

ATPESC 2025 Intro and Orientation

Ray Loy

ATPESC Program Director, ANL

ATPESC

Founded by Paul Messina in 2013. ATPESC 2025 is #13 !



Welcome



Argonne National Laboratory



ATPESC Logistics



Tour

Welcome!

ATPESC 2025

50 Institutions

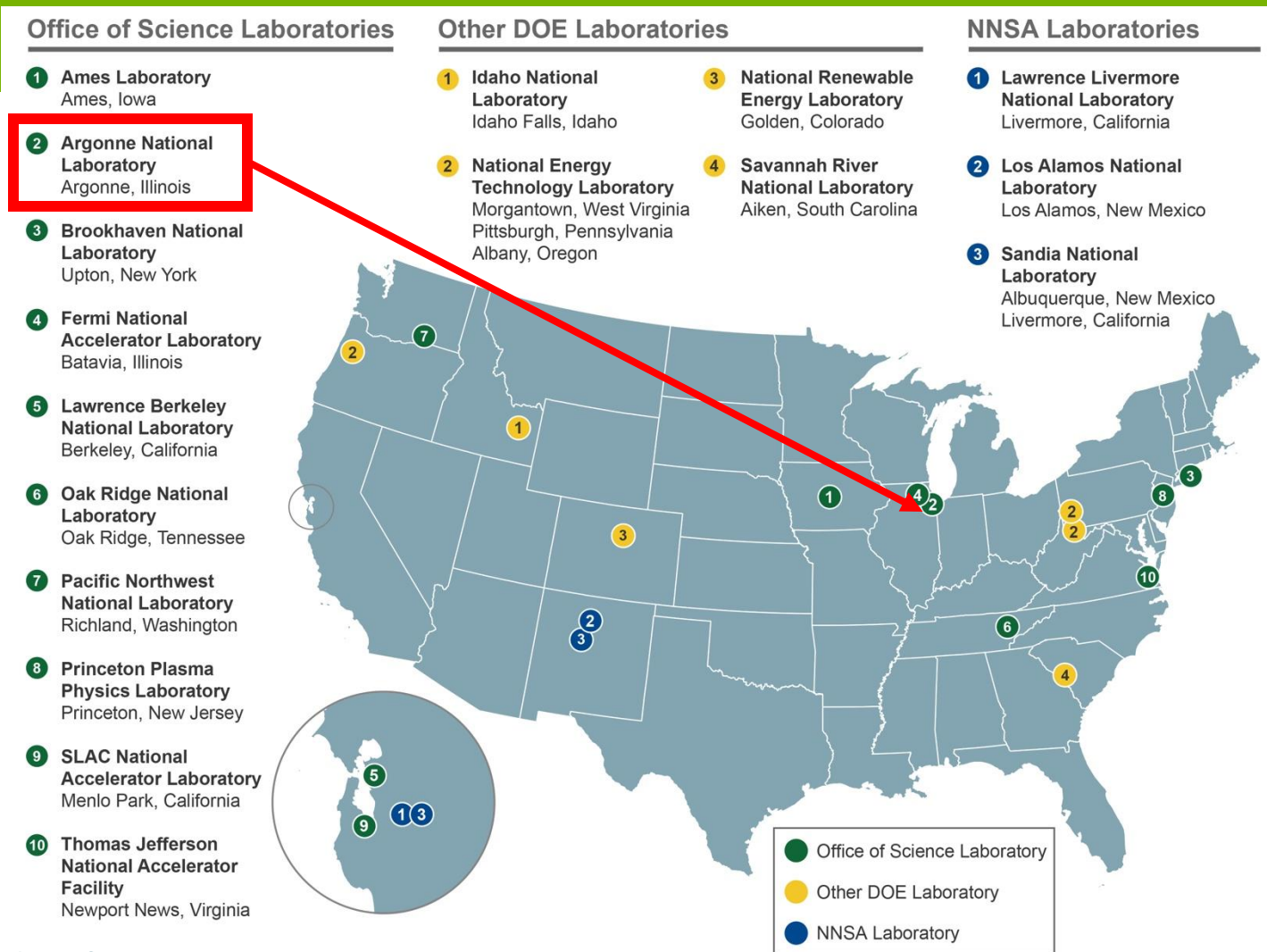
ANL
ANU
Altair Engineering Inc
BNL
BP
CEA Saclay
CMU
Convergent Science Inc
FNAL
Florida State U.
Georgia Inst. of Tech.
IU Bloomington
Jefferson Lab
KAUST
KTH Royal Inst. of Tech.
LANL
LBNL

LLNL
LSU
Loyola Univ. Chicago
MIT
Missouri U. of Sci. and Tech.
NASA
NC State
NETL
NREL
NexGen Analytics
ORNL
Penn State
RPI
SMU
Saint Louis Univ.
Salk Institute
Stanford

Texas Tech
U. Wisconsin–Madison
U. Chicago
U. Michigan
UC Boulder
UIC
UIUC
UMass Dartmouth
USC
UT Austin
UT Knoxville
Univ. Of Cambridge
Univ. of Delaware
Univ. of Pittsburgh
Washington U. St. Louis
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Argonne National Laboratory

Argonne – a part of DOE National Laboratory System

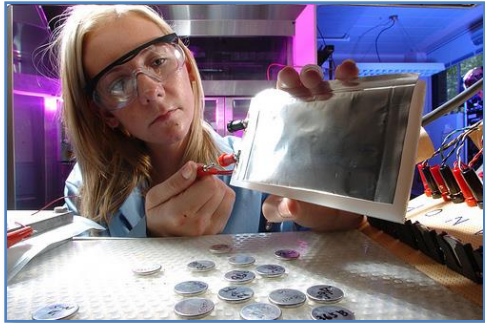


[Image Source](#)

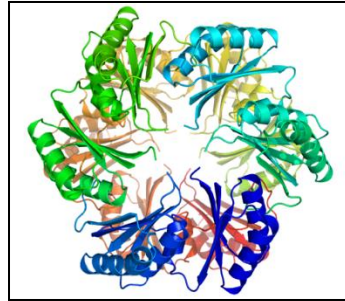
Together, the **17 DOE laboratories** comprise a preeminent federal research system, providing the Nation with strategic scientific and technological capabilities. The laboratories:

- 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.

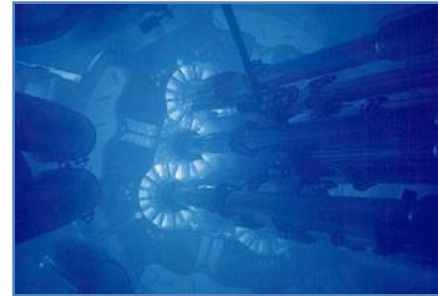
Argonne's mission: Provide science-based solutions to pressing global challenges



Energy Science



Environmental Sustainability



Nuclear and National Security

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

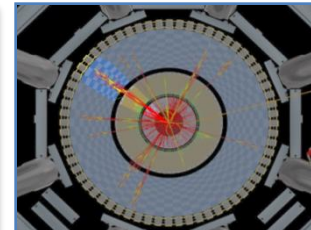
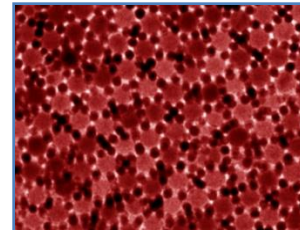
Centers and Joint Institutes

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

*Use-Inspired Science and Engineering ...
... Discovery and transformational Science and Engineering*



Major User Facilities



Science and Technology Programs

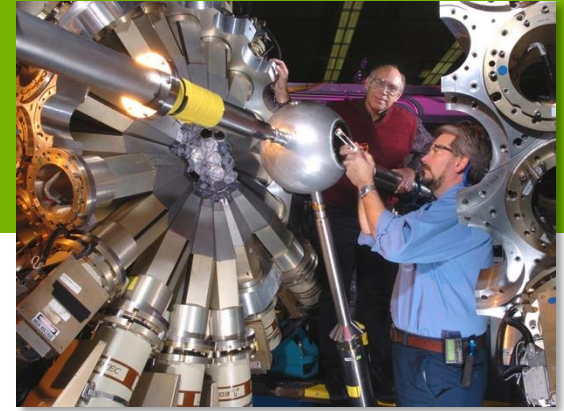
<https://www.anl.gov>

Major Scientific User Facilities at Argonne

**Advanced
Photon
Source**



**Argonne Tandem Linear
Accelerator System**



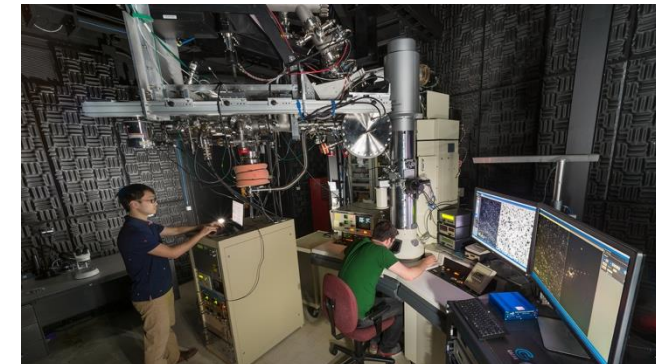
**Center for
Nanoscale Materials**



**Argonne
Leadership
Computing
Facility**



**Intermediate
Voltage Electron
Microscope**

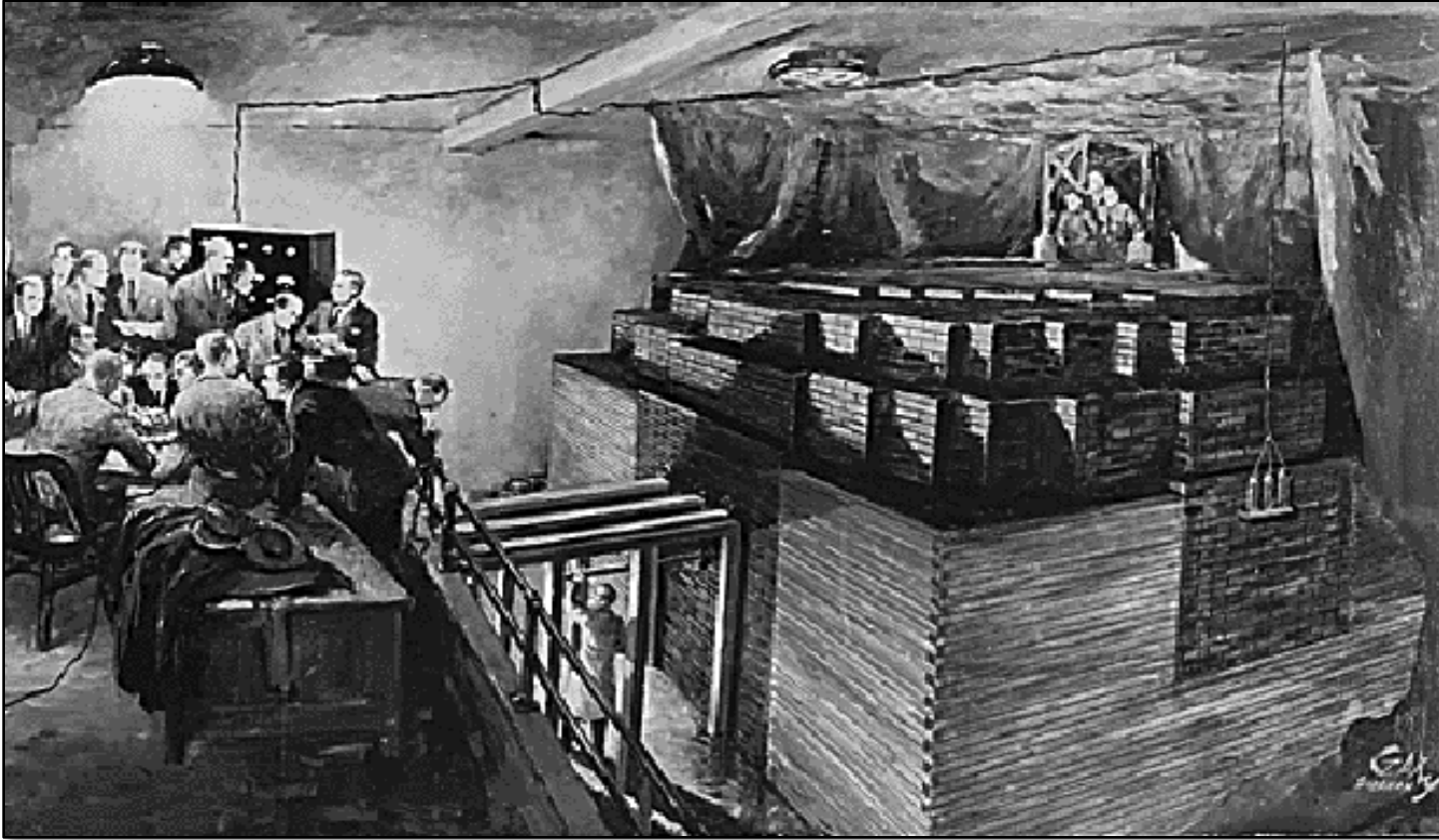


**Atmospheric
Radiation
Measurement**



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*](#)

Early Computing at Argonne



Donald "Moll" Flanders, Director
Jeffrey Chu, Chief Engineer

- **AVIDAC (1949-1953)**: based on a prototype at the Institute for Advanced Study in Princeton
 - 100,000 times as fast as a trained "Computer" using a desk calculator



Mathematician Margaret Butler (ANL)
and ORNL Engineer Rudolph Klein

- **ORACLE (1953)**
 - Designed at Argonne, constructed at Oak Ridge.
 - World's fastest computer, multiplying 12-digit numbers in .0005 seconds (2Kop/s)

ALCF Timeline

2006-2008 Blue Gene/L
2008-2013 Blue Gene/P – Intrepid
2012-2019 Blue Gene/Q – Mira
2017-2023 Theta (KNL)
2022- Polaris
2023- Aurora

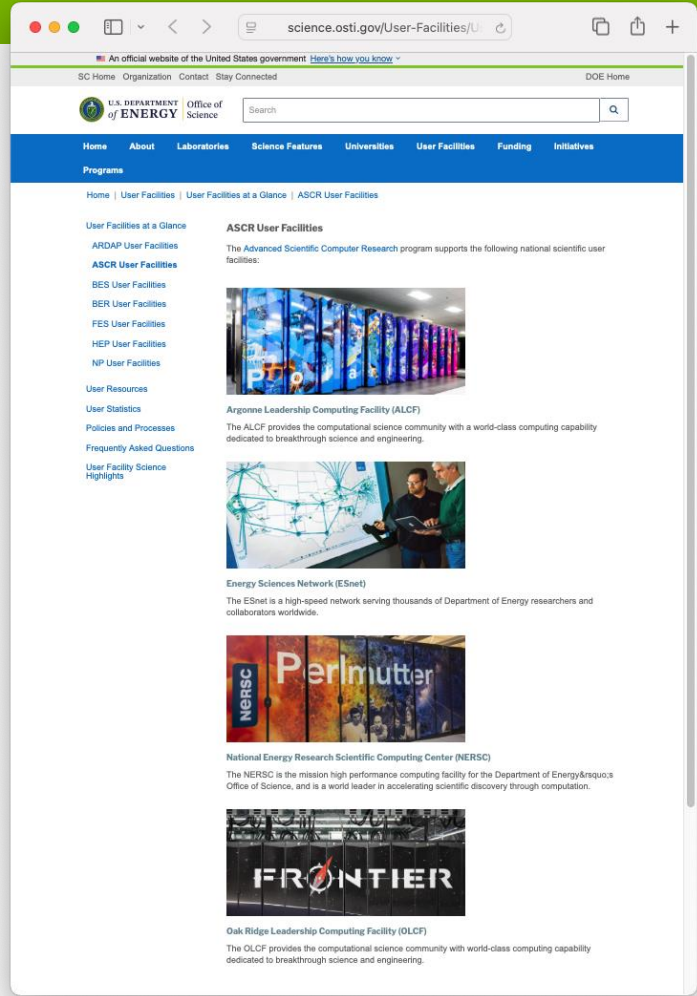
[TOP500 \(May 2024\):](#)

#2 HPL 1.012 EFlop/s

#1 HPL-MxP 10.6 EFlop/s



ATPESC Computing Resources



- **ALCF** – Aurora, Polaris, Sambanova, Cerebras, Graphcore, Groq
- **NERSC** – Perlmutter
- **OLCF** – Odo

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

Curriculum Tracks and their leaders

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

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Agenda 2025

[[Introductions](#) | [Track 1](#) | [Track 2](#) | [Track 3](#) | [Tour](#) | [Track 4](#) | [Track 5](#) | [Track 6](#) | [Track 7](#) | [Track 8](#)] [\[MACHINE RESERVATIONS\]](#)

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

Sunday — July 27, 2025

1:00 p.m.	Registration opens	
2:00 p.m.	Welcome and Introduction to ATPESC	Ray Loy, ANL
2:30 p.m.	Quick Start on ATPESC Computing Resources	JaeHyuk Kwack, ANL
4:30 p.m.	Participant Introductions	All
6:30 p.m.	Adjourn; Dinner	

Monday — July 28, 2025

Track 1 — Hardware Architectures

8:30 a.m.	Aurora	Brice Videau, ANL
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ATPESC Slack

- alcf-workshops.slack.com
- #announce
- #atpesc-2025-general for discussion and Q&A during the program
- Topic-related channels (e.g. #atpesc-2025-track-1-hw)
 - See #announce channel pinned items for a list
 - Or Channels + option to browse
- #atpesc-2025-helpdesk
 - Assistance ALCF login issues (**see next slide for OLCF and NERSC)
- Try to not DM me unless you can't avoid it 😊
 - You will get help faster via #atpesc-2025-helpdesk

Help!

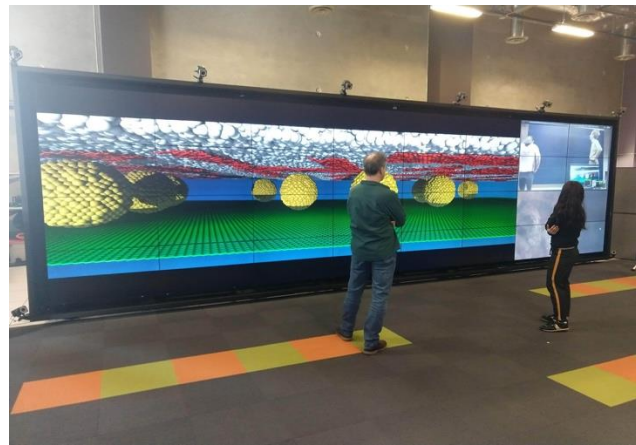
- ALCF accounts (Aurora, Polaris, SambaNova, Cerebras, Graphcore)
 - support@alcf.anl.gov (put ATPESC in subject) and slack #atpesc-2025-helpdesk
- OLCF accounts (Odo)
 - Token issues, call: 865-241-6536 (24/7). Other questions, email: help@olcf.ornl.gov (put ATPESC in subject)
- NERSC accounts (Perlmutter)
 - accounts@nersc.gov (put ATPESC in subject) or call 1-800-666-3772
- ATPESC general support
 - support@extremecomputingtraining.anl.gov
 - #atpesc-2025-helpdesk

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, telecons, phonecalls*
- After dinner, please return to the Amphiteater **on time** for the after-dinner dinner speaker.
- *In case of illness or other unexpected problems – please talk to me.*

Argonne National Laboratory Tour (Sat 8/2)

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



Aerial view of Argonne National Laboratory

**Advanced
Photon
Source
(APS)**

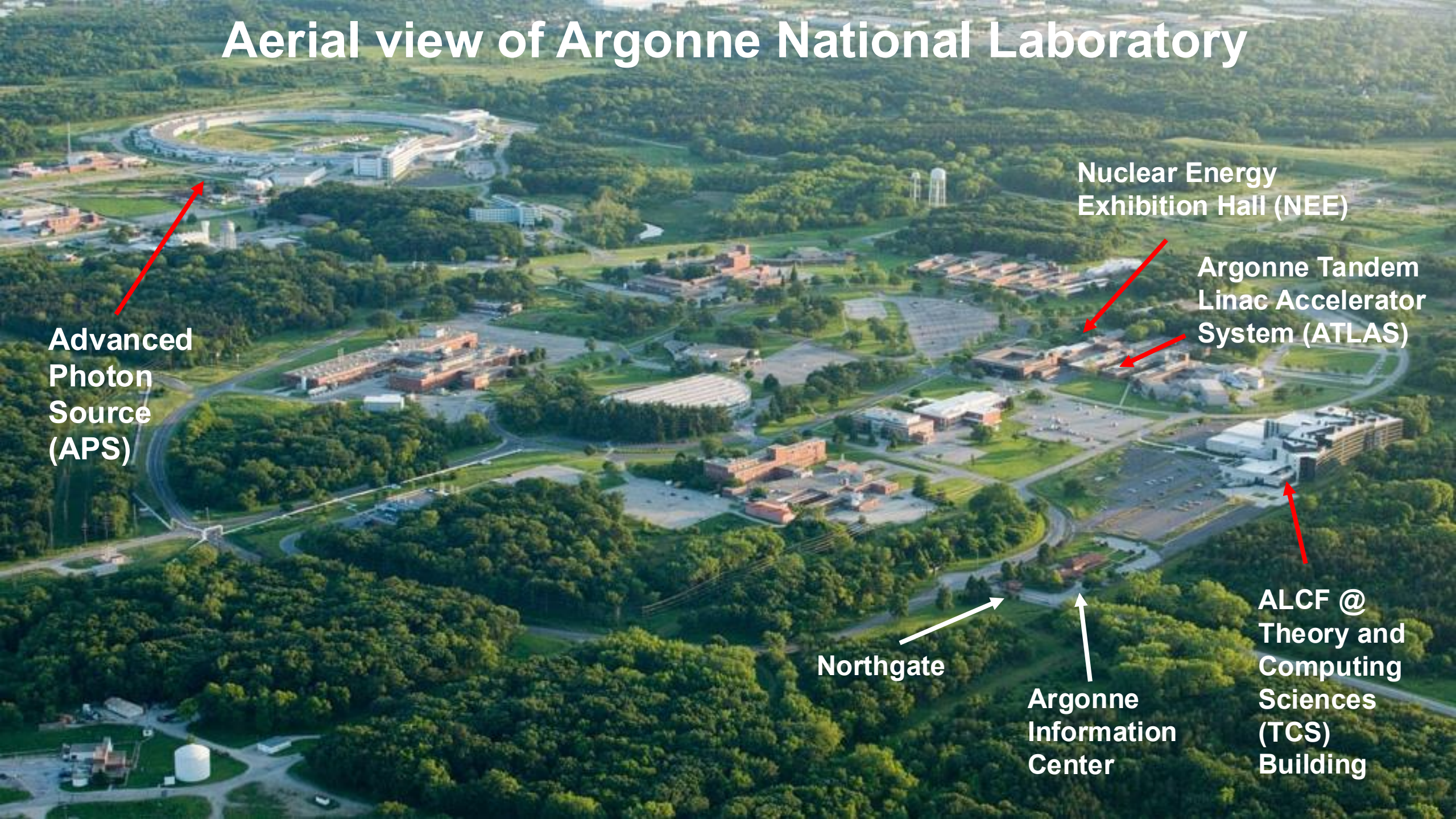
**Nuclear Energy
Exhibition Hall (NEE)**

**Argonne Tandem
Linac Accelerator
System (ATLAS)**

Northgate

**Argonne
Information
Center**

**ALCF @
Theory and
Computing
Sciences
(TCS)
Building**





ARGONNE TRAINING PROGRAM ON EXTREME-SCALE COMPUTING

Produced by Argonne National Laboratory, a U.S. Department of Energy Laboratory managed by UChicagoArgonne, LLC under contract DE-AC02-06CH11357.

Special thanks to the National Energy Research Scientific Computing Center (NERSC) and Oak Ridge Leadership Computing Facility (OLCF) for the use of their resources during the training event.

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