ARGONNE
ATPESC2023
EXTREME-SCALE COMPUTING

Introduction to ATPESC

Ray Loy
ATPESC Program Director, ANL

Outline

Welcome

Argonne National Laboratory

ATPESC Overview

Logistics

Tour

Welcome!

ATPESC 2023

47 Institutions

ANL
ANU
ARL
Boise State
Brown
Colorado State
Cornell
CU Anschutz
Duke
Federal U Rio de Janeiro
FNAL
Hebrew U of Jerusalem
Iowa State
KTH Royal Inst of Tech
LANL
LBNL
MIT
NASA Langley
NCAR
NERSC
North Carolina State
NREL
Oklahoma State
ORNL
PNNL
Politecnico di Milano
Princeton
Purdue
RPI
Stanford
Stony Brook
TEXAS A&M
Tulane
U Chicago
U Maryland
U Michigan Ann Arbor
U Minnesota
U Pittsburgh
U. Alabama Birmingham
UC Boulder
UC Irvine
UIUC
USC
UT Arlington
UT Austin
UT Knoxville
Washington U St Louis

Argonne National Laboratory

Argonne – a part of DOE National Laboratory System

Office of Science Laboratories

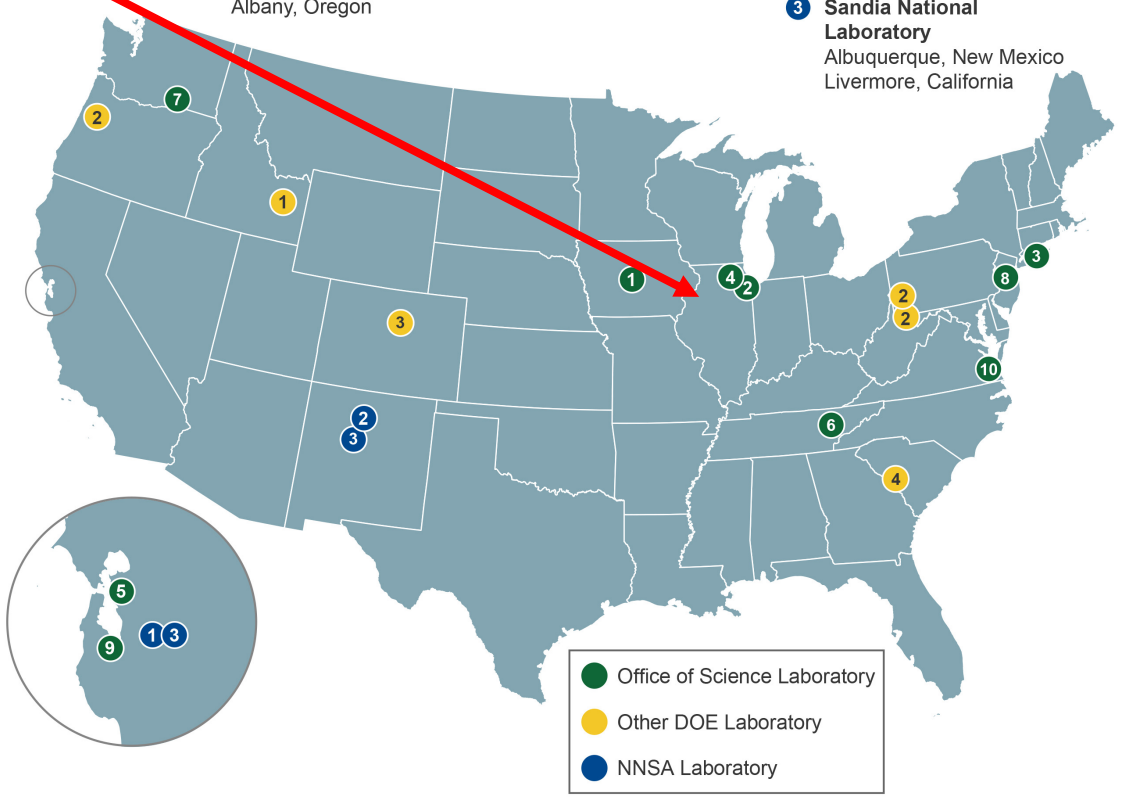
1. **Ames Laboratory**
   Ames, Iowa
2. **Argonne National Laboratory**
   Argonne, Illinois
3. **Brookhaven National Laboratory**
   Upton, New York
4. **Fermi National Accelerator Laboratory**
   Batavia, Illinois
5. **Lawrence Berkeley National Laboratory**
   Berkeley, California
6. **Oak Ridge National Laboratory**
   Oak Ridge, Tennessee
7. **Pacific Northwest National Laboratory**
   Richland, Washington
8. **Princeton Plasma Physics Laboratory**
   Princeton, New Jersey
9. **SLAC National Accelerator Laboratory**
   Menlo Park, California
10. **Thomas Jefferson National Accelerator Facility**
    Newport News, Virginia

Other DOE Laboratories

1. **Idaho National Laboratory**
   Idaho Falls, Idaho
2. **National Energy Technology Laboratory**
   Morgantown, West Virginia
   Pittsburgh, Pennsylvania
   Albany, Oregon
3. **National Renewable Energy Laboratory**
   Golden, Colorado
4. **Savannah River National Laboratory**
   Aiken, South Carolina

NNSA Laboratories

1. **Lawrence Livermore National Laboratory**
   Livermore, California
2. **Los Alamos National Laboratory**
   Los Alamos, New Mexico
3. **Sandia National Laboratory**
   Albuquerque, New Mexico
   Livermore, California

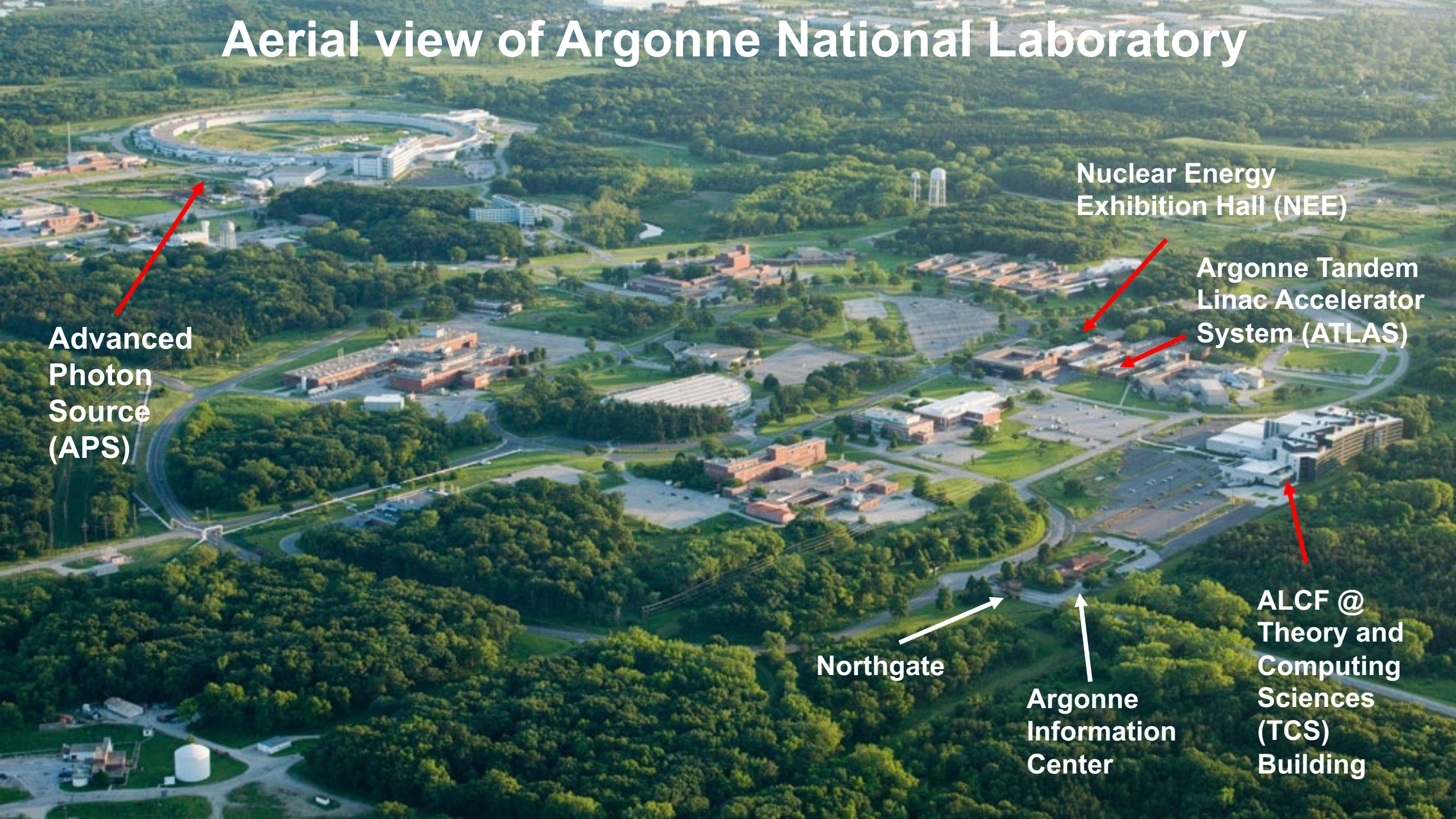


[Image Source]

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

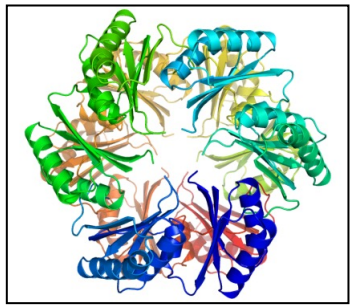
- Execute long-term government scientific and technological missions, often with complex security, safety, project management, or other operational challenges;
- Develop unique, often multidisciplinary, scientific capabilities beyond the scope of academic and industrial institutions, to benefit the Nation's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

Aerial view of Argonne National Laboratory



Argonne's mission: Provide science-based solutions to pressing global challenges

Energy Science



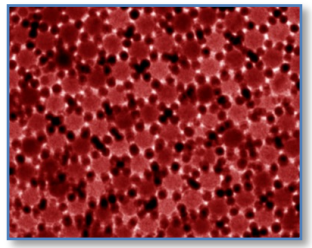
Environmental Sustainability

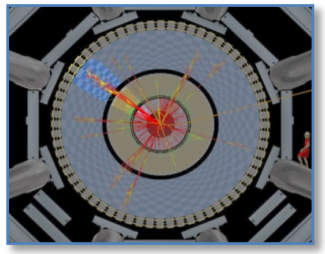
Nuclear and National Security

Use-Inspired Science and Engineering …

... Discovery and transformational Science and Engineering

Major User Facilities





Science and Technology Programs

RESEARCH DIVISIONS

Computing, Environment and Life Sciences

BIO	Biosciences
EVS	Environmental Science
MCS	Mathematics and Computer Science

Energy and Global Security

ES	Energy Systems
GSS	Global Security Sciences
NE	Nuclear Engineering

Photon Sciences

ASD	Accelerator Systems
AES	APS Engineering Support
XSD	X-ray Science

Physical Sciences and Engineering

CSE	Chemical Sciences and Engineering
HEP	High Energy Physics
MSD	Materials Science
NST	Nanoscience and Technology
PHY	Physics

FACILITIES, CENTERS, AND INSTITUTES

User Facilities

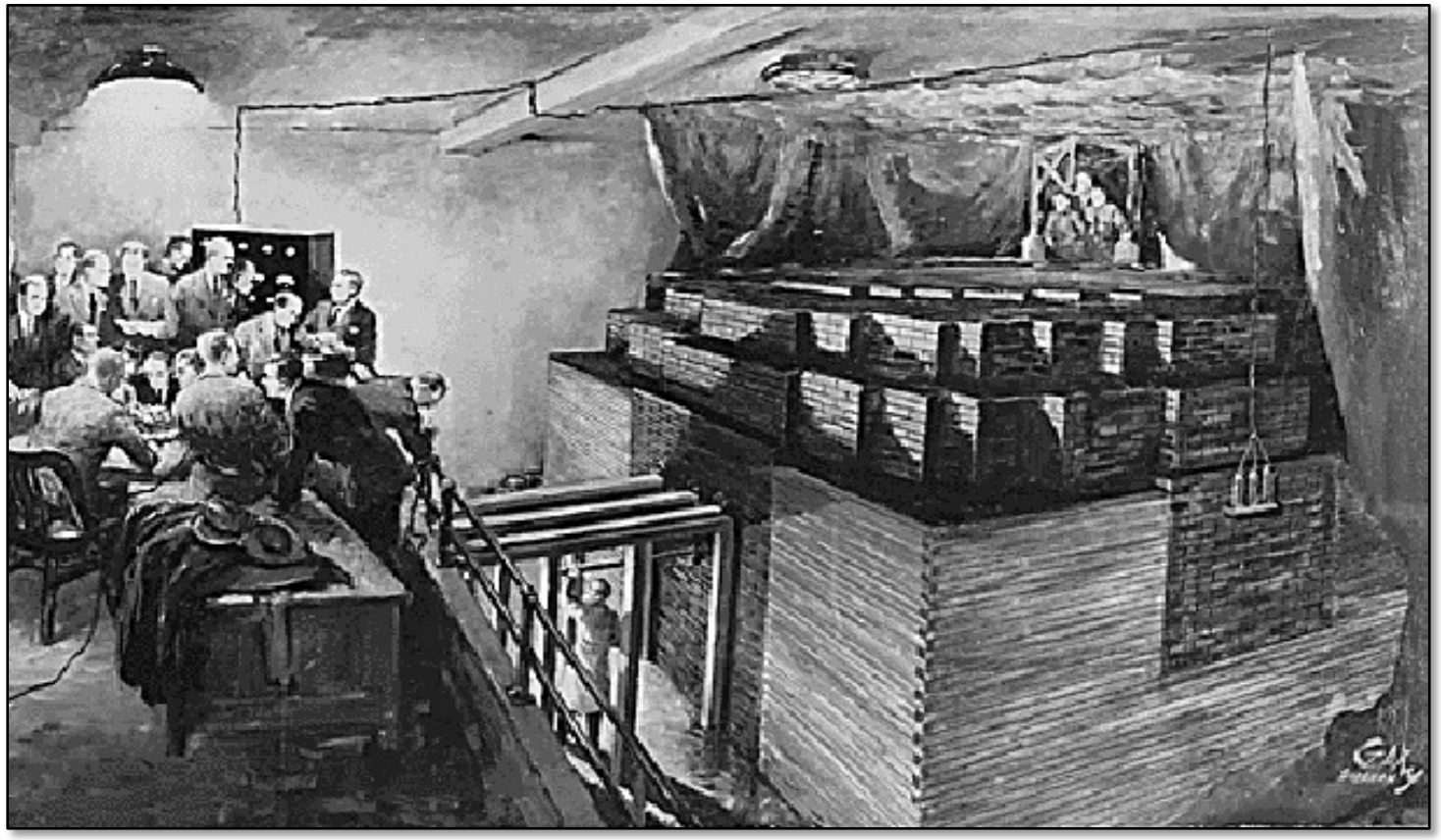
APS	Advanced Photon Source
ALCF	Argonne Leadership Computing Facility
ATLAS	Argonne Tandem Linear Accelerator System
ARM	ARM Southern Great Plains
CNM	Center for Nanoscale Materials

Centers and Joint Institutes

AAI	Argonne Accelerator Institute
ACCESS	Argonne Collaborative Center for Energy Storage Science
ADW	Argonne Design Works
ALI	Argonne Leadership Institute
CEES	Center for Electrochemical Energy Science
CTR	Center for Transportation Research
CRI	Chain Reaction Innovations
CI	Computation Institute
IACT	Institute for Atom-Efficient Chemical Transformations
IGSB	Institute for Genomics and Systems Biology
IME	Institute for Molecular Engineering
JCESR	Joint Center for Energy Storage Research
MCSG	Midwest Center for Structural Genomics
NSP	National Security Programs
NAISE	Northwestern-Argonne Institute for Science and Engineering
RISC	Risk and Infrastructure Science Center
SBC	Structural Biology Center

https://www.anl.gov

The origin of Argonne National Laboratory
CP-1 under the bleachers of Stagg field at U. Chicago



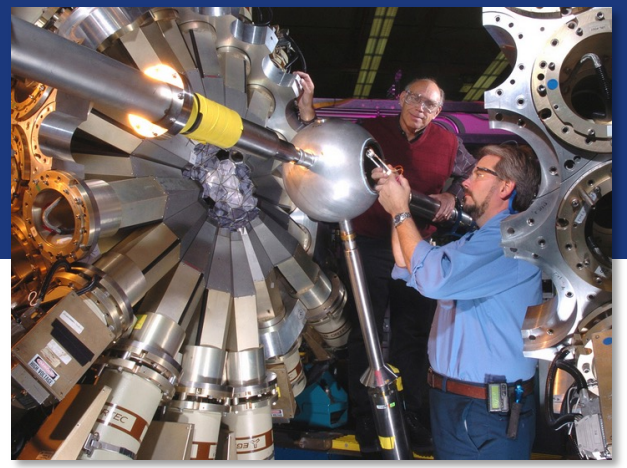
Chicago Pile-1 was the world's first artificial nuclear reactor. The first man-made self-sustaining nuclear chain reaction was initiated on December 2, 1942

See also
Chicago Pile-1: A Brick History

Major Scientific User Facilities at Argonne

Advanced Photon Source

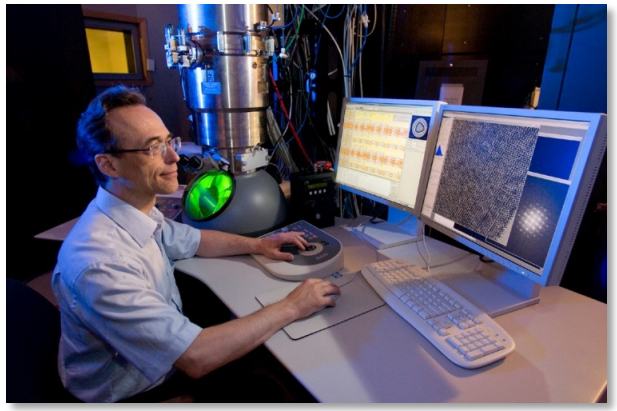
Argonne Tandem Linear Accelerator System



Center for Nanoscale Materials

Argonne Leadership Computing Facility

Electron Microscopy Center



AVIDAC (1949-1953)
Argonne's Version of the Institute's Digital Arithmetic Computer

"Moll" Flanders, Director
Jeffrey Chu, Chief Engineer

- **AVIDAC:** based on a prototype at the Institute for Advanced Study in Princeton
- **Margaret Butler wrote AVIDAC's interpretive floating-point arithmetic system**
  - Memory access time: 15 microsec
  - Addition: 10 microsec
  - Multiplication: 1 millisec
- **AVIDAC press release:**
  100,000 times as fast as a trained "Computer" using a desk calculator

Early work on computer architecture

Margaret Butler helped assemble the ORACLE computer with ORNL Engineer Rudolph Klein

In 1953…

ORACLE was the world's fastest computer, multiplying 12-digit numbers in .0005 seconds (2Kop/s).

Designed at Argonne, it was constructed at Oak Ridge.

ALCF Timeline

2006-2008 Blue Gene/L

2008-2013 Blue Gene/P – Intrepid

2012-2019 Blue Gene/Q – Mira

2017 Theta (KNL)

2022 Polaris

2023 Aurora - *Exascale!*

Motivation for ATPESC

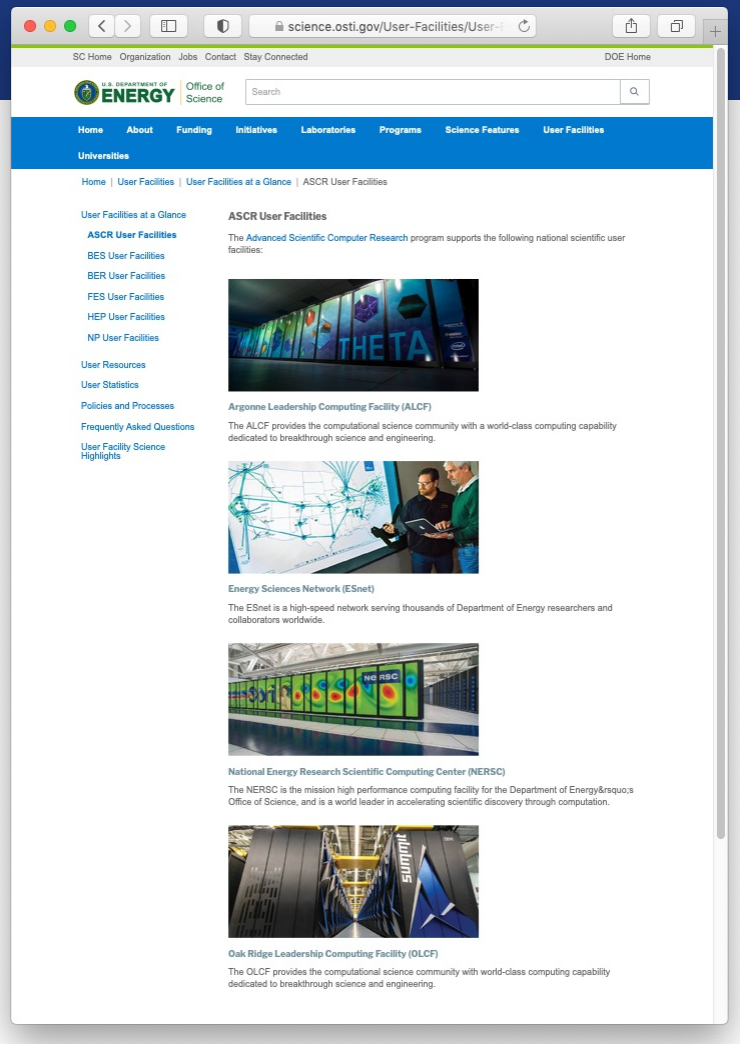
Founded by Paul Messina in 2013. This year is #11 !

- 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

Curriculum Tracks and their leaders

- **Track 1: Hardware Architectures –** Kalyan Kumaran, Vitali Morozov
- **Track 2: Programming Models and Languages –** Rajeev Thakur, Yanfei Guo, Thomas Applencourt
- **Track 3: Software Productivity and Sustainability –** Anshu Dubey
- **Track 4: Visualization and Data Analysis –** Joseph Insley and Silvio Rizzi
- **Track 5: Numerical Algorithms and Software for Extreme-Scale Science –** Richard Tran Mills
- **Track 6: Performance Tools and Debuggers–** JaeHyuk Kwack
- **Track 7: Data-intensive Computing and I/O –** Rob Latham and Phil Carns
- **Track 8: Machine Learning and Deep Learning for Science –** Bethany Lusch

ATPESC Computing Resources



ALCF – Polaris, Theta, ThetaGPU, Cooley, Sambanova, Cerebras, Graphcore

NERSC – Perlmutter

OLCF – Ascent

AMD Devcloud

https://science.osti.gov/User-Facilities/User-Facilities-at-a-Glance/ASCR

https://extremecomputingtraining.anl.gov/agenda-2023/

Agenda 2023

[Introductions | Track 1 | Track 2 | Track 3 | Track 4 | Tour | Track 5 | Track 6 | Track 7 | Track 8]

[MACHINE RESERVATIONS]

ALL TIMES ARE U.S. CENTRAL DAYLIGHT TIME (UTC-5)

SUNDAY, July 30, 2023

1:00PM	Registration opens.	
2:00PM	Welcome and Introduction to ATPESC	Ray Loy, ANL
2:30PM	Quick Start on ATPESC Computing Resources	JaeHyuk Kwack, ANL
3:15PM	*Break*	All
3:45PM	Hands-on	All
4:30PM	Participant Introductions	All
6:30PM	Adjourn/Dinner	

ATPESC Slack

alcf-workshops.slack.com

#announce

#atpesc-2023-general for discussion and Q&A during the program

Topic-related channels (#track-1-hardware)

- See #announce channel pinned items for a list
- Or Channels + option to browse

#atpesc-2023-helpdesk

- Assistance with Zoom or ALCF login issues (see next slide for OLCF and NERSC)

Please do not DM if you can avoid it

- You will get help faster via #atpesc-2023-helpdesk

Help!

ALCF accounts (Polaris, Theta, ThetaGPU, Cooley)

support@alcf.anl.gov (put ATPESC in subject) and slack #help-desk-general

OLCF accounts (Ascent)

Token issues, call: 865.241.6536 (24x7). Other questions, email: help@olcf.ornl.gov (put ATPESC in subject)

NERSC accounts (Perlmutter)

accounts@nersc.gov (put ATPESC in subject) or call 1-800-666-3772

ATPESC general support

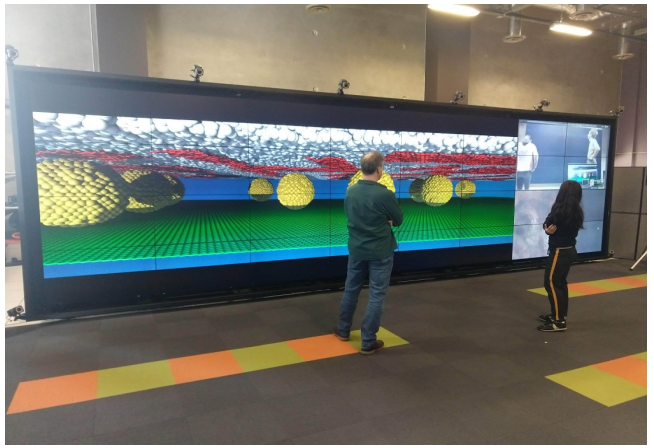
support@extremecomputingtraining.anl.gov

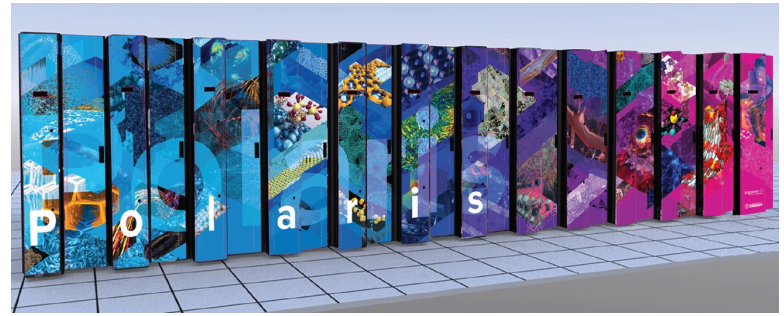
#atpesc-2023-helpdesk

Behind the scenes at ATPESC support

Argonne National Laboratory Tour (Sat 8/5)

- APS – Advanced Photon Source (synchrotron)
- Nuclear Engineering Exhibit
- Data Center (Machine Room) in the Theory and Computing Sciences Building (TCS)
  - Aurora, Polaris, and Theta
- ALCF Visualization Lab





ATPESC Conduct

- Over 70 speakers have taken time out to travel and speak ***for your benefit***
  - *Please give them your attention.*
- You are expected to be present when we are in session
  - *You should not be leaving ATPESC to participate in other meetings*
- After dinner, please return to the Amphiteater on time for the Dinner Speaker

In case of illness or other unexpected problems – please talk to me.

Acknowledgments

Exascale Computing Project

Website: https://exascaleproject.org

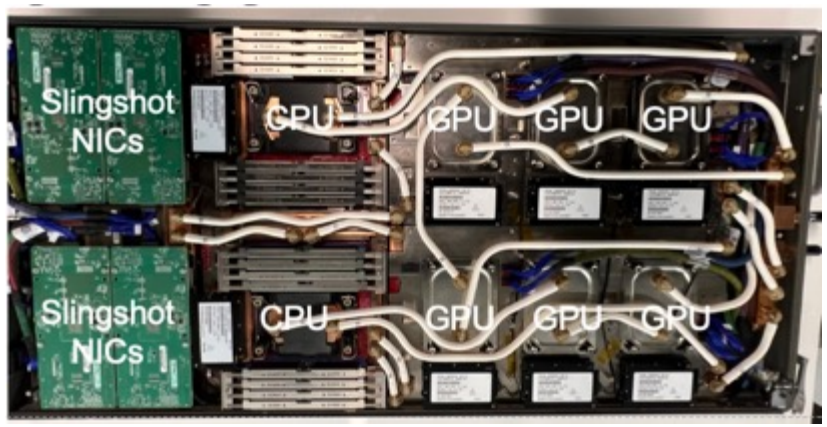
This training and research was supported by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of the U.S. Department of Energy Office of Science and the National Nuclear Security Administration.

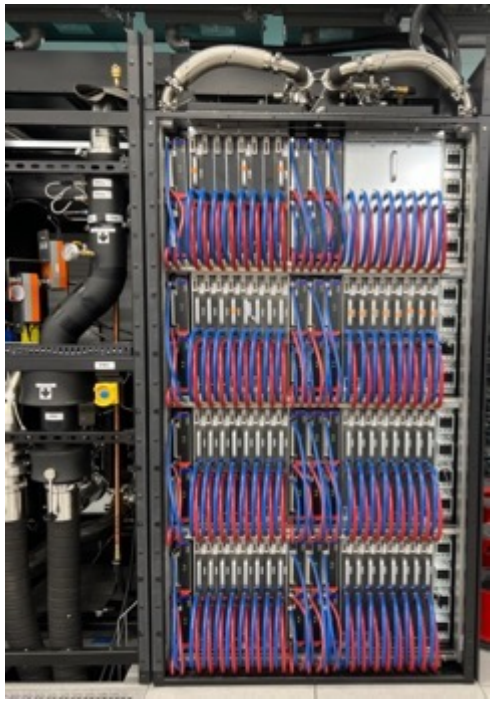
ATPESC 2024

If an associate is interested in attending

- Subscribe to mailing list https://extremecomputingtraining.anl.gov (at top and bottom of page)
- Call for applications usually opens in early January
- *Read the application instructions carefully*
  - Statement of Purpose and Letter of Recommendation should address how the candidate meets the prerequisites *in detail*. Lack of detail is the number one reason applications do not rate highly in the review.

Next up: Aurora Exascale System





Play Video