Data Explosion in Astrophysics: Web Services and Grid Computing

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Astronomers have a few hundred TB now
- 1 pixel (byte) / sq arc second ~ 4TB
- Multi-spectral, temporal, … → 1PB

They mine it looking for
new (kinds of) objects or
more of interesting ones (quasars),
density variations in 400-D space
correlations in 400-D space

Data doubles every year
Data is public after 1 year
So, 50% of the data is public
Same access for everyone
The Challenges

Exponential data growth:
Distributed collections
Soon Petabytes

Data Collection

Discovery and Analysis

New analysis paradigm:
Data federations,
Move analysis to data

Publishing

New publishing paradigm:
Scientists are publishers
and Curators
Exponential growth:
- Projects last at least 3-5 years
- Data sent upwards only at the end of the project
- Data will **never** be centralized

More responsibility on projects
- Becoming Publishers and Curators

Data will reside with projects
- Analyses must be close to the data
Data Access is Hitting a Wall

FTP and GREP are not adequate

- You can GREP 1 MB in a second
- You can GREP 1 GB in a minute
- You can GREP 1 TB in 2 days
- You can GREP 1 PB in 3 years

- You can FTP 1 MB in 1 sec
- You can FTP 1 GB / min (= 1 $/GB)
- … 2 days and 1K$
- … 3 years and 1M$

- Oh!, and 1PB ~4,000 disks

- At some point you need indices to limit search parallel data search and analysis
- This is where databases can help
Statistical analysis often deals with
- Creating uniform samples – data filtering
- Assembling relevant subsets
- Estimating completeness
- Censoring bad data
- Counting and building histograms
- Generating Monte-Carlo subsets
- Likelihood calculations
- Hypothesis testing

Traditionally these are performed on files
Most of these tasks are much better done inside a database
Move Mohamed to the mountain, not the mountain to Mohamed.
Looking for
- Needles in haystacks – the Higgs particle
- Haystacks: Dark matter, Dark energy

Needles are easier than haystacks

Global statistics have poor scaling
- Correlation functions are $N^2$, likelihood techniques $N^3$

As data and computers grow at same rate, we can only keep up with $N \log N$

A way out?
- Discard notion of optimal (data is fuzzy, answers are approximate)
- Don’t assume infinite computational resources or memory

Requires combination of statistics & computer science
The Grid will run on many web services
- It will be much more than CPU harvesting
- IETF standards Provide
  - Naming
  - Authorization / Security / Privacy
  - Distributed Objects
    - Discovery, Definition, Invocation, Object Model
  - Higher level services: workflow, transactions, DB,...
- Synergy: commercial Internet & Grid tools
- Convergence
Examples in Astrophysics

- LIGO – studying gravitational waves
- SDSS – the ‘Cosmic Genome Project’
- NVO – the National Virtual Observatory

Real data, real problems, thousands of users today!!!
Excellent opportunity to test grid tools
Ratio of CPU cycles/byte different from HEP
Data can be very distributed
Lots of database usage
Realizing the full potential of LIGO

The search for gravitational waves at hrms ~ 10^{-21}

- Revealing the full science content of LIGO data is a computationally and data intensive challenge
- Several classes of data analysis challenges require large-scale computational resources
- Search for gravitational wave (GW) analogs of electromagnetic (EM) pulsars
- GW sky is unknown, searches will need to survey a large parameter space
- All-sky search for previously unidentified periodic sources requires > 10^{15} floating point operations per second (FLOPS)
- Coalescence of compact binary systems (“inspiral chirps”) which include spin-spin interactions will cover a huge parameter space (~ 106 greater than spinless systems)

- These analyses are ideally suited for distributed (grid-based) computing
LIGO and the GRID

To date LIGO has …

✓ Developed data replication, distribution capabilities over a data analysis grid
  1. Near real time production of reduced data sets, transmission to Tier 2
     1. Tens of TB over the internet
  ✓ Provides access to reduced data, data replications, data mirrors

✓ Implemented the use of virtual data catalogs for efficient (re)utilization
  ✓ Tracking data locations, availability with catalogs
  2. Data discovery, data transformations

3. Implemented a persistent data grid for the international collaboration
  1. Access to distributed computing power - US & EU
  2. Will eventually enable CPU-limited analyses as background jobs
     1. Challenge: making full use of inherent CPU capacity
2004: transition from demos to real computations

Main Issues
- Be early adapters for grid computing
- Bring databases close to Grid Computing
- Astronomical data quite different from HEP data:
  - Object granularity rather than file granularity
  - All telescopes look at the same sky – cross-correlations important!

Particular testbed challenges from SDSS/NVO
- Cluster Finding, Galaxy Morphology, Photometric redshifts, OpenSkyQuery
- Recent accomplishments
  - Large scale computations started, Cluster Finding project driving scaling of Chimera and Pegasus
  - New SDSS-JHU cluster online
  - Several other testbed challenges under way
The dag for 1 place on the sky
Simplified DAG: later stages depend on the intermediate results of nearby dags
The DAG for the real analysis is quite extensive (100,000 nodes)
Scaling to SDSS: 4000 deg$^2$, about 10% of sky
Nonlocal!
Cluster Finding on a DB Cluster

Maria Nieto-Santisteban, A.Szalay, J.Gray, J.Annis,…

- Parallel SQL implementation over 10 nodes
- Identical problem – very different implementation
  - First database implementation finished in two days
  - Two more days of refinement
  - Two weeks spent on partitioning
- Runs 30 times faster on similar hardware
- Originally: hand-coded
- Now: Workflow with DAG in progress
- Experimenting with MapReduce look-alike in SQL
- Generalizing to Crossmatch between 1B object catalogs
  - Crossmatch performed in 2.5 hours
Physical inversion of photometric measurements!
- Adaptive template method

Computed for 50M SDSS DR1 galaxies
- Fitting many templates to data
- Currently 1sec / galaxy
- Data source in a database
- Results loaded back into DB

Currently
- SDSS DR3 has 180M objects
- Calibration now finished
- Computation is done using iVDGL resources
Measuring Dark Matter/Dark Energy from P(k)

SDSS only:
\[ \Omega_{m} h = 0.26 \pm 0.04 \]
\[ \Omega_{b}/\Omega_{m} = 0.29 \pm 0.07 \]

With \( \Omega_{b} = 0.047 \pm 0.006 \) (WMAP):
\[ \Omega_{m} h = 0.21 \pm 0.03 \]
\[ \Omega_{b}/\Omega_{m} = 0.16 \pm 0.03 \]

SDS: Pope et al. (2004)
WMAP: Verde et al. (2003), Spergel et al. (2003)

Alex Szalay  \[ \Omega_{m} h \]
Why Is Astronomy Special?

- Especially attractive for the wide public
- It has no commercial value
  - No privacy concerns, freely share results with others
  - Great for experimenting with algorithms
- It is real and well documented
  - High-dimensional (with confidence intervals)
  - Spatial, temporal
- Diverse and distributed
  - Many different instruments from
    many different places and
    many different times
- The questions are interesting
- There is a lot of it (soon petabytes)
The Virtual Observatory

- Premise: most data is (or could be) online
- So, the Internet is the world’s best telescope:
  - It has data on every part of the sky
  - In every measured spectral band: optical, x-ray, radio...
  - As deep as the best instruments (2 years ago).
  - It is up when you are up
  - The “seeing” is always great
  - It’s a smart telescope:
    - links objects and data to literature on them
- Software became the capital expense
  - Share, standardize, reuse..
NVO - Short History

- Driven by exponential data growth
- Started with SDSS + GriPhyN
- Recognized that data will never be centralized
- Continued with NVO (NSF ITR)
- International Virtual Observatory Alliance
  - Now in 15 countries
  - Closely integrated with Grid Computing efforts (iVDGL, AstroGrid, GAVO)
- Core services and standards adopted
NVO: How Will It Work?

- Based on Web Services/Grid Services
- Database connectivity and federation is essential
- Do not build “everything for everybody”
- Define commonly used core services
- Build higher level toolboxes/portals on top
- Place Grid applications behind Web Services
- Use the 90-10 rule:
  - Define the standards and interfaces, build the framework
  - Build the 10% of services that are used by 90%
  - Enable users to build the rest from components
- Show powerful demos in 2003
- Deployed Core services by Jan 2005
  - Registry, DataScope, OpenSkyQuery, WESIX
SkyQuery – Federating the Sky

- **Rationale**
  - Most astronomical data will be distributed
  - They look at the same sky
  - Cross-matching is the most common use pattern
  - Successful demo for NVO across the Atlantic
  - Understand stateless Web Services vs distributed databases

- **www.skyquery.net**
  - Built it in 5 man months, over 6 weeks, using MS.NET
  - Tanu Malik, Tamas Budavari, Ani Thakar, Alex Szalay
  - Now forms the basis of OpenSkyQuery
OpenSkyQuery

- Repeat the same functionality
  - Using VO standards and grid services (VOTable, OGSA-DAI)
  - Build interfaces also for DB2 and Oracle
- Widely distributed Grid+DB application
  - OpenSkyQuery: now reference implementation for OGSA-DAI
  - Collaboration with the Edinburgh eScience Center
    M. Westhead, R. Mann, G. Ricardi (Florida)
- MyDb-MySpace (w. Astrogrid)
  - Store custom collections (databases) next to the data set
  - Authentication, resource allocation
  - How to do it in Web Services (with S. Parastatidis)
- Now working on 17 archives on 3 continents
Outreach

- **SkyServer:** [http://skyserver.sdss.org/](http://skyserver.sdss.org/)
  - 1 TB of SDSS data server to high school students
  - Support from NSF, NASA, HP, Microsoft, FNAL
  - Goal: teach scientific exploration, use ‘hot’ data
  - 50 hours of course material, 100 teachers
  - English, German, Japanese version
  - 70 million web hits since June 2001
  - Soon: major discovery by a student will happen

- **Collaborations:**
  - Collaboration with Hands On Universe (C. Pennypacker, UCB)
  - Linking other (remote) data sets (SkyQuery.net)
  - Database cloned at 12 sites over the world (astro+CS depts)
  - Provide templates for data publishing
    - STScI, CIT, Bell Labs, ROE, IoA
  - NVO Summer School (Aspen, Sep 04): major success
## The Future

### CMB Maps
- 1990 COBE: 1000
- 2000 Boomerang: 10,000
- 2002 CBI: 50,000
- 2003 WMAP: 1 Million
- 2008 Planck: 10 Million

### Galaxy Redshift Surveys
- 1986 CfA: 3500
- 1996 LCRS: 23000
- 2003 2dF: 250000
- 2005 SDSS: 1000000

### Galaxy Angular Surveys
- 1970 Lick: 1M
- 1990 APM: 2M
- 2005 SDSS: 200M
- 2008 LSST: 2000M

### Time Domain Astronomy
*Many new experiments under way*
- QUEST
- SDSS Extension survey
- Dark Energy Camera
- PanStarrs
- SNAP
- LSST

Petabytes/year by 2010…
Challenges

- **Scaling**: lots of complex data around the world
  - SDSS today is 3TB of catalogs, 8TB imaging
  - NVO today is tens of TB, 1PB by 2012 (LSST)
  - IVOA is 15 countries around the world
  - Need $N\log N$ statistical algorithms

- **Community buy-in**: increasing pressure
  - Tech community ‘on-board’, astronomers ‘wait-and-see’
  - First production level services already deployed
  - NVO: Grid tools behind WS interfaces

- **Database–Grid interface**: still evolving
  - We are playing a leading role
  - Focusing on several challenging applications => new science