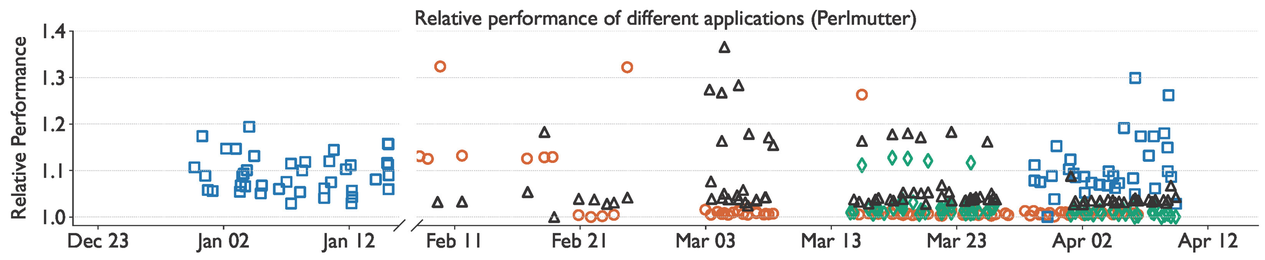
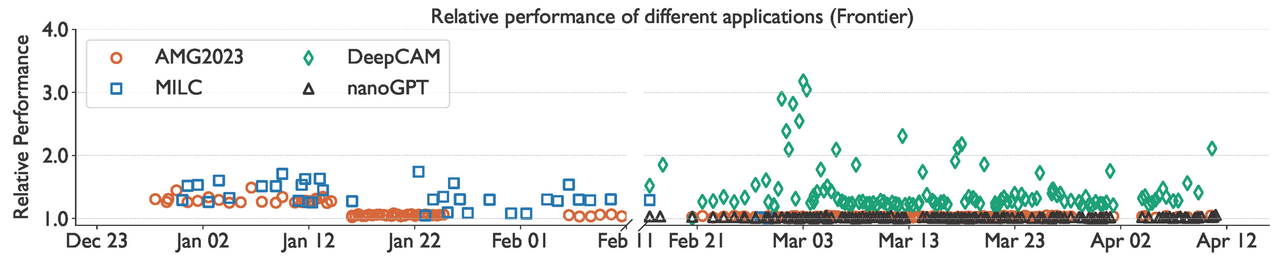
Unmasking Performance Variability in GPU Codes on Production Supercomputers

Cunyang Wei, Keshav Pradeep, Abhinav Bhatele
Department of Computer Science, University of Maryland





Abstract

Modern HPC facilities increasingly rely on GPU-accelerated clusters to drive both scientific computing and AI workloads. Performance variability is a critical issue in these systems, undermining efficiency and reproducibility. While prior studies have extensively analyzed variability in CPU-centric supercomputers, large-scale investigations on GPU clusters are lacking. To address this gap, we set up a longitudinal experiment on Perlmutter and Frontier. We benchmark representative HPC and AI applications and collect detailed performance data to assess the impact of compute variability, allocated node topology, and network conditions on overall runtime. We also use a ML based approach to identify potential correlations between these factors and to forecast the execution time. Our analysis identifies network performance as the dominant source of runtime variability.

What is Performance Variability?

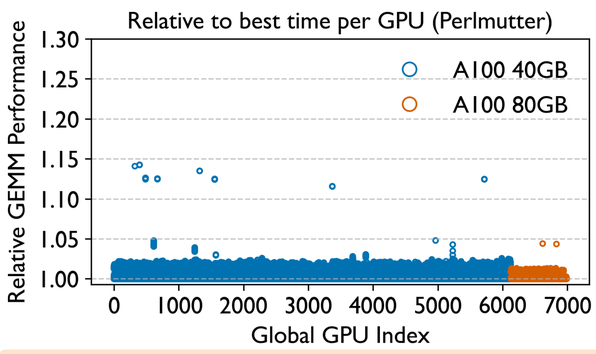
- **Performance Variability**: fluctuations in application runtime across repeated executions under seemingly identical inputs, environments, and system conditions
- Sources of variability: HW defects, network contention, job placement, OS jitter
- Prior studies focused on CPU-based systems, leaving the impact of new communication patterns on variability in GPU-based supercomputers unexplored.

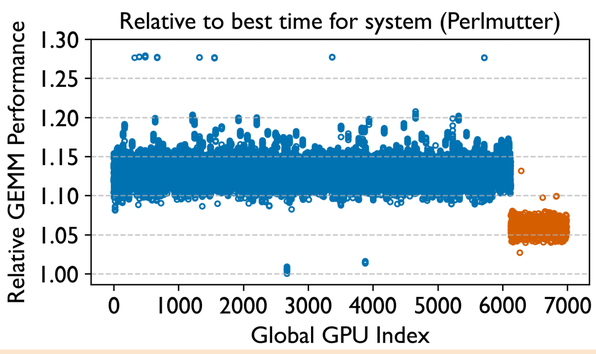
Methodology for Measuring Variability

- We measure variability for two HPC apps (AMG and MILC) and two AI apps (DeepCAM and nanoGPT)
- We collect the following features to analyze performance variability: **mpiP** for profiling HPC apps, the **PyTorch profiler** for AI workloads, **SLURM's sacct logs**, **Cassini NIC hardware counters**, and performance data from **GEMM** and **All-Reduce microbenchmarks**.
- Platforms used:

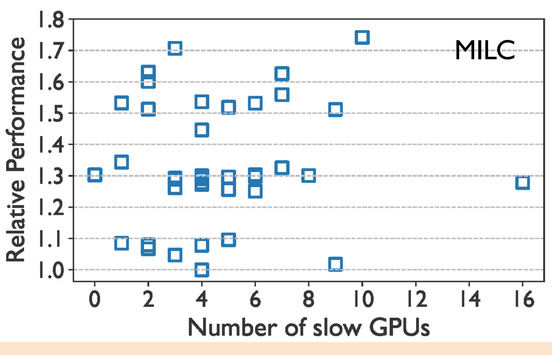
	NERSC Perlmutter	**OLCF Frontier**
GPU model	NVIDIA A100 GPU	AMD MI250X GPU
Interconnect	HPE Slingshot-11	HPE Slingshot-11
GPUs/GCDs per node	4	8

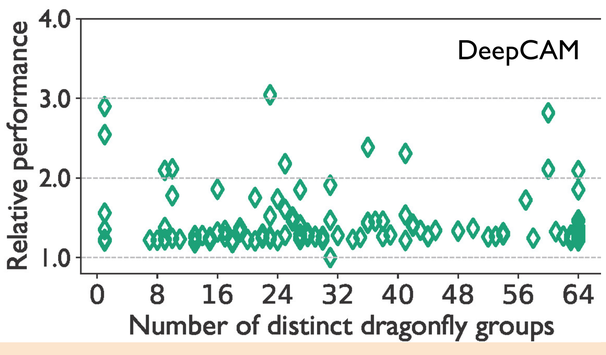
Analysis of the Data



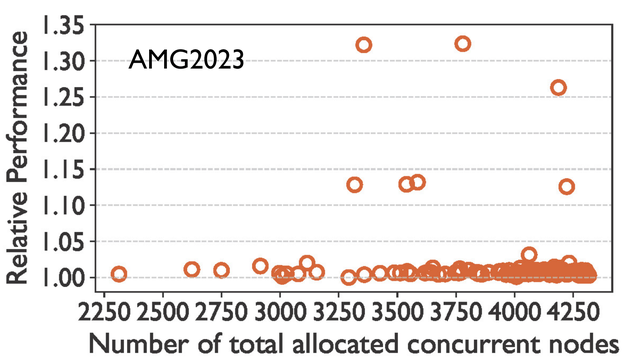


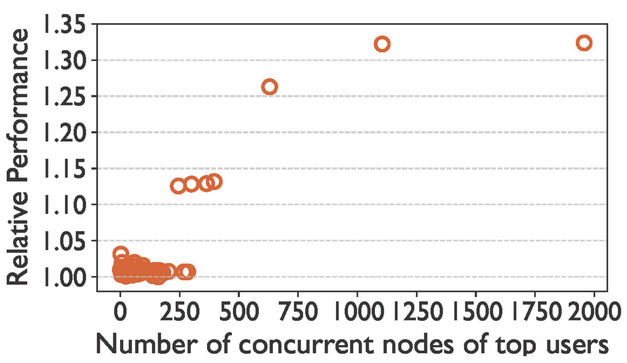
Observation: While single-GPU performance remains relatively stable over time (especially on Perlmutter), there is notable variability across different GPUs.





- **Left:** Slow GPU = # of GPUs in job allocation which fall in slowest 1% of system's GPUs. **Observation:** The quantity of "slow" GPUs has no impact on performance. **Right:** On both systems, job allocations across more Dragonfly groups does not degrade app performance, despite incurring more network hops.

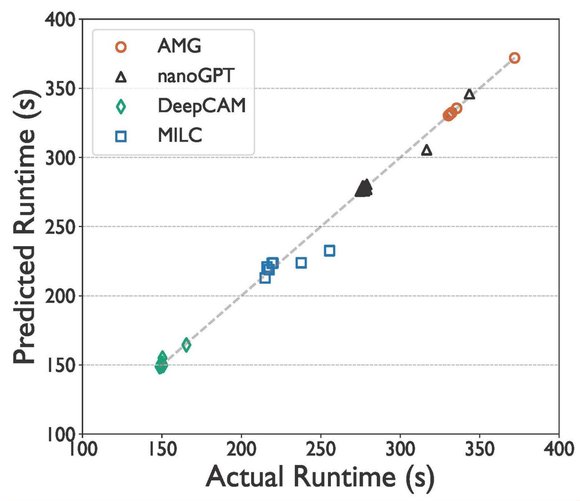


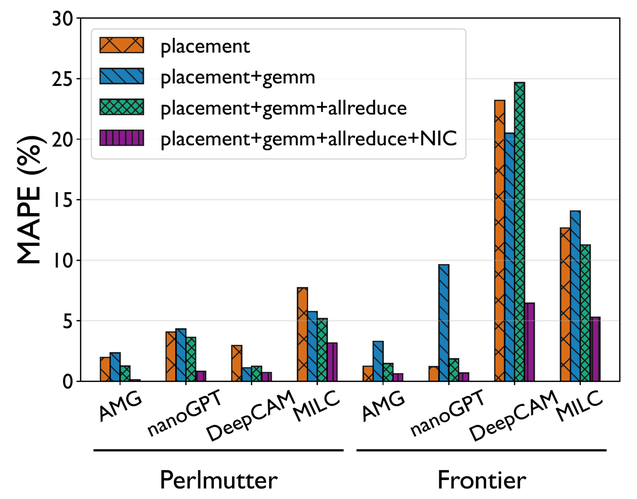


- **Top Users:** Users whose allocated number of nodes correlates with our application's performance variation and who concurrently request more than 32 nodes.
- **Observation:** Overall system utilization alone does not explain the observed performance degradation; a few specific neighbors with high communication intensity cause most of the performance variability.

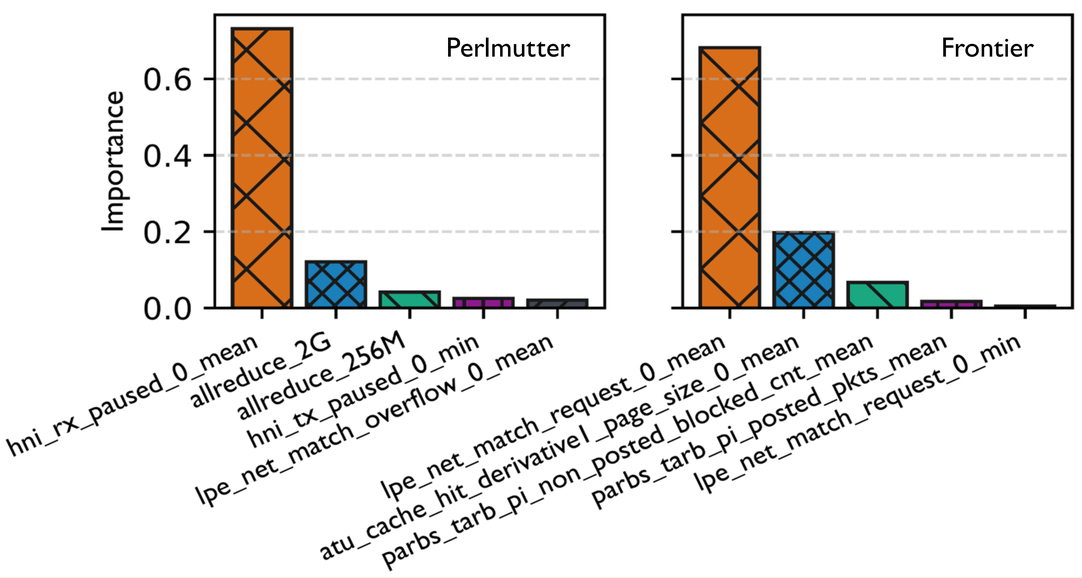
ML based Analysis and Performance Prediction

- Methodology: We train an **XGBoost** model to predict runtime. We use 90% of our runs for training data, reserving 10% of testing.
  - Summary of performance dataset features [name (feature count per run)]: Application Name (1), Placement (1), GEMM (3), MPI Allreduce (11), NCCL Allreduce (8), NIC Counters (29*3)
- Evaluation: We use Mean Absolute Percentage Error (MAPE)





- **Left:** Actual vs predicted runtime using placement, GEMM, Allreduce, and NIC counters features (Perlmutter & Frontier).
- **Right:** When NIC counter features are included in input, MAPE decreases significantly, especially for apps with more variation (e.g. DeepCAM on Frontier). This highlights the importance of NIC counters for explaining variability



- **Feature importances based on XGBoost models. Left:** On Perlmutter, most important feature is hni_rx_paused_0_mean (num cycles where recv path is paused, suggesting network pushing data quicker than NIC can read) **Right:** On Frontier, most important feature is lpe_net_match_request_0_mean (num requests matched on software endpoints)

Conclusions

- Network conditions - not GPU variability or job placement - are the primary drivers of runtime variability in large-scale GPU workloads.
- A small subset of users running communication-heavy jobs account for most of the observed performance degradation.
- Our ML model accurately predicts runtime variability, even with limited training data per application.

Recommendations for Future Efforts

- "Top User" jobs should run on isolated nodes to prevent their communication patterns from impacting network performance for others.
- Future designs need not *over-engineer* the topology for increased network hops. The dragonfly topology is very robust, essentially neutralizing the incurred penalties from nodes allocations being spread out.
- The application of ML-models (like XGBoost) for system-wide monitoring can predict runtime variability with high accuracy using features like NIC and network counters. System administrators can use these predictions to detect early signs of congestion and allow users to delay or cancel their workloads.

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