INTRODUCTION TO THE ATPESC

Presented to
ATPESC 2017 Participants

Marta García Martínez
ATPESC 2017 Program Director

Q Center, St. Charles, IL (USA)
Date 07/30/2017
Outline

Welcome

A few words about Argonne National Laboratory

Motivation of the ATPESC

The curriculum

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Welcome!

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Welcome!

45 Institutions

- Argonne National Laboratory
- Cornell University
- Georgia Institute of Technology
- Institute for Computational and Engineering Sciences
- Lawrence Livermore National Laboratory
- Michigan State University
- National Renewable Energy Laboratory
- Northwestern University
- Princeton Plasma Physics Laboratory
- Sandia National Laboratories
- Technische Universität Wien
- University of California, Irvine
- University of Florida
- University of Michigan
- University of Virginia
- Brown University
- CTTC - Heat and Mass Transfer Technological Center
- IBM Research
- KTH Royal Institute of Technology
- Los Alamos National Laboratory
- NASA Langley Research Center
- NOAA / Engility
- Oak Ridge National Laboratory
- Princeton University
- Stanford University
- The University of Texas at Austin
- University of California, Los Angeles
- University of Illinois at Urbana-Champaign
- University of Pittsburgh
- University of Wisconsin-Madison
- California Institute of Technology
- Geophysical Fluid Dynamics Laboratory
- INRIA
- Lawrence Berkeley National Laboratory
- Massachusetts Institute of Technology
- National Center for Atmospheric Research
- North Carolina State University
- Old Dominion University
- Purdue University
- Technical University of Ostrava
- University of California, Berkeley
- University of Colorado Boulder
- University of Massachusetts Dartmouth
- University of Southern California
- University of Wyoming
You are here: **Time**...

**Argonne Training Program on Extreme-Scale Computing**

**ATPESC 2017**
- 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.
Argonne’s mission: To 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
- Computing, Environment and Life Sciences
  - BIO Biosciences
  - EVS Environmental Science
  - MCS Mathematics and Computer Science
- Energy and Global Security
  - ES Energy Systems
  - GSS Global Security Sciences
  - NE Nuclear Engineering
- Photon Sciences
  - ASD Accelerator Systems
  - AES APS Engineering Support
  - XSD X-ray Science
- Physical Sciences and Engineering
  - CSE Chemical Sciences and Engineering
  - HEP High Energy Physics
  - MSD Materials Science
  - NST Nanoscience and Technology
  - PHY Physics

FACILITIES, CENTERS, AND INSTITUTES
- User Facilities
  - APS Advanced Photon Source
  - ALCF Argonne Leadership Computing Facility
  - ATLAS Argonne Tandem Linear Accelerator System
  - ARM ARM Southern Great Plains
  - CMM Center for Nanoscale Materials
- Centers and Joint Institutes
  - AAI Argonne Accelerator Institute
  - ACCESS Argonne Collaborative Center for Energy Storage Science
  - ADW Argonne Design Works
  - ALI Argonne Leadership Institute
  - CEES Center for Electrochemical Energy Science
  - CTR Center for Transportation Research
  - CRI Chain Reaction Innovations
  - CI Computation Institute
  - IACT Institute for Atom-Efficient Chemical Transformations
  - IGSB Institute for Genomics and Systems Biology
  - IME Institute for Molecular Engineering
  - JCESR Joint Center for Energy Storage Research
  - MCSES Midwest Center for Structural Genomics
  - NSE National Security Programs
  - NSEI Northwestern-Argonne Institute for Science and Engineering
  - RISE Risk and Infrastructure Science Center
  - SBC Structural Biology Center

Argonne NATIONAL LABORATORY
E-CP EXASCALE COMPUTING PROJECT
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 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

“Moll” Flanders, Director
Jeffrey Chu, Chief Engineer
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 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 Exhibit (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 by the numbers

- 70 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 – Katherine Riley and Anshu Dubey
- **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

Edward Seidel
UIUC

Francine Berman
RPI

Michael J. Franklin
UChicago

Rick Stevens
ANL

Rupak Biswas
NASA

Tom Evans
ORNL

Cleve Moler
MathWorks

Peter Kogge
Univ. of Notre Dame

Narayanan Kasthuri
ANL
ATPESC Resources

+ AWS & qwiklabs (NVIDIA)
+ IBM Quantum Computing
+ Jupyter

ALCF – Mira, Cetus, Vesta, Cooley and Theta

NERSC – Edison and Cori

OLCF – Titan

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 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
- Pick up ALCF and OLCF tokens, and NERSC account instructions
- Log in to all 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 2017

WHEN
July 30 - August 11, 2017

WHERE
St. Charles, IL
Q Center

Argonne NATIONAL LABORATORY
Go to the ATPESC agenda

Go to the ATPESC agenda

Click here: “More info”

Agenda 2017

July 30, 2017

2:00 pm - 4:00 pm
On-site Check-in
Room D L202

4:00 pm - 4:30 pm
Introduction to ATPESC
St. Charles Amphitheater

Marta Garcia Martinez, ANL
Go to the ATPESC agenda

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
- 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 (8/11) 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 1 (week 1) and 3 (week 2)
- 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**
- Scrambled eggs
- Toasted bread
- Chef's potatoes
- Hashbrowns
- Blueberry muffins

**Lunch**
- Chicken noodle soup
- Vegetable beef
- Chicken salad
- Grilled cheese sandwich
- Chicken curry
- Bean and rice salad
- Pad Thai noodles
- Grilled cheese
- Caesar salad
- Macaroni and cheese
- Butternut squash and apple salad
- Lentil soup

**Dinner**
- Baked salmon with lemon
- Macaroni and cheese
- Chicken wings
- Tacos with beef
- Grilled chicken breast
- Pasta with meat sauce
- Beef Stroganoff
- Fish tacos
- Grilled chicken and vegetables
- Grilled salmon
- Grilled chicken breast

**Nourishment Hubs**

**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 of what is offered in the dining room. Please check the app daily to see the full menu selection.
Participant Introductions

Today (7/30) after the Dinner Talk

INSTRUCTIONS FOR PARTICIPANT INTRODUCTION SLIDE

Section 1
Profile Picture
| Attach a recent photo (optional) |
Name
| First, Last Name > Example: John Doe |
Position
| Ph.D. Student, Postdoc, Engineer, etc. |
Department, Institution
| > Example: Civil Engineering, Univ. of Houston, TX (USA) |
University Logo and current institutional logo (if you have one)

Section 2
Scientific Field
| Pull field from the list below |
Research Interests
| Name three (or more) |
Personal Interests
| Name two (or more) |

Section 3
Graphic
| Attach a jpeg, png, tif or an editable file of an image of your choice about your work |

List of Scientific Fields

- Biological Sciences, Bioinformatics
- Biological Sciences, Biophysics
- Biological Sciences, Medical Science
- Biological Sciences, Neuroscience
- Chemistry, Analytical Chemistry
- Chemistry, Biochemistry
- Chemistry, Catalysis
- Chemistry, Combustion
- Chemistry, Environmental
- Chemistry, Geochemistry
- Chemistry, Organic
- Chemistry, Physical
- Chemistry, Quantum Chemistry
- Computer Science
- Earth Sciences, Environmental Sciences
- Earth Sciences, Geophysical Sciences
- Earth Sciences, Climate Research
- Earth Sciences, Geologic Sciences
- Economics
- Engineering, Material Response
- Engineering, Heat Transfer
- Engineering, Aerodynamics
- Engineering, Fluid-Structure Interaction
- Engineering, Fluids and Turbulence
- Fusion Energy, Inertial Fusion
- Fusion Energy, Magnetic Fusion
- Materials Science, Condensed Matter and Materials Physics
- Materials Science, Materials Discovery
- Materials Science, Solid State Physics
- Materials Science, Nanotechnology
- Materials Science, Nanoelectronics
- Materials Science, Nanophotonics
- Materials Science, Nanoscience
- Nuclear Energy
- Physics, Accelerator Physics
- Physics, Astrophysics
- Physics, Plasma/Molecular Physics
- Physics, Condensed Matter Physics
- Physics, High Energy Physics
- Physics, Nuclear Physics
- Physics, Space Physics
- Physics, Plasma Physics
- Physics, Energy Technologies, Bioenergy
- Physics, Energy Technologies, Wind Energy
- Physics, Energy Technologies, Solar Energy
- Physics, Energy Technologies, Energy Efficiency
- Physics, Energy Technologies, Energy Storage
- Physics, Energy Technologies, Energy Grid
- Mathematics

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
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
Raffle: 12 nights … 12 Books & 12 lanyards with flash drives

Special thanks to:

10x

James Reinders & Intel (Lecturer)

2x

Pavan Balaji (Track Lead and Lecturer)

12x

Ashley Barker (ECP 1.2.4. Developer Training and Productivity Lead)
Whom to ask for help on-site

- **Administration**
  - Office: Sue Gregurich or Renée Plzak
    Or by email to your ATPESC Contact Person

- **Computing issues**
  - **User Services**: Liza Booker / Robert Scott / Avanthi Mantrala
  - **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

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- 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