From SDSS to Simulations: Data Intensive Astrophysics

Alex Szalay
Institute for Data-Intensive Engineering and Science
The Johns Hopkins University
Gartner Hype Curve

- Gartner Hype Cycle
- Innovation Trigger
- Peak of Inflated Expectations
- Trough of Disillusionment
- Slope of Enlightenment
- Plateau of Productivity

- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
- Hot air balloon
- Balloon
- Innovation
- Hype
- Peak
- Trough
- Enlightenment
- Productivity

- Gartner Hype Cycle
Scientific Data Analysis Today

- Data grows as fast as our computing power
  - *Consequence of Moore’s Law and chip technology*
  - *Need tradeoff in analysis: best result in 1 min, 1 day, 1 month*
  - *Need randomized, incremental algorithms*
- Need both “exploratory” and “confirmatory” searches
  - *Quite different from “click-stream/ad-ware” data mining*
- Data access patterns quite different from business
  - *Structured vs unstructured data*
- Architectures increasingly CPU-heavy, IO-poor
- Most scientific data analysis done on Beowulf clusters lacking IO performance, managed in broom closets
- Universities hitting the “power wall”
If There Is Too Much Data….

- If there is too much data to handle, **collect less**
  - *What is sufficient data?*

- **Statistical** vs **systematic** errors
  - *Random sampling*
  - *How do you sample rare phenomena?*
  - *Smooth selection boundaries (sample across the threshold)*

- Most important natural phenomena are **sparse**
  - *Compressive sensing (Candes)*
  - *Importance sampling (Mahoney)*

- Collect the data that carries the **most information**
  - *How to optimize the knowledge gained / $$$ ?*
  - *Active learning and survey design (Budavari and Joseph)*
  - *Simulate surveys before you start data collection*
Non-Incremental Changes

• Multi-faceted challenges
• New computational tools and strategies
  … not just statistics, not just computer science, not just astronomy, not just genomics…
• Science is moving increasingly from hypothesis-driven to data-driven discoveries

Astronomy has always been data-driven…. now this is becoming more accepted in other areas as well
Sloan Digital Sky Survey

“The Cosmic Genome Project”

- Started in 1992, finished in 2008
- Data is public
  - 2.5 Terapixels of images => 5 Tpx of sky
  - 10 TB of raw data => 400TB processed
  - 0.5 TB catalogs => 35TB in the end

- Database and spectrograph built at JHU (SkyServer)
- Now SDSS-3, data served from JHU
Skyserver

Prototype in 21st Century data access

- 1.2B web hits in 12 years
- 200M external SQL queries
- 4,000,000 distinct users vs. 15,000 astronomers
- The emergence of the “Internet Scientist”
- Collaborative server-side analysis done by 7K astronomers

Jim Gray
MyDB: Workbench

- Registered ‘power users’, with their own server-side
- Query output goes to ‘MyDB’
- Can be joined with source database (contexts) or with other tables – *fundamental change*!!!
- Results are extracted from MyDB
- Users can collaborate!
  - *Insert, Drop, Create, Select Into, Functions*
  - *Publish/share* their tables to a group area
  - *Flexibility “at the edge”/ Read-only big DB*

- Data delivery via Web Services
  ⇒ *Sending analysis to the data!*

First example of “cloud computing” in science (2003)
NSF DIBBs

• DIBBs: Data Infrastructure Building Blocks
• Recent 5 year NSF grant to JHU to
  – Operate the SDSS Archive for 5 years
  – Upgrade the underlying infrastructure so that it can be maintained for another 10 years
  – Migrate all legacy flat files to JHU
  – Unify the SDSS 1-2-3-(4) “brands”
  – Modularize the components for easy reuse
  – Develop and deploy systems in other disciplines:
    • Turbulence, cosmology simulations, environmental science, oceanography, connectomics, genomics
  – Link the data sets and the framework to the “Long Tail”
Data in Simulations

• HPC is an instrument in its own right
• Largest simulations approach petabytes
  – from supernovae to turbulence, biology and brain modeling
• Need public access to the best and latest through interactive numerical laboratories
• Creates new challenges in
  – How to move the petabytes of data (high speed networking)
  – How to look at it (render on top of the data, drive remotely)
  – How to interface (smart sensors, immersive analysis)
  – How to analyze (value added services, analytics, …)
  – Architectures (supercomputers, DB servers, ??)
Lifecycle of Simulation Data

• Huge variations in Data Lifecycle
  – On-the fly analysis (immediate, do not keep)
  – Private reuse (short/mid term)
  – Public reuse (mid term)
  – Public service portal (mid/long term)
  – Archival and curation (long term)

• Very different from Supercomputer usage patterns
• Vacuum: also an opportunity to create a national network of data resources
• Use cases: turbulence and cosmology
Immersive Turbulence

“... the last unsolved problem of classical physics...”

• Understand the nature of turbulence
  – Consecutive snapshots of a large simulation of turbulence: $1024^4 \Rightarrow 30$ Terabytes
  – Treat it as an experiment, play with the database!
  – Shoot test particles (sensors) from your laptop into the simulation, like in the movie Twister

• New paradigm for analyzing simulations!

with C. Meneveau, S. Chen (Mech. E), G. Eyink (Applied Math), R. Burns (CS)
Turbulence Data Sets

- Isotropic turbulence JHU 30TB in use
- MHD1 JHU 50TB in use
- Channel flow UT 96TB in use
- MHD2 ANL 500TB data in xfer
- Rotating flow LANL 20TB data arrived
- 2 fluid mix LANL 20TB running
- Isotropic 6K^3 LANL 1000TB in planning

More than 50 papers published in elite journals on the first data set
Cosmology Simulations

• Millennium DB is the poster child/success story
  – 600 registered users, 17.3M queries, 287B rows
    http://gavo.mpa-garching.mpg.de/Millennium/
  – Dec 2012 Workshop at MPA: 3 days, 50 people

• Data size and scalability
  – PB data sizes, trillion particles of dark matter
  – Where is the data stored, how does it get there

• Value added services
  – Localized (SED, SAM, SF history, posterior re-simulations)
  – Rendering (viz, lensing, DM annihilation, light cones)
  – Global analytics (FFT, correlations of subsets, covariances)

• Data representations
  – Particles vs hydro grid
  – Particle tracking in DM data
  – Aggregates, uncertainty quantification
The Milky Way Laboratory

- Use cosmology simulations as an immersive laboratory for general users
- Via Lactea-II (22TB) as prototype, then Silver River (50B particles) as production (15M CPU hours)
- 800+ hi-rez snapshots => 800TB in DB
- Users can insert test particles (dwarf galaxies) into system and follow trajectories in pre-computed simulation (Wayne Ngan, Toronto)
- Users interact remotely with a PB in ‘real time’

Madau, Rockosi, Szalay, Wyse, Silk, Kuhlen, Lemson, Westermann, Blakeley
Dark Matter Annihilation

• Data from the Via Lactea II Simulation (400M particles in core)
• Compute the dark matter annihilation
• Original code by M. Kuhlen runs in 8 hours for a single image
• New GPU based code runs in 24 sec, OpenGL shader language (Lin Yang, JHU)
• Interactive service
  – Design your own cross-section and pick your view
• Technique would apply very well to lensing and image generation
Changing the Cross Section

Annihilation (No Correction)

Annihilation (1/ν Correction)

Annihilation (1/ν² Correction)

Decay Map (No Correction)

Yang, Silk, Szalay, Wyse, Bozek and Madau arxiv 1312.0006
The Indra Simulations

- Quantifying cosmic variance
- Suite of dark matter $N$-body simulations
  - Gadget2
    - 512 different 1 Gpc/h boxes, $1024^3$ particles per simulation
    - Data loaded into SQL database, will be available to the public
    - Random initial conditions, WMAP7 cosmology
- Particle data:
  - Ids, positions, velocities for 64 snapshots of each simulation
  - 35T particles total, 1.1PB total, currently 20% complete
- Halo catalogs
- Fourier modes:
  - Course density grid for 512 time steps of each run

Bridget Falck (ICG Portsmouth), Tamás Budavári (JHU), Shaun Cole (Durham), Daniel Crankshaw (Berkeley), László Dobos (Eötvös), Adrian Jenkins (Durham), Gerard Lemson (MPA), Mark Neyrinck (JHU), Alex Szalay (JHU), and Jie Wang (Durham/Beijing)
• How to build a system good for the analysis?
• Where should data be stored
  – Not at the supercomputers (have too expensive storage)
  – Computations and visualizations must be on top of the data
  – Need high bandwidth to data sources
• Databases are a good model, but are they scalable?
  – Google (Dremel, Tenzing, Spanner: exascale SQL)
  – Need to be augmented with value-added services
  – Cannot beat them for fine grained, indexed access
• Scale out!
  – Cosmology simulations are not hard to partition
  – Use fast, cheap storage, GPUs for some of the compute
  – Consider a layer of large memory systems
JHU Data-Scope

- Funded by NSF MRI to build a new ‘instrument’ to look at data
- Goal: ~100 servers for $1M + about $200K switches+racks
- Two-tier: performance (P) and storage (S)
- Mix of regular HDD and SSDs
- Large (6.5PB) + cheap + fast (500GBps), but …
  ..a special purpose instrument

<table>
<thead>
<tr>
<th>Final configuration</th>
</tr>
</thead>
<tbody>
<tr>
<td>1P</td>
</tr>
</tbody>
</table>
| --- | --- | ----- | ----- | -----
| servers | 1 | 1 | 90 | 6 | 102 |
| rack units | 4 | 34 | 360 | 204 | 564 |
| capacity | 24 | 720 | 2160 | 4320 | 6480 TB |
| price | 8.8 | 57 | 8.8 | 57 | 792 $K |
| power | 1.4 | 10 | 126 | 60 | 186 kW |
| GPU* | 1.35 | 0 | 121.5 | 0 | 122 TF |
| seq IO | 5.3 | 3.8 | 477 | 23 | 500 GBps |
| IOPS | 240 | 54 | 21600 | 324 | 21924 kIOPS |
| netwk bw | 10 | 20 | 900 | 240 | 1140 Gbps |
The Long Tail

- The “Long Tail” of a huge number of small data sets
  - The integral of the “long tail” is big!
- Facebook: bring many small, seemingly unrelated data to a single place and new value emerges
  - What is the science equivalent?
- The Dropbox lesson
  - Simple interfaces are more powerful than complex ones
  - API public
- Ideally suited for the cloud
  - SQL Share (Bill Howe)
  - SciDrive: drag-and-drop, automatically upload into DB, automatically harvest searchable metadata, group shares
SciDrive

- Help the Long Tail of astronomy (and other science) data
- Looks like DropBox+MyDB+ plugins
- Use a simple framework to provide
  - Cloud storage for small data in various science communities
  - Link these data sets to each other and to analysis services
  - Link SciDrive to searchable databases and MS Azure
  - Automatically harvest the metadata and build contexts
  - Enable data sharing and collaborations
  - 400TB+ both at JHU and SDSC operational

- Dmitry Mishin, Dmitry Medvedev, Tamas Budavari, AS (JHU), Ray Plante (NCSA), Matthew Graham (Caltech)
- Funded by the Alfred P. Sloan Foundation
- Recently major new NSF DIBBs grant
Sociology

• Broad sociological changes
  – Convergence of Physical and Life Sciences
  – Data collection in ever larger collaborations
  – Virtual Observatories: CERN, VAO, NCBI, NEON, OOI,…
  – Analysis decoupled, off archived data by smaller groups
  – Emergence of the citizen/internet scientist

• Need to start training the next generations
  – П-shaped vs I-shaped people
  – Early involvement in “Computational thinking”
Summary

- Science is increasingly driven by data (big and small)
- Changing sociology – surveys analyzed by individuals
- From hypothesis-driven to data-driven science
- We need new instruments: “microscopes” and “telescopes” for data
- There is a major challenge on the “long tail”
- A new, Fourth Paradigm of Science is emerging…
- Astronomy has been at the cusp of this transition
“If I had asked people what they wanted, they would have said faster horses…”

―Henry Ford