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

acmqueue HOW WILL ASTRONOMY ARCHIVES SURVIVE THE DATA TSUNAMI?

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.[17]

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]

http://queue.acm.org/detail.cfm?id=2047483 (http://arxiv.org/abs/1111.0075)

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

http://www.nrao.edu/meetings/bigdata/agenda.shtml

The Early Years: Delivering Montage

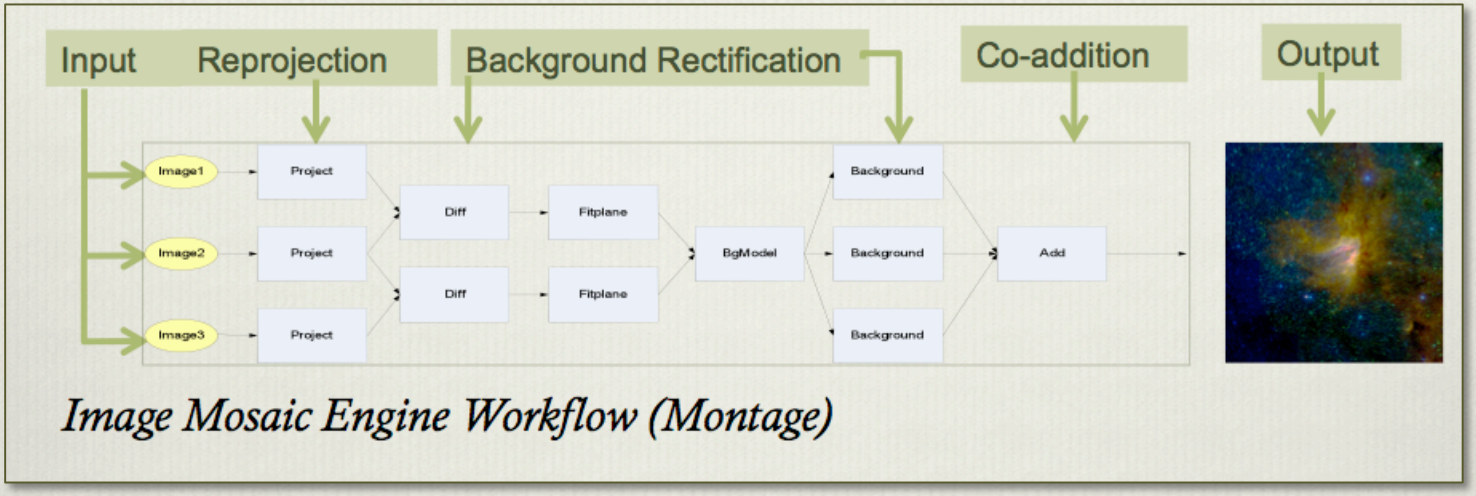
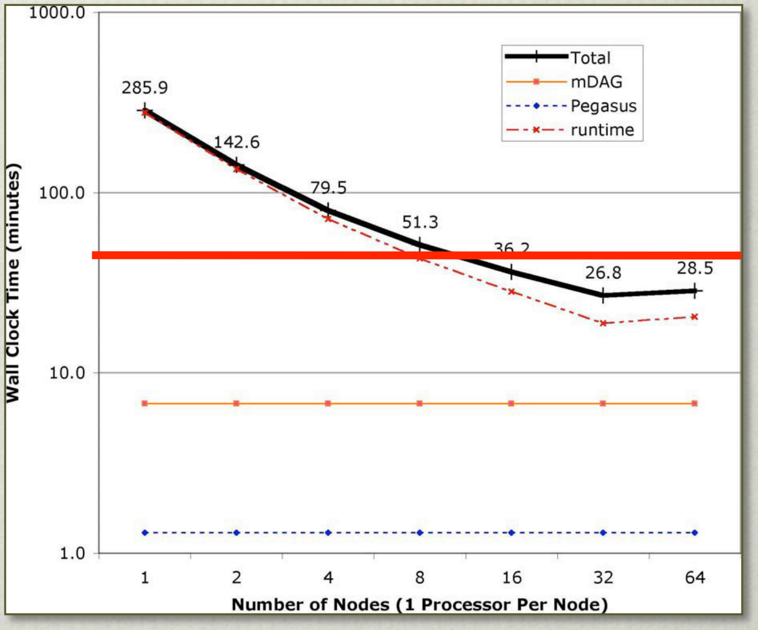


Image Mosaic Engine Workflow (Montage)

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



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

Pegasus	Maps tasks and data to executable resources; Performance optimizer
DAGMan	Workflow engine - Tracks dependencies, releases tasks, retries tasks
Condor Schedd	Task manager; schedules and dispatches tasks (and data) to resources

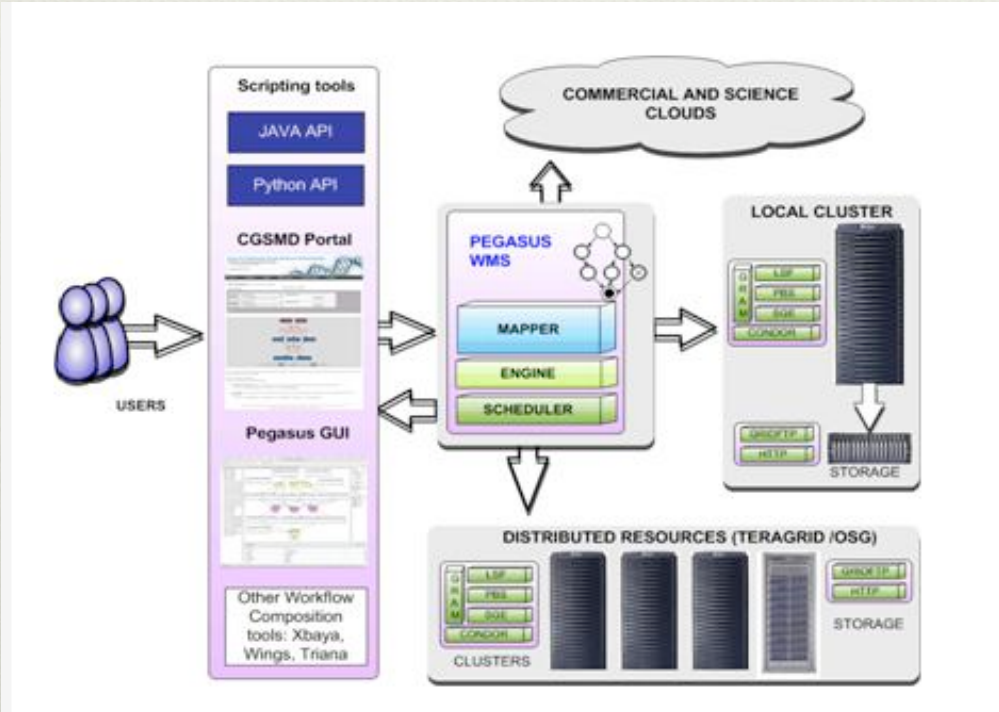
Cyberinfrastructure: Local machine, cluster, Condor pool, Grid, Cloud,…

Science Driven Cyber Infrastructure

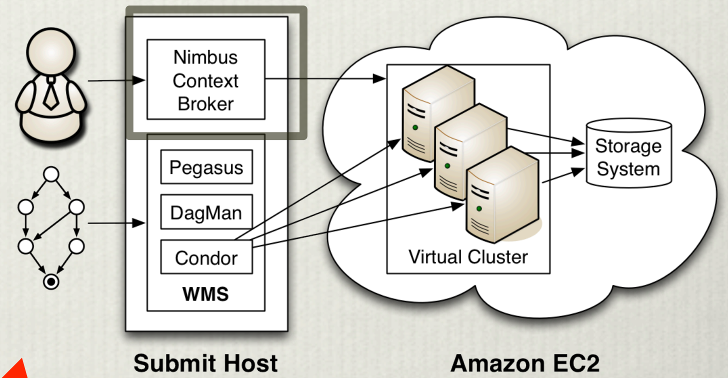
- Task scheduling in distributed environments (performance focused).
- Designing job schedulers for the grid.
- Designing fault tolerance techniques for job schedulers.
- Exploring issues of data provenance in scientific workflows.
- Developing high-performance workflow restructuring techniques.
- Developing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

Berriman, Good, Deelman and Alexov
Phil. Trans. R. Soc. A 2011 ***369, 3384-3397*** doi: 10.1098/rsta.2011.0136

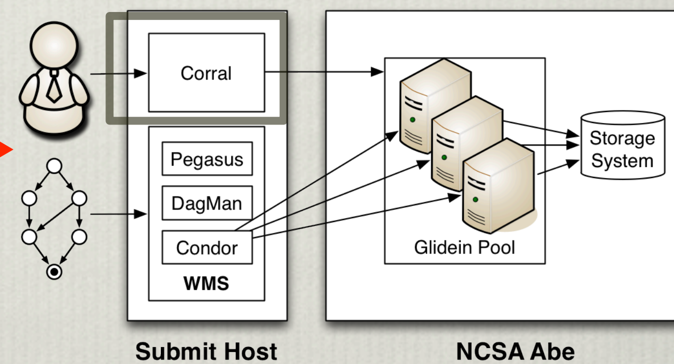
Comparing Grids With Clouds



Amazon EC2



NCSA Abe - high-performance cluster.

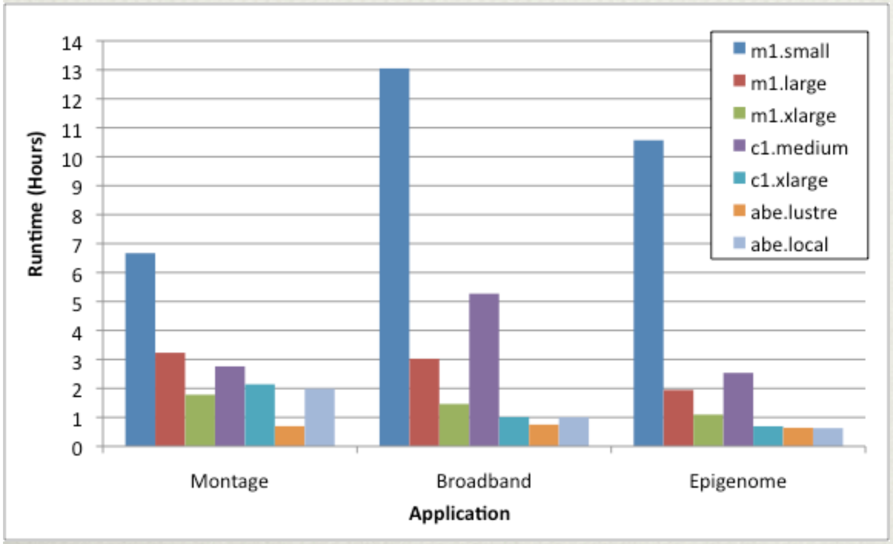


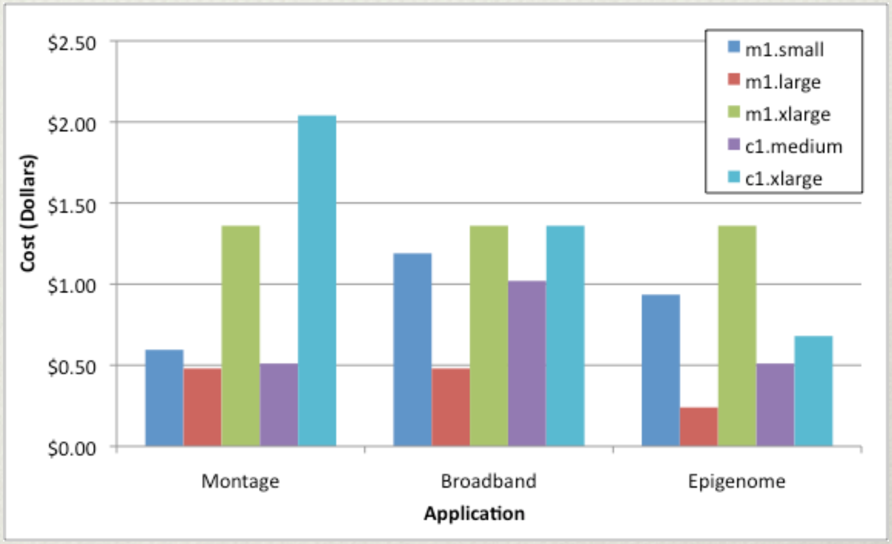
Set up computationally equivalent configurations on Amazon and Abe

Nimbus Context Broker – toolkit for configuring virtual clusters.

Corral – resource provisioning tool for grids.

How Did They Do and How Much Did It Cost?





Montage mosaic engine. I/O-bound

Broadband calculates seismograms from simulated earthquakes. Memory bound.

Epigenome maps DNA segments to a reference genome. CPU-bound.

Montage Results:

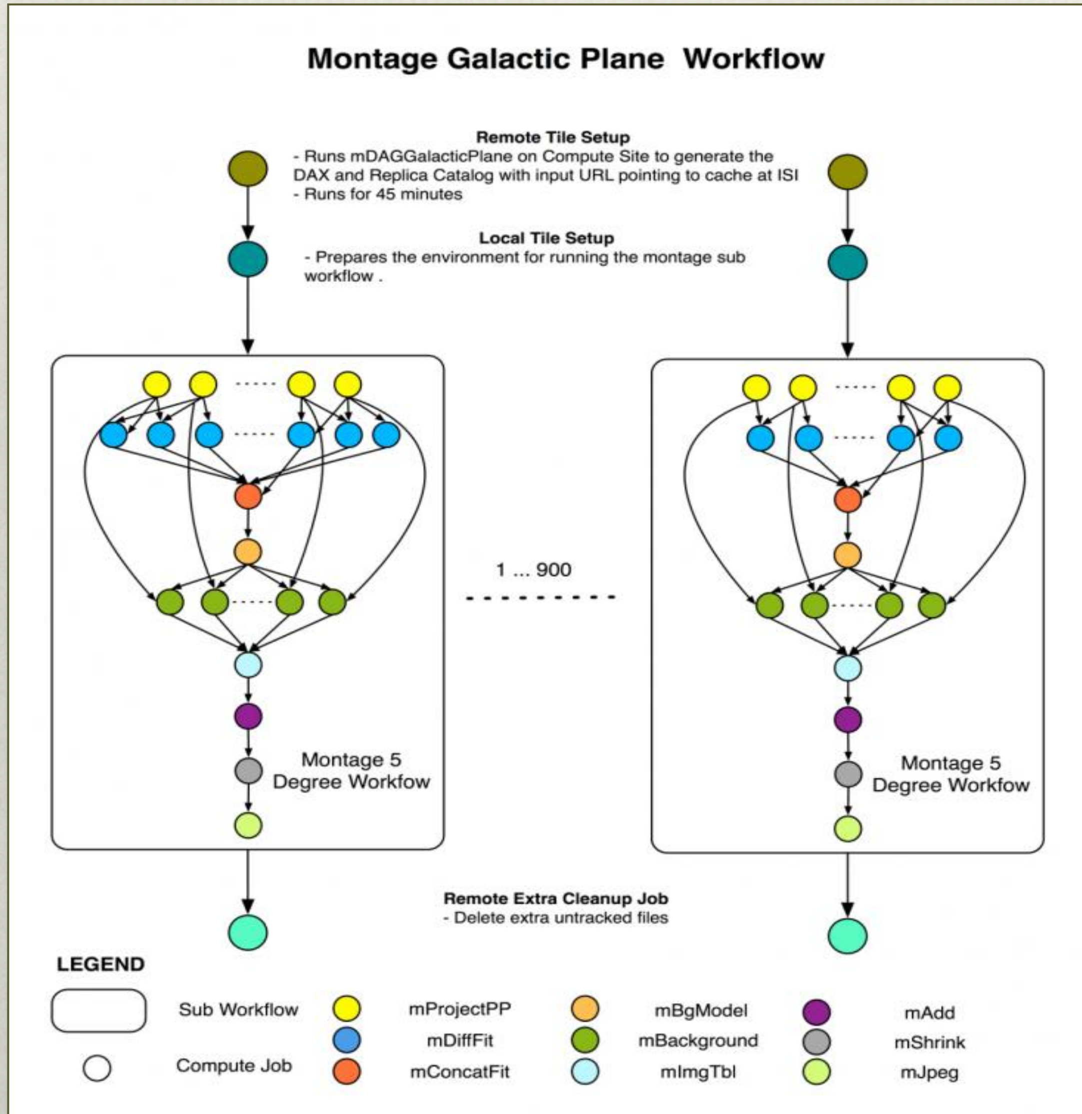
- Most powerful processor *c1.xlarge* offers 3x the performance of *m1.small* – but at 4x the cost.
- Most cost-effective processor is *c1.medium* – 20% performance loss over *c1.xlarge* but 5x lower cost.
- Parallel file system gives big performance advantage

When Should I Use Commercial Clouds?

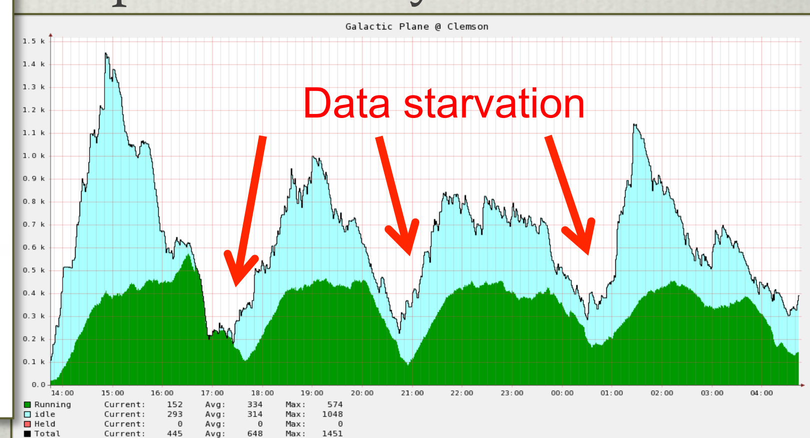
- **The answer is….it depends on your application and use case.**
- **Recommended best practice: Perform a cost-benefit analysis to identify the most cost-effective processing and data storage strategy. Tools to support this would be beneficial.**
- Amazon offers the best value for
  - Compute- and memory-bound 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

See "Scientific Workflow Applications on Amazon EC2,"
Juve et al. (2009) e-Science 2009. http://arxiv.org/abs/1010.4822

How Do We Build Mosaics of the Galactic Plane?

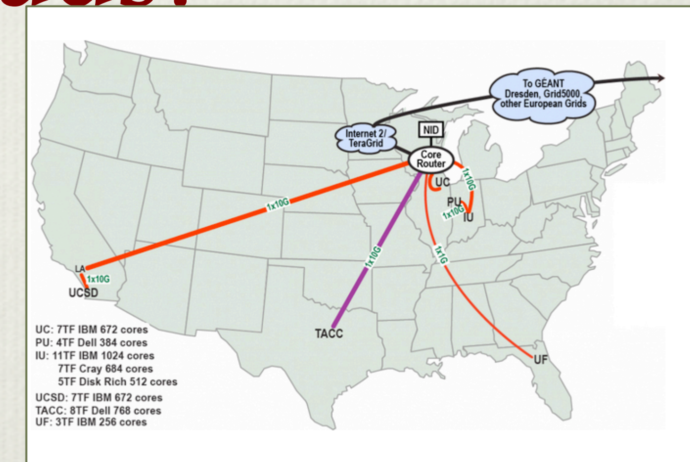


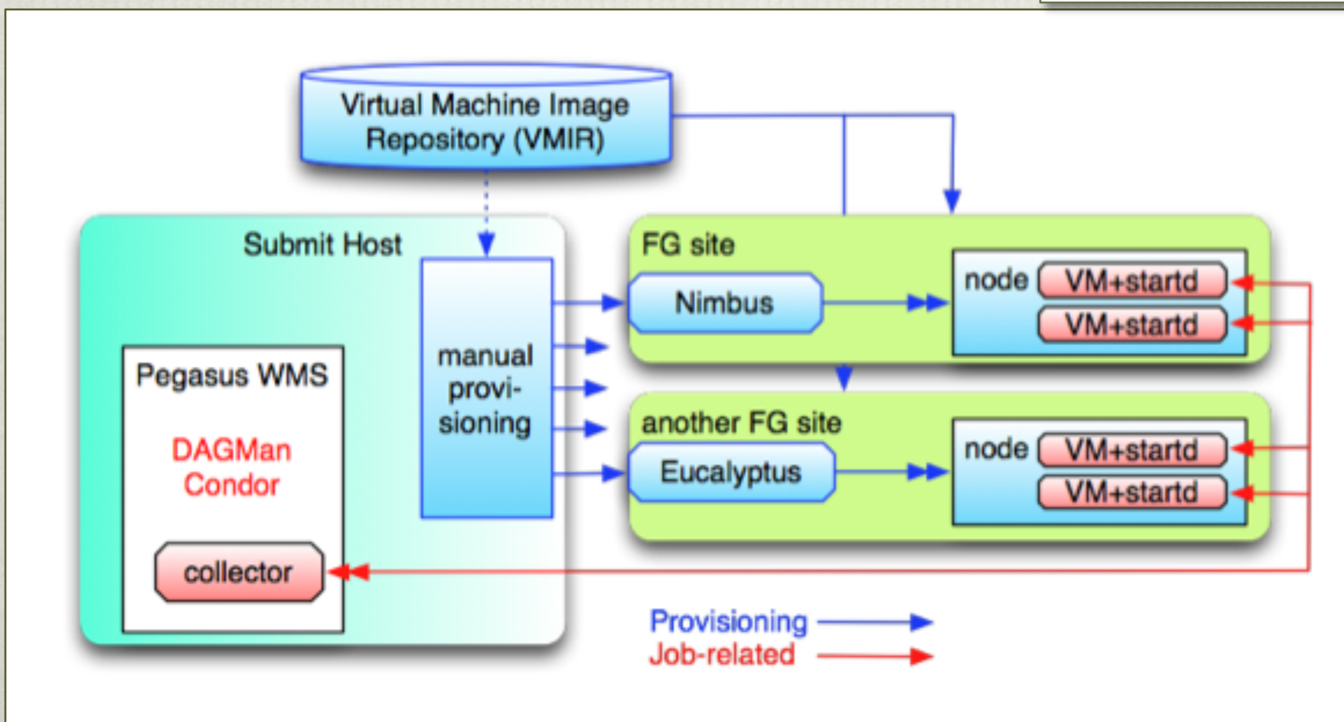
- ❖ 300 cores (average)
- ❖ 900 tiles; 5° x 5° with 1° overlap; 2MASS J and H bands.
- ❖ Takes 30 CPU hours
- ❖ Managing I/O is the major bottleneck – transfers, parallel file system



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/

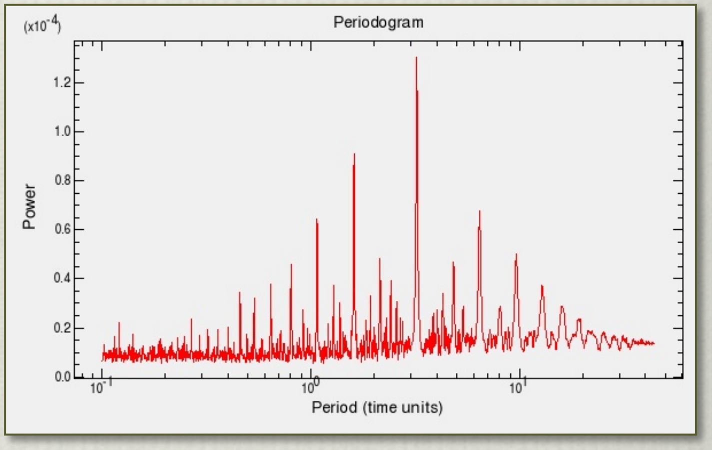




Computing Periodograms on Academic Clouds

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

- 33,000 Kepler periodograms with *Plavchan* algorithm
- Given 48 physical cores
  - Speed-up ≈ x40+
  - AWS cost ≈ $31:
    - 7.2 h x 6 x c1.large ≈ $29
    - 1.8 GB in + 9.9 GB out ≈ $2



"The Application of Cloud Computing to Astronomy: A Study of Cost and Performance." Berriman et al. e-Science 2010. (http://arxiv.org/abs/1010.4813).
"Experiences Using Cloud Computing for A Scientific Workflow Application." 2011 Vöckler et al. 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