Argonne Training Program on Extreme-Scale Computing

Introduction to the ATPESC

Marta García Martínez
ATPESC 2019 Program Director

Q Center, St. Charles, IL (USA)
July 28 – August 9, 2019
Outline

- Welcome
- A few words about Argonne National Laboratory
- Motivation of the ATPESC
- The curriculum
- Logistics and reminders
WELCOME
Welcome!

73 ATPESC 2019 Participants

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<th>Alberto</th>
<th>Alexander</th>
<th>Ángel Manuel</th>
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<td>Logan</td>
<td>Luca</td>
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<td>Matti</td>
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<td>Peng</td>
<td>Petro Junior</td>
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Welcome!

ATPESC 2019
49 Institutions

- Argonne National Laboratory
- Brookhaven National Laboratory
- CEA, Saclay
- Duke University
- Georgia Institute of Technology
- Illinois State University
- Iowa State University
- IT4Innovations National Supercomputing Center, VSB - TU Ostrava
- Lawrence Berkeley National Laboratory
- Los Alamos National Laboratory
- Massachusetts Institute of Technology
- NASA
- Naval Nuclear Laboratory
- Politecnico di Milano
- Rensselaer Polytechnic Institute
- Stanford University
- Texas A&M University
- The University of North Carolina at Chapel Hill
- University of California, Berkeley
- University of Cambridge
- University of Colorado Boulder
- University of Illinois at Urbana-Champaign
- University of Michigan
- University of Minnesota
- University of Washington
- BP America Inc.
- Brown University
- Courant Institute of Mathematical Science
- Fermi National Accelerator Laboratory
- Hardvard University
- Instituto de Astrofísica de Canarias
- ISAE-SUPAERO
- King's College London
- Lawrence Livermore National Laboratory
- Marquette University
- Michigan State University
- National Renewable Energy Laboratory
- Northwestern University
- Queen Mary University of London
- SLAC National Accelerator Laboratory
- Technical University of Munich
- The Ohio State University
- University of Tennessee
- University of California, Irvine
- University of Cambridge
- University of Delaware
- University of Illinois at Urbana-Champaign
- University of Michigan
- University of Southern California
You are here: **Space …**

Source: Google Maps, shutterstock, NASA
You are here: **Time…**

Argonne Training Program on Extreme-Scale Computing

**ATPESC 2019**

- Two-weeks training program
- Once-in-a-lifetime experience
- Conceived as a retreat
A few words about 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.
The origin of Argonne National Laboratory

CP-1 under the stands of Stagg field of 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
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
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

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

The Advanced Photon Source (APS) is one of the most technologically complex machines in the world. The APS provides the brightest high-energy X-ray beams in the Western Hemisphere to more than 6,000 scientists each year from every U.S. state, the District of Columbia, Puerto Rico, and countries in the world.

The Argonne Tandem Linac Accelerator System (ATLAS) is the world's first ion accelerator using superconducting devices for the energy gain. It is capable of accelerating ions of all elements, both stable and radioactive, from hydrogen to uranium for research into the properties of the nucleus, the core of matter, the fuel of stars.

The Nuclear Energy Exhibition Hall (NEE) showcases Argonne's rich heritage in the development of nuclear reactors and its current role in the development of next-generation reactors and fuel cycle technologies.
Motivation of the ATPESC
Motivation of the 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** that are tackled with 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 2019 by the numbers

73 participants
100 h courses & hands-on
$0 no cost to attend
$1.4M 2019-2021
>100 staff

Domestic airfare, meals and lodging provided

- Lecturers
- Reviewers
- Admins
- On-site support
- Organizers
- …
The Curriculum
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 and Joseph Insley
- **Track 5**: Numerical Algorithms and Software for Extreme-Scale Science – Lois McInnes and Mark Miller
- **Track 6**: Performance Tools and Debuggers – Ray Loy and JaeHyuk Kwack
- **Track 7**: Software Engineering – Anshu Dubey and Katherine Riley
- **Track 8**: Machine Learning and Deep Learning for Science – Venkatram Vishwanath and Prasanna Balaprakash
Dinner Talks

- Purpose: present additional topics that will probably be relevant to your research at some point in your career – but in any case interesting

- Rommie Amaro
  UC San Diego

- Rob Schreiber
  Cerebras

- Mark Miller
  LLNL

- Jeffrey Vetter
  ORNL

- Katrin Heitmann
  ANL

- Ian Foster
  ANL

- Michela Taufer
  ACM

- Mark Jackels
  DreamWorks

- Yuri Alexeev
  ANL
ATPESC Resources

Source: https://science.energy.gov/user-facilities/user-facilities-at-a-glance/ascr/
Yes, the ATPESC is an intensive program

- Many lectures every day, followed by evening hands-on sessions
- Ideally we would cover all topics in more depth but the result would be a six-week program
  - But few people’s schedules would allow them to participate
- Note the **8:30 am** starting time, dinner at **5:30 pm** right after the end of the afternoon lectures, evening sessions
ATPESC Deliverables

• Presentations
The slides of the Lectures will be available before the talk with the exception of the Dinner Talks (to keep some mystery)

All presentations will be available under a Box folder at the end of the program

• Videos
The videos of the Lectures will be available in September on the Argonne Youtube Channel and the ATPESC website

NEW!

https://www.youtube.com/user/ArgonneNationalLab

• Audio-only files
MP3 audio files of the Lectures (2017-2019) will be available in September on the ATPESC website

https://extremecomputingtraining.anl.gov
Goals for today

Check-in (hotel and program)

ATPESC Resources

- Pick up ALCF and OLCF tokens, and NERSC account instructions, log in to JLSE
- Log in to all ATPESC Resources

Introductions and discussions

Plan your time at ATPESC

- Agenda, tracks, breaks …
- Location, activities, food …
Goals for the next two weeks

- Get inspired
- New ideas
- Challenge your science and codes

- Take advantage of ATPESC Resources

- Talk with Lecturers, Participants, Support Staff…

- & Enjoy!
Logistics and reminders
ATPESC Website

extremecomputingtraining.anl.gov

ATPESC
ARGONNE TRAINING PROGRAM ON EXTREME-SCALE COMPUTING

AGENDA

WHEN
July 28 - August 9, 2019

WHERE
Q Center, St. Charles, IL (USA)
Go to the ATPESC agenda


<table>
<thead>
<tr>
<th>Agenda 2019</th>
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<tbody>
<tr>
<td><strong>July 28, 2019</strong></td>
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</table>
| 2:00 pm - 4:00 pm | **On-site Check-in**  
Entrance 4 Lobby / Room D L202 |
| 4:00 pm - 4:30 pm | **Presentation: Introduction to the ATPESC**  
St. Charles Amphitheater  
Marta García Martínez, ANL |
| 4:30 pm - 5:30 pm | **Presentation: Quick Start on ATPESC Computing Resources**  
St. Charles Amphitheater  
Ray Loy, ANL |
Go to the ATPESC agenda

Click here: “More info”
Go to the ATPESC agenda

Presentation: Introduction to the ATPESC

Click here
ATPESC Pocket Folder

Contains information about:

- Maps of the Q Center (Conference Area, Guest, Aerobic Mile Chart)
- Restaurants around Q Center
- Some flyers of the systems that you will be using
- ANL tour flyers
- Argonne Now magazine
- Information about tokens and what to do in case of problems (provided during check-in)
General Logistics

- **Breakfast & Lunch in the Q Tower Dining**

- **Menus** will be sent after this talk.

- A photographer will stop by one day to take a **group photo**. We will let you know in advance.

- An Argonne team might conduct brief **interviews** with some participants.

- **Buses location** for ANL Tour and ORD transportation (8/10) will depart from the South Entrance (close to the Gift Shop)
General Logistics

- All lectures and hands-on sessions in the Lecturer Room in the St. Charles Amphitheater
- Dinner Talks in the Fox River Ballroom 3 and 6
- Nourishment Hubs available; 8 – 11 am and 2 – 5 pm
- Office hours: 8 am – 5 pm (lunch break closed: 12 – 1 pm)
**Mens sana in corpore sano**

*Mens sana in corpore sano* is a Latin phrase, usually translated as "a healthy mind in a healthy body". The phrase is widely used in sporting and educational contexts to express the theory that physical exercise is an important or essential part of mental and psychological well-being. (*)

Source: [https://en.wikipedia.org/wiki/Mens_sana_in_corpore_sano](https://en.wikipedia.org/wiki/Mens_sana_in_corpore_sano)


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**Aerobic Mile Chart @ Q Center**

# Meals

## Breakfast

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<th>Item</th>
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**Note:** All menu items are subject to change without notice.

The MOD lunches that are attached are VERY limited to what will be available in the dining room. This is only for the private meals which are based off of what is offered in the dining room. Please check the app daily to see the full menu selection.

## Lunch

### 2018 spring and summer MOD Items

<table>
<thead>
<tr>
<th>LUNCH MOD - WEEK 1</th>
<th>Monday</th>
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### 2018 Spring and Summer MOD Items

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## Dinner

<table>
<thead>
<tr>
<th>Function: Dinner</th>
<th>Room: Fox River Ballroom 6</th>
<th>Time: 5:30 PM to 7:00 PM</th>
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<tbody>
<tr>
<td>MOD Dinner</td>
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<tr>
<td>Creamy Chipotle Potato Soup</td>
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<tr>
<td>Toasted Green Salad with Assorted Dressings</td>
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<tr>
<td>Artisan Bread and Rolls with Butter</td>
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<td></td>
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<tr>
<td>Honey Ginger Tsoi with Brokkoli</td>
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<tr>
<td>Herb Roasted Chicken</td>
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<tr>
<td>Spicy Sesame Beef with Scallions</td>
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<tr>
<td>Ginger Cilantro Rice</td>
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<td>Roasted Asparagus</td>
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<td>Lemon Bit</td>
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<tr>
<td>Assorted Hot and Cold Beverages</td>
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Menu items are subject to change without notice.

Included in Package

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Participant Introductions

Today (7/28) during Dinner

John Doe
Ph.D. Student
Civil Engineering, University of Houston, Houston, TX (USA)

Scientific Field | Mathematics

Research Interests
- Subsurface flow and transport
- Finite Element Methods
- High-Performance Computing

Personal Interests
- Tennis
- Fishing
Marta García Martínez

Scientific Field | Computational Fluid Dynamics

Research Interests
- Two-phase Flows
- High-Performance Computing
- Partitioning Algorithms

Personal Interests
- Reading
- Traveling
Feedback

Help us improve the training program
• Track evaluations
• Overall program evaluation
• Conversations or emails to any of us

- Tour of Argonne
- More hands-on exercises during lectures
- Participant introductions
Whom to ask for help on-site

- **Administration**
  - Office: Virginia Doyle, Monica White & Julie Smagacz (week 1)
    Karen VanMeerten (week 2)
  Or by email to your ATPESC Contact Person

- **Computing issues**
  - **User Services**: Robert Scott / Haritha Som
  - **Operations**: Adam Scovel / Ben Lenard / Mark Fahey / Frank Willmore / Gordon McPheeters
  Or by email to support@alcf.anl.gov

- **General**
  - Email: support@extremecomputingtraining.anl.gov
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.
Acknowledgments

- This research used resources of the Argonne Leadership Computing Facility, which is a DOE Office of Science User Facility supported under Contract DE-AC02-06CH11357

- This research used resources of the Oak Ridge Leadership Computing Facility at the Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725

- This research used resources of the National Energy Research Scientific Computing Center, a DOE Office of Science User Facility supported by Office of Science of the U.S. Department of Energy under Contract DE-AC02-05CH11231
Thank you for your attention!

& for taking two weeks of your summer to participate in this program

Questions