DS 7347
High-Performance Computing (HPC) and Data Science
Session 2

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April 28, 2022

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Outline

Session Question

HPC and Data Science

Semester Project

Assignment

Session Question

Session Question

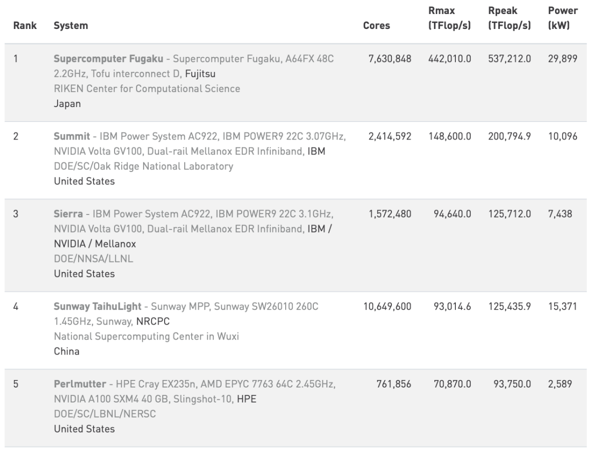
Why does data science at scale need HPC?

HPC and Data Science

Top500

- top500.org
- Twice yearly lists of the top 500 supercomputers in the world
    - Top500, based on HPL performance
    - HPCG, based on HPCG performance
    - Green500, based on HPL performance per watt
- Lists have been kept since 1993

Nov. 2021 Top500 Top Five



Rank	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	**Supercomputer Fugaku** - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science Japan	7,630,848	442,010.0	537,212.0	29,899
2	**Summit** - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM DOE/SC/Oak Ridge National Laboratory United States	2,414,592	148,600.0	200,794.9	10,096
3	**Sierra** - IBM Power System AC922, IBM POWER9 22C 3.1GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM / NVIDIA / Mellanox DOE/NNSA/LLNL United States	1,572,480	94,640.0	125,712.0	7,438
4	**Sunway TaihuLight** - Sunway MPP, Sunway SW26010 260C 1.45GHz, Sunway, NRCPC National Supercomputing Center in Wuxi China	10,649,600	93,014.6	125,435.9	15,371
5	**Perlmutter** - HPE Cray EX235n, AMD EPYC 7763 64C 2.45GHz, NVIDIA A100 SXM4 40 GB, Slingshot-10, HPE DOE/SC/LBNL/NERSC United States	761,856	70,870.0	93,750.0	2,589

Figure 1: Top five supercomputers.

Fugaku

- COVID-19 Projects
- SALMON (Scalable Ab initio Light-Matter simulator for Optics and Nanoscience)
  - Optimized the simulation computer code to maximize its performance
  - Modeled light-matter interactions in a thin film of amorphous silicon dioxide, composed of more than 10,000 atoms
  - Simulations were carried out using almost 28,000 nodes

Summit

- Air Flow with Classrooms
- Deep Learning to Predict Protein Functions at Genome Scale
  - Datasets of $\sim 45,000$ proteins
  - Use of DeepMind’s AlphaFold 2 for genome sequence to structure converstion

Sierra

- HPC4Mfg project targets more energy-efficient steelmaking
  - Goal is to reduce emissions and defects from inclusions in steel manufacturing
  - Computer vision
  - Machine learning
  - HPC resources
- COVID-19 Risks for Cancer Patients
  - Dataset $\sim 50,000$ patients with cancer
  - Identified a higher risk from COVID-19 due to a specific group of rarer blood cancers and two cancer medications

Sunway TaihuLight

- Millimeter-Scale and Billion-Atom Reactive Force Field Simulation
  - Simulate chemical reactions (ReaxFF)
  - $1,358,954,496$ atoms
  - $4,259,840$ cores
  - Performance of 0.015 ns/day
- Extreme-Scale Earthquake Simulations
  - Simulate Tangshan and Wenchuan earthquakes
  - Leading spatial resolution
  - Memory bandwidth constraints yielded 8% to 16% efficiency

Perlmutter

- November 2020 - July 2021: Cabinets containing GPU compute nodes and service nodes for the Phase 1 system arrived on-site and are being configured and tested
- Summer 2021: When the Phase 1 system installation completed, NERSC started to add users in several phases, starting with NESAP teams
- June and November 2021: The Phase 1 system was ranked at No. 5 in the Top500 lists in June and November, 2021
- June 2, 2021 and January 5-7, 2022: User trainings were held to teach NERSC users how to build and run jobs on Perlmutter
- January 19, 2022: The system is available to all users who want to use GPUs with the start of the allocation year 2022

Semester Project

Semester Project Goal

Produce single-submit, end-to-end, performant pipeline for a complex and computationally intensive data analysis workflow.

Semester Project Details

- The analysis and dataset, possibly generative, needs to be sufficiently computationally intensive such that a resonable performance analysis can be conducted.
- The specific dataset, analysis, and performance analysis will be agreed to at various stages during the semester.
- The pipeline should be single-submit, meaning that a single job is submitted to the queue system and then entire pipeline is run with each stage run on appropriate hardware with appropriately optimized software stacks.

Semester Project Details

- The deliverable will be a ready to present slide deck in your GitHub repo, *i.e.* a job will be submited on an SMU HPC cluster and then, sometime later with zero human interaction, a PDF presentation will appear in your GitHub repo.
- The presentation should discuss both the dataset analysis and performance analysis.
- Specific compute resources will be reserved for final testing and the production run.

Finding Datasets

- ERNESTO.net
- KDnuggets
- Data Is Plural
- Open Data on AWS

Group Discussion

- Discuss ideas
- Find some interesting datasets

Assignment

Assignment 2

Readings

- Eijkhout sections [1.0–1.4]

Assignment

- Find three HPC and Data Science example articles or papers using three, non-top five of the Top500, supercomputers (can be decomissioned machines)
- Briefly discuss the research workflow, specific hardware used, and cite the sources
- Commit `assignments/assignment_02.md` to your class repo
- Due 12:00 AM Central, Tuesday, May 3, 2022