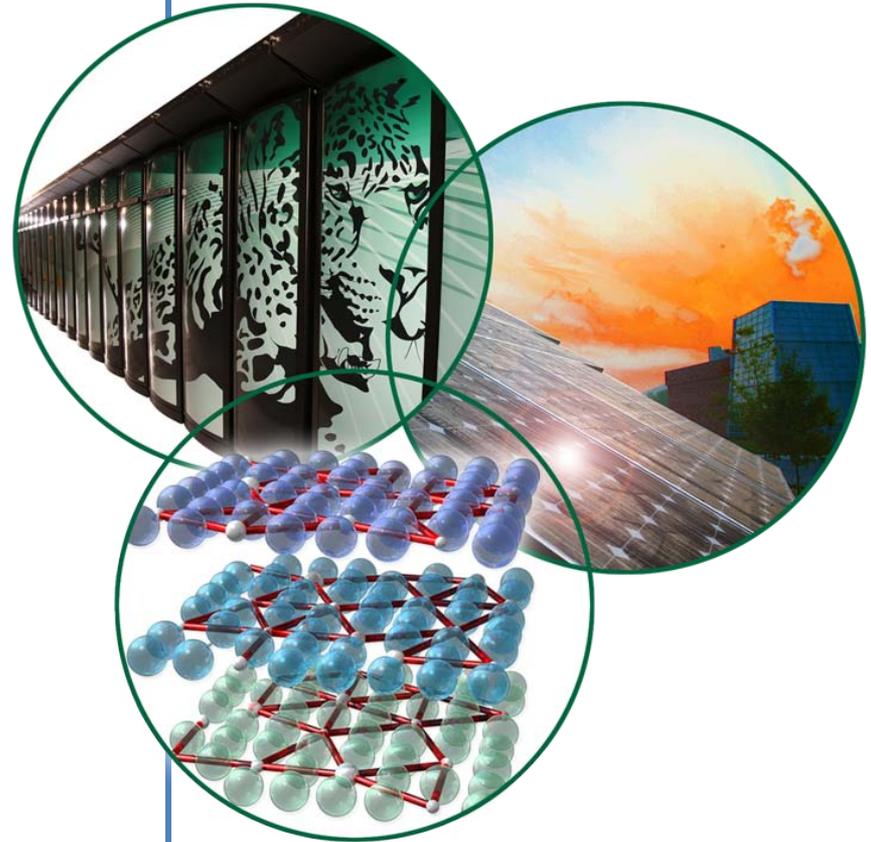


CSMD Division All Hands Meeting

- Barney Maccabe
- December 14, 2011



Personnel

Service Anniversaries

Name	Years
Chongle Pan	5
Stephen Poole	5
Andrey Gorin	10
Line Pouchard	10

New Hires

Computational Engineering and Energy Sciences	
Ross Bartlett	07/25/2011

Computational Chemistry and Materials Sciences	
Matt Reuter	08/29/2011

Computational Earth Sciences	
Ben Mayer	09/12/2011

Org Chart

Computation at Scale

Computer Science and Mathematics Division

Computer Science and Mathematics Division
Barney Maccabe

John Cobb, Teragrid

Thomas Schulthess, Europe

Steve Poole, Chief Scientist
Director of Special Programs

Robert Harrison, Director of Computational Science Programs

Apply
Computation for Science

Computational Astrophysics
Anthony Mezzacappa

Computational Chemical and Material Sciences
Bobby Sumpter

Computational Earth Sciences
Danny McKenna

Computational Engineering and Energy Sciences
John Tumer

Center for Computational Molecular Biophysics
Jeremy Smith

Experimental Computing Laboratory
Jeffrey Vetter

Center for Engineering Science Advanced Research
Jacob Barhen

Institute for Advanced Architectures and Algorithms
Jeff Nichols

EASI Math/CS Institute
Al Geist

Extreme Scale System Center
Steve Poole

Centers and Institutes

Explore
Computational Approaches

Computational Mathematics
Ed D'Azevedo (Interim)

Statistics and Data Science
Scott Klasky

Complex Systems
Jacob Barhen

Build
Computational Systems

Future Technologies
Jeffrey Vetter

Computer Science Research
Al Geist

Application Performance Tools
Rich Graham

Groups

Highlights

2011 INCITE Awards–New

Type: New

Title: —Cellulosic Ethanol: Simulation of Multicomponent Biomass System

Principal Investigator: Jeremy Smith, Oak Ridge National Laboratory

Co-Investigators: Xiaolin Chang, Oak Ridge National Laboratory and Loukas Petridis, Oak Ridge National Laboratory

Scientific Discipline: Biological Sciences: Biophysics

INCITE Allocation: 30,000,000 processor hours

Site: Oak Ridge National Laboratory

Machine (Allocation): Cray XT (30,000,000 processor hours)

Type: New

Title: —Three Dimensional Simulations for Core Collapse Supernovae

Principal Investigator: Anthony Mezzacappa, Oak Ridge National Laboratory

Co-Investigators: John Blondin, North Carolina State University; Stephen Bruenn, Florida Atlantic University; Christian Cardall, Oak Ridge National Laboratory; William Raphael Hix, Oak Ridge National laboratory; Jirina Stone, Oak Ridge National Laboratory

Scientific Discipline: Physics: Astrophysics

INCITE Allocation: 60,000,000 processor hours

Site: Oak Ridge National Laboratory

Machine (Allocation): Cray XT (60,000,000 processor hours)

Type: New

Title: —Petascale Modeling of Chemical Catalysts and Interfaces

Principal Investigator: Robert Harrison, Oak Ridge National Laboratory

Co-Investigators: Edoardo Apra, Oak Ridge National Laboratory; David Dixon, University of Alabama; Karol Kowalski, Pacific Northwest National Laboratory; William Shelton, Oak Ridge National Laboratory; David Sherrill, Georgia Institute of Technology; Bobby Sumpter, Oak Ridge National Laboratory

Scientific Discipline: Chemistry: Catalytic

INCITE Allocation: 75,000,000 processor hours

Site: Oak Ridge National Laboratory

Machine (Allocation): Cray XT (75,000,000 processor hours)

2011 INCITE Awards–New (cont.)

Type: New

Title: —Climate-Science Computational Development Team: The Climate End Station II

Principal Investigator: Warren Washington, National Center for Atmospheric Research

Co-Investigators: Philip Cameron-Smith, Lawrence Livermore National Laboratory; Scott Elliott, Los Alamos National Laboratory; David Erickson, Oak Ridge National Laboratory; Steven Ghan, Pacific Northwest National Laboratory; James Hack, Oak Ridge National Laboratory; Jim Hurrell, University Corporation for Atmospheric Research; Rob Jacob, Argonne National Laboratory; Philip Jones, Los Alamos National Laboratory; Jean-Francois Lamarque, University Corporation for Atmospheric Research; L. Ruby Leung, Pacific Northwest National Laboratory; Bette Otto-Bliesner, University Corporation for Atmospheric Research; Steven Pawson, NASA; Mark Taylor, Sandia National Laboratories; Peter Thornton, Oak Ridge National Laboratory

Scientific Discipline: Earth Science: Climate Research

INCITE Allocation: 110,000,000 processor hours

Site: Oak Ridge National Laboratory

Machine (Allocation): Cray XT (70,000,000 processor hours)

Site: Argonne National Laboratory

Machine (Allocation): IBM Blue Gene/P (40,000,000 processor hours)

Type: New

Title: —Advanced Simulations of Plasma Microturbulence at the Petascale and Beyond

Principal Investigator: William M. Tang, Princeton University

Co-Investigators: Mark F. Adams, Columbia University; Stéphane Ethier, Princeton Plasma Physics Laboratory; Scott Klasky, Oak Ridge National Laboratory; Bruce Scott, Max-Planck Institute for Plasma Physics; Weixing Wang, Princeton University

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation: 8,000,000 processor hours

Site: Argonne National Laboratory

Machine (Allocation): IBM Blue Gene/P (8,000,000 processor hours)

Type: Renewal

Title: —High Fidelity Tokamak Edge Simulation for Efficient Confinement of Fusion Plasma

Principal Investigator: C.S. Chang, New York University

Co-Investigators: Scott Klasky, Oak Ridge National Laboratory; Scott Parker, University of Colorado; Linda Sugiyama, Massachusetts Institute of Technology

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation: 50,000,000 processor hours

Site: Oak Ridge National Laboratory

Machine (Allocation): Cray XT (50,000,000 processor hours)

2011 INCITE Awards–Renewals

Type: Renewal

Title: —Performance Evaluation and Analysis Consortium End Station

Principal Investigator: Patrick Worley, Oak Ridge National Laboratory

Co-Investigators: David H. Bailey, Lawrence Berkeley National Laboratory; Jack J. Dongarra, University of Tennessee; William D. Gropp, University of Illinois at Urbana-Champaign; Jeffrey K. Hollingsworth, University of Maryland; Robert F. Lucas, University of Southern California ; Allen D. Malony, University of Oregon; John Mellor-Crummey, Rice University; Barton P. Miller, University of Wisconsin at Madison; Leonid Oliker, Lawrence Berkeley National Laboratory; Allan Snavely, University of California at San Diego; Jeffrey S. Vetter, Oak Ridge National Laboratory; Katherine A. Yelick, University of California at Berkeley; Bronis R. de Supinski, Lawrence Livermore National Laboratory

Scientific Discipline: Computer Science

INCITE Allocation: 30,000,000 processor hours

Site: Oak Ridge National Laboratory

Machine (Allocation): Cray XT (20,000,000 processor hours)

Site: Argonne National Laboratory

Machine (Allocation): IBM Blue Gene/P (10,000,000 processor hours)

Type: Renewal

Title: —Magnetic Structure and Thermodynamics of Low Dimensional Magnetic Structures

Principal Investigator: Markus Eisenbach, Oak Ridge National Laboratory

Co-Investigators: Paul Kent, Oak Ridge National Laboratory; Malcolm Stocks, Oak Ridge National Laboratory

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation: 50,000,000 processor hours

Site: Oak Ridge National Laboratory

Machine (Allocation): Cray XT (50,000,000 processor hours)

Type: Renewal

Title: —Investigation of Multi-Scale Transport Physics of Fusion Experiments Using Global Gyrokinetic Turbulence Simulations

Principal Investigator: Weixing Wang, Princeton Plasma Physics Laboratory

Co-Investigators: Mark Adams, Columbia University; Stephane Ethier, Princeton Plasma Physics Laboratory; Scott Klasky, Oak Ridge National Laboratory; Wei-li Lee, Princeton Plasma Physics Laboratory

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation: 20,000,000 processor hours

Site: Oak Ridge National Laboratory

Machine (Allocation): Cray XT (20,000,000 processor hours)

2011 INCITE Awards–Renewals (cont.)

Type: Renewal

Title: —**Ultrascale Simulation of Basin-Scale CO₂ Sequestration in Deep Geologic Formations and Radionuclide Migration using PFLOTRAN**

Principal Investigator: Peter Lichtner, Los Alamos National Laboratory

Co-Investigators: Glenn Hammond, Pacific Northwest National Laboratory and Richard Mills, Oak Ridge National Laboratory

Scientific Discipline: Earth Science: Environmental Sciences

INCITE Allocation: 15,000,000 processor hours

Site: Oak Ridge National Laboratory

Machine (Allocation): Cray XT (15,000,000 processor hours)

SEA Winners

- **Revolutionary Computing Paradigm in MADNESS (Multiresolution Adaptive Numerical Environment for Scientific Simulations)**
 - Robert Harrison, **George Fann**, **Judith Hill**, **Jun Jia**, Rebecca Hartman-Baker, **Diego Galindo**
- **New Educational Appointment Application**
 - Tracey Lawson, Cecilia Rowe, Robert Tannert, Becky Wagner, Justin Keck, David Hetrick, **Cindy Sonewald**, Irene Sharp, Jennifer Seiber, Nancy Wright, and Valentina Moore

Awards Night Winners

Laboratory Operations, Administrative Support Award - Tracey Lawson, Cecilia Rowe, Robert Tannert, Becky Wagner, Justin Keck, David Hetrick, **Cindy Sonewald**, Irene Sharp, Jennifer Seiber, Nancy Wright, and Valentina Moore

For transforming, automating, and improving the ORISE educational appointment hiring process, thereby promoting outstanding customer satisfaction, significant time reductions, and substantial cost savings

Secretarial Support – Lora Wolfe

For exemplary administrative secretarial support to the Computer Science and Mathematics Division and to the ORNL SciDAC proposal process.

Achievement Award



ORNL's Dave Hetrick, Charlotte Barbier and **Sreekanth Pannala** were part of a multi-agency team of researchers cited with an Achievement Award for their contribution to the Deepwater Horizon oil spill in summer 2010.

The three represented ORNL in efforts that included Lawrence Berkeley, Lawrence Livermore, Los Alamos and Pacific Northwest national laboratories, the National Energy Technology Laboratory, National Institute of Standards and Technology, University of Pittsburgh and West Virginia University. The multi-agency's effort was deemed critical to estimating the rate of oil flowing into the Gulf of Mexico and, in turn, developing options to cap the well.

Distinguished Employee Program

- **November 2011: Eric Lingerfelt** - For his agile development of the Bellerophon software platform. October's release of Bellerophon (1.1.8) not only included the usual group of bug fixes, etc., but also included significant new functionality to help computational scientists glean insight from simulation. New caching techniques and expanded VisIt functionality through Bellerophon are the chief improvements. These new features have set the stage for the generalization of Bellerophon for other code teams.
- **October 2011: Antonios Danalis** - For being a Good Samaritan - What happened: I was taking a walk around the pond (only to fight off 2:00 sleepiness so I can be more productive :-)), when I suddenly saw huge sparks and heard violent sounds from behind the trees across the road (where the intersection of the power lines is). Shortly after, I saw a car slowly coming from the electric tower toward the pond, very close to where I was. The car continued through the grass, over the road and into the pond. I couldn't see anybody in the driver's seat, but I assumed that somebody had to be driving this car, so I ran, jumped in the pond, opened the back door that was still above the water, got in the car, saw the lady laying on her side (semiconscious) and started pulling her up and trying to wake her up. Her leg was stuck between the seat and the console, so I couldn't set her free, but another guy helped me open the front door and then we moved the seat back and set her leg free. Soon the fire department, police and paramedics came and they took over. Donna walked away, so she is probably not in too much medical trouble. She was lucky though; given how long it took us to set her free and that she was semiconscious at best, if the pond was deep enough to swallow the whole car, I don't know that we would have managed to get her out in time.
- **September 2011: Terry Jones** - As part of ASCR funded research, Terry Jones worked to develop I/O forwarding capabilities for the Cray. Terry also worked with the Technical University of Dresden and NCCS, in the context of the OLCF-3 project, to incorporate the I/O forwarding capabilities into the Vampir performance analysis tool suite. With these new capabilities, trace-based performance analysis was performed on an application sized at about 200,000 processes, which is an order of magnitude increase in the job size for which such analysis is feasible. This work is helping the OLCF meet its goal of being able to analyze full user applications at system scale.

Distinguished Employee Program (cont.)

- **August 2011: Collin McCurdy** - Developed Memphis - a tool for pinpointing memory-related performance problems in multithreaded applications. Collin has used Memphis to optimize several important DOE applications, and has had those optimizations integrated into several applications. For example, with Memphis, this work led to a ~25% performance improvement of the XGC1 fusion application at scale on Jaguar.
- **July 2011: George Fann** – George Fann initiated, derived, and developed many of the mathematical results and numerical methods in Multiresolution Adaptive Numerical Environment for Scientific Simulation (MADNESS) that recently won an R&D 100 award. He also co-developed and prototyped the numerical methods for solving singular and pseudo-differential operators in applications in collaboration with Professor Gregory Beylkin at the University of Colorado at Boulder and Professor Robert Harrison of Joint Institute for Computational Sciences (JICS). He continues to derive and prototype new computational methods and scalable numerical algorithms. He was also an instrumental player in the application of MADNESS to computational chemistry (with Professor Robert Harrison) and nuclear physics (with Dr Witold Nazarewicz in Physics Division). He continues to be a principal investigator and a collaborator of numerous projects to further develop and enhance the algorithmic and mathematical capabilities of MADNESS and its applications to other disciplines.

MADNESS is a free open-source general purpose user-friendly numerical framework and software for the development scientific simulations from laptops to massively parallel supercomputers. MADNESS utilizes the latest parallel computing and solution methodologies to solve many dimensional integral and differential equations accurately and precisely for real-world problems. MADNESS provides a new platform for scientists and engineers to easily create new applications with assurance in the exactness of their results.

Research Support Award from ESD given in recognition of sustained, outstanding computer programming contributions to the AmeriFlux data center



Barbara Jackson has

Written over 1000 SAS codes to read, check, and merge a multitude of data streams from over 40 AmeriFlux site teams

Assembled the “AmeriFlux Network database,” which now contains over 300 million observations and 700 variables

Developed web documents detailing CDIAC’s site-specific QA/QC contributions to the AmeriFlux database

Created a web-based interface for users to query the AmeriFlux database

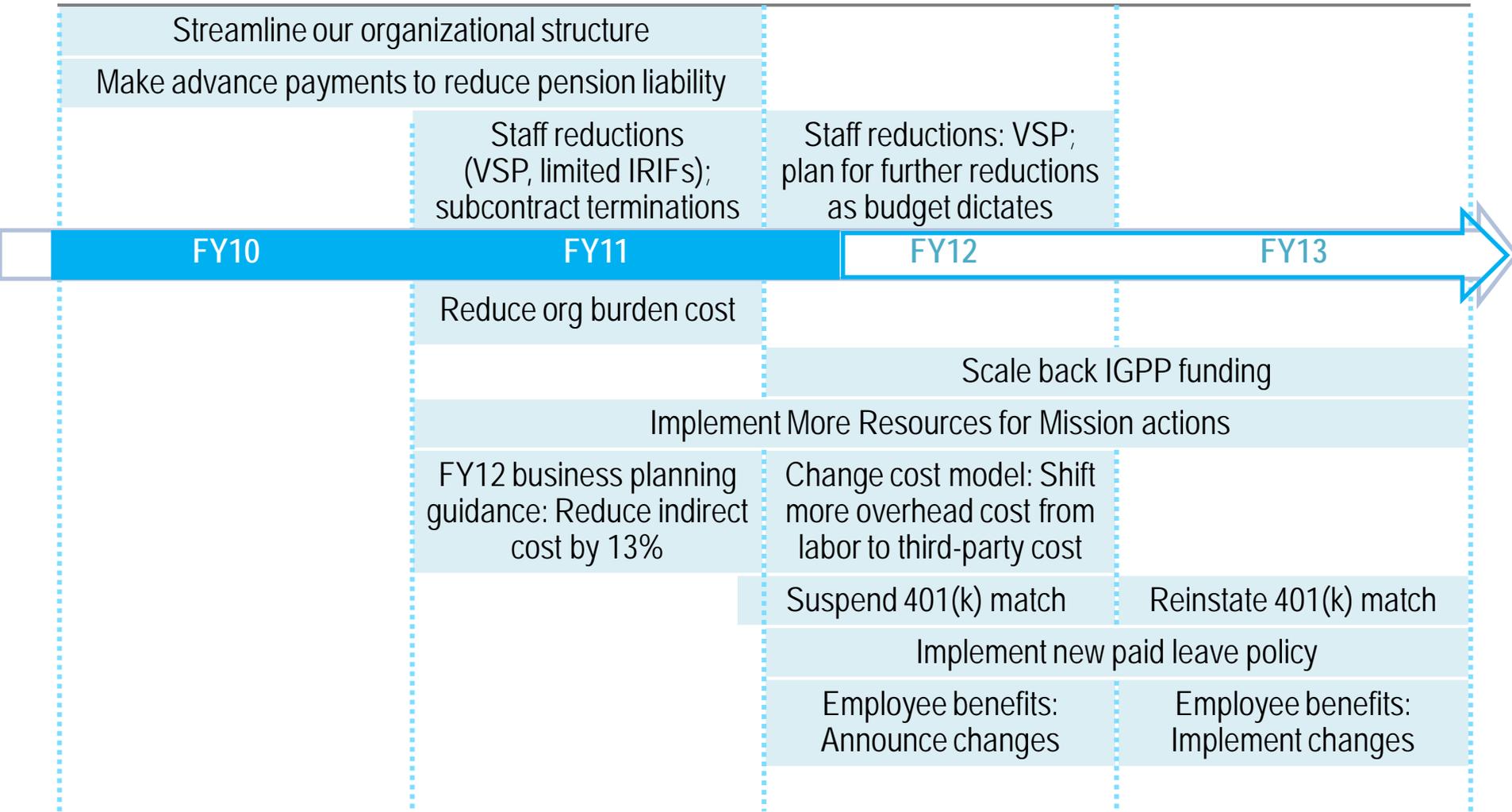
Produced standardized AmeriFlux data products fundamental to terrestrial climate change modeling and synthesis activities

DOE Early Career Award

- Gonzalo Alvarez-Campot
Computational Chemistry and Materials
Sciences Group
- Diagonalization Solvers for Electronic
Collective Phenomena in Nanoscience

Other

Reducing indirect costs and increasing value



The more things change . . .

“ORNL continues to make important contributions to energy R&D. In recent years, however, budget uncertainties and a lack of direction on the national scale have hampered the Laboratory’s programs.”

“Faced with the prospects of such large cuts, Laboratory management was forced to make contingency plans for staff reorganization and to monitor, on a daily basis, budget-related actions by Congressional committees.”

“Uncertainties such as these seriously impair ORNL’s efforts to plan for its future needs.”

“[Planning] is becoming a more important activity for programs and divisions, as well as the Laboratory as a whole.”



January 1981

Excellence in S&T: Possible performance indicators

Customer view	Facility use	Knowledge generation	Knowledge application	Recognition	R&D management
<ul style="list-style-type: none"> • Customer ratings (previous FY) • Projected customer ratings (current FY) • Business volume (BV) 	<ul style="list-style-type: none"> • Unique users • Unique Science • Reliability • Availability 	<ul style="list-style-type: none"> • Publications • Highly cited publications • Intellectual property • Invention disclosures 	<ul style="list-style-type: none"> • Patent awards • Licenses • Spin-offs • Software use ("exposure") 	<ul style="list-style-type: none"> • Awards • Prizes • External appointments • Media exposure 	<ul style="list-style-type: none"> • Status of major projects • R&D staff with annual BV >\$1M • R&D staff turnover rate • R&D staff development • Direct/indirect ratio • LDRD costing

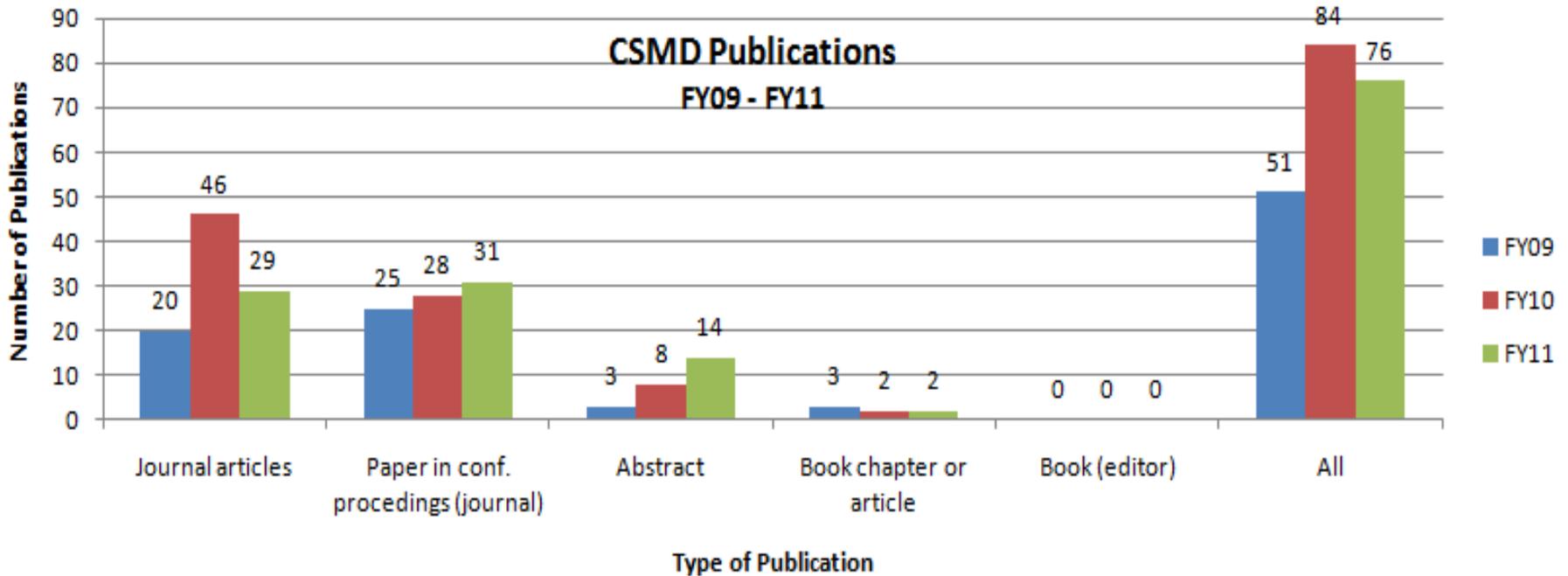
For each indicator, we should have access to:

- Snapshot for current period or complete data set
- Trending over time

CCSD Publications FY09 - FY11

From PTS on 9Nov11

	CCSD			NCCS			CSED			CSMD			ITSD			Total		
	FY09	FY10	FY11	FY09	FY10	FY11												
Journal articles	0	0	0	4	1	0	14	12	17	20	46	29	0	0	0	38	59	46
Paper in conf. proceedings (journal)	0	0	1	1	3	6	35	39	29	25	28	31	0	0	0	61	70	67
Abstract	0	1	0	0	0	0	0	5	20	3	8	14	0	0	0	3	14	34
Book chapter or article	0	0	0	0	0	0	4	3	1	3	2	2	0	0	0	7	5	3
Book (editor)	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	1	1	0
All	0	1	1	5	4	6	54	60	67	51	84	76	0	0	0	110	149	150



Thank you!



Ursula had surgery on December 1, 2011 and is recuperating well. She is scheduled to return to work in mid to late January 2012.

Safety

Sharing the Road

Sharing the Road: Motorists

Drive Cautiously:

- Reduce speed when encountering cyclists
- Don't tailgate, especially in bad weather
- Recognize hazards cyclists may face and give them space

Yield to Cyclists:

- Bicycles are considered vehicles and in most jurisdictions are prohibited from riding on the sidewalk
- Cyclists should be given the appropriate right of way
- Allow extra time for cyclists to get through intersections

Be Considerate:

- Scan for cyclists in traffic and at intersections
- Do not blast your horn in close proximity to cyclists
- Look for cyclists when opening doors

Pass with Care:

- When passing, leave at least three feet between you and a cyclist
- Wait for safe road and traffic conditions before you pass
- Check over your shoulder before moving back

Watch for Children:

- Children on bicycles are often unpredictable
- Expect the unexpected and slow down
- Don't expect children to know traffic laws
- Because of their size children can be harder to see
- Watch for children on bicycles crossing intersections from sidewalks

Sharing the Road: Cyclists

On the Road:

- The same laws that apply to motorists apply to cyclists
- Obey all traffic control devices
- Use hand signals to indicate stops and turns other users
- Wear a helmet, no matter how short the trip

Ride on the Right:

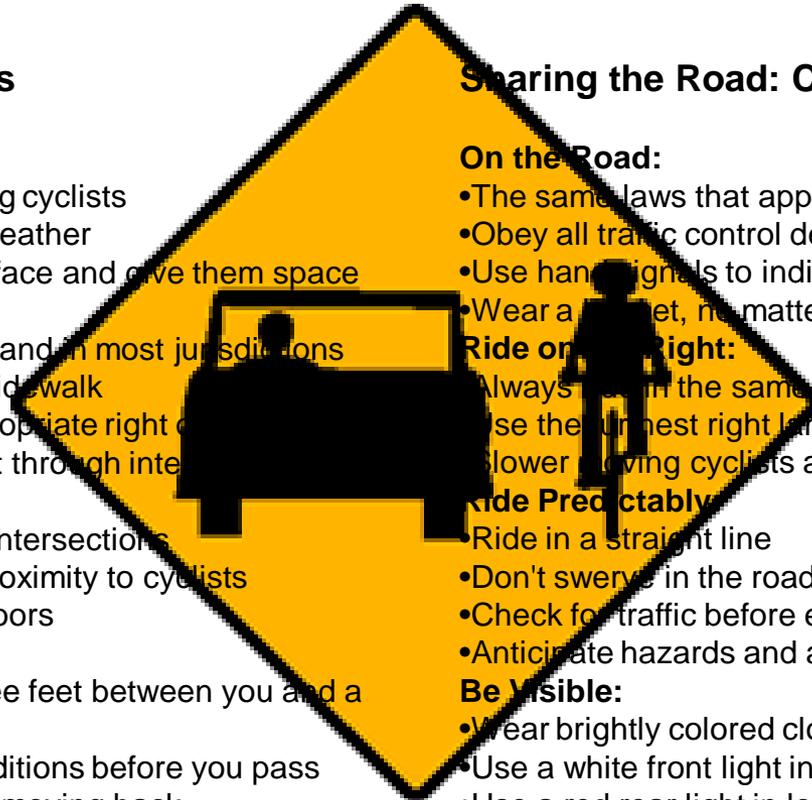
- Always ride in the same direction as traffic
- Use the furthest right lane that heads to your destination
- Slower moving cyclists and motorists stay to the right

Ride Predictably:

- Ride in a straight line
- Don't swerve in the road or between parked cars
- Check for traffic before entering street or intersection
- Anticipate hazards and adjust your position accordingly

Be Visible:

- Wear brightly colored clothing that provides contrast
- Use a white front light in low light conditions
- Use a red rear light in low light conditions
- Use a reflector or reflective tape or clothing anytime
- Announce yourself by making eye contact with motorists



Thanks