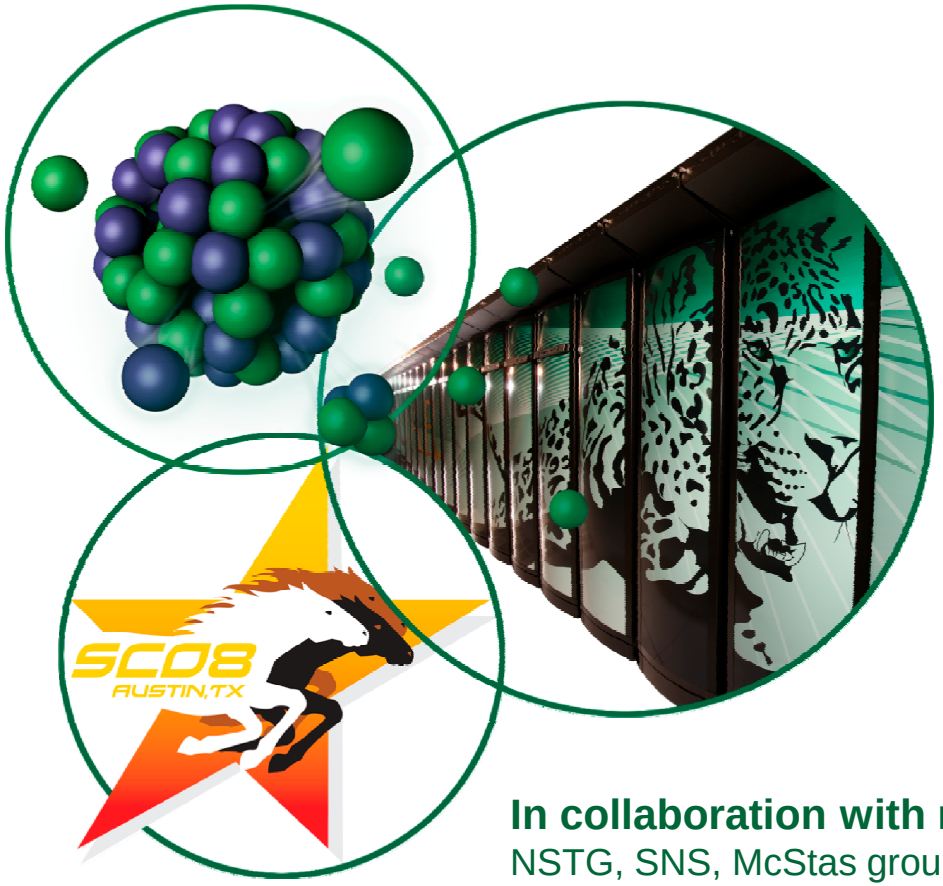
The Neutron Science TeraGrid Gateway: TeraGrid Cyberinfrastructure at ORNL



Presented by

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Computer Science and Mathematics
Office of Cyberinfrastructure
National Science Foundation

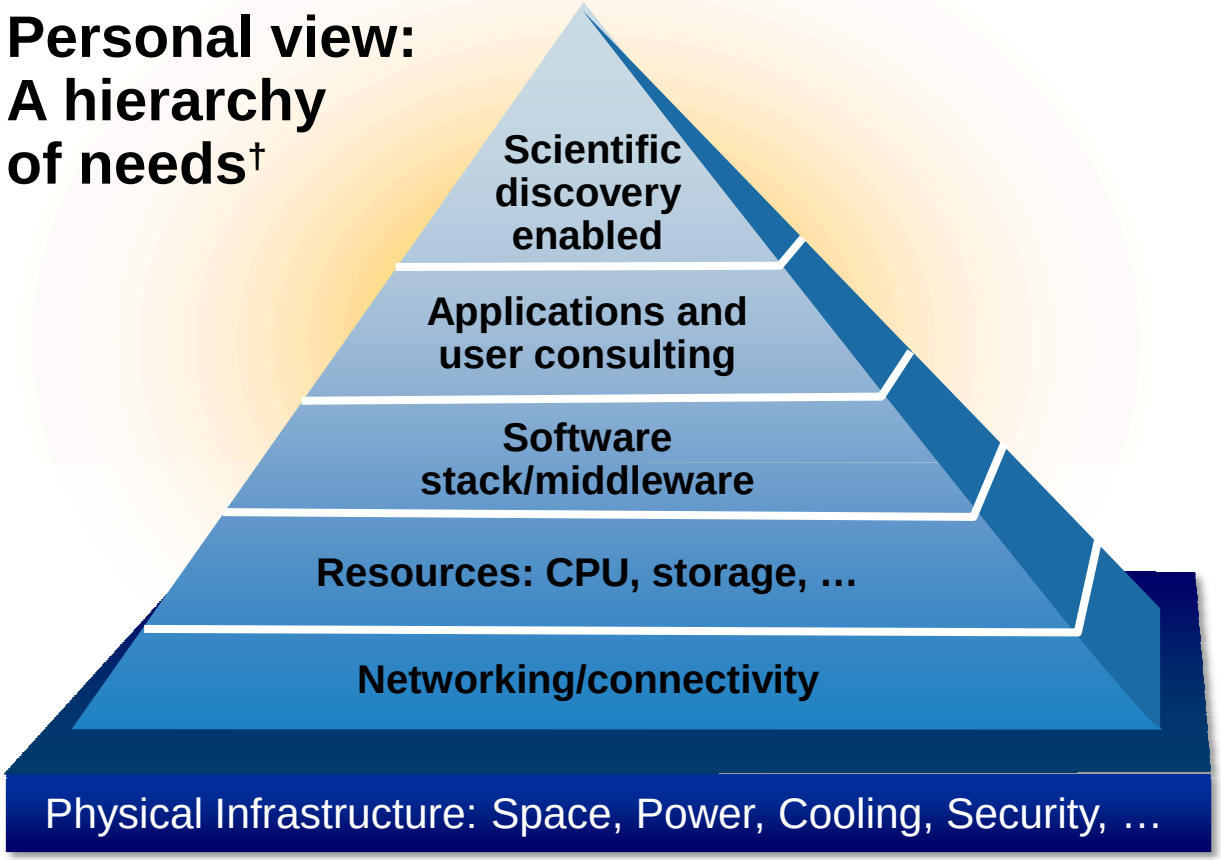
In collaboration with many teams:
NSTG, SNS, McStas group, Open Science Grid, Earth Systems Grid, TechX Corp, OGCE, UK eScience effort, and the TeraGrid Partners teams.

Outline

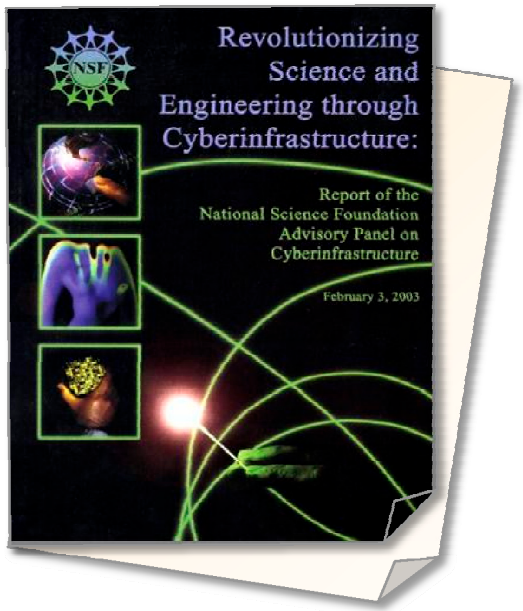
1. Cyberinfrastructure (CI)
2. TeraGrid
3. The Spallation Neutron Source
4. The Neutron Science TeraGrid Gateway
5. Other collaborations

Cyberinfrastructure overview

Personal view: A hierarchy of needs†



2003 Blue Ribbon Panel: "Atkins Report"



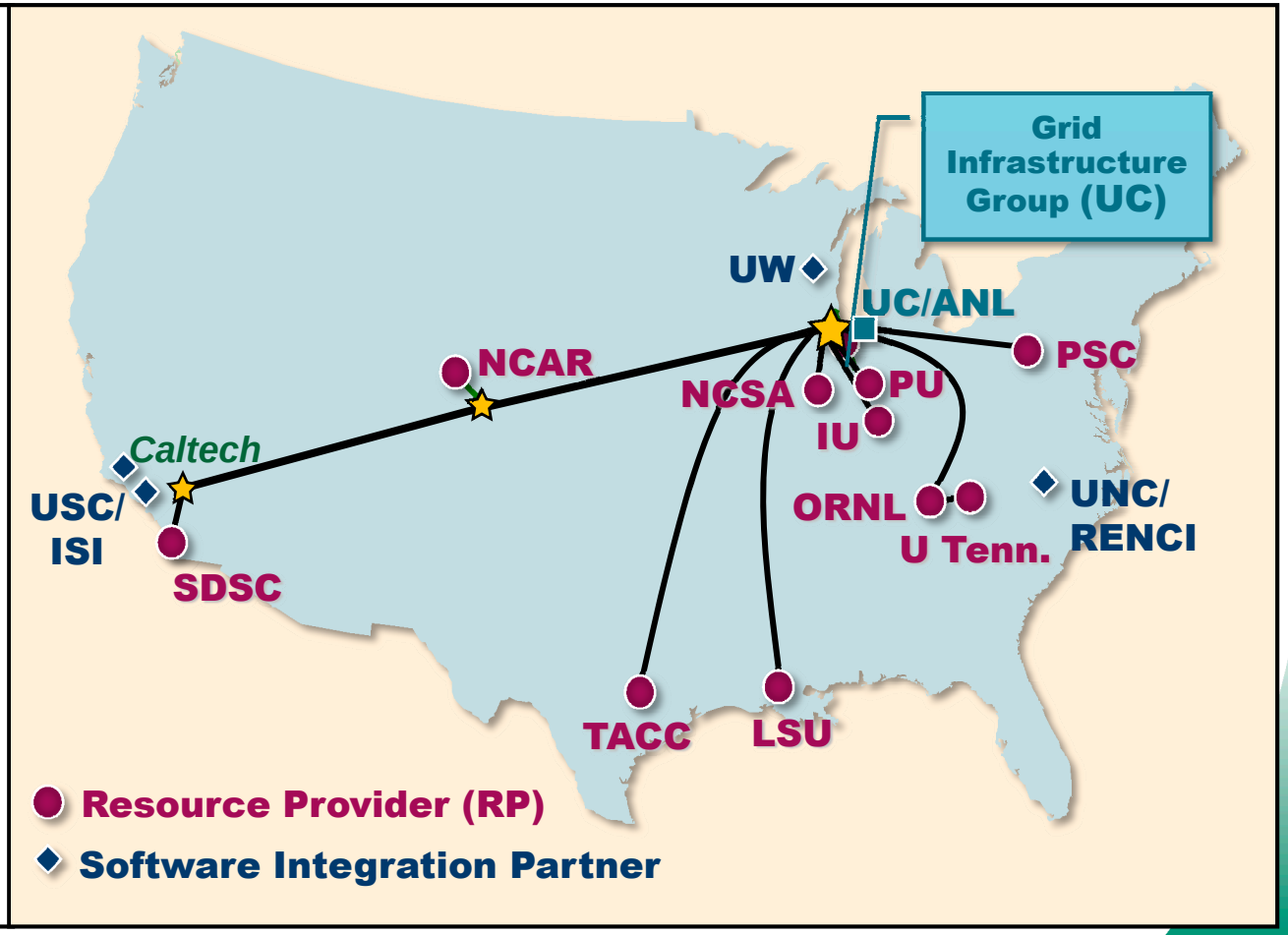
"Like the physical infrastructure of roads, bridges, power grids, telephone lines, and water systems that support modern society, **Cyberinfrastructure** refers to the distributed computer, information and communication technologies combined with the personnel and integrating components that provide a long-term platform to empower the modern scientific research endeavor ." ‡

†A. H. Maslow. "A Theory of Human Motivation," *Psychological Review*, **50**, 370−396 (1943)

‡ David Hart in NCSA News release "National Science Foundation Releases New Report from Blue-Ribbon Advisory Panel on Cyberinfrastructure" February 3, 2003 http://access.ncsa.uiuc.edu/Releases/03Releases/02.03.03_National_S.html as quoted on Cyberinfrastructure Wikipedia entry.

TeraGrid resource providers

- Dedicated links
- Resource to resource
- Bandwidth unit: 10 Gbps
- Substrate for high-performance high-quality data movement and communications



TeraGrid resources

TeraGrid Systems Monitor

HPC Systems | Storage Systems | Advanced Vis Systems | Special Purpose Systems

High Performance Systems

Name	Institution	System	Peak TFlops	Memory TBytes	Status	Load	Running Jobs	Queued Jobs	Other Jobs
Ranger	TACC	Sun Constellation	579.40	123.00	Up		392	3	53
Kraken	NICS	Cray XT4	166.00	18.04	Up		28	7	19
Abe	NCSA	Dell Intel 64 Linux Cluster	89.47	9.38	Up		162	23	47
Lonestar	TACC	Dell PowerEdge Linux Cluster	62.16	11.60	Up		142	79	4
Steele	Purdue	Dell Intel 64 Linux Cluster	60.00	12.40	Up		597	52	38
Queen Bee	LONI	Dell Intel 64 Linux Cluster	50.70	5.31	Up		90	39	0
Big Red	IU	IBM e1350	30.60	6.00	Up		310	156	791
BigBen	PSC	Cray XT3	21.50	4.04	Up		26	25	41
TeraGrid Cluster	NCSA	IBM Itanium2 Cluster	10.23	4.47	Up		134	72	0
Cobalt	NCSA	SGI Altix	6.55	3.00	Up		78	256	0
Frost	NCAR	IBM BlueGene/L	5.73	0.51	Up		10	0	1
Pople	PSC	SGI Altix 4700	5.00	1.54	Up		26	39	30
TeraGrid Cluster	SDSC	IBM Itanium2 Cluster	3.10	1.02	Up		8	0	6
TeraGrid Cluster	UC/ANL	IBM Itanium2 Cluster	0.61	0.24	Up		54	14	0
NSTG	ORNL	IBM IA-32 Cluster	0.34	0.07	Up		1	0	1
		Total:	**1091.39**	**200.62**			**2058**	**765**	**1031**

**Indicates failure of one or more status test.*
Hover mouse pointer over Resource Name, Resource Status, and headings to see additional information.

- **11 distributed centers**
- **> 1 petaflop**
  On path to double every year
- **2.9 petabyte disk**
- **6 petabyte archive**
- **Different resource types**
  - **Capability**
  - **Capacity**
  - **High throughput**
  - **Visualization**
  - **Specialized use**
- **Common user environments**
- **Tuned data transfer over dedicated 10+ gbs network**

Science gateways

- TeraGrid size: How can we manage it?
  - Today: 4000+ user accounts across 20 resources
  - Target: 10–100× increase in user base; increase in number of resources
- **TeraGrid science gateways**
  1. Web portal with users in front and TeraGrid services in back
  2. Grid-bridging gateways: Extending the reach of a community grid (devoted to a single area of science) so it can use TeraGrid resources
  3. Application programs running on users' machines (e.g., workstations and desktops) that access TeraGrid (and other) services
- The Neutron Science TeraGrid Gateway NSTG is one of 32 existing gateways

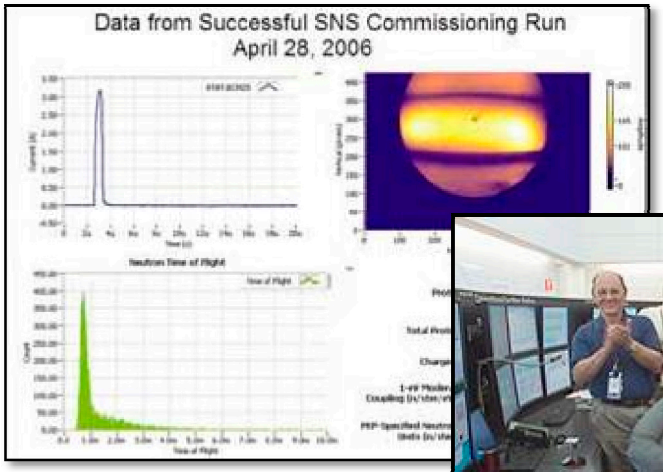
Charting new territory for wide cyberinfrastructure services

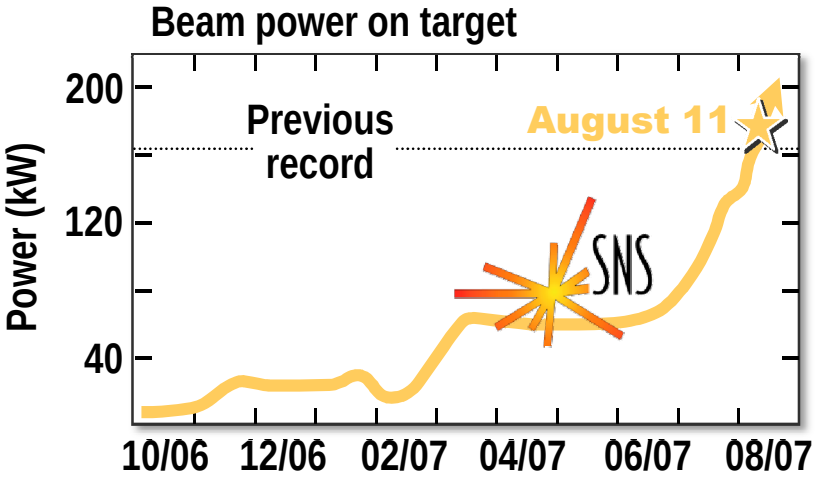
- Federated user management
- Callback end-user identification with automated service auditing across federated identity space "gateway community accounts"
- Grid interoperability
- Participation in attribute-based authorization

Spallation Neutron Source

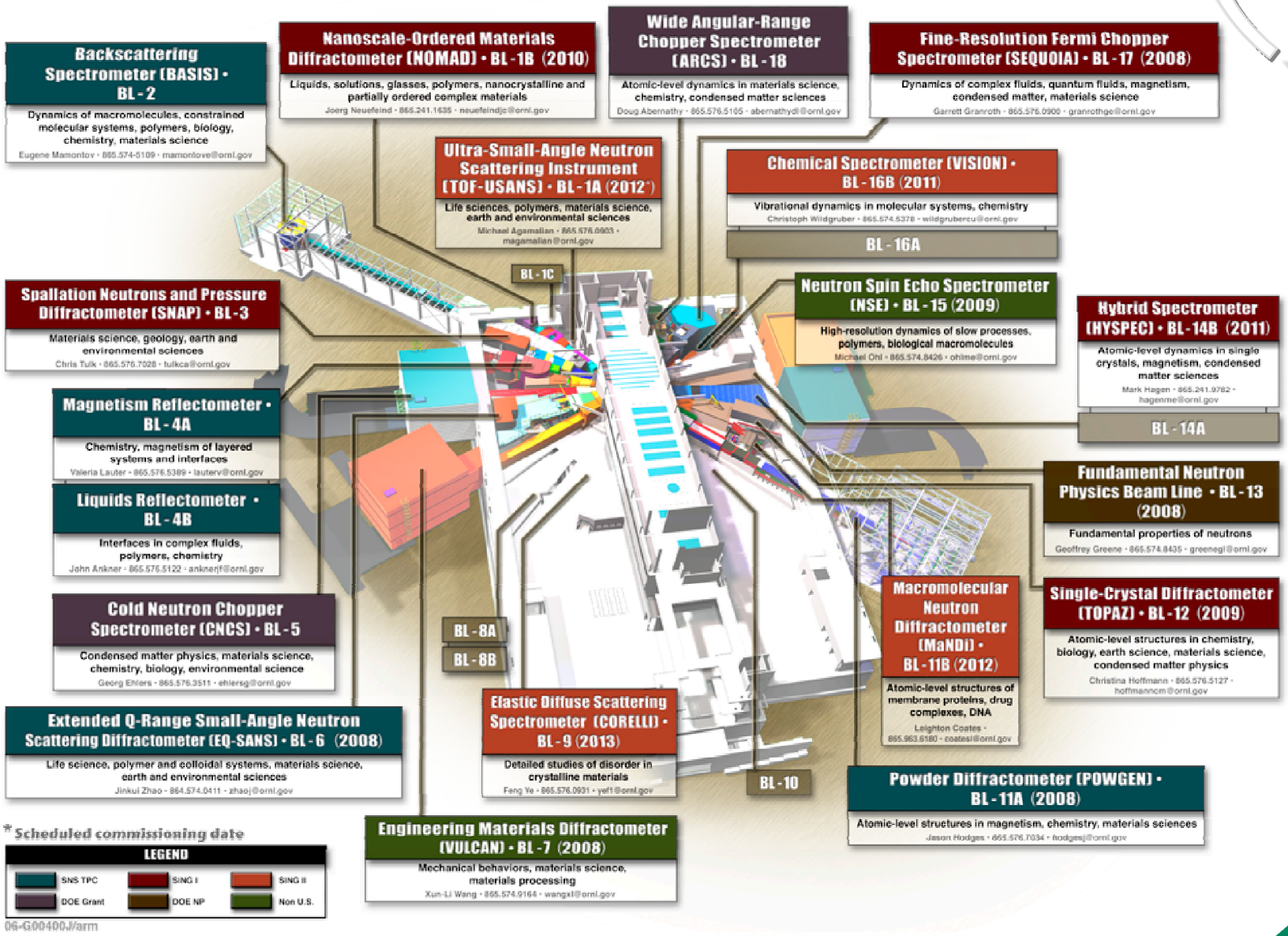
"The next generation of materials research"

Large world-class user facility	• Neutrons as a probe of matter
Construction complete	• 1998–2006, TPC $1.4 billion
Accelerator power-up	• Ongoing— 183 kW record set in August 2007; over 600 kW now
Instruments	• Commissioning 3 to 4 per year • 6 in user program • 13 under construction • Additional under consideration
User program	• 73 allocated experiments already





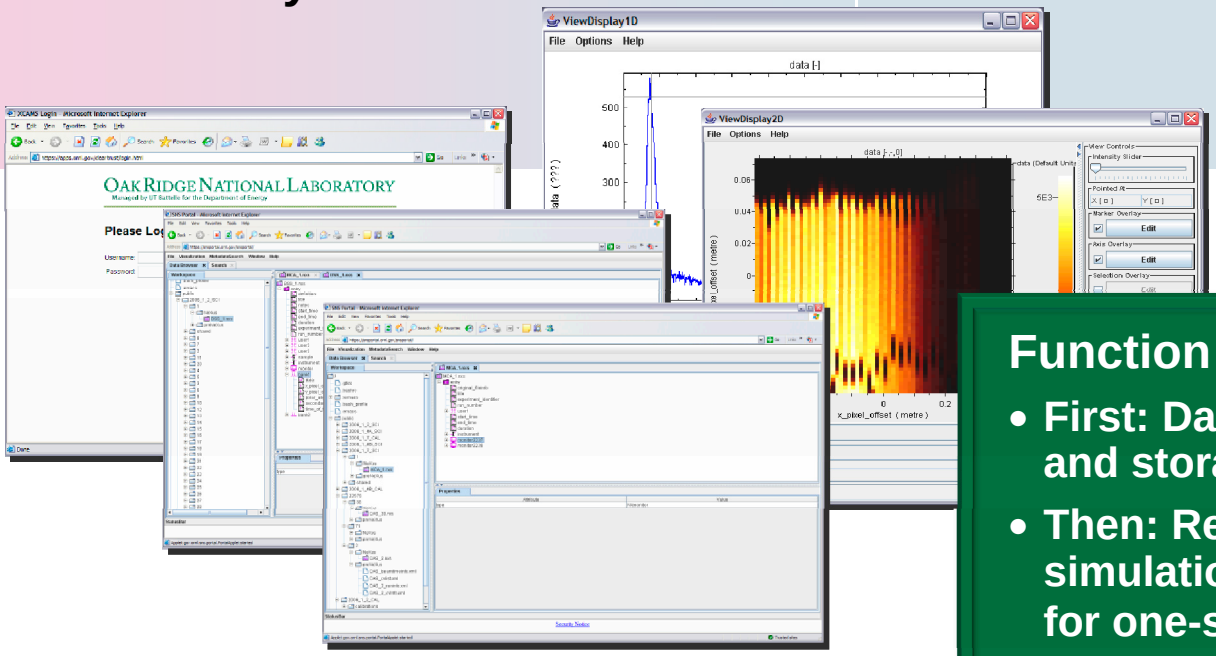
SNS instrument suite



SNS data access via portal
(Reduction, analysis, and simulation as well)

Turnkey solutions are being requested by users and user groups

Problem	SNS approach
Providing advanced tools in an easy fashion while retaining customizability	• Neutron Science User Portal – Totally in Java



Function deployment order

- First: Data acquisition and storage/stewardship
- Then: Reduction, analysis, simulation, proposals for one-stop access

Acknowledgement: S. Miller and SNS Advisory SW group;
J. Kohl, S. Vazhkudai, and ORNL/CSM division)

Neutron science portal view

Currently hosts data from five different facilities

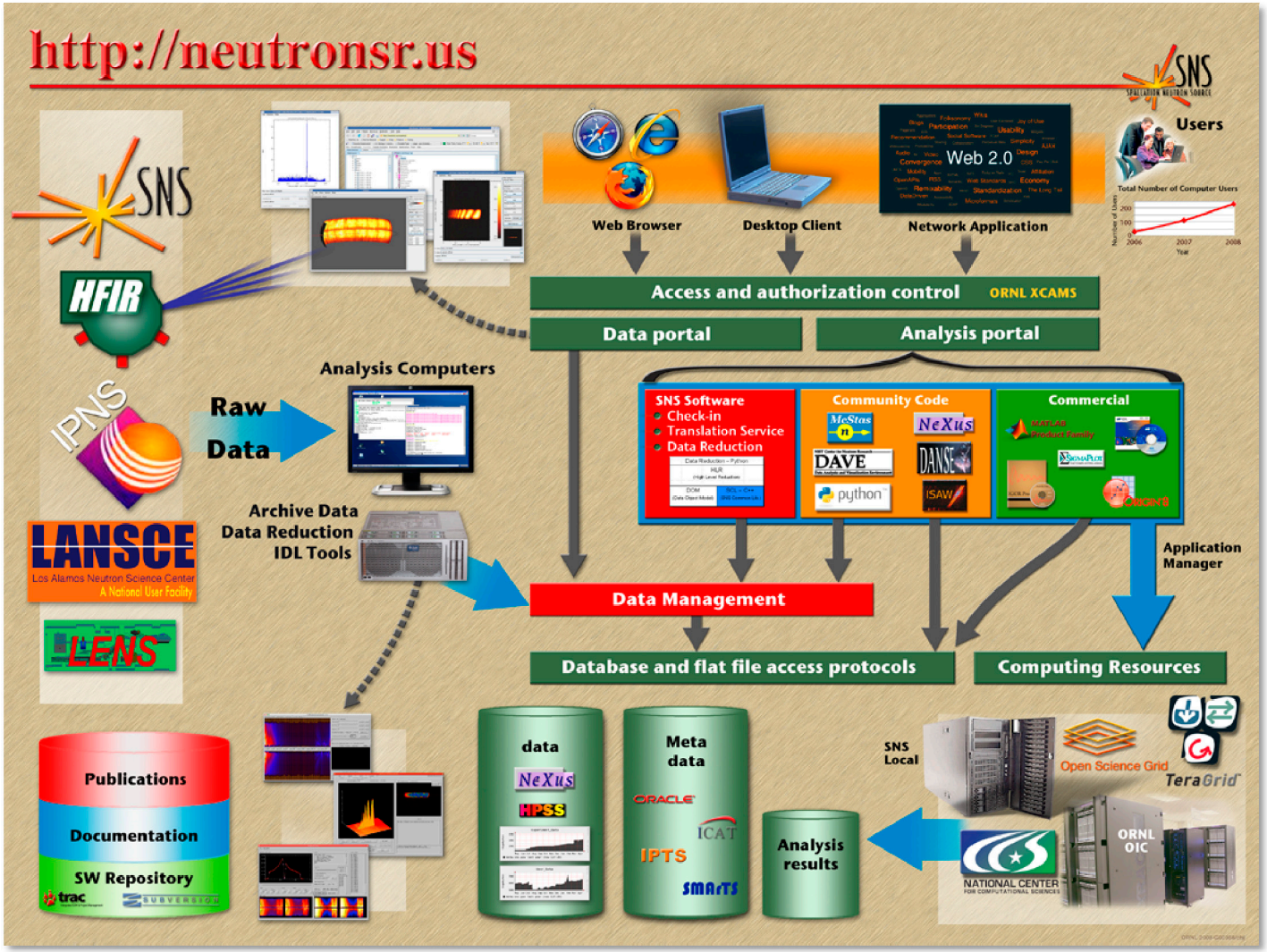
SNS

HFIR

IPNS

LANSCE

LENS



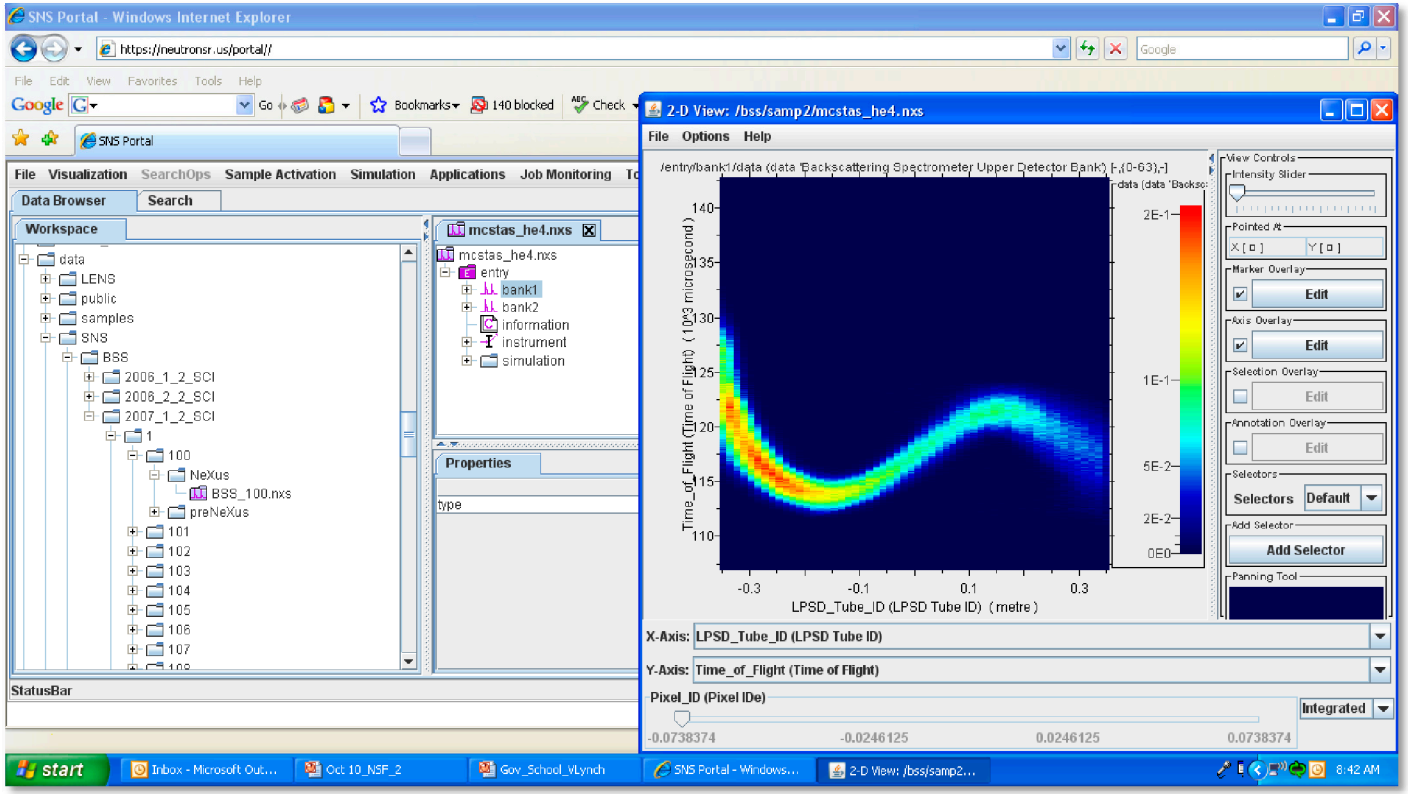
Acknowledgement: From SNS ASG

Simulation available from portal

Simulation of inelastic scattering off of He_4 sample in Backscattering Spectrometer (BASIS)

- Using McStas
- 1010 simulation neutrons
- Performed on NSTG cluster

Acknowledgement: V. E. Lynch, M. Hagen



NeXus
A community-driven standards process

- Data format for neutron, X-ray, and muon science
- Based on HDF5 (http://www.hdfgroup.org)
- Self-describing
- Compression
  - Data: 95% compression
  - Metadata remain uncompressed (more easily searchable)
- Use increasing as new facilities come on line
  - SNS
  - OPAL at ANSTO
  - ISIS second target station
  - J-SNS
- McStas (neutron Monte Carlo ray-trace simulation tool) can read and write NeXus format

NeXus

http://www.nexusformat.org/

Neutron Science TeraGrid Gateway

One of 11 TeraGrid partner resource providers

Focus areas	Resources provided
• Neutron science • Connecting facilities with cyberinfrastructure • Bridging cyberinfrastructures • Data movement within and across TeraGrid	• Outreach to a specific science community (neutron science) – Expertise – Technology transfer – Education, in a broad sense – User outreach • A science gateway interface for neutron science • Exploration of large science facility integration with national-scale cyberinfrastructure • Combine TeraGrid computational resources with available neutron scattering datasets for analysis and simulation comparison

NSTG operational components

- Wide-area network connections to TeraGrid
- Local connections, at maximum bandwidth, to local facilities (SNS and HFIR)
- Modest local cluster with complete TeraGrid environment for small local TeraGrid jobs
- Long-term High-Performance Storage system archival storage via ORNL's LCF/NCCS
- System operations
- Application consulting

NSTG results: Highlights

First principles sample kernel simulations of experimentally relevant materials (E. Farhi, ILL)

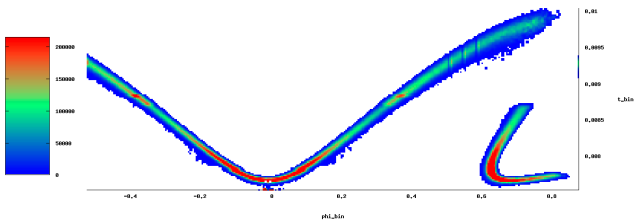
- Ability to launch McStas neutron Monte Carlo ray tracing instrument simulations on the TeraGrid directly from neutron science portal
- Production use of TeraGrid community account "Jimmy Neutron"
  - New TeraGrid science gateway scaling technology
- In development: A generalized fitting service for experimental data integrated into neutron science portal and using TeraGrid computational resources
- Outreach: mentored RAMS summer Student: Jessica Travierso (Austin Peay State University). Implemented XML-driven fitting service GUI. First prize undergraduate research at TeraGrid'08

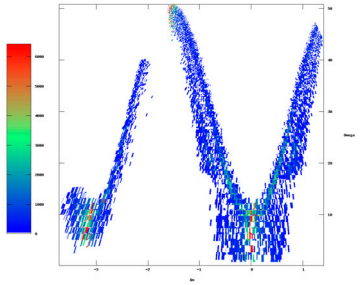
Neutron science simulations

Next step: Provide analysis and relevant simulations in support of neutron science

Instrument design optimization

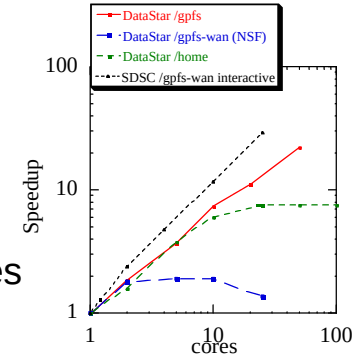
Moving simulations to TeraGrid allows larger runs and faster turnaround. Assisted in effort to redesign instrument to lower cost. Simulations provided confidence that resolution would not be sacrificed

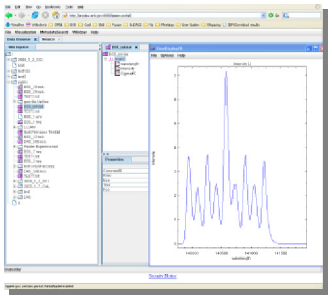


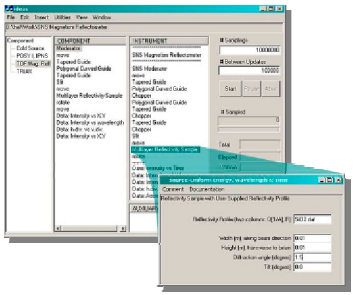


Porting and deployment of simulation tools to TeraGrid cyber-infrastructure: McStas

Many codes currently I/O limited. Next step is to modify I/O strategy in codes to take advantage of I/O architectures

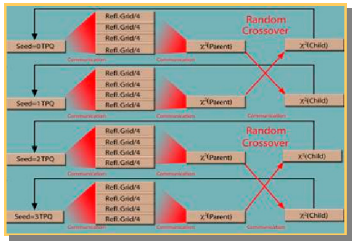


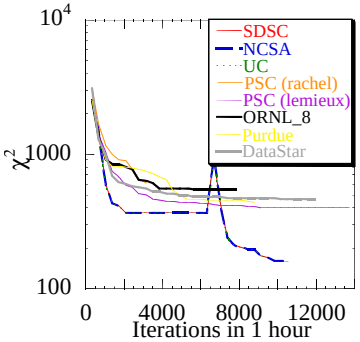




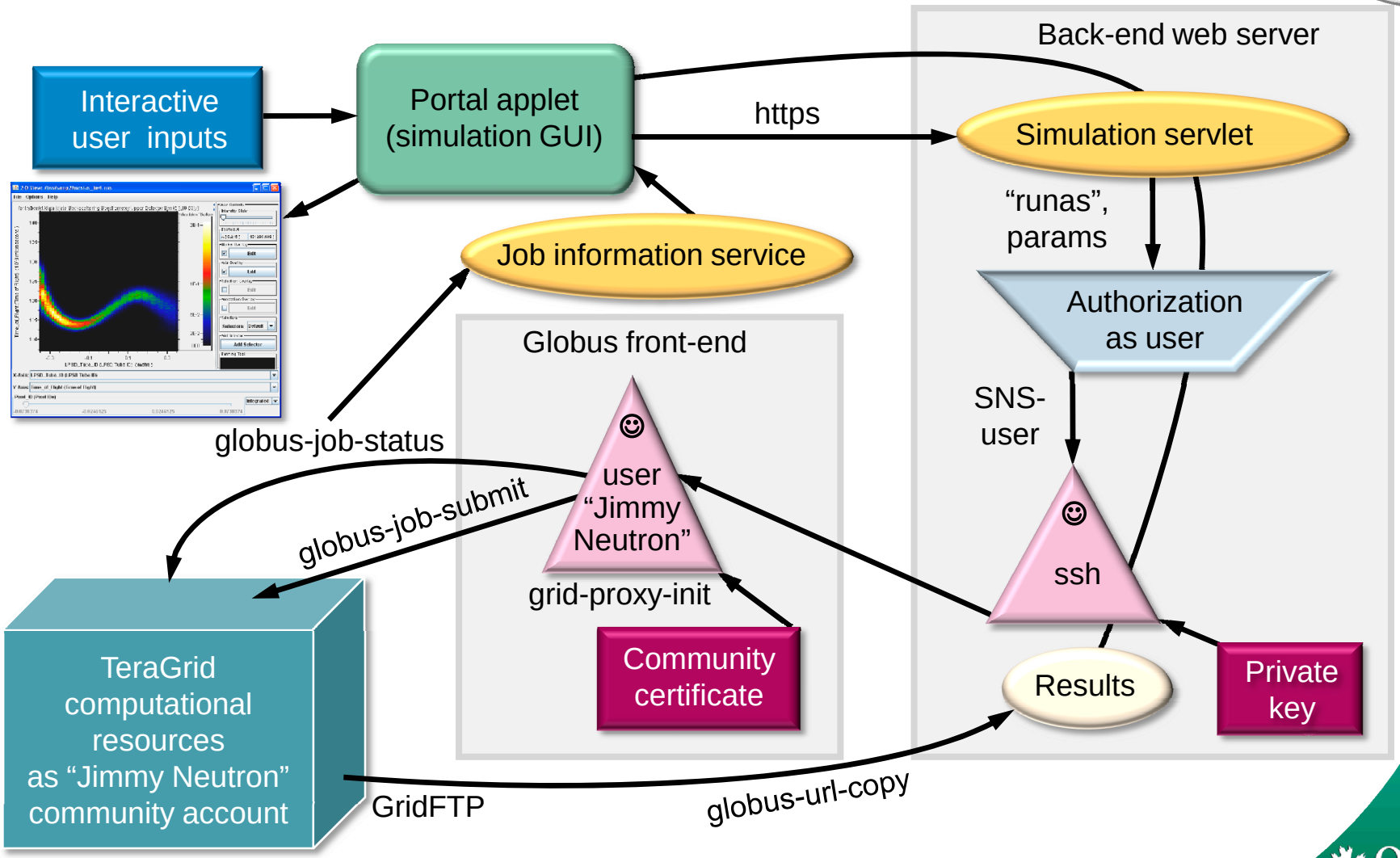
Improved and faster data analysis: Reflectometry

Faster and better χ^2 minimization





Portal-initiated simulations . . . under the covers!



NSTG was and is "postured as a pathfinder"

- Proposed a Science Gateway as part of ORNL RP in 2003, before creation of TeraGrid Science Gateways Program
- Included a focus on cyber-enabled science from the outset: Enabling neutron science
- One of the first intergrid production operations
- Early (but not first) concentration on intra-TeraGrid high-performance wide area data transfer
- Concentration on high-performance transfer between TeraGrid and external endpoints
- Early adopter and pathfinder postures fit with NSTG RP role

NSTG participates in several collaborative areas

Neutron science

- SNS and other facilities
- McStas instrument simulation software
- Portal development tools and deployments
  - OGCE, Eclipse Rich Client Platform

Data transport

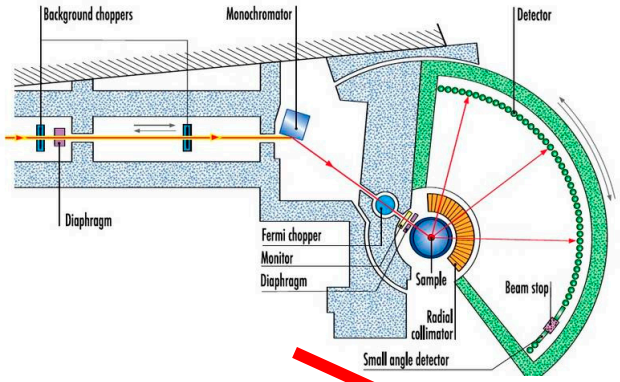
- Within TeraGrid network
- In wider area (REDDnet)

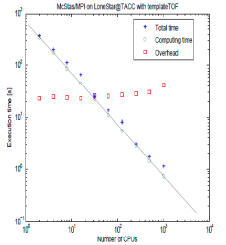
Intergrid operation

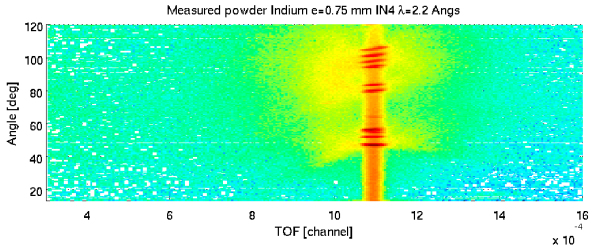
- Open Science Grid
- Earth Systems Grid

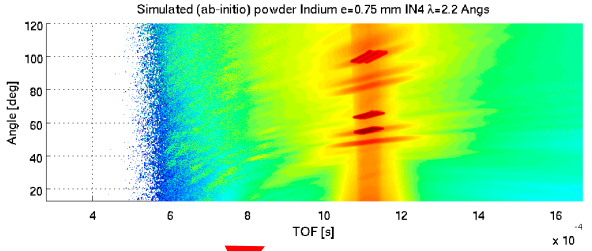
McStas

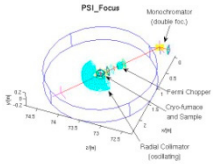
- Widely used Monte Carlo neutron ray tracing neutron instrument simulation package for instrument design and experiment planning
- Developed at Risø National Laboratory (Denmark) and Institut Laue-Langevin (France)
- Simulations from moderator through sample to detectors agree with experimental results
- Use cases:
  - Instrument design and construction
  - Experiment interpretation
  - Experiment planning
  - Experiment proposal evaluation
- E. Farhi has completed a preliminary study to computationally compute scattering kernels using VASPE
- McStas scalable: 1024+ cores





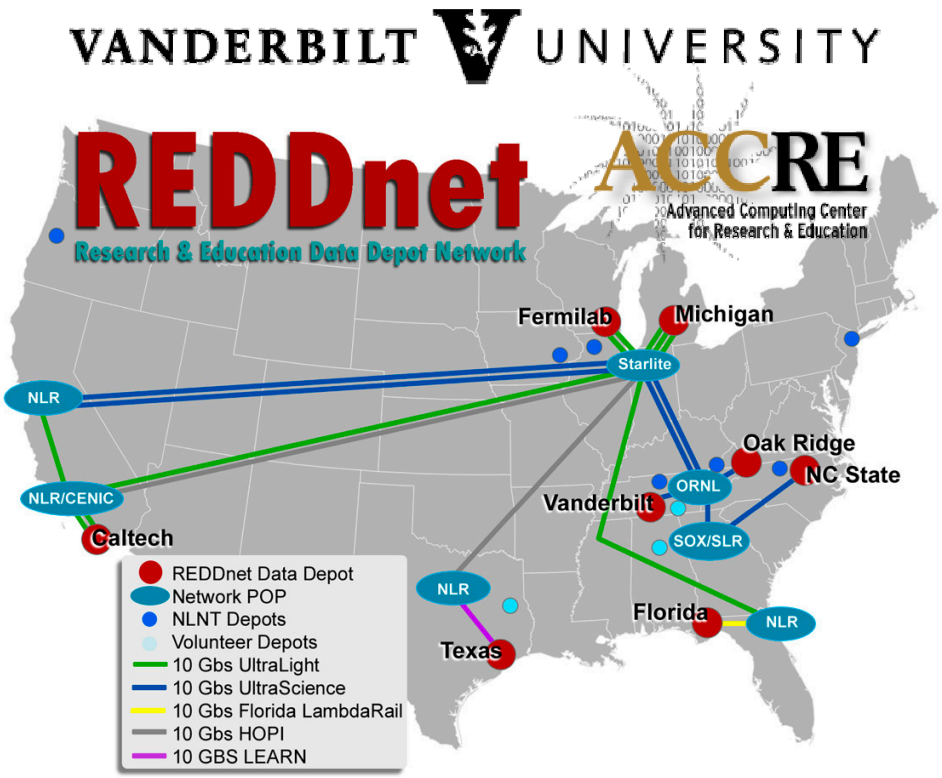






McStas – A neutron ray–trace simulation package

REDDnet
Research and Education Data Depot Network



ORNL REDDnet nodes in NSTG and LCF

See Vanderbilt research booth for SC'08 demo, bandwidth challenge and more details

http://www.reddnet.org/

- **National-scale logistical storage network**
- **Distributed** (but acts local!)
- Funding from NSF and Library of Congress
- >700 TB (500 disk, 200 tape)
- Multiple application domains
  - Satellite imagery (AmericaView)
  - High energy physics: LHC
  - Terascale Supernova Initiative
  - Structural biology
  - Vanderbilt TV news archive
  - National Geospatial Data Archive
- **Data everywhere** (under the cover tools to manage movement, replication, …)

Acknowledgements and thanks

Staff and Effort

- **NSTG:** M. Chen[1], J. Cobb[1], D. Giles[1], V. Hazlewood[7], S. Hicks[1], G. Hinkel[1], D. Hudson[1], V. Lynch[1], P. Newman[1], J. Nichols[1], D. Pack[1], G. Pike[1], J. Rome[1], J. Travierso[9], W. Wing[1]
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Organization

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