

OUTREACH AND COMMUNICATIONS PROJECT FOR ASCR

James Corones
Krell Institute
February 28, 2007



What are We Trying to Do?

The purpose of this activity is to communicate clearly and crisply the **value**, the **importance** and the **quality** of the **facilities**, **research** and **people** supported by **OASCR**.

Audiences

Decision Makers

Interested Public

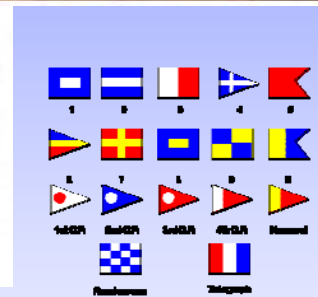
**Technical
Communities**

Context

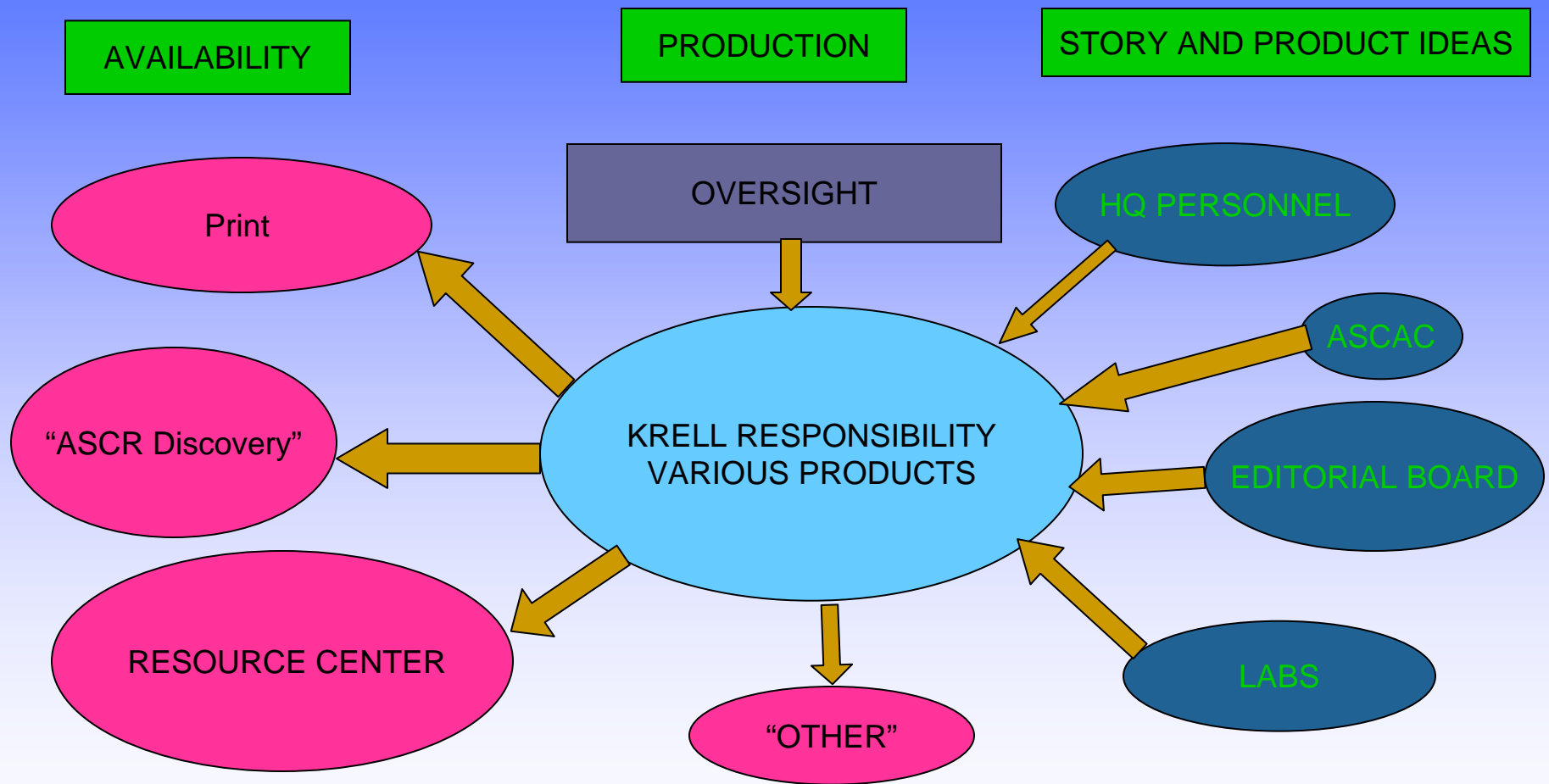
- Science within DOE
- DOE laboratory credit
- Joint funding of many activities
- Balancing “end use” and research
- Historical deficit

Approach

- Create a broad range of accessible materials that **communicate to wide but selected audiences.**
- Make these materials **widely and easily available** to the target audiences.
- Organize and archive this material for **multiple use in multiple forms.**



HOW WILL THIS GET DONE?



Editorial Board Members

Bill	Gropp	ANL	Chris	Johnson	Utah
Jim	Davenport	BNL	Randy	Bramley	Indiana
David	Moulton	LANL	Marc	Snir	UIUC
Adolphy	Hoisie	LANL	Marsha	Berger	NYU
Juan	Meza	LBNL	Linda	Petzold	UCSB
Kathy	Yelick	LBNL	David	Keyes	Columbia
Lori	Diachin	LLNL	David	Brown -Chair	LLNL
David	Bernholdt	ORNL	Jim	Corones – ex officio	
Debbie	Gracio	PNNL			Krell
Scott	Collis	SNL			
Ron	Brightwell	SNL			

First Product

- ASCR Discovery
 - Feature Story
 - Research at the Labs (mostly base program)
 - University Research
 - Large Scale Computing
 - Collaborative Work
 - Development of ideas
 - New Faces
 - Notable News
- <http://www.sc.doe.gov/ascr/Misc/ASCRDiscovery.html>

ASCR Discovery

ASCR | ORGANIZATION | NEWS | CONTACT US

 U.S. DEPARTMENT OF ENERGY

 Office of Science

 **ascr discovery**
UNDERSTANDING SCIENCE THROUGH COMPUTING

FEATURE
[Top Story](#)

KERNELS
[Core Research](#)

BIG IRON
[Highest-End Computing](#)

AT THE UNIVERSITIES
[University Research](#)

SYNCHRONIZED
[Working Together](#)

GENEALOGY
[Lineage Of Ideas](#)

NEW FACES
[Future Of Science](#)

NOTABLE
[Community News](#)

feature story *Updated 2.08.07*

Burning questions
Powerful computers are simulating how turbulence enhances – or retards – combustion in clean, efficient engines. A grant of 2.5 million processor hours from the Department of Energy's INCITE program made the model possible.

[HOME](#) | [COMMENT ONLINE](#) | [EMAIL UPDATES](#) | [A SCR HOME](#) | [ABOUT ASCR](#) | [PRESS ROOM](#)

Search ASCR Discovery Site

[Web Policies](#) | [No Fear Act](#) | [Site Map](#) | [Privacy](#) | [Phone Book](#) | [Employment](#)



U.S. DEPARTMENT OF
ENERGY



Office of
Science



FEATURE

[Top Story](#)

KERNELS

[Core Research](#)

BIG IRON

[Highest-End Computing](#)

AT THE UNIVERSITIES

[University Research](#)

SYNCHRONIZED

[Working Together](#)

GENEALOGY

[Lineage Of Ideas](#)

NEW FACES

[Future Of Science](#)

kernels

Updated 2.23.07

MADNESS makes sense

A mathematical software framework called MADNESS could help scientists study and simulate systems previously thought nearly impossible. It has potential applications in energy, drug development and other fields.

Putting the pieces together

Scientists are redefining the computer operating system concept to provide a framework for custom systems efficient enough for the next generation of high-performance computers.

[HOME](#) | [COMMENT ONLINE](#) | [EMAIL UPDATES](#) | [ASCR HOME](#) | [ABOUT ASCR](#) | [PRESS CENTER](#)

Search ASCR Discovery Site



U.S. DEPARTMENT OF
ENERGY



Office of
Science



ASCR **kernels** [core research]

FEATURE

INCITE ignites combustion simulation

KERNELS

MADNESS calms chemistry on computers
Building an operating system from the ground up

BIG IRON

INCITE collaboration boosts combustion simulation

AT THE UNIVERSITIES

Error estimation improves multiscale models

Cyber Forensics "Robots" Clean Up Infected Code

SYNCHRONIZED

Collaborative Effort Helps Optimize Cavities In Accelerators

GENEALOGY

MPI – enabling the world's fastest computers

NEW FACES

The need for speed pushes optimization researcher

MADNESS calms chemistry on computers

George Fann of Oak Ridge National Laboratory says there's no hidden meaning behind the name he and his fellow researchers chose for their scientific software framework. MADNESS was a catchy play on words for **M**ultiresolution **A**daptive **N**umerical Scientific Simulation and, perhaps, a reflection of the project's ambitious nature.



[Click here to read more](#)

*A base of fundamental work in applied mathematics and computer science makes advanced scientific computing possible. **Kernels** looks at the development of these engines, which power software for scientific and engineering simulation, performance analysis, high-performance computing and other high-level research.*

Building an operating system from the ground up

In a project that harks back to the days of computer pioneer John Von Neumann, scientists at Sandia National Laboratories in Albuquerque, N.M., are breaking down the entire concept of an operating system (OS) and rebuilding it.



[Click here to read more](#)





U.S. DEPARTMENT OF
ENERGY



Office of
Science



ASCR
kernels [core research]

FEATURE

INCITE ignites combustion simulation

KERNELS

MADNESS calms chemistry on computers
Building an operating system from the ground up

BIG IRON

INCITE collaboration boosts combustion simulation

AT THE UNIVERSITIES

Error estimation improves multiscale models

Cyber forensics "Robots" Clean Up Infected Code

SYNCHRONIZED

Collaborative Effort Helps Optimize Cavities In Accelerators

GENEALOGY

MPI – enabling the world's fastest computers

NEW FACES

The need for speed pushes optimization researcher

MADNESS calms chemistry on computers

Posted February 23, 2007

George Fann says there's no hidden meaning behind the name he and his fellow researchers chose for their scientific software framework. MADNESS was a catchy play on words for Multiresolution Adaptive Numerical Scientific Simulation and, perhaps, a reflection of the project's ambitious nature.

Unusual name aside, MADNESS could cause a stir in the scientific modeling community. The mathematical methods behind it could allow scientists to attack problems previously considered computationally impossible. They also could let scientists solve such problems with a previously unattainable level of precision.

Fann, a senior researcher at the Department of Energy's Oak Ridge National Laboratory, is collaborating on the project with University of Colorado applied mathematician Gregory Beylkin and Robert Harrison, leader of Oak Ridge's Computational Chemical Sciences Group.

The work, supported by DOE's Office of Advanced Scientific Computing Research through the Scientific Discovery through Advanced Computing (SciDAC) program, could have uses in energy technology, drug development, and other fields.

The researchers are applying the mathematical methods encompassed in MADNESS to computational chemistry with a focus on solving the electronic structures of atoms, molecules and nanoscale systems. They're also preparing their models to run on the next generation of high-performance computers.

Modeling in many dimensions

Scientists running such models often must limit their size. The algorithms – mathematical recipes computers use – that are practical in one dimension demand too much computer time for high-accuracy applications in the multiple dimensions needed to represent big systems of many atoms or molecules.

To do such computations, "usually you're using a reduced model so you actually compute in three dimensions (instead of more) and you're assuming certain things," Fann says.

1 | 2 | 3 | Print

CONTACT:

George I. Fann
Oak Ridge National Lab
fanngi@ornl.gov
Personal web page

COLLABORATORS:

Martin Mohlenkamp
Ohio University

Fernando Perez
University of Colorado

Jun Jia
Oak Ridge National Lab

Rebecca Hartman-Baker
Oak Ridge National Lab

Takashi Yanai
Cornell University

APPLIED MATHEMATICS PROGRAM MANAGER:

Anil Deane
deane@ascr.doe.gov

RELATED LINKS:

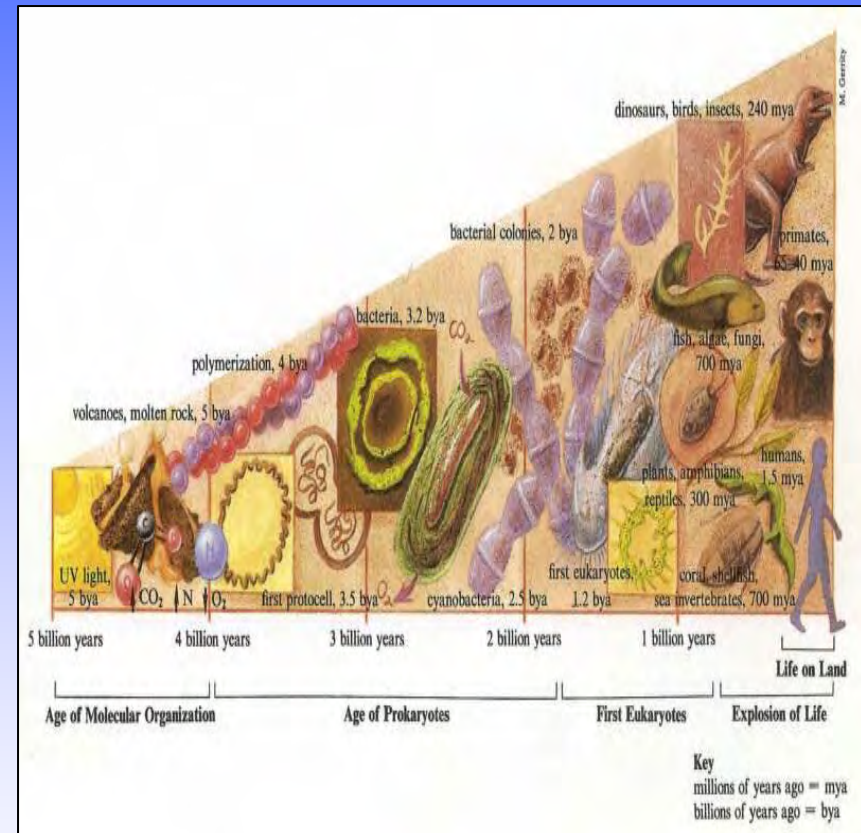
MADNESS project website

SciDAC SAP in Computational Chemistry



Evolution

- ASCR Discovery
 - Distribution issue
 - Add content elements e.g. notes by PI, linked dictionary,...
 - Evolve delivery e.g. audio clips, podcasts, rss, ...
- Other modalities
 - Print versions of stories
 - Large graphics
 - Aggregates
 - Other (of course)



Evolution, Yes but...

... with an intelligent design.

We value your comments and ideas on this project

CORONES@KRELLINST.ORG

703-413-1677

515-556-1191 (CELL)