

Exploring Deep Learning for Science Benchmarks on DOE Supercomputers

Aristeidis Tsaris¹, Jacob Balma², Murali Emani³, Steve Farrell⁴, Geoffrey C Fox⁶, Yin Junqi¹, Thorsten Kurth⁷, Abid Malik⁵, Prabhat⁴, Mallikarjun Shankar¹, Venkatram Vishwanath³
¹Oak Ridge National Lab, ²Cray Inc., ³Argonne National Laboratory, ⁴Lawrence Berkeley National Laboratory, ⁵Brookhaven National Laboratory, ⁶Indiana University Bloomington, ⁷NVIDIA



Introduction

High-performance computing is seeing an upsurge in workloads with data in unprecedented scale that require **data analysis**:

- Deep Learning models are used in several domains such as cosmology, particle physics and biology
- Problems typically include image detection, segmentation, synthetic data generation

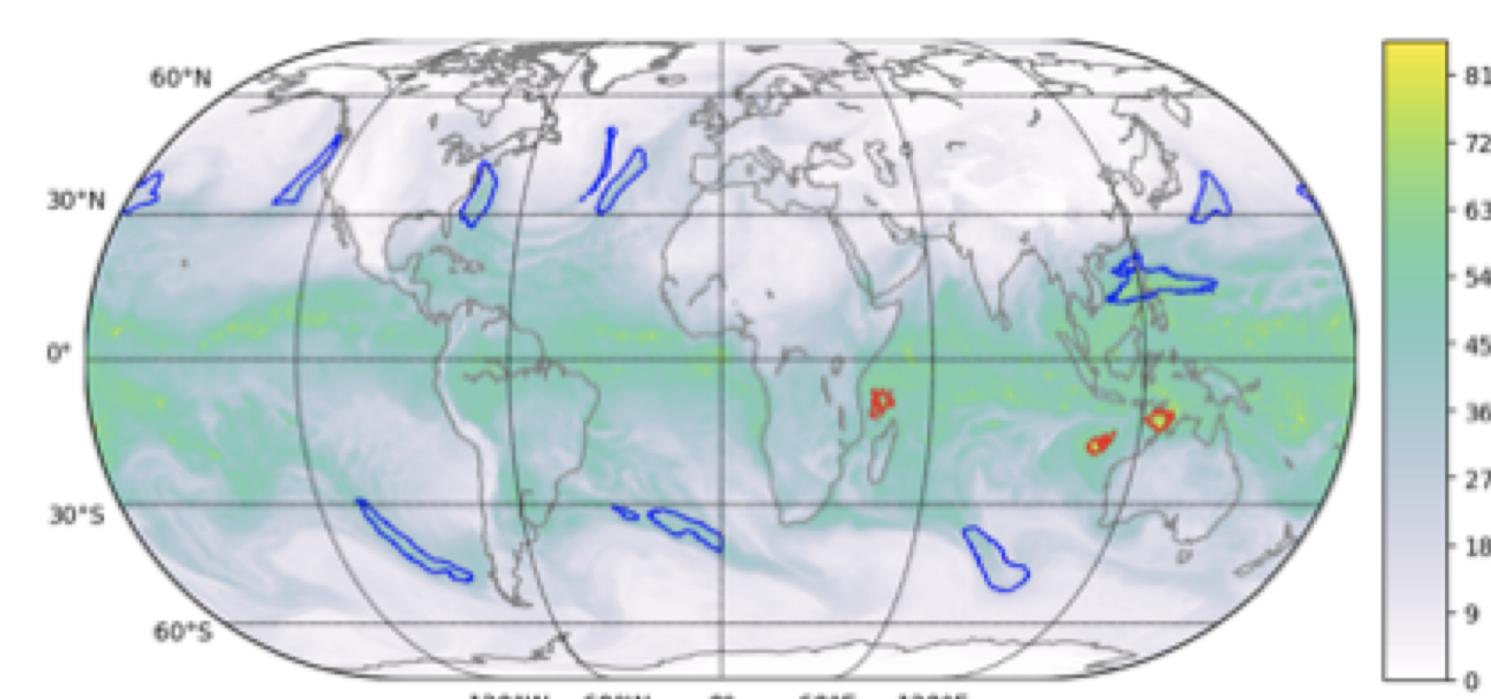
It is critical to understand the **performance of deep learning models on HPC systems** on the exascale era and beyond.

We are designing an **HPC ML benchmark suite**, that will help:

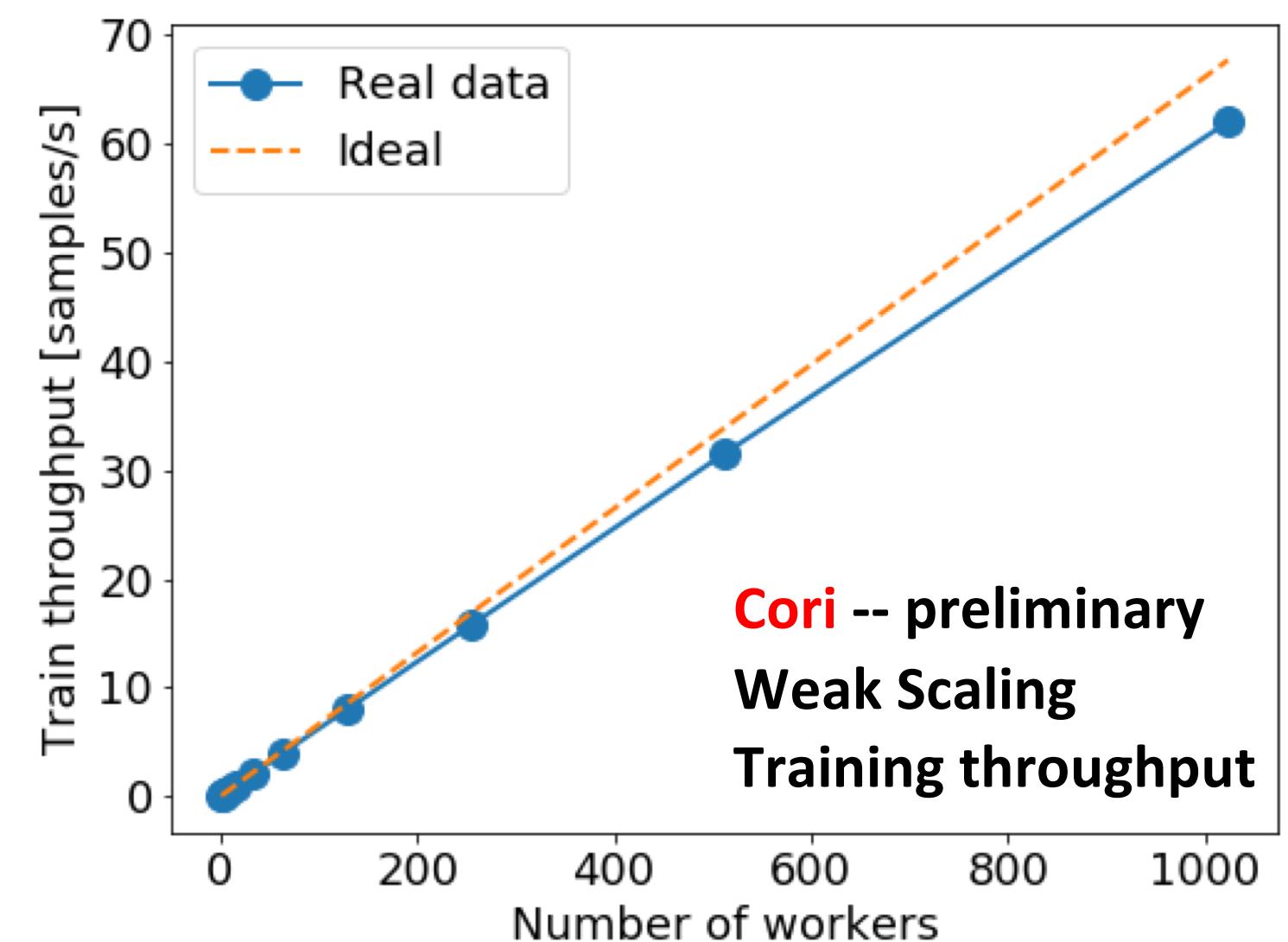
- Better understand the model-system interactions
- Better understand the deep learning workloads, optimize them and identify potential bottlenecks
- Quantify the scalability for different deep learning methods, frameworks and metrics on hardware diverse HPC systems

Climate segmentation

Segmentation of extreme weather phenomena in climate simulation (768 x 1152 x 16 image shape) [arXiv:1808.04728](https://arxiv.org/abs/1808.04728)

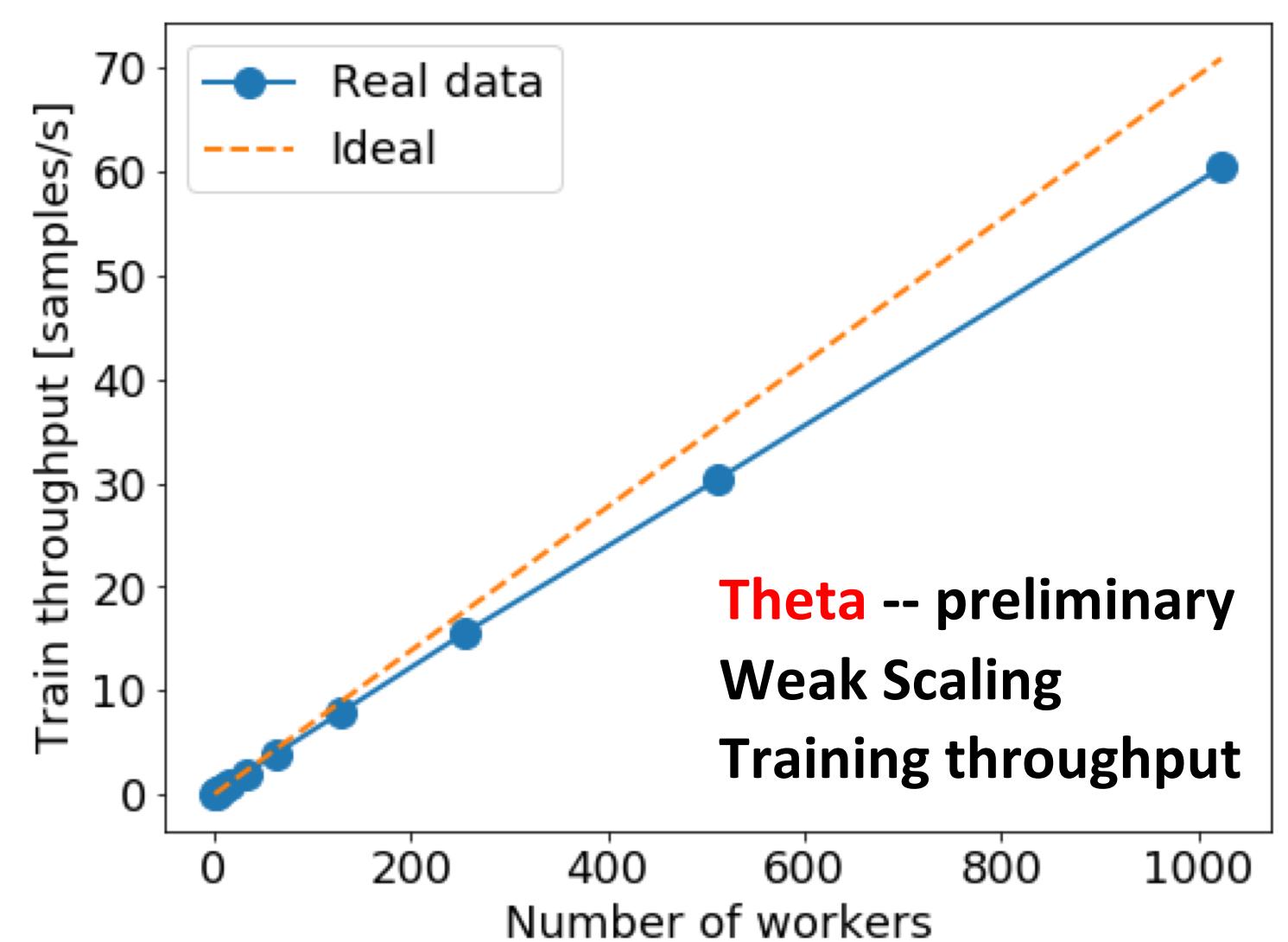


- High-dimensional inputs and multi-label targets
- 16-channel 2D images of size (768, 1152, 16), 3-class per-pixel
- **Large dataset (20 TB) stresses I/O subsystem**



Measurements on target systems with mini-dataset

- **Cori**: 1024 KNL nodes, 1.33 PF/s peak, 1.14 PF/s sust [FP32]
- **Theta**: 1024 KNL nodes, 1.11 PF/s peak, 1.09 PF/s sust [FP32]
- **Summit**: 170 nodes (x6 v100s) 48.08 PF/s peak, 38.71 PF/s sust [FP16]
- Further analysis underway



Reference implementation:
<https://github.com/sparticlesteve/climate-seg-benchmark>

What's done

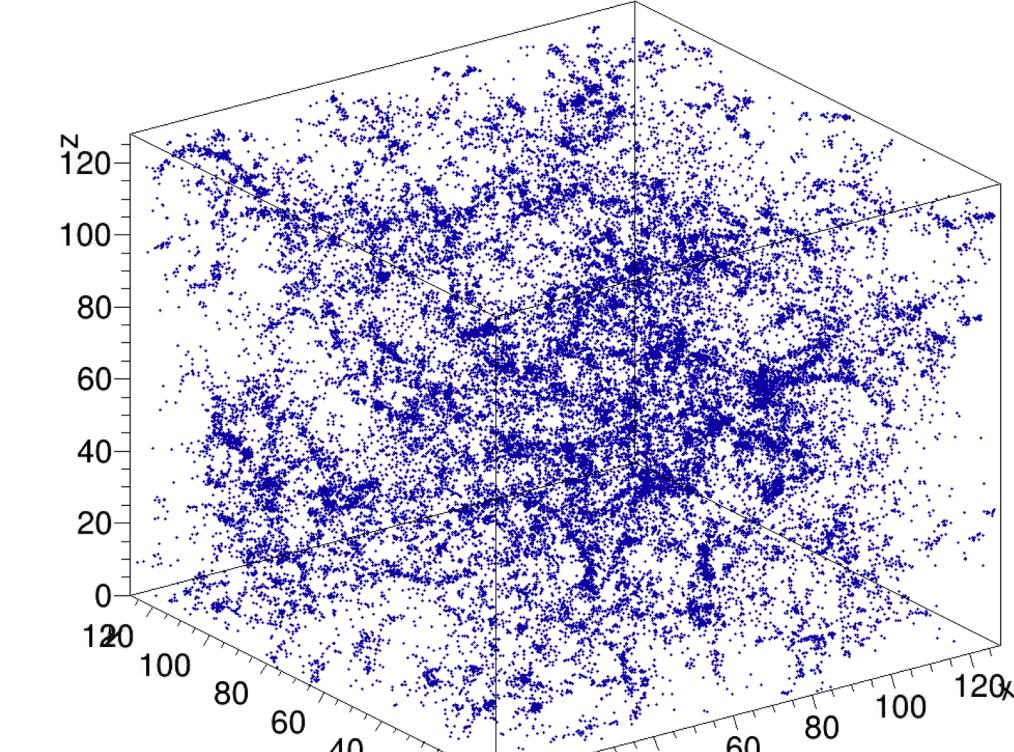
- Work is done within MLPerf-HPC working group
- Identify initial target systems: [Summit@OLCF](#), [Cori@NERSC](#), [Theta@ALCF](#)
- Select a list of candidate workloads. Not shown here, but in the works:
 - Language modeling on OpenWebText dataset: utilize communication patterns unique to sequence model-parallelism
 - Large scale multi-label image classification on TenCent dataset

What's next

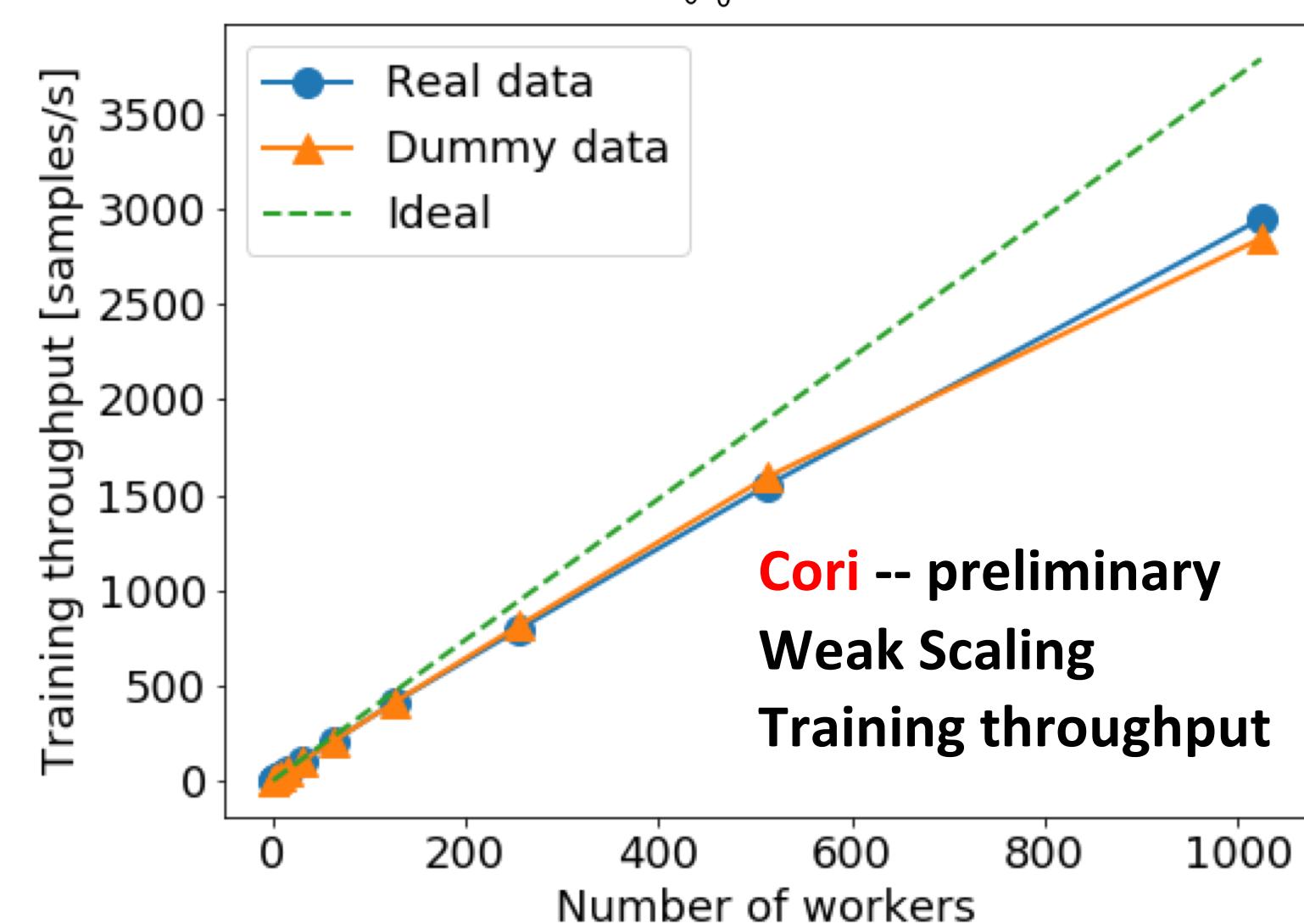
- Systematic study of the two benchmarks on the 3 target systems
- Finalize metrics collection and software tool for system performance (flops, I/O, communication) across all 3 systems
- Get the language modeling and the Image classification benchmark up and running
- Identify and pursue commonalities with main track MLPerf, best practices for data, model and pipelining parallelism
- Use our benchmarks to evaluate next-generation HPC systems
- Update suite with new benchmarks

CosmoFlow

Predict cosmology parameters from whole-universe dark matter simulations (128 x 128 x 128 x 4 crops) [arXiv:1810.01993](https://arxiv.org/abs/1810.01993)

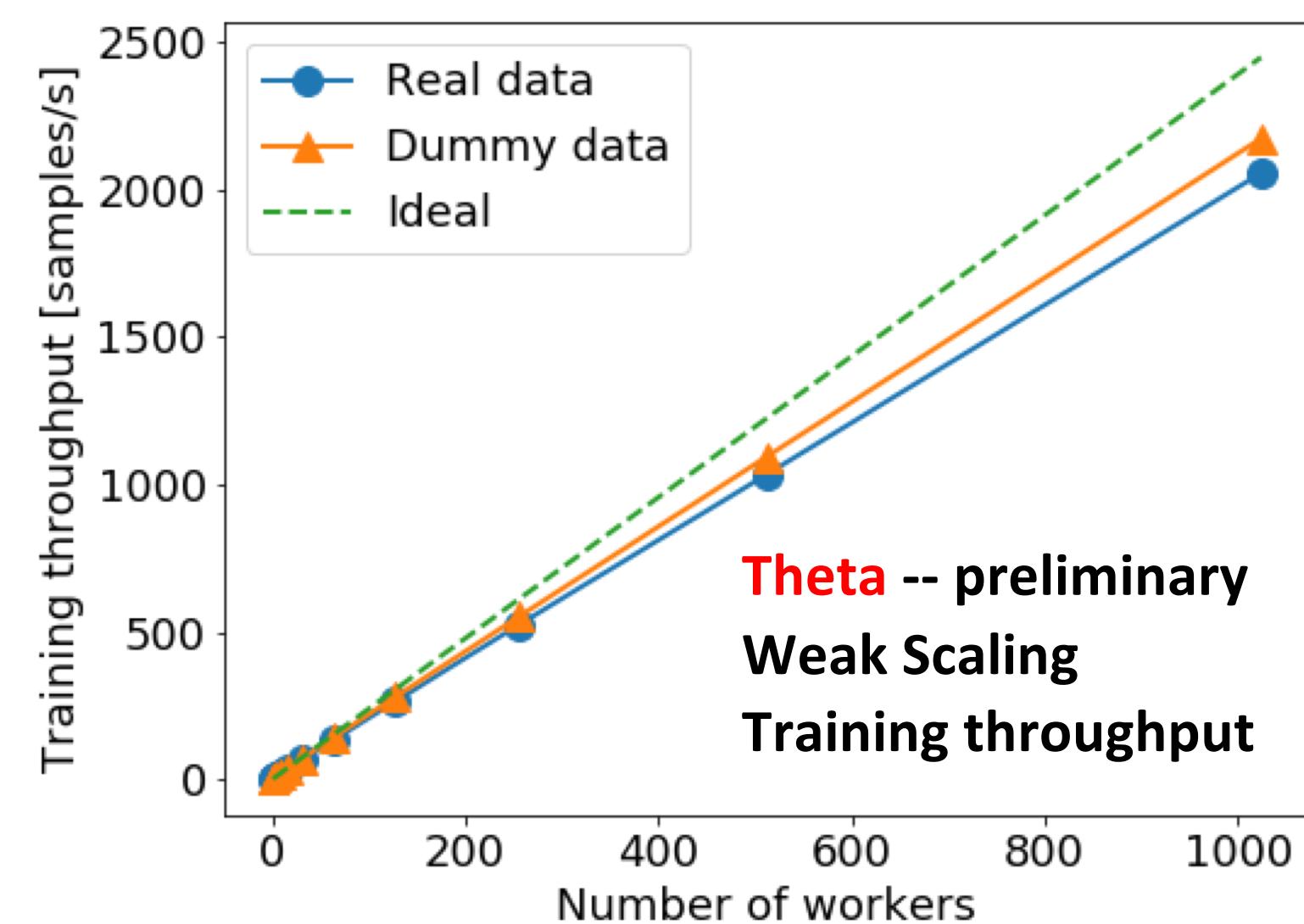


- Data-parallel implementation across 3D Convolutions
- **Multi-channel Volumetric input data stresses on-node bandwidths and memory capacities**
- **Communication patterns unique to convolutional model-parallelism**



Measurements on target systems

- **Cori**: 1024 KNL nodes, --78% scaling eff
- **Theta**: 1024 KNL nodes, -- 84% scaling eff
- **Summit**: 170 nodes (x6 v100s), -- 72% scaling eff
- Further studies underway



Reference implementation:
<https://github.com/sparticlesteve/cosmoflow-benchmark>

