

NERSC User's Group (NUG) Monthly Community Call



29 February, 2024

Science Engagement @ NERSC



Lipi Gupta, PhD



Science Engagement Engineer in the User Engagement Group (UEG) at NERSC

Background: PhD in Physics, University of Chicago

Research Interests: applying Machine Learning techniques to improve particle accelerator operation and control

Eating Preferences/Fav Foods: any noodle based dish!

Favorite Sci-Fi Movie: The Martian (2015 - Matt Damon and Jessica Chastain)

Charles Lively III, PhD



Science Engagement Engineer in the User Engagement Group (UEG) at NERSC

Background: PhD in Computer Engineering, Texas A&M University

Research Interests: Energy-Aware Computing, Performance Modeling and Optimization, Applications of Game Theory

Eating Preferences/Fav Foods: Vegan but seafood on rare occasions

Favorite Sci-Fi Movie: Contact (1997 - Jodie Foster and Matthew McConaughey)

Welcome to NUG Community Calls



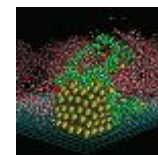
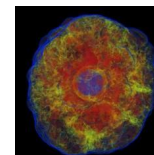
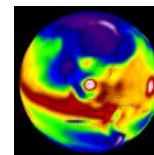
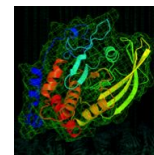
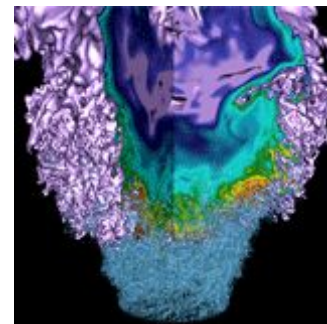
- What is a NUG Community Call?
- How will this be different from the previous NUG meetings?
- What will the future of NUG Community Calls look like?

Today's Pipeline



- Interactive - please participate!
 - [NERSC User Slack](#) (link in chat)
 - **#webinars** channel
- Agenda:
 - Introductions - Charles Lively and Lipi Gupta (NERSC)
 - ICE Breakers - NERSC Edition
 - General NERSC Updates/Announcements
 - Calls for Participation and Upcoming Scheduled NERSC Trainings
 - Topic(s) of the Day:
 - Documentation Tree Testing (Annette Greiner, NERSC)
 - Towards Large-Scale Materials Modeling at Quantum Accuracy (Bikash Kanungo, the University of Michigan)
 - High Impact Scientific Achievement NERSC Early-Career Award Winner

NUG Breakers



NUG Breakers (1)



What did you
want to be
when you
grew up (if
not what you
are now!)

Can you guess Lipi's answer?



Image by macrovector on Freepik

Can you guess Charles' answer?



Image by vectorpocket on Freepik

NUG Breakers (2)



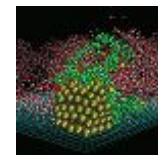
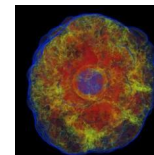
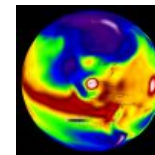
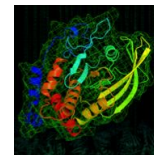
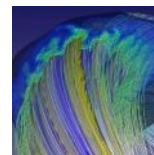
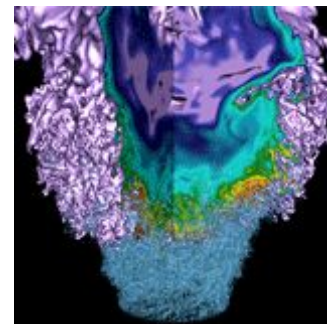
Will you be seeing Dune 2
this weekend? (if you
haven't already!)

Have you read the book?

If you are not going to see it,
why not!?



Announcements/Updates/Calls



Announcements - NERSC Updates



- Apply for Quantum Information Science Research Allocations by Friday!
 - NERSC is soliciting new project proposals in the area of quantum information science using the Perlmutter supercomputer. Open call, not limited to current NERSC users.
- Attention Students: NERSC Summer Internships Available!
 - Undergraduate or Graduate students who will be enrolled as a student in the fall? Qualifications/pay vary depending on the project and years of education completed.
- Announcing 2024 NESAP Pathfinding Projects!
 - 23 teams were selected as "pathfinding teams". Teams will have access to a total of 25 NERSC staff, 10 Postdocs, and 200K GPU node hours on the Perlmutter supercomputer.
- Attention VASP Users: VASP 6 for GPUs Available at NERSC!
 - VASP application performs ab initio quantum-mechanical molecular dynamics (MD) using pseudopotentials and a plane wave basis set. You can use NERSC-installed binaries that are optimized for Perlmutter. Request Access.

Reminder: Please see the Weekly Email for Links!

Announcements - Calls for Participation



- **Nominations for George Michael Memorial HPC Fellowship Now Open!**
 - Honors exceptional PhD students throughout the world whose research focus is on high-performance computing areas.
 - The Fellowship includes a \$5000 honorarium, recognition on the ACM, IEEE CS, and ACM SIGHPC websites, and paid travel expenses to attend SC24, where recipients will be honored at the SC Conference Awards Ceremony.
 - must be enrolled in a full-time PhD program at an accredited college or university
 - Nominations Due May 1, 2024

Reminder: Please see the Weekly Email for Links!

Announcements - Perlmutter



- **Perlmutter Scratch Purge Now Enforced**
 - NERSC began enforcing its Perlmutter scratch purge policy on February 1. As part of the policy, NERSC reserves the right to delete any files on the scratch file system that have not been accessed for 8 weeks or longer.
- **Podman-HPC Available Again on Perlmutter**
 - Rolling reboot of Perlmutter last month included a fix for the issue, and Podman has been re-enabled.
- **NERSC@50-Save the Date: Celebrate 50 Years of NERSC with Us October 22-24**
 - In honor of NERSC's fiftieth anniversary, we are planning an exciting program of anniversary-related events culminating with the annual NERSC User Group meeting, to be held October 22-24, 2024

Reminder: Please see the Weekly Email for Links!

Announcements - Trainings



- NERSC Training - Forge Toolset for Debugging & Profiling, March 13
 - The goal of this training is to teach useful features of these tools and demonstrate how to use them for debugging and profiling tasks on Perlmutter. Linaro Forge combines DDT for parallel HPC application
- Performance Portability Series: AMReX Tutorial, March 14
 - As part of the OLCF/NERSC/ALCF Performance Portability training series, will cover an overview of AMReX and its applications, focusing on features to solve multiphysics problems.
- Learn Parallel Programming in Fortran, March 26-27
 - A two-day, virtual, hands-on training, "Introduction to Parallel Programming in Fortran," March 26th-27th from 9:00 am to 1:30 pm (Pacific Time) each day, hosted by the Fortran Users of NERSC (FUN) Special Interest Group.
- Debugging Challenging Memory and GPU Problems with TotalView, May 13, 2024
 - NERSC is hosting a training event on effectively using TotalView to debug challenging memory and NVIDIA GPU problems.

Reminder: Please see the Weekly Email for Links!

Announcements - Scheduled Outages

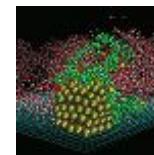
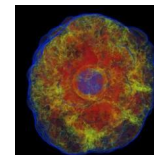
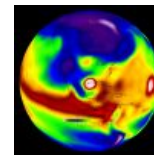
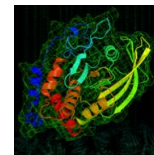
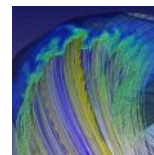
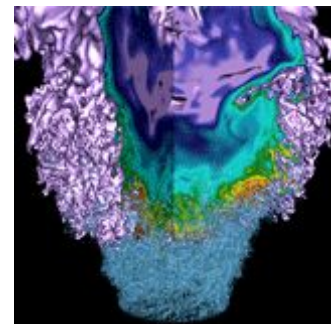


Please see the Weekly Email for Links!

- **Perlmutter**
 - 03/20/24 06:00-16:00 PST, Scheduled Maintenance
 - Perlmutter will be unavailable during the listed times due to scheduled maintenance.
 - 04/17/24 06:00-16:00 PST, Scheduled Maintenance
 - Perlmutter will be unavailable during the listed times due to scheduled maintenance.
 - 05/15/24 06:00-16:00 PST, Scheduled Maintenance
 - Perlmutter will be unavailable during the listed times due to scheduled maintenance.
- **HPSS Regent (Backup)**
 - 03/06/24 09:00-13:00 PST, Scheduled Maintenance
 - System down for quarterly maintenance
- **HPSS Archive (User)**
 - 03/13/24 09:00-13:00 PST, Scheduled Maintenance
 - System down for quarterly maintenance

<https://www.nersc.gov/live-status/motd/>

Tree Testing



Annette Greiner, NERSC

Annette Greiner, NERSC UX Lead



Background: Member of Data and AI Services group at NERSC. Web developer and data wrangler since 1994. Formerly at ALS and JGI. At NERSC since 2010. Dubbed UX Lead in 2023.

Research Interests: User interface design and development, data visualization, FAIR data

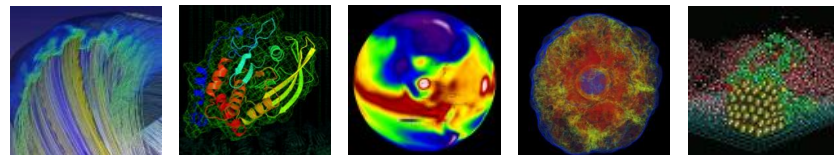
Eating Preferences/Fav Foods: Basic omnivorous human, especially fond of Thai food

Favorite Movie: Buster Keaton's *The General* (1926)

- We're testing a possible new organization for our user documentation. (We're not testing you!)
- You'll have 10 brief tasks, and you can provide additional feedback at the end.
- You can quit anytime. You can skip any task with the "Skip" button.
- We'll see the path you took and learn from it.
- Find the URL and the password in the chat.

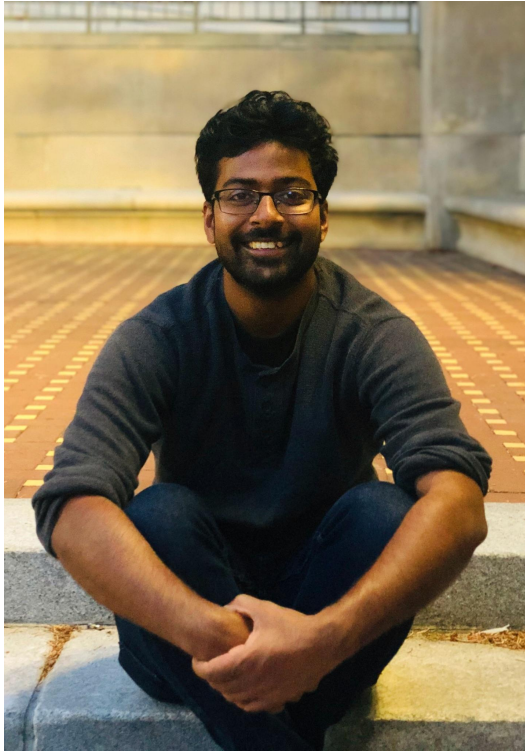
2023-2024 NERSC EARLY CAREER WINNER TALK:

Towards Large-Scale Materials Modeling at Quantum Accuracy



Bikash Kanungo, University of Michigan

Early Career Award Winner - High Impact Scientific Achievement

The NERSC logo features the letters "NERSC" in a bold, white, sans-serif font. The text is set against a dark blue background with a radial light effect emanating from behind the letters, creating a sense of energy and technology.

- Bikash Kanungo is a research scientist at the University of Michigan, Ann Arbor. His research focuses on various theoretical and numerical aspects of density functional theory (DFT) and time-dependent DFT(TDDFT).
- His work involves developing machine-learned exchange-correlation functionals in DFT by drawing connections to quantum many-body (QMB) methods.
- He also develops fast and scalable numerical methods, ranging from efficient mixed basis to accelerated time propagators to high performance computing innovations, to enable exascale DFT/TDDFT calculations.
- He received his Ph.D in Mechanical Engineering and Scientific Computing from the University of Michigan (2019). Prior to being a research scientist, he worked as a postdoc at the University of Michigan (2019-2021).

Coming up



Upcoming topics:

- Power/Energy Consumption Series @ NERSC
- Security @ NERSC
- Community needs/ideas (e.g. new groups/topics, “get to know” <blank>, new docs/training options, career?)
- Other topic suggestions/requests?

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>

Science Highlights Submission:

<https://docs.google.com/forms/d/e/1FAIpQLScP4bRCtcde43nqUx4Zsz780G9HsXtpecQqIPKvGafDVVKQ/viewform>

Lightning Talks



Highlights



Until Next Time!



Thank You