

Introduction to the Argonne Training Program on Extreme-Scale Computing (ATPESC)

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Argonne National Laboratory

Outline

- **Welcome**
- **A few words about Argonne National Laboratory**
- **Motivation of the ATPESC**
- **The curriculum**
- **Logistics**



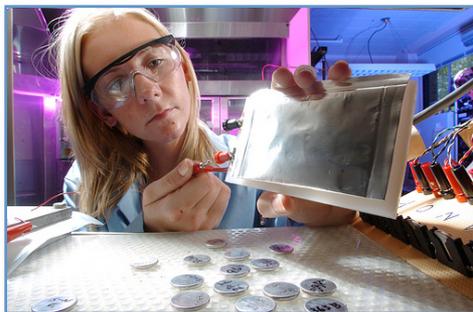
Argonne – a part of DOE National Laboratory System



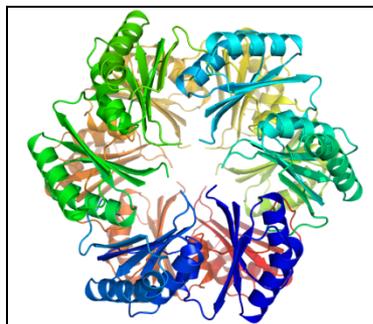
- Office of Science laboratory
- National Nuclear Security Administration laboratory
- Office of Fossil Energy laboratory
- Office of Energy Efficiency and Renewable Energy laboratory
- Office of Nuclear Energy, Science and Technology laboratory
- Office of Environmental Management laboratory



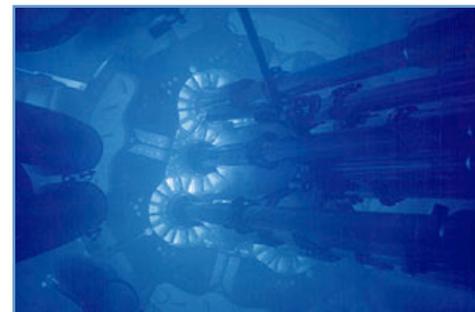
Argonne's mission: To provide science-based solutions to pressing global challenges



Energy
Science



Environmental
Sustainability



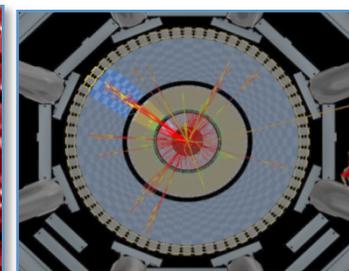
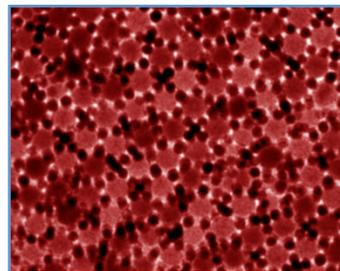
Nuclear and
National Security

Use-Inspired Science and Engineering...

...Discovery and Transformational Science and Engineering



Major User Facilities



Science and Technology Programs



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**

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.

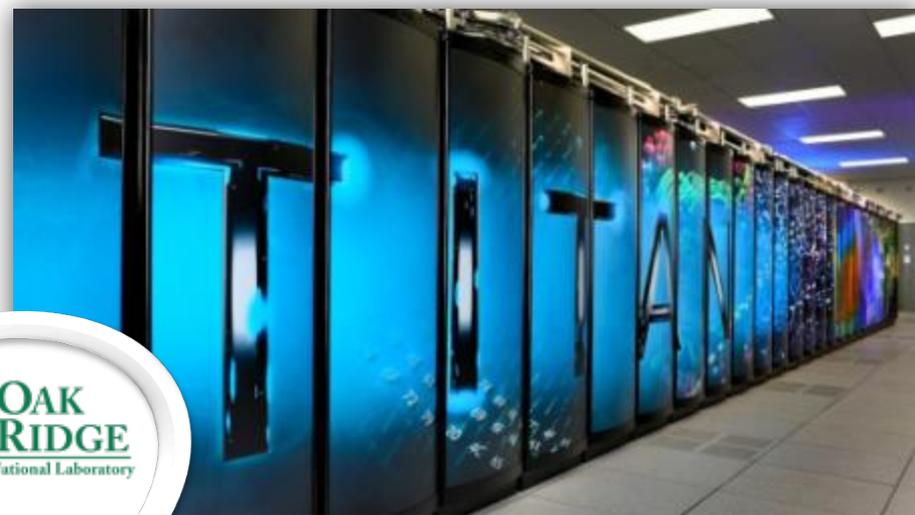
Motivation for the ATPESC

- **Today's most powerful supercomputers have complex hardware architectures and software environments**
 - and even greater complexity is on the horizon from 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**



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).



Leadership Computing Facility systems

	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



10 Petaflops Blue Bene/Q - Mira

■ *Mira* – BG/Q system

- 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 system

- 2,048 nodes / 32,768 cores
- 32 TB of memory
- Peak flop rate: 420 TF

■ *Tukey* – Nvidia system

- 100 nodes / 1600 x86 cores/ 200 M2070 GPUs
- 6.4 TB x86 memory / 1.2 TB GPU memory
- Peak flop rate: 220 TF

■ Storage

- Scratch: 28.8 PB raw capacity, 240 GB/s bw (GPFS)
- Home: 1.8 PB raw capacity, 45 GB/s bw (GPFS)
- Storage upgrade planned in 2015



Mira's Ecosystem

Mira

48 racks/768K cores
10 PF



I/O

Cetus

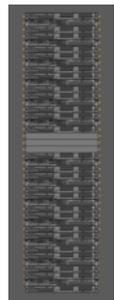
4 racks/64K cores
832 TF



I/O

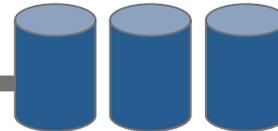
Tukey (Viz)

100 nodes/1600 cores
200 NVIDIA GPUs
220 TF

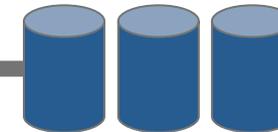


Infiniband Switch Complex

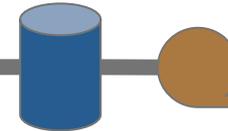
(16) DDN 12Ke couplets – Scratch – 28 PB (raw), 240 GB/s



(3) DDN 12Ke couplets – Home – 1.8 PB (raw), 45 GB/s



Tape Library – 16 PB (raw)



(1) DDN 12Ke – 600 TB (raw), 15 GB/s

IB Switch



Networks – 100Gb
(via ESnet, internet2
UltraScienceNet,)

Vesta (Dev)

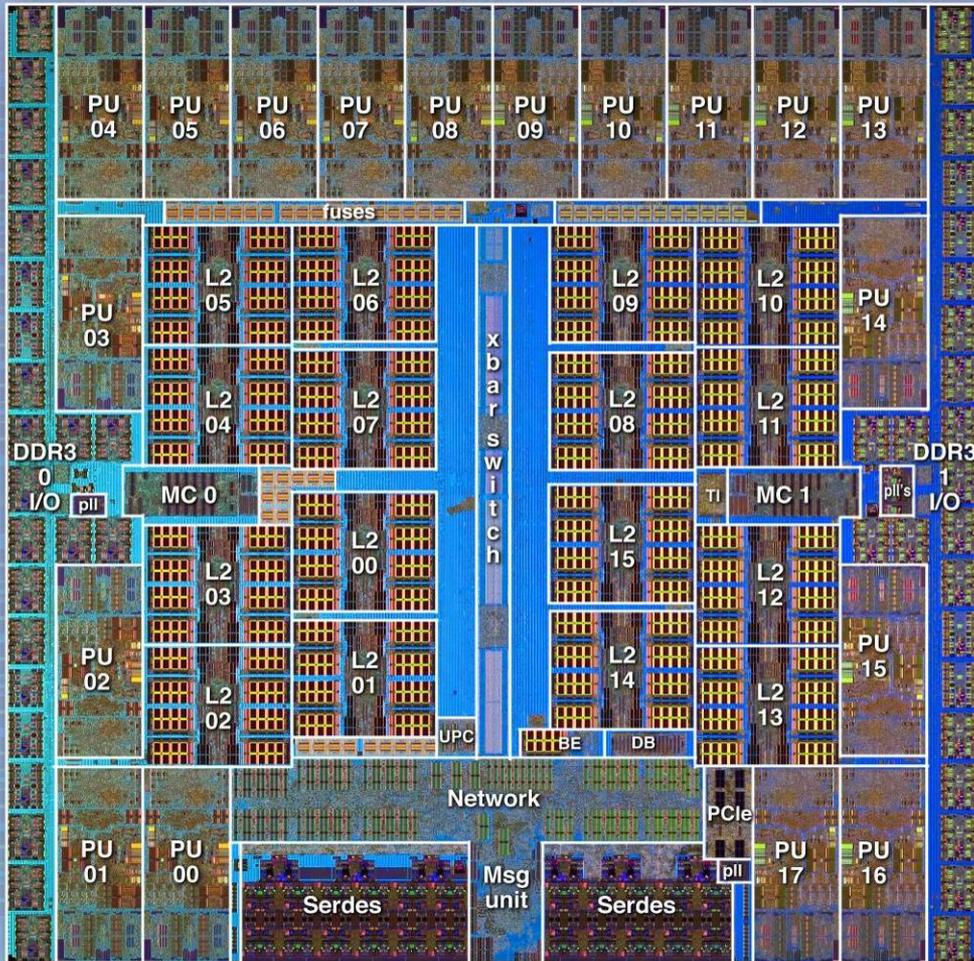
2 racks/16K cores
416 TF



I/O

BlueGene/Q Compute Chip

System-on-a-Chip design : integrates processors, memory and networking logic into a single chip



- **360 mm² Cu-45 technology (SOI)**
 - ~ 1.47 B transistors
- **16 user + 1 service processors**
 - plus 1 redundant processor
 - all processors are symmetric
 - L1 I/D cache = 16kB/16kB
 - L1 prefetch engines
- **Crossbar switch**
 - Connects cores via L1P to L2 slices
- **Central shared L2 cache**
 - 32 MB eDRAM
 - 16 slices
- **Dual memory controller**
 - 16 GB external DDR3 memory
 - 42.6 GB/s
- **Chip-to-chip networking**
 - Router logic integrated into BQC chip
 - DMA, remote put/get, collective operations
 - 11 network ports
- **External IO**
 - PCIe Gen2 interface

CORAL Joint NNSA & SC Leadership Computing Acquisition Project

Objective - Procure 3 leadership computers to be sited at ANL, ORNL, and LLNL in CY17-18

Current DOE Leadership Computers

Titan (ORNL)



Sequoia (LLNL)



Mira (ANL)



Leadership Computers run the most demanding DOE mission applications and advance HPC technologies to assure continued US/DOE leadership

Approach

Competitive process - one RFP (issued by LLNL) leading to 3 computer procurement contracts

For risk reduction and to meet a broad set of requirements,
2 architectural paths will be selected

Each lab manages and negotiates its own computer procurement contract, and may exercise options to meet their specific needs

Understanding that **long procurement lead time may impact architectural characteristics and designs** of procured computers



ALCF-3 Project Description

- **Acquire and deploy a 75 – 200PF Leadership Computing system for the Department of Energy's Office of Science Leadership Computing Facility**
 - Procure the compute and storage system
 - Prepare site for system power and cooling needs
 - Select and prepare Early Science Program code teams for the system
 - Prepare for general users
 - Deploy, test, and accept the system integrated in the ALCF environment



NERSC's Cori* System: on the path to exascale

**Gerty Cori was the first American woman to receive the Nobel Prize in Science*

- **Gerty Cori was the first American woman to receive the Nobel Prize in Science (bio-chemistry)**
- **Cori will be a Cray XC system whose nodes are based on Intel's next-generation Intel® Xeon Phi™ processor -- code-named "Knights Landing"**
 - on-package high bandwidth memory
 - 3 teraFLOPS of double-precision peak performance per single socket node
- **The Knights Landing processor will have 72cores, each with multiple hardware threads**
- **Cori is cheduled for delivery in mid-2016**



Curriculum tracks/sessions and their leaders

- **Architectures – Pete Beckman**
- **Programming models and languages – Rusty Lusk and Rajeev Thakur**
- **Numerical algorithms and software -- Lois McInnes and Lori Diachin**
- **Toolkits and frameworks – Kalyan Kumaran and Scott Parker**
- **Visualization and data analysis – Mike Papka and Joe Insley**
- **Data-intensive computing and I/O – Rob Ross and Rob Latham**
- **Community codes and software engineering – Katherine Riley and Anshu Dubey**



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**



Yes, the ATPESC is an intense 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**



Thank you, DOE Office of Advanced Scientific Computing Research (ASCR)

- **This training program was made possible by funding from the Research Division of the Advanced Scientific Computing Research program of the Department of Energy's (DOE) Office of Science**
- **The funding is for three years**
 - The training program will be offered again in 2015
 - And we may ask for funding for 2016ff
- **Help us improve the training program**
 - Track evaluations
 - Overall program evaluation
 - Conversations or emails to any of us



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
 - Respond by the morning of the next day to be eligible for the prize raffle
 - Chel Lancaster is coordinating the evaluations and will be available to answer questions or help



Suggestions from last year's surveys adopted this year

- **Suggested reading before the ATPESC**
- **Participant introductions**
 - Details during dinner



Paul Messina

- **Position: Ph.D. student, applied mathematics, University of Cincinnati**
- **Research background:**
 - Solution of elliptic PDEs with singularities
 - Mathematical software
- **Research interests:**
 - Parallel computer architectures
- **Personal interests**
 - Sailing
- **Personal background:**
 - Had lived in four countries by the time I was 14 years old



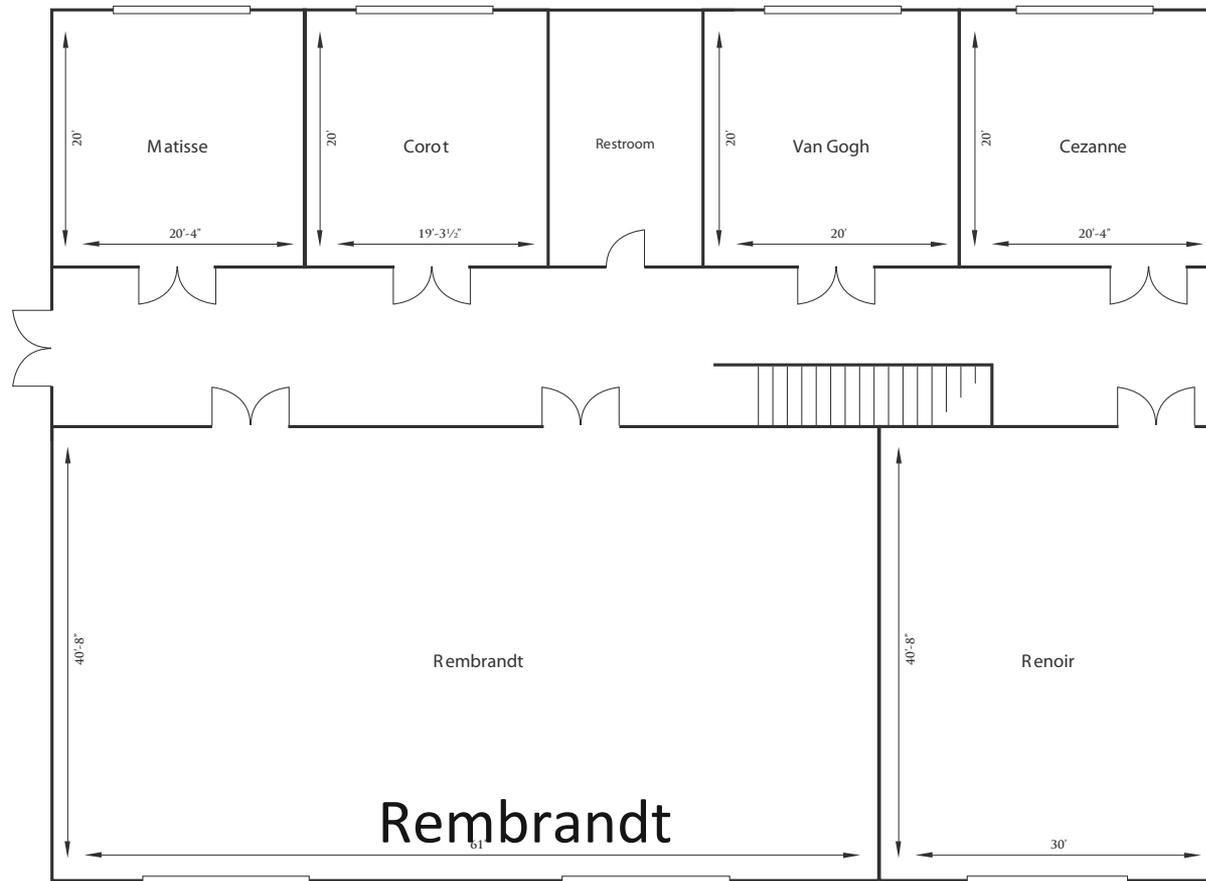
Logistics

- All lectures and hands-on sessions in Rembrandt room
- All meals in Utrillo room on ground floor
 - Lunch and dinner presentations will be in this room
- Other rooms in ground floor might be used as needed
- Wi-fi SSID in this building is **Argonne**
- Password is **argonne14**



Diagram of Meeting Rooms: Second Floor

GALLERY HALL (SECOND FLOOR)



SCALE IN FEET
0 5 10



Diagram of meeting rooms: Ground floor

GALLERY HALL (FIRST FLOOR)



Whom to ask for help

- Local arrangements
 - Cheryl Zidel
 - Ashley Boyle
 - Ginny Doyle
 - (sometimes they will be in Picasso room on ground floor)
- Surveys
 - Chel Lancaster
- Computing issues
 - Ray Loy
 - Robert Scott
 - Adam Scovel
 - Others TBD



Summary

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

