Argonne Training Program on Extreme-Scale Computing

Introduction to ATPESC

Ray Loy
ATPESC 2021 Program Director
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  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
Argonne National Lab
Battelle Memorial Inst.
CEA Saclay
CMU
Cornell U.
Duke U.
Frederick National Lab
Indiana U.
KAUST
LBNL
MIT
NERSC
NREL
North Carolina A&T
Northwestern U.
PNNL
RPI
Rice U.
Stanford U.
TU Dresden
Texas A&M
U. Wisconsin Madison
U. Udine
UC Berkeley
UI Urbana-Champaign
UT Austin

Aramco Americas
BP
Boston U.
CERN
Carleton U.
DESY
Environment and Climate Change Canada
Harvard U.
Inst. de Astrofísica de Canarias
LANL
LSU
NASA Langley
NETL
New York U.
North Carolina State
Oak Ridge National Lab
Queen's U.
Reservoir Labs
SLAC National Accelerator Lab
Stony Brook U.
TU Vienna
U. Nacional de San Luis
U. Basel
U. Wyoming
UC Riverside
USC
Wayne State
Argonne National 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.
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

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)
- ALCF @ Theory and Computing Sciences (TCS) Building
- Northgate
- Argonne Information Center
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

- **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 milliseck

- **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 – *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
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

Goals for Attendees

- Exposure to New ideas
- Take advantage of ATPESC Resources
- Talk F2F (virtually) with Lecturers, other Participants, Support
Box Folder

Linked at

ATPESC Home Page
Agenda
Class Materials
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

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ATPESC 2022

• If you or an associate is interested in attending
  – Subscribe to mailing list [https://extremecomputingtraining.anl.gov](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