

Scientific Computing Group



Judith Hill
Liaison Task Lead, Scientific Computing Group
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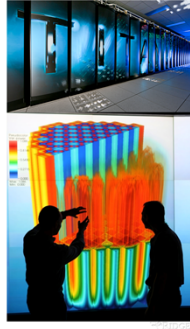
OLCF Users Meeting
July 22, 2014
Oak Ridge National Laboratory



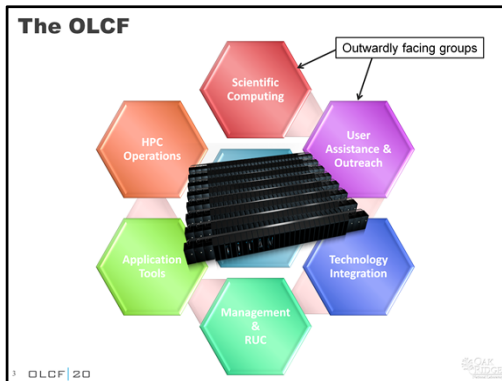
Oak Ridge Leadership Computing Facility Mission

The OLCF is a DOE Office of Science National User Facility whose mission is to enable breakthrough science by:

- Fielding the most powerful capability computers for scientific research,
- Building the required infrastructure to facilitate user access to these computers,
- Selecting a few time-sensitive problems of national importance that can take advantage of these systems,
- And partnering with these teams to deliver breakthrough science.



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User Assistance and Outreach

User Assistance & Outreach	
A. Carlyle	D. Levy ⁶
D. Daniels ¹	S. Parete-Koon
A. DiGirolamo	L. Rael
F. Foerster	S. Ray
R. French	B. Renaud
C. Fuson	D. Rose
B. Gajus ⁵	A. Simpson
J. Gary	J. Smith ²
S. Jones ³	R. Whitten ¹⁰
T. Metcalf ¹	L. Williams ¹¹
	J. Wynne ¹

- Often your first stop when you enter the OLCF
 - Account setup
 - Training events
 - Website documentation
 - Technical support
 - Communications


help@olcf.ornl.gov

Ashley Barker will speak more to this shortly

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OLCF

SciComp Group



M. Abbas ¹	J. Larkin ¹
S. Ahern ^{1,5}	Y. Li
V. Anantharaj	D. Liskov ²
M. Benini	M. Matheson
J. Carillo ²	B. Messer
J. Choi ²	H. Nam
M. Chen ²	M. Norman
J. Daniel	G. Ostroichov ⁶
E. D'Azevedo ³	N. Podhorski ³
M. Eisenbach	D. Pugmire ³
M. Fahey ^{1,5}	D. Rosenberg
J. Hill ^{1,5}	R. Sankaran
W. Joubert	A. Tharrington
S. Klasky ⁴	
S. Laosooksathit ¹	

- ~ 20 staff members
 - Some matrixed into our group
- 5 post-docs
- Expertise across a breadth of application domains
 - Common denominator is HPC

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SCAR

SciComp Group Tasks

Scientific Computing	
M. Abbas ¹	J. Larkin ¹
S. Ahern ^{1,5}	Y. Li
V. Anantharaj	D. Lisk ²
M. Benini	M. Matheson
J. Carillo ²	B. Messer
J. Chai ²	H. Nam
M. Chen ¹	M. Norman
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M. Eisenbach	D. Pugmire ³
M. Fahey ^{1,5}	D. Rosenberg
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S. Klasky ⁴	
S. Laosooksathit ¹	

- Liaison
 - Visualization
- } User-facing

- Acceptance
 - Performance
- } Internal

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Inwardly-Focused Tasks

- Acceptance Task
 - *Ensuring that new machines satisfy requirements*
 - Team across OLCF groups, including ~5 SciCompers
 - Very intensive testing schedule during acceptance period
- Performance Task
 - *Understanding how to use the machine and how the machine is used*
 - Improve performance of code
 - Study usage of machine
 - Inform next-generation architectures

Outwardly-Focused Tasks

- Liaison Task
 - *Furthering scientific accomplishments*
 - Collaborate with users to make codes run more efficiently, and produce more science
 - Advocate for users on center policies
- Visualization Task
 - *Enabling scientific discovery through visualization*
 - Creating tools for visualization
 - Developing visualizations in collaboration with users

About Liaisons

- PhD-level scientists with expertise in computation
 - Astrophysics, biology, chemistry, climate, computer science, engineering, materials science, mathematics, nuclear physics, plasma physics, etc.
 - Experienced computational scientists with one thing in common
- Liaisons matched with INCITE projects based on science, mathematical, and algorithmic expertise
 - Can't always match for science first, e.g., I am not a chemist, but I am generally familiar with their math and algorithms
- **Our motto: Whatever it takes!**

SciComp Liaisons



Valentine Ananthanaj
Climate



Mark Berni
CFD



Ed O'Azevedo
Applied Math



Markus Eisenbach
Materials



Mark Fahney
Scientific Computing



Judy Hill
Applied Math



Wayne Joubert
Scientific Computing



Ying Via Li
Materials



Bronson Messer
Astrophysics



Hai An Nam
Nuclear Physics



Matt Norman
Climate



Duane Rosenberg
Turbulence



Ramanan Sankaran
Combustion



Tjerk Straatsma
Group Leader
Chemistry



Arnold Tharrington
Biophysics



Sean Ahern
Visualization



Jamison Daniel
Visualization



Mike Matheson
Visualization

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Liaison Role

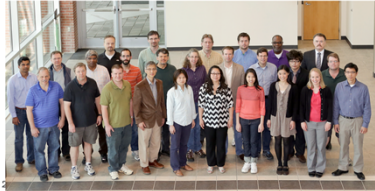
- Liaisons are collaborators whose unique expertise with leadership-level computers can enhance your experience and help you get more science done
- Levels of liaison support
 - Level 1: User support +
 - Level 2: Paratrooper – fix a specific problem in your code, O(1 month)
 - Level 3: Embedded member of code development team and science collaborator

Opportunities for Engagement

- Typical liaison activities
 - Collaborate scientifically
 - Profile code performance, providing feedback to code team
 - Code porting
 - Implement solutions to problems experienced by application scientists
 - Advocate for users regarding tools, libraries, etc.

Conclusions

- Liaisons are a valuable resource for INCITE projects
- Liaisons have unique HPC skills that projects can take advantage of
- *Whatever it takes!*



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Questions?



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