



Argonne Training Program on Extreme-Scale Computing

Introduction to ATPESC

Ray Loy
ATPESC 2020 Program Director

Thanks to Marta Garcia, ATPESC 2016-2019 Program Director



Outline



Welcome



Argonne National Laboratory



ATPESC Overview



Logistics



Tour(?)

Welcome!

73 ATPESC 2020 Participants

Alan
Ana
Denis
Evan
Ian
Jorge Luis
Komal
Massimiliano
Michelle
Nathaniel
Ral
Valeria
Zongcai

Albert
Antonin
Derek
Francois
Igor
Joseph
Kyle
Matthew
Ming
Neil
S M
Victor

Alberto
Ashka
Dmitry
Georgios
Imanuel
Juan Diego
Ligia Diana
Md Fazlay
Muaaz
Neil
Soonpil
Yangzesheng

Aleksandra
Bruce
Dossay
Giuseppe
Jacob
Justin
Łukasz
Melisa
Muhong
Niels
Steven
Yiban

Amanda
Carlos
Dylan
Henry
Jared
Kento
Maciej
Michael
Mukund
Patrick
Suyash
Zac

Amil
Choah
Eremey
Hugo
Jeremy
Kevin
Malik
Michael
Nathan
Philippe
Thomas
Zhi

Welcome!

ATPESC 2020

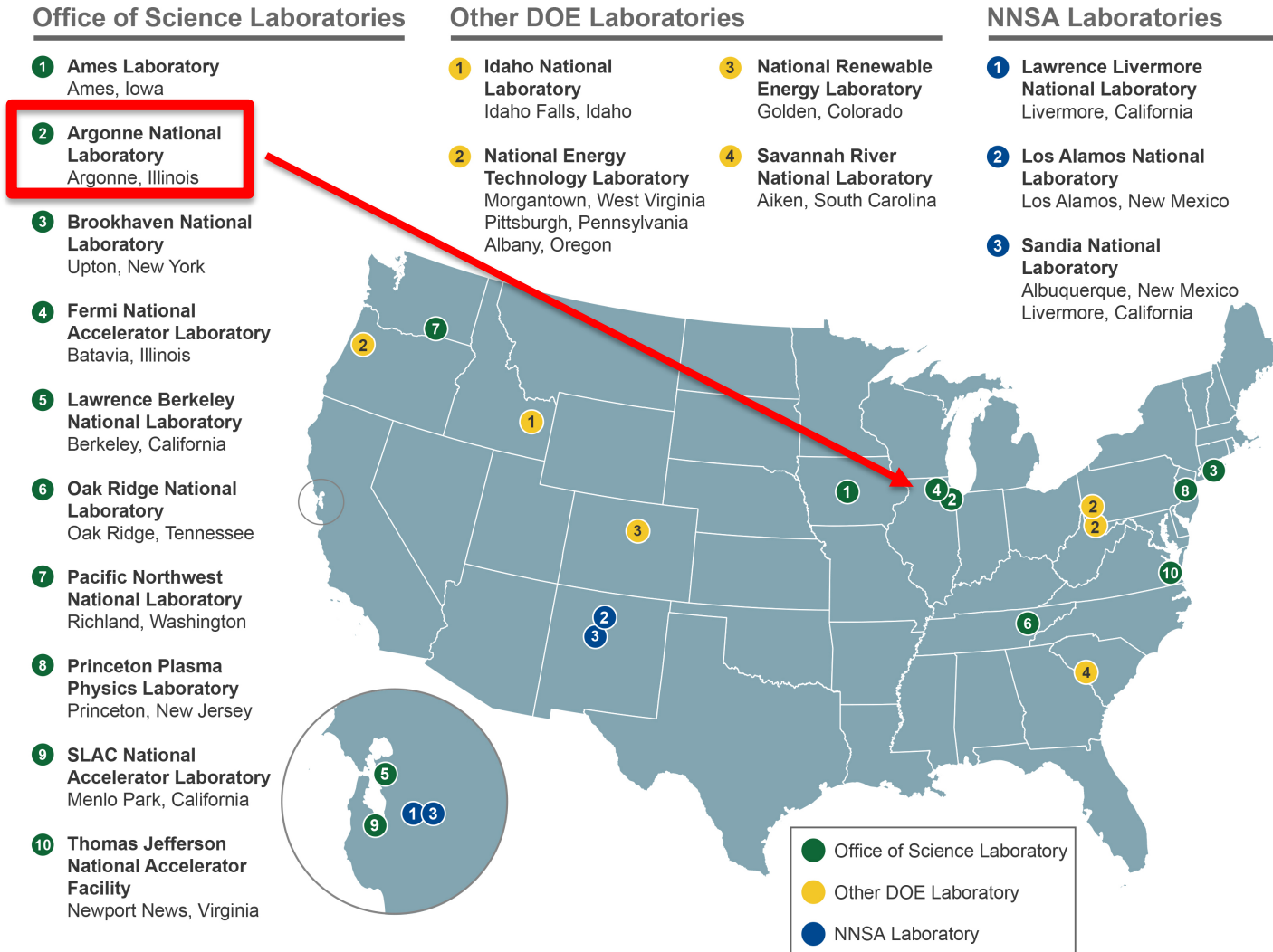
45 Institutions

Argonne National Laboratory
CEA Saclay
Canadian Nuclear Laboratories
Colorado State University
Cornell University
Iowa State University
LUT University
Lawrence Livermore National Laboratory
Michigan State University
NASA Langley Research Center
National Renewable Energy Laboratory
Naval Surface Warfare Center
Oak Ridge National Laboratory
Princeton Plasma Physics Laboratory
Rensselaer Polytechnic Institute
Stanford University
The Australian National University
University of Colorado Boulder
University of Illinois at Urbana-Champaign
University of Minnesota
University of Saskatchewan
University of Tennessee
Westinghouse Electric Company, LLC

BP
CU Boulder
Carnegie Mellon University
Columbia University
Environment and Climate Change Canada
KTH Royal Institute of Technology
Lawrence Berkeley National Laboratory
Los Alamos National Laboratory
NASA Ames Research Center
NERSC
Naval Postgraduate School
Numerical Algorithms Group (NAG)
Oregon State University
Purdue University
Sandia National Lab
Texas A&M University
University of Chicago
University of Florida
University of Michigan
University of Notre Dame
University of Southern California
University of Warsaw

Argonne National Laboratory

Argonne – a part of DOE National Laboratory System

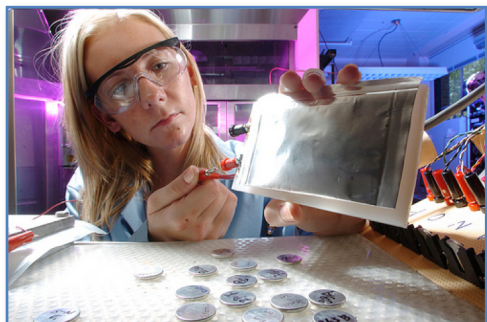


Together, the **17 DOE laboratories** comprise a preeminent federal research system, providing the Nation with strategic scientific and technological capabilities. The laboratories:

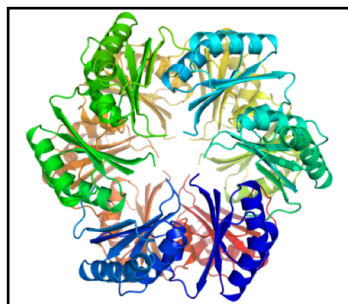
- Execute long-term government scientific and technological missions, often with complex security, safety, project management, or other operational challenges;
- Develop unique, often multidisciplinary, scientific capabilities beyond the scope of academic and industrial institutions, to benefit the Nation's 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

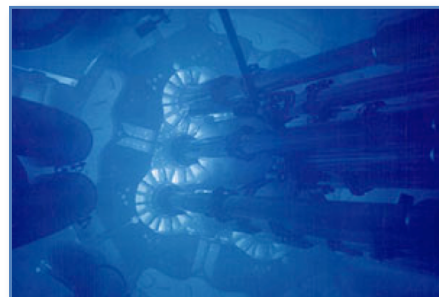
Argonne's mission: Provide science-based solutions to pressing global challenges



Energy Science



Environmental Sustainability

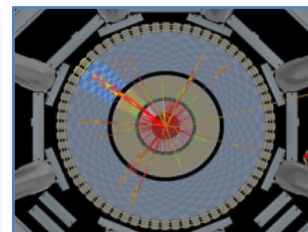
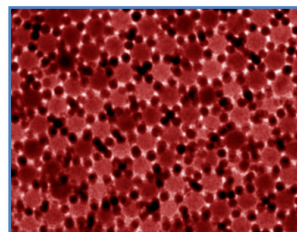


Nuclear and National Security

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



Major User Facilities



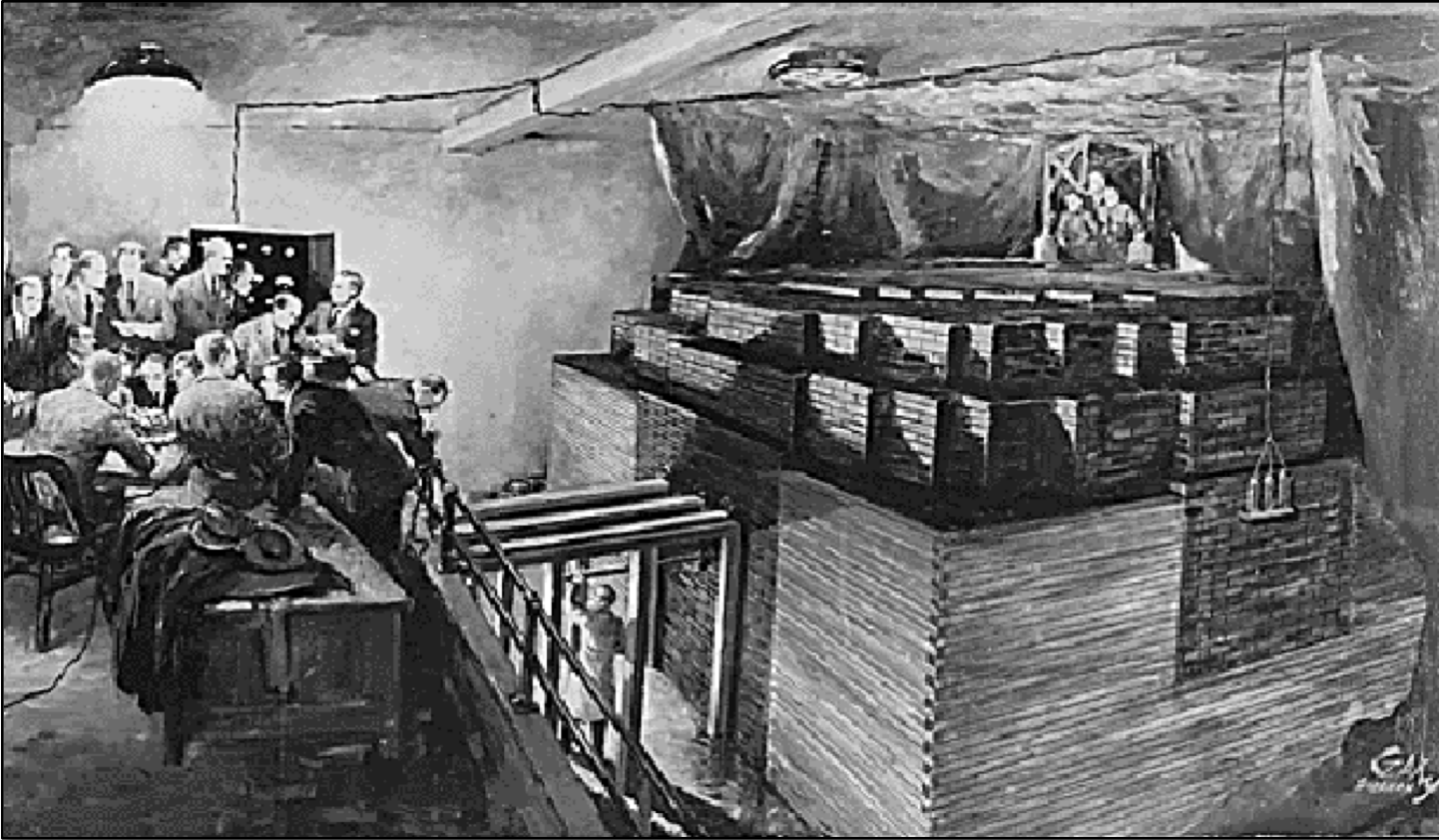
Science and Technology Programs

RESEARCH DIVISIONS	FACILITIES, CENTERS, AND INSTITUTES
Computing, Environment and Life Sciences	User Facilities
BIO Biosciences	APS Advanced Photon Source
EVS Environmental Science	ALCF Argonne Leadership Computing Facility
MCS Mathematics and Computer Science	ATLAS Argonne Tandem Linear Accelerator System
Energy and Global Security	ARM ARM Southern Great Plains
ES Energy Systems	CNM Center for Nanoscale Materials
GSS Global Security Sciences	Centers and Joint Institutes
NE Nuclear Engineering	AAI Argonne Accelerator Institute
Photon Sciences	ACCESS Argonne Collaborative Center for Energy Storage Science
ASD Accelerator Systems	ADW Argonne Design Works
AES APS Engineering Support	ALI Argonne Leadership Institute
XSD X-ray Science	CEES Center for Electrochemical Energy Science
Physical Sciences and Engineering	CTR Center for Transportation Research
CSE Chemical Sciences and Engineering	CRI Chain Reaction Innovations
HEP High Energy Physics	CI Computation Institute
MSD Materials Science	IACT Institute for Atom-Efficient Chemical Transformations
NST Nanoscience and Technology	IGSB Institute for Genomics and Systems Biology
PHY Physics	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

**Advanced
Photon
Source
(APS)**

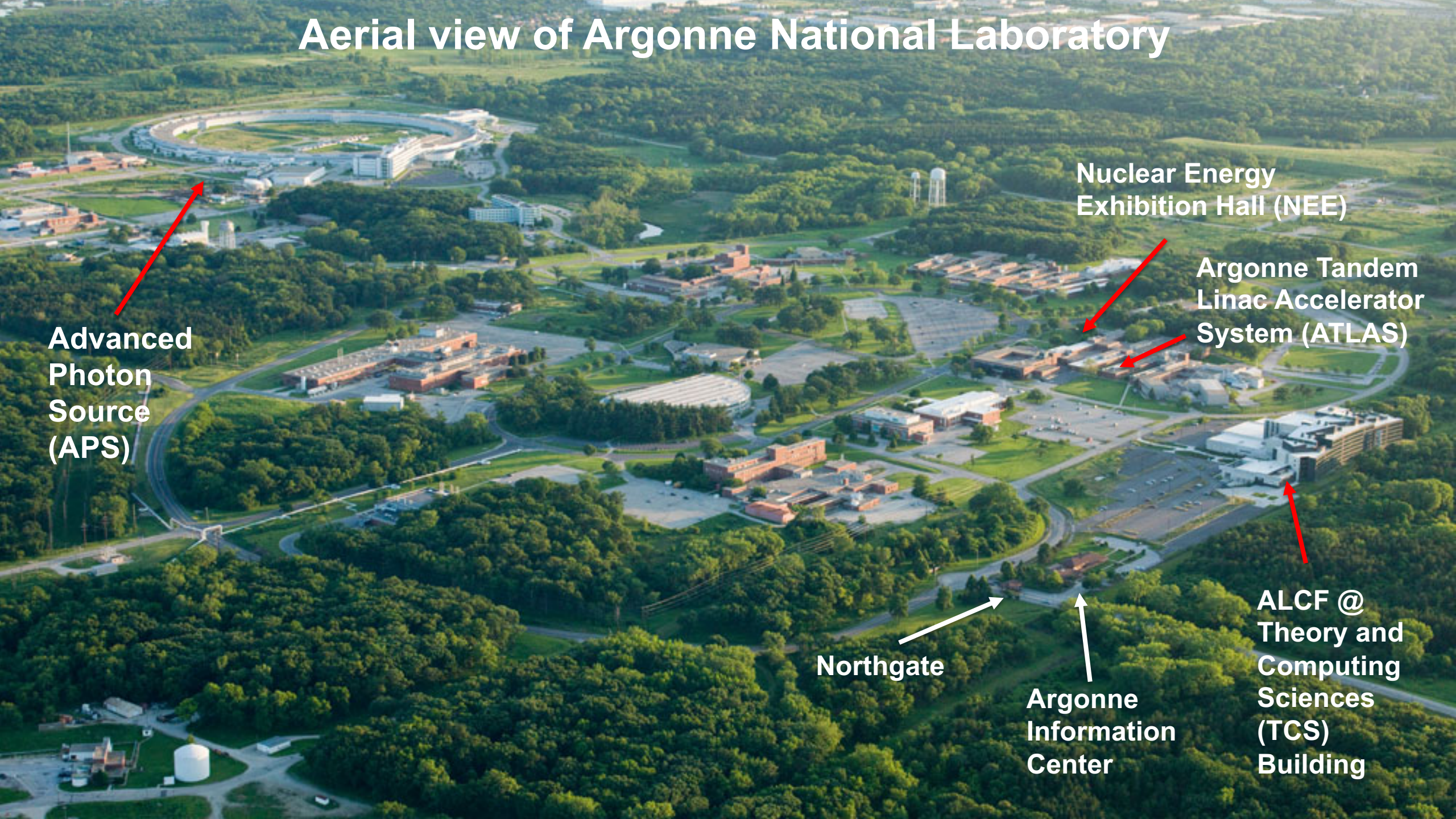
**Nuclear Energy
Exhibition Hall (NEE)**

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

Northgate

**Argonne
Information
Center**

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



Major Scientific User Facilities at Argonne

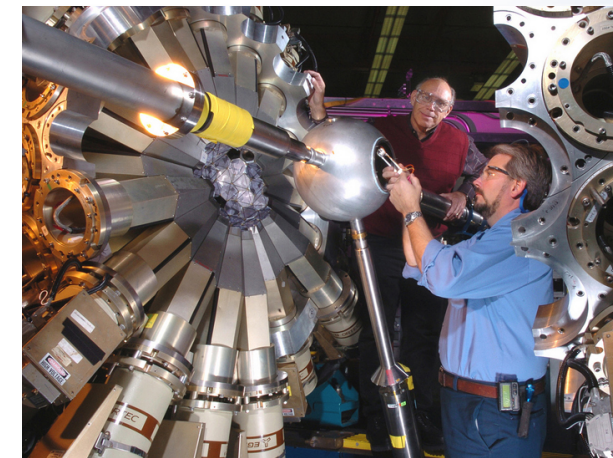
**Advanced
Photon
Source**



**Argonne
Leadership
Computing
Facility**

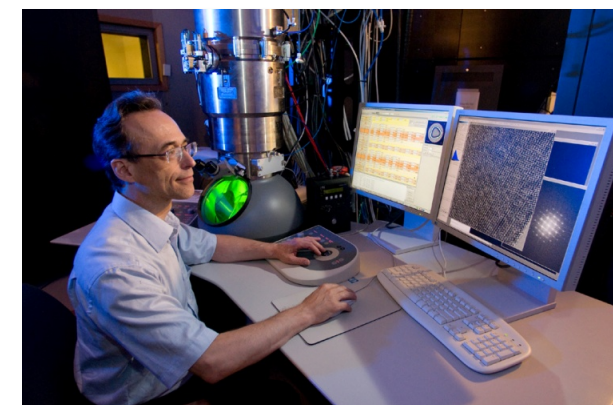


**Argonne Tandem Linear
Accelerator System**



**Center for
Nanoscale
Materials**

**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.

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

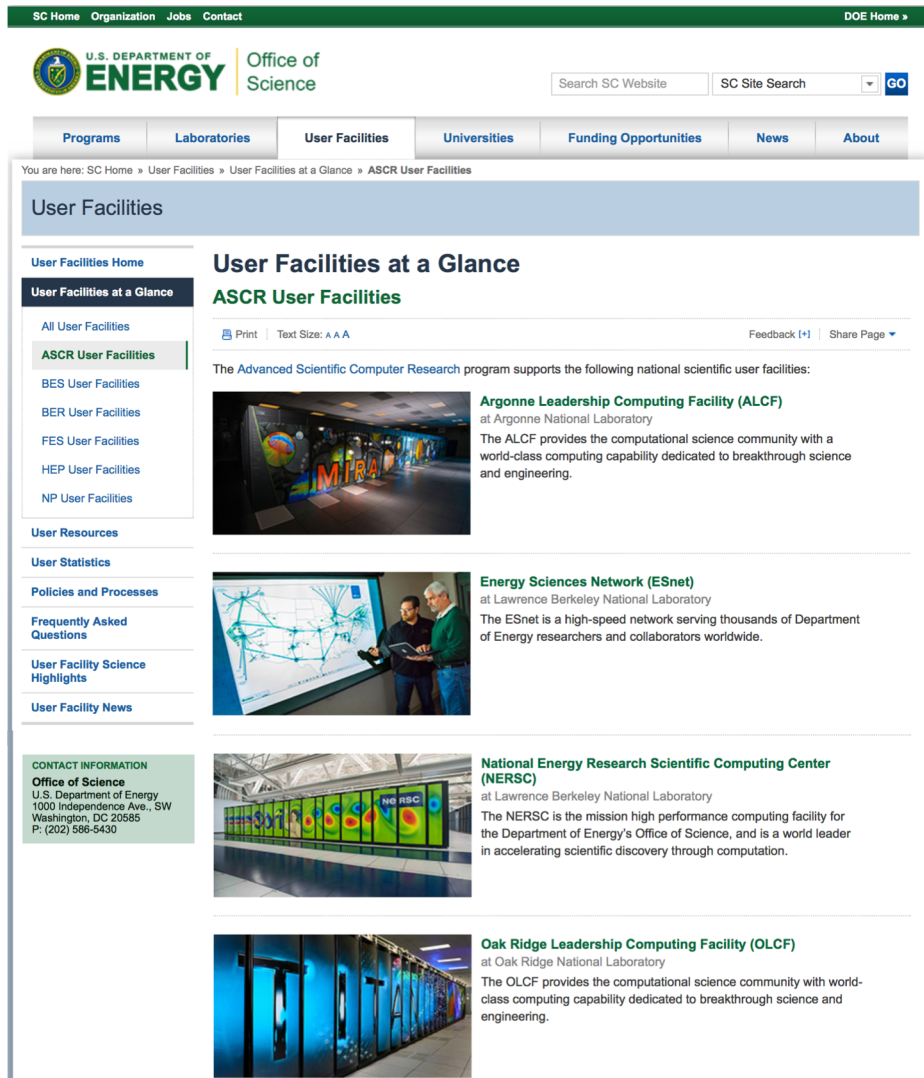
ATPESC Overview

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

Curriculum Tracks and their leaders

- **Track 1: Hardware Architectures** – Pete Beckman
- **Track 2: Programming Models and Languages** – Rajeev Thakur and Yanfei Guo
- **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 Engineering** – Anshu Dubey and Katherine Riley
- **Track 8: Machine Learning and Deep Learning for Science** – Venkatram Vishwanath


ATPESC Computing Resources



The screenshot shows the 'User Facilities at a Glance' page on the ATPESC website. The page is titled 'User Facilities at a Glance' and 'ASCR User Facilities'. It lists several user facilities: ALCF, BES, BER, FES, HEP, and NP. The page also includes a sidebar with links to 'User Resources', 'User Statistics', 'Policies and Processes', 'Frequently Asked Questions', 'User Facility Science Highlights', and 'User Facility News'. The main content area features a section titled 'User Facilities at a Glance' and 'ASCR User Facilities'. It includes a list of user facilities and a description of the Advanced Scientific Computing Research program. The page also features a contact information section for the Office of Science, U.S. Department of Energy, and a list of user facilities with their descriptions and images.

 **ALCF** – Theta and Cooley

 **OLCF** - Ascent

 **NERSC** – Cori et al.

 **Intel Devcloud**

Source: <https://science.energy.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

Agenda 2020 « Argonne Training X +

https://extremecomputingtraining.anl.gov/agenda-2020/

Argonne NATIONAL LABORATORY

HOME ATPESC NEWS ABOUT ATPESC PAST PROGRAMS

Agenda 2020

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

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

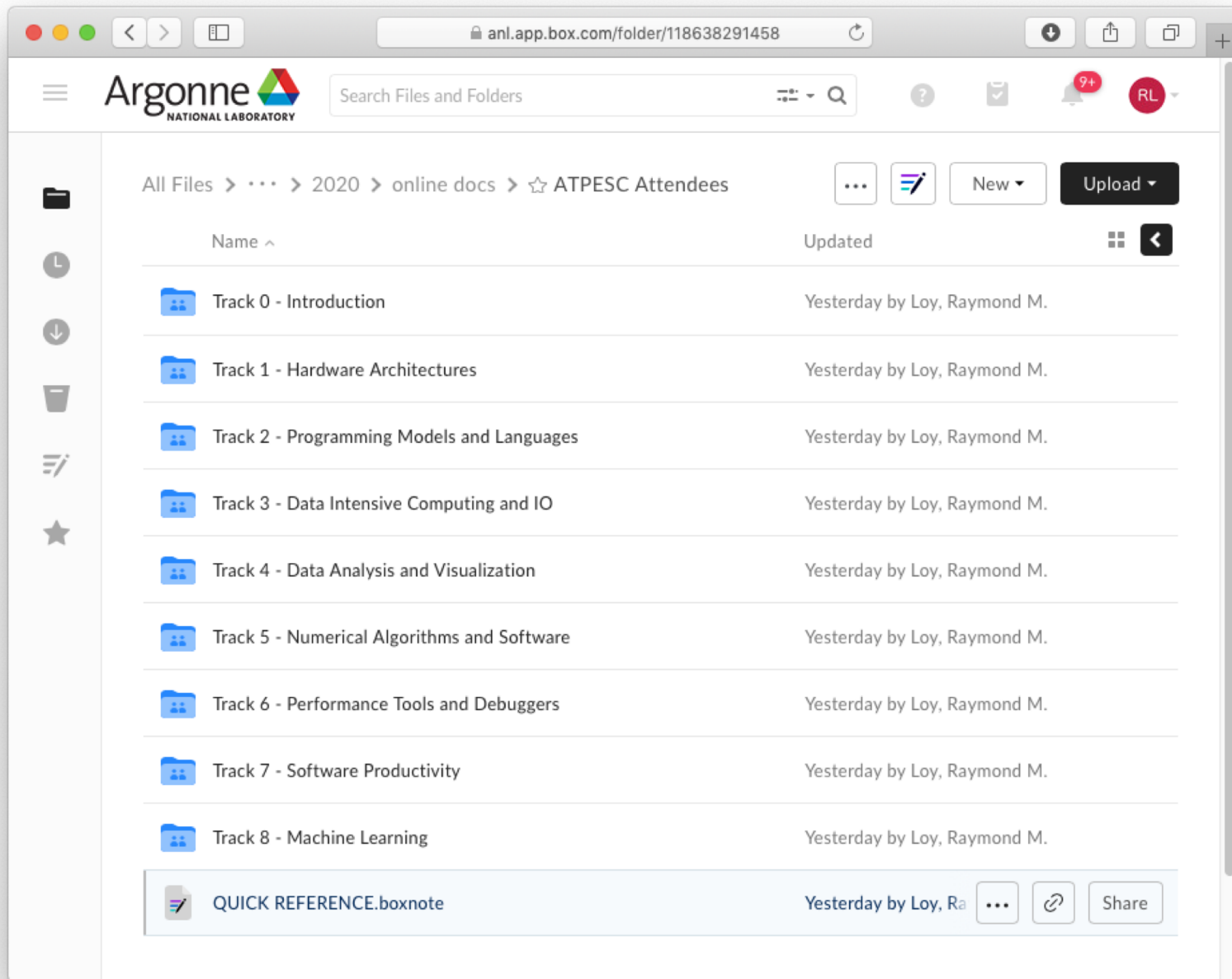
[MEETING CONNECTION INFO AND HANDOUTS](#)

SUNDAY, July 26, 2020

11:00	Introduction to ATPESC	Ray Loy, ANL
11:30	Quick Start on ATPESC Computing Resources	JaeHyuk Kwack, ANL
1:00 p.m.	Participant Introductions	All
2:00	Adjourn	

MONDAY, July 27, 2020

X Highlight All Match Case Match Diacritics Whole Words



anl.app.box.com/notes/695095101259

New

QUICK REFERENCE

Agenda <https://extremecomputingtraining.anl.gov/agenda-2020/>

Zoom Meeting Links

Main Room <---- ALL DAYS WILL START IN THE MAIN ROOM
<https://exascaleproject.zoomgov.com/j/1608499706?pwd=NFhkdlldzZmpjSmRTWWJVdUkzTGV3Zz09>
Meeting ID: 160 849 9706
Password: 626483

Room B (Used by break-outs as listed in the Agenda)
<https://exascaleproject.zoomgov.com/j/1601131634?pwd=SDRSNEtKT3daQ0xqL0FSOC9rMG5yQT09>
Meeting ID: 160 113 1634
Password: 9pgW.M

Room C (Used by break-outs as listed in the Agenda)
<https://exascaleproject.zoomgov.com/j/1610856640?pwd=SHRINKpGWGY2RDFFPeUs2SmJRby9nUT09>
Meeting ID: 161 085 6640
Password: 21DRKC

Slack Workspace

<https://alcf-workshops.slack.com>

This Quick Reference Document: <https://anl.app.box.com/notes/695095101259>

ATPESC Slack

- alcf-workshops.slack.com
- #announce
- #general for Q&A during the program
 - There are also topic-related channels
 - See Channels + option to browse the list
- #alcf-account-support ← help with Theta and Cooley accounts
- #atpesc-support ← other logistical help

Getting help

- ALCF accounts (Theta, Cooley)
 - support@alcf.anl.gov and slack #alcf-account-support
- OLCF accounts
 - Token issues, call: 865.241.6536 (24x7). Other questions, email: help@olcf.ornl.gov (mention ATPESC in subject)
- NERSC accounts
 - accounts@nerosc.gov (mention ATPESC in subject) or call 1-800-666-3772
- ATPESC general support including Slack, Box
 - support@extremecomputingtraining.anl.gov
 - #atpesc-support

(**TENTATIVE**) Virtual Argonne National Laboratory Tour

Saturday, August 1 11AM-2PM (expected one hour in this range, watch for updates)

The **Argonne Leadership Computing Facility (ALCF)** is one half of the U.S. Department of Energy's (DOE) Leadership Computing Facility, which deploys diverse high-performance computer architectures that are 10 to 100 times more powerful than typical research computing.



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 2021

- 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

