
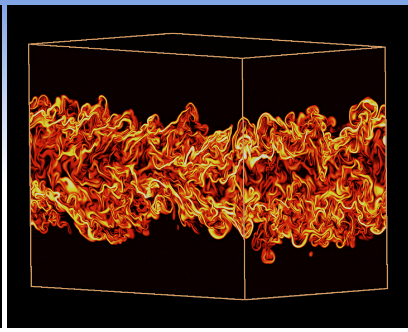
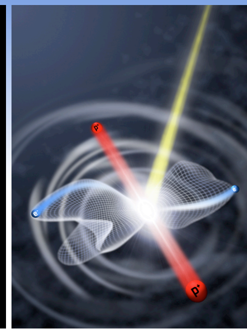
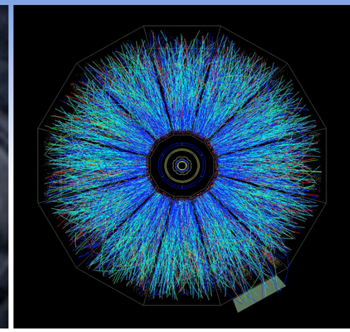
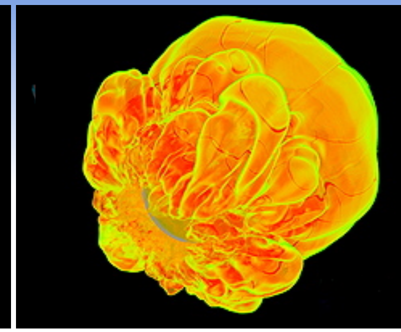

Extreme Scale Data Intensive Computing at NERSC

Harvey Wasserman

NERSC User Services Group

Los Alamos Computer Science Symposium

Workshop on Workshop on Performance Analysis of Extreme-Scale Systems and Applications

October 14, 2009

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U.S. DEPARTMENT OF ENERGY

NERSC

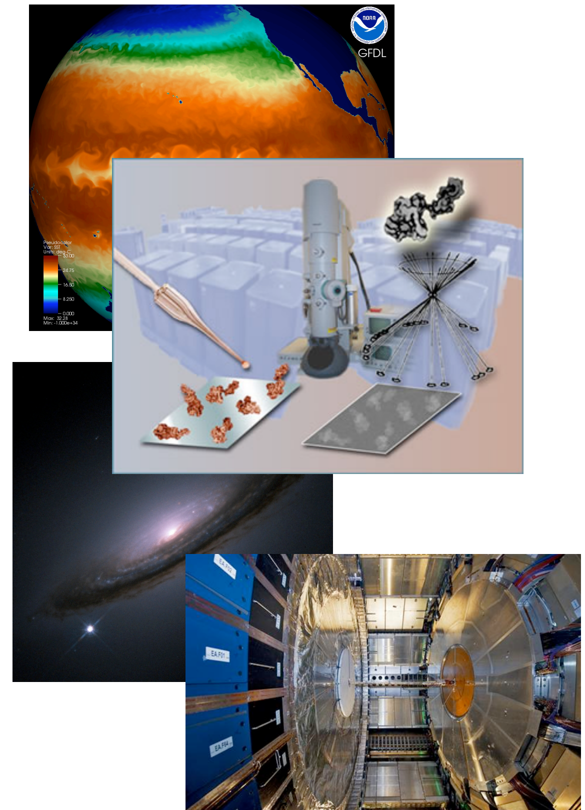
BERKELEY LAB

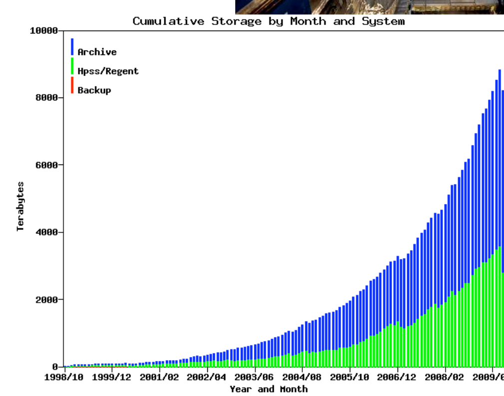
Outline

- **The need: project examples**
  - **Current & potential future**
- **The response: architecture and methods**
- **Results**
- **N.B., Many additional projects at LBNL**

Data Driven Science

- Ability to generate data is challenging our ability to store, analyze, & archive it.
  - Some observational devices grow in capability with Moore's Law.
  - Data sets are growing exponentially.
- Petabyte (PB) data sets soon will be common:
  - *Climate:* next IPCC estimates 10s of PBs
  - *Genome:* JGI alone will have .5 PB this year and double each year
  - *Particle physics*: LHC projects 16 PB / yr
  - *Astrophysics*: LSST, others, estimate 5 PB / yr
- Redefine the way science is done?
  - One group generates data, different group analyzes
- Turning point: in 2003 NERSC changed from being a data source to a data sink





Data Intensive Computing

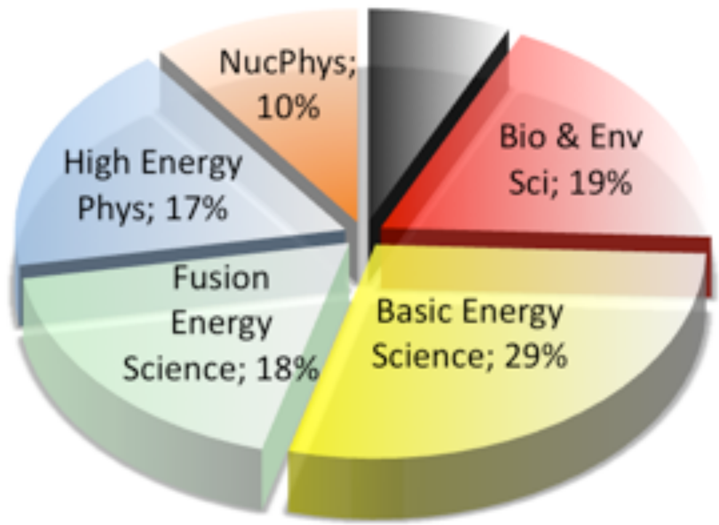
- Data mining: process of extracting hidden patterns from data
  - de novo genome assembly
  - Analysis of cosmological observations
  - Combine various DBs (protein/genome)
- Data-Intensive Predictive Science: simulations that generate lots of data
- Overarching need: fast I/O but not just BW

Nick Wright (~~SDSC~~/NERSC)

Intro to NERSC

- National Energy Research Scientific Computing Center
- Production computing for all DOE Office of Science (SC) research.
- ~ 2,000 users

2009 Allocations



- DOE allocated ~225M hours for ~370 projects at NERSC for 2010
  - ~ 50% of what users requested
  - Plus ~ 56M from SC, NERSC reserve
  - Plus ~ 60M “Storage Resource Units”

Selected NERSC Data Intensive Projects

Project	Category	Compute Hours	Storage RUs
Supernovae Factory	HEP/ Astro	14k	1.8M
Palomar Transient Factory	HEP/ Astro	36k	1M
ALICE	NP/ Astro	10k	2.2M
CCSM	Climate	12M	2M
STAR	Nuclear Physics	-	8M
CMB: PLANCK +	HEP/ Astro	680k	500k
20th Century ReAnalysis	Climate	8M	4M
John Bell	Chem/Comb/Math	5.5M	7.5M
Lattice QCD	NP	1.4M	2M
PCMDI	Climate	20k	2M
KamLAND	NP / Astro	-	4M
JGI	Biological Science	10k	2M

Cosmic Microwave Background

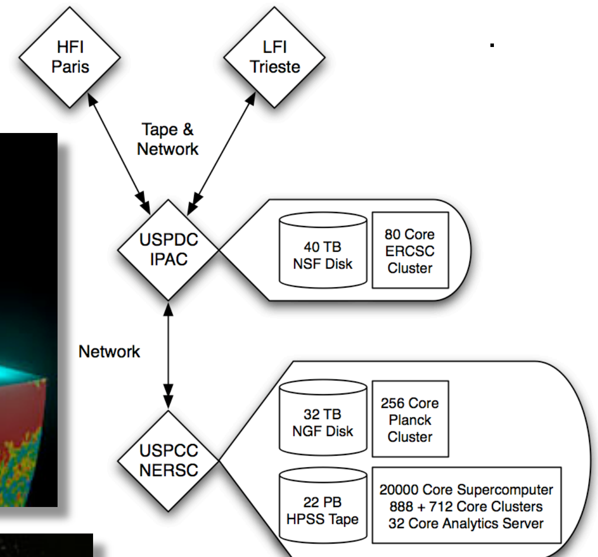
Objective: Analyze data from the Planck satellite -- definitive Cosmic Microwave Background (CMB) data set.

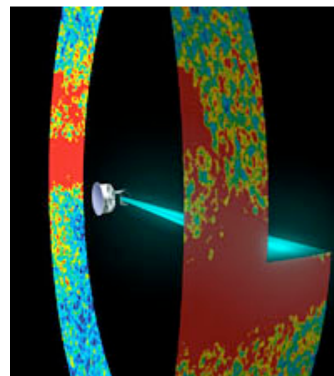
Implications: CMB: image of the universe at 400k years, relic radiation from Big Bang

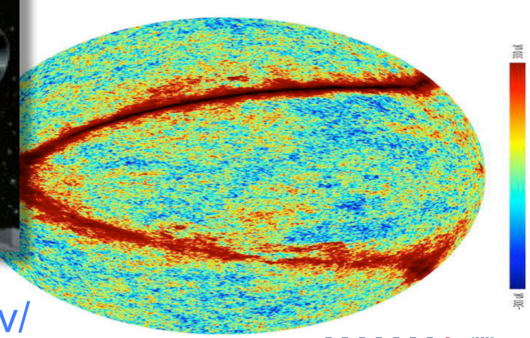
Accomplishments: NERSC provides the components of the data pipeline for noise reduction, map-making, power spectrum analysis, and parameter estimation

- 2006 Nobel Prize in Physics
- 32 TB final data set size, ~400 users
- data sets analyzed as a whole because complex data correlations
- Extensive use of NGF / PDSF
- Launched May09, first “light” Sept09
- Also ~10k-core Cray XT4 MonteCarlo calibration runs, produce ~10X data
- Anticipate Moore’s law growth in data set size for *15 years*

PI: J. Borrill (LBNL)







https://c3.lbl.gov/

PDSF / NGF

- Parallel Distributed Systems Facility
  - Heterogeneous commodity Linux cluster
    - GigE, I/B, several OSs, several CPUs
  - Open Science Grid
  - “Sub” clusters, data vaults for experiments
  - Funding comes from NERSC, NP and HEP
- NERSC Global File System (.45PB -> ~ 1PB)
  - Common global filesystem for all NERSC systems
  - GPFS
  - Extremely stable (zero unscheduled outages past two years)

KamLAND

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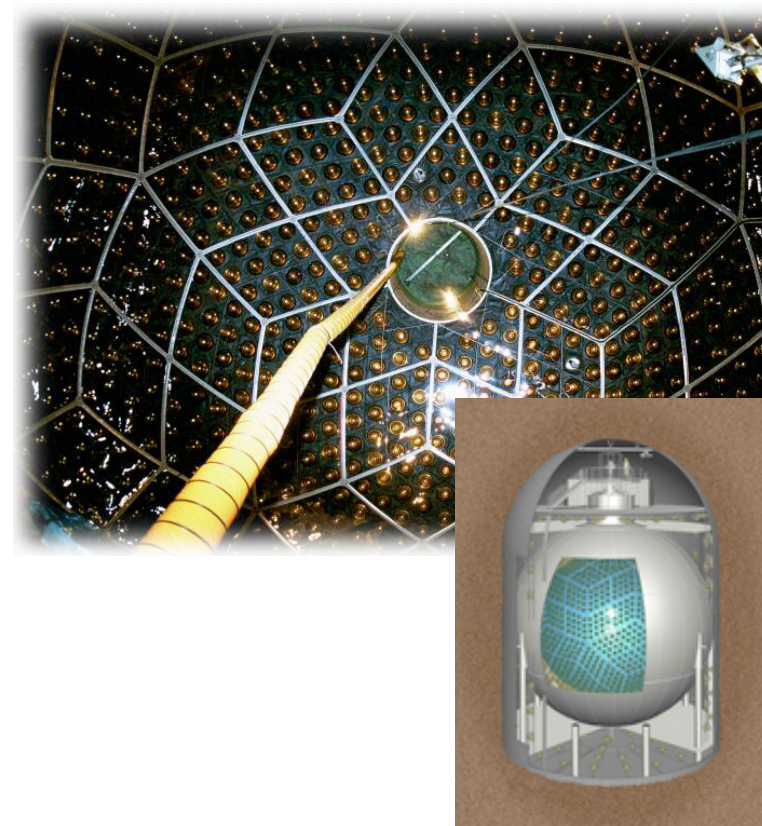
Objective: **Archive, analyze all stages of the US data from Kamioka Liquid Scintillator Anti-Neutrino Detector**

Implications: **Substantially increase our scientific knowledge of neutrinos**

Accomplishments: **Many significant physics milestones – neutrino oscillation, precise value for the neutrino oscillation parameter, etc.**

- **NERSC resources instrumental in reactor neutrino analysis and the preparations for the solar phase;**
- **Currently recording data at trigger rate of 100Hz, data rate of 200GB/day, 365 days/yr**
- **0.6 PB of data stored from 6 years; plan to read large fraction of this in 2010**

PI: S. Freedman (UCB)



http://kamland.lbl.gov/

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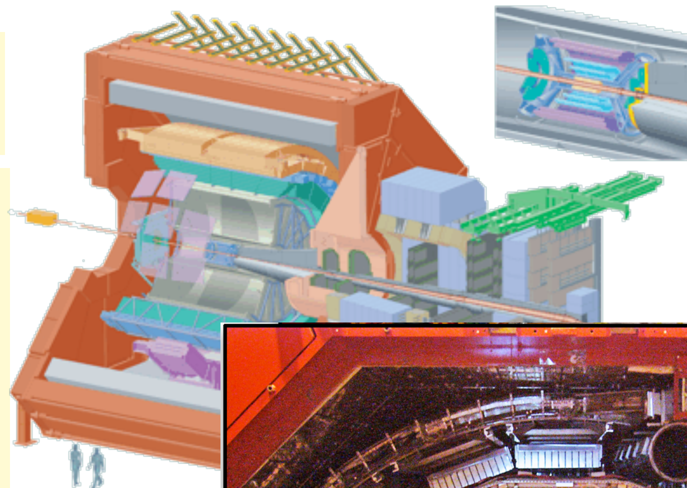
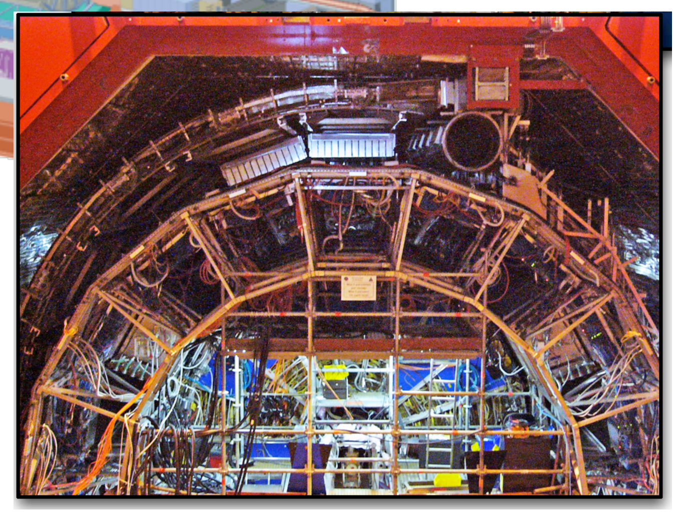
ALICE

Objective: Data analysis and simulations for the ALICE heavy-ion detector experiment at the LHC.

PI: P. Jacobs (LBNL)

Implications: Understanding of dense QCD matter.





Notes: Uses (primarily) NERSC's PDSF cluster + LLNL + Grid resources;

- Expect ~600TB of data distributed over 1GB files, ~25% of USA obligation in 2010.
- Challenge of providing direct-charged resources for experimentation that might be delayed.
- Simulation resources to reconstruct and analyze detector events prior to the experiment.
- Longer term: Estimate 3.8 PB of disk space and 5.31 PB of HPSS in 2013, accessible by international community.

http://aliceinfo.cern.ch/Collaboration/

Program for Climate Model Diagnosis and Intercomparison

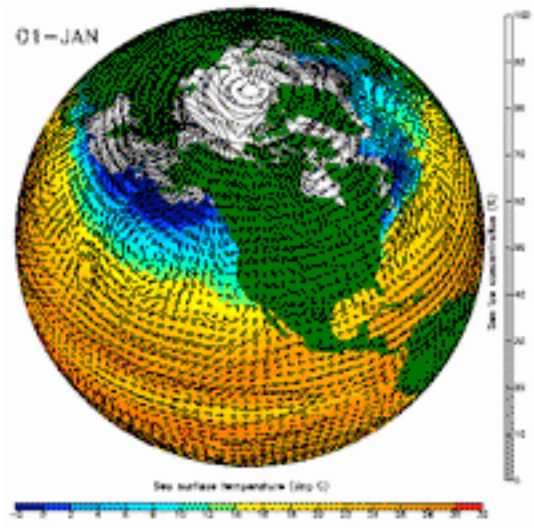
Objective: Compare forecasts made by global climate models (GCMs) with varying initial conditions based on detailed observations to assess GCM accuracy.

Implications: Improved climate prediction; support for IPCC.

Accomplishments: Archived European observational data at NERSC mass storage facility;

- Extensive CAM runs on Franklin;
- New, very high resolution (~100 meters) Large Eddy Simulation (LES) model to be added in 2010.
- LES results in 2X storage increase
- Small time scale (~20 min) produces many files

PI: C. Covey (LLNL)



https://ccpp.llnl.gov/

Cloud-Resolving Climate Model

PI: D. Randall, Colo. St

Objective: Climate models that fully resolve key convective processes in clouds; ultimate goal is 1-km resolution.

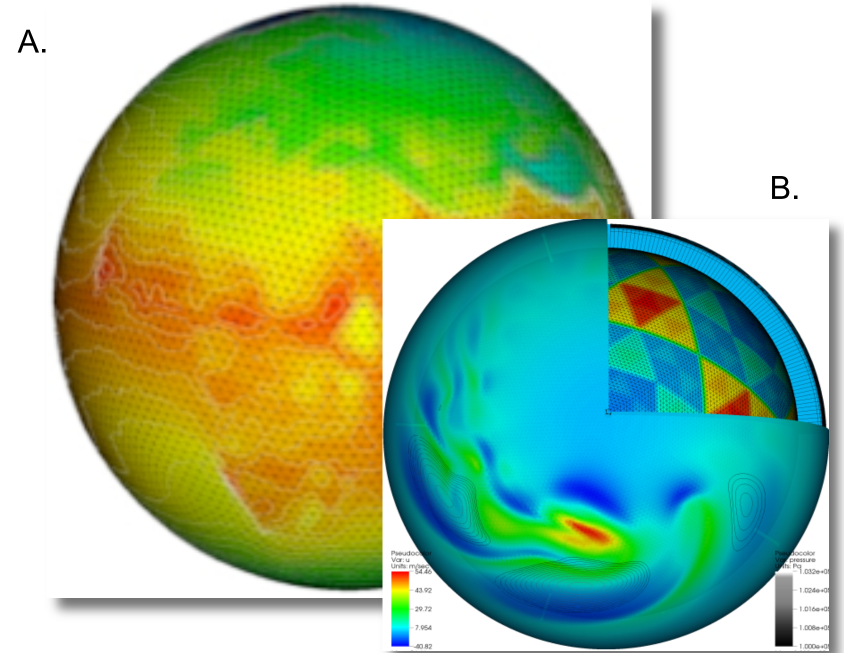
Implications: Major transformation in climate/weather prediction, likely to be standard soon, just barely feasible now.

Accomplishments: Developed a coupled atmosphere-ocean-land model based on geodesic grids.

- Multigrid solver scales perfectly on 20k cores of Franklin using grid with 167M elements.
- Invited lecture at SC09.

NERSC:

- 3-km 24-hr run, 30k cores = 10TB output
- NERSC/LBNL played key role in developing critical I/O code & Viz infrastructure to enable analysis of ensemble runs and icosohedral grid.



A. Surface temperature showing geodesic grid.
B. Composite plot showing several variables: wind velocity (surface pseudocolor plot), pressure (b/w contour lines), and a cut-away view of the geodesic grid.

Joint Genome Institute

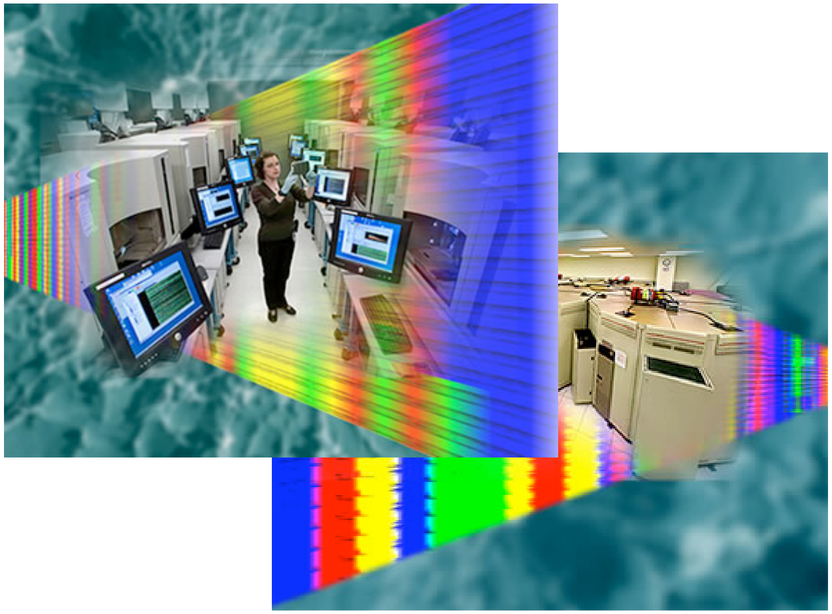
Objective: Archive all production and R&D data from three sequencing platforms at JGI

Implications: One of the world's largest public DNA sequencing facilities.

Accomplishments: NERSC, JGI staff collaborated to set up nightly back-up pipeline using ESnet's new Bay Area MAN.

- Archiving sequencing data at NERSC allowed JGI to scale up infrastructure with minimal additional DOE investment.
- Data import expected to grow nearly exponentially in 2010; impossible to maintain data onsite at the JGI HQ.
- NERSC/DOE JGI collaboration to develop improved techniques for data access, handling.
- Note: additional Microbial Genome project

PI: E. Rubin (LBNL)



JGI is producing sequence data at increasing rate: 2 million files per month of trace data (25 to 100 KB each) plus 100 assembled projects per month (50 MB to 250 MB); total about 2 TB per month on average.

Palomar Transient Factory

Objective: Process, analyze & make available data from Palomar Transient Sky survey (~300 GB / night) to expose rare and fleeting cosmic events.

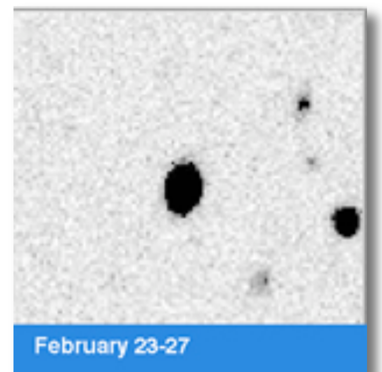
Implications: First survey dedicated solely to finding transient events.

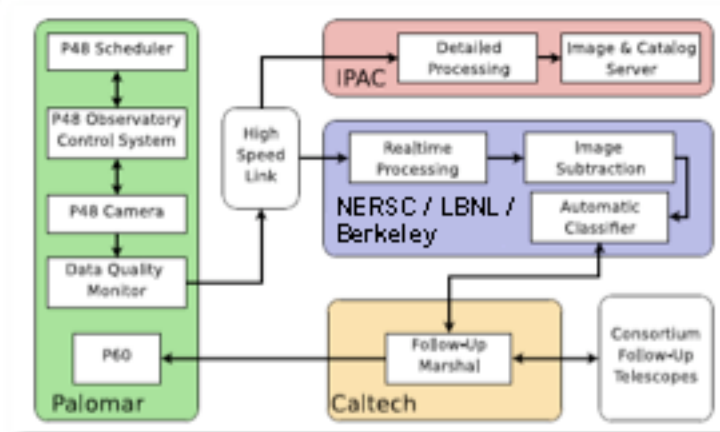
Accomplishments: Automated software for astrometric & photometric analysis and *real-time* classification of transients.

- Analysis at NERSC is fast enough to reveal transients *as data are collected.*
- Has *already uncovered* more than 40 supernovae explosions since Dec., 2008.
- Uncovering a new event about *every 12 minutes.*

- 40k MPP allocation + 1M HPSS in 2009; Stored on NERSC's 450-TB NGF + gateway (other slide)

PI: P. Nugent (LBNL)

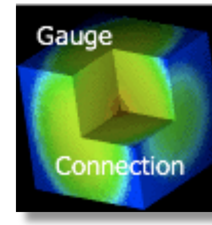




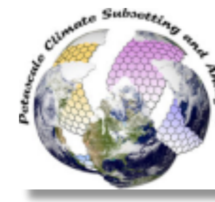
PTF project data flow

Two manuscripts submitted to Publications of the Astronomical Society of the Pacific

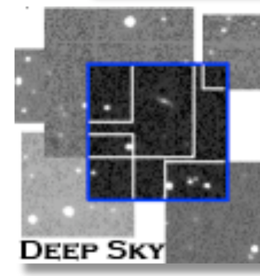
Science Gateways



- Create scientific communities around data sets
  - NERSC HPSS, NGF accessible by broad community for exploration, scientific discovery, and validation of results
  - Increase value of existing data



- *Science gateway: custom (*hardware/software) to provide remote data/computing services
  - Deep Sky – “Google-Maps” for astronomical image data
    - Discovered 36 supernovae in 6 nights during the PTF Survey
    - 15 collaborators worldwide worked for 24 hours non-stop
  - GCRM – Interactive subselection of climate data (pilot)
  - Gauge Connection – Access QCD Lattice data sets
  - Planck Portal – Access to Planck Data



- New models of computational access
  - Projects with mission-critical time constraints require guaranteed turn-around time.
  - Reservations for anticipated needs: Computational Beamlines
  - Friendly interfaces for applications and workflows

Deep Sky Science Gateway

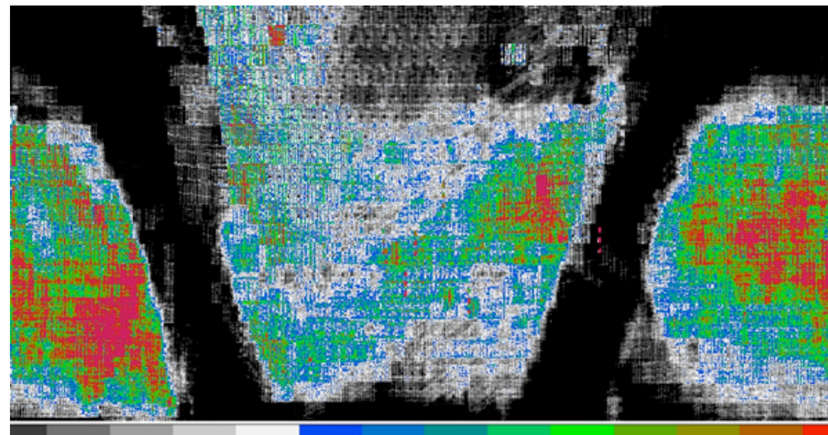
Objective: Pilot project to create a richer set of compute- and data-resource interfaces for next-generation astrophysics image data, making it easier for scientists to use NERSC and creating world-wide collaborative opportunities.

Implications: Efficient, streamlined access to massive amounts of data – some archival, some new -- for broad user communities.

Accomplishments: Open-source Postgres DBMS customized to create Deep Sky DB and interface: www.deepskyproject.org

- 90TB of 6-MB images stored in HPSS / NGF (biggest NGF project now)
  - -- images + calibr. data, ref. images, more
  - -- special storage pool focused on capacity not bandwidth
- Like "Google Earth" for astronomers?

PI: C. Aragon (NERSC)



Map of the sky as viewed from Palomar Observatory; color shows the number of times an area was observed

See Peter Nugent's NUG2009 Talk

- **Other NERSC gateways: GCRM (climate), Planck (Astro), Gauge Connection (QCD)**

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Molecular Dynameomics

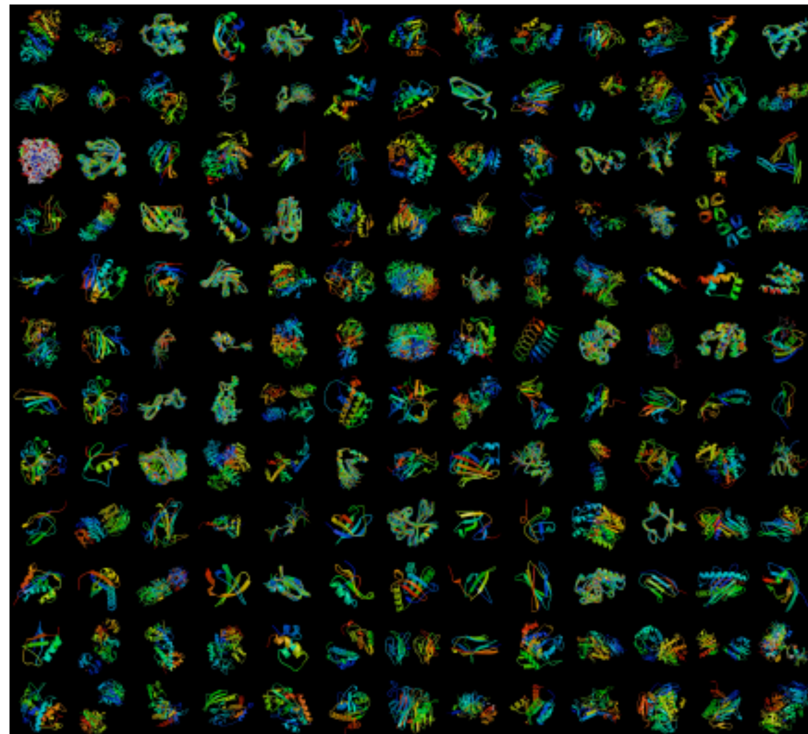
PI: V. Daggett (U. Wash.)

Objective: **Create & mine a database of molecular dynamics structures to identify similarities between native and unfolded states across all secondary and tertiary structure types and sequences.**

Implications: **Improved protein structure prediction algorithms by identifying patterns and general features of transition, intermediate and denatured states.**

Accomplishments: **To date, performed more than 6,000 simulations of nearly a 1,000 proteins for a combined simulation time of >140 microseconds.**

- **Continued data mining to identify similarities / differences between native and unfolded states across all 2° and 3° structure types and sequences.**
- **Expect repository similar to Protein DB, 100+ TB relational database**



The first 156 dynameomics simulation targets

http://www.dynameomics.org

Observations

- It's not just about providing tapes / disk / fiber
  - It's about organization & intelligent, secure, public access using modern tools
- Simulation output becomes too large to move "home."
  - However, some science groups lack agreement on how much data needs to be available and where
- Kathy Yelick: Tape archives, vital to efficient science, use 2-3 orders of magnitude less power than disk
- Beyond "enormous growth," precise requirements sometimes elusive
  - NERSC XT4 increased HPSS use 50% - why?
  - Data needs linked to machine reliability
  - Observational projects easier to characterize storage needs?
- Value of data varies: observations may be irreplaceable; rarely touched; processing raw data may result in 10X larger volume
- Manipulation and analysis of data is becoming a problem that can be addressed only by large HPC systems.
- Few projects are purely simulation or observation.
- Fast I/O is key

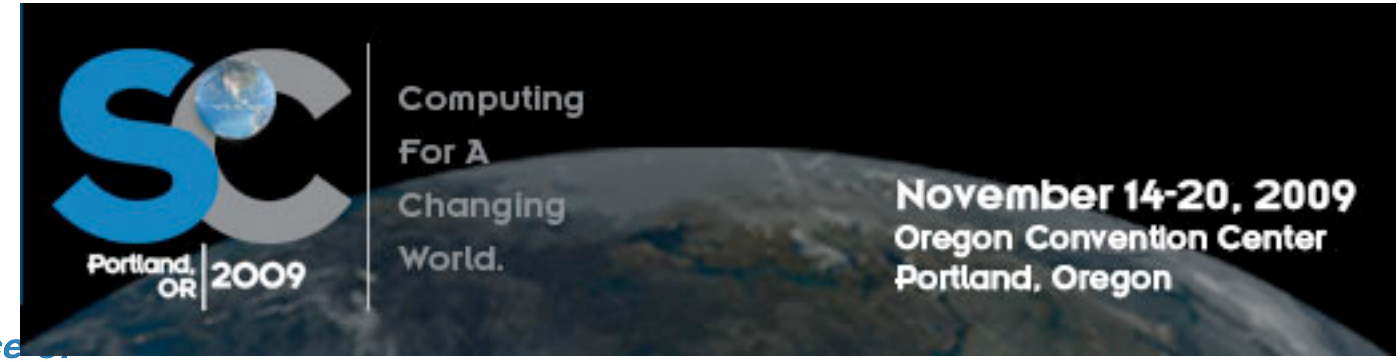
NERSC Response

- Upgrade I/O capability in NERSC-5*
- Increased I/O capability in NERSC-6
- Improved user access in NERSC-5/6
- User support for improved I/O

*NERSC-5 is "Franklin," Cray XT4

But first…

- SC09 Masterworks: Data intensive computing and lots more!
- http://sc09.supercomputing.org/?pg=masterworks.html
- Talks from Google, Facebook
- Data Challenges in Genome Analysis
- Talks are Tu, Weds, Thurs; Portland Ballroom



I/O Benchmarking

- Difficulty is in finding tests that accurately capture the workload but are easy to use
- LBNL CRD research, using IOR to accurately capture I/O in applications (Oliker/Shalf/Borrill/Shan, SC07)
- NERSC-6 procurement approach:
  - One application writes checkpoint files
  - IOR and Metadata kernel tests
- Additional applications: GTC, Flash, S3D, POP
- Vary sizes, method (POSIX / MPI-IO / HDF / netCDF)
- Metrics: % of runtime / % of peak / % of relative peak
- Frequently asked to provide I/O “stress tests”

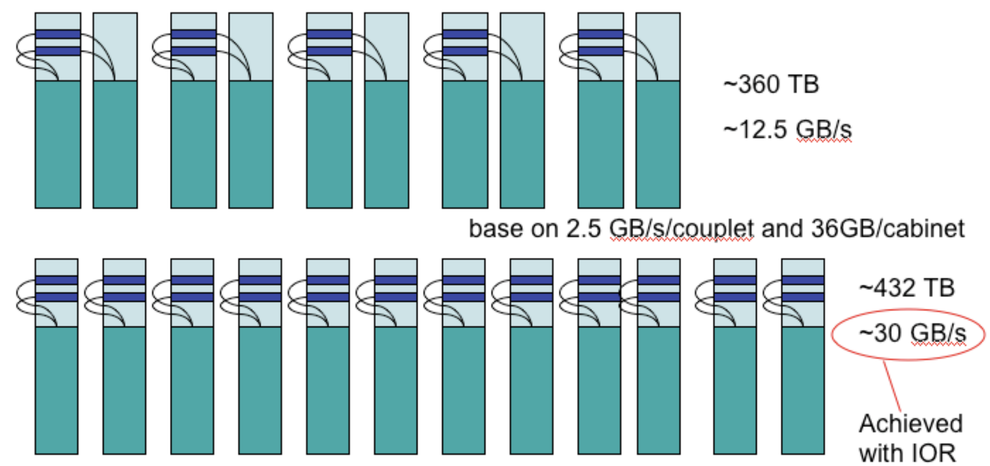
NERSC XT4 I/O Improvement: HW

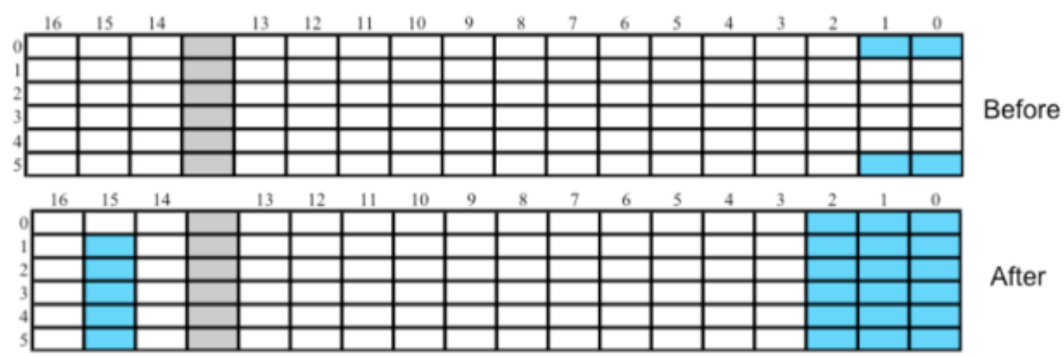
- **Congestion in the I/O subsystem had been a major cause of instability, poor achieved I/O rates.**

	Before	After
Compute Nodes	9,660	9,572
Login Nodes	10	10
MOM Nodes	16 (also serve as login nodes)	6 (distinct MOM nodes)
Lustre OSS / OST	20 / 80 per filesystem	24 / 48 per 2 filesystems
DVS Nodes	0	20
Filesystems	/scratch	/scratch /scratch2
Capacity	346 TB	420 TB (210 TB ea.)
I/O adaptors	PCI	PCI-e
Peak I/O perf.	~ 12.5 GB/s	~ 30 GB/s

NERSC XT4 I/O Improvement: HW

- 2nd scratch filesystem added
  - reduce I/O congestion among simultaneous user jobs
- Disks better distributed, 2X # of controllers
- Service nodes redistributed.





indicates that this cabinet contains service nodes

NERSC XT4 I/O Improvement: HW

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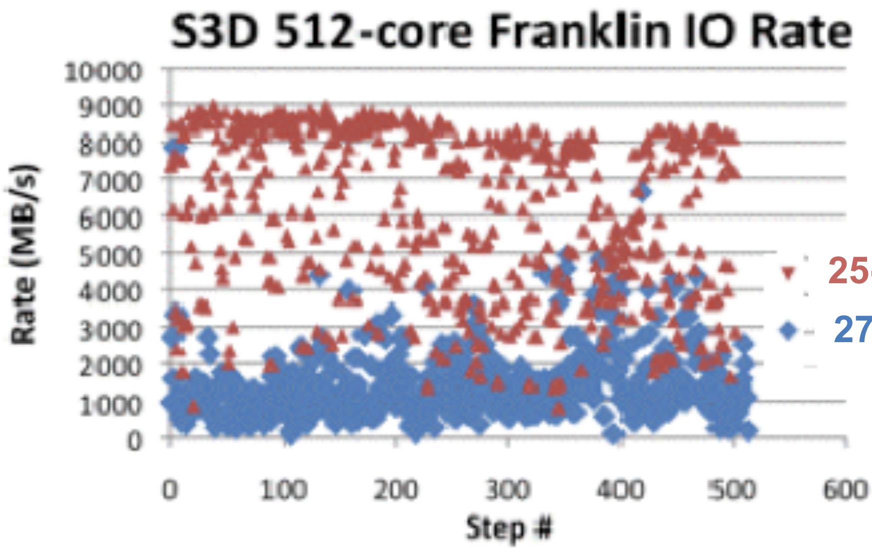


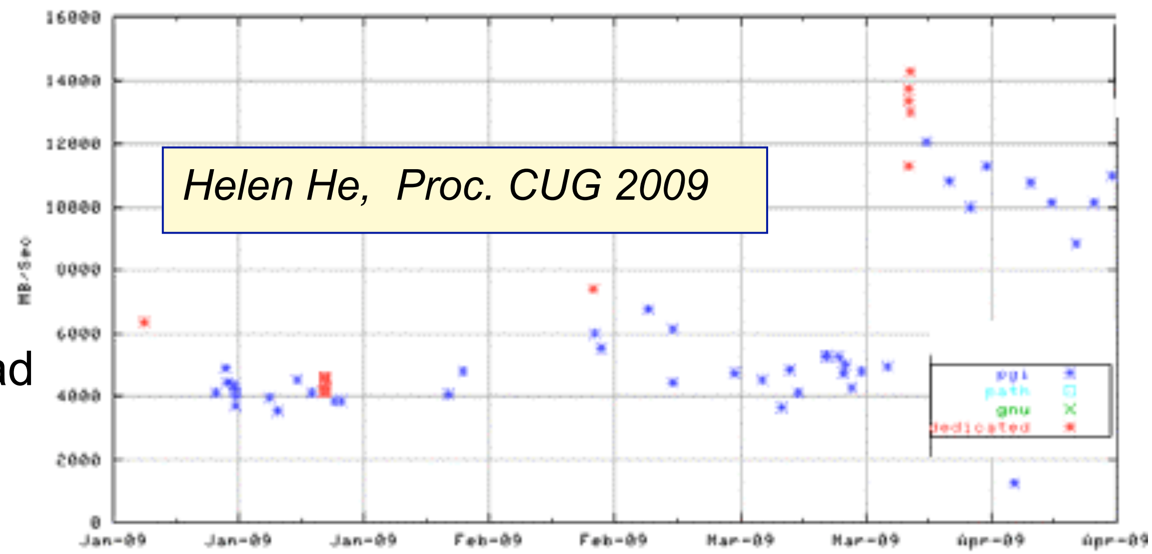
25-Mar Harmonic Mean = 4,972 MB/s

27-Feb Harmonic Mean = 955 MB/s

	BlueGene	Jaguar	FranklinBefore	FranklinAfter
%I/O 16000	24%	15%	29%	5%
%I/O 4096	7%	9%	7%	1%
%I/O 512	2%	<1%	1%	<1%

S3D aggregate performance, unpublished results

IOR benchmark aggregate read performance



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NERSC XT4 I/O Improvement: SW

- Users report < 1 GB/s write bandwidth
- K. Antypas and A. Uselton (NERSC), *CUG09*
- Identify Sub-optimal MPI-IO implementation
- Study via IOR, Flash, MadBench
- Compare:
  - file-per-proc vs. shared file
  - Lustre block boundary alignment (1e6 *vs.* 2^{20} bytes)

Tools

- **IPM**
  - **David Skinner (NERSC), Noel Keen (LBNL), Mark Howison (NERSC)**
  - **intercept** libc **`open`, `close`, `read` and `write` calls**
  - **http://www.nersc.gov/projects/ipm/**

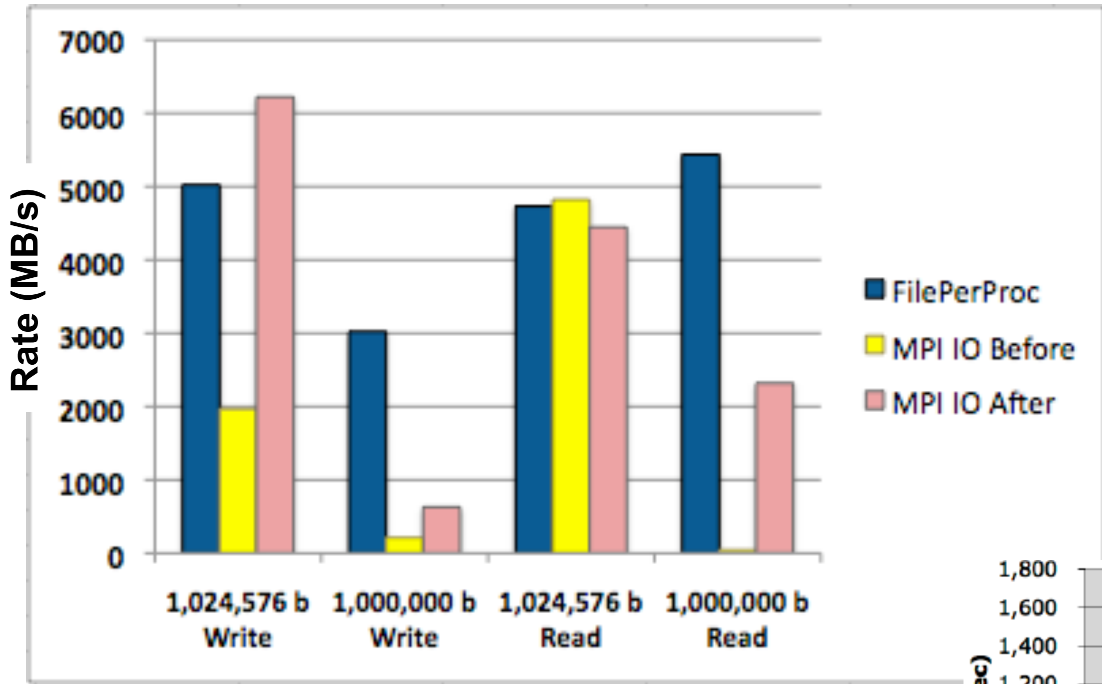
Antypas and Uselton, Proc. CUG 2009

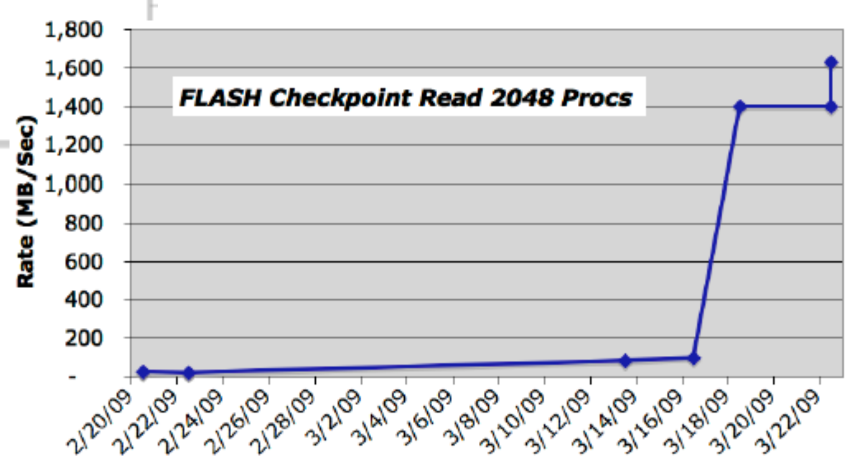
- **Lustre Monitoring Tool (Andrew Uselton, NERSC) http://code.google.com/p/lmt**

NERSC XT4 I/O Improvement: SW

- Adjust default stripe width to 4 MB (4x)
- Cray revised collective buffering algorithm to issue write calls that respect stripe boundaries
- Set # of writer nodes equal to the number of stripes (via trial & error using IOR)
  - led to an optimal OST assignment; performance on par with file-per-proc
- Result:
  - collective write bandwidths ~ 6.5 GB/s

NERSC XT4 I/O Improvement: SW



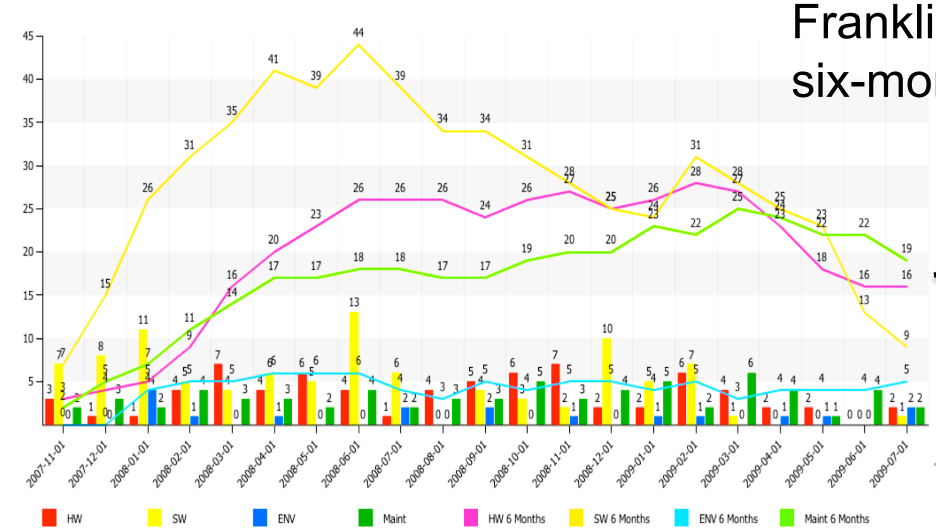


Antypas and Uselton, Proc. CUG 2009

Improved XT4 Stability

- **I/O improvements yield stability improvement**

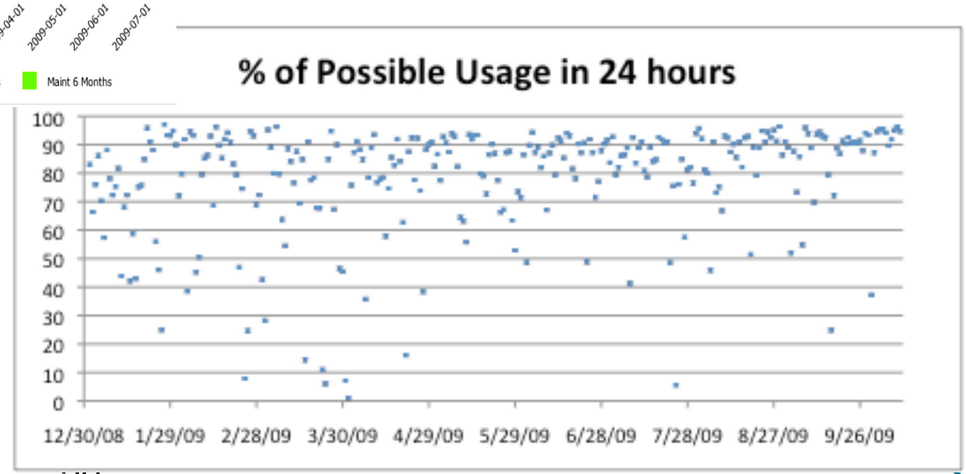
Franklin Outages Nov07 - Jul09 with six-month moving averages



HW 6-mo

SW 6-mo

HW SW



NERSC-6 (Hopper) System

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Phase 1 – Cray XT5

- 668 nodes, 5,344 cores
- 2.4 GHz AMD Opteron (Shanghai, 4-core)
- 50 TF peak
- 5 TF SSP
- 11 TB DDR2 memory total
- Seastar2+ Interconnect
- 2 PB disk, 25 GB/s
- Air cooled

Phase 2 Cray <?>

- > 6,000 nodes > 150,000 cores
- 12-core AMD Opteron (Magny-Cours)
- > 1 PF peak
- > 100 TF SSP
- > 200 TB DDR3 memory total
- Gemini Interconnect
- 2 PB disk, 80 GB/s*
- Liquid cooled

* measurable, sustained aggregate filesystem I/O bandwidth between the external parallel filesystem and the computational nodes using IOR.

3Q09	4Q09	1Q10	2Q10	3Q10	4Q10

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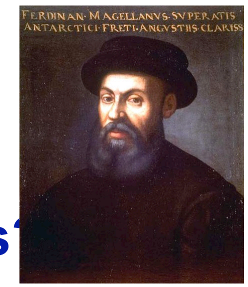
Testbeds, etc.

- **GPU/Accelerator Testbed** Hank Childs (NERSC)
  - Large-memory (.5 TB RAM) with Nvidia Tesla (1 TF) GPU accelerators
  - Experiment with GPU accelerated sequence matching and OpenCL/CUDA programming model
  - Gain experience with administration of this kind of platform
- **Cloud Computing Testbed (NERSC/ANL: Magellan)**
  - Distributed, multi-institution dynamically expandable computing resource
  - Experiment with cost effectiveness of cloud computing paradigm, including Amazon EC2 evaluation
- **Solid State/FLASH Accelerated I/O**
  - Next slide Shane Canon /Jason Hick (NERSC)
- **FPGA Accelerator Testbed (LBL Computing Research Division)**
  - Convey HC1 FPGA accelerator with 80GB/s vector memory subsystem: can be programmed with "custom personalities" for, e.g., bioinformatics applications John Shalf (NERSC)

DOE Explores Cloud Computing

- ASCR Magellan Project
  - $32M project at NERSC and ALCF
  - ~100 TF/s compute cloud testbed (across sites)
  - Petabyte-scale storage cloud testbed
- Cloud questions to explore on Magellan:
  - Can a cloud serve DOE's mid-range computing needs?
    → More efficient than cluster-per-PI model
  - What part of the workload can be served on a cloud?
  - What features (hardware and software) are needed of a "Science Cloud"? (Eucalyptus at ALCF; Linux at NERSC)
  - How does this differ, if at all, from commercial clouds?



Flash Storage Testbeds

- ~ 10TB in NERSC Global Filesystem (NGF)
  - Metadata acceleration
  - High bandwidth, low-latency storage class
- ~ 16TB as local SSD in one ScalableUnit (~7 TF) of new "Magellan" cloud testbed
  - Data analytics
  - Local read-only data
  - Local temp storage
- ~ 2TB in HPSS (metadata acceleration)

Shane Canon, Jason Hick (NERSC)

Other NERSC Efforts

- Increase in I/O Bandwidth for GCRM project
  - Mark Howison (NERSC), PNNL
  - recently achieved aggregate write bandwidth of 5 GB/sec on XT4
- HDF5 I/O Library Performance Analysis, Optimization, and HDFPart API layer
  - Mark Howison, John Shalf (NERSC)
  - See NUG talk, Oct2009

Acknowledgments

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- Shane Canon, NERSC Data Systems Group Lead
- John Shalf, NERSC SDSA Group Lead
- Wes Bethel, NERSC Analytics Group Lead
- David Skinner, NERSC SW Integration Group Lead
- Brent Draney, NERSC Networking Group Lead

- http://www.nersc.gov

Backup Slides

NERSC
NATIONAL ENERGY RESEARCH SCIENTIFIC COMPUTING CENTER

NERSC 2009 Configuration

Large-Scale Computing System

Franklin (NERSC-5): Cray XT4

- 9,740 nodes; 38,288 Opteron cores,
- 8 GB of memory per node
- 26 Tflop/s sustained SSP (355 Tflops/s peak)

NERSC-6 (XT5) planned for 2010 production

- 3-4x NERSC-5 in application performance

Clusters

- Bassi IBM Power5 (888 cores)
- Jacquard LNXI Opteron (712 cores)
- New Nehalem / IB Cluster
- PDSF (HEP/NP)
  - Linux cluster (~1K cores)

NERSC Global Filesystem (NGF)

400 TB; 5.5 GB/s

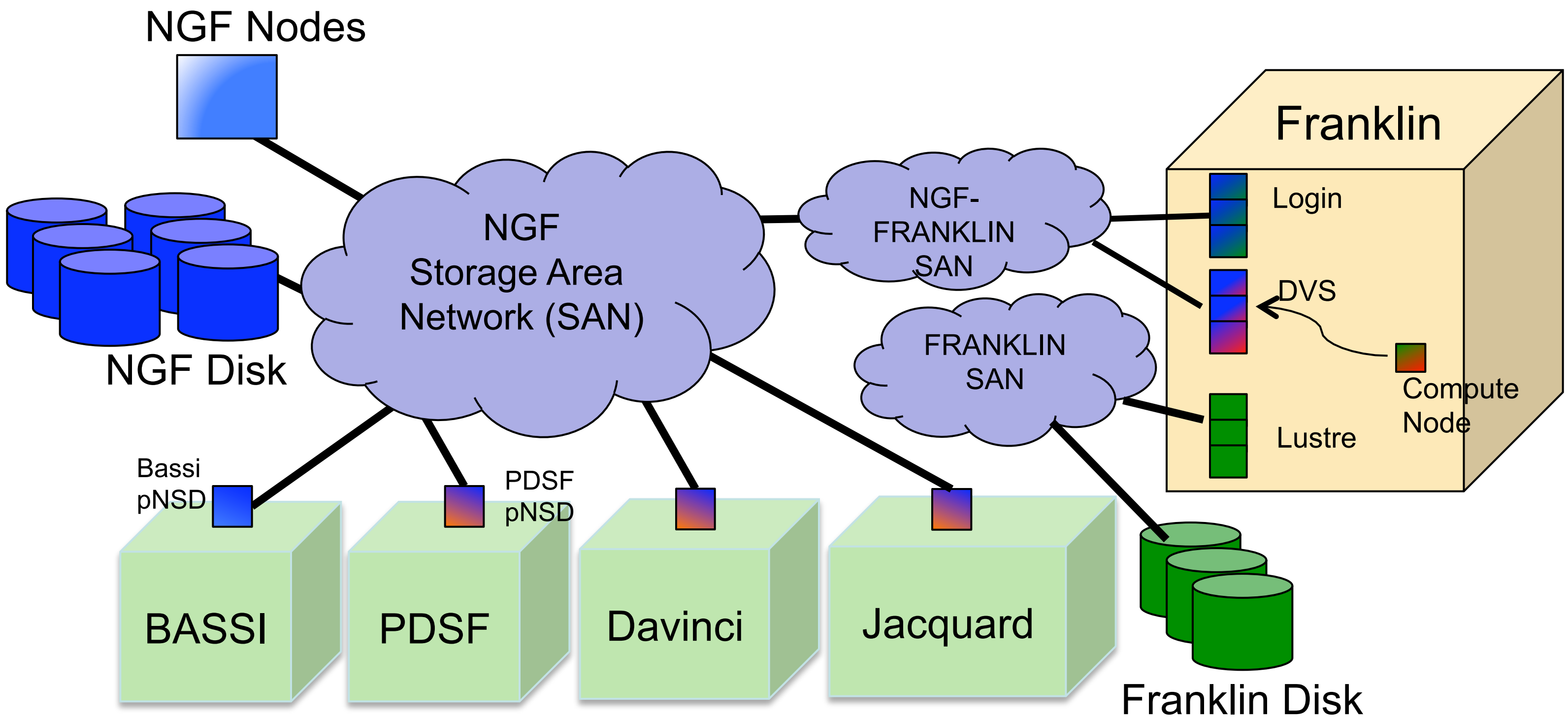
HPSS Archival Storage

- 60 PB capacity
- 10 Sun robots
- 130 TB disk cache

Analytics / Visualization

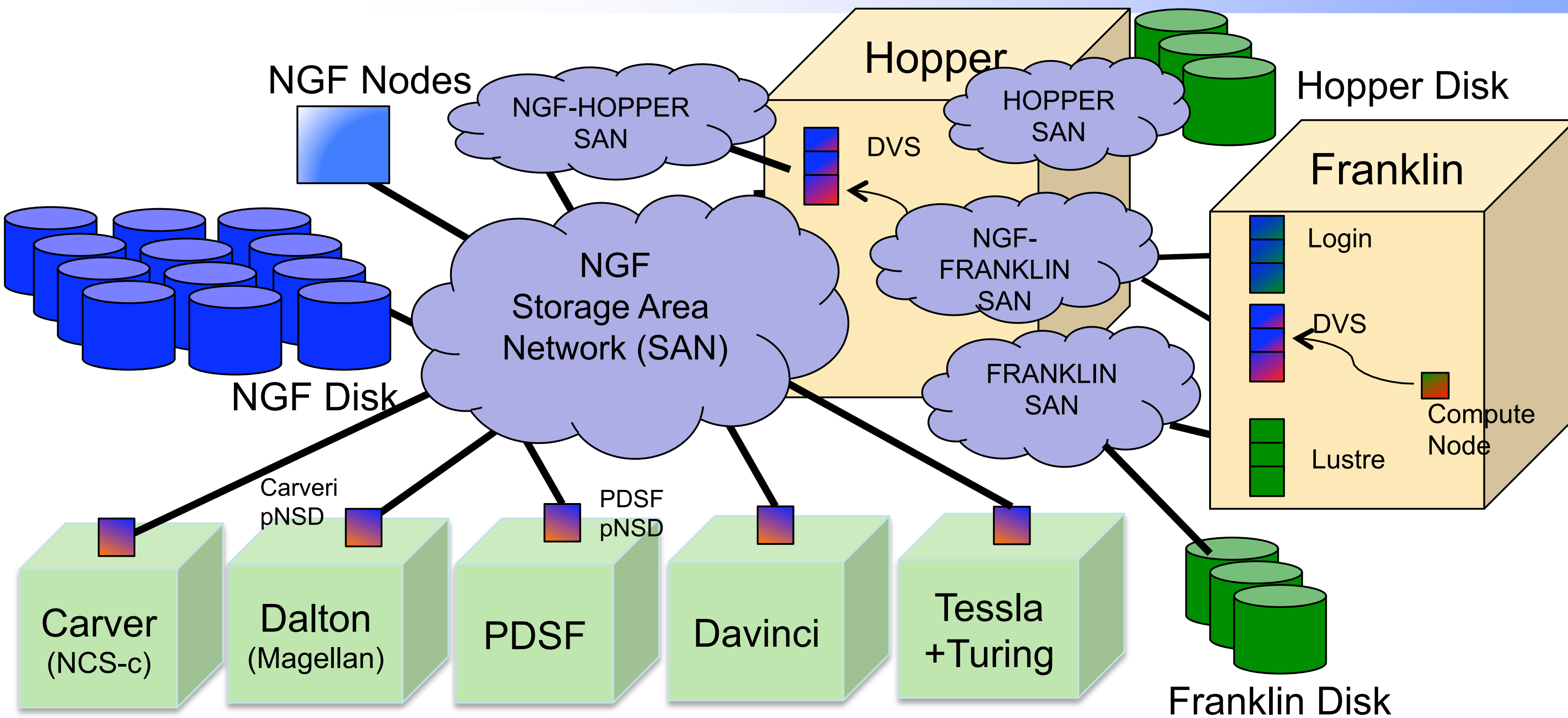
- Davinci (SGI Altix)

NERSC Global File system (NGF)



- A facility-wide, high performance, parallel file system
  - Uses IBM's GPFS technology for scalable high performance
  - Designed for user productivity

NERSC Global File system (NGF)



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20th Century Climate Reanalysis

NERSC
NATIONAL ENERGY RESEARCH SCIENTIFIC COMPUTING CENTER

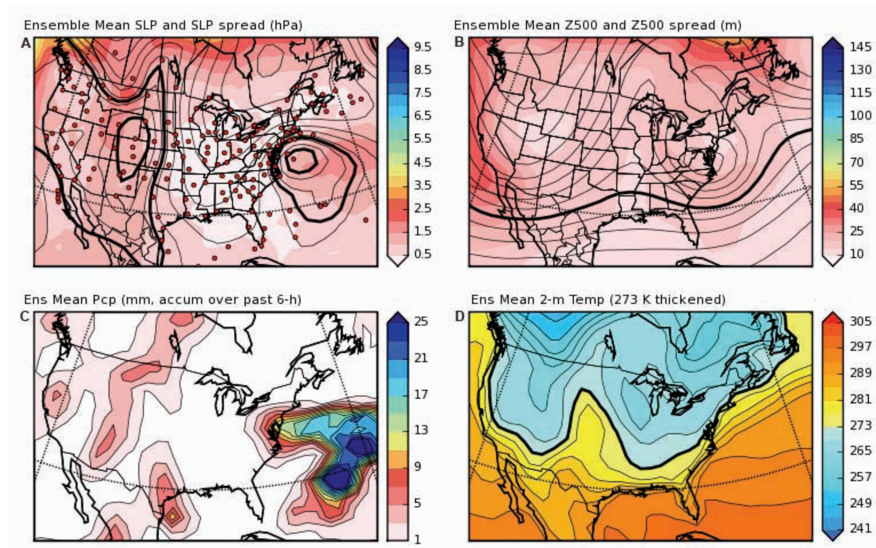
PI: G. Compo (U. Colorado)

Objective: **Use an Ensemble Kalman filter to reconstruct global weather conditions in six-hour intervals from 1871 to the present.**

Implications: **Validate tools for future projections by successfully recreating – and explaining – climate anomalies of the past.**

Accomplishments: **First complete database of 3-D global weather maps for the 19th to 21st centuries.**

- **Provide missing information about the conditions in which extreme climate events occurred.**
- **Reproduced 1922 Knickerbocker storm, comprehensive description of 1918 El Niño**
- **Data can be used to validate climate and weather models**



Sea level pressures with color showing uncertainty (a&b); precipitation (c); temperature (d). Dots indicate measurements locations (a).

Monthly Weather Review Vol 137(6) 2009;
Bull. Am. Meteorological Soc. (2009)

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