NUG Monthly Meeting

19 November, 2020
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
  • Announcements/CFPs
  • Topic of the day: NERSC and NERSC Users at SC20
  • Coming meetings: topic suggestions/requests?
  • Last month's numbers
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/)

Tell us what you did, and what was the key insight?
Dilip Asthagiri had a paper published in J Physical Chemistry Letters shows that temperature influences protein folding, perhaps prompts a re-thinking partitioning proteins into hydrophilic/hydrophobic groups.

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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
Announcements and CFPs

Check latest weekly email for these:

- NERSC User Survey - invitation coming this week!
  - You’ll see an email from NBRI on behalf of NERSC
  - Please give feedback! The survey is short, and important for NERSC - both for reporting and for identifying what we should keep doing and what we should improve
- Maintenance yesterday: PE defaults unchanged, new 20.10 PE replaces old 20.03 one
- Upcoming training events for NVidia HPC SDK and for Totalview HPC debugger, Dec 8-10
The final power upgrade for the Perlmutter installation will take place December 15-20. During most of this time, power will be cut to the building where NERSC is housed. You can expect that for the duration of the outage, all NERSC resources will not be available.

Especially: we expect power to be out from Tuesday Dec 15 to Friday Dec 18.
Changes to Premium Charging for 2021

• When to use premium
  • For a scientific emergency (i.e. not expiring allocation)
    • Unexpected scientific event, review that needs results right away
    • Infrequently
  • Starting in AY2021, projects can use premium at x2 charge factor until they’ve spent 20% of their allocation on premium jobs
  • Then charge increases to x4
    • NERSC may change this in response to premium usage
• PIs will be able to toggle permissions for users in their project to charge a job to premium in iris
  • Instructions will be posted on the web page shortly
New Julia kernel for jupyter.nersc.gov

- Added support for IJulia to jupyter.nersc.gov
  - Kernel has access to all officially-supported packages (in /global/common/cori_cle7/software) as well as the user packages (in ~/.julia)

- Looking for folks to kick the tires
Most NERSC users use computational science to advance research in another field.

But a number of NERSC users, and NERSC itself, contribute to the field of High Performance Computing itself.

This week and last, SC20 - the International Conference for High Performance Computing, Networking, Storage and Analysis - has been happening, and NERSC and a number of NERSC users have been involved.

So for today, we have a brief showcase of how NERSC participates in the field of HPC.
NERSC staff and users presented:

- **Performance Tuning** with the Roofline Model on GPUs and CPUs
- In Situ Analysis and **Visualization** with SENSEI and Ascent
- **Parallel I/O** In Practice
- The **OpenMP** Common Core: A Hands-On Introduction
- **Deep Learning** at Scale
- **UPC++**: An Asynchronous RMA/RPC Library for Distributed C++ Applications
- Using **Containers** to Accelerate HPC
Workshops

NERSC staff and users either organized or presented in:

- Women in HPC
- First International Workshop on Quantum Computing Software
- 5th Deep Learning on Supercomputers Workshop
- HUST-20: 7th International Workshop on HPC User Support Tools
- Seventh SC Workshop on Best Practices for HPC Training and Education
- WORKS20: 15th Workshop on Workflows in Support of Large-Scale Science
- CANOPIE-HPC: Containers and New Orchestration Paradigms for Isolated Environments in HPC
NERSC staff and users either organized or presented in:

- Fifth International **Parallel Data Systems** Workshop
- The 11th International Workshop on **Performance Modeling, Benchmarking and Simulation** of High-Performance Computer Systems
- Seventh Workshop on **Accelerator Programming** Using Directives
- Fourth Workshop on **Interactive** High-Performance Computing
- 2nd Workshop on **Machine Learning** for Computing Systems
- 2nd Annual Workshop on Extreme-Scale **Experiment-in-the-Loop-Computing**
NERSC staff presented a few papers:
(plus more at workshops)

Iris: Allocation Banking and Identity and Access Management for the Exascale Era

Gabor Torok
Mark R. Day

Tuning Floating-Point Precision Using Dynamic Program Information and Temporal Locality

Hugo Brunie*, Costin Iancu*, Khaled Z. Ibrahim*, Philip Brisk1, Brandon Cook*
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Abstract—We present a methodology for precision tuning of full applications. These techniques must select a search space composed of either variables or instructions and provide a scalable search strategy. In full application settings one cannot assume compiler support for practical reasons. Thus, an additional important challenge is enabling code refactoring. We argue for an instruction-based search space and we show: 1) how to exploit dynamic program information based on call stacks; and 2) how to exploit the iterative nature of scientific codes, combined with temporal locality. We applied the methodology to tune the implementation of scientific codes written in a combination of Python, NERSC's compute resources, and Fortran. In this paper, we present the results of this study and discuss the implications for future scientific code development.


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Accelerating Large-Scale Excited-State GW Calculations on Leadership HPC Systems

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2CDE, University of California, Berkeley, CA, USA
3and Jack Deslippe
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Abstract—Large-scale GW calculations are the state-of-the-art approach to accurately describe many-body excited-state phenomena in complex materials. This is critical for novel device design but due to their extremely high computational cost, these calculations often run at a limited scale. In this work, we present algorithms and implementations enhancements made in the materials science code BerkeleyGW to scale calculations to the order of over 10,000 electrons utilizing the entire Summit at ORNL. Excellent strong and weak scaling is observed, and a 108.9 PFILOP/s double-precision performance is achieved on 27,648 V100 GPUs, reaching 32.7% of the peak. This work for the first time demonstrates the possibility to perform GW calculations at such scale within minutes on current HPC systems, and leads the way for future efficient HPC software development in materials, electronic, physical, chemical, and engineering sciences.

Index Terms—GW, GW method, electronic engineering, GW, electronic, excited state, excited state, electronic, GW, electronic, excited state, excited state.
NERSC Users presented even more

Foresight: Analysis That Matters for Data Redu

1st Pamela Gross: Data Science at Scale, CCS-3 Los Alamos National Laboratory Las Alamos, USA pacmgross@lanl.gov

Arvind T. Mohan: CCS-2 Computational Physics and Methods Los Alamos, USA arvinde@lanl.gov

7th Traverse: Tartan

2nd Christopher M. Brown: Data Science at Scale, CCS-3 Los Alamos National Laboratory Las Alamos, USA cbrown@lanl.gov

5th Ryan Bowers: Data Science at Scale, CCS-3 Los Alamos, USA syan@lanl.gov

9th John Pace: Data Science at Scale, CCS-3 Los Alamos National Laboratory Las Alamos, USA jpace@lanl.gov

10th David H. Rees: Los Alamos National Laboratory Los Alamos, USA drees@lanl.gov

Task Bench: A Parameterized Benchmark for Evaluating Parallel Runtime Performance

Elliot Slaughter1, Wei Wu1,2, Yuankun Fu1, Legend Brandenburg1, Nicolai Garcia1, Wilhem Kautz1, Emily Mare1, Kalile S. Morris1, Qinglei Cao3, George Bosilca3, Sooma Mirchandaney1, Wonchun Lee1, Sean Treichler1, Patrick McCormick1, Alex Aiken3

1SLAC National Accelerator Laboratory, 2Los Alamos National Laboratory, 3Purdue University, 4University of Tennessee, Knoxville, 5NVidia

Contact: elliot.slaughter@slac.stanford.edu

ABSTRACT

We present Task Bench, a parameterized benchmark designed to explore the performance of all parallel programming systems under a variety of application scenarios. Task Bench dramatically lowers the barrier to benchmarking and comparing multiple programming systems by making the implementation for a given system orthogonal to the benchmarks themselves: every benchmark constructed with Task Bench runs on every Task Bench implementation. Furthermore, Task Bench’s parameterization enables a wide variety of benchmark scenarios that distill the key characteristics of larger applications.

To assess the effectiveness and overheads of the tested systems, we introduce a novel metric, minimum effective and maximum effective. We evaluate this metric benchmark with

distributed Many-to-Many Protein Sequence Alignment using Sparse Matrices

Oguz Selmioğlu1, Saliya Ekanayake1, Giulia Guidi1, Georgios A. Pavloupolos1, Arifal Azad2, Aydin Buluç3

1Computational Research Division, Lawrence Berkeley National Laboratory, USA 2Microsoft Corporation, USA 3Erkeks, USA

Using All-to-Many Personalized Communication in Two-Phase I/O

Qiao Kang1, Robert Ross1, Robert Latham2, Sumos Lee3, Ankit Agrawal4, Alok Choudhary4, and Wei-keng Liao4

*University
NERSC staff and users presented at least a few posters
Students

- NERSC staff and users contributed to the Students@SC program
- Pic below is leaderboard for Virtual Student Cluster Competition (winner to be announced today!)
BoFs, Panels and more

NERSC staff were involved in:

- State-of-the-Practice talks
- Spack Community BoF
- Panels:
  - Exotic Computation and System Technology
  - Diverse Approaches to Tiering HPC Storage
  - The Inner Workings of SCinet as Told by Four Alumni of the Women in IT Networking at SC (WINS) Program
- SCinet
- Committees
NERSC at SC20

Key take-home here is:

NERSC is heavily involved in the development of HPC as a field
More than just a provider of compute resources

Our users are a key part of this
Coming up

Topic requests/suggestions?

• Eg:
  • Deep(ish) dive into NERSC's Slurm setup
  • HPSS tips, and stories of the move from Oakland to Berkeley

We'd love to hear some lightning talks from NERSC users about the research you use NERSC for!
Last month's numbers - October

Scheduled and overall availability:

<table>
<thead>
<tr>
<th></th>
<th>Scheduled</th>
<th>Overall</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cori</td>
<td>95.9%</td>
<td>94.2%</td>
</tr>
<tr>
<td>HPSS</td>
<td>100.00%</td>
<td>100.0%</td>
</tr>
<tr>
<td>CFS</td>
<td>100.00%</td>
<td>99.8%</td>
</tr>
</tbody>
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Cori:
- Big cscratch1 crash
- Monthly maintenance
- Effects of a downed cabinet
Last month's numbers - October

Cori Utilization: 91.4%
Large jobs: 28.0%

New Tickets: **669**
Closed Tickets: **711**
Backlog at 1 Oct: **594**
Thank You