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
Immanuel
Juan Diego
Lidia
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
Ereemy
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
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

Advanced Photon Source (APS)
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 millisecond

- **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

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

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

**MEETING CONNECTION INFO AND HANDOUTS**

#### SUNDAY, July 26, 2020

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Speaker(s)</th>
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<tbody>
<tr>
<td>11:00</td>
<td>Introduction to ATPESC</td>
<td>Ray Loy, ANL</td>
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<tr>
<td>11:30</td>
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<td>JaeHyuk Kwack, ANL</td>
</tr>
<tr>
<td>1:00 p.m.</td>
<td>Participant Introductions</td>
<td>All</td>
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<tr>
<td>2:00</td>
<td>Adjourn</td>
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#### MONDAY, July 27, 2020

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<tr>
<td>0 - Introduction</td>
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<td>Yesterday by Loy, Raymond M.</td>
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<tr>
<td>1 - Hardware</td>
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<td>Yesterday by Loy, Raymond M.</td>
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<td>2 - Programming</td>
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<td>Yesterday by Loy, Raymond M.</td>
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<td>3 - Data Intensive</td>
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<td>4 - Data Analysis</td>
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<td>5 - Numerical</td>
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<td>6 - Performance</td>
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<td>7 - Software</td>
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<td>8 - Machine</td>
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Quick Reference: boxnote

Yesterday by Loy, Raymond M.
QUICK REFERENCE

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

Zoom Meeting Links

Main Room  ALL DAYS WILL START IN THE MAIN ROOM
https://exascleproject.zoomgov.com/j/1608499706?pwd=NPhkdldzZmgjSmRTWVJvdxUkzTGV3Ze09
Meeting ID: 160 849 9706
Password: 6264B3

Room B (Used by break-outs as listed in the Agenda)
https://exascleproject.zoomgov.com/j/1601131634?pwd=5DRSNEtKT3daQ0xl0F3OCmMG5yQT09
Meeting ID: 160 113 1634
Password: 9pgW.M

Room C (Used by break-outs as listed in the Agenda)
https://exascleproject.zoomgov.com/j/1610856640?pwd=SHRlbipGWGY2RDFPeUs25mJRby9niUT09
Meeting ID: 161 085 6640
Password: 21DRKC

Slack Workspace
https://alf-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@nersc.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