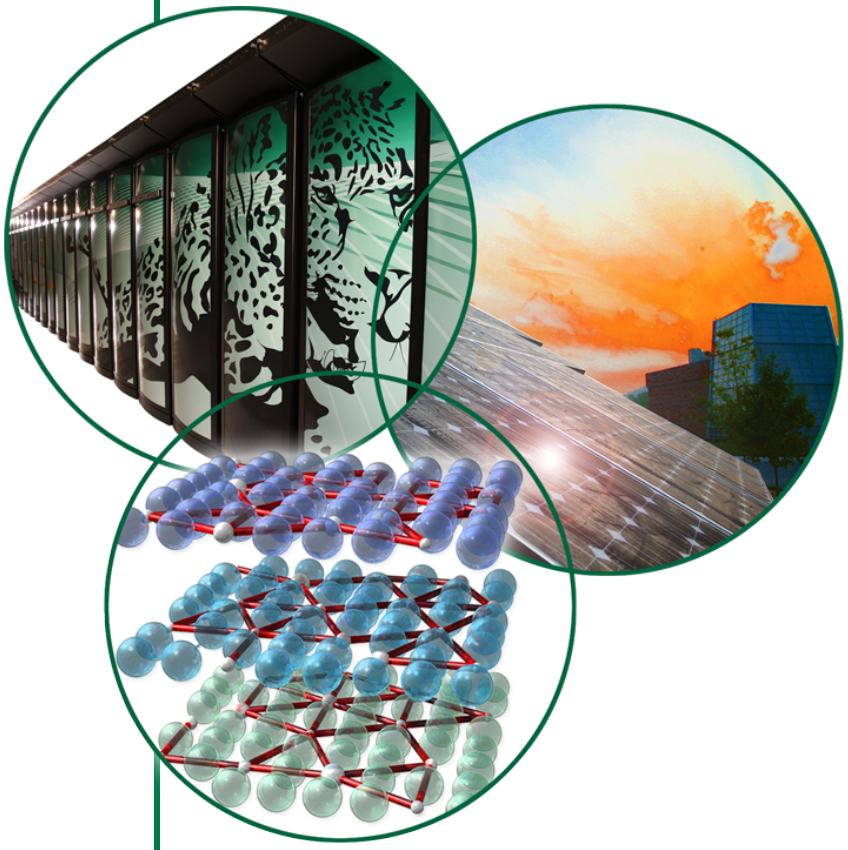
CSMD Division All Town Hall*

Barney Maccabe

July 21, 2011



*quarterly, more interactive than an “All Hands”

U.S. DEPARTMENT OF ENERGY

OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

AWARDS AND RECOGNITIONS

R&D 100 Award

MADNESS: Multiresolution ADaptive Numerical Environment for Scientific Simulations, submitted and developed by ORNL with a team led by

- **Robert Harrison and George Fann with Judith Hill, Diego Galindo and Jun Jia of the Computer Science and Mathematics Division and**
- **Rebecca Hartman-Baker of the Oak Ridge Leadership Computing Facility.**

Significant Event Achievement Award

Support to DOE in response to the Fukushima Dai-ichi damaged reactors

- **Bill Cochran,**
- **Srikanth Allu,**
- **Sreekanth Pannala,**
- **Bobby Philip, and**
- **John Turner**

DOE Mentor Awards

DOE recognizes the service of DOE's scientific staff in training the next generation of scientists. The following ORNL mentors have been *chosen by their students* to be honored through this award program.

- **Patrick Worley**
- **Ralf Deiterding**
- **John Cobb, and**
- **George Ostrouchov**

Distinguished Contributor Awards

- **Jingsong Huang**
  Leadership in multiscale computational tools for investigating and optimizing key variables of supercapacitors based on nanoporous carbon materials. This work bridges three different divisions at ORNL: NCCS, CNMS, and CSMD.

- **Ralf Deiterding**
  Development of a new method for simulating ultra-short light pulses in fiber-optical networks.

- **Pratul Agarwal**
  Received patent for fast computational methods for predicting protein structure from primary amino acid sequence.

Service Awards

Name	Years
Don Nicholson	25
Ed D'Azevedo	20
Sreekanth Pannala	10
Edo Apra	5

New Hires

Computational Engineering and Energy Sciences	
Srikanth Allu	Rahul Sampath
Clayton Webster	

Computational Earth Sciences
Moetasim Ashfaq

Future Technologies
Seyong Lee

ASCR HIGHLIGHTS

"MADNESS-Multiresolution Adaptive Numerical Environment for Scientific Simulations" – George Fann and Robert Harrison, ORNL

ASCR- Applied Mathematics Highlight

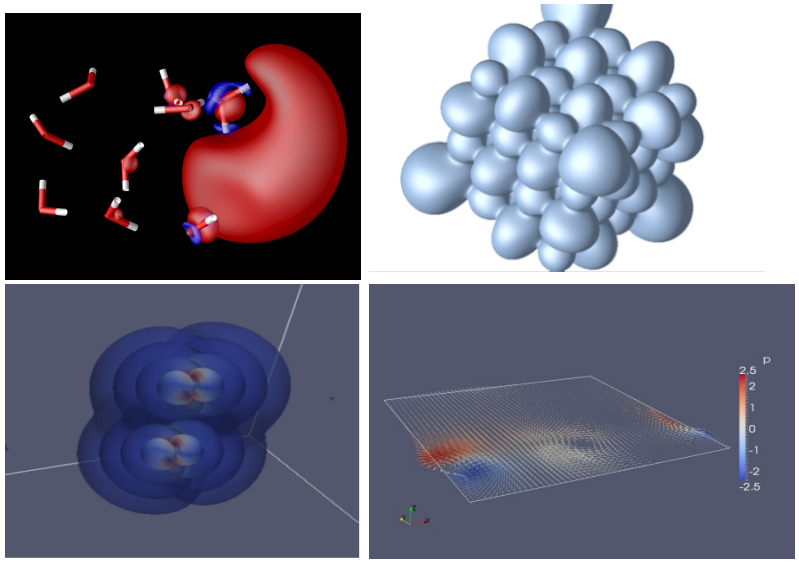
Objectives

- General purpose numerical environment for reliable, fast and scalable scientific simulations
- **General purpose parallel programming environment scalable to petascale and exascale computers**
- **Provide guaranteed precision with adaptive high order bases expansions and controlled approximations**

Impact

- Provide researchers a scalable and easy to program environment for scalable simulations
- First 1-6D adaptive pseudo-spectral and multiresolution analysis based solver for integral and differential equations
- Each function or operator has its own adaptive spectral representation for computation. Composition of operators and functions
- C++ Object Oriented to increase productivity and high programming complexity

Computational Chemistry, Material Science and Nuclear Physics



2011 Progress and Accomplishments

- **2011 R&D100 Prize**
- **First 4-D simulation with quantum nuclei and non-collinear fields, 3 electronic + inter-nuclear coordinate (Krystic and Harrison et. al.), in progress**
- **"Multiresolution Representation of Operators with Boundary Conditions on Simple Domain," G. Beylkin, G. Fann, R. Harrison, C. Kurcz and L. Monzon, submitted to J. Appl. and Comp. Harmonic Analysis**
- **"Solving PDEs in Irregular Geometries with Multiresolution Methods I: Embedded Dirichlet Boundary Conditions," M. Reuter, J. Hill, and R. J.Harrison. Computer Physics Communications. Accepted.**

"Advanced Dynamically Adaptive Algorithms for Stochastic Simulations on Extreme Scales"

PI: R. Archibald, R. Deiterding, C.Hauck (ORNL), D. Xiu (Purdue)

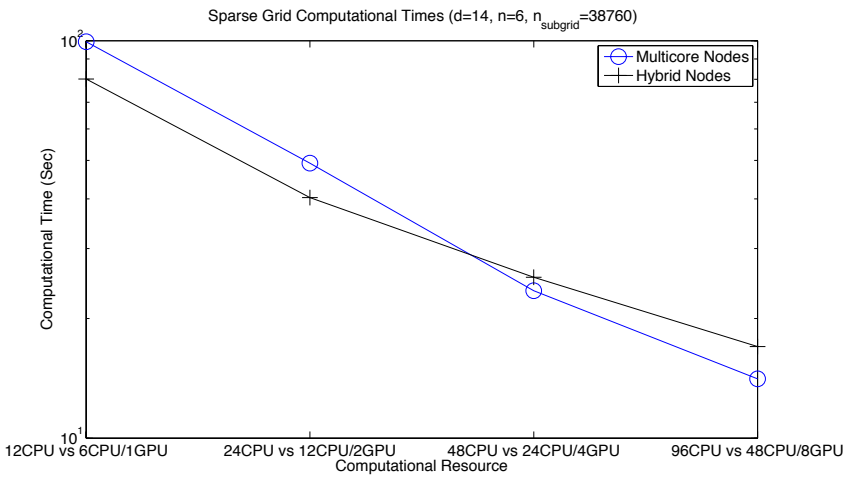
ASCR- Applied Mathematics Highlight

Objectives

- Extend deterministic adaptive mesh refinement (AMR) algorithms to high dimensional random space to facilitate adaptive stochastic simulations.
- Develop stochastic edge-detection methods to locate discontinuities in high dimensional random space.
- Develop advanced, dynamically adaptive, scalable and parallel stochastic collocation methods for extreme-scale computing.

Impact

- Enable application scientists in high-performance computing (HPC) to conduct stochastic simulation on the next-generation computer architecture on extremely large scales.
- Provide capability for *optimal* uncertainty quantification simulation in high dimensions
- Essential for predictive modeling and simulation-based decision-making.



Hybrid node vs. Multi-core node scaling across a GPU-based cluster at ORNL

Accomplishments

- Developed serial prototype library to support adaptive sparse grid algorithm to characterize complex functions in random space with optimal efficiency---its simulation cost grows linearly with dimensionality. ***No curse-of-dimensionality***.
- Developed prototype for efficient sparse grid approximation in parallel for emerging hybrid architectures that utilizes graphics processing units (GPU) efficiently (first of a kind, see left figure for a benchmark)
- *J. Jakeman, R. Archibald, and D. Xiu. Characterization of discontinuities in high-dimensional stochastic problems on adaptive sparse grids. J. Comput. Phys., Vol. 230, 2011.*
- *R. Archibald, R. Deiterding and J. Jakeman. Extending adaptive sparse grids for stochastic collocation to hybrid parallel architectures. SciDAC Procedings, 2011.*

DE-FG02-10ER26023 (ORNL)
DE-SC0005173 (Purdue)

"Numerical Linear Algebra Techniques for Scientific Computing"
Ed D'Azevedo, Oak Ridge National Laboratory

ASCR- Applied Mathematics Highlight

Objectives

- Develop high performance algorithms for numerical linear :
  - Adapt out-of-core dense matrix factorization algorithms for GPU to solve problems larger than available memory on GPU device

Impact

- Much higher performance computing over multi-core CPUs on dense matrix computations by taking advantage of Graphics Processing Unit (GPU)
- Dense matrix computations arising in modeling response of fusion plasma to radio frequency (RF) waves, modeling radiation heat transfer, boundary element method, and large scale linear least squares problems

Accomplishments

	MAGMA 1.0	Out of core
N=25,000	266 Gflop/s	246 Gflop/s
N=35,000	Failed – out of memory	263 Gflop/s

Comparison of MAGMA 1.0 to new out-of-core Cholesky factorization (DPOTRF) using only 1 Gbytes of device memory on Nvidia M2070

- Developed algorithms for LU and Cholesky factorization for large matrices on GPU. A matrix taking up 10 GBytes can be factored on GPU with 1 Gbytes of device memory.
- Achieves over 95% performance of best all in-memory MAGMA library. Overhead for data movement accounts for about 5% of time.
- **Algorithm enhancement: column oriented left-looking algorithm with variable column panel width to take full advantage of available device memory.**

Scalable Graph Decompositions & Algorithms to Support the Analysis of Petascale Data

Blair D. Sullivan, Chris Groër, Oak Ridge National Laboratory

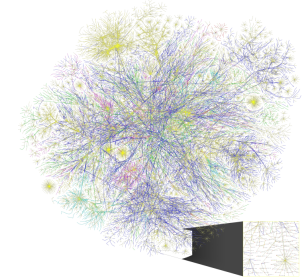
ASCR- Applied Mathematics Highlight

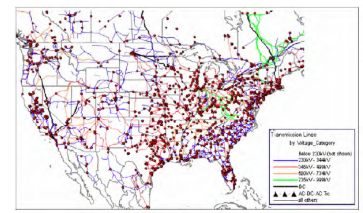
Objectives

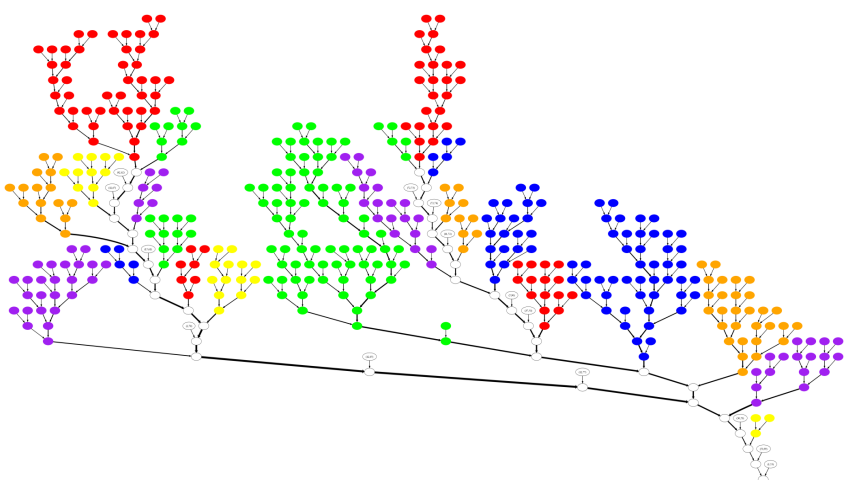
- Demonstrate viability of graph decomposition-based algorithms for large combinatorial optimization problems
- Exploit parallelism to enable dynamic programming (DP) speed-up
- Provide computational evidence that exponential worst-case running times predicted in theory are not realized in practice

Impact

- Provide computationally efficient alternative method for solving discrete optimization problems
- Enable optimal solutions on graphs with width an order of magnitude larger than previously believed possible
- Crucial new strategies for memory reduction in DP tables







Processing a decomposition in parallel using subtrees

Accomplishments

- Developed efficient software library to generate tree decompositions and provide framework for running TD-based dynamic programming algorithms
- Using maximum weighted independent set as a prototypical dynamic programming application, solved problems on graphs with width > 400
- Fixed parameter tractability-type scaling enables exact solutions on graphs with over a million nodes
- Working parallel implementation using MPI and pthreads

“Runtime system for I/O staging” – S. Klasky, ORNL

ASCR - Computer Science Highlight

Objectives

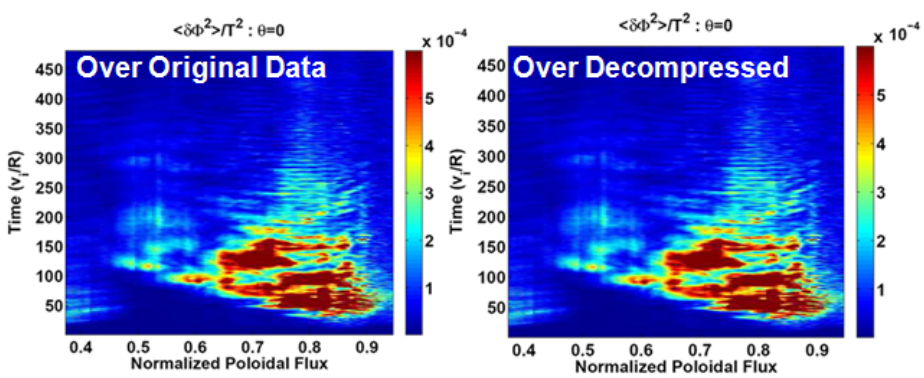
- Develop a lossy compression methodology to reduce “incompressible” spatio-temporal double precision scientific data.
- Ensure high compression rates with ISABELA, while adhering to user-controlled accuracy bounds.

Impact

- Up to 85% reduction in storage on data from petascale simulation applications: S3D, GTS, XGC, Climate, and Groundwater.
- Guaranteed bounds in per-point error, and overall 0.99 correlation, and 0.01 NRMSE with original data.
- Superior compression and accuracy compared to widely used Wavelet compression.

ISABELA Compression Accuracy at 75% reduction in size

Analysis of XGC1 Temperature Data



Progress (and/or Accomplishments w/FY)

- **Communication-free, minimal overhead technique easily pluggable into any simulation application.**
- **Drastic reduction in size, while being highly accurate and robust.**
- **"*Compressing the Incompressible with ISABELA: In-situ Reduction of Spatio-Temporal Data*“ by Lakshminarasimhan. S, Shah. N, Ethier. S, Klasky. S, Latham. R, Ross. R, Samatova . N. F, nominated for distinguished paper award at Int’l European Conf. on Parallel and Distributed Computing, 2011.**
- **Contact: Nagiza Samatova, samatova@csc.ncsu.edu**

ASCR NEWS

Three Exascale Co-Design Centers Awarded

Exascale Co-Design Center for Materials in Extreme Environments (ExMatEx)

Director: Timothy Germann (LANL)

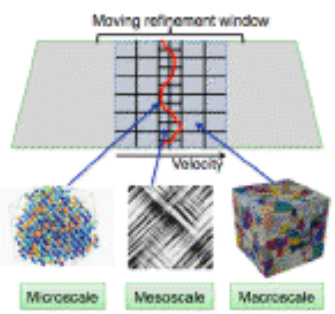
Center for Exascale Simulation of Advanced Reactors (CESAR)

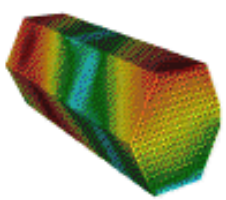
Director: Robert Rosner (ANL)

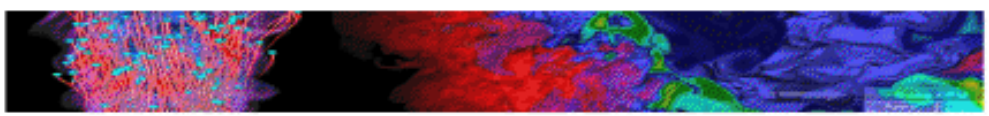
Combustion Exascale Co-Design Center (CECDC)

Director: Jacqueline Chen (SNL)

	ExMatEx (Germann)	CESAR (Rosner)	CECDC (Chen)
National Labs	LANL	ANL	SNL
	LLNL	PNNL	LBNL
	SNL	LANL	LANL
	ORNL	ORNL	ORNL
		LLNL	LLNL
			NREL
University & Industry Partners	Stanford	Studsvik	Stanford
	CalTech	TAMU	GA Tech
		Rice	Rutgers
		U Chicago	UT Austin
		IBM	Utah
		TerraPower	
		General Atomic	
		Areva	







THE OFFICE OF

ADVANCED SCIENTIFIC COMPUTING RESEARCH

Functional Organization Chart

The Office Of

The Associate Director of Advanced Scientific Computing Research

Daniel Hitchcock, Acting Associate Director
Barb Helland – Senior Advisor
Walt Polansky – Senior Advisor
Robert Lindsay – Special Projects
Julie Scott – Financial Analyst
Lori Jernigan - Program Support Specialist
Melea Baker – Administrative Assistant

Budget and Planning
Christine Chalk – Budget Formulation
Julie Scott – Budget Execution
Dan Hitchcock – Budget Planning
Barb Helland – Budget Planning

ASCAC
Christine Chalk – DFO
Lucy Nowell – Committee Manager
Melea Baker – Admin Support

Operations
Barb Helland – Ops Lead
Melea Baker – Admin Lead

Facilities Division
Dan Hitchcock - Director
Sally McPherson - Administrative Support

Computational Science Research and Partnerships (SciDAC) Division
William Harrod - Director
Teresa Beachley – Grants and Contracts
Angie Thevenot – Administrative Support

Facilities
- Oak Ridge Leadership Computing Facility — **Barb Helland** (Acting)
- Argonne Leadership Computing Facility — **Betsy Riley**
- NERSC — **Yukiko Sekine**
- ESnet — **Vince Dattoria**
- Physical Scientist (User Programs) — **Dave Goodwin**

Applied Math
- Base, Multiscale Math — **Sandy Landsberg**
- Base, Multiscale Math — **Karen Pao**
- CSGF — **Barb Helland**

Computer Science
- Computer Science — **Lenore Mullin**
- Data & Visualization — **Lucy Nowell**
- Extreme Scale — **Sonia Sachs**
- File Systems — **Vacant**
- HPC Sci & Apps — **Vacant**

Computational Partnerships
- Biology SAPs — **Christine Chalk**
- Non-SC Program SAPs — **Randall Laviolette**
- SC Program SAPs — **Ceren Susut**
- Non-SC Program SAPs — **Vacant**
- Math – SciDAC Centers & Institutes — **Steven Lee**
- CS – SciDAC Centers & Institutes — **Vacant**

Distributed Network Environment
- Network Research — **Thomas Ndousse-Fetter**
- Collaboratories/ Middleware — **Rich Carlson**

-Battelle
artment of Energy

April 2011

OAK RIDGE National Laboratory

Other ASCR News

- SciDAC Institutes
  - should be announced any day now
- SciDAC Applications
  - FOAs should appear August to September
  - Individual FOAs from individual offices
- Upcoming workshops
  - Programming Challenges: end of July
  - Architecture I and II: first two weeks of August
- Anticipated FOAs
  - SDM & Visualization Institute
  - Tools
  - Programming models and Architecture

DIVISION INITIATIVES AND ACTIVITIES

Initiatives from Offsite Planning: Strategy

- ASCR Interactions
  - With all of the changes at ASCR, we need a communication strategy
- ORNL Exascale Science Vision
  - Includes Science, Mathematics, and Computer Science
- Costs: ORNL charge-out costs are increasing
  - How do we compare with peer institutions? How can we impact the process that has led to these changes?
- Awards
  - Which awards/recognitions do we value? How do we recognize accomplishments?
- OLCF
  - How do we improve this relationship?
- ITSD
  - How do we ensure that the division needs are addressed?

DIVISION DASHBOARD

PROJECTING FUNDING COVERAGE

Project Hours

http://portal.ornl.gov/sites/ccsd/csmd/Lists/Project Hours/My Items.aspx

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Complex Systems

Computational Astrophysics

Computational Earth Sciences

Computational Engineering & Energy Sciences

- CEES Wiki

Computational Materials Science

Computational Mathematics

Computer Science Research

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There are no items to show in this view of the "Project Hours" list. To create a new item, click "New" above.

Project Hours

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OK | Cancel

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CSMD Staff Member *	ORNL\Your 3 character id (ex. ORNL\jpk)
Project Name	A name to help you identify the project.
FWP/IAN Number	For example: ERKJ###
WBS Number	For example: 3410-####
% of Hours	What percent of the year do you expect work on this project?

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CSMD Staff Member *	ORNL\3np ORNL\Your 3 character id (ex. ORNL\jpk)
Project Name	Collaborative Space Development A name to help you identify the project.
FWP/IAN Number	ERKJCSD For example: ERKJ###
WBS Number	3410-COLB For example: 3410-####
% of Hours	10 What percent of the year do you expect work on this project?

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WBS Number	3410-COLB For example: 3410-####
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Last modified at 7/20/2011 9:15 AM by Pack, Daniel L.

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Inside CSM

Inside CSM

http://www.csm.ornl.gov/IAO/

CSM Computer Science and Mathematics
Oak Ridge National Laboratory

Internal Home

CSM Internal Homepage -- information specific to CSM.
(Some frequently used ORNL links are included on the category pages.)

Town Hall Meeting Presentations (pdfs)

- July 21st 2011

Links from Town Hall Meetings

- CSMD Dashboard
- Projecting Funding Coverage

General Information

- **SciDAC 3 Information**

- **Employee Info**
  Bomb Threats, **Handbook**, **Jobs**, **Training**...
  New Employee Orientation Checklist (doc) updated 6/2006
  Bldg. maps and Evacuation routes
  Willful Misconduct Presentation

- **Who, What, Where?**
  Operations Council
  Calendar

- **Computing Info**
  Server (CSM) Accounts, **Cluster (TORC) Accounts**
  HPC (CCS)Accounts, **Export control**,
  access to new webservers, **Webtips**

- **ORNL Connections**
  Division reps, **Inside ORNL**, ...

- **News/Results**
  Highlights, **Publications**, **PR**...

Off-Site Presentation (9/21/09)

Division (All hands) meeting notes and Strategic Plans | Barney's weekly staff meeting notes (Beginning 1/6/09)

inside-csm | employee info | computing info | development | who, what, where? | ornl connections | news/results
ornl | ccs | csm | disclaimer | search

URL *http://www.csm.ornl.gov/IAO/index.html*
Updated: *Thursday, 21-Jul-2011 12:02:27 EDT*
webmaster

THANKS