Argonne Training Program on Extreme-Scale Computing (ATPESC)

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



A few words about Argonne National Laboratory





Logistics and reminders





WELCOME





Welcome!

70 ATPESC 2017 Participants

Aditya Alexey Alessandro Alessio Alexander Alexander Benjamin Amelia Anand Ben Carlo Ben Cheng-Yu Carola Chris Christos Daniel **Eric Eric** Ferran Forrest Gabriele Gaddiel Forrest Gopal Guillaume *I-Te* Jakub Johann Jon Jonathan Jonathan Julien Justin Kuo-Chuan Kurt Kyle Lindsay Lisa Marc Matthew Maxence Nathan Mikhail Nadish **Nicholas** Ozan Philipp Polykarpos Rahulkumar Richard Sergi Robert Saumil Sumathi Sergio Shikhar Shinhoo Sidafa Som Sunwoo Théophile Thilina Thomas Tom Swarnava Vishal Xavier Yuliana Zahra





Welcome!

- Argonne National Laboratory
- Cornell University
- Georgia Institute of Technology
- Institute for Computational and Engineering Sciences
 KTH Royal Institute of Technology
- 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

- 45 Institutions
- Brown University
- CTTC Heat and Mass Transfer Technological Center
- IBM Research
- 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-Madisor

- 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



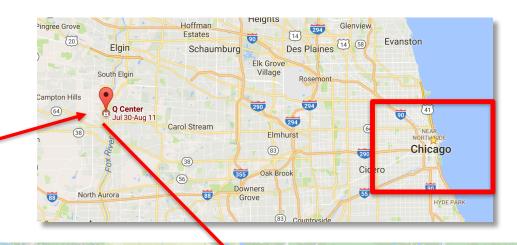


You are here: Space ...











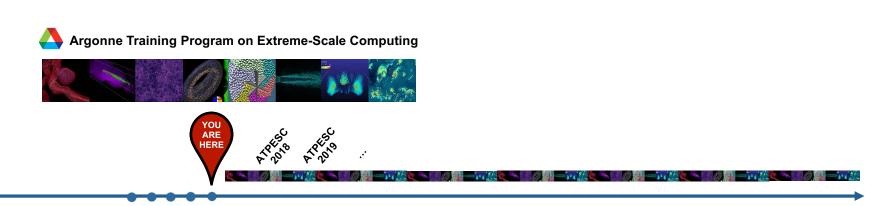




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Source: Google Maps, shutterstock, NASA

You are here: Time...



ATPESC 2017

- Two-weeks training program
- Once-in-a-lifetime experience
- Conceived as a retreat



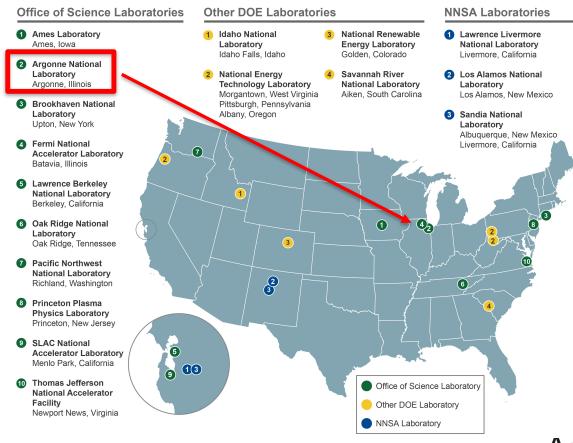


A few words about Argonne National Laboratory





Argonne – a part of DOE National Laboratory System



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.

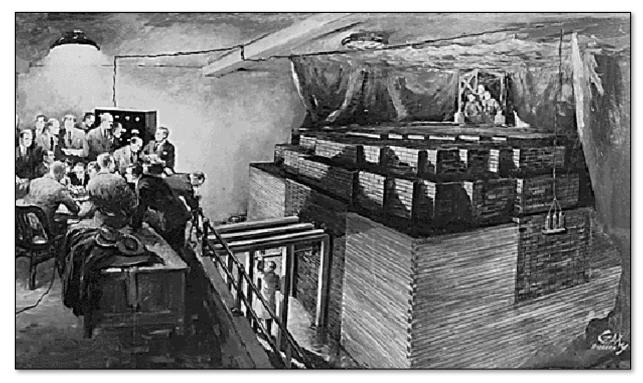
Source: https://science.energy.gov/~/media/_/images/laboratories/DOE_Laboratories_Map_2014_Hi-res.jpg

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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

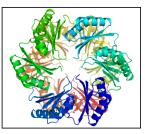




Argonne's mission: To provide science-based solutions to pressing global challenges







Environmental Sustainability



Nuclear and **National Security**

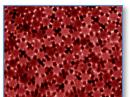
Use-Inspired Science and Engineering Discovery and transformational Science and Engineering



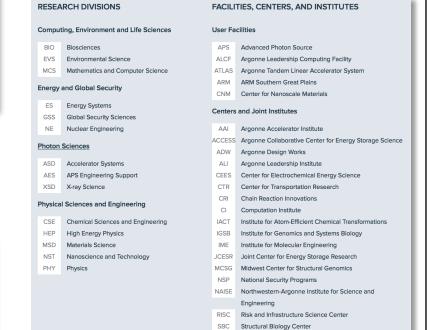




Major User Facilities



Science and Technology Programs







Major Scientific User Facilities at Argonne

Advanced Photon Source



Argonne Tandem Linear Accelerator System



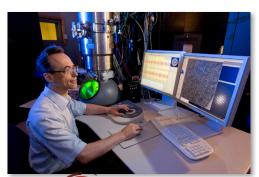
Center for Nanoscale Materials

Argonne Leadership Computing Facility



Electron Microscopy Center







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AVIDAC (1949-1953) Argonne's Version of the Institute's Digital Arithmetic Computer



"Moll" Flanders, Director Jeffrey Chu, Chief Engineer

- AVIDAC: based on prototype at the Institute for Advanced Study in Princeton
- Margaret Butler wrote AVIDAC's interpretive floatingpoint arithmetic system

Memory access time: 15 microsec

Addition: 10 microsecMultiplication: 1 millisec

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.





Argonne National Laboratory Tour (if you signed in)

Saturday, August 5 12:30 pm - 5:30 pm (round-trip from Q Center to Argonne by bus with stop at downtown St. Charles on the way back)



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

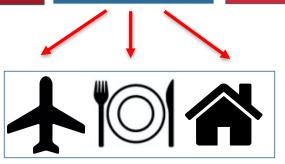
\$0
no cost to attend

\$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

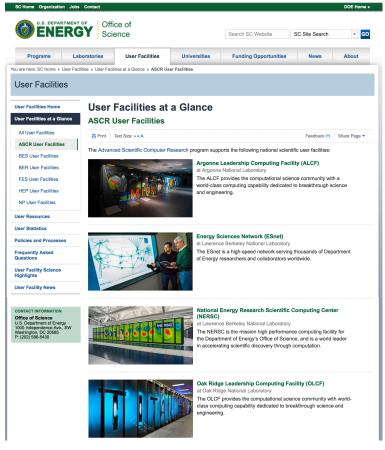


Narayanan Kasthuri ANL

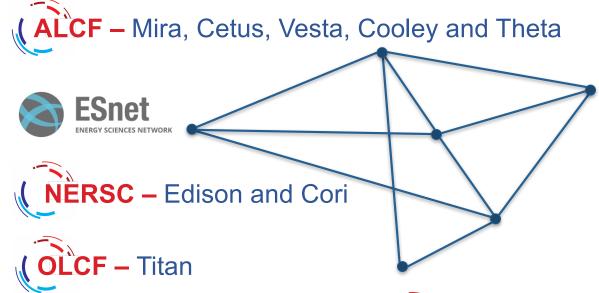




ATPESC Resources



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



Source: https://science.energy.gov/user-facilities/user-facilities-at-a-glance/ascr/

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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





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



Plan your time at ATPESC

- Agenda, tracks, breaks ...
- Location, activities, food ...





Goals for the next two weeks



New ideas

Challenge your science and codes



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









Logistics and reminders

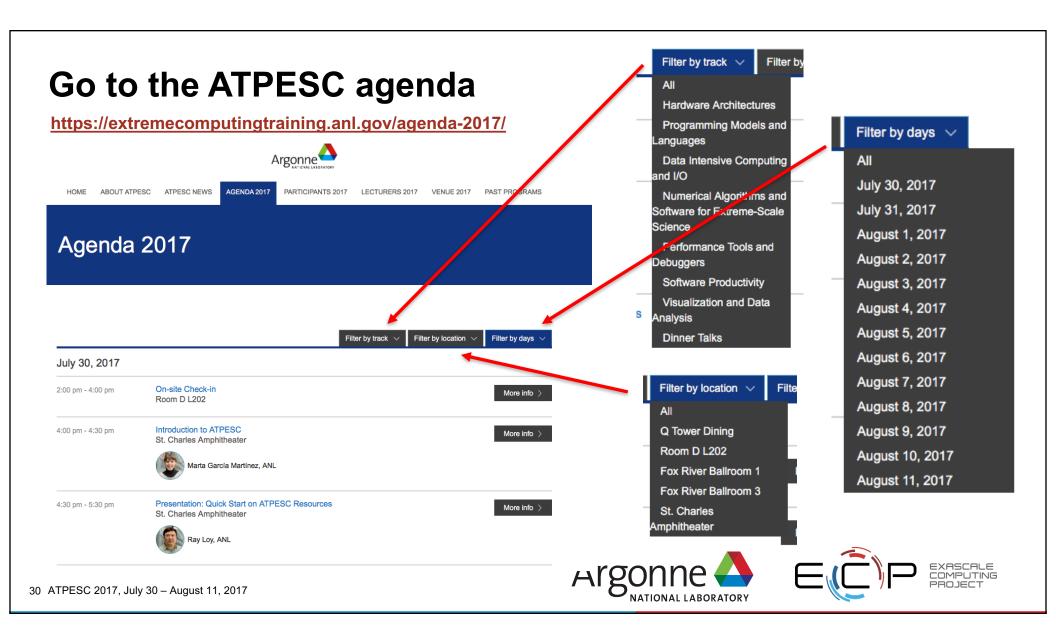




ATPESC Website

extremecomputingtraining.anl.gov



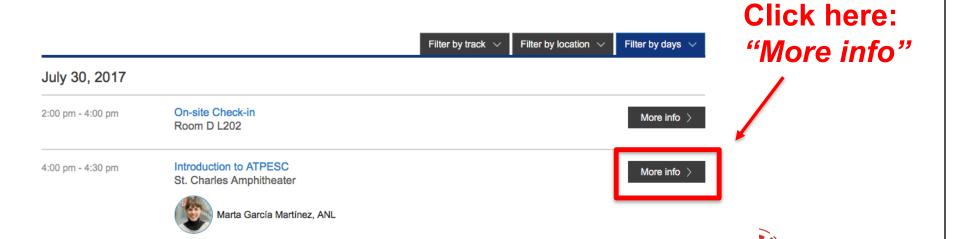


Go to the ATPESC agenda



HOME ABOUT ATPESC ATPESC NEWS AGENDA 2017 PARTICIPANTS 2017 LECTURERS 2017 VENUE 2017 PAST PROGRAMS

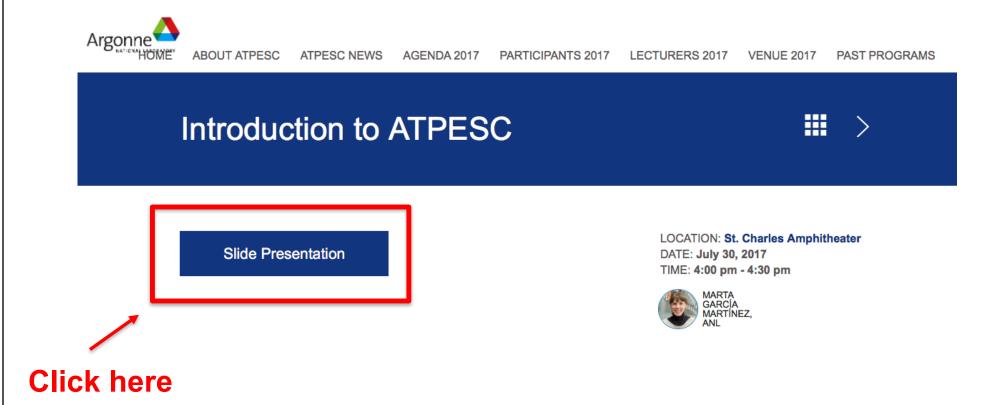
AGENDA 2017 PAST PROGRAMS





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Go to the ATPESC agenda







ATPESC Pocket Folder

Contains information about:

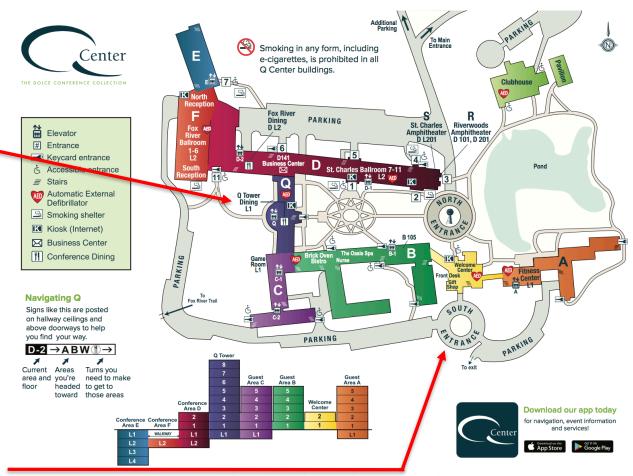
- Maps of the Q Center (Conference Area, Guest, Aerobic Mile Chart)
- Restaurants around Q Center
- Some flyers of the systems that you will be using
- WIFI connection
- ANL tour flyers
- Argonne Now magazine
- Information about tokens and what to do in case of problems (provided during check-in)





General Logistics

- Breakfast & Lunch in theQ 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)









EXASCALE COMPUTING PROJECT

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)



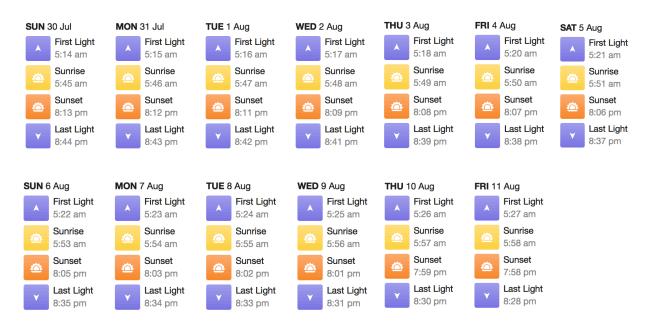




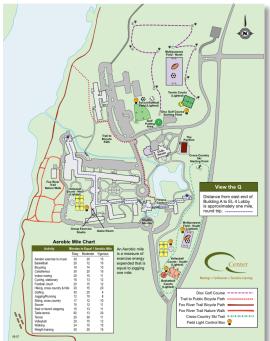
Mens sana in corpore sano

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



Aerobic Mile Chart @ Q Center



 $\textbf{Source}: \underline{\text{http://sunrisesunset.willyweather.com/il/kane-county/st-charles.html}}$





Meals



MONDAY	TUESDAY	WEDNESDAY	THURSDAY	FRIDAY	SATURDAY	SUNDAY
Scrambled Eggs	Scrambled Eggs	Scrambled Eggs	Scrambled Eggs	Scrambled Eggs	Scrambled Eggs	Scrambled Eggs
Chef's Potatoes	hashbrowns	Chef's Potatoes	hashbrowns	Chef's Potatoes	Chef's Potatoes	Chef's Potatoes
Hickory Smoked Bacon	Pork Sausage	Hickory Smoked Bacon	Chicken Apple Sausage	Hickory Smoked Bacon	Sausage Links	Hickory Smoked Bacon
Blueberry Scones	Cheese Blintz	Belgian Waffles	blueberry Pancakes	apple Crepes	Belgian Waffles	Pancakes

All Breakfast MOD's Include Bakery Breads and Pastries, Milk, Dry Cereal, Yogurt, Toast & Seasonal Fruit.
Freshly Brewed Regular and Decaffeinated Coffees, Specialty Teas, Milk, Assorted Juices, and Assorted Sodas.



		THURSDAY	FRIDAY	SA	TURDAY	SUNDAY				
nicken Noodle Soup	Vegetable Beef	Tomato Basil Soup	oup Cheddar Broccoli		ef's Choice	Chef's Choice				
ossed Salad du Jour with 2 Dressings	Tossed Salad du Jour with 2 Dressings	Tossed Salad du Jour with 2 Dressings	Tossed Salad du Jour with 2 Dressings			Tossed Salad du Jour with 2 Dressings				
seera Stuffed Shell P	Roasted Portobello		_							
neese starred strent	MONDAY	TUESDAY	WEDNESE	WEDNESDAY		THURSDAY		RIDAY	SATURDAY	SUNDAY
Spicy tilapia with Pineapple Relish	toamto Dill and White Bean				Toamto Basil Soup		Swiss Chicken Noodle		Chef's Choice	Chef's Choice
Chicken Enchilada	Tossed Salad du Jour with 2 Dressings	Tossed Salad du Jou with 2 Dressings				Tossed Salad du Jour with 2 Dressings		Tossed Salad du Jour with 2 Dressings	Tossed Salad du Jour with 2 Dressings	
Fiesta Lime Rice	Polenta with a Vegetabl Ragout	cheese Enchilasa	Baked Penne Flo	orentine Vegetable Lasagna		Lasagna	Vegetable Frittata		Chef's Choice	Chef's Choice
eet Poached Carror	Glaze over Homney			Red Curried Cod with Pineapple/Mango Salsa		Mustard Crusted Salmon			Chef's Choice	Chef's Choice
ple Chocolate Cook	Puree		псаррісутан					ac sauce		
Macadamia Nut Cookie Triple Criscolate Couk		Tacos al Pasor	Orange BBQ Por	Orange BBQ Pork Chops		Chicken Shawarama		en Vesuvio	Chef's Choice	Chef's Choice
		Saffron Cous Cous wi Peas	th Roasted Yukon I	Roasted Yukon Potatoes		basmati Rice		ans and rice	Chef's Choice	Chef's Choice
[Sauteed Zucchini and Yellow Squash	Mexican Corn	Chimimichurri Ca	ulifower	Steamed A	sparagus			Chef's Choice	Chef's Choice
[White Chocolate Macadamia Nut Cookie	Triple Chocolate Cook	ie Peanut Butter	Cookie	Heath Crun	ch Cookie	Chocolat	e Chip Cookie	Assorted Cookies	Assorted Cookies
S P	with 2 Dressings wese Stuffed Shell spicy tilapia with spicy ti	with 2 Dressings with 2 Dressings sees Stuffed Sheh picy stapia with trenspoke Rainh Rainh trenspoke Rainh Rainh trenspoke Rainh trenspoke t	with 2 Dressings with 2 Dressings with 2 Dressings Sees Suffed Shell Bostered Emmobility Supplies of Shell Bostered Emmobility Supplies Shell Bostered Emmobility Supplies Shell Bostered Emmobility Supplies Shell Bostered Emmobility Supplies Shell	with 2 Dressings with 2	with 2 Dressings Supplication of the 2 Dressings with 2 Dressings Supplication of the 2 Dressings with 2 Dressings wit	with 2 Dressings Sould Date of Dill and Vinite Bean Chicken Tortilla Sould Date of Dill and Vinite Bean Chicken Tortilla Sould Date of Dill and Vinite Dressings with 2 Dressings Sould Date of Dill and Vinite Dressings with 2 Dr	with 2 Dressings with 2	with 2 Dressings with 2	with 2 Dressings with 2	with 2 Dessirgs with 2 Dessirg

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.



	Monday	Tuesday	Wednesday	Thursday	Friday	Saturday	Sunday
Serving Times	All Day						
lavored Waters	Cucumber / Kiwi	Watermelon	Orange	Pineapple / Basil	Lemon / Mint	Orange	Pineapple
Serving Times	7:30a-9:30a						
	Homemade granola*	Homemade granola					
Serving Times	7:30a-11a						
	Trail Mix*						
Sliced Fresh Fruit	Watermelon	Honey Dew	Cantaloupe	Watermelon	Honey Dew	Cantaloupe	Honey Dew
Additional Sweet Item	Donut Holes						
Morning Pastry	Gluten Free Mango Swirl Cake**	Mini Blueberry Muffins*	Gluten Free Marble Coffeecake*	Mini Chocolate Chip Muffin*	Lemon Scone*	Chef's Choice	Chef's Choice
Baked Breakfast Bread	Chocolate Breakfast Bread*	Pineapple Coconut Bread*	Cherry Vanilla Bread*	Raspberry Orange Bread* Banana Bread*		Banana Bread*	Cherry Vanilla Bread
Baked Breakfast Item	Croissants with jam, whipped butter	Fresh baked biscuits w/ jam, whipped butter	Croissants with jam, whipped butter	Fresh baked biscuits w/ jam, whipped butter	Croissants with jam, whipped butter	Fresh baked biscuits w/ jam, whipped butter	Croissants with jam whipped butter
Power bars	Peanut Butter and Oatmeal Energy Bar*	Chocolate Energy Bar*	Lemon Energy Bar*	Cashew & Apricot Bar*	Brownie Energy Bar*	Chef's Choice Energy Bar	Chef's Choice Energy Bar
Serving Times	9:30a - 11a						
Protein Item	Hard cooked eggs with hot sauce and salt & pepper	Hard cooked eggs with hot sauce and salt & pepper	Hard cooked eggs with hot sauce and salt & pepper	Hard cooked eggs with hot sauce and salt & pepper	Hard cooked eggs with hot sauce and salt & pepper	Hard cooked eggs with hot sauce and salt & pepper	Hard cooked eggs with hot sauce and salt & pepper
Serving Times	2p-5p	2p-5p	2p-5p	2p-5p	2p-5p	2p -5p	2p-5p
	Agave Roasted Chickpeas***	Garlic & Parm Roasted Chickpeas	Lime, Cumin & Cilantro Roasted Chickpeas	Honey Cinnamon Roasted Chickpeas	Sweet & Spicy Roasted Chickpeas w/ Rosemary	Garlic & Parm Roasted Chickpeas	Honey Cinnamon Roasted Chickpeas
Witchen Station	Hummus	Ranch Dip Cucumber	Pico de Gallo	Peanut Butter	Nutella spread	Ranch Dip Cucumber	Peanut Butter
	Carrots	Celery	Corn Tortilla Chips	Celery Sticks	Cinnamon Sugar Crisps	Celery	Celery Sticks
Serving Times	2p - 5p						
	Ice Cream Novelties						
Baked Cookle	Chocolate Chip Cookie*	Sugar Cookie*	Chewy Chocolate Cookie*	M & M Cookie*	Oatmeal Raisin Cookie*	Sugar Cookie*	M & M Cookie*
Baked Treats	Orange Texas Sheet Cake*	Chocoalte Shortbread*	Rice Krispy Treats	Brownies*	Cherry Bar*	Rice Krispy Treats	Shortbread*







Participant Introductions

Today (7/30) after the Dinner Talk

INSTRUCTIONS FOR PARTICIPANT INTRODUCTION SLIDE

Profile Picture Attach a recent photo (optional) First, Last Name > Example: John Doe Name Ph.D. Student, Postdoc, Engineer, etc. Position Department, Institution | > Example: Civil Engineering, Univ. of Houston, TX (USA)

University Logo and/or current Institutional Logo (if you have one)

Scientific Field Research Interests Personal Interests

Pull field from the list below Name three (or more) Name two (or more)

Section 3

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

List of Scientific Fields

- Biological Sciences, Bioinfomatics · Chemistry, Physical Biological Sciences, Biophysics
 Biological Sciences, Medical Science
- Biological Sciences, Neuroscience Biological Sciences, Proteomics
 Biological Sciences, Systems Biology
- · Chemistry, General
- Chemistry, Biochemistry
 Chemistry, Catalytic
- · Chemistry, Combustion

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- Chemistry, Inorganic
- Chemistry, Environmental
 Chemistry, Geochemistry
- Chemistry, Quantum Chemistry Computer Science Earth Science, Environmental Sciences Earth Science, Agricultural Sciences Earth Science, Climate Research
- Earth Science, Geological Sciences Economics Engineering, Material Response
- Engineering, Heat Transfer Engineering, Aerodynamics Engineering, Fluid-Structure Interaction
- · Engineering, Fluids and Turbulence
- Fusion Energy, Inertial Fusion
- Nuclear Energy Physics, Accelerator Physics Physics, Astrophysics Physics, Atomic/Molecular Physics Physics, Condensed Matter Physics Argonne Argonatory

Fusion Energy, Magnetic Fusion
 Materials Science, Condensed Matter and Materials Physics

Materials Science, Materials Discovery

Design, and Synthesis Materials Science, Nanoelectronics

Materials Science, Nanomechanics

Materials Science, Nanophotonics Materials Science, Nanoscience





Physics, High Energy Physics Physics, Nuclear Physics

Physics, Space Physics Physics, Particle Physics Physics, Plasma Physics

Physics, Plasma Physics
 Energy Technologies, Bloenergy
 Energy Technologies, Wind Energy
 Energy Technologies, Solar Energy
 Energy Technologies, Solar Energy
 Energy Technologies, Energy Stroage
 Energy Technologies, Energy Stroage
 Energy Technologies, Energy Grid

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Section 1

John Doe

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





Section 3

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)

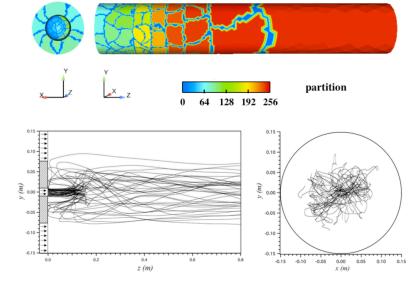
Scientific Field | Computational Fluid Dynamics

Research Interests

- **Two-phase Flows**
- **High-Performance Computing**
- **Partitioning Algorithms**

Personal Interests

- Reading
- Traveling



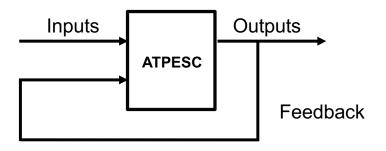




Feedback

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

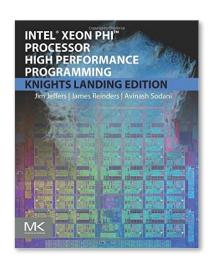




Raffle: 12 nights ... 12 Books & 12 lanyards with flash drives

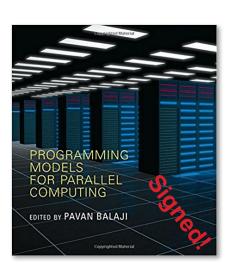
Special thanks to:

10x



James Reinders & Intel

2x



Pavan Balaji
(Track Lead and Lecturer)



12x

Ashley Barker
(ECP 1.2.4. Developer Training and Productivity Lead)





(Lecturer)

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

- 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

