Enabling Data Intensive Science with PetaShare

Tevfik Kosar

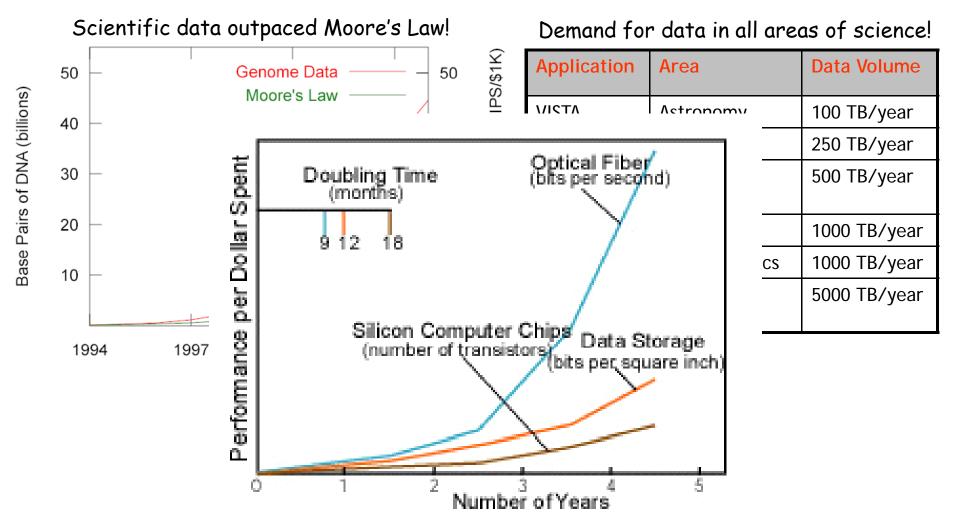
Center for Computation & Technology Louisiana State University

April 6, 2007





The Imminent Data "deluge"



LONI

- Since September 2004, the State of Louisiana has committed \$50M for a statewide optical network.
- 40Gb/sec bandwidth
- Spanning 6 Universities and 2 Health Centers:
 - LSU
 - Latech
 - UL-Lafayette
 - Tulane
 - UNO
 - Southern University
 - LSU Health Centers in
 - New Orleans
 - Shreveport



- 112 processor IBM P5 servers being deployed at each site
- 540 processor Linux clusters will follow
- 100 TFlops in a couple of years

DONE?..

- We will have one of the
 - Fastest networks
 - Most powerful computational grids
 - in the world..
- But this solves only part of the problem!
- Researchers at these institutions still not be able to share and even process their own data



Home Page

Applications:

NSF Funds LSU \$1 Million for PetaShare Development

The National Science Foundation (NSF) recently funded Louisiana State University (LSU) \$1 million for the development of PetaShare, which is seen as "a system might become an important testbed for future grids, and a leading site in next-generation petascale research."

The unbounded increase in the size of data generated by scientific applications necessitates collaboration and sharing among the nation's education and research institutions. Simply purchasing high capacity, high performance storage systems and adding them to the existing infrastructure of the collaborating institutions does not solve the underlying and highly challenging data handling problem. Scientists are compelled to spend a great deal of time and energy on solving basic data-handling issues, such as the physical location of data, how to access it, and/or how to move it to visualization and/or compute resources for further analysis.

LSU assistant professor Tevfik Kosar and his team aim to develop an innovative distributed data archival, analysis and visualization cyberinfrastructure for data intensive collaborative research, which they call PetaShare. PetaShare will enable transparent handling of underlying data sharing, archival and retrieval mechanisms, and will make data available to scientists for analysis and visualization on demand. PetaShare will enable scientists to focus on their primary research problem, assured that the underlying infrastructure will manage the low-level data handling issues.



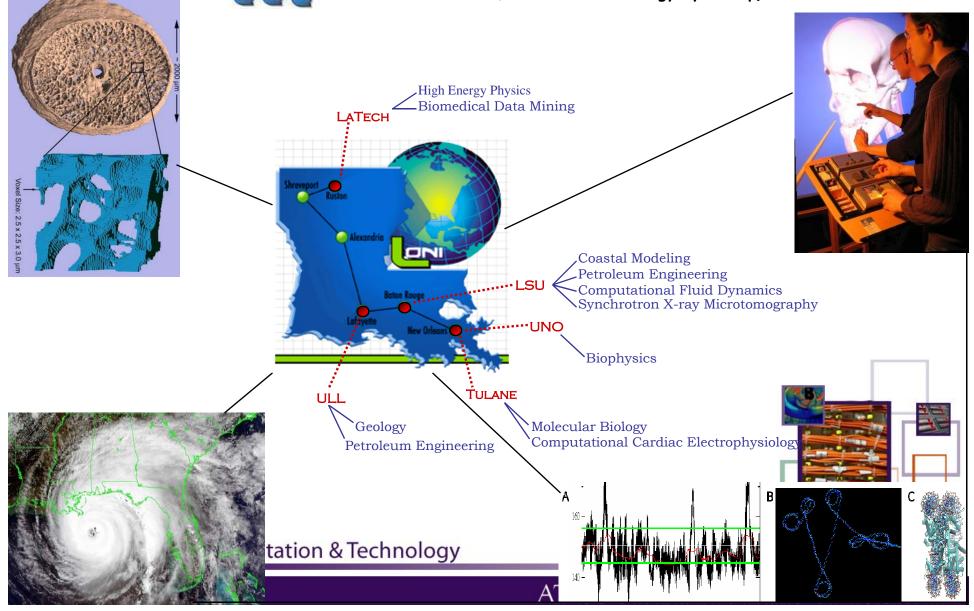
- Goal: enable domain scientists to focus on their primary research problem, assured that the underlying infrastructure will manage the low-level data handling issues.
- Novel approach: treat data storage resources and the tasks related to data access as first class entities just like computational resources and compute tasks.
- Key technologies being developed: data-aware storage systems, data-aware schedulers (i.e. Stork), and crossdomain meta-data scheme.
- Provides and additional 200TB disk, and 400TB tape storage



- PetaShare exploits 40 Gb/sec LONI connections between 5 LA institutions: LSU, LaTech, Tulane, ULL, and UNO.
- PetaShare links more than fifty senior researchers and two hundred graduate and undergraduate research students from ten different disciplines to perform multidisciplinary research.
- Application areas supported by PetaShare include coastal and environmental modeling, geospatial analysis, bioinformatics, medical imaging, fluid dynamics, petroleum engineering, numerical relativity, and high energy physics.



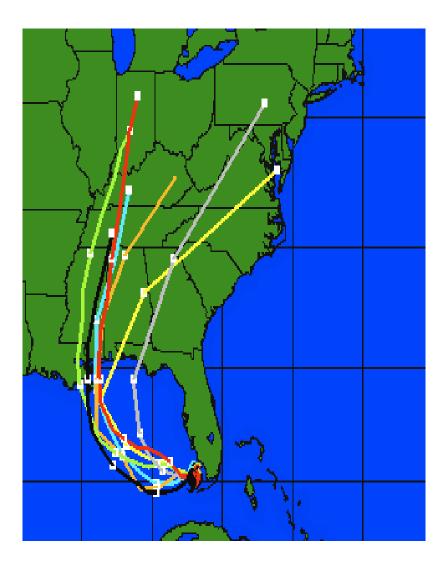
Participating institutions in the PetaShare project, connected through LONI. Sample research of the participating researchers pictured (i.e. biomechanics by Kodiyalam & Wischusen, tangible interaction by Ullmer, coastal studies by Walker, and molecular biology by Bishop).



PetaShare Science Drivers

Coastal Studies

- Walker, Levitan, Mashriqui, Twilley (LSU)
- The Earth Scan Lab: with its three antennas, it captures 40GB of data from six satellites each day. (→ 15 TB/year)
- Hurricane Center
 - Storm surge modeling, hurricane track prediction
- Wetland Biochemistry
 Institute
 - Coastal Ecosystem preservation
- SCOOP data archive



Petroleum Engineering

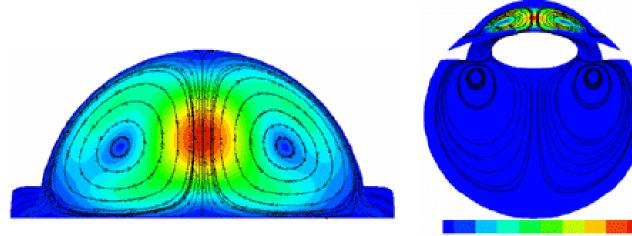
- White, Allen, Lei et al. (LSU, ULL, SUBR)
- UCoMS project reservoir simulation and uncertainty analysis
- 26M simulations, each generating 50MB of data
 → 1.3 PB of data total



 Drilling processing and real-time monitoring is data-intensive as well → real-time visualization and analysis of TB's of streaming data

Computational Fluid Dynamics

- Acharya et al. (LSU)
- Focusing on simulation of turbulent flows including Direct Numerical Simulations (DNS), Large Eddy Simulations (LES), and Reynolds-Averaged Navier Stokes Simulations (RANS).
- In DNS, ~10,000 instances of flow field must be stored and analyzed, each instance may contain 150M discrete variables. Resulting data set ~ 10 TB.



5.00E-06 1.50E-05 2.50E-05 3.50E-05 4.50E-05

Molecular Biology

•Winters-Hilt (UNO)

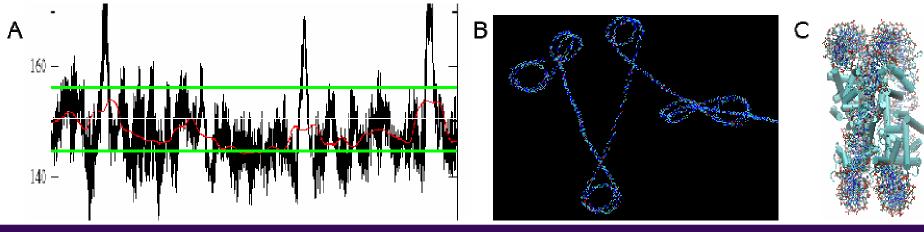
- •Biophysics and molecular biology gene structure analysis
- •Generates several terabytes of channel current measurements per month
- •Generated data being sent to UC-Santa Cruz, Harvard and other groups

•Bishop (Tulane)

•Study the structure and dynamics of nucleosomes using all atom molecular dynamics simulations

 Each simulation requires 3 weeks of run time on a 24-node cluster, and 50-100 GB of storage → 1-2 TB data per year

* Both access to the Genome database but separately!



And Others...

- Numerical Relativity Seidel et al (LSU)
- High Energy Physics Greenwood, McNeil (LaTech, LSU)
- Computational Cardiac Electrophysiology Trayanova (Tulane)
- Synchrotron X-ray Microtomography Wilson, Butler (LSU)
- Bio Data Mining Dua (LaTech)

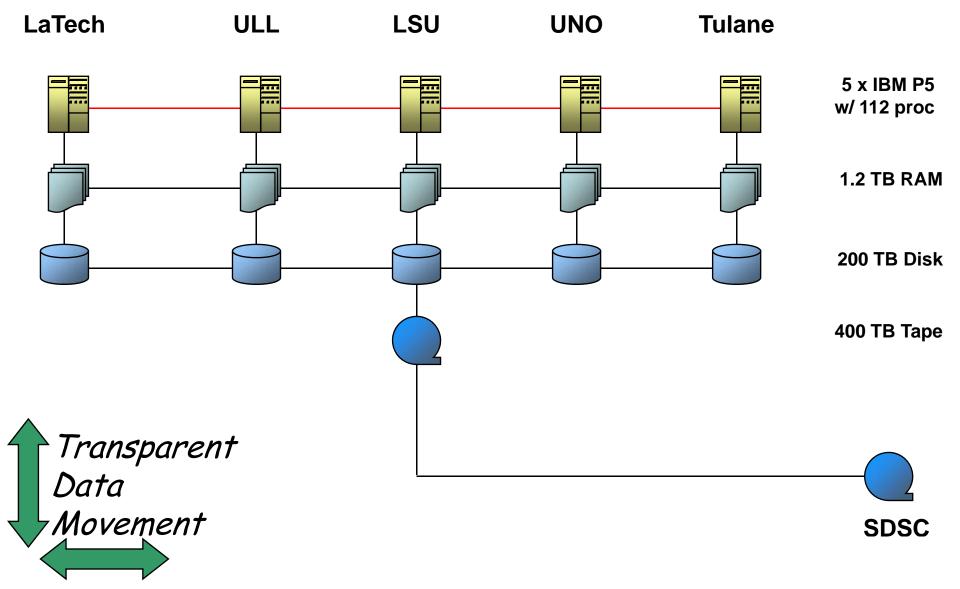
CS Research

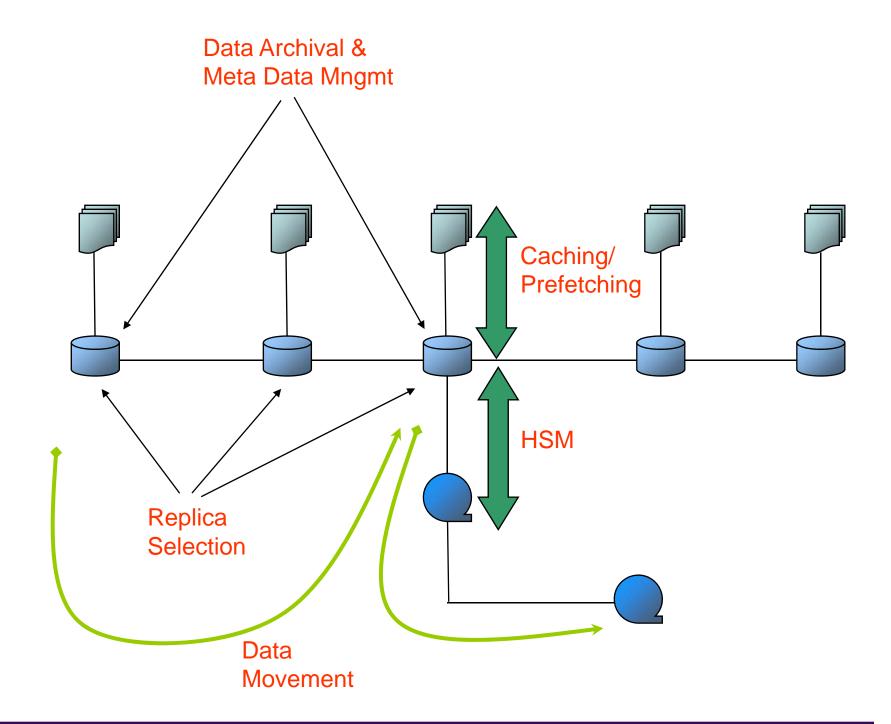
- Distributed Data Handling (Kosar)
- Grid Computing (Allen, Kosar)
- Visualization (Hutanu, Karki)
- Data Mining (Dua, Abdelguerfi)
- Database Systems (Triantaphyllou)

People involved with PetaShare Development and Usage

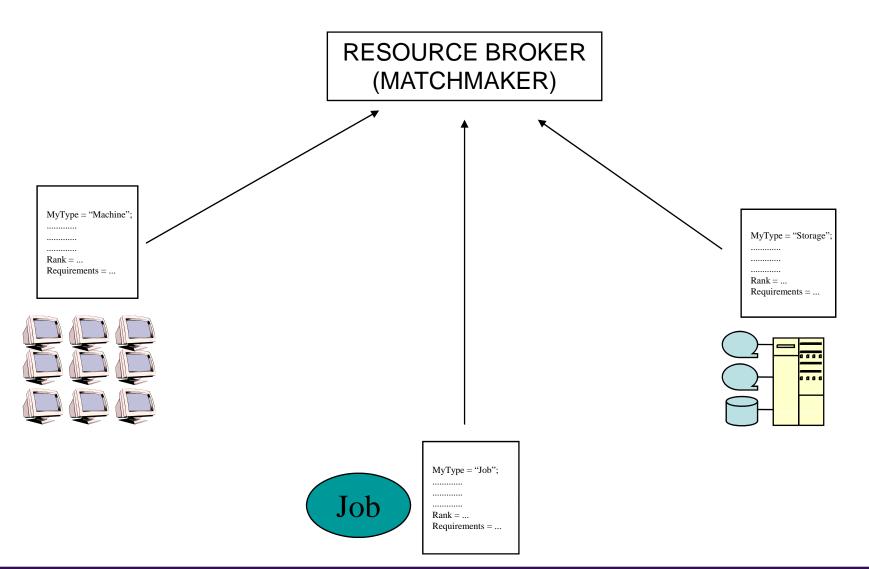
	Senior Personnel			Postdocs			Graduate Students			Undergraduates		
	Women	Minority	Total	Women	Minority	Total	Women	Mincrity	Total	Women	Minority	Total
LaTech			2						5			2
LSU	3		27			5	5	4	47	2	2	24
Tulane	1		3			2	3	5	11		1	3
ULL	7	4	18			8	13	5	31			4
UNO			7				5	4	32	3	8	17
Total	11	4	57			15	26	18	126	5	11	50

PetaShare Overview





Storage Systems as First Class Entities



Data-Aware Storage

- Storage server advertises:
 - Metadata information
 - Location information
 - Available and used storage space
 - Maximum connections available (eg. Max FTP conn, Max GridFTP conn, Max HTTP conn)
- Scheduler takes these into account
 - Allocates a connection before data placement
 - Allocates storage

Data-Aware Schedulers

 Traditional schedulers not aware of characteristics and semantics of data placement jobs

> Executable = genome.exe Arguments = a b c d

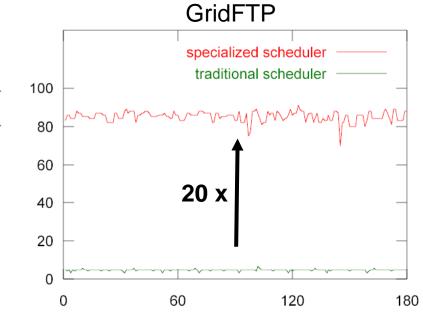
Executable	=	globus-url-copy
Arguments	=	gsiftp://host1/f1
		gsiftp://host2/f2
		-p 4 -tcp-bs 1024

Any difference?

[ICDCS'04]

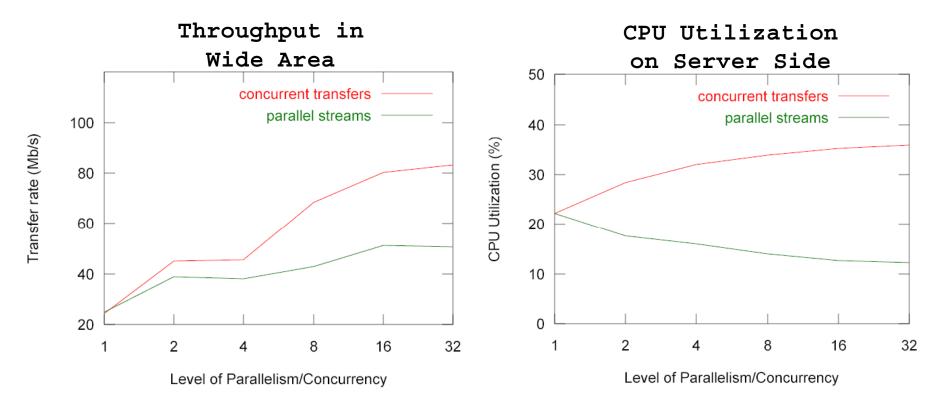
Data-Aware Schedulers

- What type of a job is it?
 - transfer, allocate, release, locate...
- What are the source and destination?
- destination? Which protocols to use? What is available storage space? What is best concurrency level?
- What is best concurrency level?
- What is the best route?
- What are the best network parameters?
 - tcp buffer size
 - I/O block size
 - # of parallel streams



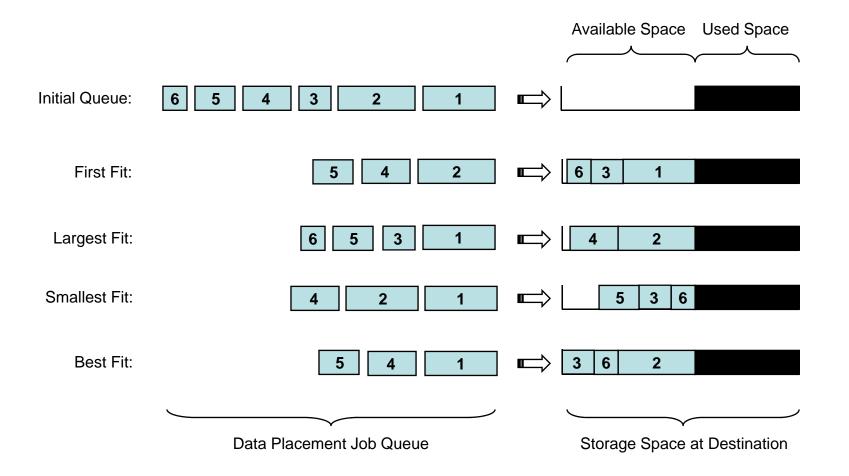
Time (minutes)

Optimizing Throughput and CPU Utilization at the same Time



- Definitions:
 - Concurrency: transfer n files at the same time
 - Parallelism: transfer 1 file using n parallel streams

Storage Space Management





A system driven by the local needs (in LA), but has potential to be a generic solution for the broader community!

