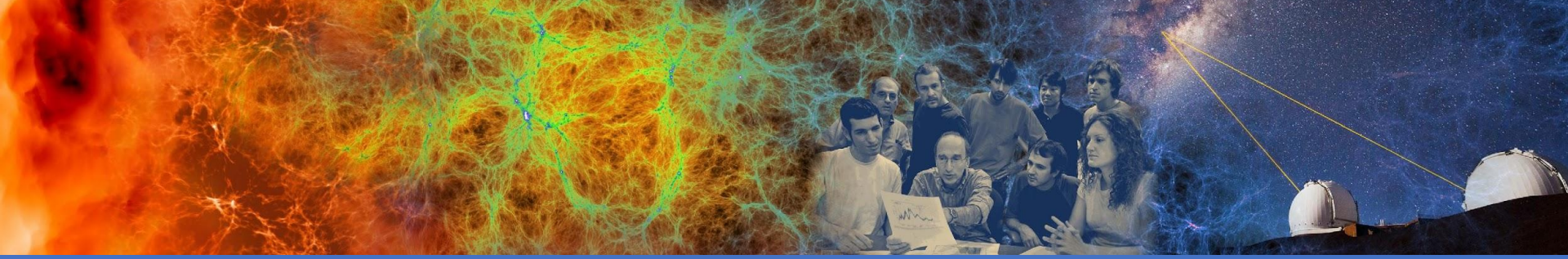

NERSC User's Group (NUG) Community Call

January 09, 2025

NERSC

BERKELEY LAB

U.S. DEPARTMENT OF ENERGY | Office of Science

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
  - Topic(s) of the Day:
    - Everything You Need to Know About the Allocation Year Transition and More
      - Understanding NERSC Updated Appropriate Use Policy
      - PI Focus: Tips and Guidance
    - 2024 NERSC Early Career Award Winners

Announcements - Calls for Participation

Please see the Weekly Email for Links!

- Applications to Attend the International HPC Summer School Now Open
  - Are you a graduate student or postdoctoral scholar from an institution in Canada, Europe, Japan, Australia, or the United States who is interested in learning more in computational sciences with major state-of-the-art aspects of HPC and Big Data Analytics for a variety of scientific disciplines, advancing the formation of professional networks, being provided with advanced mentoring, facilitating international exchange and opening up further career options?

- Applications for DOE Computational Science Graduate Fellowship Now Open! (Due Jan 16, 2025)

Announcements - Meetings/Trainings

Please see the Weekly Email for Links!

- Webinar: High-Performance Computing and Software Sustainability: Toward Green Software Development
  - This webinar will take place Jan 15, 2025 from 10 to 11 AM PST and requires free registration.

- TotalView Debugging Office Hours, January 24, 2025
  - The office hours will be held from 10 to 11 am (Pacific time) on Friday, January 24, 2025. Zoom connection information is provided at the event webpage (login required).

Announcements - Meetings/Trainings

Please see the Weekly Email for Links!

- (NEW/UPDATED) Join NERSC for HPC Horizons Event, February 12
  - NERSC's annual GPUs for Science Day event is evolving and will now be called HPC Horizons. This evolution reflects the event's focus on exploring the future of high-performance computing (HPC) through the lens of both cutting-edge technology and the diverse community driving its advancement.
  -
- (NEW/UPDATED) NERSC New User Training and Updated Best Practices on Perlmutter on February 13-14, 2025 (Virtual)
  - NERSC is hosting a two half-day virtual training event for new users and existing users on efficiently using NERSC resources and Perlmutter. This also allows for our existing users to learn more about best practices for using Perlmutter as well. This virtual event will occur on Thursday and Friday, February 13-14, 2025.

Announcements - Scheduled Outages

Please see the Weekly Email for Links!

- NERSC Site-Wide Outage Rescheduled for Week of January 27, 2025
  - A site-wide outage, previously scheduled for the week of December 2, has now been rescheduled to the week of January 27, 2025.
  - An outage of NERSC resources is required while power equipment maintenance and upgrades are being performed. The outage is currently expected to begin in the afternoon (Pacific time) on Monday, January 27, 2025, and conclude on Friday, January 31, 2024.
    - Every effort will be made to minimize the total downtime, but please plan for the fact that Perlmutter will be unavailable for the week, and other NERSC resources will likely be unavailable for extended periods during this outage event.
    - We will provide more details as the planning continues.

Topic of the Day

Everything You Need to Know About the Allocation Year Transition and More

Understanding NERSC Updated Appropriate Use Policy

PI Focus: Tips and Guidance

NERSC Early Career Awards Winners

NERSC Early Career Award for High Impact Scientific Achievement

This award recognizes work that has had or is expected to have an exceptional impact on scientific understanding, engineering design for scientific facilities, and/or a broad societal impact.

2024 High Impact Scientific Achievement (1)

Ronald Kouski
Graduate Student
Iowa State University;
Department of the Earth, Atmosphere, and Climate

For research that has shed new light on the influence of African easterly waves (AEWs) on tropical cyclone (TC) genesis and landfall in the Atlantic, uncovering that TC frequency and spatial distribution significantly change in the absence of AEWs.

Ronald Kouski's groundbreaking research has shed new light on the influence of African easterly waves (AEWs) on tropical cyclone (TC) genesis and landfall in the Atlantic, uncovering that TC frequency and spatial distribution significantly change in the absence of AEWs. His analysis of a 50-member ensemble of TC-permitting climate simulations revealed a 10-44% increase in TC activity under AEW suppression, linked to enhanced mid-tropospheric humidity. Leveraging NERSC's Perlmutter supercomputer, Ronald ran 500 simulations, using ~10,000 CPU node hours and generating 300 TB of data, to achieve statistically robust conclusions.

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2024 High Impact Scientific Achievement (2)

Vinicius Mikuni
NESAP Post-Doctoral Fellow
NERSC
Lawrence Berkeley National Laboratory

For developing solutions in the application of deep learning in particle, nuclear, and astrophysics and developing innovative computational workflows.

Vinicius is revolutionizing the application of deep learning in particle, nuclear, and astrophysics by developing cutting-edge solutions to complex challenges, particularly in the realm of denoising or "unfolding" for differential cross-section measurements. His groundbreaking methodologies, encapsulated in the widely-used PyPI package OmniFold, have enabled unprecedented scientific insights and fostered collaborations across experimental, theoretical, and computational domains. Utilizing NERSC's Perlmutter, Vinicius has innovated computational workflows, leveraging GPUs to train thousands of networks for robust uncertainty quantification and introducing a foundation model that doubles training speed without compromising performance.

NERSC Early Career Awards Winners

NERSC Early Career Award for Innovative Use of High Performance Computing

This award honors the innovative use of NERSC's HPC resources. Examples include introducing HPC to a new science domain or a novel use of HPC resources. Anything that puts a fresh perspective on HPC or presents a new way to solve a problem is considered.

2024 Innovative Use of High-Performance Computing (1)

Kyla De Villa
PhD Student
University of California, Berkeley; Department of Earth and Planetary Science

For groundbreaking contributions to computational materials through the discovery of a new state of matter, double superionicity, using GPU-accelerated molecular dynamics simulations at NERSC.

Kyla de Villa has made groundbreaking contributions to computational material science through her discovery of a new state of matter, double superionicity, using GPU-accelerated molecular dynamics simulations at NERSC. Her work, published in *Nature Communications*, revealed this hybrid state where hydrogen and another heavier nucleus become mobile under extreme conditions, significantly advancing our understanding of the interiors of Uranus and Neptune and their magnetic field generation. Kyla independently performed all simulations and analyses, overcoming rigorous challenges to demonstrate the robustness and planetary relevance of her findings. Beyond her research, Kyla is a dedicated mentor, educator, and community builder, revitalizing peer mentoring programs, leading STEM outreach efforts, and organizing graduate seminars, fostering a supportive and inclusive academic environment.

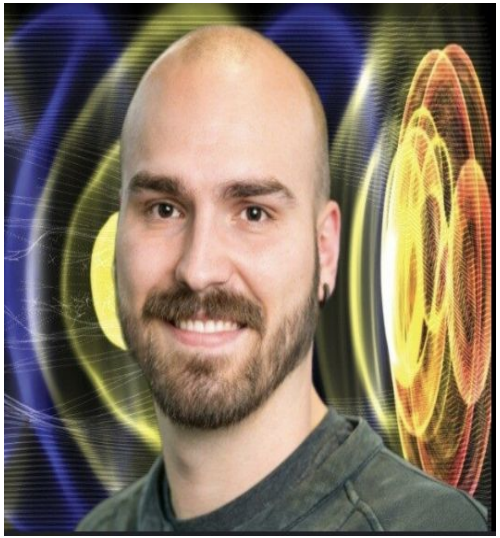
2024 Innovative Use of High-Performance Computing (2)

Massimiliano Pasini
Staff Data Scientist
Oak Ridge National Laboratory;
Computational Coupled Physics Group

For groundbreaking contributions to Scientific Machine Learning through the development of HydraGNN

Dr. Massimiliano Lupo Pasini's groundbreaking contributions to scientific machine learning, particularly through the development of HydraGNN, exemplify innovative use of high-performance computing (HPC). His work achieved unprecedented scalability, processing 154 million atomistic structures with near-linear strong scaling on systems like Perlmutter and Frontier, and addressed critical challenges in data management and energy optimization. By integrating multi-task learning, uncertainty quantification, and energy-efficient hyperparameter optimization into HydraGNN, Dr. Lupo Pasini set new benchmarks in computational efficiency and accuracy for materials science applications. His leadership in leveraging NERSC resources and fostering collaborations across national laboratories underscores his commitment to advancing HPC and delivering impactful solutions across scientific domains.

2024 Innovative Use of High-Performance Computing (3)



Axel Huebl
Staff Scientist
Lawrence Berkeley National Laboratory;
Accelerator Technology & Applied Physics Division

For groundbreaking contributions in developing computational workflows, including the WarpX particle-in-cell code the pyAMRex Python Interface

Dr. Axel Huebl's groundbreaking contributions to high-performance computing (HPC) have transformed accelerator modeling and computational workflows, making him a highly deserving recipient of the 2024 NERSC Early Career Achievement Award. His leadership in developing the WarpX particle-in-cell code and the pyAMReX Python interface has not only advanced the capabilities of block-structured adaptive mesh refinement but also benefitted a wide array of scientific disciplines. By integrating GPU-accelerated simulations with in-the-loop AI/ML methods, Dr. Huebl achieved a remarkable 750x speedup in accelerator workflows, a feat recognized with the PASC24 Conference Best Paper Award. His innovative synthesis of computational techniques exemplifies excellence in HPC and ensures future scientific productivity at an unprecedented scale.

Coming up

Upcoming topics:

- 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