The results of HPCWorld: Best practice on peer-review

JULIA WHITE, INCITE PROGRAM MANAGER

CINECA/PRACE MEETING

BOLOGNA, ITALY

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Goal of HPCWorld

Through close understanding of the details of allocation review processes in use by a number of HPC infrastructures worldwide, derive a general review methodology that ensures that allocation proposals are reviewed in a fair, competitive, transparent, and in-depth manner.

Participants

HPCW consortium
Sanzio Bassini, CINECA Francesca Garofalo, CINECA Claudio Gheller, CINECA
Sergi Girona, BSC Montserrat Gonzalez, BSC
Eric Boyer, GENCI/CINES
Thomas Eickermann, FZJ
Tony Dale, BlueFern
Mike Norman, SDSC

HPCW working group
Julia White, INCITE
Alison Kennedy, EPCC
J-C Desplat, ICHEC
Philip Webster, NASA
Dave Hart, NCAR
John Towns, NCSA
Ana Bela Dias, NWO
Abani Patra, University of Buffalo

Allocation of HPC resources

A small number of projects are granted very large awards of compute time.

INCITE
10 and 20 PF
5B core-hours
Jan – Dec '13

PRACE
10 PF
2B core-hours
May '12 – April '13
Nov '13 – Oct '14

Time awarded through allocation programs is equivalent to billions of dollars/euros.

Best practices gathered

From 2009 – 2011, representatives shared best practices for allocation of large-scale resources.

Although members were predominantly HPC, practices are relevant to non-HPC resources.

Allocations hierarchy defined

Table 1. Organizational entities engaged in the allocations process

Level 0	Government	This is the top level of the RI. It is represented by the governing entities, such as national ministries and the European Commission At this level, overall decisions about budgets and global policies are made
Level 1	Funding agencies	This is the institutional level, entities that manage funds (e.g., ESRF, NSF, DOE, NASA), allocates them to specific research themes, manages the lower levels, supervises the whole resource allocation procedure, appoints an allocation committee (Level 2), and announces opportunities, usually in the form of calls. At European level PRACE can be considered to be Level 1 with the difference that at present PRACE does not manage funds; it manages computer cycles contributed by members that host HPC resources in their countries
Level 2	Allocation committee or similar (e.g., scientific steering committee in collaboration with access committee)	According to the rules defined at Levels 0 and 1, the Level 4 entity defines the calls; specifies the evaluation and resource allocation criteria and priorities; appoints the panels; and manages the entire review, allocation, and assessment procedure
Level 3	Technical and scientific panels	The technical panel evaluates the technical feasibility of the project. The scientific panel evaluates the scientific merit, timeliness and impact. Possible thematic panels can be formed for the review of specific research areas
Level 4	Resource infrastructure management	Level 4 management is expected to follow up the project during its execution and to provide the necessary technical support. It can also be responsible for collecting and providing the information required for the assessment phase but can also delegate this responsibility to an administrative group
Level 5	User-project management	Proposals and subsequent projects have management structures, typically the principal investigator or proposer, but alternatively a designated project leadership team. User-project management receives notifications regarding allocations and is the primary point of contact for the project

Basis for allocations

The peer review process has been selected as the most successful and effective best practice, based on its widespread use within funding agencies, a large number of production infrastructures, and scientific publications. [Reference Levels 2 & 3]

Review principles

Transparency—The review process should be transparent, both to proposers and stakeholders.

Expert assessment—Peer reviewers should be experts with appropriate knowledge and experience.

Confidentiality—The identity of proposers and reviewers should be protected.

Right of appeal—Proposal submitters should be able to appeal to the reviewers for reconsideration of unsuccessful proposals.

Prioritisation—Proposals should be ranked according to the evaluation criteria defined for the call and completed according the ranking.

Management of conflicts of interests—Reviewers and members of the review panels should not have a conflict of interest with proposals assigned to them. Conflicts of interest can be personal, professional or intellectual.

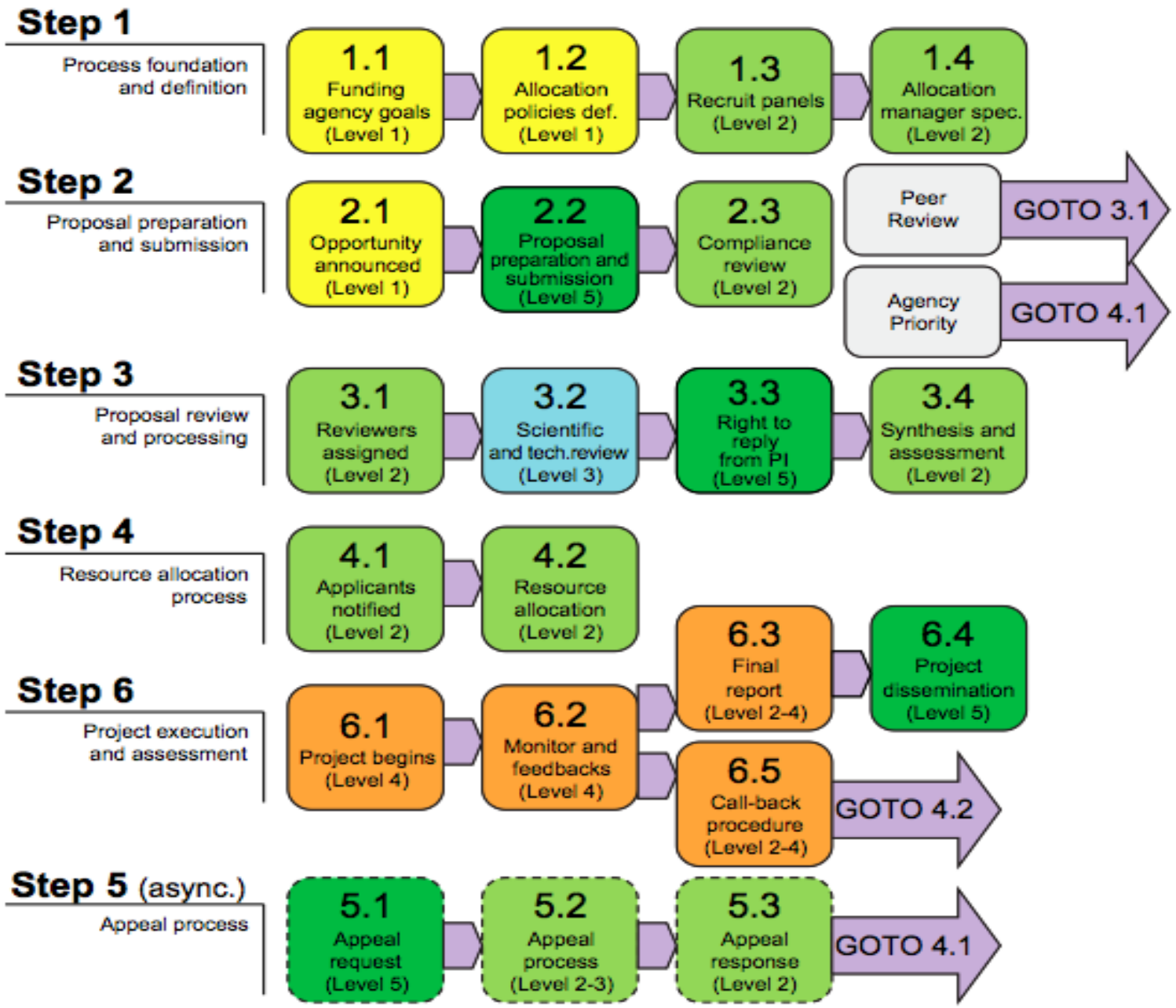
Review principles cont.

No parallel assessment—There should be a single and unique assessment; i.e., all proposals should be assessed according to the same criteria. (Submitters have the right to appeal when their proposals are rejected.)

Fairness to the science proposed—Managers of the review process should ensure that there is no favoritism toward any scientific disciplines and that all proposals are evaluated on the basis of scientific excellence.

Avoidance of parochialism—The review process should ensure that proposals from particular regions, institutions, or countries are not favored.

Good communication channels—The RI should be prompt in notifying the PI or user-project management of the outcome of the allocation process and in providing all other necessary information regarding the project and its progress.



Allocation life cycle

Technical review

The technical review is compulsory and is deployed by the Technical Panel, which is typically composed by experts local to the infrastructure.

In general, the technical review provides a yes/no response that precedes the scientific evaluation.

The technical review should base its comments on:

- the justification of the need of accessing to the research infrastructure
- the suitability of requested resources (both software and hardware)
- the timeframe of the workplan
- the applicant's experience and the probability to fulfil the project aims

Technical evaluation does not consider any evaluation of the purposed activity but only technical aspects.

Scientific review

The scientific review is performed by the Scientific Panels, composed by experts in different scientific domains, which have to evaluate the proposals in terms of scientific relevance and impact of the project in the specific scientific field.

The scientific review should base its comments on:

- the objective of the scientific project that frames the activity requested in the application
- the relevance and impact in an specific scientific area
- the researcher team curriculum

Scientific assessment has a completely different significance than the technical one.

Applications of best practices

These best practices are employed by many HPC sites…

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…as well as non-HPC facilities. For example, the $1.4B Spallation Neutron Source; the Advanced Photon Source; and the Center for Nanophase Materials Science.

Practical considerations

The process described represents an idealized outline of the major components of the general best practices for allocations.

Each resource institution must customize the general process for its specific situation and stakeholders.

Practical considerations

Overall Concerns

- Process bottlenecks
- Adaptation to numbers of proposals and frequency of process
- Record keeping

Step 1: Process Foundation and Definition

- “Quotas” per science domains
- Industry Access
- "Juste retour" principle and exchange of resources

Practical considerations

Step 2: Proposal Preparation and Submittal

- Programme access and other types of research efforts
- Allocation of ancillary resources
- Contingent allocations and submissions to multiple RIs

Step 3: Proposal Review and Processing

- Double jeopardy (science twice)
- Competing proposals on same topic
- Allocation committee election and evaluation (e.g. recursion)
- Reviewer pool and quality

Practical considerations

Step 4: Resource Allocation Process

- Over- and under-allocation
- Ranking procedures and reconciliation (programme goals, ex. Grand challenge scale vs. Community)
- User agreement
- Legal issues (IP, conflicts, privacy)

Practical considerations

Step 5: Appeal Process

- Successful appeals (timing, where does time come from)

Step 6: Project Execution and Assessment

- Operational policies and resource management (queueing, reservations, workflow)
- Supplemental requests for time and resources

Continuation of HPCworld

An MoU is underway with interested centers for "*Maintainance of the HPCWorld model for access to RIs*."

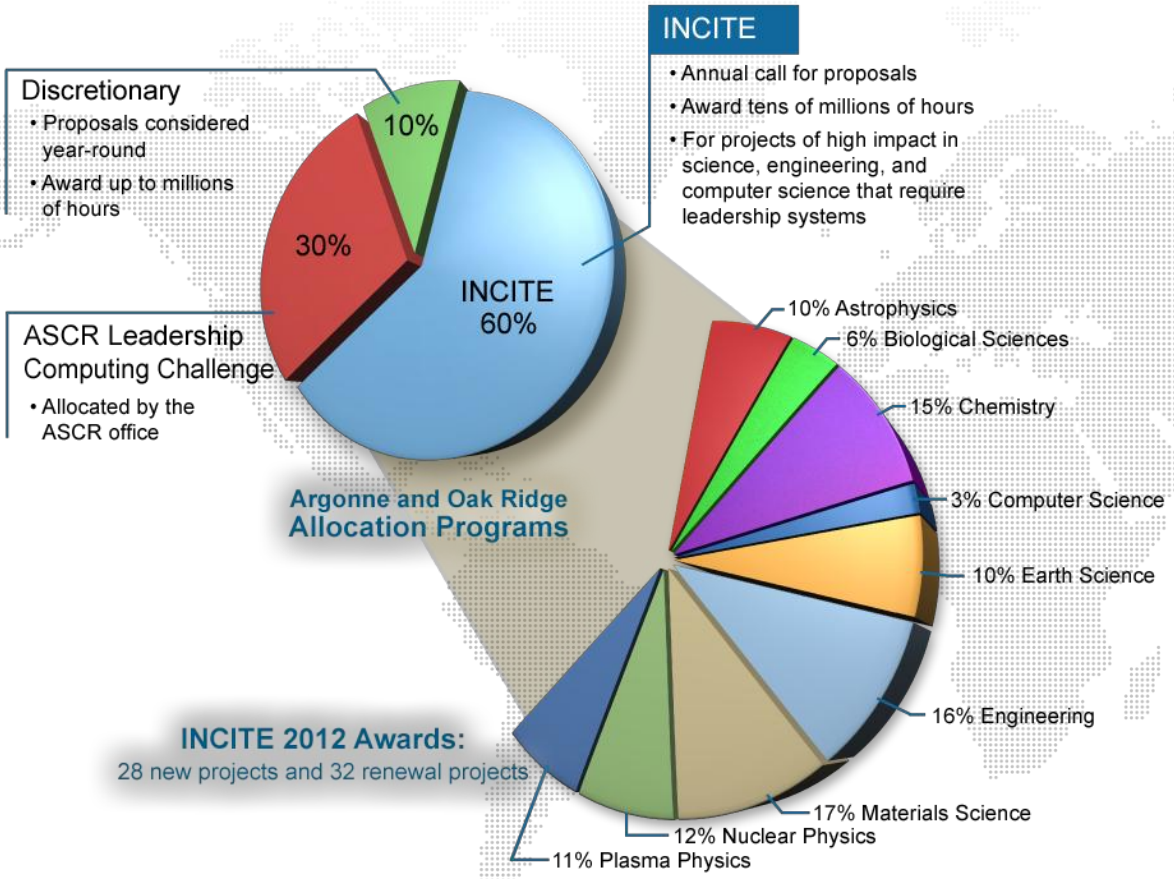
- Act as "observatory" of the changes and evolutions of the practices in the peer review processes.
- Keep the handbook updated.
- Provide support to the ongoing programmes, agencies, and research infrastructures implementing models of peer review.

INCITE

INNOVATIVE AND NOVEL COMPUTATIONAL IMPACT ON THEORY AND EXPERIMENT

INCITE IS ENTERING ITS 10TH YEAR

INCITE provides awards of time on the Oak Ridge and Argonne Leadership Computing Facility systems for researchers to pursue transformational advances in science and technology: **1.7 billion core hours** were awarded in 2012.



Call for Proposals

The INCITE program seeks proposals for high-impact science and technology research challenges that require the power of the leadership-class systems. Allocations will be for calendar year 2013.

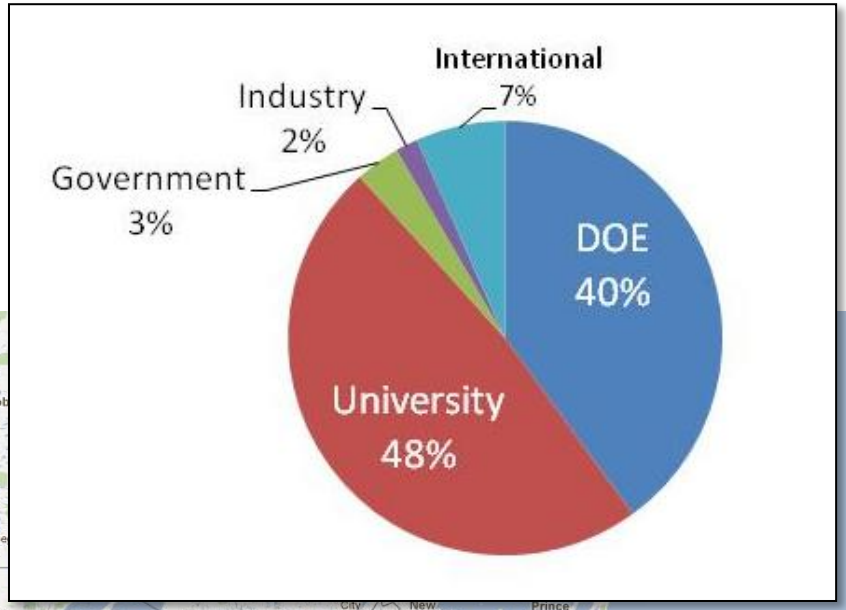
April 11 – June 27, 2012

Contact information
Julia C. White, INCITE Manager
whitejc@DOEleadershipcomputing.org

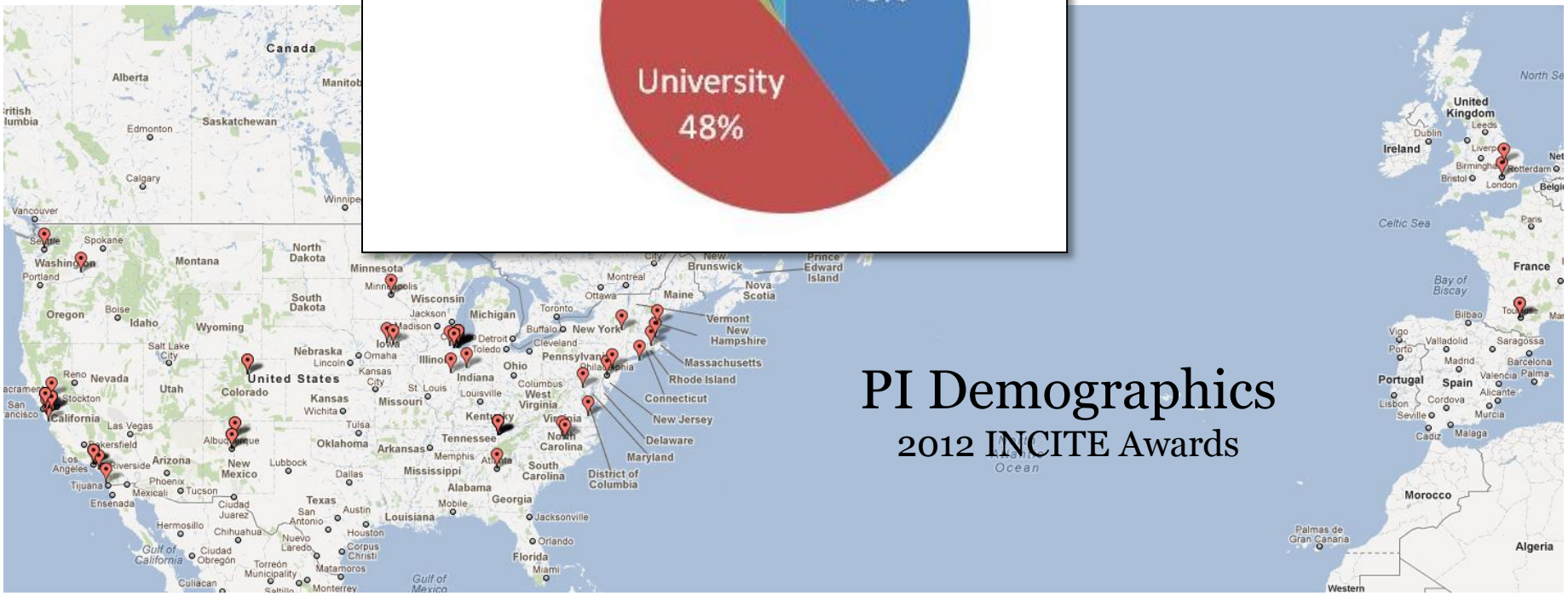
INCITE criteria

1	**Impact criterion**
	High-impact science and engineering
2	**Computational leadership criterion**
	Computationally intensive runs that cannot be done anywhere else
3	**Eligibility criterion**
	• INCITE grants allocations regardless of funding source (ex. DOE, international agency, private, etc) • Non-US-based researchers are welcome to apply

2012 INCITE award demographics

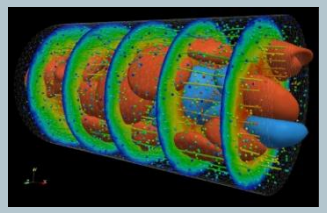


PI Affiliations
2012 INCITE Awards



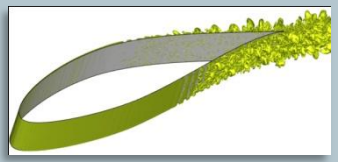
PI Demographics
2012 INCITE Awards

Simulating a flow of healthy (red) and diseased (blue) blood cells with a Dissipative Particle Dynamics method.
- George Karniadakis, Brown University

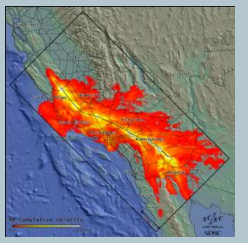


Provide new insights into the dynamics of turbulent combustion processes in internal-combustion engines.
-Jacqueline Chen and Joseph Oefelein, Sandia National Laboratories

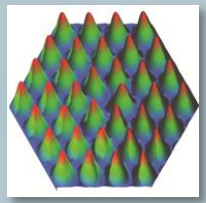
Demonstration of high-fidelity capture of airfoil boundary layer, an example of how this modeling capability can transform product development.
- Umesh Paliath, GE Global Research



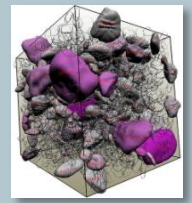
Calculating an improved probabilistic seismic hazard forecast for California.
- Thomas Jordan, University of Southern California



Modeling charge carriers in metals and semiconductors to understand the nature of these ubiquitous electronic devices.
- Richard Needs, University of Cambridge, UK



High-fidelity simulation of complex suspension flow for practical rheometry.
- William George, National Institute of Standards and Technology



Other INCITE research topics

- Glimpse into dark matter
- Supernovae ignition
- Protein structure
- Creation of biofuels
- Replicating enzyme functions
- Global climate
- Regional earthquakes
- Carbon sequestration
- Turbulent flow
- Propulsor systems
- Membrane channels
- Protein folding
- Chemical catalyst design
- Combustion
- Algorithm development
- Nano-devices
- Batteries
- Solar cells
- Reactor design
- Nuclear structure

Opportunities for collaboration

At this meeting and elsewhere (e.g. ISC12) there are opportunities to discuss potential coordination of activities.

- Joint advertising of calls for proposals
- Co-sponsored workshops and training events
- Others…

Contacts

For details about the INCITE program:

www.doeleadershipcomputing.org
INCITE@DOEleadershipcomputing.org

U.S. DEPARTMENT OF ENERGY
INCITE
LEADERSHIP COMPUTING

For details about the centers:

www.olcf.ornl.gov
help@nccs.gov, 865-241-6536

OAK RIDGE
National Laboratory

www.alcf.anl.gov
support@alcf.anl.gov, 866-508-9181

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