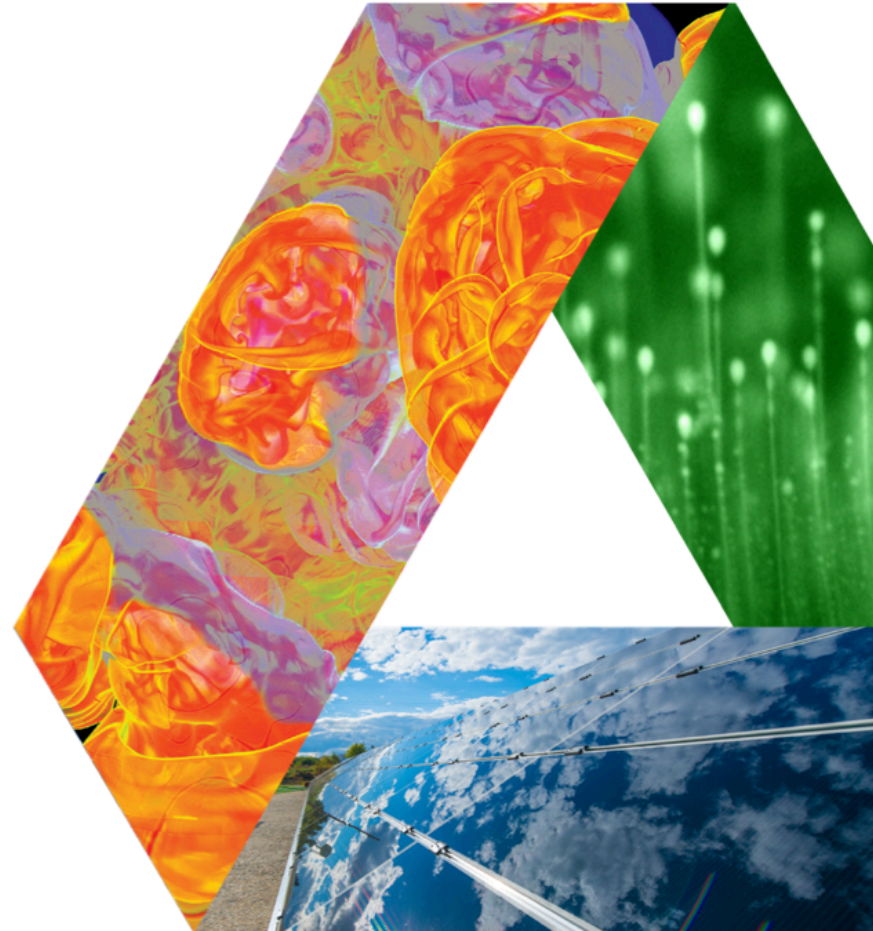




Argonne Training Program on Extreme-Scale Computing (ATPESC)

Introduction to ATPESC

**Paul Messina, Argonne National
Laboratory**
Former ATPESC Program Director

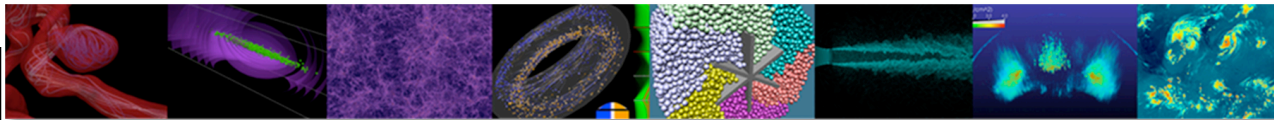


Outline

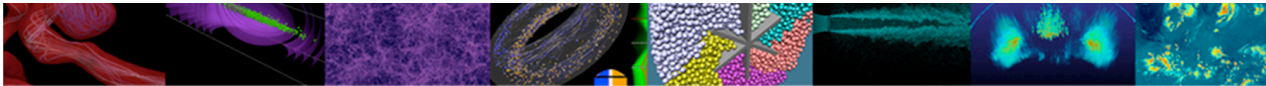
- Welcome
- Thank you
- A few words about Argonne National Laboratory
- Motivation of the ATPESC
- Logistics and reminders



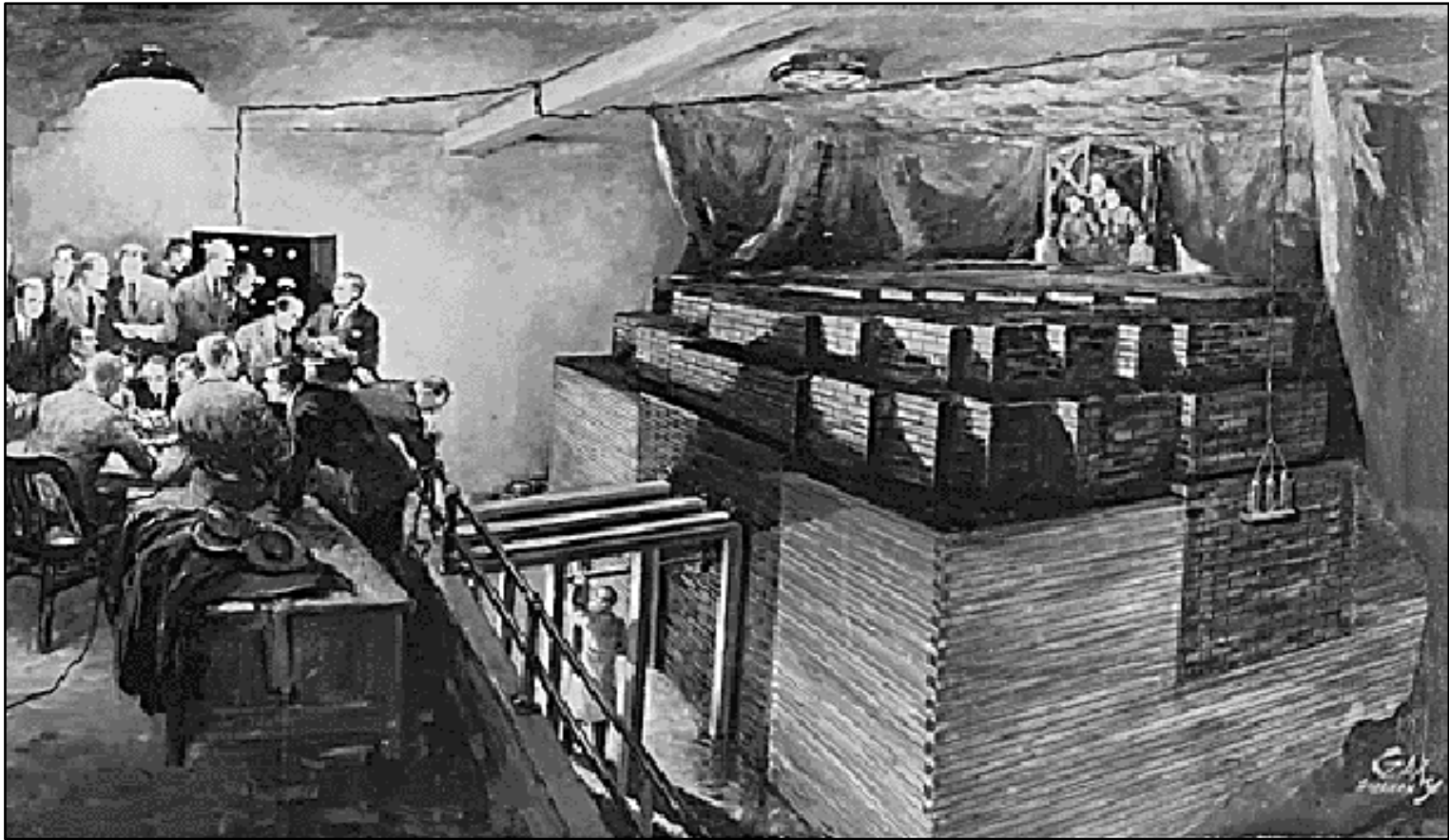
Argonne Training Program on Extreme-Scale Computing



Argonne – a part of DOE National Laboratory System



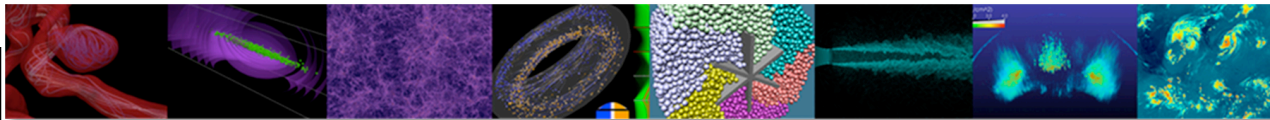
The origin of Argonne National Laboratory: CP-1 under the stands of Stagg field of U. Chicago



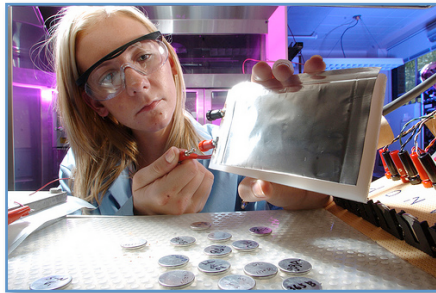
Chicago Pile-1 was the world's first artificial nuclear reactor. The first man-made self-sustaining nuclear chain reaction was initiated on December 2, 1942



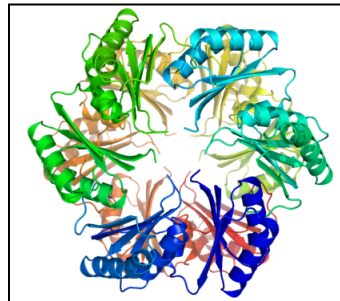
Argonne Training Program on Extreme-Scale Computing



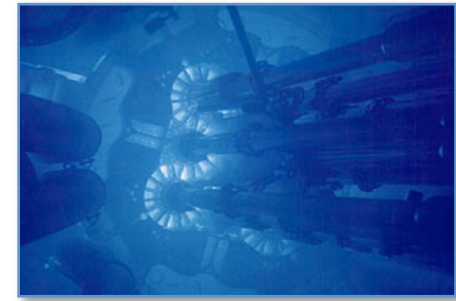
Argonne's mission: To provide science-based solutions to pressing global challenges



Energy Science



Environmental Sustainability

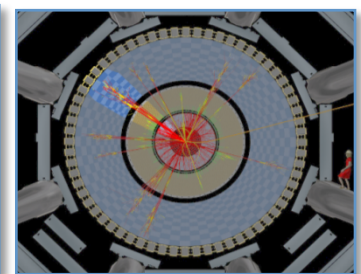
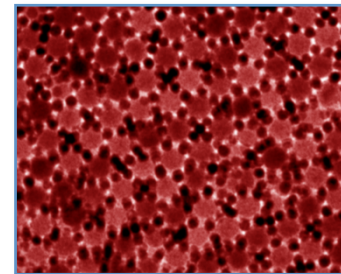


Nuclear and National Security

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



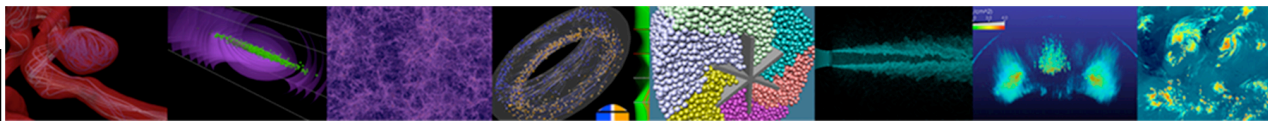
Major User Facilities



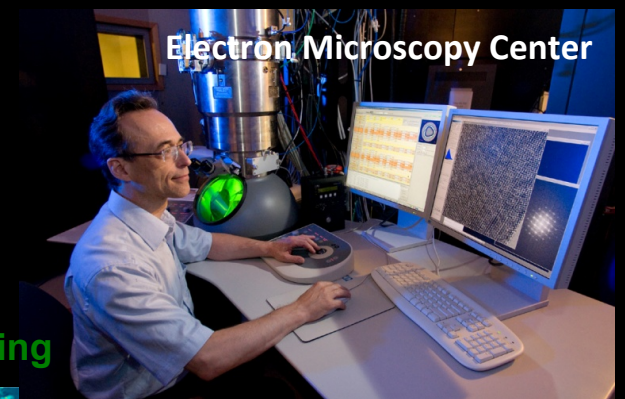
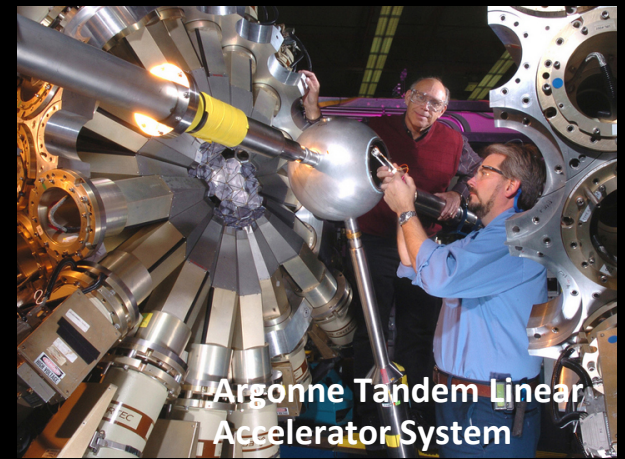
Science and Technology Programs



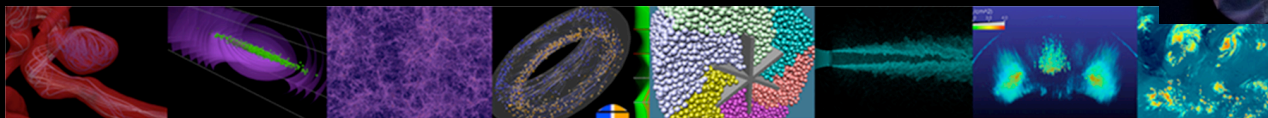
Argonne Training Program on Extreme-Scale Computing



Major Scientific User Facilities at Argonne



Argonne Training Program on Extreme-Scale Computing



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

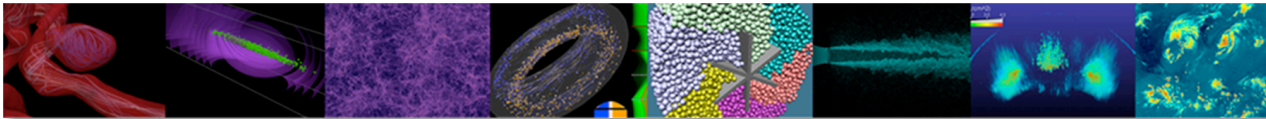


"Moll" Flanders, Director
Jeffrey Chu, Chief Engineer

- **AVIDAC: based on prototype at the Institute for Advanced Study in Princeton**
- **Margaret Butler wrote AVIDAC's interpretive floating-point arithmetic system**
 - Memory access time: 15 microsec
 - Addition: 10 microsec
 - Multiplication: 1 millisc
- **AVIDAC press release: 100,000 times as fast as a trained "Computer" using a desk calculator**



Argonne Training Program on Extreme-Scale Computing



Early work on computer architecture

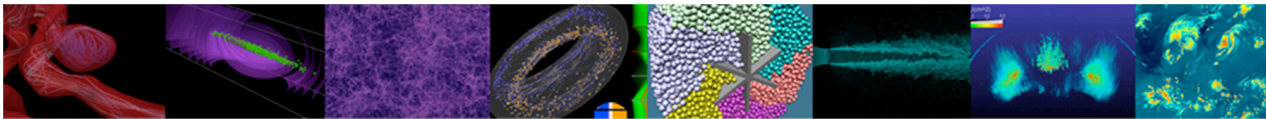


Margaret Butler helped assemble the ORACLE computer with ORNL Engineer Rudolph Klein

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 Training Program on Extreme-Scale Computing



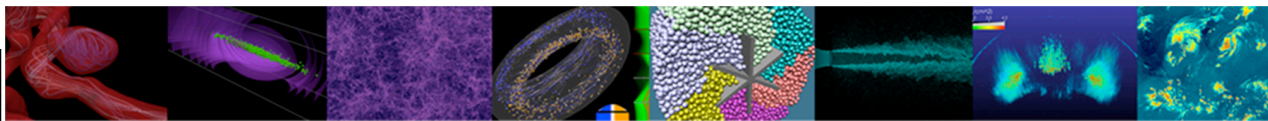
Argonne National Laboratory Tour

Saturday, August 6 1:00 – 6:00 pm

- **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 Nuclear Energy Exhibit (building 208)** 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.
- **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 systems
- **Round-trip from Pheasant Run to Argonne by bus**
(if you signed in)



Argonne Training Program on Extreme-Scale Computing



Aerial view of Argonne National Laboratory

Advanced Photon Source (APS)

Nuclear Energy Exhibit

Argonne Information Center

Theory and Computing
Sciences (TCS) Building

Northgate

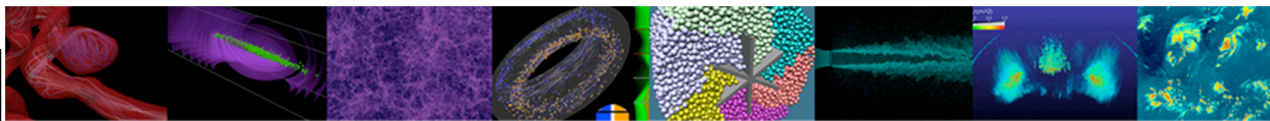


Motivation for the ATPESC

- **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**



Argonne Training Program on Extreme-Scale Computing



The DOE Leadership Computing Facility

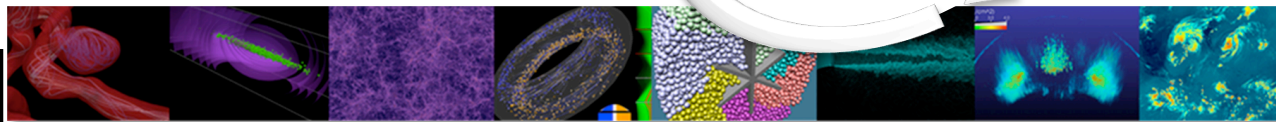
- Collaborative, multi-lab, DOE/SC initiative ranked top national priority in *Facilities for the Future of Science: A Twenty-Year Outlook*.
- Mission: Provide the computational and data science resources required to solve the most important scientific & engineering problems in the world.
- Highly competitive user allocation program (INCITE, ALCC).
- Projects receive 100x more hours than at other generally available centers.
- LCF centers partner with users to enable science & engineering breakthroughs (Liaisons, Catalysts).



Argonne Training Program



Computing

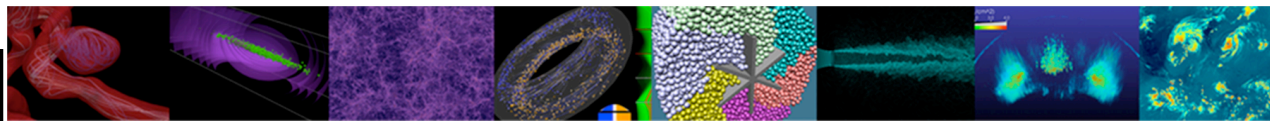


Leadership Computing Facility System

	Argonne LCF	Oak Ridge LCF
System	IBM Blue Gene/Q	Cray XK7
Name	Mira	Titan
Compute nodes	49,152	18,688
Node architecture	PowerPC, 16 cores	AMD Opteron, 16 cores NVIDIA K20x (Kepler) GPU
Processing Units	786,432 Cores	299,008 x86 Cores + 18,688 GPUs
Memory per node, (gigabytes)	16	32 + 6
Peak performance, (petaflops)	10	27



Argonne Training Program on Extreme-Scale Computing



ALCF Systems

▪ ***Mira* – BG/Q**

- 49,152 nodes / 786,432 cores
- 786 TB of memory
- Peak flop rate: 10 PetaFLOPs
- 3,145,728 hardware threads

▪ ***Vesta (T&D)* - BG/Q**

- 2,048 nodes / 32,768 cores

▪ ***Cetus (debug)* - BG/Q**

- 4,096 nodes / 65,536 cores

▪ ***Cooley (visualization & data analysis)* – Cray CS**

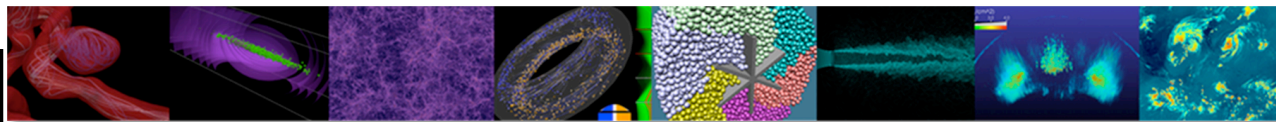
- 126 nodes, each with
 - Two Intel Xeon E5-2620 Haswell 2.4 GHz 6-core processors
 - NVIDIA Tesla K80 graphics processing unit with 24 GB memory
 - 384 GB DDR4 memory

• **Storage**

- Scratch: 28.8 PB raw capacity, 240 GB/s bw (GPFS)
- Home: 1.8 PB raw capacity, 45 GB/s bw (GPFS)

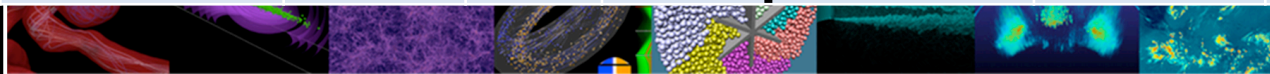


Argonne Training Program on Extreme-Scale Computing



DOE ASCR Computing Upgrades At a Glance

System attributes	NERSC Now	OLCF Now	ALCF Now	NERSC Upgrade	OLCF Upgrade	ALCF Upgrades	
Name Planned Installation	Edison	TITAN	MIRA	Cori 2016	Summit 2017-2018	Theta 2016	Aurora 2018-2019
System peak (PF)	2.6	27	10	> 30	150	>8.5	180
Peak Power (MW)	2	9	4.8	< 3.7	10	1.7	13
Total system memory	357 TB	710TB	768TB	~1 PB DDR4 + High Bandwidth Memory (HBM) +1.5PB persistent memory	> 1.74 PB DDR4 + HBM + 2.8 PB persistent memory	>480 TB DDR4 + High Bandwidth Memory (HBM)	> 7 PB High Bandwidth On- Package Memory Local Memory and Persistent Memory
Node performance (TF)	0.460	1.452	0.204	> 3	> 40	> 3	> 17 times Mira
Node processors	Intel Ivy Bridge	AMD Opteron Nvidia Kepler	64-bit PowerPC A2	Intel Knights Landing many core CPUs Intel Haswell CPU in data partition	Multiple IBM Power9 CPUs & multiple Nvidia Volta GPUs	Intel Knights Landing Xeon Phi many core CPUs	Knights Hill Xeon Phi many core CPUs
System size (nodes)	5,600 nodes	18,688 nodes	49,152	9,300 nodes 1,900 nodes in data partition	~3,500 nodes	>2,500 nodes	>50,000 nodes
System Interconnect	Aries	Gemini	5D Torus	Aries	Dual Rail EDR- IB	Aries	2 nd Generation Intel Omni-Path Architecture
File System	7.6 PB 168 GB/s, Lustre®	32 PB 1 TB/s, Lustre®	26 PB 300 GB/s GPFS™	28 PB 744 GB/s Lustre®	120 PB 1 TB/s GPFS™	10PB, 210 GB/s Lustre initial	150 PB 1 TB/s Lustre®

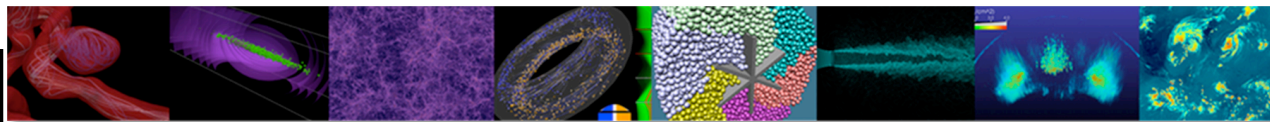


Systems available during ATPESC

- **ALCF** – Mira, Cetus, Vesta and Cooley
 - **Project name:** **ATPESC2016**
 - **Note:** use your ALCF Username. The password will be your old/newly established PIN + token code displayed on the token.
 - **Support:** on-site ALCF staff available to help you!! and support@alcf.anl.gov
 - **Reservations:** 6:30 pm – 9:30 pm for hands-on on Mira (8 racks), Cetus (1 rack) and Vesta (512 nodes). Specific reservations on Cooley for some tracks. Please check the details of the reservations directly on each machine (**command:** showres)



Argonne Training Program on Extreme-Scale Computing



Systems available during ATPESC

▪ OLCF – Titan

- **Project name:** **TRN001**
- **Note:** use the Username printed on the envelope the token came in. It will be csep01, csep02, etc. The password will be your newly established PIN + token code displayed on the token.
- **Support:** help@olcf.anl.gov or call 1-865-241-6536
- See documents in your Argonne Folder for additional information

▪ NERSC – Edison and Cori

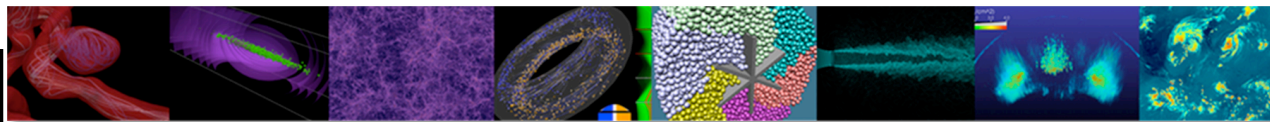
- **Project name:** **ntrain**
- **Note:** *ssh machine_name.nersc.gov*
- **Support:** accounts@nersc.gov or call 1-800-666-3772

Edison: <http://www.nersc.gov/users/computational-systems/edison/running-jobs/>

Cori: <http://www.nersc.gov/users/computational-systems/cori/running-jobs/>



Argonne Training Program on Extreme-Scale Computing



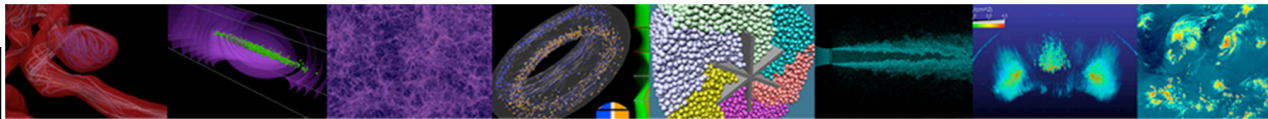
Aurora



- Homogeneous
- Many-core
 - Four hardware threads/core
- Self-hosted
- Water cooled
- 18x *Mira* speed
- 2.7x *Mira* peak power consumption
- Similar node count to *Mira*
- Intel Architecture (x86-64) Compatibility



Argonne Training Program on Extreme-Scale Computing



Theta



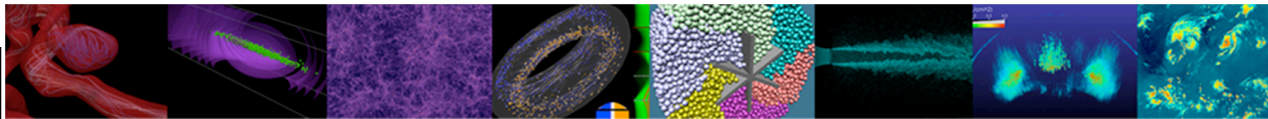
Theta has arrived!



- Homogeneous
- Many-core
 - Four hardware threads/core
- Self-hosted
- Water cooled
- 0.85x *Mira* speed
- 0.35x *Mira* peak power consumption
- >2500 nodes
- Intel Architecture (x86-64) Compatibility



Argonne Training Program on Extreme-Scale Computing

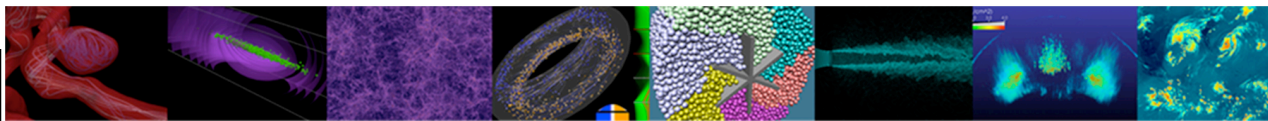


Curriculum tracks/sessions and their leaders

- **Hardware Architectures** – Pete Beckman
- **Programming Models and Languages** – Rusty Lusk and Rajeev Thakur
- **Numerical Algorithms and FASTMath** – Lois McInnes, Lori Diachin and Mark Miller
- **Community Codes and Software Engineering** – Katherine Riley and Anshu Dubey
- **Toolkits and Frameworks** – Ray Loy and Scott Parker
- **Visualization and Data Analysis** – Mike Papka and Joe Insley
- **Data-intensive Computing and I/O** – Rob Latham and Phil Carns



Argonne Training Program on Extreme-Scale Computing



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
- **Nine dinner talks**



Paul Messina,
ANL



Seth Darling,
ANL



Gabrielle Allen,
NCSA



Douglas Kothe,
ORNL



Frank Cappello,
ANL



Jamie Dixon,
Hammerhead
Productions, Inc.



Paul Fischer,
UIUC



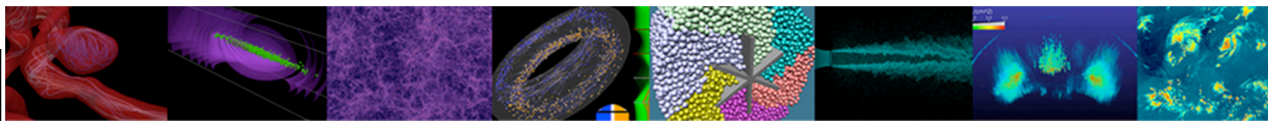
Mike Heroux,
SNL



Subramanian
Sankaranarayanan,
ANL



Argonne Training Program on Extreme-Scale Computing

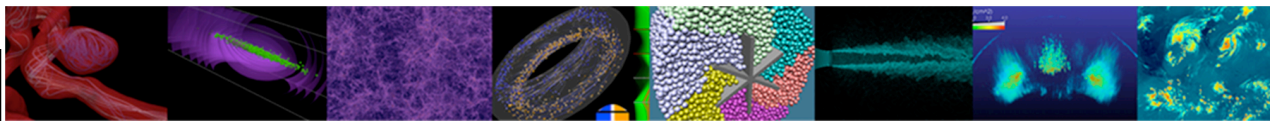


Yes, the ATPESC is an intensive program

- 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 a.m. starting time, dinner at 5:30 p.m. right after the end of the afternoon lectures, evening sessions
- Slides will be posted online as soon as available
 - **Show how to find the slides on the agenda**



Argonne Training Program on Extreme-Scale Computing



Go to the ATPESC Agenda

[HOME](#) [ABOUT ATPESC](#) [AGENDA 2016](#) [LECTURERS 2016](#) [PARTICIPANTS 2016](#) [VENUE](#) [PAST PROGRAMS](#)

AGENDA 2016

Click here:
“More info”

Filter by track ▾

Filter by days ▾

August 1, 2016

7:30 am - 8:30 am

Continental Breakfast

[More info](#)

Dining Room

8:30 am - 8:45 am

Introduction to Session: Hardware Architectures/Overview

[More info](#)

Lecturer Room



Pete Beckman, ANL

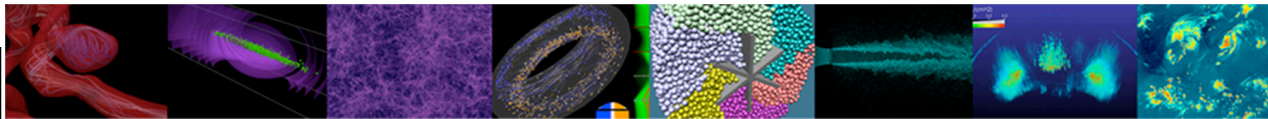
8:45 am - 9:30 am

Presentation: Extreme-Scale Interconnects and Impacts for Applications

[More info](#)



Argonne Training Program on Extreme-Scale Computing



Then click on: “Slide Presentation”

[HOME](#) [ABOUT ATPESC](#) [AGENDA 2016](#) [LECTURERS 2016](#) [PARTICIPANTS 2016](#) [VENUE](#) [PAST PROGRAMS](#)

Introduction to Session: Hardware Architectures/Overview

Click here



Hardware Architectures

Slide Presentation

Location: **Lecturer Room**

Date: **August 1, 2016**

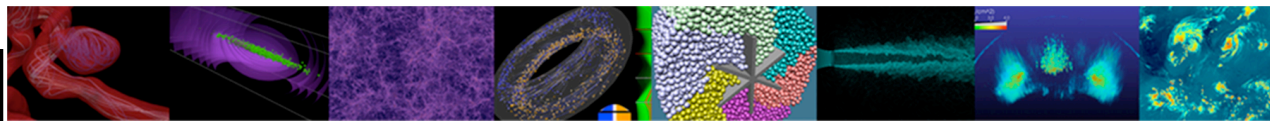
Time: **8:30 am - 8:45 am**



Pete Beckman, ANL



Argonne Training Program on Extreme-Scale Computing



Thank you

- DOE Office of Advanced Scientific Computing Research (ASCR)



U.S. DEPARTMENT OF

ENERGY

Office of
Science

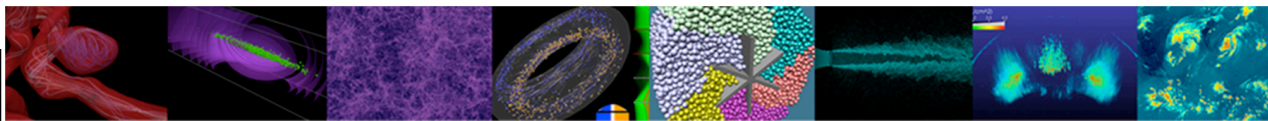
- Exascale Computing Project



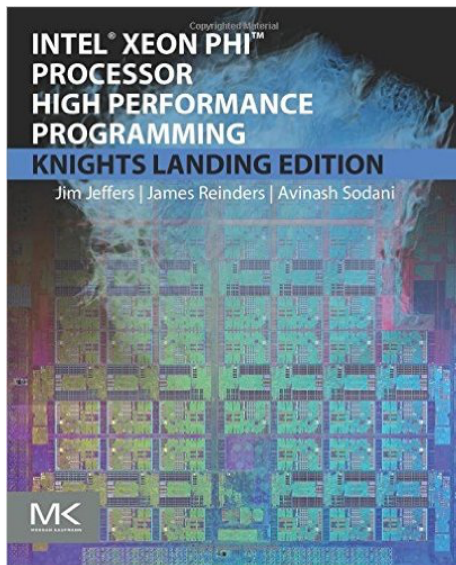
EXASCALE COMPUTING PROJECT



Argonne Training Program on Extreme-Scale Computing



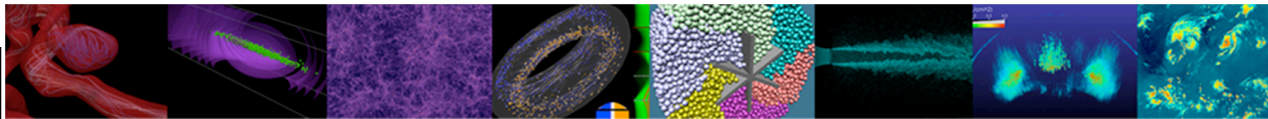
Special thanks to: **James Reinders and Intel**



For the individual copy of their book
to all ATPESC 2016 Participants!



Argonne Training Program on Extreme-Scale Computing

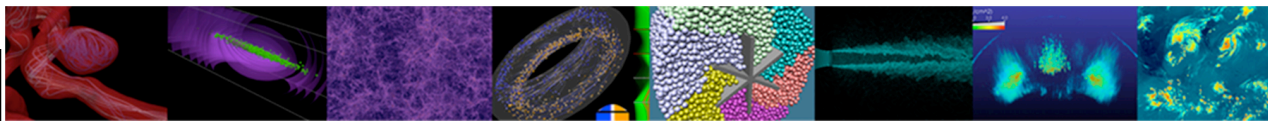


Acknowledgments

- 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



Argonne Training Program on Extreme-Scale Computing



ATPESC Folder

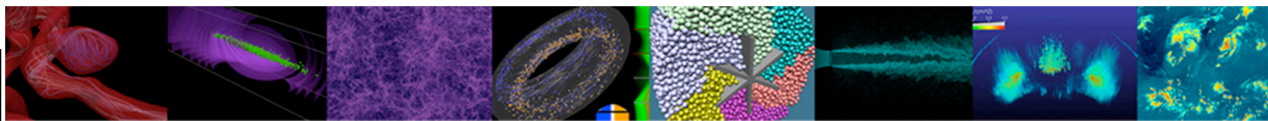
Contains information about:

- A map of the Pheasant Run Resort with directions
- The agenda of the event
- The Network and Password for WIFI connection
- Some flyers of the systems that you will be using.
- Information about tokens and what to do in case of problems.

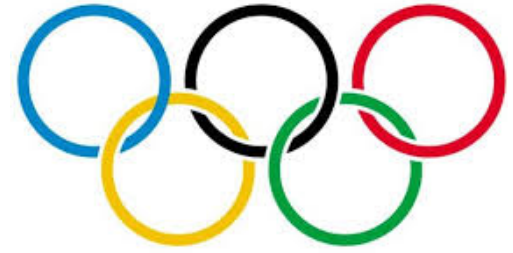
Help us improve it! please tell us what else would be useful to include!



Argonne Training Program on Extreme-Scale Computing



ATPESC Games

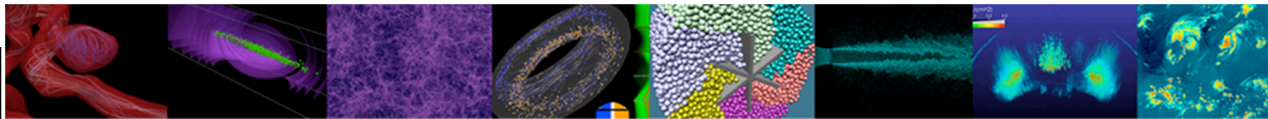


Some fun during the Olympics year!

- Some simple games related to the tracks to look at HPC from a different angle
- **1st, 2nd and 3rd prizes:** a book, an ATPESC cap and an Argonne flash drive, respectively
- Send your reply to:
support@ExtremeComputingTraining.anl.gov
- If your response is correct, you will be eligible for the prize raffle of each game



Argonne Training Program on Extreme-Scale Computing

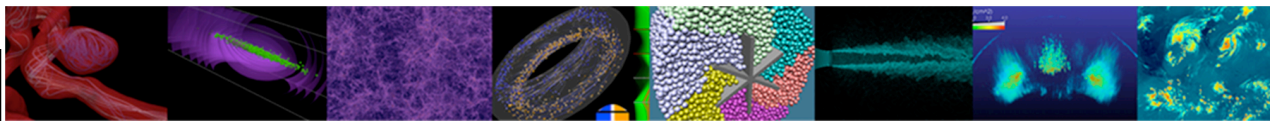


Surveys

- **Help us improve the training program**
 - Track evaluations
 - Overall program evaluation
 - Conversations or emails to any of us
- **Please fill out the online evaluation surveys on each track and the overall program**
 - At the end of each track, you will receive an email from chel@alcf.anl.gov with a link to that track's evaluation
 - Please respond by the morning of the next day. Your input is very valuable!
 - Chel Lancaster is coordinating the evaluations and will be available to answer questions or help



Argonne Training Program on Extreme-Scale Computing

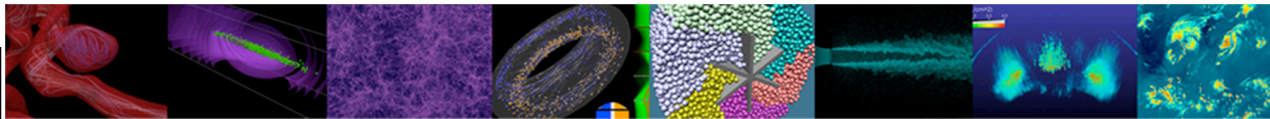


Suggestions from previous years' surveys

- Tour of Argonne
- Pre-event exercise
- More hands-on exercises during lectures
- Participant introductions



Argonne Training Program on Extreme-Scale Computing

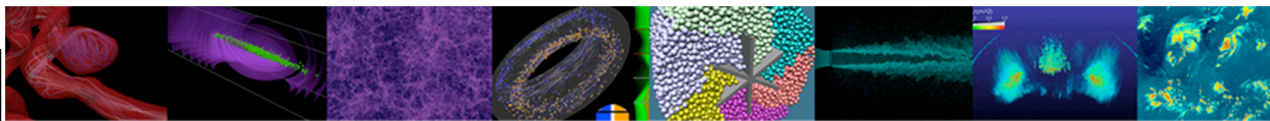


Participant Introductions

- One minute (60 seconds) to say something about yourself so that participants will know who has common interests.
- Your introduction slide will be displayed during the first week of the program with the rest of the slides in several boards at the end of the Lecture Room.
- The slides will be ordered alphabetically and the chairman of the session will call you to the podium to present it.



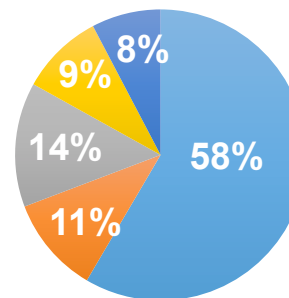
Argonne Training Program on Extreme-Scale Computing



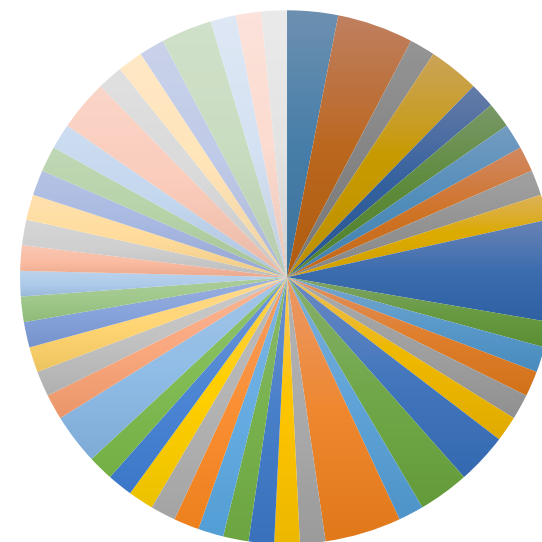
Statistics ATPESC 2016

- Aramco Services Company
- Barcelona Supercomputing Center
- California Institute of Technology
- CERFACS
- Colorado School of Mines
- Cornell University
- George Washington University
- Heat and Mass Transfer Technological Center
- Iowa State University
- LBNL-NERSC
- Middle Tennessee State University
- National Cancer Institute
- Oak Ridge National Laboratory
- Polytechnic University of Catalonia
- RWTH Aachen University
- Stanford University
- U.S. Army Research Laboratory
- University of Arizona
- University of Colorado
- University of Kansas
- University of Massachusetts Dartmouth
- University of Rochester
- University of Tennessee
- University of Utah
- University of Wyoming
- Virginia Tech

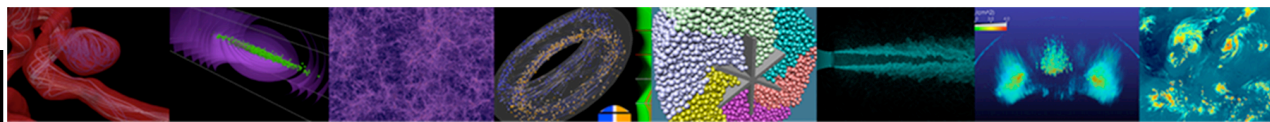
- Argonne National Laboratory
- Brown University
- CEA
- Clarkson University
- Convergent Science, Inc
- Geo Imaging Solutions / UFRJ
- Harvard Medical School
- IBM India Research Laboratory
- Lawrence Livermore National Laboratory
- Los Alamos National Laboratory
- Mississippi State University
- NERSC
- Oklahoma State University
- Princeton Plasma Physics Laboratory
- Southern Methodist University
- The University of Texas at Austin
- University of Alabama in Huntsville
- University of Berkeley
- University of Illinois at Urbana-Champaign
- University of Leeds
- University of Minnesota & Sandia National Labs
- University of Southern California
- University of Udine
- University of Wisconsin - Madison
- UTC SimCenter



- **Ph.D. student**
- **Postdoc academia**
- **Postdoc Nat'l Labs**
- **Industry**
- **Other**



Argonne Training Program on Extreme-Scale Computing



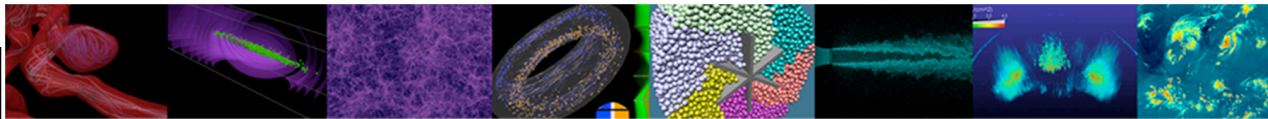
ATPESC Social Media

Like Us on Facebook

- Share your experience on the **ATPESC Facebook page**
 - Share your photos
 - Share something that you didn't know before
 - Share how this will help your career
 - Share how wonderful the lecturers are
 - Share interesting articles on Computational Science using HPC
 - **facebook.com/atpesc**
- The page is open to the public and allows anyone to add postings, photos, and videos. All posts will be moderated by ALCF staff.



Argonne Training Program on Extreme-Scale Computing

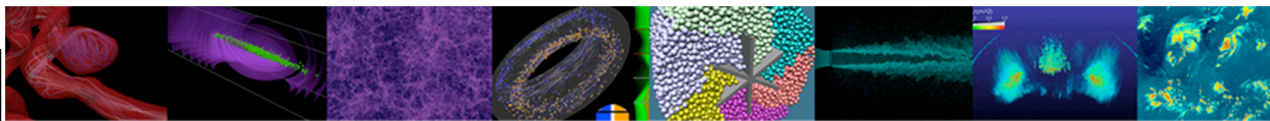


General Logistics

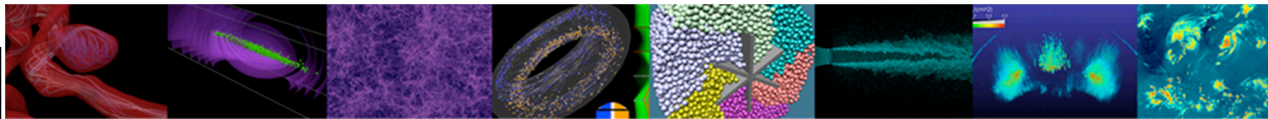
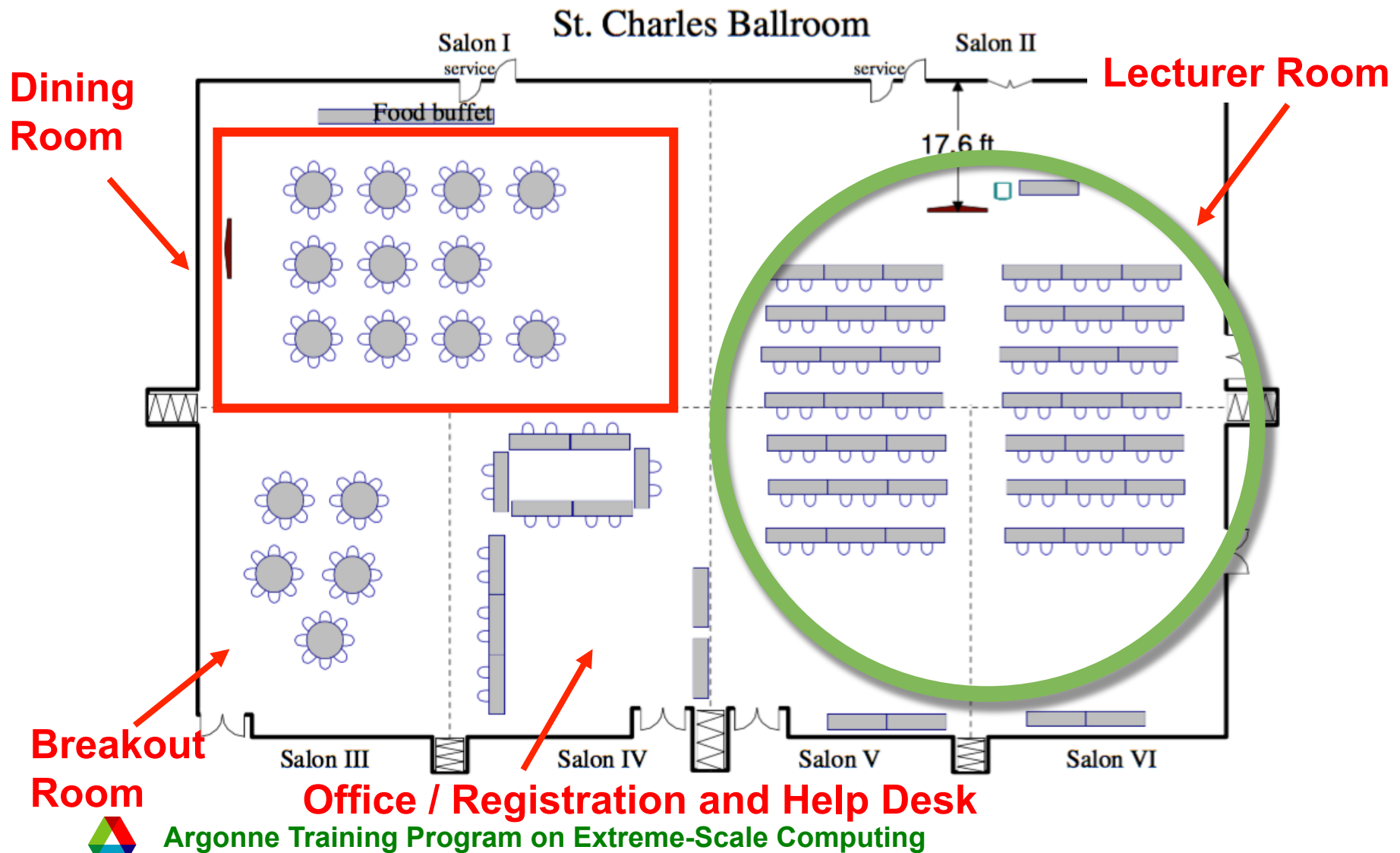
- All lectures and hands-on sessions in the Lecturer Room in the St. Charles ballroom
- All meals in the Dining room
 - Lunch and dinner presentations will be in this room
- A Break-out room is available for your discussions
- Wi-fi Network and password included in your Argonne Folder
- [atpesc2016-attendees](#) and [atpesc2016-discuss](#) lists in place to share information by the instructors and to discuss with them.
- A photographer will stop by one day to take a group photo. We will let you know in advance.
- An Argonne video team will conduct brief video-camera interviews with some participants during the lunch break on Tuesday, Aug. 9



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Lodging at Pheasant Run – Rooms



Whom to ask for help on-site

- **Local arrangements**

- Ashley Boyle
- Ginny Doyle
- Sue Gregurich

Or by email to your ATPESC Contact Person

- **Surveys**

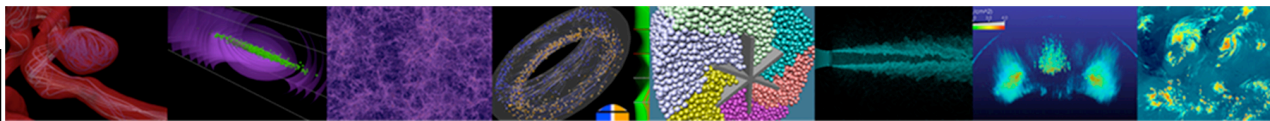
- Chel Lancaster

- **Computing issues**

- Ray Loy
- **User Services:** Robert Scott / Avanthi Mantrala / Liza Booker
- **Operations:** Ben Lenard / Tommie Jackson / John 'Skip' Reddy



Argonne Training Program on Extreme-Scale Computing



Summary

- Thanks in advance to all of you for taking two weeks of your summer to participate in this program

Questions?



Argonne Training Program on Extreme-Scale Computing

