Argonne Training Program on Extreme-Scale Computing

Introduction to ATPESC

Ray Loy
ATPESC Program Director

Outline

- Overview of the ATPESC program
- Application Guidance
- Questions/Discussion

Motivation for ATPESC

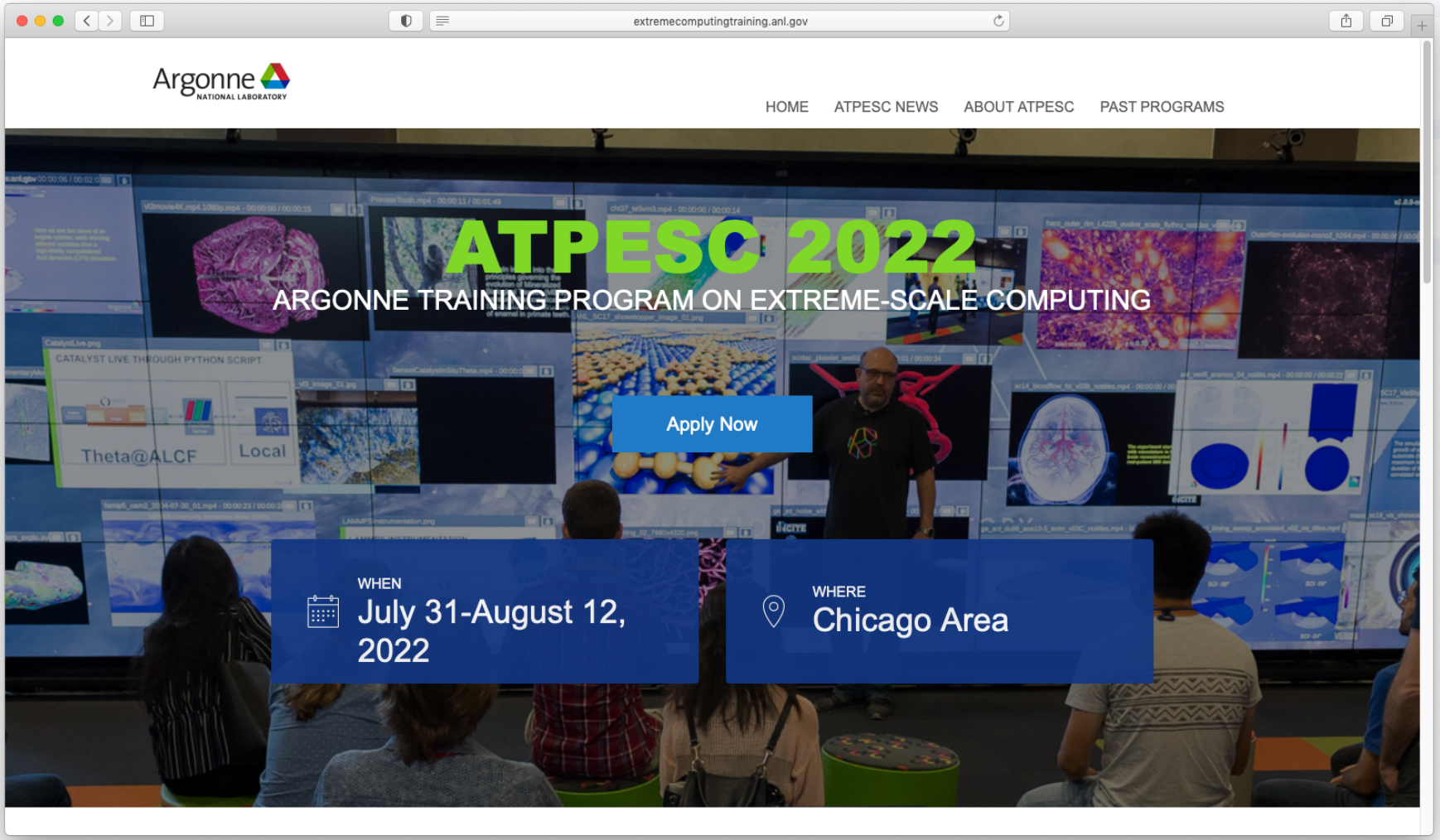
- Today's most **powerful supercomputers** have **complex hardware architectures** and **software environments**
  - and even greater complexity is on the horizon on next-generation and exascale systems
- The **scientific and engineering applications** developed for these systems are themselves **complex**
- There is a **critical need for specialized, in-depth training for the computational scientists** poised to facilitate breakthrough science and engineering using these systems

ATPESC Overview

- Founded by Paul Messina in 2013
- Conceived as a 2-week retreat
- Renowned computer scientists and HPC experts from US national laboratories, universities, and industry serve as lecturers and guide hands-on sessions.
- Target audience: advanced doctoral students, postdocs, and early career computational scientists
- No fee to participate. Domestic travel, meals, and lodging provided.
- Competitive application process reviewed by committee
  - Must have experience in MPI and/or OpenMP and/or Data Science frameworks
  - Experience with at least one HPC system
  - Concrete plans to conduct CSE research on large-scale computers

ATPESC Website

extremecomputingtraining.anl.gov



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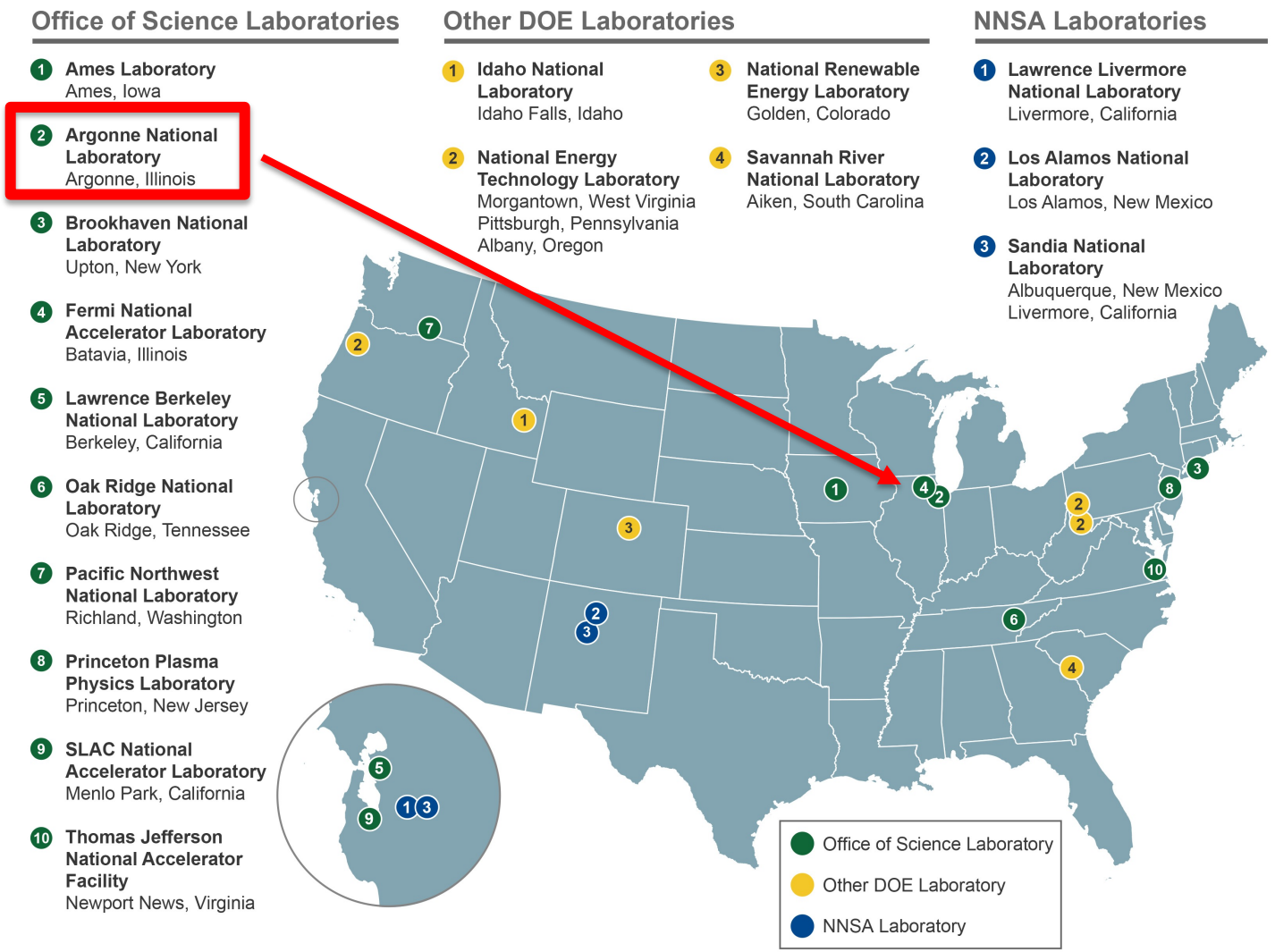
ECP EXASCALE COMPUTING PROJECT

Argonne – a part of DOE National Laboratory System



Together, the **17 DOE laboratories** comprise a preeminent federal research system, providing the Nation with strategic scientific and technological capabilities. The laboratories:

- Execute long-term government scientific and technological missions, often with complex security, safety, project management, or other operational challenges;
- Develop unique, often multidisciplinary, scientific capabilities beyond the scope of academic and industrial institutions, to benefit the Nation's researchers and national strategic priorities; and
- Develop and sustain critical scientific and technical capabilities to which the government requires assured access.

Source: https://science.energy.gov/~/media/_/images/laboratories/DOE_Laboratories_Map_2014_Hi-res.jpg

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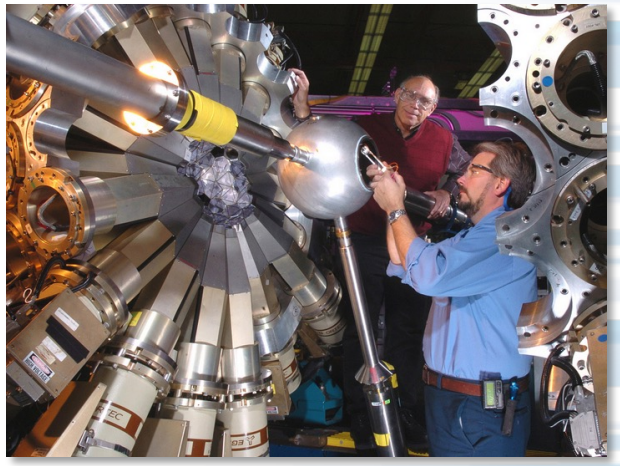
Major Scientific User Facilities at Argonne

Advanced Photon Source

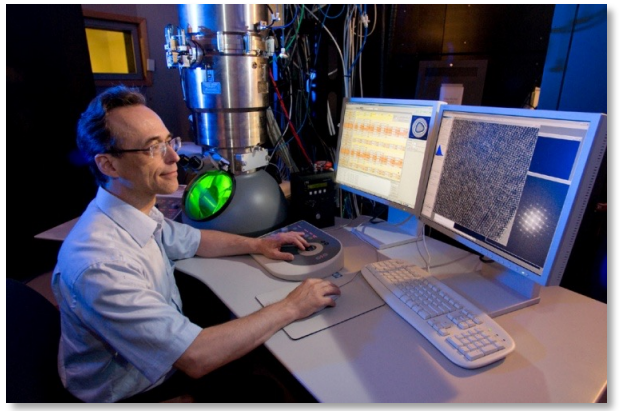
Argonne Tandem Linear Accelerator System



Center for Nanoscale Materials

Argonne Leadership Computing Facility

Electron Microscopy Center



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The future… Aurora Exascale System

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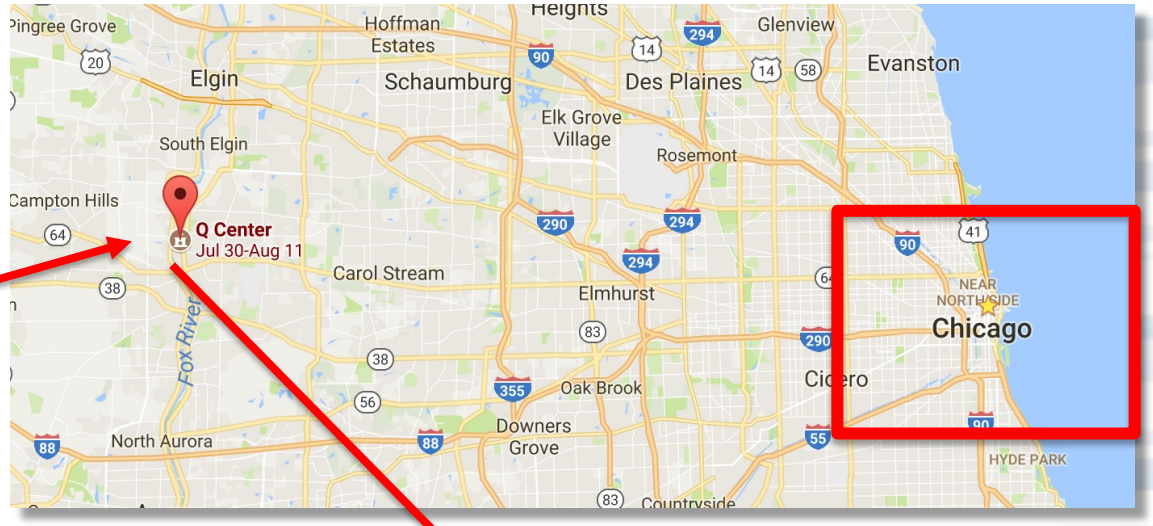
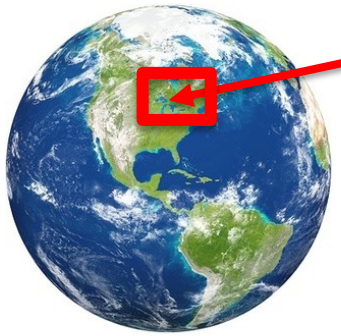
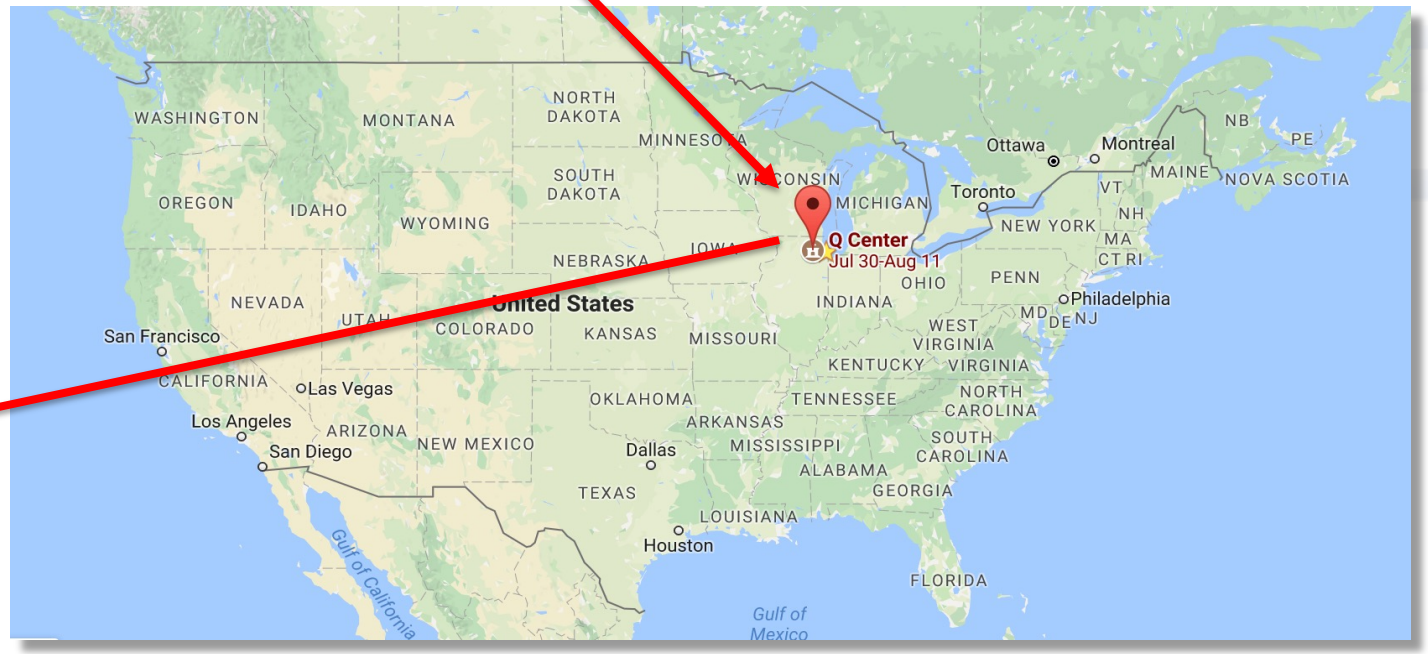
ATPESC 2019 Venue







Source: Google Maps, shutterstock, NASA

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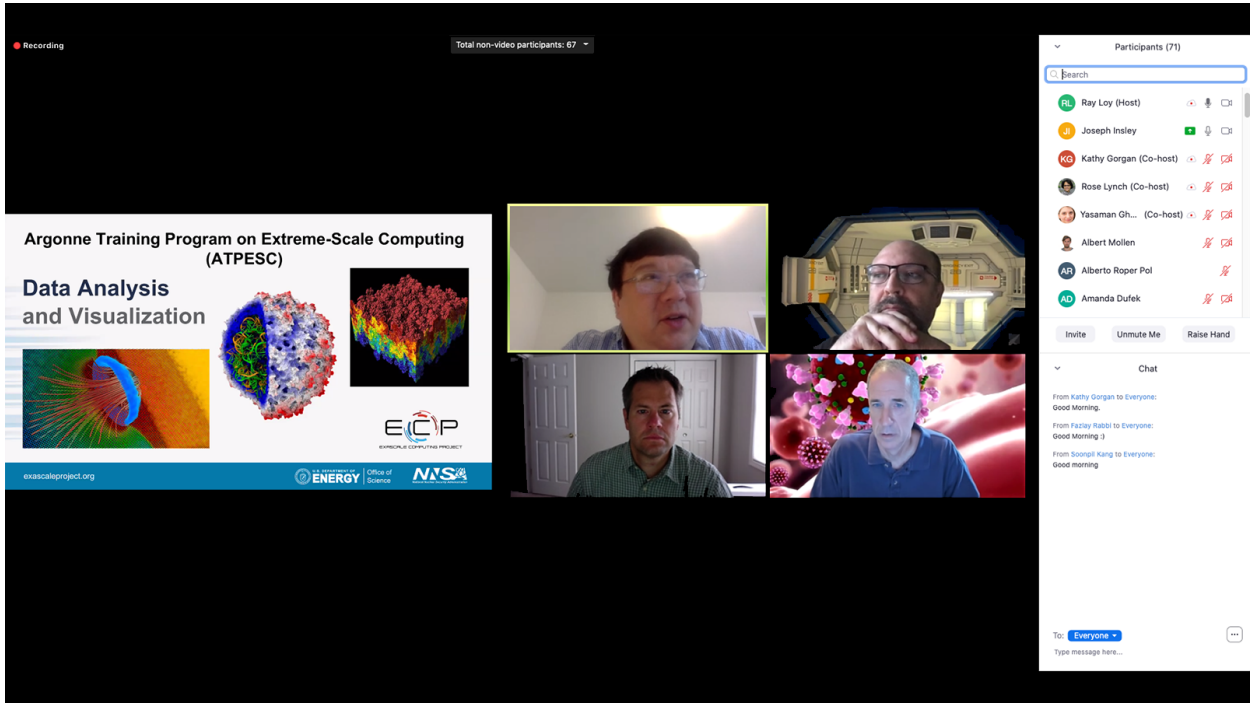
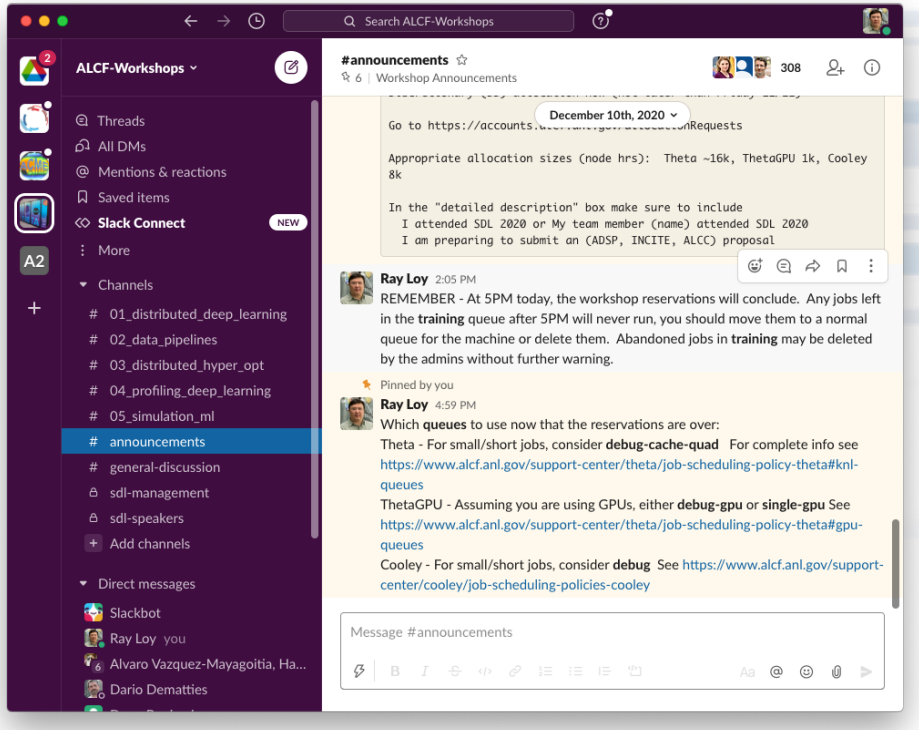
ATPESC 2020, 2021 – Virtual Events





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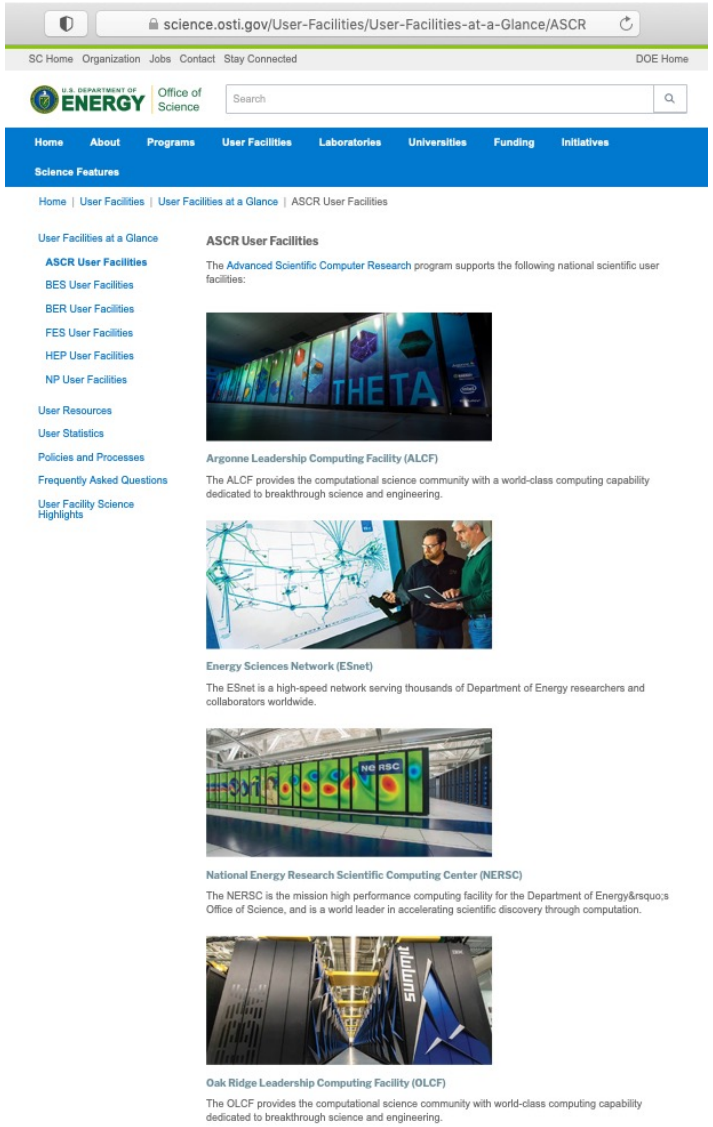
Curriculum Tracks *(over 100 hours of content)*

- **Track 1:** Hardware Architectures
- **Track 2:** Programming Models and Languages
- **Track 3:** Data-intensive Computing and I/O
- **Track 4:** Visualization and Data Analysis
- **Track 5:** Numerical Algorithms and Software for Extreme-Scale Science
- **Track 6:** Performance Tools and Debuggers
- **Track 7:** Software Engineering
- **Track 8:** Machine Learning and Deep Learning for Science

ATPESC Computing Resources



- **ALCF** – Theta/ThetaGPU and Cooley
- **OLCF** - Ascent
- **NERSC** – Cori et al.
- **Intel Devcloud**

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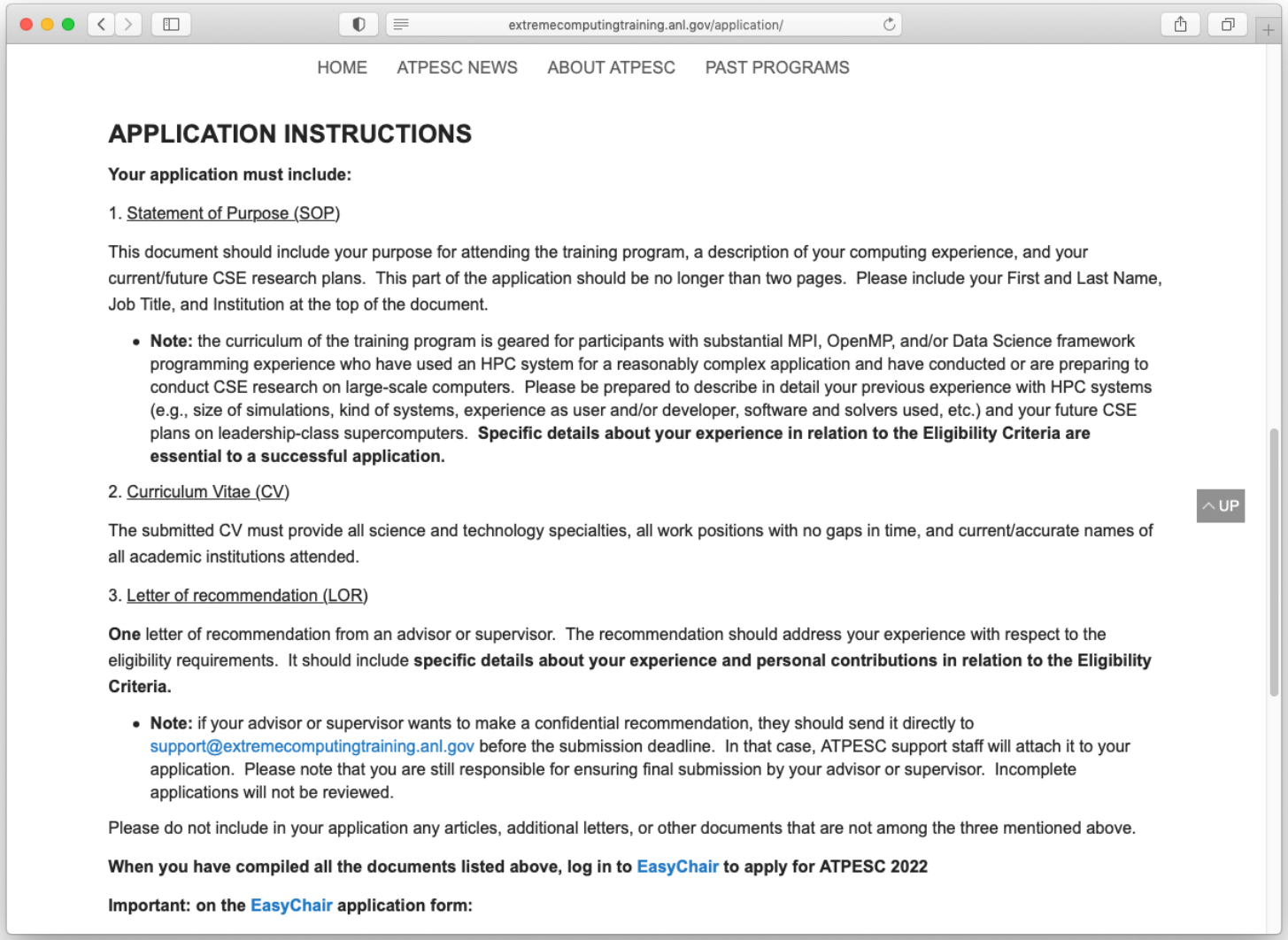
Other ATPESC Content

- Dinner Speakers
  - https://extremecomputingtraining.anl.gov/dinner-talks/
- Tour of selected Argonne National Lab Facilities
  - https://extremecomputingtraining.anl.gov/atpesc-argonne-national-laboratory-tour/

Goals for Attendees

- Exposure to New ideas
- Take advantage of ATPESC Resources
- Talk F2F with Lecturers, other Participants, Support

Application Instructions



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Eligibility

- Substantial experience in MPI and/or OpenMP programming. Equivalent experience with Data Science frameworks will also be considered.
- Experience using at least one HPC system for a reasonably complex application.
- Plans to conduct computational science and engineering (CSE) research on large-scale computers.

Application Components

- Statement of Purpose
- Curriculum Vitae (CV)
- Letter of Recommendation (LOR)

The Key to success

Provide details

The #1 problem a reviewer faces is trying to guess your qualifications when the materials are not clear.

1. Substantial experience in MPI and/or OpenMP programming. Equivalent experience with Data Science frameworks will also be considered.

- Weak statements
  - "I took a class on MPI"
  - "I ran a code that uses MPI"
- Stronger statements
  - "I work on the ___ code. I implemented, tested, and benchmarked the message-passing routines for the boundary exchange of the ___ solver which has a communication pattern that communicates between ___ and the observed scaling was ___ …"
  - "I set up the machine learning framework ___ to solve the ___ problem, using a training data set of size ___ and run on ___ nodes. This was then applied to ___ thousand data sets of size ___ …"
- If you are part of a group-developed code or working on a community code, be specific about your individual contribution.

Experience using at least one HPC system for a reasonably complex application.

- We do not expect that you have access to a world-class system
  - University/corporate clusters are relevant
- Be clear if you are developing code and running it vs. running an existing code that you did not develop.
- What types of runs have you accomplished?
  - Core/node counts are informative
  - Did you perform scaling studies or other performance inquiries?
- What type of queuing system(s) were involved?
  - Did you construct job scripts?
  - Did you run a large campaign and employ any workflow techniques to manage jobs?

Plans to conduct computational science and engineering (CSE) research on large-scale computers.

- The training should be put to good use
- What is your current situation?
  - Are you currently part of a research effort?
  - What specific ways do you anticipate applying your ATPESC training?
- Where are you headed in your career?
  - If you are a student, what types of positions are you applying to?
  - In what ways do you expect your current work to carry over?

ATPESC 2022 Updates

- Subscribe to mailing list linked from the homepage
  - https://extremecomputingtraining.anl.gov (bottom of page)
- Direct inquiries to
  - support@extremecomputingtraining.anl.gov

Acknowledgments

Exascale Computing Project

Website: https://exascaleproject.org

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Questions/Discussion