Argonne Training Program on Extreme-Scale Computing

Introduction to the ATPESC

Marta García Martínez
ATPESC 2018 Program Director

Q Center, St. Charles, IL (USA)
July 29 – August 10, 2018
Outline

Welcome

A few words about Argonne National Laboratory

Motivation of the ATPESC

The curriculum

Logistics and reminders
Welcome!

<table>
<thead>
<tr>
<th>Aaron</th>
<th>Aaron</th>
<th>Agnieszka</th>
<th>Amelia</th>
<th>Andrew</th>
<th>Anthony</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ashleigh</td>
<td>Bo</td>
<td>Brendan</td>
<td>Bryce</td>
<td>Christopher</td>
<td>Chunlei</td>
</tr>
<tr>
<td>Daniel</td>
<td>Dario</td>
<td>Davide</td>
<td>Duoming</td>
<td>Elizabeth</td>
<td>Giovanni</td>
</tr>
<tr>
<td>Haithem</td>
<td>Henry</td>
<td>Hilario</td>
<td>Hyun</td>
<td>Jack</td>
<td>Jared</td>
</tr>
<tr>
<td>Jeremy</td>
<td>Jinxun</td>
<td>Johannes</td>
<td>Jonas</td>
<td>Julian</td>
<td>Jun</td>
</tr>
<tr>
<td>Kai-Yuan</td>
<td>Karima</td>
<td>Kenneth</td>
<td>Kevin</td>
<td>Kristi</td>
<td>Laurie</td>
</tr>
<tr>
<td>Leandro</td>
<td>Lukas</td>
<td>Maria</td>
<td>Massimiliano</td>
<td>Matias</td>
<td></td>
</tr>
<tr>
<td>Matthew</td>
<td>Md</td>
<td>Michael</td>
<td>Nicole</td>
<td>Oguz</td>
<td>Oscar Luis</td>
</tr>
<tr>
<td>Petr</td>
<td>Priyanka</td>
<td>Robert</td>
<td>Rudradatt</td>
<td>Ryan</td>
<td>Satyam</td>
</tr>
<tr>
<td>Sayan</td>
<td>Shafigh</td>
<td>Socratis</td>
<td>Srinivasan</td>
<td>Stefan</td>
<td>Stephen</td>
</tr>
<tr>
<td>Storm</td>
<td>Thomas</td>
<td>Timothy</td>
<td>Timur</td>
<td>Tong</td>
<td>Umesh</td>
</tr>
<tr>
<td>Valentina</td>
<td>Victor</td>
<td>Vivek</td>
<td>William</td>
<td>Yao-Lung</td>
<td>Yeqing</td>
</tr>
<tr>
<td>Yu</td>
<td>Yu Hong</td>
<td>Yuzhi</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Welcome!

ATPESC 2018
52 Institutions

- Ames Laboratory
- Argonne National Laboratory (3)
- Bates College
- BP America Inc.
- Brookhaven National Laboratory
- Carnegie Mellon University
- Emory University
- Illinois Institute of Technology
- Iowa State University
- King’s College London
- Lawrence Livermore National Laboratory (2)
- Massachusetts Institute of Technology
- NASA Langley Research Center (4)
- Northeastern University
- Numerical Algorithms Group
- Polytechnic University of Catalonia
- Purdue University
- SISSA
- Stony Brook University
- The University of Tennessee, Knoxville (2)
- University of Alabama
- University of California, Berkeley
- University of Campinas
- University of Oregon (2)
- University of Wyoming
- USGS
- Aramco Services Company
- Barcelona Supercomputing Center
- Bilkent University
- Brigham Young University
- Brown University
- CEA Saclay France
- Georgia Institute of Technology (2)
- Indiana University Bloomington
- IT4Innovations, VSB - Technical University of Ostrava (2)
- Lawrence Berkeley National Laboratory (6)
- Los Alamos National Laboratory
- Michigan State University
- Naval Nuclear Laboratory (2)
- Northwestern University (2)
- Oak Ridge National Laboratory
- Princeton Plasma Physics Laboratory
- Rensselaer Polytechnic Institute
- Stanford University
- Technische Universität Wien
- The University of Texas at Austin (3)
- University of Buenos Aires
- University of Cambridge
- University of Illinois at Chicago (2)
- University of Southern California (2)
- UNSW Sydney
- Washington State University (2)
You are here: **Space ...**

Source: Google Maps, shutterstock, NASA
ATPESC 2018

- 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=mTPIkJ2bKS0
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
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
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
Argonne National Laboratory Tour

Saturday, August 4  8:30 pm – 12:50 pm

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.

(round-trip from Q Center to Argonne by bus with stop at downtown St. Charles on the way back)

(if you signed in)
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
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 by the numbers

- **74** participants
- **100 h** courses & hands-on
- **$0** no cost to attend
- **$1.25M** 2016-2018
- **>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 Pavan Balaji
- **Track 3:** Data-intensive Computing and I/O – Rob Latham and Phil Carns
- **Track 4:** Numerical Algorithms and Software for Extreme-Scale Science – Lois McInnes, Lori Diachin and Mark Miller
- **Track 5:** Performance Tools and Debuggers – Ray Loy and Scott Parker
- **Track 6:** Software Engineering – Anshu Dubey and Katherine Riley
- **Track 7:** Visualization and Data Analysis – Mike Papka and Joe Insley
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
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 by mid-September on the Argonne Youtube Channel

https://www.youtube.com/user/ArgonneNationalLab
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
Go to the ATPESC agenda

Go to the ATPESC agenda

Click here: “More info”
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
- WIFI connection
- 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 2 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)

## Meals

### Breakfast

**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

<table>
<thead>
<tr>
<th>Item</th>
<th>MONDAY</th>
<th>TUESDAY</th>
<th>WEDNESDAY</th>
<th>THURSDAY</th>
<th>FRIDAY</th>
<th>SATURDAY</th>
<th>SUNDAY</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soup</td>
<td>Cream of Asparagus and Basil Soup</td>
<td>Chicken Noodle Soup</td>
<td>Beef Barley Soup</td>
<td>Tomato Basil Soup</td>
<td>Shrimp Bisque</td>
<td>Chef's Choice</td>
<td>Chef's Choice</td>
</tr>
<tr>
<td>Salad du Jour</td>
<td>Tossed Salad du Jour with 2 Dressings</td>
<td>Tossed Salad du Jour with 2 Dressings</td>
<td>Tossed Salad du Jour with 2 Dressings</td>
<td>Tossed Salad du Jour with 2 Dressings</td>
<td>Tossed Salad du Jour with 2 Dressings</td>
<td>Tossed Salad du Jour with 2 Dressings</td>
<td></td>
</tr>
<tr>
<td>Enhanced Salad</td>
<td>(Add'l Charge)</td>
<td>Chopped Romaine with Peppers, Baby Corn and Balsamic Vinaigrette</td>
<td>Chopped Romaine with Black Beans, Corn, Tomato, Red Onion and Cilantro Lime Vinaigrette</td>
<td>Field Greens with Red Onion, Olives, Asparagus with Herb Vinaigrette</td>
<td>Iceberg Lettuce with Slice Turkey, Tomato, Bacon, Bleu Cheese and Sun-Dried Tomato Vinaigrette</td>
<td>Mixed Greens with Asparagus Tomato, Peppers, and Lemon Dill Vinaigrette</td>
<td>Chopped Romaine with Parmesan Cheese, Croutons and Caesar Dressing</td>
</tr>
<tr>
<td>Vegetarian Option</td>
<td>Vegetarian Gratin</td>
<td>Vegetable Fajitas</td>
<td>Vegetable Pancit</td>
<td>Penne Pasta with Lentil Bolognese</td>
<td>Green Chili Corn Casserole</td>
<td>Chef's Choice</td>
<td>Chef's Choice</td>
</tr>
<tr>
<td>Entrée</td>
<td>Honey Mustard Glazed Artic Char</td>
<td>Seared Mahi with Spicy Papaya Relish</td>
<td>Tilapia in Hot and Sour Sauce</td>
<td>Sole Meuniere</td>
<td>BBQ Salmon with an Andouille Hash</td>
<td>Chef's Choice</td>
<td>Chef's Choice</td>
</tr>
<tr>
<td>Starch</td>
<td>Basil and Brown Rice Pilaf</td>
<td>Arroz Verde</td>
<td>Garlic Rice</td>
<td>Roasted Potatoes</td>
<td>Fried Rice</td>
<td>Chef's Choice</td>
<td>Chef's Choice</td>
</tr>
<tr>
<td>Side</td>
<td>Pork Sausage Links</td>
<td>Hickory Smoked Bacon</td>
<td>Hickory Smoked Bacon</td>
<td>Hickory Smoked Bacon</td>
<td>Hickory Smoked Bacon</td>
<td>Hickory Smoked Bacon</td>
<td>Hickory Smoked Bacon</td>
</tr>
</tbody>
</table>

### Dinner

**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.
Participant Introductions

Today (7/29) after the Dinner Talk
Marta García Martínez
Principal Project Specialist – Computational Science
Argonne National Laboratory
Argonne, IL (USA)

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: Sue Gregurich (week 1) or Teresa Rodriguez (week 2)
    Or by email to your ATPESC Contact Person

- **Computing issues**
  - **User Services**: Liza Booker / Robert Scott / Avanthi Madduri
  - **Operations**: Adam Scovel / Ben Lenard / John ‘Skip’ Reddy
    Or by email to support@alcf.anl.gov

- **General**
  - Marta García
    Or by email to 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