NERSC User's Group (NUG) Monthly Community Call

NERSC

21 March, 2024

U.S. DEPARTMENT OF ENERGY | Office of Science

BERKELEY LAB
Lawrence Berkeley National Laboratory

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

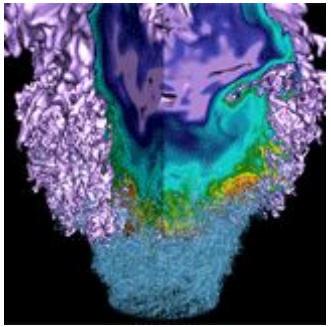
Eating Preferences/Fav Foods: Vegan but seafood on rare occasions

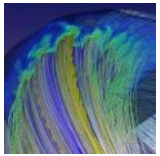
Favorite Sci-Fi Movie: Contact (1997 - Jodie Foster and Matthew McConaughey)

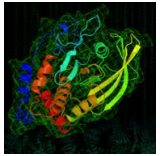
Today's Pipeline

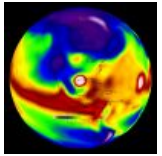
- Interactive - please participate!
  - **NERSC User Slack** (link in chat)
  - **#webinars** channel
- Agenda:
  - General NERSC Updates/Announcements
  - Calls for Participation and Upcoming Scheduled NERSC Trainings
  - Topic(s) of the Day:
    - Documentation Tree Testing (Annette Greiner, NERSC)
    - Trap-assisted Auger-Meitner recombination from first principles (Fangzhou Zhao, Max Planck Institute)
      - High Impact Scientific Achievement NERSC Early-Career Award Winner

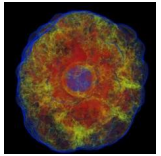
NUG Breakers

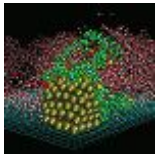












NERSC

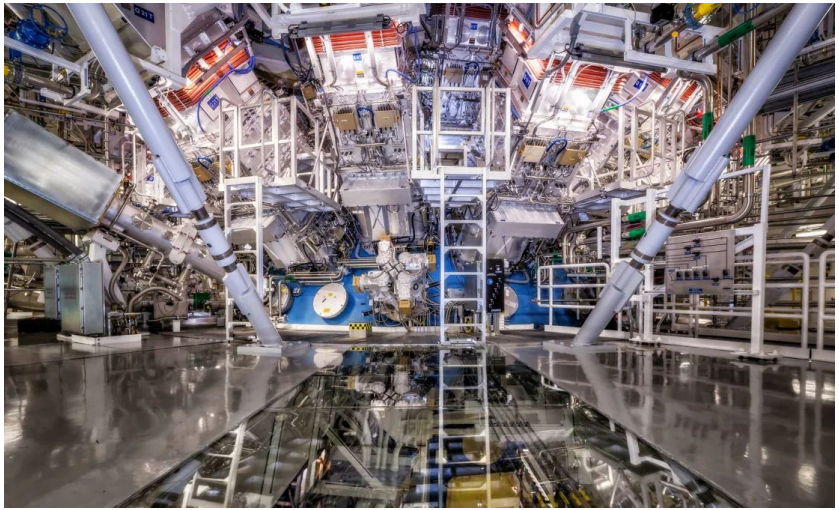
U.S. DEPARTMENT OF ENERGY | Office of Science

BERKELEY LAB
Lawrence Berkeley National Laboratory

NUG Breakers (1)

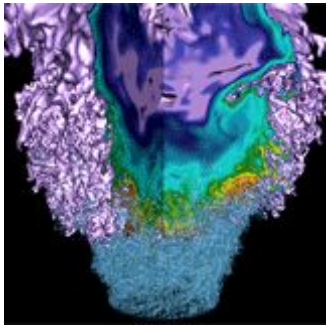
What recent scientific breakthrough in 2024 are you most excited to see progress?

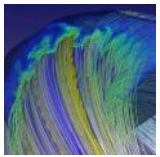
Can you guess Lipi's answer?

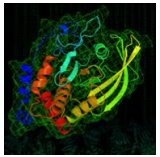


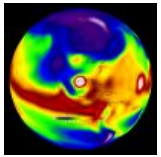
Can you guess Charles' answer?

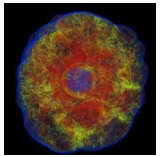
Announcements/Updates/Calls

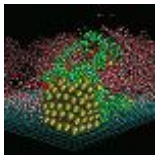












NERSC

Announcements - NERSC Updates

- 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.
- 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.
- 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 - Calls for Participation

- **Nominations for George Michael Memorial HPC Fellowship Now Open! (Due May 1, 2024)**
  - Honors exceptional PhD students throughout the world whose research focus is on high-performance computing areas and includes a $5000 honorarium
    - must be enrolled in a full-time PhD program at an accredited college or university
- **Call for Proposals for Generative AI for Science Applications**
  - NERSC has a new Call For Proposals for projects that will leverage Perlmutter to push the state of the art in Generative AI and deep learning for science and produce novel science outcomes. Submit by April 1, 2024
- **(NEW/UPDATED) BOF, Workshop, & Tutorial Submissions for US Research Software Engineer Association Conference Open through April 1**
  - Submissions are now open for the second annual US Research Software Engineer Association Conference (US-RSE'24), which will be held October 15-17, 2024, in Albuquerque, New Mexico.
- **(NEW/UPDATED) Submit a Proposal for August NERSC/OLCF/NVIDIA Hackathon by May 8!**
  - NERSC, in conjunction with NVIDIA and OLCF, will be hosting a Open Hackathon from August 20th-22nd with an opening day on August 13th as part of the annual Open Hackathon Series.

Reminder: Please see the Weekly Email for Links!

Announcements - Perlmutter (3/21/2024)

- **Are you planning to use Perlmutter for a submission for the Gordon Bell Prize?**
  - If so, please let us know of your plans, by submitting a reservation request at least one week before the requested date (if applicable), or via a ticket.
- **Make the Most of Your Allocation: Submit Jobs on Perlmutter Now Rather than Later!**
  - While NERSC allocations are good for an entire year -- mid-January to mid-January the following year -- for best results, NERSC recommends running jobs throughout the allocation year, and especially at the beginning.

Reminder: Please see the Weekly Email for Links!

Announcements - Trainings(3/21/2024)

- 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.
- Dask Training on Perlmutter March 28 and 29
  - NERSC has contracted with OpenTeams to hold a training event Thursday, March 28 and Friday, March 29 on Dask, a Python library for parallel and distributed computing
- 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.
- (NEW/UPDATED) Apply by April 21 for May 7-9 NERSC End-to-End LLM Bootcamp
  - NERSC will be co-organizing the end-to-end Large Language Model (LLM) bootcamp with OpenACC and NVIDIA. The bootcamp will be hosted virtually for three days from May 7-9, 2024
- (NEW/UPDATED) Apply early for May-Jun ALCF AI Testbed Training Workshops
  - ALCF is offering four individual workshops to introduce participants to the architecture and software of AI testbed systems in May-June, 2024. Notice early registration deadlines, some as early as April 1
- (NEW/UPDATED) Apply by May 8 for Aug 13-22 NERSC GPU Hackathon
  - NERSC will be co-organizing hybrid GPU Hackathon with NVIDIA and OLCF from August 20th-22nd with an opening day on August 13th as part of the annual Open Hackathon Series.
  -

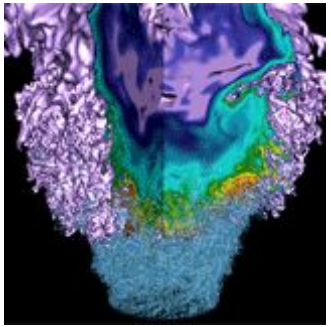
Announcements - Scheduled Outages

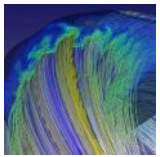
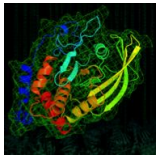
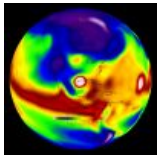
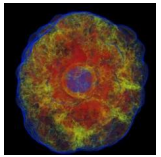
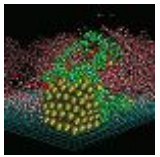
Please see the Weekly Email for Links! (3/21/2024)

- **Perlmutter**
  - 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.

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

Tree Testing(Part 2)



Annette Greiner, NERSC

U.S. DEPARTMENT OF ENERGY | Office of Science

BERKELEY LAB

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

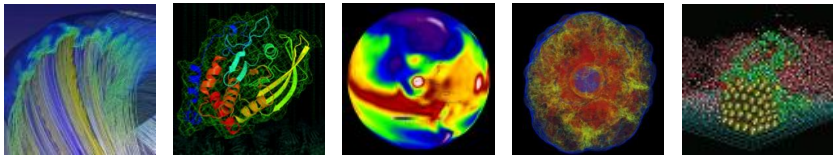
Favorite Movie: Buster Keaton's *The General* (1926)

Improving docs.nersc.gov

- We're testing a possible new organization for our user documentation. (We're not testing you!)
- You'll have 10 brief tasks.
- 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:

Trap-Assisted Auger-Meitner Recombination from First Principles



Fangzhou Zhao, PhD- *Humboldt Fellow*
Max Planck Institute for the Structure and Dynamics of Matter in Hamburg, German

U.S. DEPARTMENT OF ENERGY | Office of Science
BERKELEY LAB

Early Career Award Winner - High Impact Scientific Achievement

- Fangzhou Zhao is now a Humboldt Fellow at the Max Planck Institute for the Structure and Dynamics of Matter in Hamburg, Germany
- Fangzhou obtained his Ph.D. in Physics from UC Berkeley with Prof. Steven G. Louie in 2021, and he obtained his B.S. degree in Physics from Zhiyuan College, Shanghai Jiao Tong University in 2015.
- His graduate work consists of topological electronic and optical properties of quasi-one-dimensional nanomaterials like graphene nanoribbons and carbon conjugated systems
- His postdoctoral work as an Elings Prize Postdoc Fellow focuses on first-principles calculations modeling of nonradiative recombination process in semiconductors.
- He has recently developed a first-principles calculation formalism and code to calculate the rate of trap-assisted Auger-Meitner recombination in semiconductors and was honored with the Corbett Prize at the 32nd International Conference on Defects in Semiconductors.
- Fangzhou has published papers in top journals such as 2 Nature, 3 Physical Review Letters, 2 Nano Letters, and 1 Journal of the American Chemical Society papers.

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/1FAIpQLScP4bRCtcde43nqUx4Z_sz780G9HsXtpecQ_qIPKvGafDVVKQ/viewform

Lightning Talks

Highlights

Until Next Time!

Thank You