   **1980**   **1990**   **2000**

supports
spectroscopy, environmental
management, nuclear fuel
reprocessing,
and programming assistance

Robotics

Summit:
World's "smartest" supercomputer
optimized for AI

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AI transforming science and national security
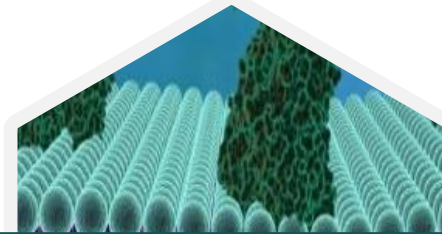Accelerating scientific discovery, fortifying energy infrastructure, and enhancing national security

Spallation Neutron Source

Manufacturing Demonstration Facility

Center for Structural Molecular Biology

Oak Ridge Leadership Computing Facility

Cyber Science Research Facility

High Flux Isotope Reactor

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Grand challenges in AI for science

nature

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EDITORIAL | 27 September 2023

AI will transform science — now researchers must tame it

A new *Nature* series will explore the many ways in which artificial intelligence is changing science — for better and for worse.

OCTOBER 30, 2023

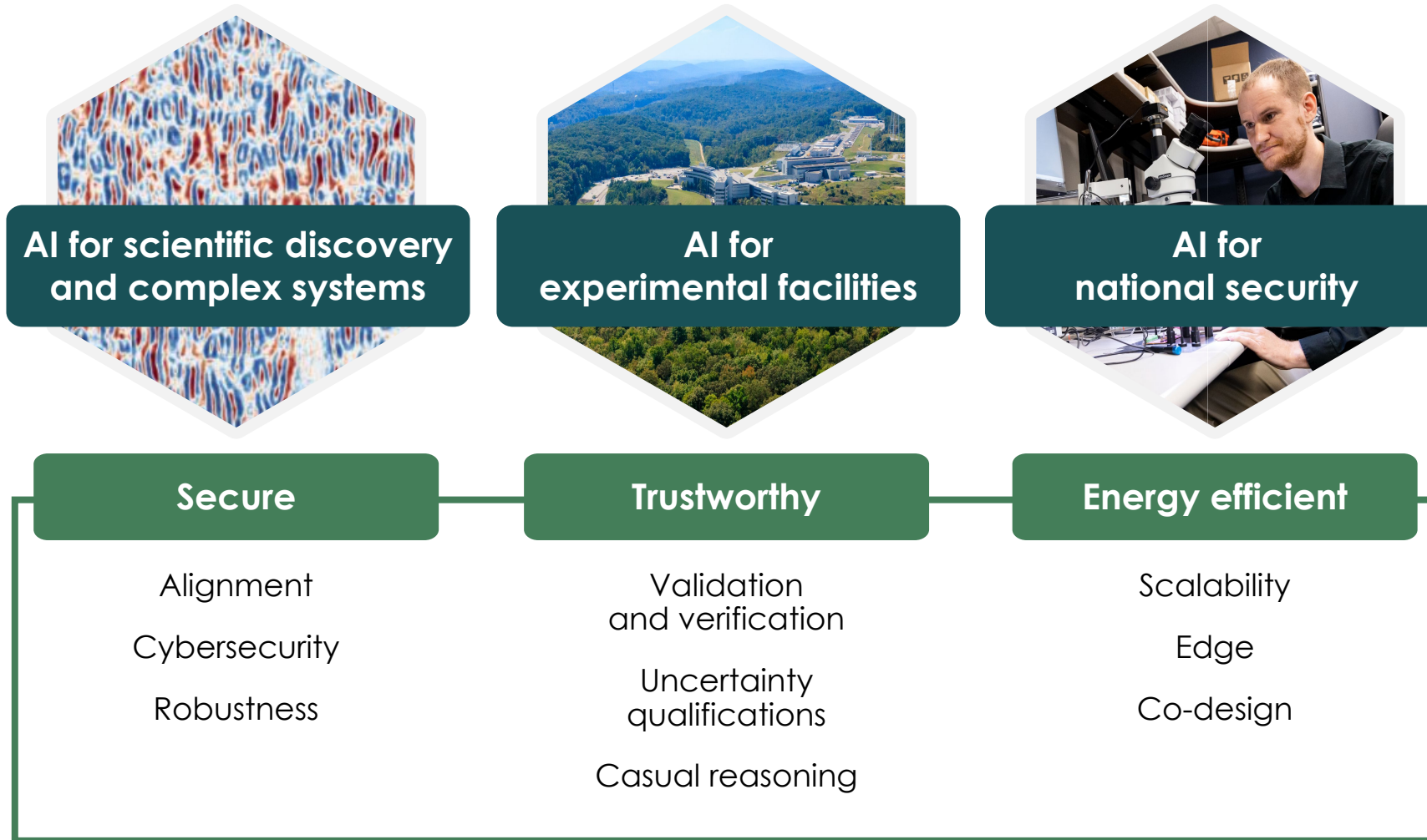## Executive Order on the Safe, Secure, and Trustworthy Development and Use of Artificial Intelligence

🏛 ▸ BRIEFING ROOM ▸ PRESIDENTIAL ACTIONS

By the authority vested in me as President by the Constitution and the laws of the United States of America, it is hereby ordered as follows:
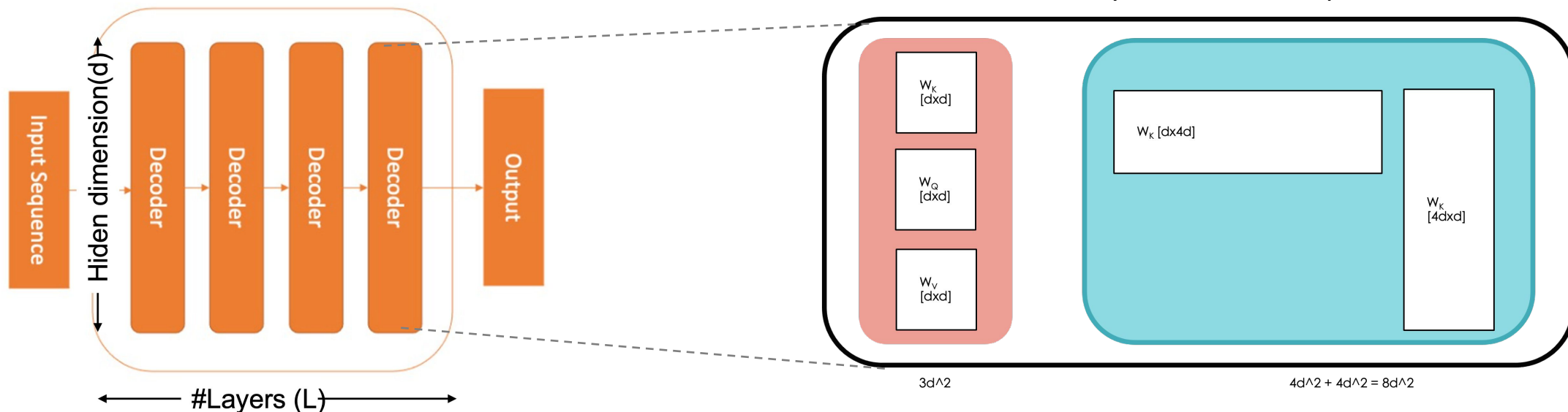
ORNL's AI initiative
Secure, trustworthy, and energy-efficient AI

AI for scientific discovery and complex systems

AI for experimental facilities

AI for national security

Secure	Trustworthy	Energy efficient
Alignment	Validation and verification	Scalability
Cybersecurity	Uncertainty qualifications	Edge
Robustness	Casual reasoning	Co-design

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Resources needed to train LLM-like models

One layer has $11d^2$ parameters

- GPT like models grows linearly with #Layers and quadratically with #Hidden dimensions

- Total parameters is roughly $12*L*d^2$

- Training one parameter needs 20 Bytes of memory and 120 FLOPs

- Need a minimum of 8, 55, and 313 MI250X GCDs to fit models of size 22B, 175B, and 1T

|	Memory Requirement		
Values	22B Model	175B Model	1T Model
Parameters (6x)	132 GB	1050 GB	6 TB
Gradients (4x)	88 GB	700 GB	4 TB
Optimizer States (8x)	176 GB	1.4 TB	8 TB
Total Memory (20x*)	440 GB	3.5 TB	20 TB

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Optimizing distributed training strategies

- Ported SOTA LLM training frameworks and libraries to Frontier (Megatron-DeepSpeed, FlashAttention 1&2)

- GPT model can be trained with a combination of Tensor (TP), Pipeline (PP), and Data parallelism (DP)

- TP slices model horizontally, PP vertically, and DP replicates

- TP should limit within node, PP should use large #micro-batches
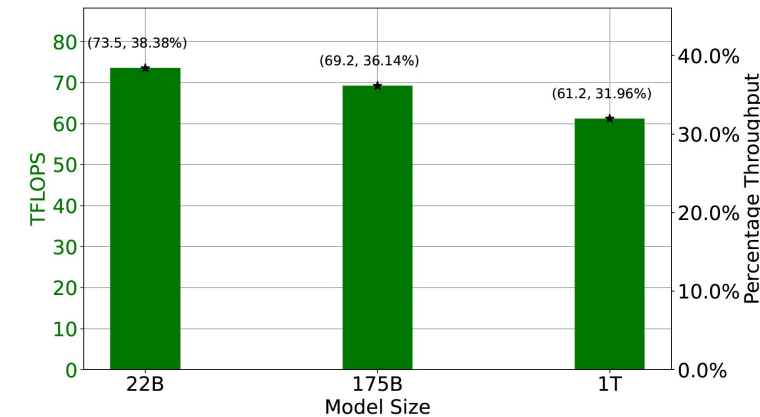
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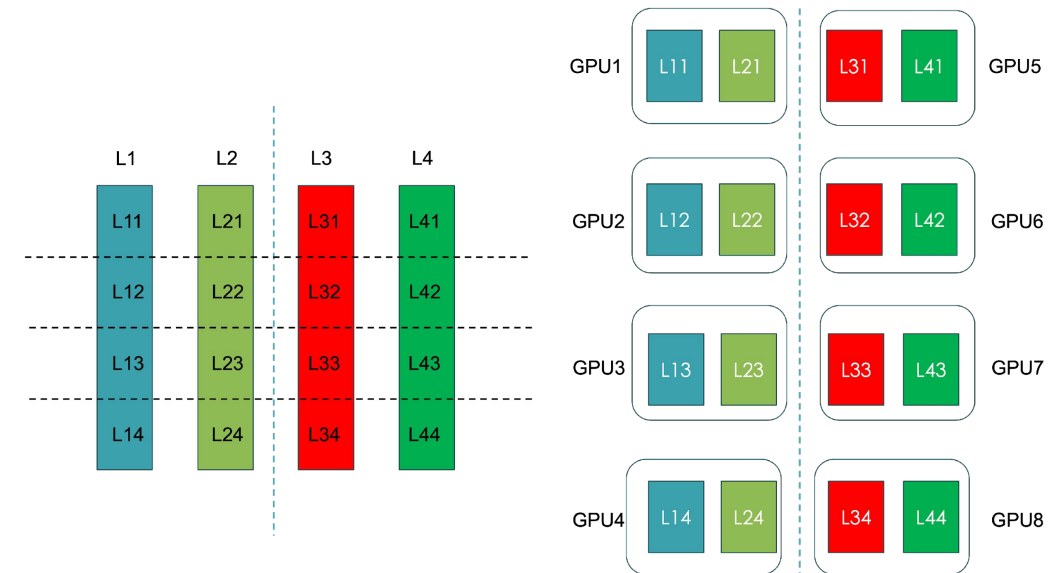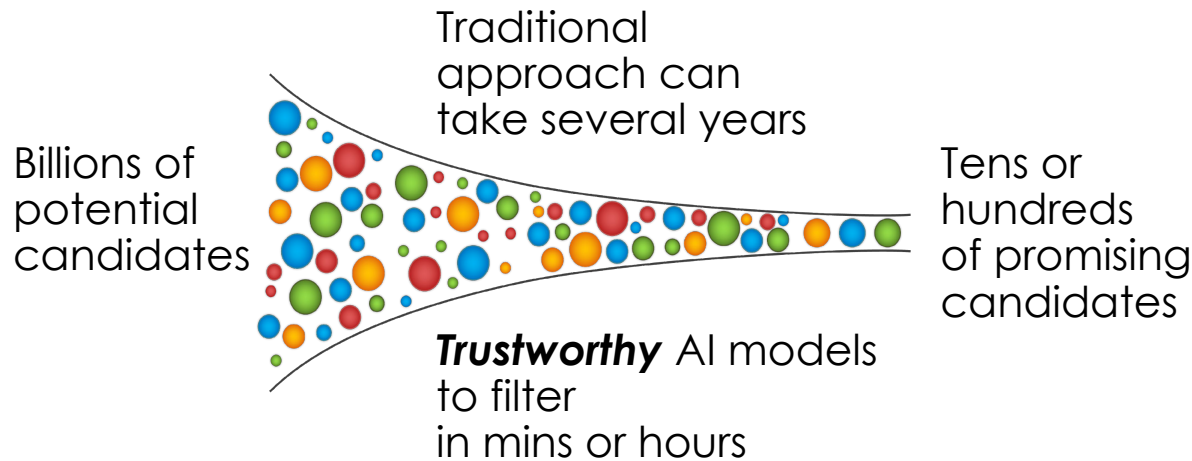
Training LLMs with 1 trillion parameters

- Automatically identify the best distribution strategies to achieve high GPU throughput and scaling efficiency

- Achieved 100% weak scaling efficiency and 87.05% strong scaling efficiency at 3072 GPUs.

- Trained the models for 10-100 iterations instead of training till completion.
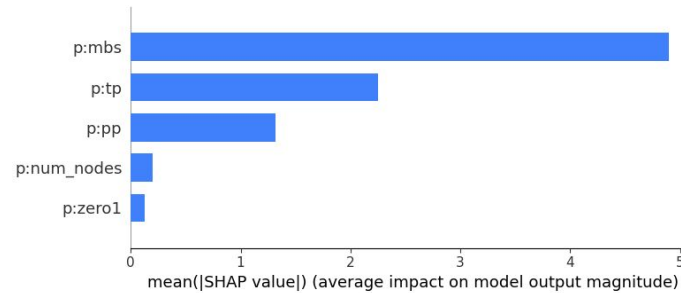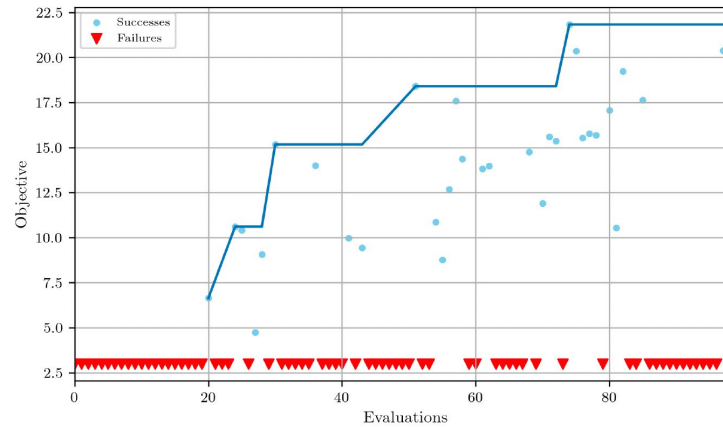
Hyperparameters	Value	
	175B Model	1T Model
TP	4	8
PP	16	64
MBS	1	1
GBS	640	1600
ZeRO Stage	1	1
Flash Attention	v2	v2
Precision	fp16	fp16
checkpoint-activations	True	True

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Accelerated materials discovery via trustworthy AI models on Frontier

Traditional approach can take several years

Billions of potential candidates

Tens or hundreds of promising candidates

Trustworthy AI models to filter in mins or hours

AI model training on 32 GPUs takes 100 hours

AI model training on 1,024 GPUs takes 10 hours

Chromophores
Biomedical, MRIs, Quantum circuits
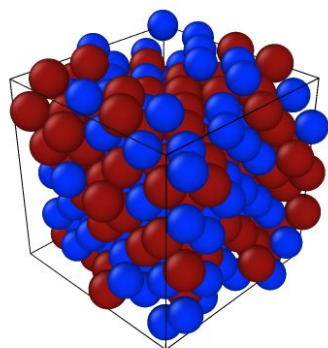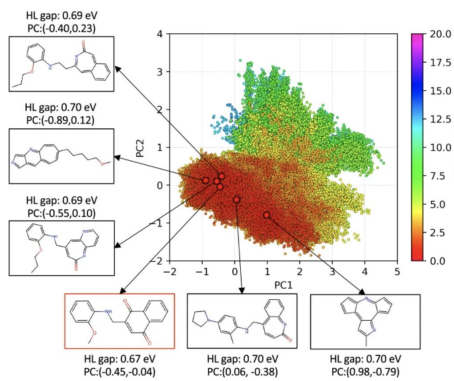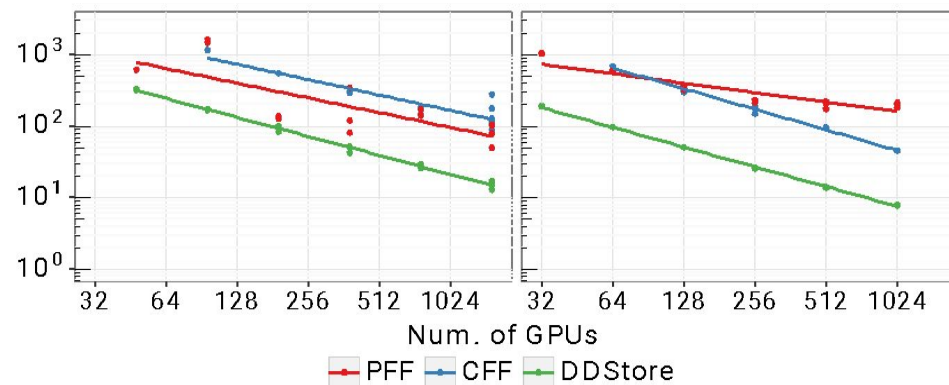
High-entropy alloy
Aerospace, mechanical manufacturing, biomedicine

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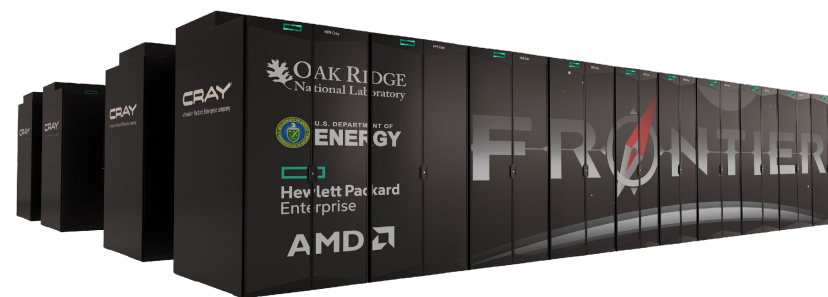
Foundation model for climate and weather forecasting

Variable 2m_temperature, at time: 2017-01-04 02:00, lead time: 72 hrs
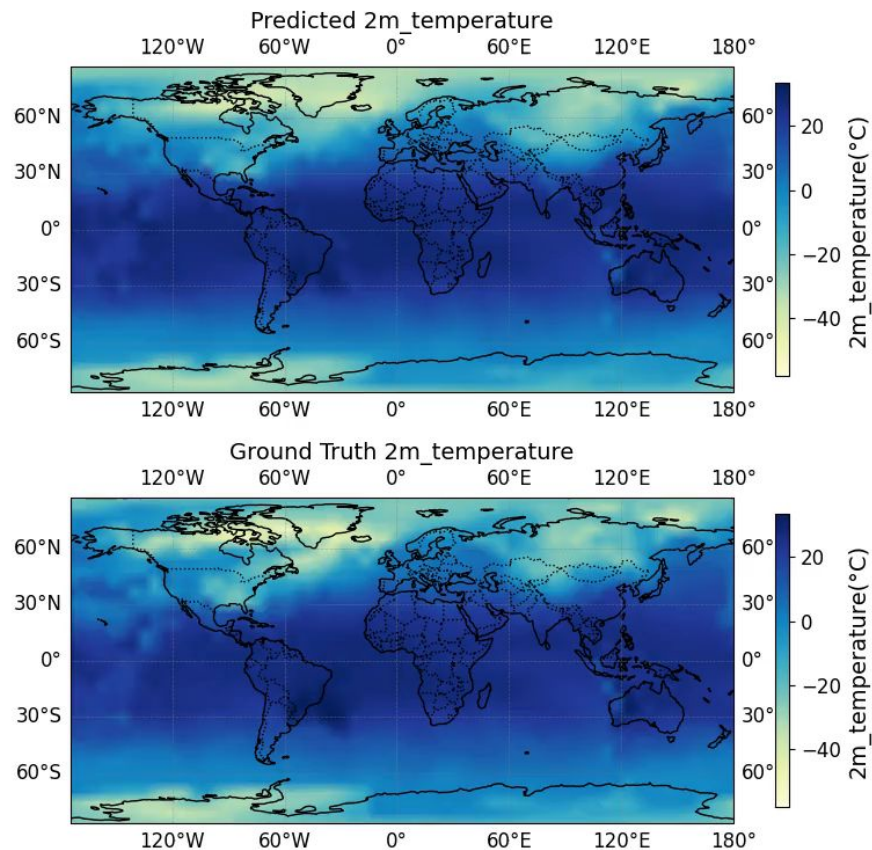
- Scaled our AI foundation model with 1B to 5B parameters on Frontier supercomputer;
- 87% scaling efficiency.
- Our AI foundation model accurately forecasts weather 72 hours ahead.

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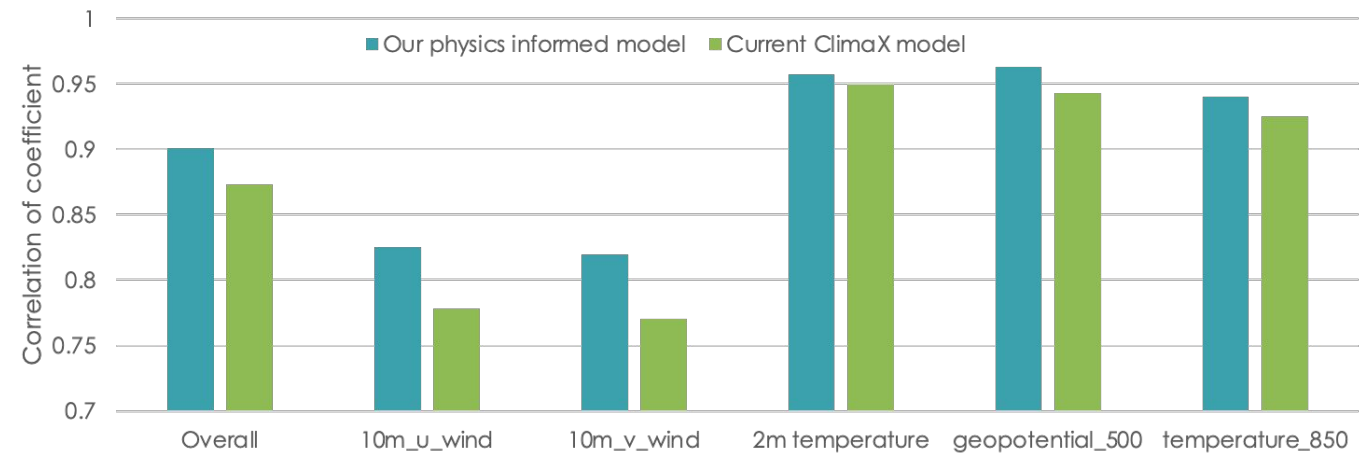
Foundation models for fluid dynamics
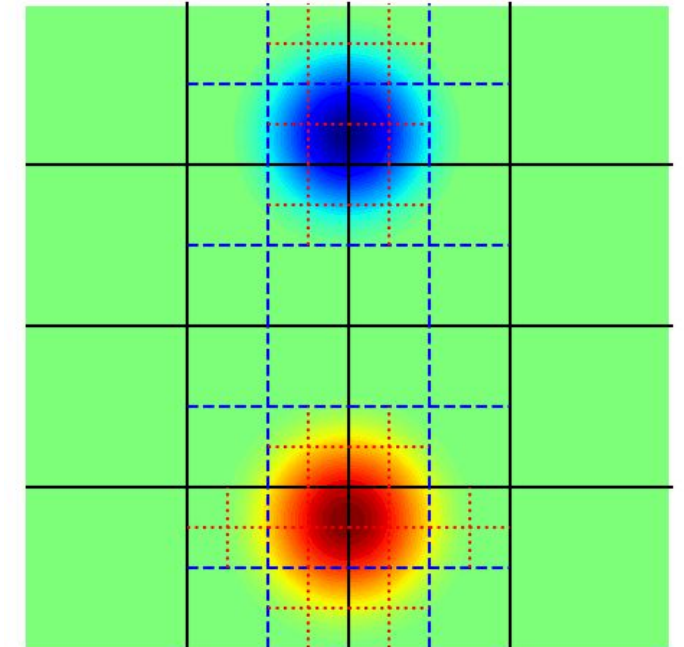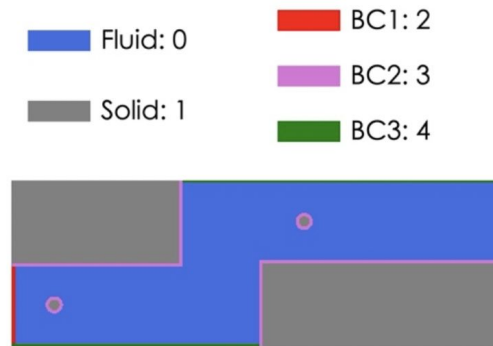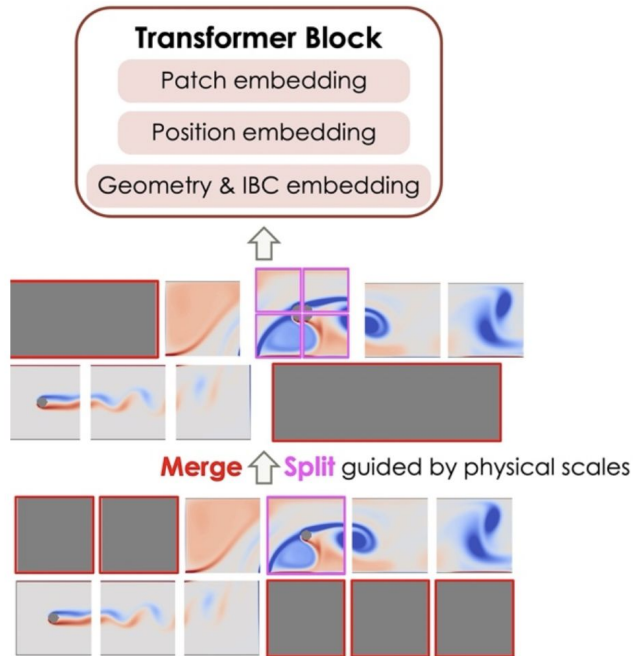
- Multiscale vision transformer models ⮕ efficient representation & computing resources distribution
  - Adaptivity guided by physics, like Adaptive Mesh Refinement (AMR)
  - Hierarchical transformers: Transformers at various scales with a two-way coupling

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Frontier first indicates path for energy efficient scaling

Glenn K. Lockwood
—
Oakland, California, United States
—
I am a supercomputing enthusiast who writes opinions on industry trends and technologies. I was once a materials scientist and played with high-performance computers in my free time, but I've been fortunate enough pursue that hobby as a paid profession since 2012. Don't take that to mean I know what I'm talking about though; I'm still trying to figure out all this computing

GLENN K. LOCKWOOD

Personal perspectives of a supercomputing enthusiast

HPC · STORAGE · PERSONAL · ABOUT ME · MY WEBSITE

Labels

ai

applications

January 13, 2024

A CLOSER LOOK AT "TRAINING" A TRILLION-PARAMETER MODEL ON FRONTIER
—

A paper titled "Optimizing Distributed Training on Frontier for Large Language Models" has been making its rounds over the last few weeks with sensational taglines saying the authors trained a trillion-parameter model using only a fraction of the Frontier supercomputer. The superficiality of the discourse around this paper seemed suspicious to me, so in the interests of embracing my new job in AI systems design, I decided to sit down with the manuscript and figure out exactly what the authors did myself.

- First time in open science setting and on non-NVIDIA hardware
  - So far, large runs on only NVIDIA hardware
- No heroic effort in software engineering
  - Largely dependent on existing software like Megatron-DeepSpeed
- Train massive LLMs with good efficiency using an entirely NVIDIA-free supercomputer
- Don't need an army of researchers at a national lab to make productive use of AMD GPUs for training large LLMs

Frontier trained a ChatGPT-sized large language model with only 3,000 of its 37,888 Radeon GPUs — the world's fastest supercomputer blasts through one trillion parameter model with only 8 percent of its MI250X GPUs

News By Matthew Connatser published January 07, 2024

Now you're playing with AI power!

Comments (19)

(Image credit: ORNL)

Researchers at Oak Ridge National Laboratory trained a large language model (LLM) the size of ChatGPT on the Frontier supercomputer and only needed 3,072 of its 37,888 GPUs to do it. The team published a research paper that details

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