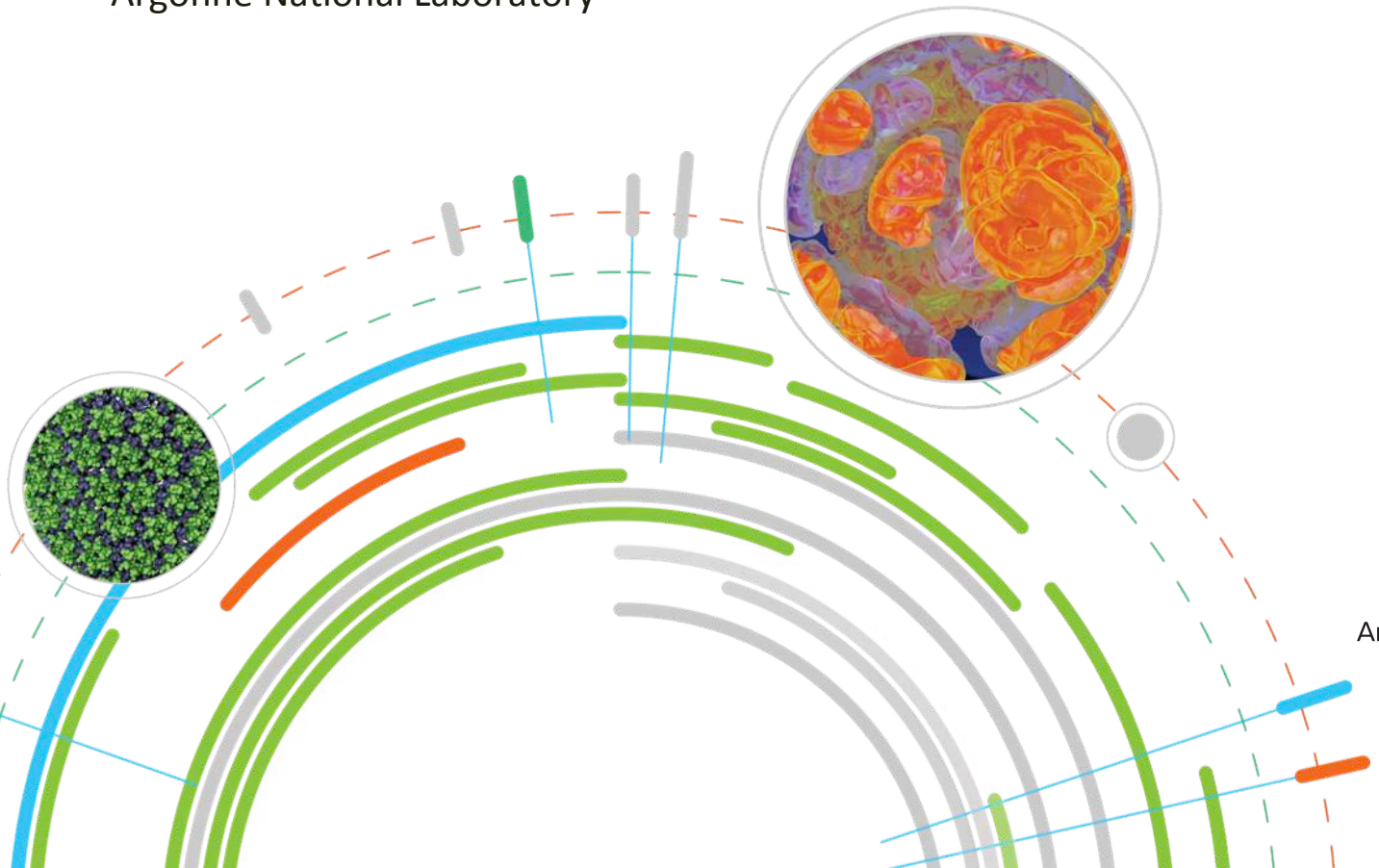
Overview of Allocations Programs at ALCF

Nichols A. Romero
Assistant Computational Scientist
Argonne Leadership Computing Facility
Argonne National Laboratory



Argonne **Leadership Computing** Facility

Argonne NATIONAL LABORATORY

What is the Leadership Computing Facility?

- Two centers/two architectures to address diverse and growing computational needs of the scientific community.
- Highly competitive user allocation programs (INCITE, ALCC).
- Projects receive computational resources typically 10-100x greater than generally available.
- LCF centers partner with users to enable science & engineering breakthroughs.

ALCF Computing Resources

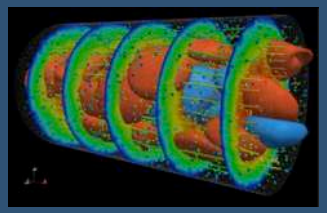
- *Mira* – Blue Gene/Q system
  - 49,152 nodes / 786,432 cores
  - 786 TB of memory
  - Peak flop rate: 10 petaFLOP/s
  - 3,145,728 hardware threads
- *Cetus (debug)* - Blue Gene/Q system
  - 4,096 nodes / 65,536 cores
  - 64 TB of memory
  - Peak flop rate: 840 teraFLOP/s
- *Vesta (T&D)* - Blue Gene/Q system
  - 2,048 nodes / 32,768 cores
  - 32 TB of memory
  - Peak flop rate: 420 teraFLOP/s
- *Tukey* – Nvidia system
  - 96 nodes, each with two 2-GHz, 8-core x86 cores/ 200 NVIDIA Tesla GPUs
  - 6.4 TB x86 memory / 1.2 TB GPU memory
  - Peak flop rate: 220 teraFLOP/s
- Storage
  - Scratch: 28.8 PB raw capacity, 240 GB/s BW (GPFS)
  - Home: 1.8 PB raw capacity, 45 GB/s BW (GPFS)

Allocation Programs at the LCFs

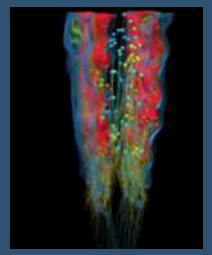
	60% INCITE		30% ALCC		10% Director's Discretionary	
Mission	High-risk, high-payoff science that requires LCF-scale resources		High-risk, high-payoff science aligned with DOE mission		Strategic LCF goals	
Call	1x/year – (Closes June)		1x/year – (Closes February)		Rolling	
Duration	1-3 years, yearly renewal		1 year		3m,6m,1 year	
Typical Size	30 - 40 projects	50M - 500M core-hours/yr.	5 - 10 projects	10M – 300+M core-hours/yr.	100s of projects	.5M – 10M core-hours
Review Process	Scientific Peer-Review	Computational Readiness	Scientific Peer-Review	Computational Readiness	Strategic impact and feasibility	
Managed By	INCITE management committee (ALCF & OLCF)		DOE Office of Science		LCF management	
Readiness	**High**		**Medium to High**		**Low to High**	
Availability	Open to all scientific researchers and organizations 5 billion core hours available in 2014 ***Capability > 131,072 cores (16.7% of Mira)***					

Diversity of INCITE science

Simulating a flow of healthy (red) and diseased (blue) blood cells with a Dissipative Particle Dynamics method.
- George Karniadakis, Brown University

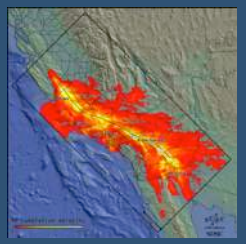


Provide new insights into the dynamics of turbulent combustion processes in internal-combustion engines.
-Jacqueline Chen and Joseph Oefelein, Sandia National Laboratories

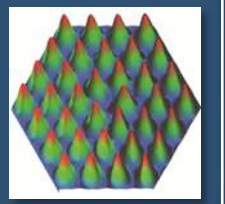


Demonstration of high-fidelity capture of airfoil boundary layer, an example of how this modeling capability can transform product development.
- Umesh Paliath, GE Global Research

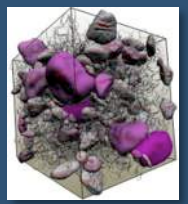
Calculating an improved probabilistic seismic hazard forecast for California.
- Thomas Jordan, University of Southern California



Modeling charge carriers in metals and semiconductors to understand the nature of these ubiquitous electronic devices.
- Richard Needs, University of Cambridge, UK



High-fidelity simulation of complex suspension flow for practical rheometry.
- William George, National Institute of Standards and Technology



Other INCITE research topics

- Glimpse into dark matter
- Supernovae ignition
- Protein structure
- Creation of biofuels
- Replicating enzyme functions
- Global climate
- Regional earthquakes
- Carbon sequestration
- Turbulent flow
- Propulsor systems
- Membrane channels
- Protein folding
- Chemical catalyst design
- Combustion
- Algorithm development
- Nano-devices
- Batteries
- Solar cells
- Reactor design
- Nuclear structure

Sample of Community Codes

-- and ALCF Application Expertise

Application	Field
FLASH	Astrophysics
MILC,CPS	Lattice QCD
Nek5000	CFD
Rosetta	Protein structure
ANGFMC	Nuclear structure
Qbox	Electronic structure
LAMMPS	Molecular dynamics
NWChem	Quantum chemistry
GAMESS	Quantum chemistry
MADNESS	Electronic structure
NAMD	Molecular dynamics
QMCPACK	Electronic structure
MPQC	Quantum chemistry
UNIC	Neutron Transport

Application	Field
AVBP	Combustion
GTC	Fusion
IRHMD	Plasma Physics
CPMD	Electronic Structure
CCSM3	Climate
HOMME	Climate
WRF	Climate
Gromacs	Molecular dynamics
Enzo	Astrophysics
Falkon	Computer science/HTC
GPAW	Electronic structure
OpenFOAM	CFD
FHI-AIMS	Electronic structure
HACC	Astrophysics

How to Apply for Director's Discretionary Account?

Director's Discretionary (DD) P...

www.alcf.anl.gov/directors-discretionary-dd-program

Contact Us | Careers | Staff Directory | User Support

Argonne Leadership Computing Facility

an Office of Science user facility

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ABOUT | RESOURCES & EXPERTISE | SCIENCE AT ALCF | NEWS & EVENTS | USER SERVICES | GETTING STARTED | USER GUIDES

- how to get an allocation
- new user guide
- intrepid to mira: key changes
- incite program
- alcc program
- director's discretionary program

Getting Started

- How to Get an Allocation
- New User Guide
- Intrepid to Mira: Key Changes
- INCITE Program
- ALCC Program
- Director's Discretionary Program

Director's Discretionary (DD) Program

Start-up time through the Director's Discretionary (DD) program ers in academia, industry, and other research institutions who can demonstrate a ship-class resources. These awards are primarily a "first step" for projects working tow C allocation.

DD awards are available year 'round and are usually between th uration. Award sizes generally range from the low tens of thousands to the low millior

- **Purpose:** Start-up and preflight projects. Primarily a "first st toward an INCITE or ALCC allocation.
- **Eligibility:** Available to researchers in academia, industry, and other research institutions. DOE sponsorship is not required.
- **Review Process:** Projects must demonstrate a need for high-performance computing resources. Reviewed by ALCF.
- **Application Period:** ongoing (available year round)
- **Award Size:** Low tens of thousands to the low millions of compute hours
- **Award Duration:** 3 - 6 months, renewable

www.alcf.anl.gov/directors-discretionary-dd-program

How to Apply for Director's Discretionary Account? (cont'd)

Discretionary Allocation Requ...

www.alcf.anl.gov/getting-started/apply-for-dd

Electronic Struc... GPAW ASCR LCRC MPI Math libraries LCF ANL OS X Programming Python Plotting Programs LAMMPS QMCPACK Most Visited

Project Institution *

List any funding agencies that support this project. *

Principal Investigator (PI): Name of the project owner *

PI Email *

The project website (if any)

Description of other systems on which your code has run. (e.g., NCSA-tungsten, SDSC-BG/L, Argonne-BG/P, etc) *

Scientific Field *

- Select -

Application (code) Name [The software that you will be running] *

Requested Allocation (Number of hours of computation desired) *

How should I compute this?

Requested Quota (Vesta Default=500GiB. Mira Default=1000GiB. Request alternate amounts in GiB.) *

Requested Duration *

- 3 Months
- 6 Months

Give a detailed description of the project, its goals, and its plan. *

What should I write here?

Verification *

Mention: QMC Training Program 2014

Acknowledgements

Most of the slides borrowed from Beth Cerny, Paul Messina, Scott Parker, and Katherine Riley.

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- Additional info: www.alcf.anl.gov