ARGONNE
ATPESC2024
EXTREME-SCALE COMPUTING

ATPESC 2024 Intro and Orientation

Ray Loy
ATPESC Program Director, ANL

ATPESC

Founded by Paul Messina in 2013. ATPESC 2024 is #12 !

Welcome

Argonne National Laboratory

ATPESC Overview

Logistics

Tour

Welcome!

ATPESC 2024

54 Institutions

Actalent
AMA / NASA Ames
ANL
ANU
Calif Inst Tech
CEA
CeNAT
Cornell
Dassault
Duke U
Env and Climate Change
INAF
LBNL
Massey U
Michigan State
MIT
NASA Langley
NIST
Northwestern U
NREL
NYU
ORNL
PNNL
Politecnico Milano
Polymath Research
PSI
RIT
Samsung Adv Inst Tech
Stanford
Stony Brook U
TACC
TPS
U Chicago
U Delaware
U Kentucky
U Michigan
U MN Twin Cities
U North Texas
U NSW
U Ottawa
U Seville
U Udine
U Utah
U WI Milwaukee
UC Berkeley
UCLA
UIUC
US NRL
USNA
UT Arlington
UT Austin
UTK
Virginia Tech
WUSTL

Argonne National Laboratory

Argonne – a part of DOE National Laboratory System

Office of Science Laboratories

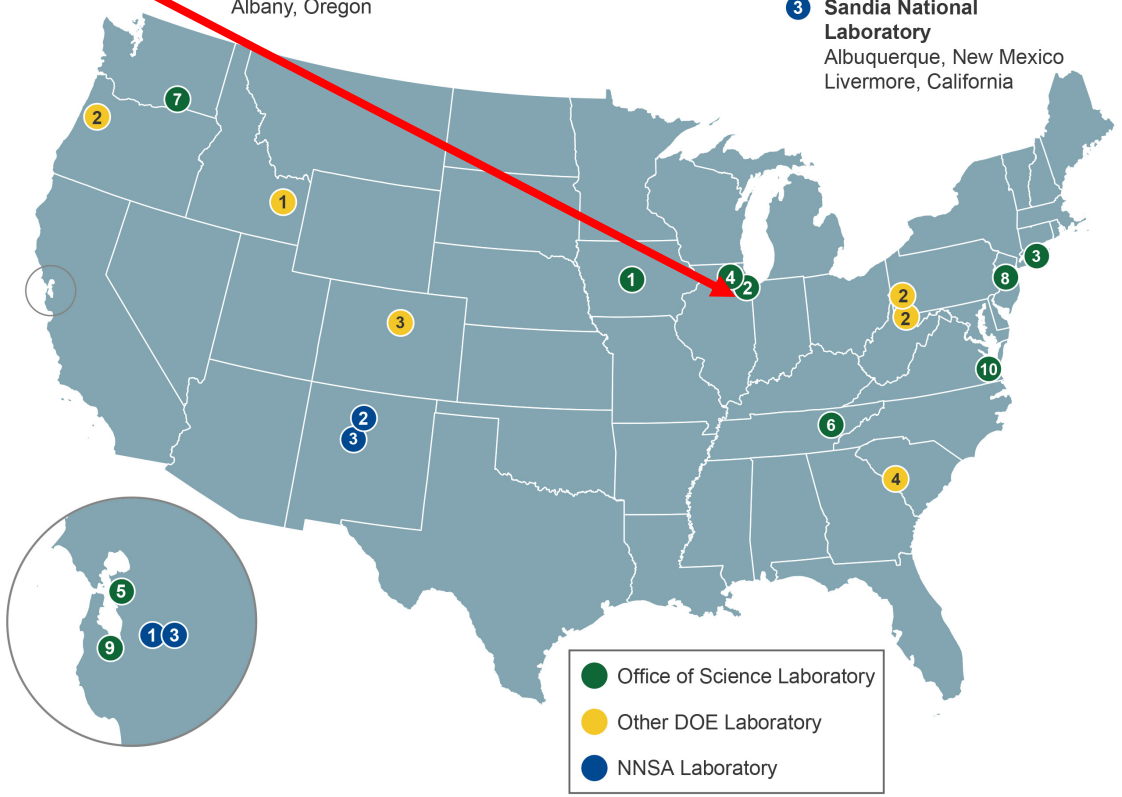
1. **Ames Laboratory**
   Ames, Iowa
2. **Argonne National Laboratory**
   Argonne, Illinois
3. **Brookhaven National Laboratory**
   Upton, New York
4. **Fermi National Accelerator Laboratory**
   Batavia, Illinois
5. **Lawrence Berkeley National Laboratory**
   Berkeley, California
6. **Oak Ridge National 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



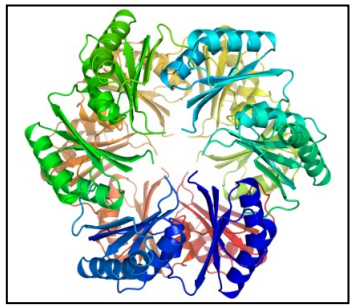
[Image Source]

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.

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

Energy Science



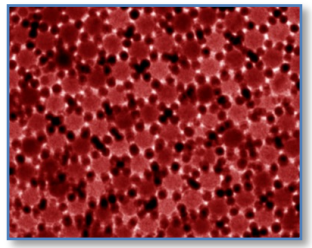
Environmental Sustainability

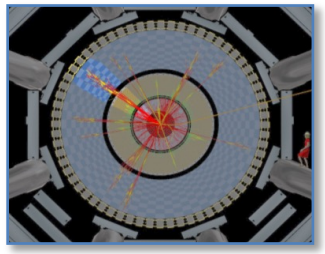
Nuclear and National Security

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

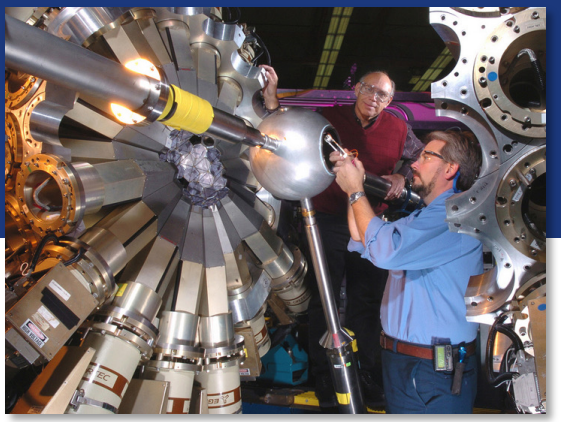
AAI	Argonne Accelerator Institute
ACCESS	Argonne Collaborative Center for Energy Storage Science
ADW	Argonne Design Works
ALI	Argonne Leadership Institute
CEES	Center for Electrochemical Energy Science
CTR	Center for Transportation Research
CRI	Chain Reaction Innovations
CI	Computation Institute
IACT	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

Major Scientific User Facilities at Argonne

Advanced Photon Source

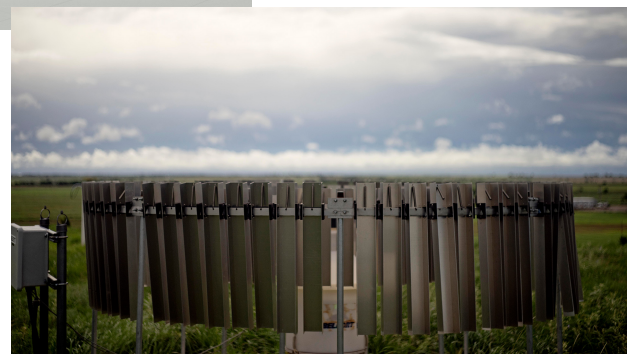
Argonne Tandem Linear Accelerator System



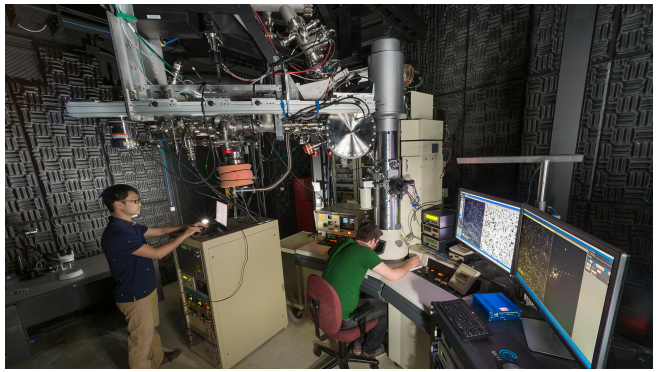
Argonne Leadership Computing Facility

Center for Nanoscale Materials

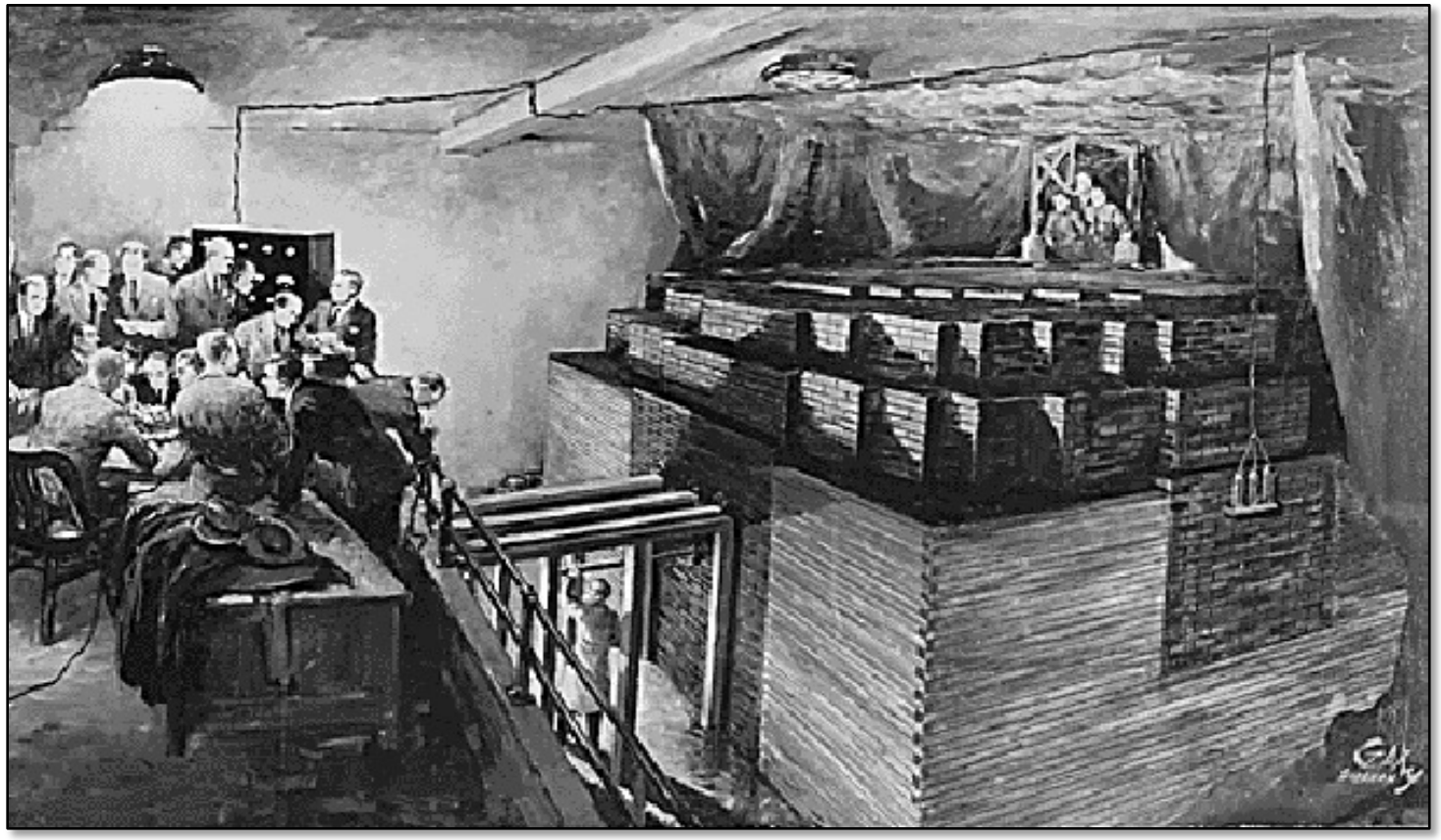
Atmospheric Radiation Measurement



Intermediate Voltage Electron Microscope



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

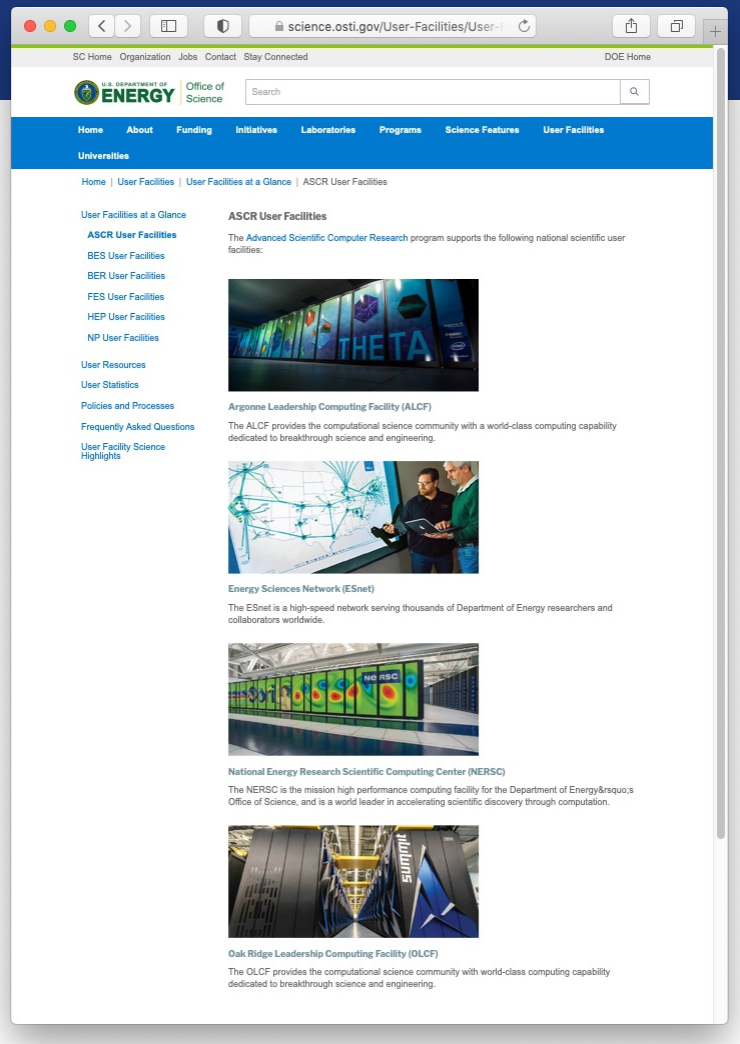
2023- Aurora

TOP500 (May 2024):

#2 HPL 1.012 EFlop/s

#1 HPL-MxP 10.6 EFlop/s

ATPESC Computing Resources



- **ALCF –** Polaris, Sambanova, Cerebras, Graphcore
- **NERSC –** Perlmutter
- **OLCF –** Odo, Ascent
- **Intel Devcloud**
- **AMD Devcloud**

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

Curriculum Tracks and their leaders

- **Track 1: Hardware Architectures –** Kalyan Kumaran, Vitali Morozov
- **Track 2: Programming Models and Languages –** Thomas Applencourt, Yanfei Guo
- **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 –** 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: Machine Learning and Deep Learning for Science –** Marieme Ngom

https://extremecomputingtraining.anl.gov/agenda-2024/

Agenda 2024

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

[MACHINE RESERVATIONS – TBA]

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

SUNDAY, July 28, 2024

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
4:30PM	Participant Introductions	All
6:30PM	Adjourn/Dinner	

ATPESC Slack

alcf-workshops.slack.com

#announce

#atpesc-2024-general for discussion and Q&A during the program

Topic-related channels (e.g. #atpesc-2024-track-1-hw)

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

#atpesc-2024-helpdesk

- Assistance ALCF login issues (***see next slide for OLCF and NERSC)

Please do not DM me if you can avoid it ☺

- You will get help faster via #atpesc-2024-helpdesk

Help!

ALCF accounts (Polaris, SambaNova, Cerebras, Graphcore)

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

OLCF accounts (Odo, Ascent)

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-2024-helpdesk

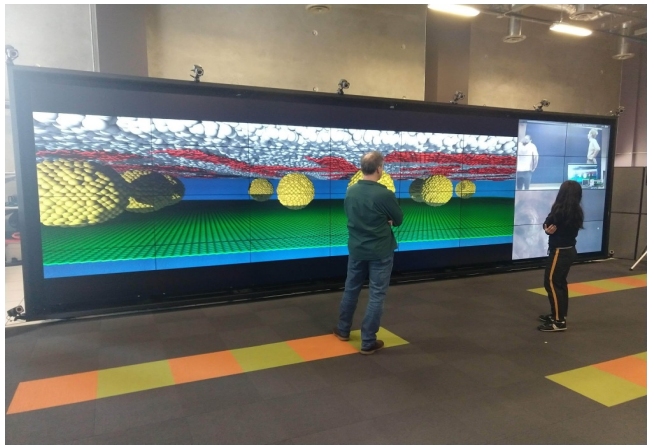
ATPESC Conduct

- 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.

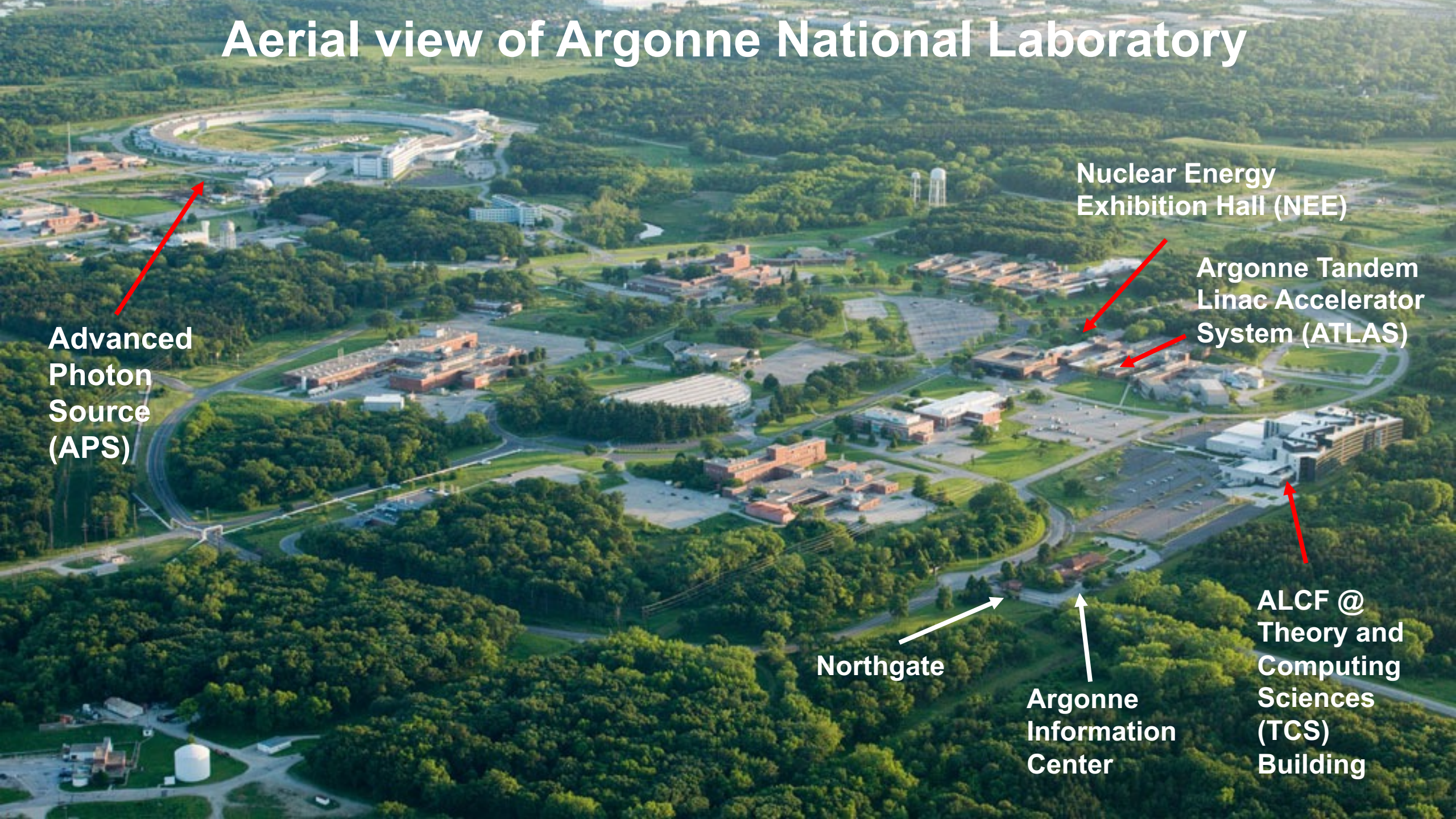
In case of illness or other unexpected problems – please talk to me.

Argonne National Laboratory Tour (Sat 8/3)

- 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



ARGONNE

ATPESC2024

EXTREME-SCALE COMPUTING

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.