NUG Monthly Meeting

16 March, 2023
Today's plan

- Interactive - please participate!
  - Raise hand or just speak up
  - [NERSC User Slack](link in chat), #webinars channel

- Agenda:
  - Win-of-the-month
  - Today-I-learned
  - User Community Survey
  - Announcements/CFPs
  - Topic of the day: **Science Highlights**
  - Coming meetings: topic suggestions/requests?
Win of the month

Show off an achievement, or shout out someone else's achievement, e.g.:

- Had a paper accepted
- Solved a bug
- A scientific achievement (maybe candidate for Science Highlight, or High Impact Scientific Achievement award)
- An Innovative Use of High Performance Computing (also a candidate for an award) ([https://www.nersc.gov/science/nersc-hpc-achievement-awards/](https://www.nersc.gov/science/nersc-hpc-achievement-awards/))

Please let us know of award-worthy work from you or your colleagues - tell us what you did, and what was the key insight?
Today I learned

What surprised you that might benefit other users to hear about? (and might help NERSC identify documentation improvements!)

Eg:

- Something you got stuck on, hit a dead end, or turned out to be wrong about
  - Give others the benefit of your experience!
  - Opportunity to improve NERSC documentation
- A tip for using NERSC
- Something you learned that might benefit other NERSC users

"If we knew what it was we were doing, it would not be called research, would it?" - Einstein
Perlmutter charging holiday (See email yesterday)

- (Yesterday) we temporarily disabled a SS11 feature for performant GPU-RDMA to mitigate a critical issue leading to node failures. This is expected to substantially affect performance of applications using GPU-RDMA capabilities for inter-node communication (such as CUDA-Aware MPI or GASNet), but will allow jobs that were previously crashing to run. **We expect to be able to remove this mitigation during the next scheduled maintenance on March 22, 2023.**

- For the **two weeks** starting (yesterday) and ending at 11:59:59 pm (Pacific time) on March 29, **all CPU and GPU jobs on Perlmutter will run free of charge** against your allocation to encourage you to use the system. Please let us know if you see problems via a ticket at [https://help.nersc.gov](https://help.nersc.gov).
Announcements and CFPs

NERSC Appropriate Use Policy and Code of Conduct

- Many users have still not read and agreed to these!
- To read and sign it - just log into Iris.nersc.gov - if you haven't signed it yet, a dialog will pop up with it
- Users who have (had) not signed were sent an email about it this week
Cori Retirement end of April

- Migrating from Cori to Perlmutter - office hours March 31
- Training last week - materials and recordings are available via [https://www.nersc.gov/users/training/events/migrating-from-cori-to-perlmutter-training-march2023/](https://www.nersc.gov/users/training/events/migrating-from-cori-to-perlmutter-training-march2023/)
Announcements and CFPs

See weekly email for these upcoming events:

• Attention Students: NERSC Summer Internships Available!
  • https://www.nersc.gov/research-and-development/internships/

• US Research Software Engineer Association Conference - submissions open
  • Oct 16-18, Chicago IL - https://us-rse.org/usrse23/

• DOE Cross-facility Workflows Workshop April 12, 2023

• NERSC is hiring! Several open positions, see
  https://lbl.referrals.selectminds.com/page/nersc-careers-85
Announcements and CFPs

Others?
What are these "Science Highlights"?

- What does one look like?
- Why does it matter?
- What sort of thing gets highlighted?
- Where to find them?
- How do I get my work into that collection?
What does one look like?

Can take the form of:

- A short summary slide
- A longer news article

Describes, in non-domain-expert terms:

- A scientific achievement
- The significance and impact of that achievement

For work that used NERSC resources:

- Compute, storage or other systems
- Collaborations with NERSC staff
Why does it matter?

It's what we're here for!

- Paying attention to the science being done helps keep focus on our mission

Presented to DOE in regular reports, and used in our annual report

- Visibility for NERSC
- Visibility for NERSC users
Some recent examples

Hot off the press:

- NERSC Users in Mathematics for Experimental Data, and Earth and Environmental Science, devised an approach to Gaussian Processes that distributes a large-but-sparse covariance matrix over many Perlmutter GPU nodes, computes the locally-small submatrices on the GPUs, then reassembles the result.
- Applied the method to a large climate dataset, and demonstrated an ability to accommodate the huge volumes of data collected in climate science.
- Breaking the matrix down into submatrices small enough to fit in a GPU enabled a ~25x speedup over Cori.
- Published in Nature Scientific Reports (March 2023).
Some recent examples

Investigating energy (heat) transfer through 2 layers of 2D semiconductor materials

- Experimentally discovered that directing light at one layer increased heat dissipation >100x
- Ran ab-initio simulations on Cori to understand the mechanism
- May enable new, smaller semiconductors
- Published in Nature Nanotechnology
FourCastNet: AI-accelerated weather modeling

Scientific Achievement
- First deep learning model to model atmospheric phenomena close to resolution and skill of operational numerical weather prediction models

Significance and Impact
- State-of-the-art transformer architecture accurately forecasts wind, temperature, precip, and water vapor up to 10 days in advance
- Hybrid data-/model-parallel training scales to 4000 GPUs on Perlmutter
- Forecasts can be made with single GPU up to 44,000x faster than conventional approaches

Pathak et al 2022 [arXiv:2202.11214]
Kurth et al 2022 [arXiv:2208.05419]
Some recent examples

Plasma accelerators are a promising development for shrinking the size and cost of particle accelerators.

- "WarpX enables computational explorations of key physics questions in the transport and acceleration of particle beams in long chains of plasma channels, which could yield significant savings in the design and characterization of plasma-based colliders before they are built"
- ECP Project, built on AMReX, and Adaptive Mesh Refinement library
- Ran successfully at scale on Frontier, Fugaku, Summit, and Perlmutter - which earned it the 2022 Gordon Bell Prize
First Exascale *Ab-Initio* MD Calculation

**Breaking the Exaop Barrier for the Electronic Structure Problem in *Ab-Initio* Molecular Dynamics**

(mixed FP16/FP32)

- Team showed that for certain problems, mixed precision arithmetic can achieve scientifically valid results in electronic structure calculations.
- The non-orthogonal local submatrix method applied to electronic-structure based molecular dynamics simulations exceeds 1.1 EOP/s in FP16/FP32 mixed floating-point arithmetic.
- Used 4,400 NVIDIA A100 GPUs on Perlmutter.
- The method achieves a sustained fraction of peak performance of about 80%.
- Example calculations are performed for SARS-CoV-2 spike proteins with up to 83 million atoms.

*SARS-CoV-2 spike protein in aqueous solution: full cell (left) and without hydrogen and oxygen atoms (right).*

Robert Schade, Tobias Kenter, Hossam Elgabarty, Michael Lass, Thomas D. Kühne, Christian Plessl, Paderborn University

*arXiv:2205.12182v1 24 May 2022*
Some recent examples

NERSC Users simulating the SARS-CoV-2 spike protein used a submatrix method to distribute a large sparse-matrix problem as a parallel set of small dense-matrix problems.

And demonstrated using mixed-precision methods (FP16 for some parts of the problem, FP32 for other parts), can give valid results alongside the ability to use the tensor cores in Perlmutter's GPUs.

With these methods, they achieved ExaOps ($10^{18}$ operations/second) across 4400 GPUs (1100 nodes) on Perlmutter.
Where to find Science Highlights

https://www.nersc.gov/science/science-news/
How to get my work written up here?

https://docs.google.com/forms/d/e/1FAIpQLScP4bRcRtcde43nqUx4Z_sz780G9HsXtpecQ_q1PKvGafDVVKQ/viewform
Coming up

Upcoming topics:

• April: Julia at NERSC
• May: JupyterHub

We'd love to hear more lightning talks from NERSC users about the research you use NERSC for!

Nominate a topic at https://forms.gle/WjYx7zV7SAz2CaYz7
Thank You