High-Performance Compute Infrastructure in Astronomy: 2020 Is Only Months Away

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How Do We Survive The Data Tsunami?

- Partnerships between computer scientists and astronomers. ✔
- Develop environment-agnostic services and applications ✔
- Science driven infrastructure ✔
- Investigate new technologies ✔
- Optimize derivation of new science products ✔
- Recognition of role of information technologists in astronomy.
- Education of astronomers in scalable programming techniques

Astronomers are collecting more data than ever. What practices can keep them ahead of the flood?

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Astronomy is already awash with data: currently 1 PB (petabyte) of public data is electronically accessible, and this volume is growing at 0.5 PB per year. The availability of this data has already transformed research in astronomy, and the STScI (Space Telescope Science Institute) now reports that more papers are published with archived data sets than with newly acquired data.3

This growth in data size and anticipated usage will accelerate in the coming few years as new projects such as the LSST (Large Synoptic Survey Telescope), ALMA (Atacama Large Millimeter Array), and SKA (Square Kilometer Array) move into operation. These new projects will use much larger arrays of telescopes and detectors or much higher data acquisition rates than are now used. Projections indicate that by 2020, more than 60 PB of archived data will be accessible to astronomers.9


Innovations in Data-Intensive Astronomy

NRAO, Green Bank, WV. May 2-5, 2011

http://www.nrao.edu/meetings/bigdata/agenda.shtml
The Early Years: Delivering Montage

- Portable by design:
  - ANSI-compliant
  - No-third party dependencies
  - Standalone modules controlled by an executive library

Image Mosaic Engine Workflow (Montage)

6 deg x 6 deg 2MASS mosaic in 50s
Pegasus Workflow Management System
http://pegasus.isi.edu

- Converts abstract workflow to a concrete workflow
- No special requirements on infrastructure

Cyberinfrastructure: Local machine, cluster, Condor pool, Grid, Cloud, …
Science Driven Cyber Infrastructure

- Task scheduling in distributed environments (performance focused).
- Designing job schedulers for the grid.
- Designing fault tolerance techniques for job schedulers.
- Exploring issues of data provenance in scientific workflows.
- Developing high-performance workflow restructuring techniques.
- Developing application performance frameworks.
- Developing workflow orchestration techniques.

Berriman, Good, Deelman and Alexov
Comparing Grids With Clouds

NCSA Abe - high-performance cluster.

Set up computationally equivalent configurations on Amazon and Abe

Nimbus Context Broker – toolkit for configuring virtual clusters.
Corral – resource provisioning tool for grids.

Amazon EC2

NCSA Abe - high-performance cluster.

Submit Host

Nimbus Context Broker
Pegasus
DagMan
Condor
WMS

Storage System

Virtual Cluster

Glidein Pool

Submit Host

NCSA Abe
How Did They Do and How Much Did It Cost?

Montage Results:

- Most powerful processor *c1.xlarge* offers 3x the performance of *m1.small* – but at 4x the cost.
- Most cost-effective processor is *c1.medium* – 20% performance loss over *c1.xlarge* but 5x lower cost.
- Parallel file system gives big performance advantage.
When Should I Use Commercial Clouds?

- The answer is....it depends on your application and use case.
- Recommended best practice: Perform a cost-benefit analysis to identify the most cost-effective processing and data storage strategy. Tools to support this would be beneficial.
- Amazon offers the best value for
  - Compute- and memory-bound applications.
  - One-time bulk-processing tasks, providing excess capacity under load, and running test-beds.
- Parallel file systems and high-speed networks offer the best performance for I/O-bound applications.
- Mass storage is very expensive on Amazon EC2

How Do We Build Mosaics of the Galactic Plane?

- 300 cores (average)
- 900 tiles; $5^\circ \times 5^\circ$ with $1^\circ$ overlap; 2MASS J and H bands.
- Takes 30 CPU hours
- Managing I/O is the major bottleneck – transfers, parallel file system
Digging Out Exoplanets On Academic Clouds?

- FutureGrid test bed for Cloud Computing
  - 6 centers across the U.S.
  - Nimbus, Eucalyptus, Moab “bare metal”
  - http://www.futuregrid.org/
Computing Periodograms on Academic Clouds

<table>
<thead>
<tr>
<th>Site</th>
<th>CPU</th>
<th>RAM (SW)</th>
<th>Walltime</th>
<th>Cum. Dur.</th>
<th>Speed-Up</th>
</tr>
</thead>
<tbody>
<tr>
<td>Magellan</td>
<td>8 x 2.6 GHz</td>
<td>19 (0) GB</td>
<td>5.2 h</td>
<td>226.6 h</td>
<td>43.6</td>
</tr>
<tr>
<td>Amazon</td>
<td>8 x 2.3 GHz</td>
<td>7 (0) GB</td>
<td>7.2 h</td>
<td>295.8 h</td>
<td>41.1</td>
</tr>
<tr>
<td>FutureGrid</td>
<td>8 x 2.5 GHz</td>
<td>29 (½) GB</td>
<td>5.7 h</td>
<td>248.0 h</td>
<td>43.5</td>
</tr>
</tbody>
</table>

- 33,000 Kepler periodograms with \textit{Plavchan} algorithm
- Given 48 physical cores
  - Speed-up \(\approx x40\)
  - AWS cost \(\approx \$31\):
    - 7.2 h x 6 x \texttt{c1.large} \(\approx \$29\)
    - 1.8 GB in + 9.9 GB out \(\approx \$2\)


Proceedings of Science Cloud 2011.
Conclusions

- ISI and IPAC have enjoyed a successful science-driven collaboration for ten years. A model for how astronomers and computer scientists can collaborate.

- Development of highly scalable, portable applications and environment-agnostic workflow management tools have been crucial in enabling and expanding our investigations.

  - Development of cyber infrastructure
  - Investigating applicability of cloud computing
  - Optimizing generation of new data products
  - Investigating performance of new technologies and facilities