







John McGee – mcgee@renci.org

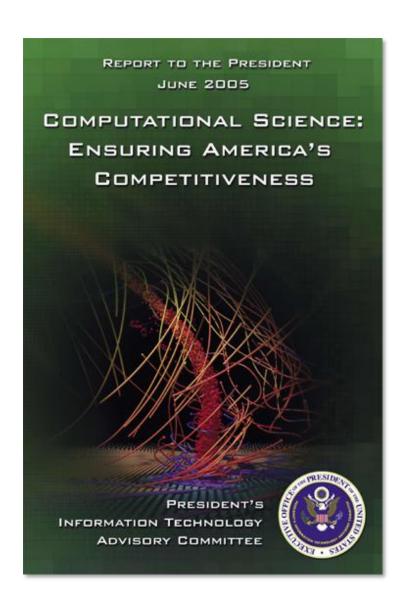
Renaissance Computing Institute
University of North Carolina, Chapel Hill







Computational Science is a critical component of discovery, and its importance is growing



http://www.nitrd.gov/pitac/reports/20050609_computational/computational.pdf





HTC vs. HPC

- High Throughput Computing (HTC)
 - simple serial jobs, mote carlo, parameter sweep
 - complex workflows with data and/or job dependencies
 - ensembles of small node count MPI jobs
 - must be able to express the work in a highly portable way
 - cannot care about exactly where pieces are executed
 - do not have SSH access to resources; many implications
 - must be able to respect the community rules of a shared infrastructure;
 "plays well with others"
 - remarkable scaling opportunities





HTC vs. HPC

- High Performance Computing (HPC)
 - top N computational scientists in the world
 - many important problems simply cannot be solved any other way
 - what does it take to successfully develop or run models at 256, or 512+ node parallelism?
 - what percentage of researchers that can benefit from computational science can realistically do this today?
 - how does grid /distributed computing fit with large scale HPC applications?



Where do researchers go for services?

- PI owned and operated cluster
- Campus Condo Computing
- Departmental Cluster
- Campus Research Computing
- Campus Condor Pool
- Regional Grids (eg NWICG)
- Communities of Practice (NanoHub, GridChem, etc)
- Open Science Grid: DOE/NSF, opportunistic access
- TeraGrid: NSF, competitively awarded allocations
- DOE ASCR: INCITE awards
- Commercial Cloud service providers
- There must be more ... what have I missed? where is NIH?

Where do researchers go for services?

Answer: wherever they can get it, with the least amount of pain

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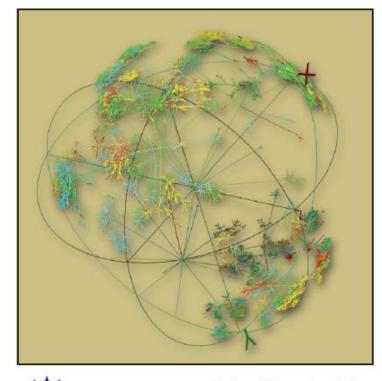
How many different:

- service interfaces
- software stacks
- policy frameworks
- identities per researcher

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where is The National Cyberinfrastructure?

CYBERINFRASTRUCTURE VISION FOR 21st CENTURY DISCOVERY



National Science Foundation Cyberinfrastructure Council March 2007

Ind cture le and sion fonission tered, tipae, and es are ognize nclusive n scis and rs in all nd rely ment, is chapgoals initia-

CI_Vision_March07.pdf - Adobe Acrobat Professional

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An effective computing environment designed to meet the computational needs of a range of science and engineering applications will include a variety of computing systems with complementary performance capabilities. NSF will invest in leadership class environments in the 0.5-10 petascale performance range. Strong partnerships involving other federal agencies, universities, industry and state government are also critical to success. NSF will also promote resource sharing between and among academic institutions to optimize the accessibility and use of HPC assets deployed and supported at the campus level. Supporting software services include the provision of intelligent development and problem-solving environments and tools. These tools are designed to provide improvements in ease of use, reusability of modules, and portable performance.

- A picosecond is 10⁻¹² second
- A petascale is 10¹⁵ operations per second with comparable storage and networking capacity

e density for iron oxide (FeO) within the local density approximation, with ors represent the spin density, showing the antiferromagnetic ordering.

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ategy to

The Open Science Grid

A framework for large scale distributed resource sharing

addressing the technology, policy, and social requirements of sharing

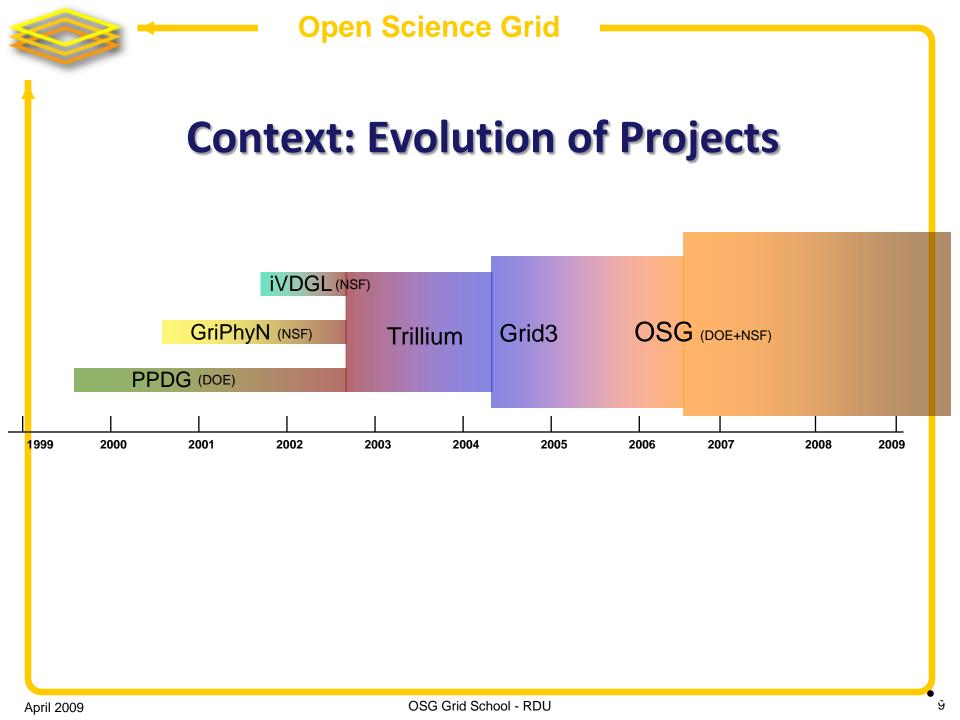
OSG is a consortium of software, service and resource providers and researchers, from universities, national laboratories and computing centers across the U.S., who together build and operate the OSG project. The project is funded by the NSF and DOE, and provides staff for managing various aspects of the OSG.

Brings petascale computing and storage resources into a uniform grid computing environment

Integrates computing and storage resources from over 80 sites in the U.S. and beyond







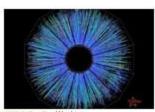


Using OSG Today

- Astrophysics
- Biochemistry
- Bioinformatics
- Earthquake Engineering
- Genetics
- Gravitational-wave physics
- Mathematics
- Nanotechnology
- Nuclear and particle physics
- Text mining
- And more...



ATLAS Detector
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STAR Collision
Image Credit Brookhaven
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Collaboration
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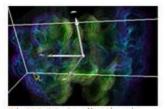
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BioMOCA Application in nanoHUB
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<u>DZero Detector</u> Image Credit Fermilab Permission Information



Why should my University facilitate (or drive) resource sharing?

- Enables new modalities of collaboration
- Enables new levels of scale
- Democratizes large scale computing
- Sharing locally leads to sharing globally
- Better overall resource utilization
- Funding agencies care about this

At the heart of the cyberinfrastructure vision is the development of a cultural community that supports peer-to-peer collaboration and new modes of education based upon broad and open access to leadership computing; data and information resources; online instruments and observatories; and visualization and collaboration services.

Arden Bement CI Vision for 21st Century introduction



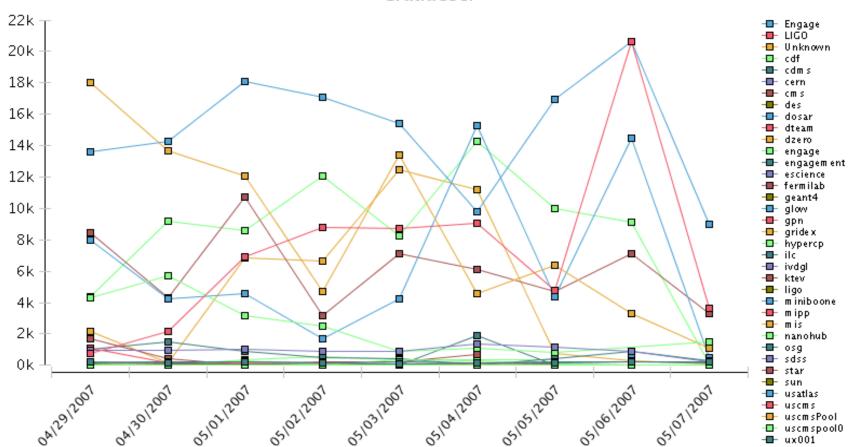


OSG Engagement Mission

- 1. Help new user communities from diverse scientific domains adapt their computational systems to leverage OSG
- 2. Facilitate University Campus CI deployment, and interconnect it with the national community
- 3. Provide feedback and new requirements to the infrastructure providers





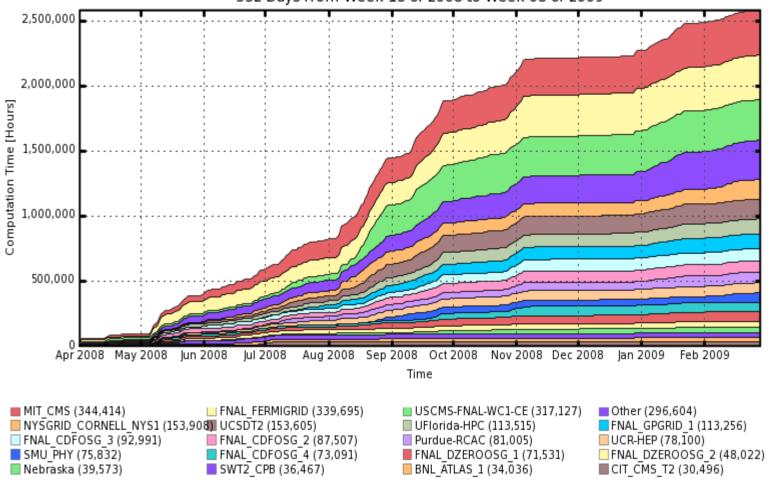


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Engaged Users Activity

Cumulative Hours Spent on Jobs By Facility





Total: 2,580,785 Hours, Average Rate: 0.09 Hours/s



Questions?

OSG Engagement VO

https://twiki.grid.iu.edu/twiki/bin/view/Engagement/WebHome

engage-team@opensciencegrid.org



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