Case Study: GGF Standards and TeraGrid

Charlie Catlett

Director, TeraGrid

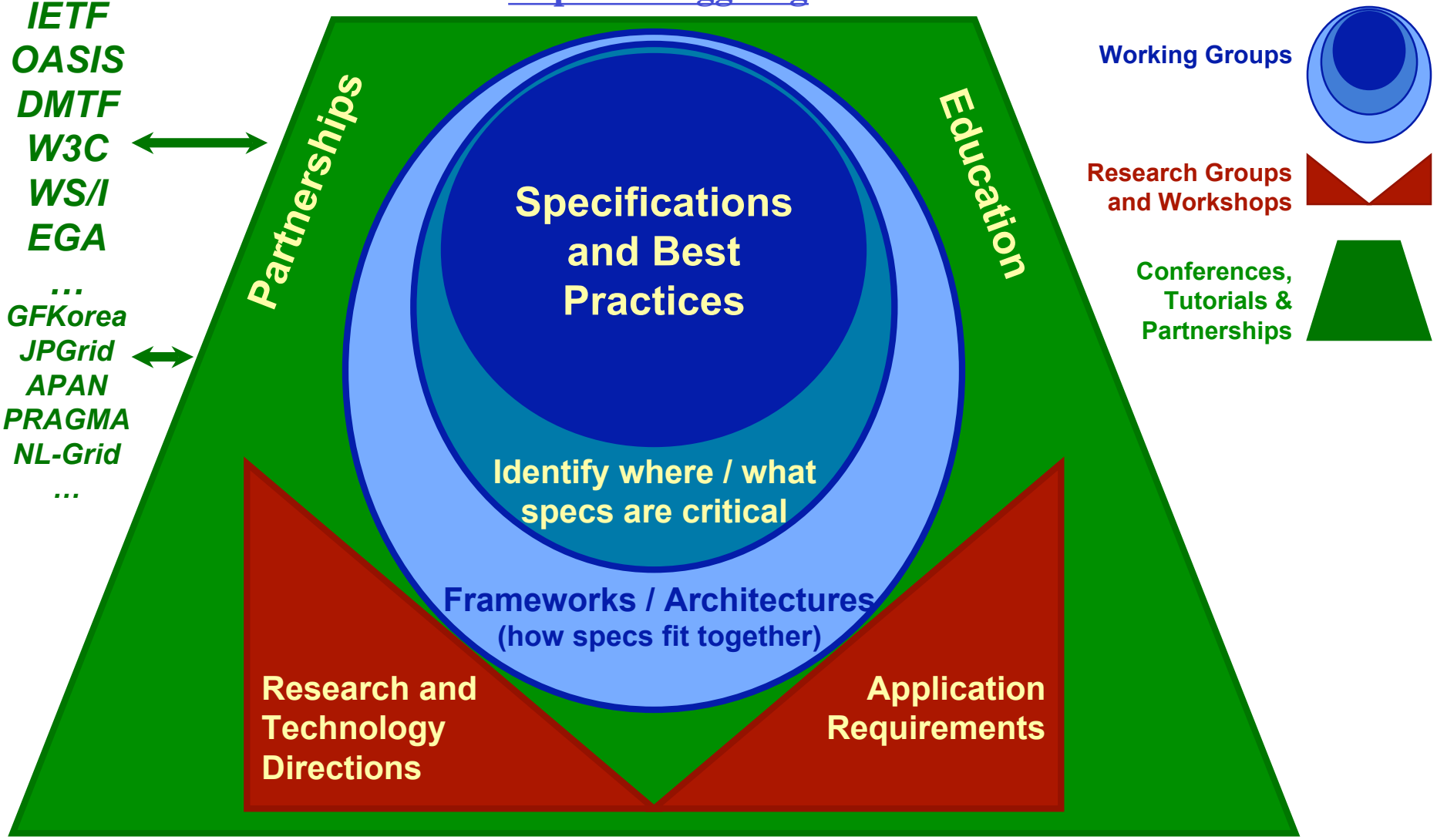
University of Chicago and Argonne National Laboratory

Founding Chair, GGF

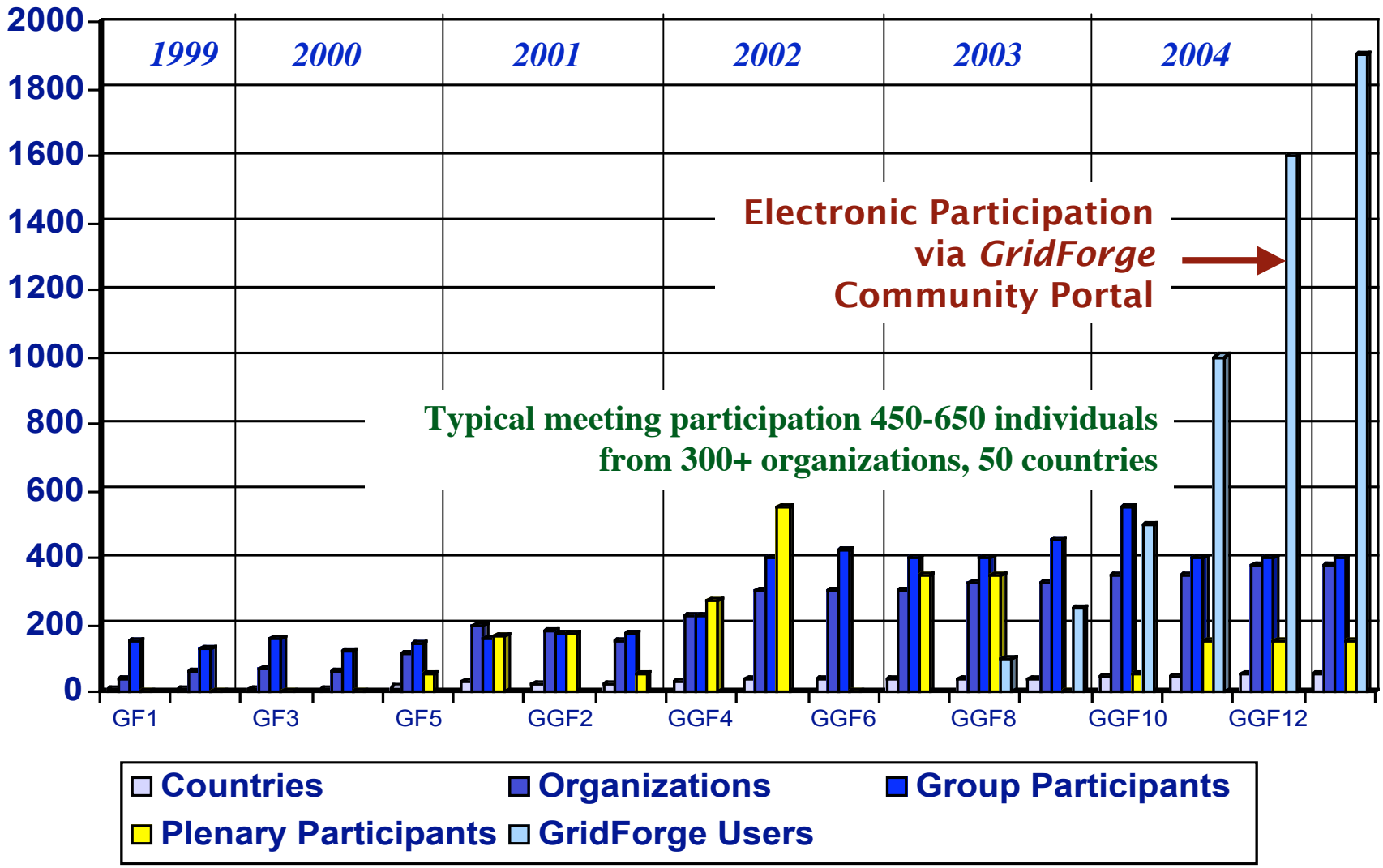
What is GGF?

Contact:
Mark Linesch, GGF Chair
(mark.linesch@hp.com)

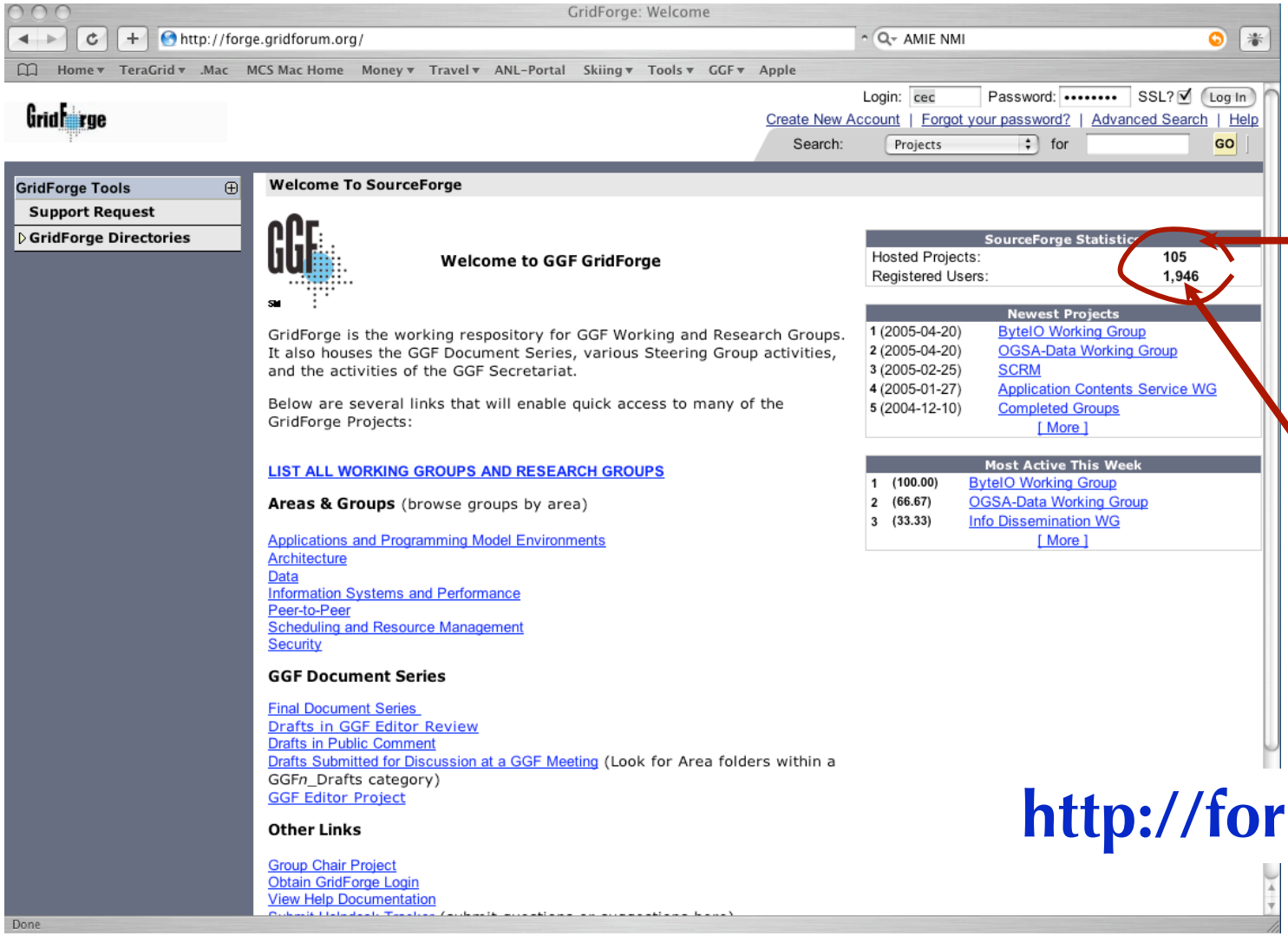
http://www.ggf.org



GGF: Six Years Sustained Growth



GridForge: Community Portal



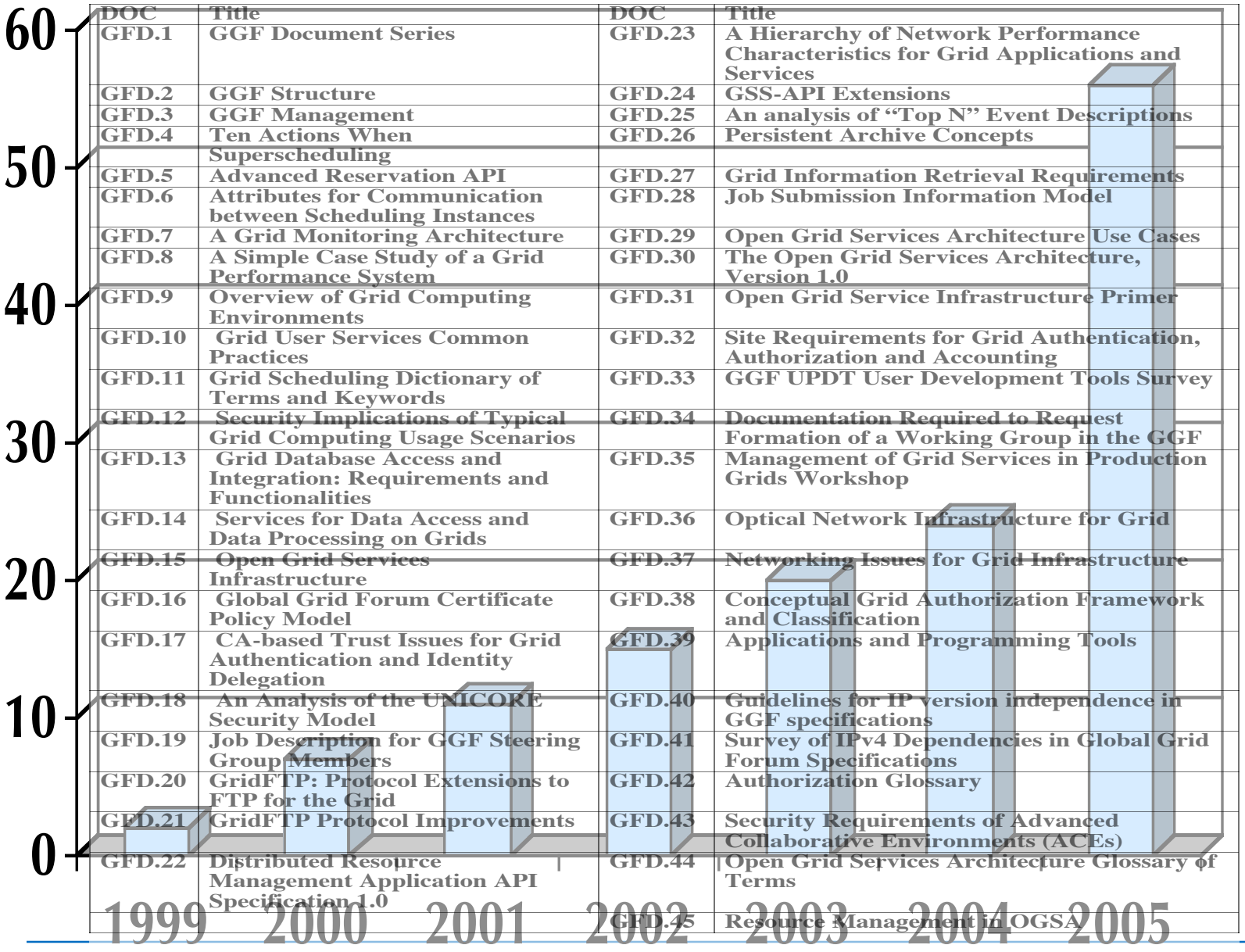
Established July 2003

Over 100 project workspaces (for all GGF groups, committees, etc.)

Over 1900 active users as of Oct 2004. (open to any interested party at no cost)

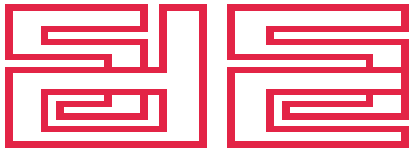
http://forge.ggf.org

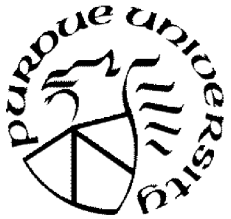
GGF Standards Document Series



DOC	Title	DOC	Title
GFD.1	GGF Document Series	GFD.23	A Hierarchy of Network Performance Characteristics for Grid Applications and Services
GFD.2	GGF Structure	GFD.24	GSS-API Extensions
GFD.3	GGF Management	GFD.25	An analysis of "Top N" Event Descriptions
GFD.4	Ten Actions When Superscheduling	GFD.26	Persistent Archive Concepts
GFD.5	Advanced Reservation API	GFD.27	Grid Information Retrieval Requirements
GFD.6	Attributes for Communication between Scheduling Instances	GFD.28	Job Submission Information Model
GFD.7	A Grid Monitoring Architecture	GFD.29	Open Grid Services Architecture Use Cases
GFD.8	A Simple Case Study of a Grid Performance System	GFD.30	The Open Grid Services Architecture, Version 1.0
GFD.9	Overview of Grid Computing Environments	GFD.31	Open Grid Service Infrastructure Primer
GFD.10	Grid User Services Common Practices	GFD.32	Site Requirements for Grid Authentication, Authorization and Accounting
GFD.11	Grid Scheduling Dictionary of Terms and Keywords	GFD.33	GGF UPDT User Development Tools Survey
GFD.12	Security Implications of Typical Grid Computing Usage Scenarios	GFD.34	Documentation Required to Request Formation of a Working Group in the GGF
GFD.13	Grid Database Access and Integration: Requirements and Functionalities	GFD.35	Management of Grid Services in Production Grids Workshop
GFD.14	Services for Data Access and Data Processing on Grids	GFD.36	Optical Network Infrastructure for Grid
GFD.15	Open Grid Services Infrastructure	GFD.37	Networking Issues for Grid Infrastructure
GFD.16	Global Grid Forum Certificate Policy Model	GFD.38	Conceptual Grid Authorization Framework and Classification
GFD.17	CA-based Trust Issues for Grid Authentication and Identity Delegation	GFD.39	Applications and Programming Tools
GFD.18	An Analysis of the UNICORE Security Model	GFD.40	Guidelines for IP version independence in GGF specifications
GFD.19	Job Description for GGF Steering Group Members	GFD.41	Survey of IPv4 Dependencies in Global Grid Forum Specifications
GFD.20	GridFTP: Protocol Extensions to FTP for the Grid	GFD.42	Authorization Glossary
GFD.21	GridFTP Protocol Improvements	GFD.43	Security Requirements of Advanced Collaborative Environments (ACEs)
GFD.22	Distributed Resource Management Application API Specification 1.0	GFD.44	Open Grid Services Architecture Glossary of Terms
		GFD.45	Resource Management in OGSA

TeraGrid





THE UNIVERSITY OF CHICAGO

TeraGrid: Foundation for NSF Cyberinfrastructure

Persistent, Reliable National Cyberinfrastructure

- Coordinated Computing Environment
- Coherent User Outreach, Training, and Support
- Common, open infrastructure services (directories, storage, authentication services)

- Science Gateways: Engaging Scientific Communities
- 90+ Community Data Collections
- 2+ PB Online Data Storage
- World's most powerful network (national footprint)
- NSF's Most powerful compute resources (40+ TF)
- National data visualization facilities

- National Science Foundation
  - $100M 3-year construction (2001-2004)
  - $150M 5-year operation & enhancement (2005-2009)

RP Resources and Services

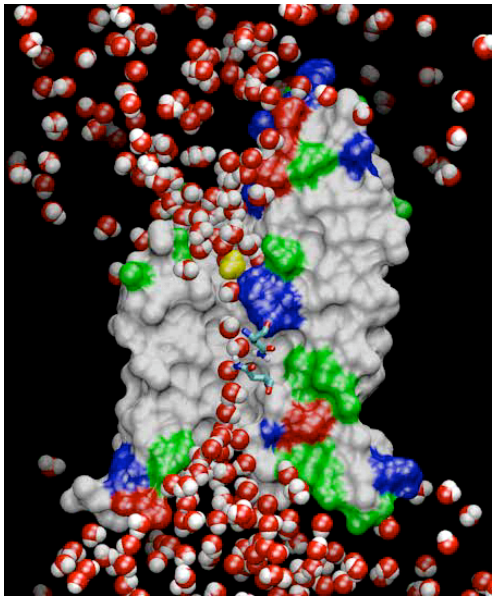
	ANL/UC	Caltech	IU	NCSA	ORNL	PSC	Purdue	SDSC	TACC
Compute Resources and User Support	Itanium2 (0.5 TF) IA-32 (0.5 TF)	Itanium2 (0.8 TF)	Itanium2 (0.2 TF) IA-32 (2.0 TF)	Itanium2 (10 TF) SGI SMP (6.5 TF)	IA-32 (0.3 TF)	XT3 (10 TF) TCS (6 TF) Marvel (0.3 TF)	Hetero (1.7 TF)	Itanium2 (4.4 TF) Power4+ (1.1 TF)	IA-32 (6.3 TF) Sun (Vis)
Network (Gb/s,Hub)	30 CHI	30 LA	10 CHI	30 CHI	10 ATL	30 CHI	10 CHI	30 LA	10 CHI
Online Storage	20 TB	155 TB	32 TB	600 TB	1 TB	150 TB		540 TB	50 TB
Archive Storage			1.2 PB	3 PB		2.4 PB		6 PB	2 PB
Data Collections			Yes	Yes			Yes	Yes	Yes
Instruments		Yes	Yes		Yes				
Visualization	Yes		Yes			Yes	Yes		Yes
Public Affairs	Yes	Yes	Yes	Yes		Yes		Yes	Yes

Grid Infrastructure Group (GIG)

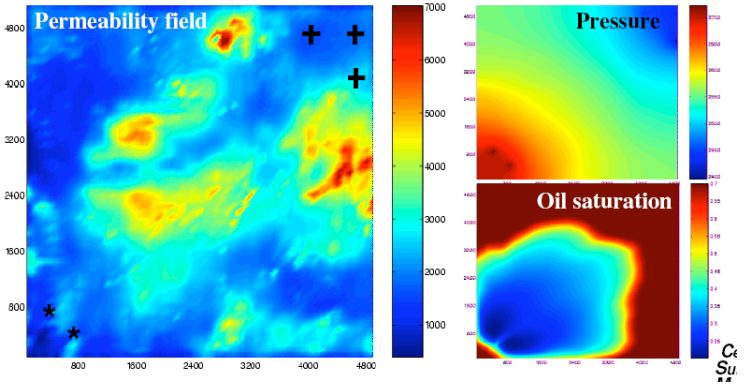
Architecture, Software, Operations, Common Services, Coordinated User Support, Science Gateways

TeraGrid: Science Examples

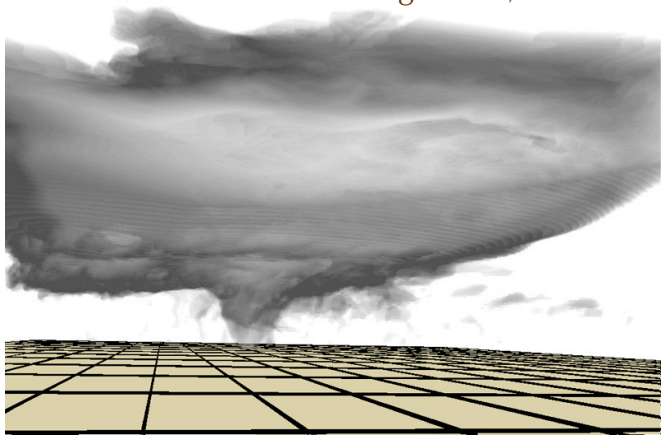
Aquaporin mechanism
Animation pointed to by 2003 Nobel chemistry prize announcement.
Klaus Schulten, UIUC



Reservoir Modeling
Joel Saltz, OSU

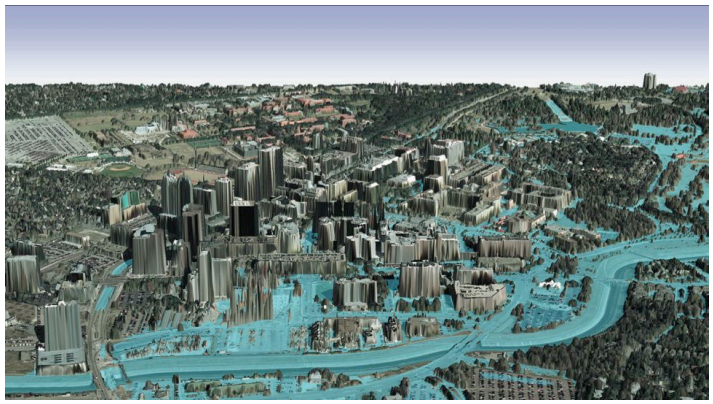


Atmospheric Modeling
Kelvin Droegemeier, OU

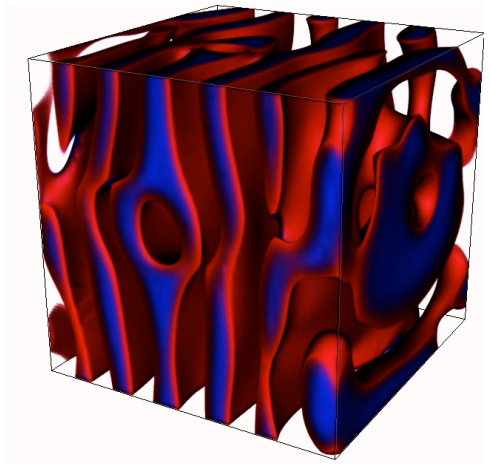


Industry Candidates currently using TeraGrid resources at individual sites:

- Engineering (vehicle design, cellular network optimization)
- Finance (risk analysis)
- Operations (transportation, fraud detection)
- Pharmaceutical (drug design)



Groundwater/Flood Modeling
David Maidment, Gordon Wells, UT



Lattice-Boltzman Simulations
Peter Coveney, UCL

The TeraGrid Vision

- TeraGrid *DEEP: Enabling the Nation's Terascale Science*
  - Make Science More Productive through a unified set of very-high capability resources.
    - *Strategy: leverage TeraGrid's unique resources to create new capabilities driven & prioritized by science partners*
- TeraGrid *WIDE: Empowering communities to leverage TeraGrid capabilities*
  - Bring TG capabilities to the broad science community (no longer just "big" science).
    - *Strategy: Science Gateways connecting communities, Integrated roadmap with peer Grids and software efforts*
- Base TeraGrid Cyberinfrastructure: *Integrating the Nation's Most Powerful Resources*
  - Provide a unified, general purpose, reliable set of services and resources.
    - *Strategy: An extensible virtual organization of people and resources across TeraGrid partner sites.*

User Types

- Expert and Advanced Users (n x 10^2)
  - Want to log into supercomputers and optimize code
    - Explicit, first-party authentication
    - Shell access with full user-level functionality
    - Resource consumption limited by allocation
  - Interest in turnaround, can use a variety of platforms
    - Actual "user" typically a graduate student willing to deal with details of computing and data management in order to fully optimize workflow
- Broad Science Community (n x 10^3)
  - Want to use specific applications provided by others, but with large variation in job size (and/or number of jobs)
    - Trusted third-party authentication
    - Limited functionality access through portal and/or restricted shell
    - Resource consumption limited by allocation
  - Interest in turnaround and avoiding details of computing and data management
  - Interest in workflow management tools to automate procedures
- Public Access (including education, n x 10^4)
  - Want to use simple applications for small (possibly fixed set of) jobs
    - Limited trust authentication
    - Limited functionality access through restricted portal methods
    - Limited resource consumption

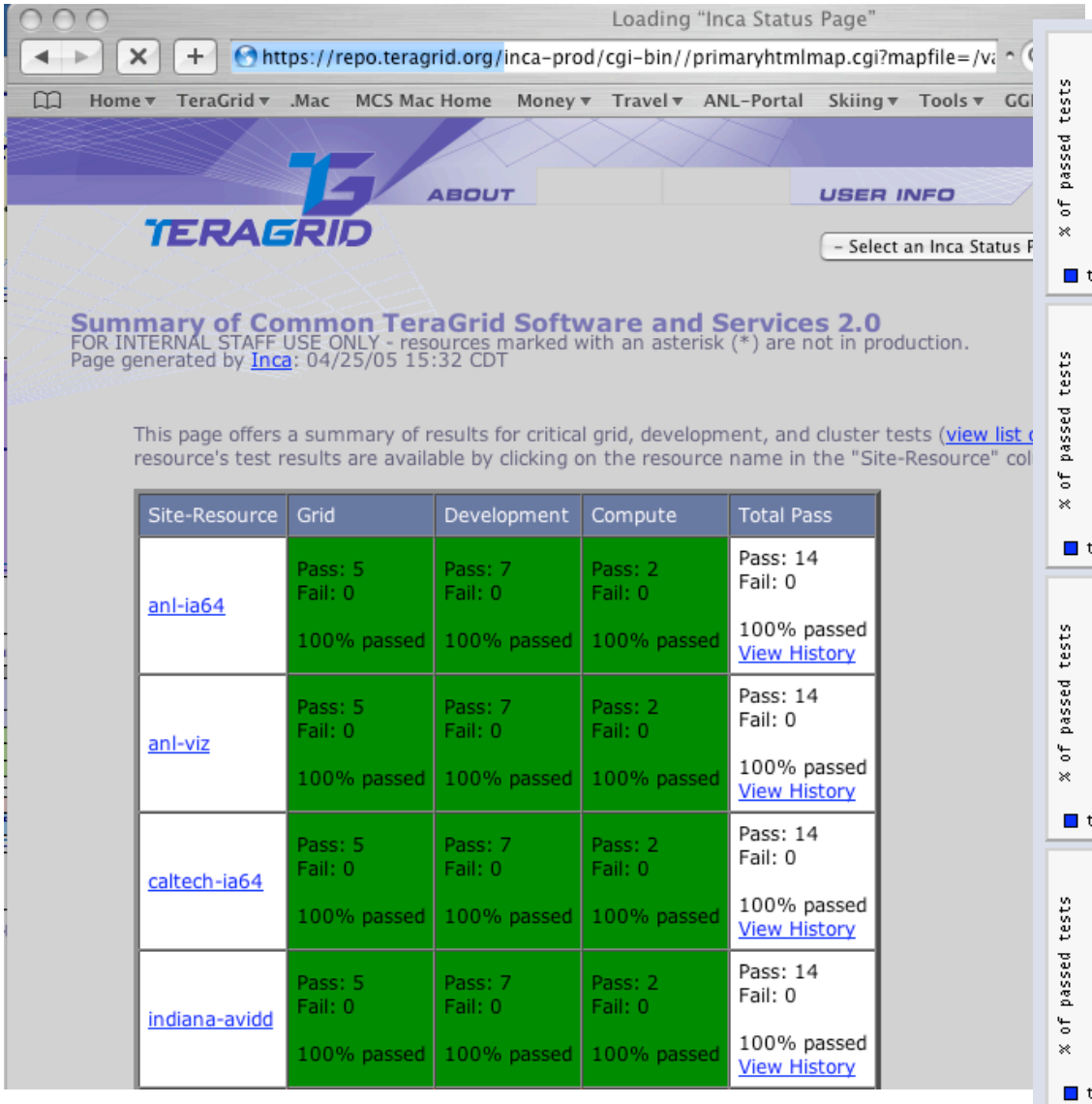
DEEP

WIDE

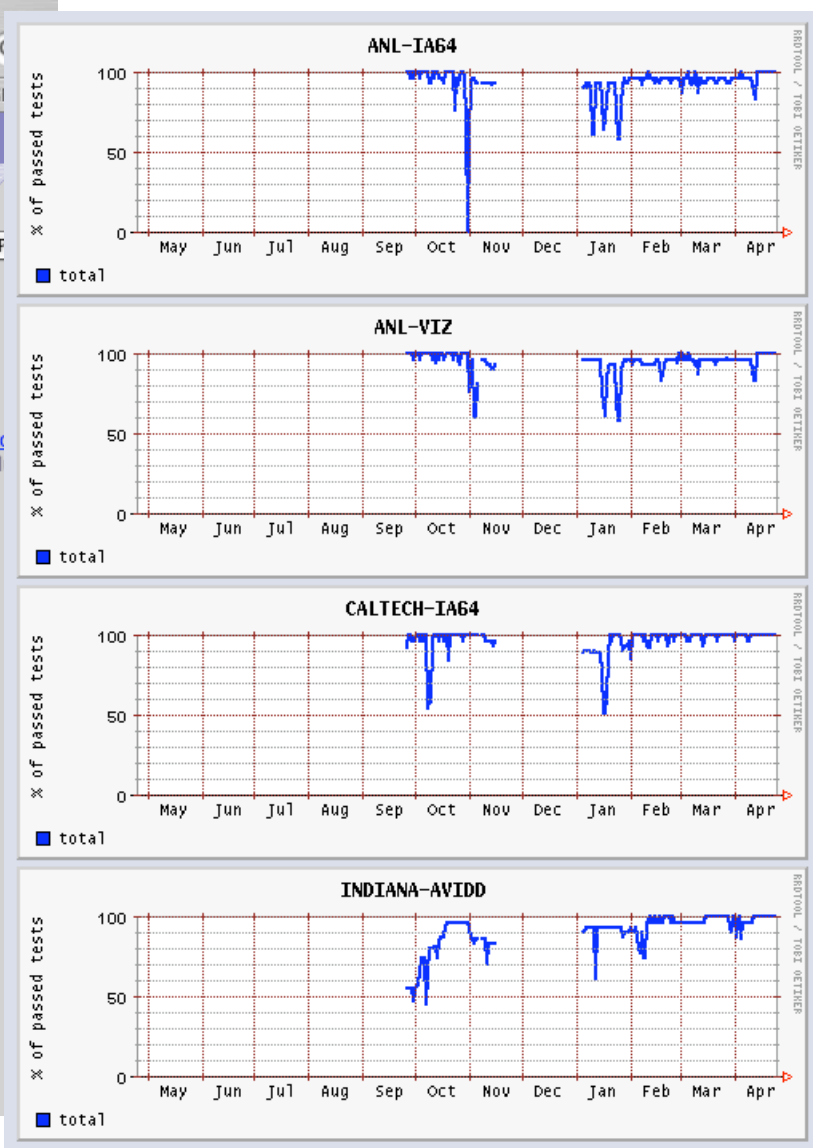
TeraGrid: Service Oriented Approach

- Defines service offerings, interactions, and "interfaces"
  - Allows local implementation decisions and approaches
- Common Integration Infrastructure
  - Verification and Validation
    - Inca (Beckman (UC/ANL), Smallen (SDSC), et. al.)
  - Account management and accounting
    - AMIE (Quinn (NCSA), et. al.)
    - GGF Resource Usage Record format standard
  - Public Key Infrastructure (system-wide) authentication,high-performance data movement & staging infrastructure
    - Globus Toolkit (GSI a GGF/IETF standard; GridFTP a GGF standard)
- Defined Services
  - Compute Service
    - Coordinated TeraGrid Software and Services (CTSS) defines the user environment baseline provided by all compute servers
    - Comprises clients, libraries, tools, $ENV variables, etc.
  - Additional Services
    - File-based archives (GridFTP interface in addition to native, e.g. HPSS)
    - Storage Resource Broker (SRB (SDSC)) archive
    - Wide area parallel file system (IBM GPFS)
    - Metascheduler (MOAB)

Inca Verification & Validation



Site-Resource	Grid	Development	Compute	Total Pass
anl-ia64	Pass: 5 Fail: 0 100% passed	Pass: 7 Fail: 0 100% passed	Pass: 2 Fail: 0 100% passed	Pass: 14 Fail: 0 100% passed View History
anl-viz	Pass: 5 Fail: 0 100% passed	Pass: 7 Fail: 0 100% passed	Pass: 2 Fail: 0 100% passed	Pass: 14 Fail: 0 100% passed View History
caltech-ia64	Pass: 5 Fail: 0 100% passed	Pass: 7 Fail: 0 100% passed	Pass: 2 Fail: 0 100% passed	Pass: 14 Fail: 0 100% passed View History
indiana-avidd	Pass: 5 Fail: 0 100% passed	Pass: 7 Fail: 0 100% passed	Pass: 2 Fail: 0 100% passed	Pass: 14 Fail: 0 100% passed View History



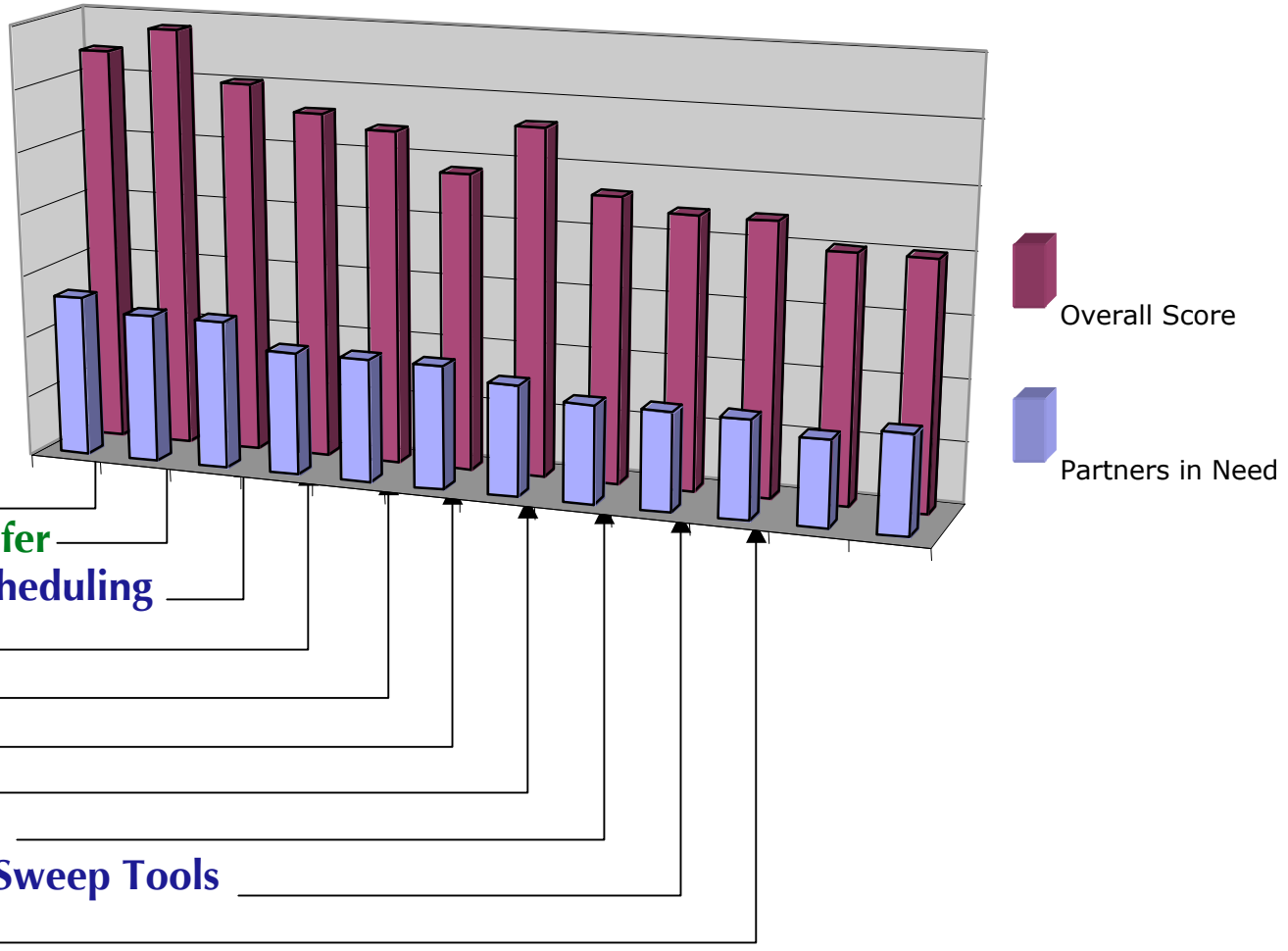
Pete Beckman (beckman@mcs.anl.gov) and Shava Smallen (ssmallen@sdsc.edu)

TeraGrid: User Driven Priorities

Data

Grid Computing

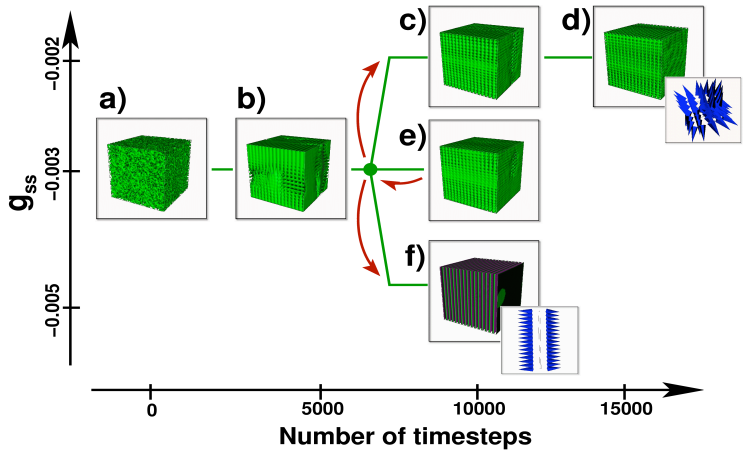
Science Gateways

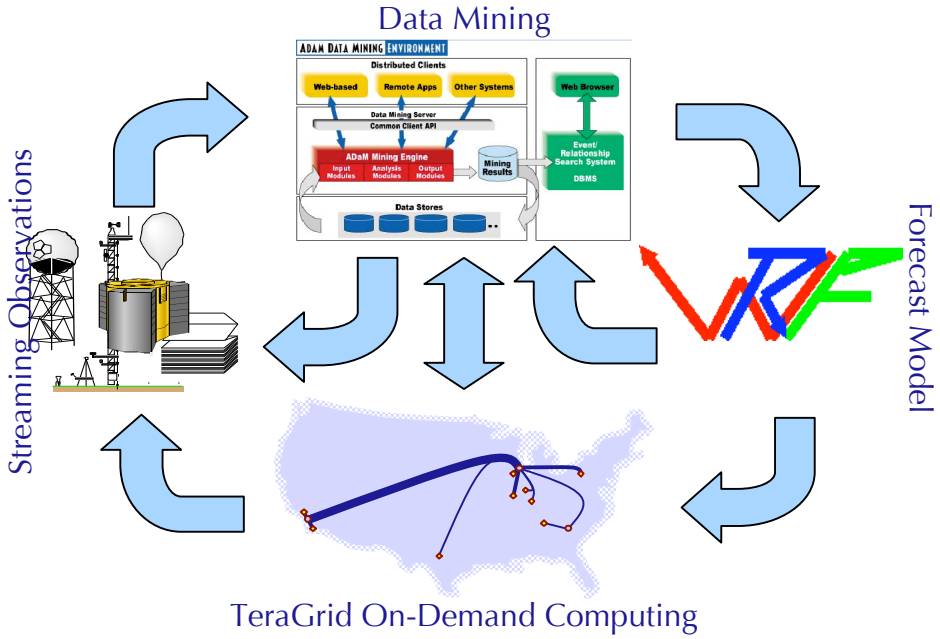


Results of in-depth discussions with 16 TeraGrid user teams.

TeraGrid DEEP: Terascale Science

- TeraGrid User Support
  - Unified team from PSC, NCSA, SDSC, TACC, Caltech, UC/ANL, ORNL, Purdue, Indiana
- Advanced Support
  - "Embedded" consultants working with application teams to enable terascale science.
- Applications exploiting unique TeraGrid resources and services



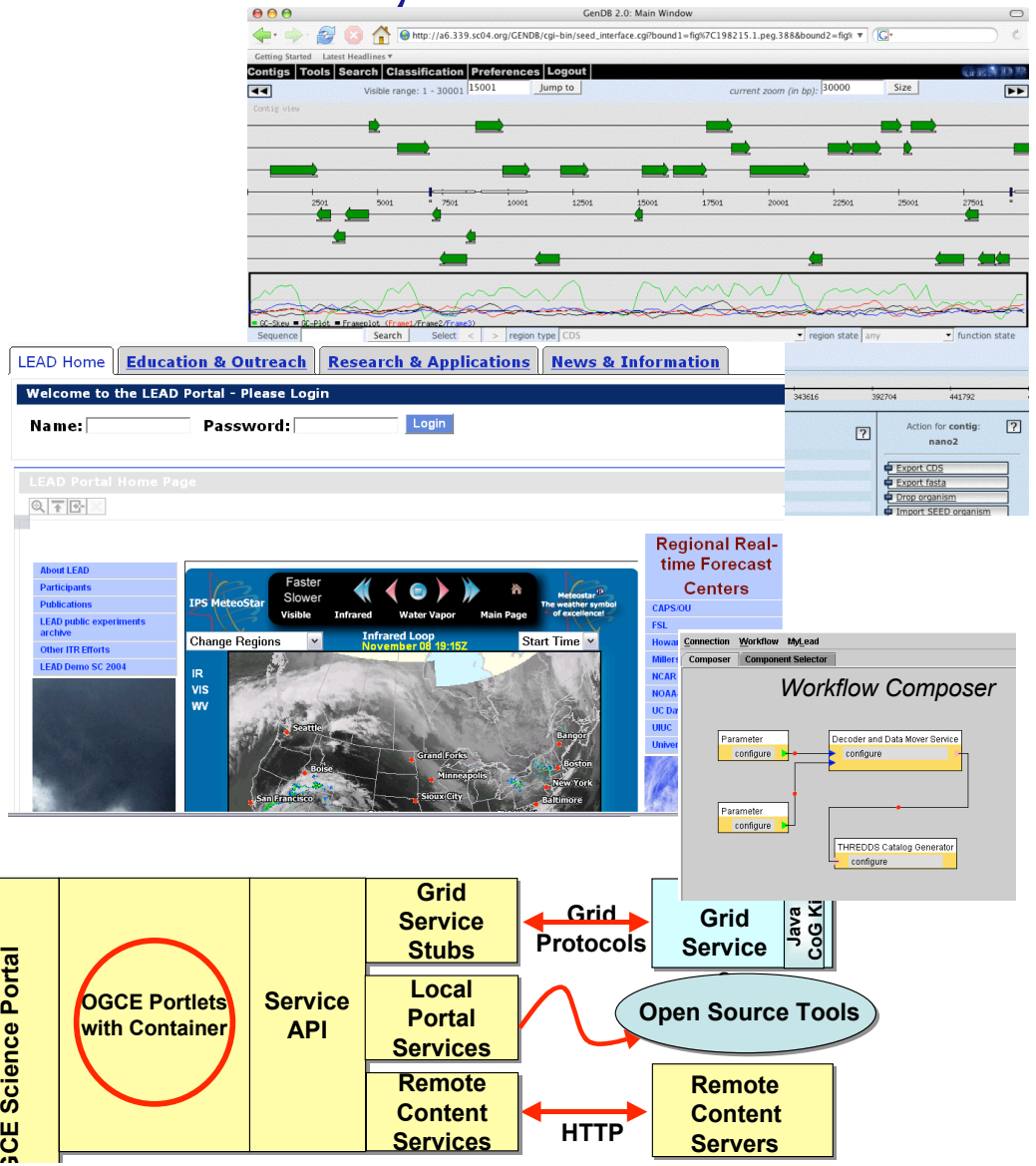


Top: Computational Steering
(Source TeraGyroid project, Peter Coveney, UCL)

Bottom: Adaptive Computational Weather Forecast
(Source LEAD project, Kelvin Droegemeier, OU)

Grid Portal Gateways

- The Portal accessed through a browser or desktop tools.
  - Provides Grid authentication and access to services
  - Provide direct access to teragrid hosted applications as services
- Required Support Services
  - Searchable Metadata catalogs
  - Information Space Management.
  - Workflow managers
  - Resource brokers
  - Application deployment services
  - Authorization services.
- Building on NSF & DOE software investments
  - Use NMI Portal Framework,
  - NMI Grid Tools
    - Condor, Globus, In-VIGO
  - OSG and HEP tools
    - Clarens, MonaLisa

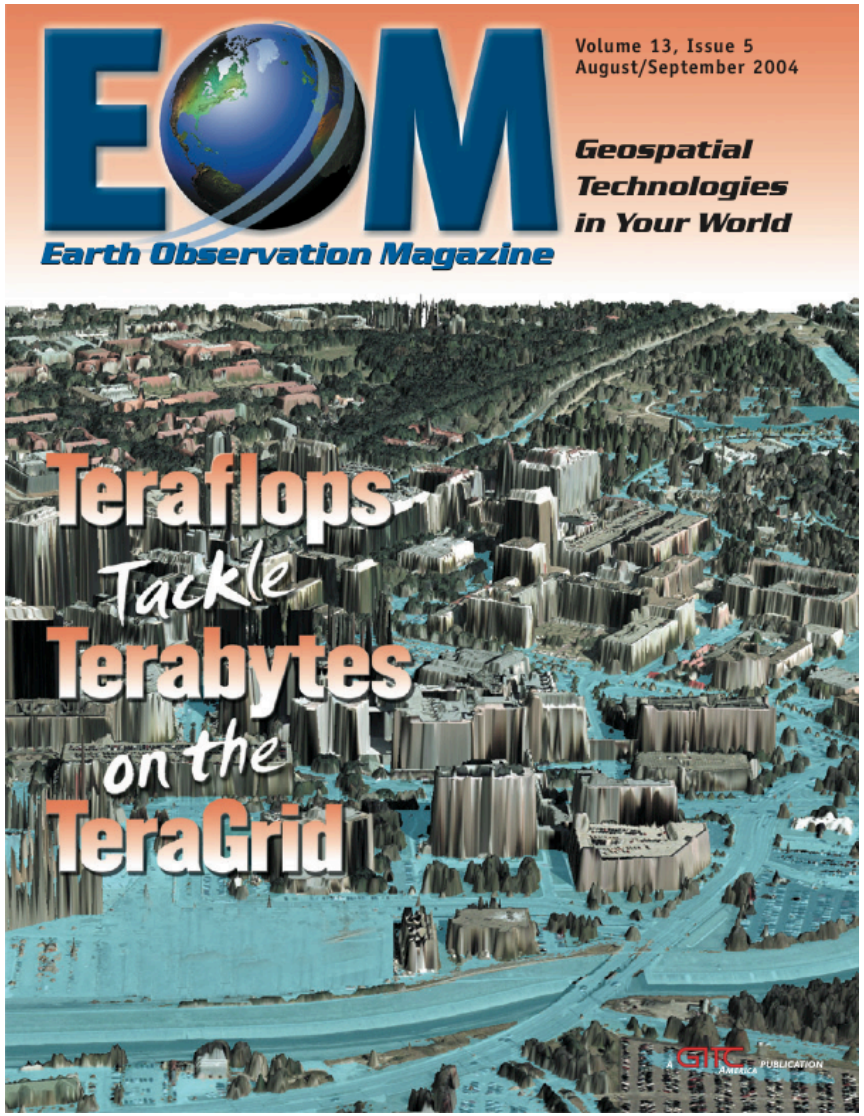


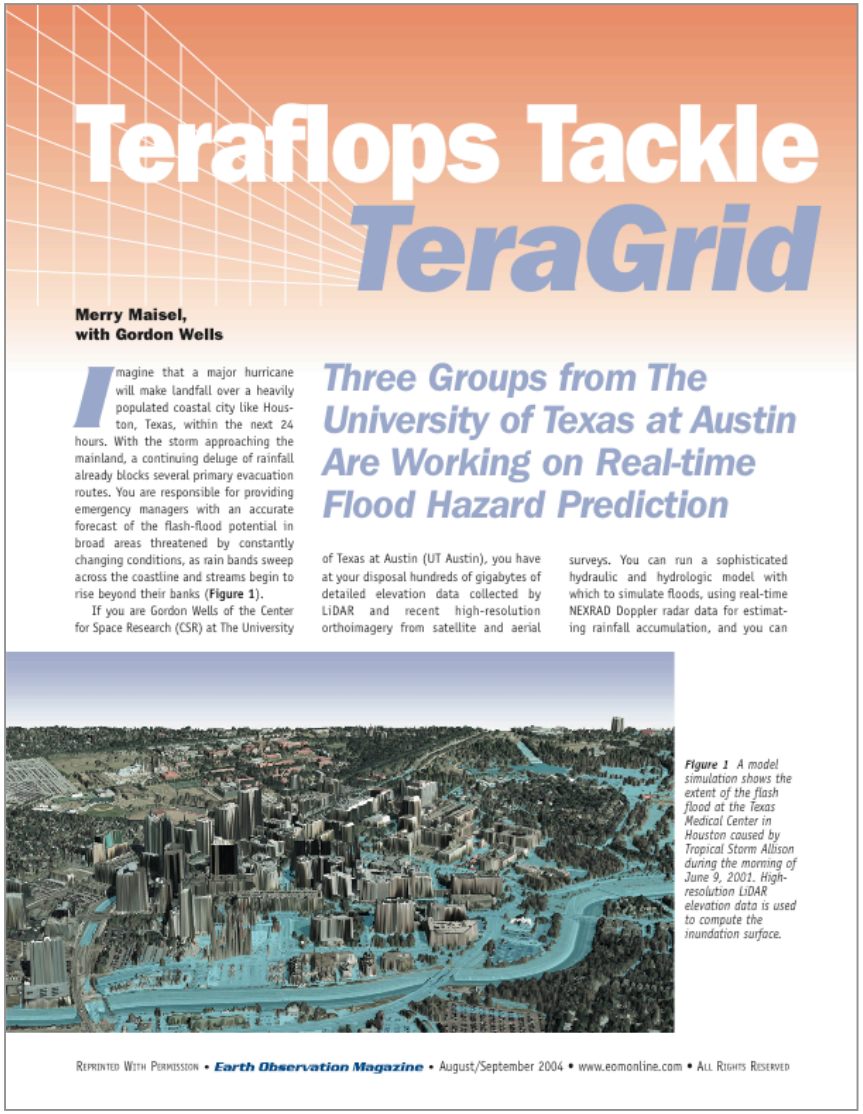
Dennis Gannon (gannon@cs.indiana.edu)

Initial TeraGrid Science Gateway Prototypes

Science Gateway Prototype	Discipline	Science Partner(s)	TeraGrid Liaison
Linked Environments for Atmospheric Discovery (LEAD)	**Atmospheric**	Droegemeier (OU)	Gannon (IU), Pennington (NCSA)
National Virtual Observatory (NVO)	**Astronomy**	Szalay (Johns Hopkins)	Williams (Caltech)
Network for Computational Nanotechnology (NCN) and "nanoHUB"	**Nanotechnology**	Lundstrum (PU)	Goasguen (PU)
National Microbial Pathogen Data Resource Center (NMPDR)	**Biomedicine and Biology**	Schneewind (UC), Osterman (Burnham/UCSD), DeLong (MIT), Dusko (INRA)	Stevens (UC/Argonne)
NSF National Evolutionary Biology Center (NESC), NIH Carolina Center for Exploratory Genetic Analysis, State of North Carolina Bioinformatics Portal project	**Biomedicine and Biology**	Cunningham (Duke), Magnuson (UNC)	Reed (UNC), Blatecky (UNC)
Neutron Science Instrument Gateway	**Physics**	Dunning (ORNL)	Cobb (ORNL)
Grid Analysis Environment	**High-Energy Physics**	Newman (Caltech)	Bunn (Caltech)
Transportation System Decision Support	**Homeland Security**	Stephen Eubanks (LANL)	Beckman (Argonne)
Groundwater/Flood Modeling	**Environmental**	Wells (UT-Austin), Engel (ORNL)	Boisseau (TACC)

Science and Multimodal: Flood Modeling





Teraflops Tackle TeraGrid

Merry Maisel, with Gordon Wells

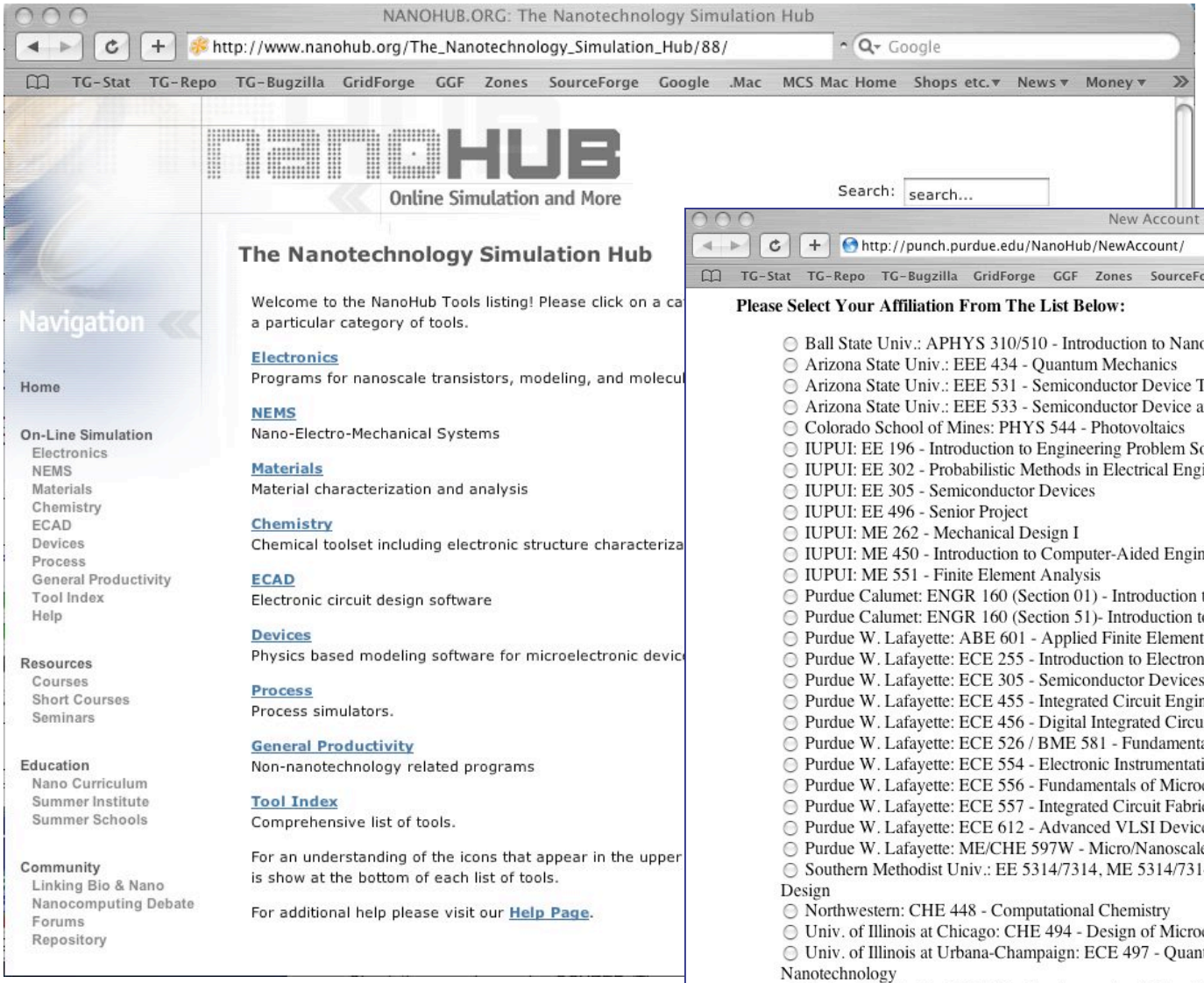
Three Groups from The University of Texas at Austin Are Working on Real-time Flood Hazard Prediction

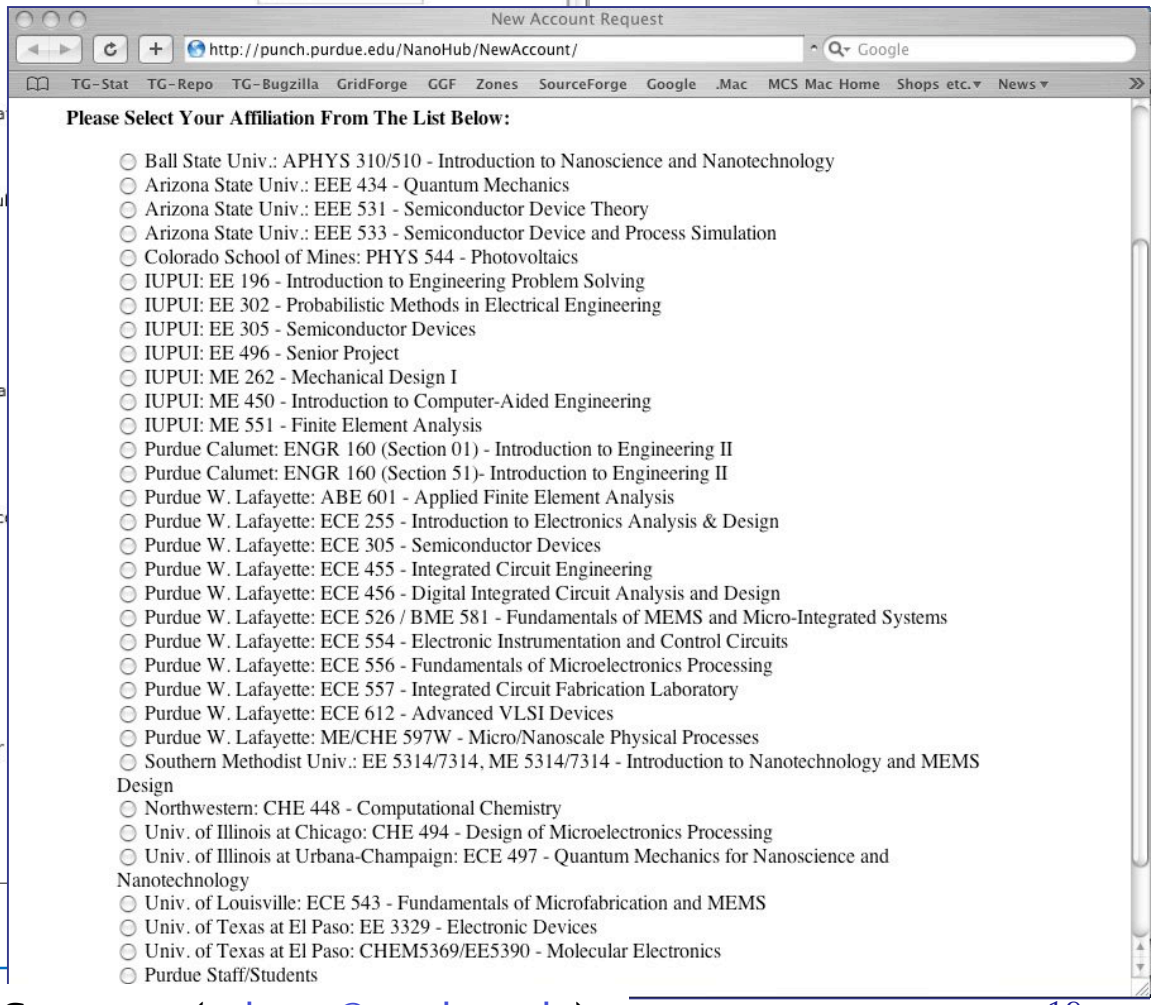
Imagine that a major hurricane will make landfall over a heavily populated coastal city like Houston, Texas, within the next 24 hours. With the storm approaching the mainland, a continuing deluge of rainfall already blocks several primary evacuation routes. You are responsible for providing emergency managers with an accurate forecast of the flash-flood potential in broad areas threatened by constantly changing conditions, as rain bands sweep across the coastline and streams begin to rise beyond their banks (**Figure 1**).

If you are Gordon Wells of the Center for Space Research (CSR) at The University of Texas at Austin (UT Austin), you have at your disposal hundreds of gigabytes of detailed elevation data collected by LiDAR and recent high-resolution orthoimagery from satellite and aerial surveys. You can run a sophisticated hydraulic and hydrologic model with which to simulate floods, using real-time NEXRAD Doppler radar data for estimating rainfall accumulation, and you can

Figure 1 A model simulation shows the extent of the flash flood at the Texas Medical Center in Houston caused by Tropical Storm Allison during the morning of June 9, 2001. High-resolution LiDAR elevation data is used to compute the inundation surface.

Adoption: Science Gateways and Education





Example: Nanohub is used to complete coursework by undergraduate and graduate students in dozens of courses at 10 universities.

Current Work: GGF and TeraGrid

- Science Gateways
  - Portal interactions with resources and Grids via Web services
    - Workshop in June 2004 (Chicago, GGF-14)
  - Discipline-specific GGF Research Groups
    - E.g. Life Sciences (pharma, bioinformatics, genomics)
- Security
  - Policy Management Authorities
    - Based on GGF Certificate Authority guidelines
  - Graduated authorization based on authentication levels
- Open Grid Services Architecture
  - Participation in development of service specifications (e.g. execution services)