Argonne Training Program on Extreme-Scale Computing

Introduction to ATPESC

Ray Loy
ATPESC 2021 Program Director

U.S. DEPARTMENT OF **ENERGY** | Office of Science

NNSA National Nuclear Security Administration

Outline

- **Welcome**
- **Argonne National Laboratory**
- **ATPESC Overview**
- **Logistics**
- **Tour**

Welcome!

79 ATPESC 2021 Participants

Tariq	Rabab	Isaac	Riccardo	Akanksha	Sagar
Pramod	Alexander	Ralph	Jingyi	Younghyun	Lisa
Saumik	Davide	Olga	Eric	Cameron	Enrico
Catherine	Angel	Jose	Lorenzo	Georgios	Elisabeth
Thomas	Dejan	Amal	Fan	Aryaman	Quang
Ryan	Mihailo	Hwancheol	Mariia	Jonas	Miriam
Dhruva	Claire	Zhi	Pinyi	Hengrui	Danylo
Michael	Vincent	Xingze	Daniel	Julio	Gabriel
John-Luke	Poornima	Matthew	Omotayo	Andrea	John
John	Roberto	Bhagyashree	Ellen	Nidia	Marcin
Gregory	Ryan	Eva	Guillem	Xiaolei	Ishan
Georgia	Christopher	Cheng-Kai	Christina	Yiltan	Josin
Guillermo	Monarin	Christopher	Stephen	Sicong	Chao
Edoardo					

Welcome!

ATPESC 2021

52 Institutions

Alabama A&M	Aramco Americas
Argonne National Lab	BP
Battelle Memorial Inst.	Boston U.
CEA Saclay	CERN
CMU	Carleton U.
Cornell U.	DESY
Duke U.	Environment and Climate Change Canada
Frederick National Lab	Harvard U.
Indiana U.	Inst. de Astrofísica de Canarias
KAUST	LANL
LBNL	LSU
MIT	NASA Langley
NERSC	NETL
NREL	New York U.
North Carolina A&T	North Carolina State
Northwestern U.	Oak Ridge National Lab
PNNL	Queen's U.
RPI	Reservoir Labs
Rice U.	SLAC National Accelerator Lab
Stanford U.	Stony Brook U.
TU Dresden	TU Vienna
Texas A&M	U. Nacional de San Luis
U. Wisconsin Madison	U. Basel
U. Udine	U. Wyoming
UC Berkeley	UC Riverside
UI Urbana-Champaign	USC
UT Austin	Wayne State

Argonne National Laboratory

ATPESC 2021, August 1-13, 2021

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

- Office of Science Laboratory
- Other DOE Laboratory
- NNSA Laboratory
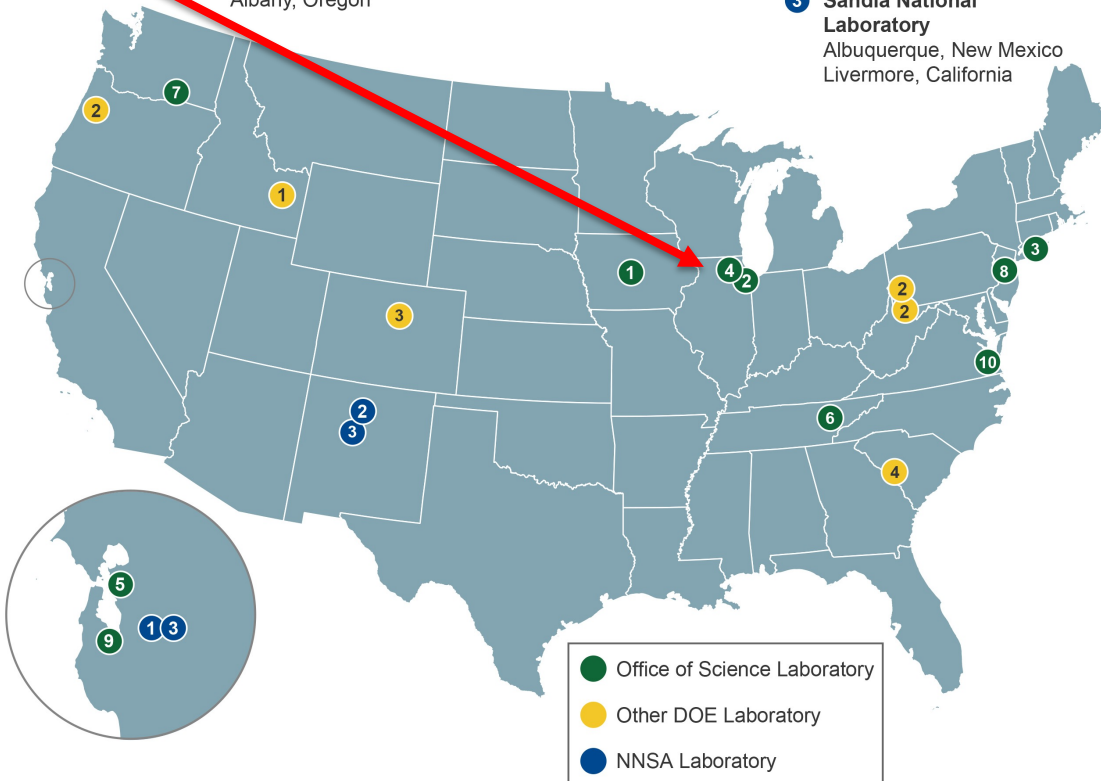
Together, the **17 DOE laboratories** comprise a preeminent federal research system, providing the Nation with strategic scientific and technological capabilities. The laboratories:

- 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

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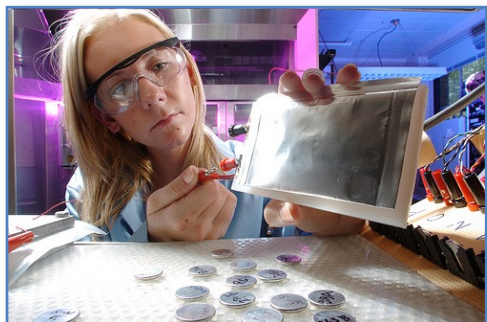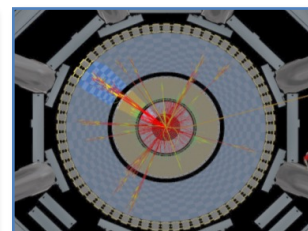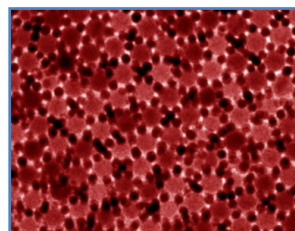

Energy Science

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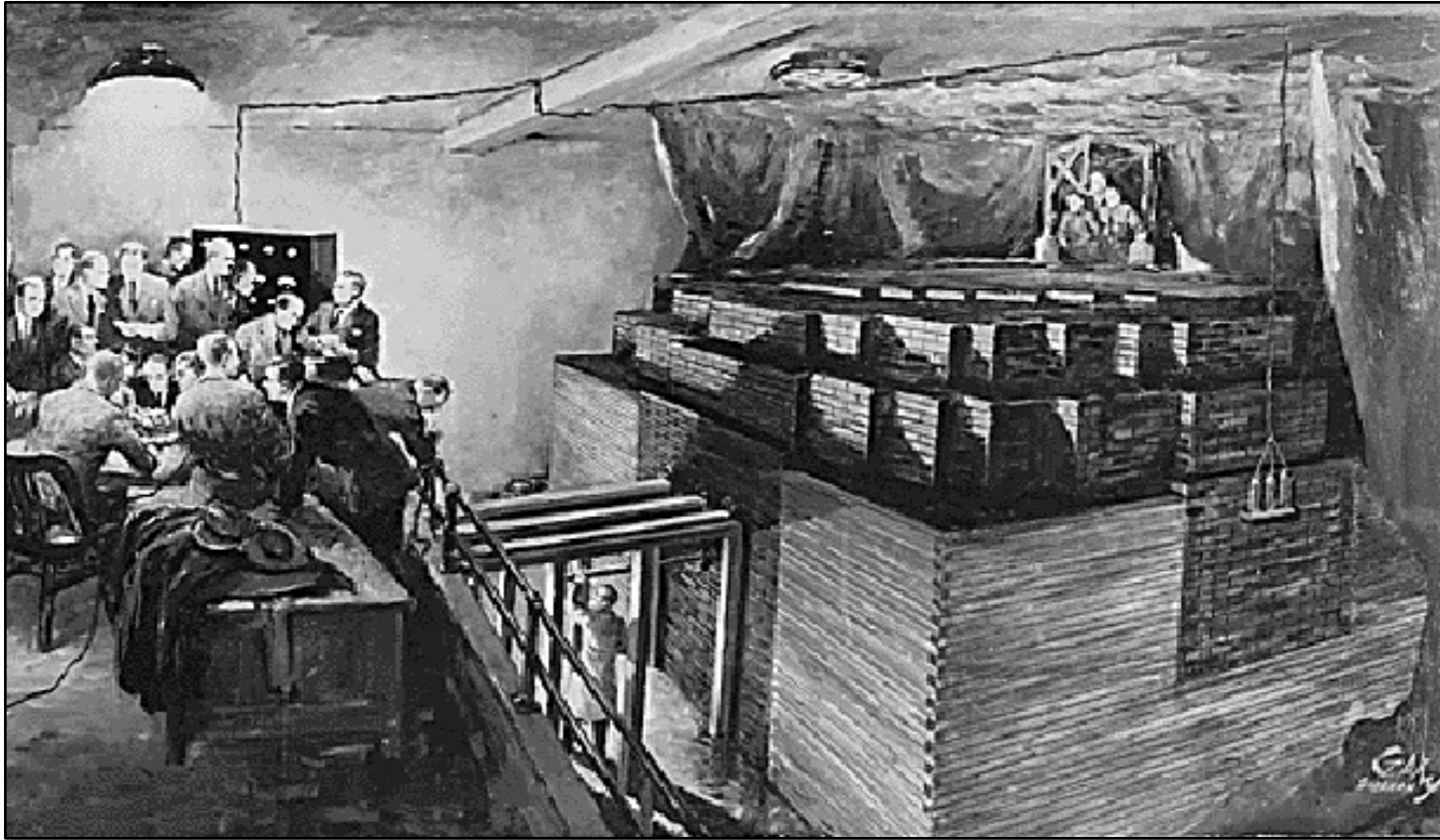
Chicago Pile-1 was the world's first artificial nuclear reactor. The first man-made self-sustaining nuclear chain reaction was initiated on December 2, 1942

Chicago Pile-1: A Brick History

https://www.youtube.com/watch?v=mTPiTJ2bKS0

Aerial view of Argonne National Laboratory

Nuclear Energy Exhibition Hall (NEE)

Argonne Tandem Linac Accelerator System (ATLAS)

Advanced Photon Source (APS)

Northgate

Argonne Information Center

ALCF @ Theory and Computing Sciences (TCS) Building
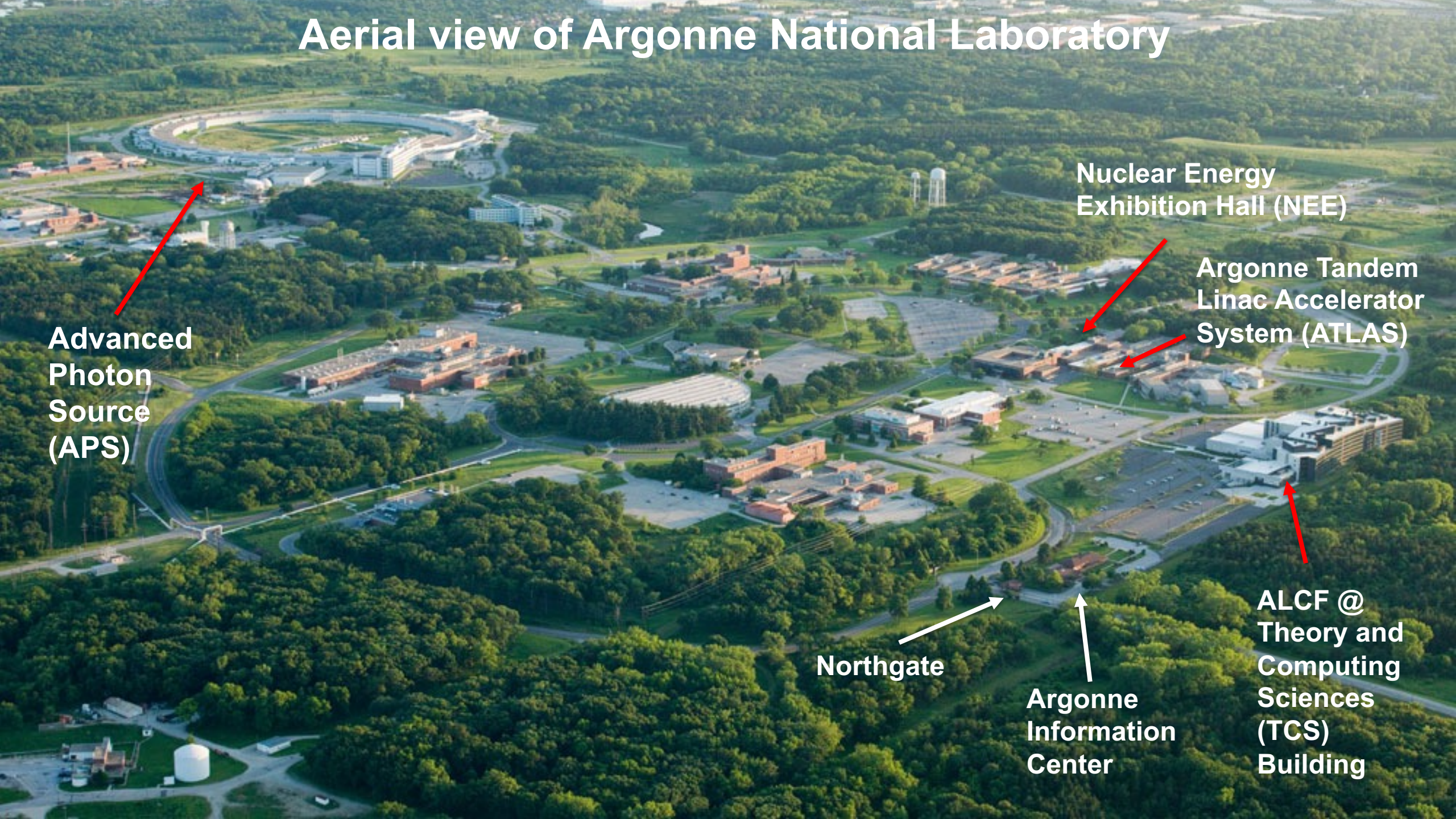
Major Scientific User Facilities at Argonne

Advanced Photon Source

Argonne Tandem Linear Accelerator System

Center for Nanoscale Materials

Argonne Leadership Computing Facility

Electron Microscopy Center
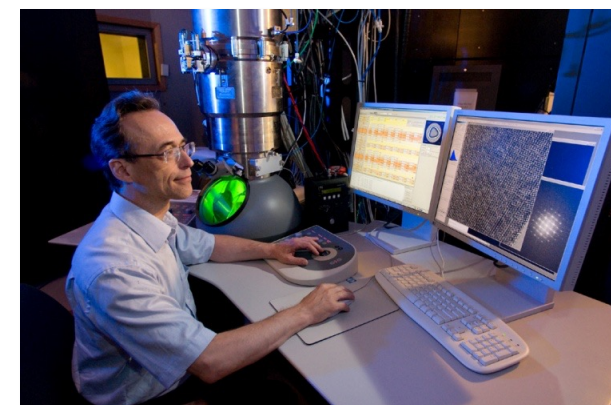
AVIDAC (1949-1953)
Argonne's Version of the Institute's Digital Arithmetic Computer
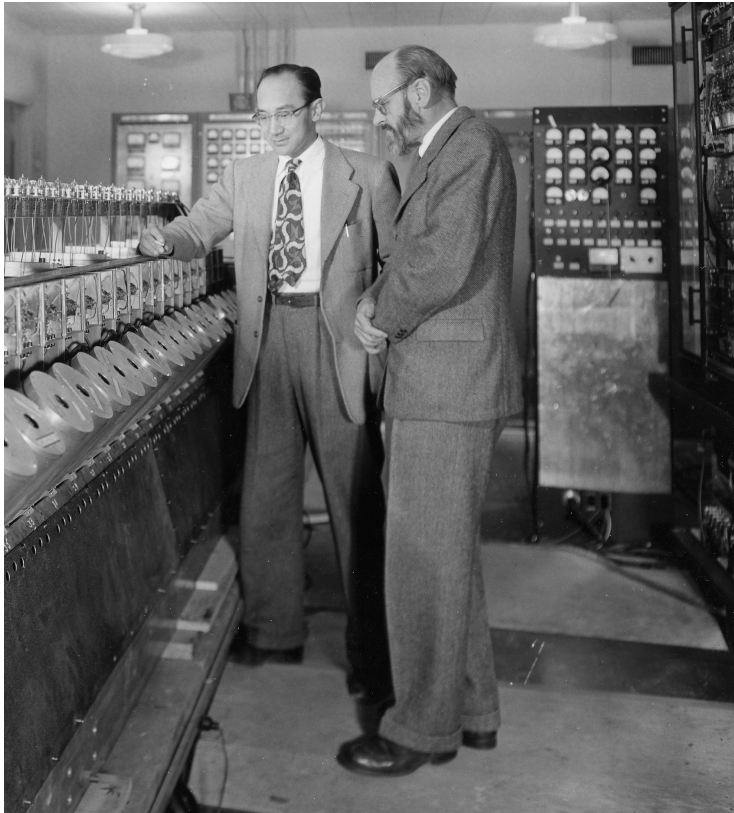
"Moll" Flanders, Director
Jeffrey Chu, Chief Engineer

- **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

Argonne NATIONAL LABORATORY

ECP EXASCALE COMPUTING PROJECT

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.

Argonne NATIONAL LABORATORY

ECP EXASCALE COMPUTING PROJECT

The future… Aurora Exascale System

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

Argonne
NATIONAL LABORATORY

ECP
EXASCALE
COMPUTING
PROJECT

ATPESC Overview

- Founded by Paul Messina in 2013 – *This year is #9 !*

- 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 with MPI and/or OpenMP and/or ML Frameworks
    - Experience with at least one HPC system
    - Concrete plans to conduct CSE research on large-scale computers

Argonne
NATIONAL LABORATORY

ECP EXASCALE COMPUTING PROJECT

Curriculum Tracks and their leaders

- **Track 1:** **Hardware Architectures –** Kalyan Kumaran

- **Track 2:** **Programming Models and Languages –** Rajeev Thakur, Yanfei Guo, and Thomas Applencourt

- **Track 3:** **Data-intensive Computing and I/O –** Rob Latham and Phil Carns

- **Track 4:** **Visualization and Data Analysis –** Mike Papka, Joseph Insley, and Silvio Rizzi

- **Track 5:** **Numerical Algorithms and Software for Extreme-Scale Science –** Lois McInnes, Mark Miller, and Alp Dener

- **Track 6:** **Performance Tools and Debuggers–** JaeHyuk Kwack and Scott Parker

- **Track 7:** **Software Productivity and Sustainability –** Anshu Dubey and Katherine Riley

- **Track 8:** **Machine Learning and Deep Learning for Science –** Bethany Lusch and Taylor Childers Vishwanath

ATPESC Computing Resources
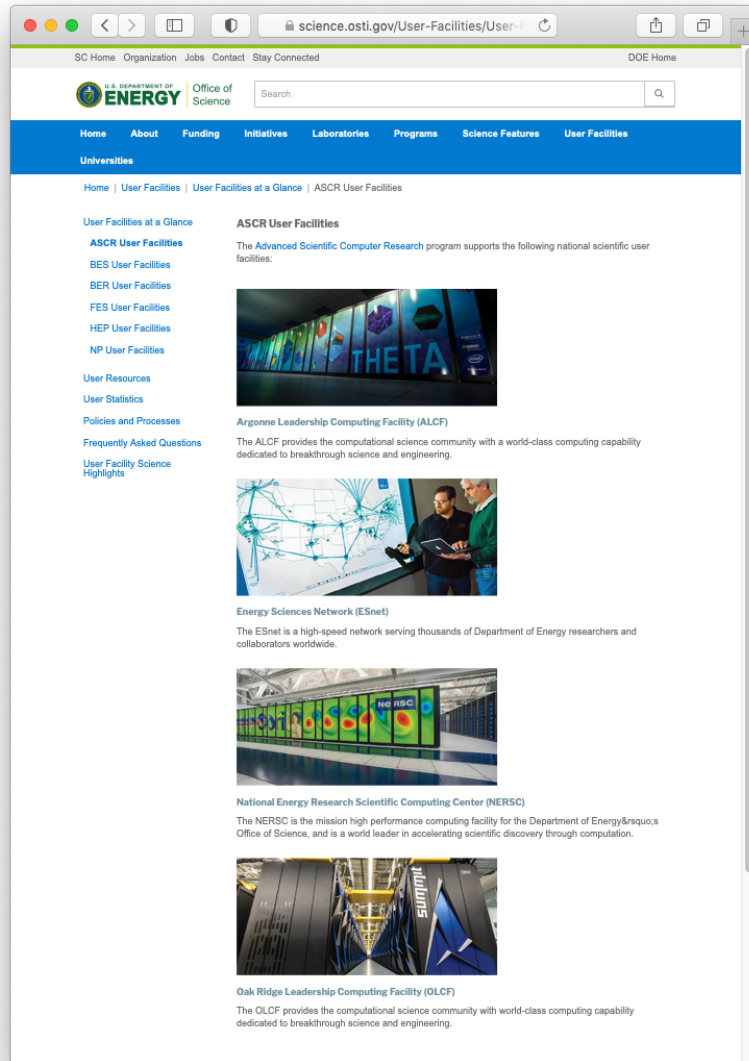
ALCF – Theta, ThetaGPU, and Cooley

OLCF - Ascent

NERSC – Cori

Intel Devcloud

AMD Devcloud

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

Goals for Attendees

Exposure to New ideas

Take advantage of ATPESC Resources

Talk F2F (virtually) with Lecturers, other Participants, Support

https://extremecomputingtraining.anl.gov/agenda-2021/

Box Folder

Linked at

ATPESC Home Page
    Agenda
        Class Materials
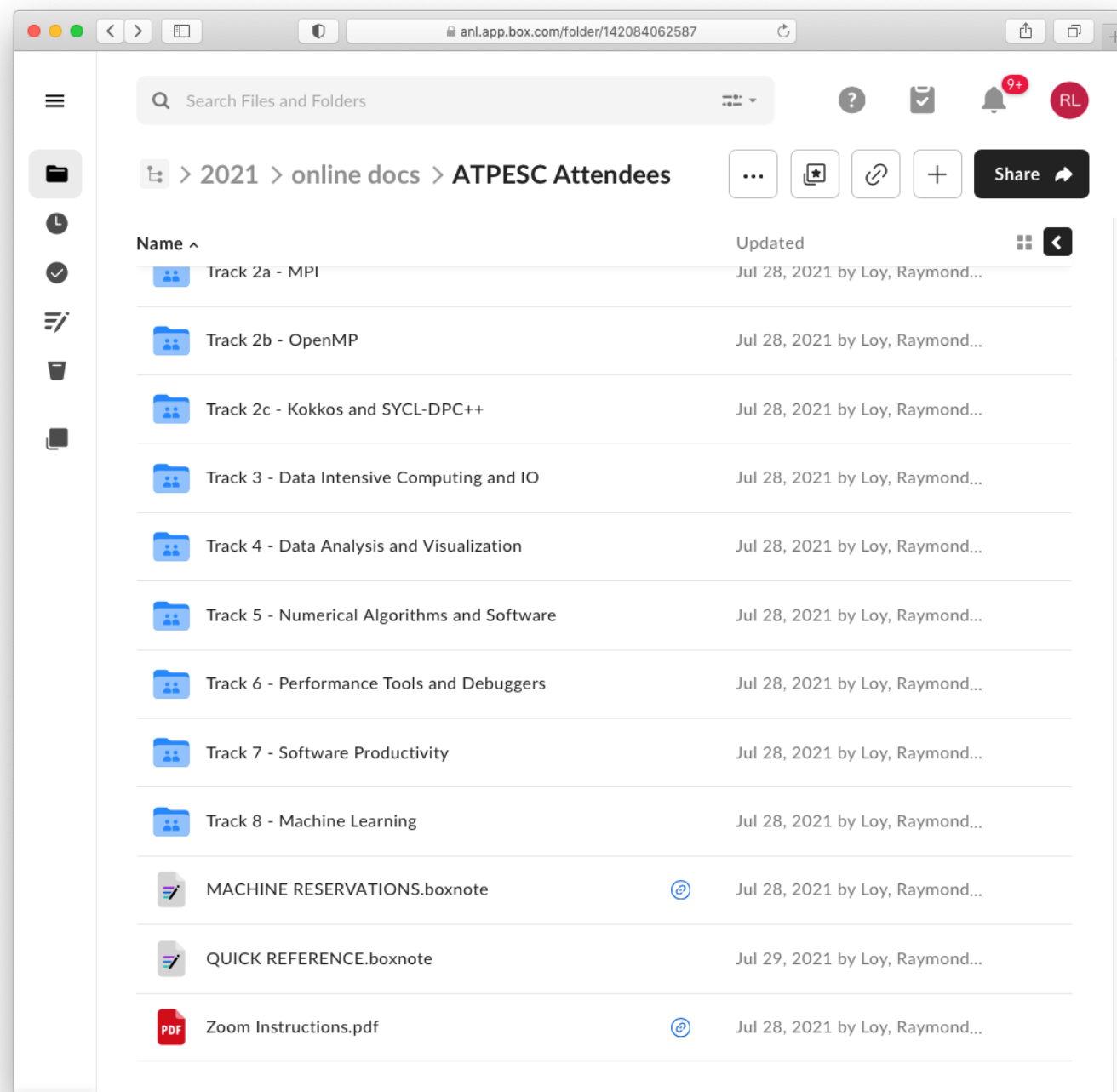
Quick Reference

In Box folder

QUICK REFERENCE

Agenda https://extremecomputingtraining.anl.gov/agenda-2021/

Zoom Meeting Links
    Main Room Meeting Link (Meeting ID: 161 625 8437   Password: 203948)
    How to set your Zoom display name and move to breakout rooms
    Numerical Track Breakout Links will be added here later

Slack Workspace
    https://alcf-workshops.slack.com

Machine Reservations
    See box note in same folder as this QUICK REFERENCE
    LCF systems location of ATPESC2021 project directory: /grand/ATPESC2021

This Quick Reference Document: https://anl.app.box.com/notes/839708419453

ATPESC Slack

- alcf-workshops.slack.com

- #announce

- #general for discussion and Q&A during the program
  - There are also topic-related channels (#track-1-hardware)
    - See Channels + option to browse the list

- #help-desk
  - Assistance with Zoom, Box, 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 #help-desk

Getting help

- ALCF accounts (Theta, ThetaGPU, Cooley)
  - support@alcf.anl.gov and slack #help-desk

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

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

- ATPESC general support including Slack, Box
  - support@extremecomputingtraining.anl.gov
  - #help-desk

Virtual Argonne National Laboratory Tour

Saturday, August 7 11AM-1PM

- **ANL Tour Guide Presentations w/Videos**
  - **APS – Advanced Photon Source**
  - **ATLAS – Argonne Tandem Linear Accelerator System**

- **ALCF Facilities (Live)**
  - **Main Machine Room in the Theory and Computing Sciences Building (TCS)**
  - **Visualization Lab**
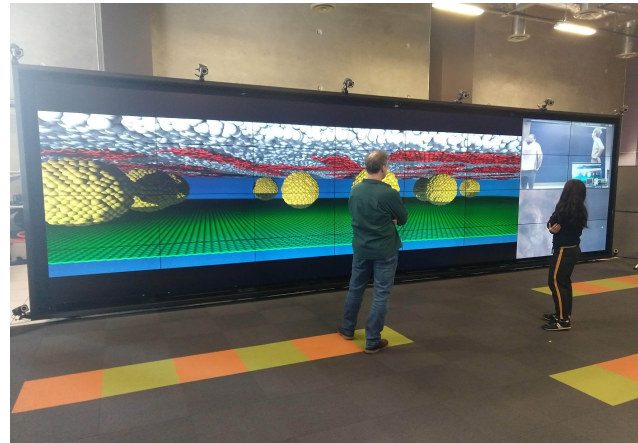
Acknowledgments

Exascale Computing Project

Website: https://exascaleproject.org

ATPESC 2022

- If you or an associate is interested in attending
    - Subscribe to mailing list https://extremecomputingtraining.anl.gov (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*.

The future… Aurora Exascale System