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.

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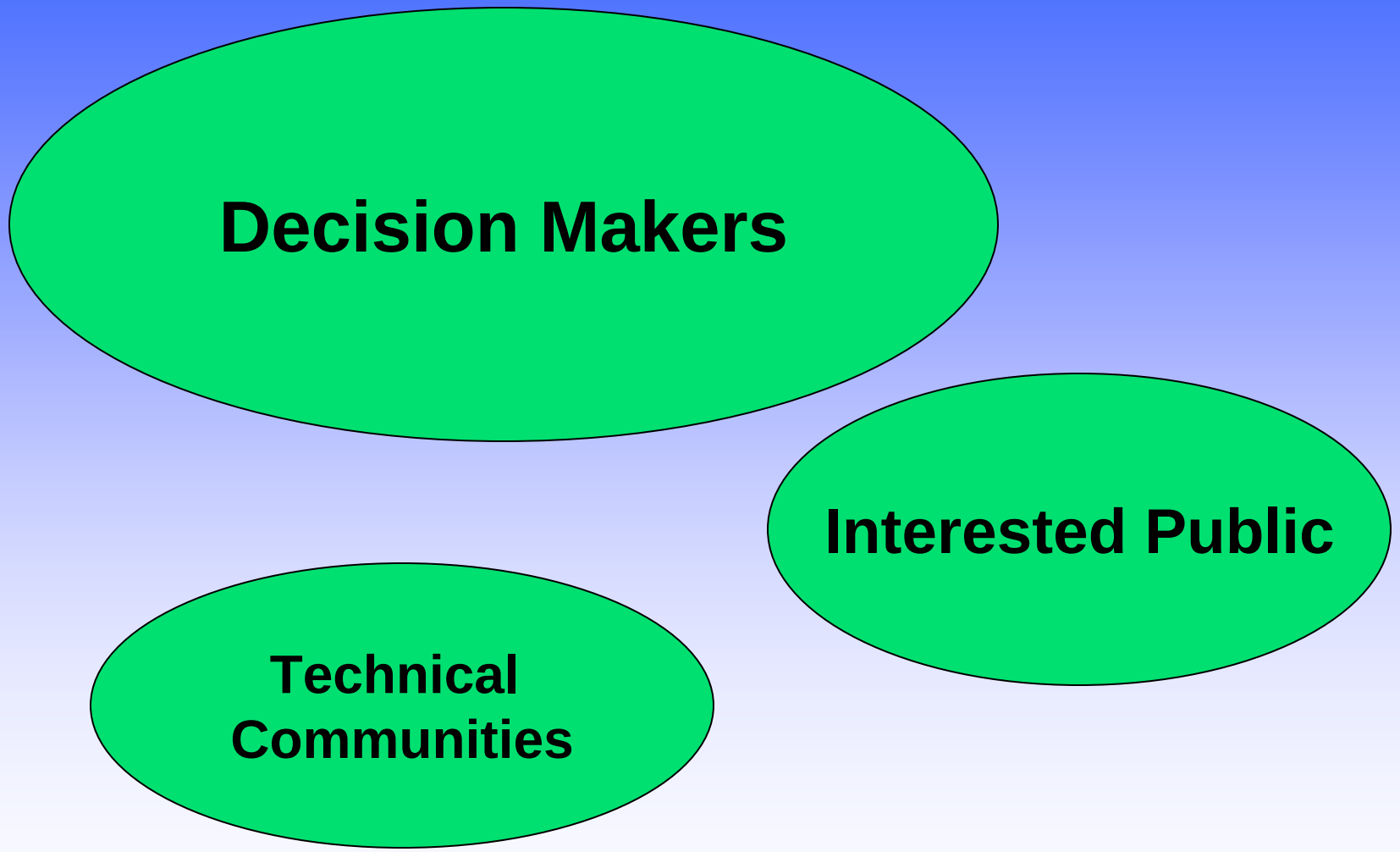
Audiences



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Context

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

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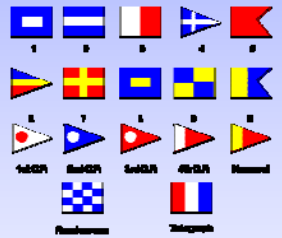
Approach

- 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.







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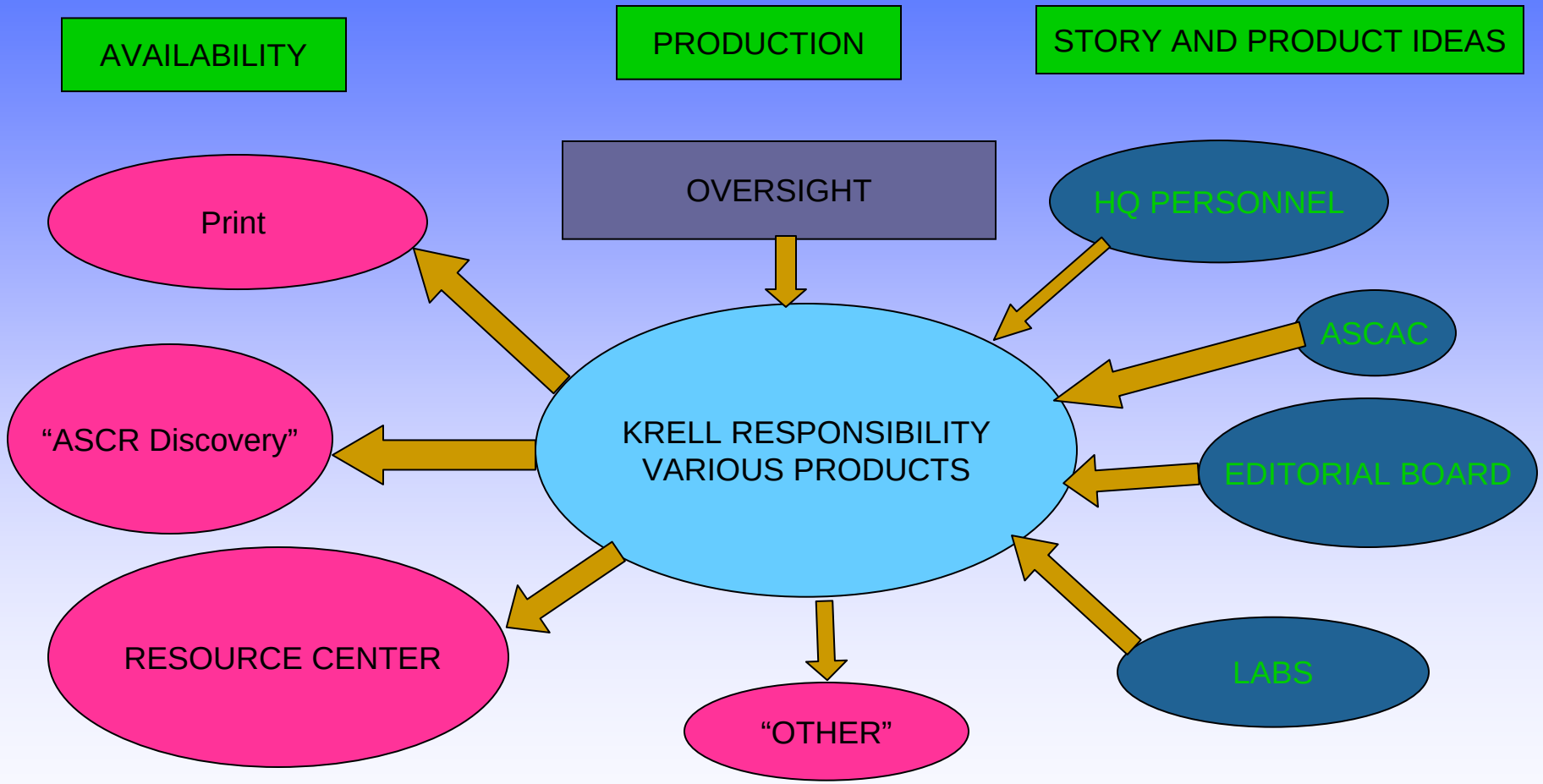
HOW WILL THIS GET DONE?



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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

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ASCR Discovery

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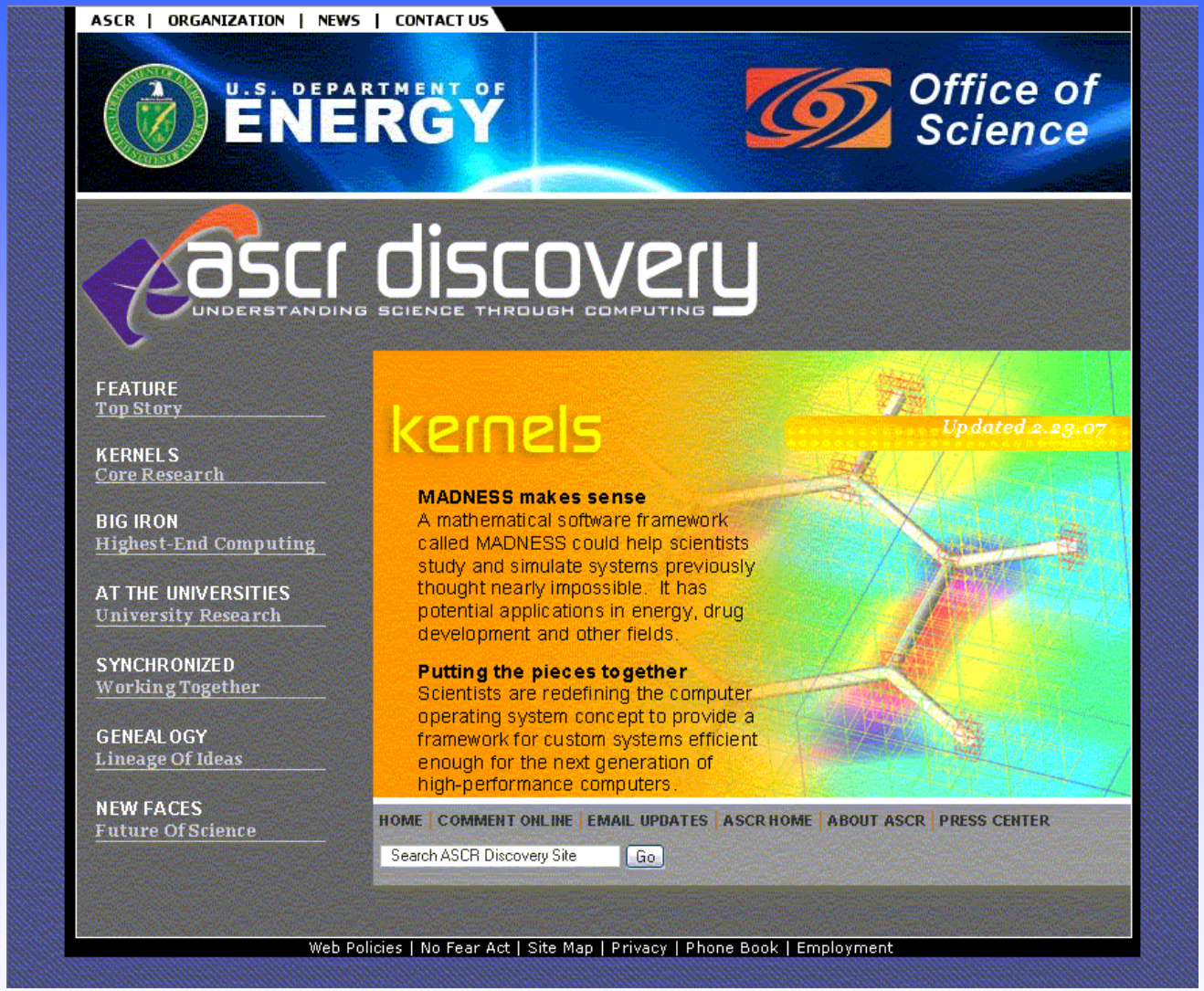

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Office of Science

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.

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RELATED LINKS:
MADNESS project website

SciDAC SAP in Computational Chemistry

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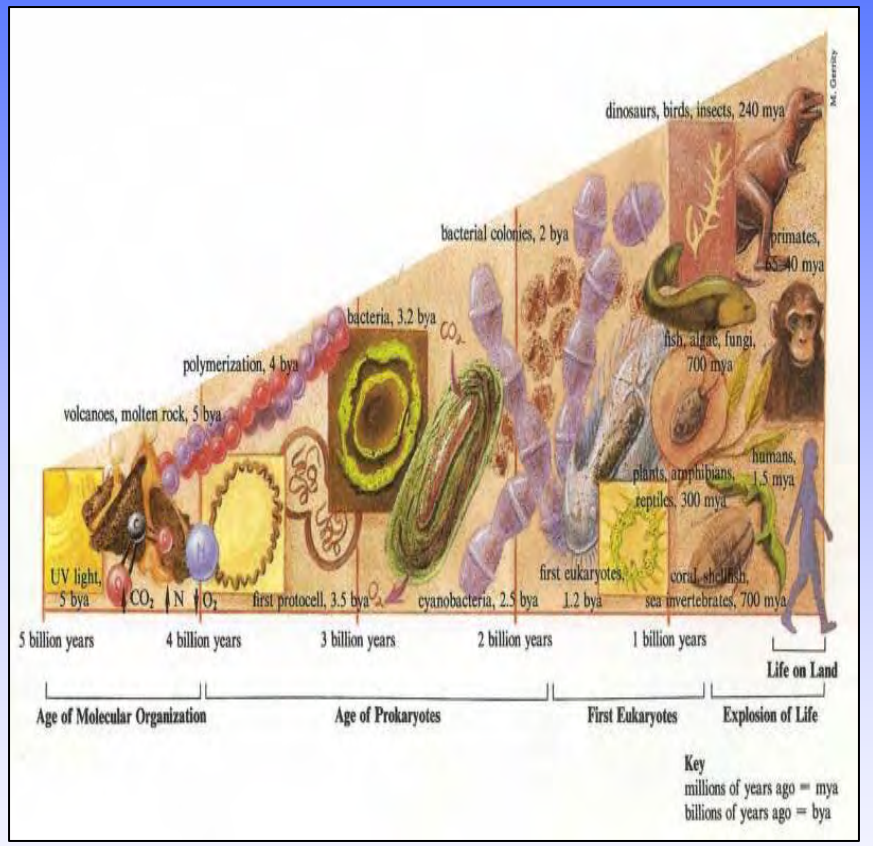
Evolution

- 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

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