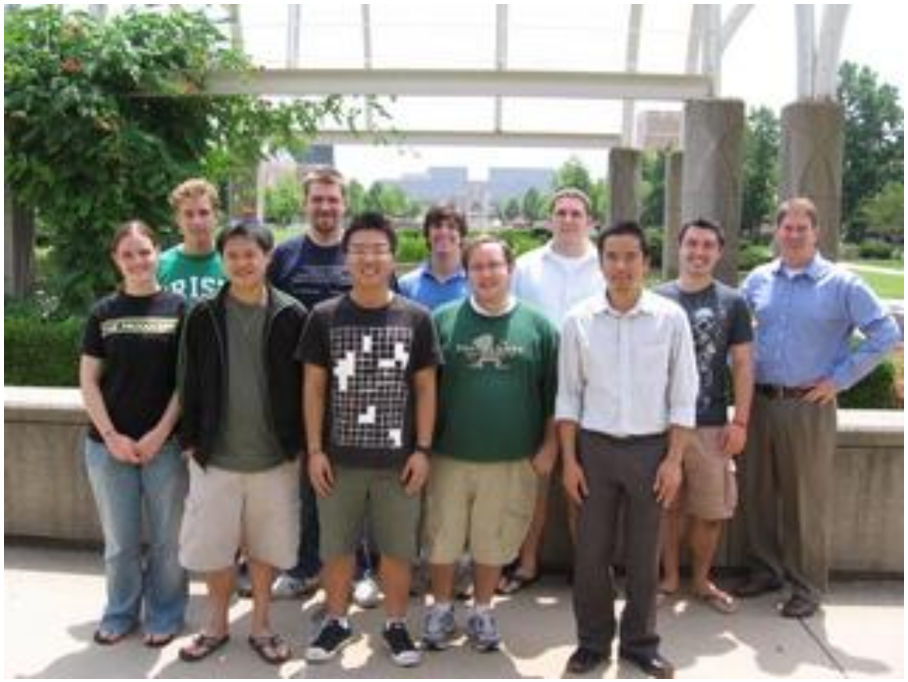
Scaling Up Without Blowing Up

Douglas Thain
University of Notre Dame

The Cooperative Computing Lab

University of Notre Dame



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Makeflow

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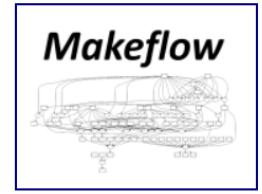

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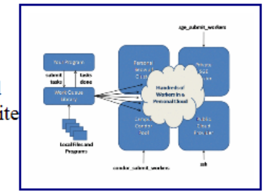

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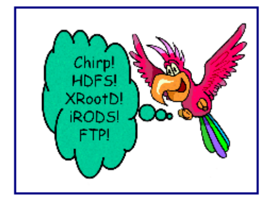

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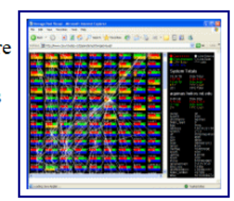


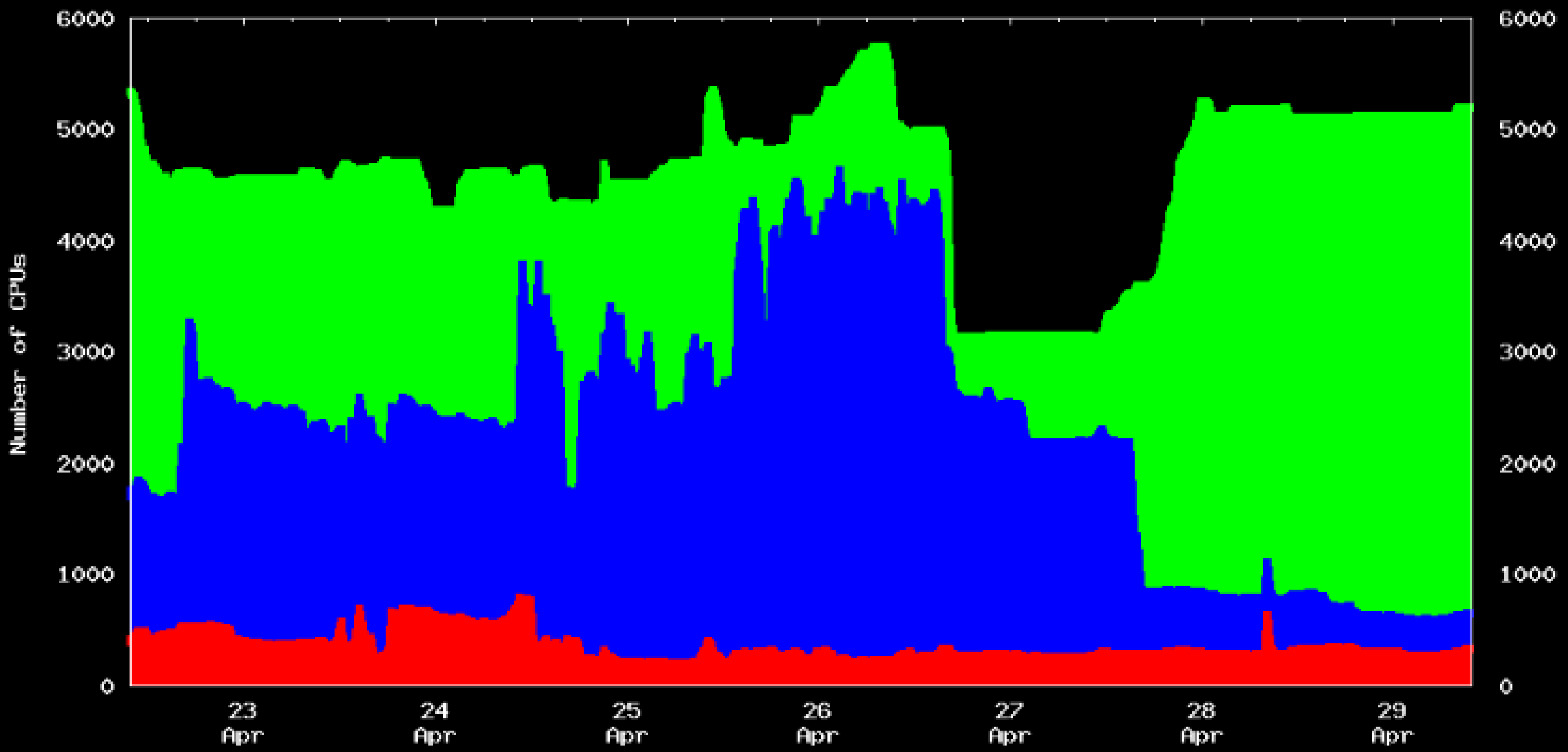
The Cooperative Computing Lab

- We *collaborate with people* who have large scale computing problems in science, engineering, and other fields.
- We *operate computer systems* on the O(10,000) cores: clusters, clouds, grids.
- We *conduct computer science* research in the context of real people and problems.
- We *release open source software* for large scale distributed computing.

http://www.nd.edu/~ccl

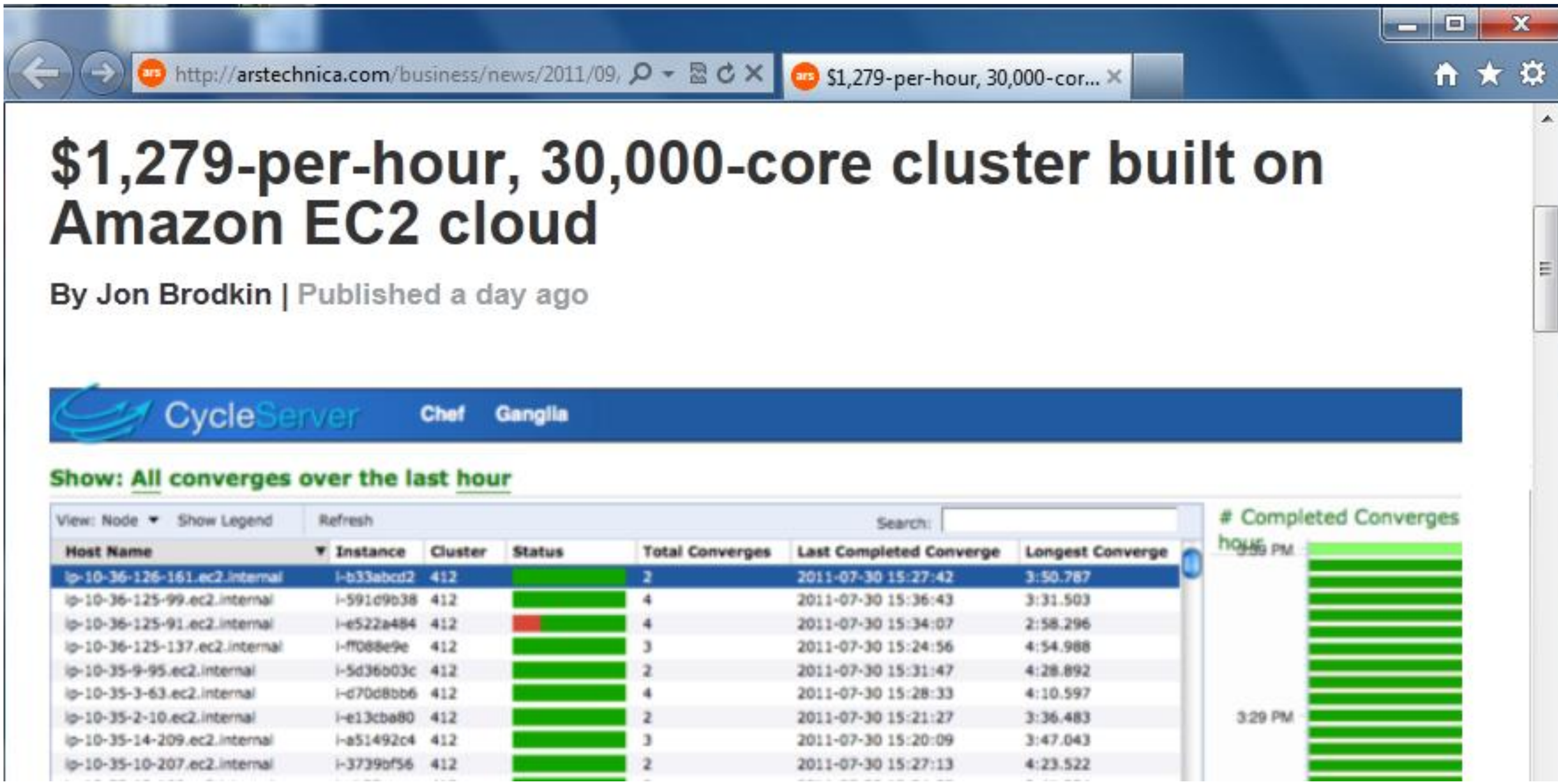
Good News:
Computing is Plentiful

CPU Utilization for the Last Week



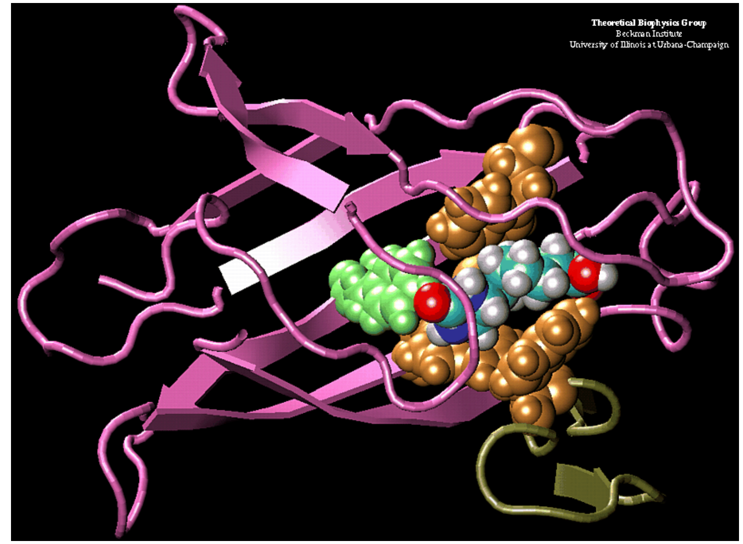
404855	(51%)	CPU-Hours Unused
328960	(41%)	CPU-Hours Used by Condor
58935	(7%)	CPU-Hours Used by Owner
792750	(100%)	CPU-Hours Total

Superclusters by the Hour

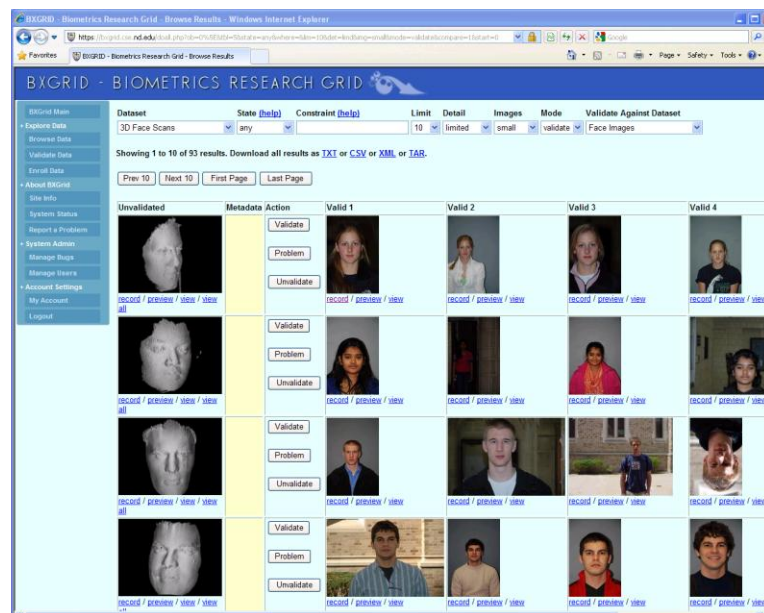


http://arstechnica.com/business/news/2011/09/30000-core-cluster-built-on-amazon-ec2-cloud.ars

Our Collaborators



AGTCCGTACGATGCTATTAGCGAGCGTGA...



The Cooperative Computing Tools

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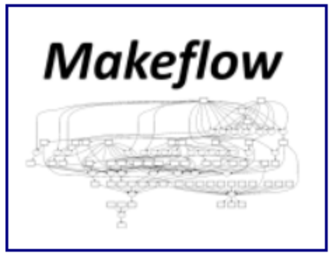

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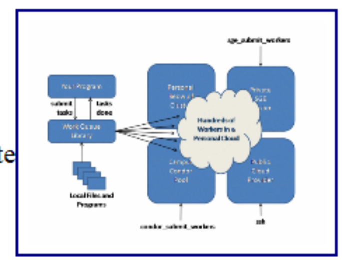

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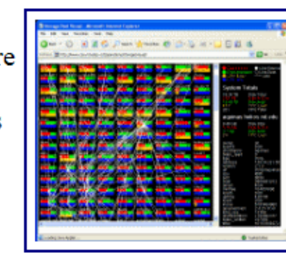

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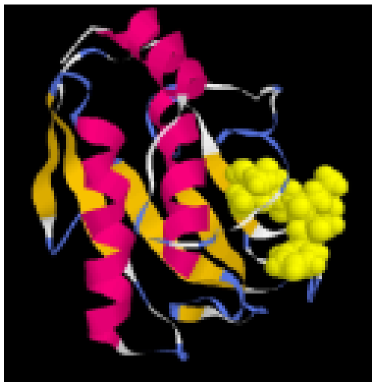
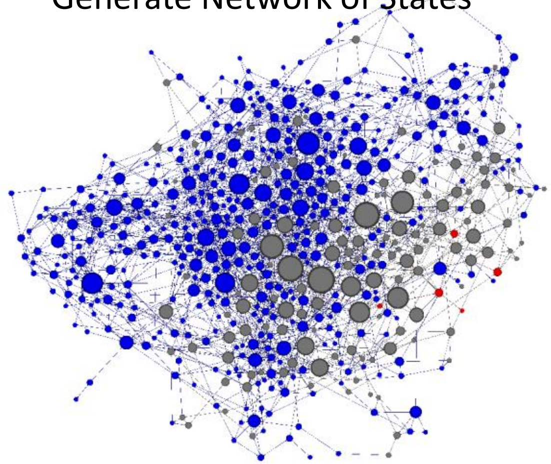
Example: Adaptive Weighted Ensemble

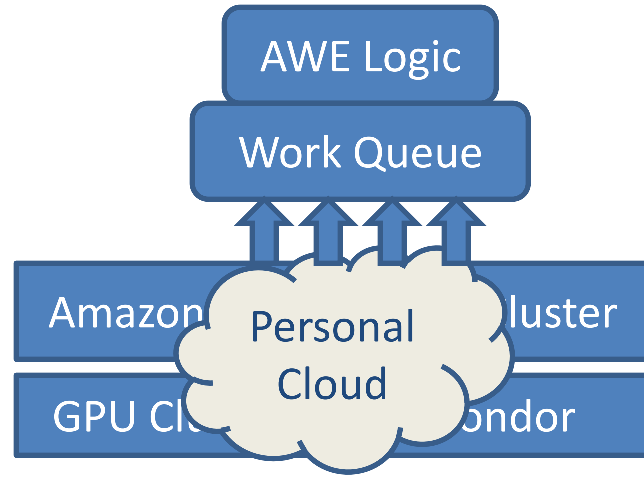
1: Start with Standard
MD Simulation



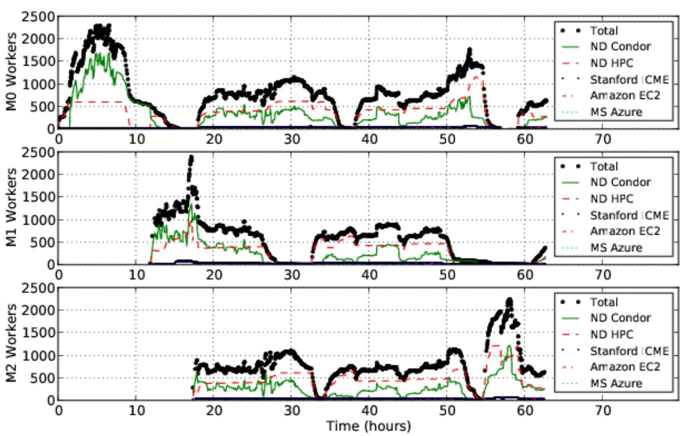
2: Research Goal:
Generate Network of States



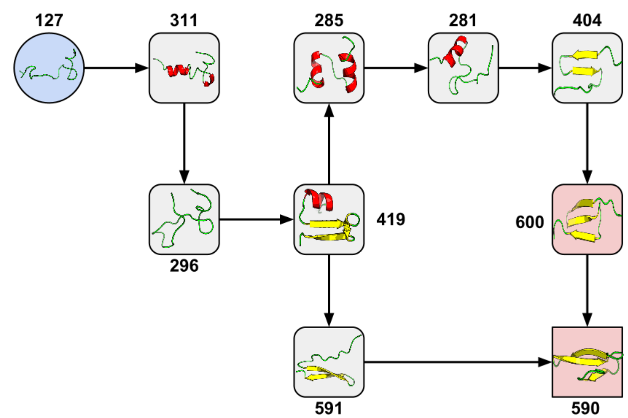
3: Build AWE Logic
Using Work Queue Library



4: Run on 2000+ CPUs/GPUs at
Notre Dame, Stanford, and Amazon

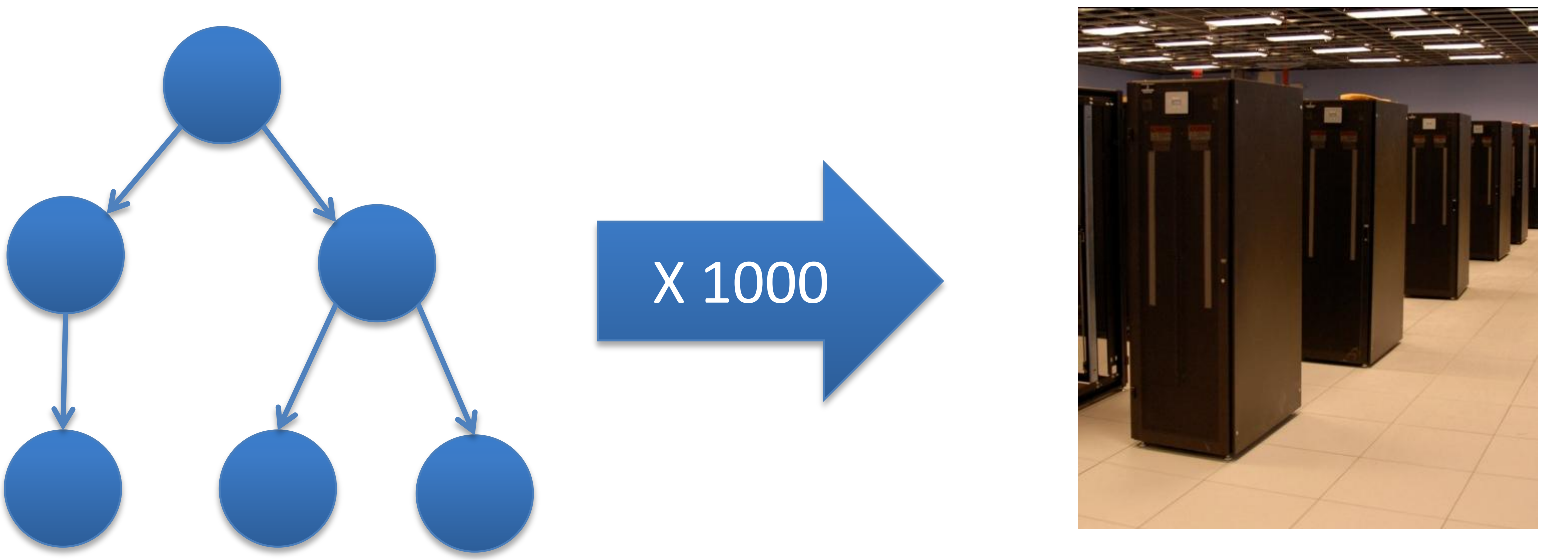


5: New State Transition Discovered!

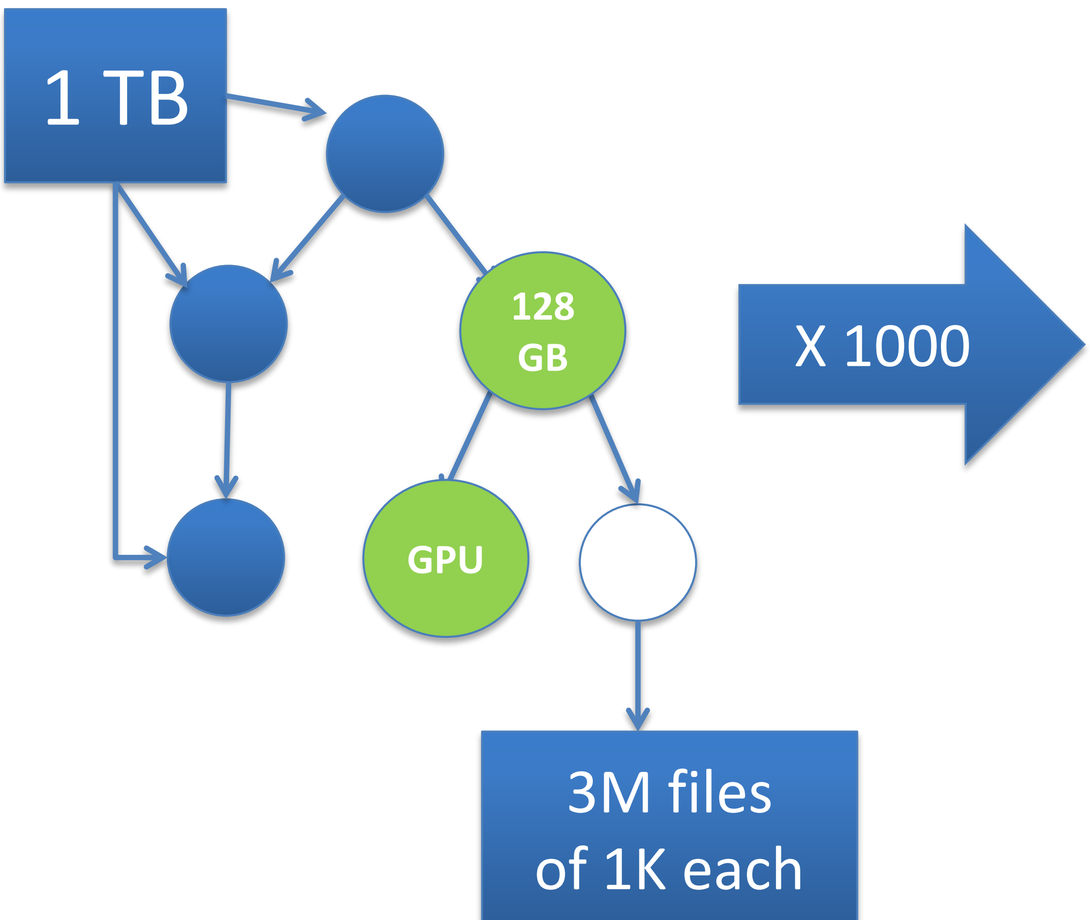


Badi Abdul-Wahid, Li Yu, Dinesh Rajan, Haoyun Feng, Eric Darve, Douglas Thain, Jesus A. Izaguirre,
Folding Proteins at 500 ns/hour with Work Queue, IEEE e-Science Conference, 2012

The Ideal Picture



What actually happens:



Some reasonable questions:

- Will this workload **at all** on machine X?
- How many workloads can I run simultaneously without running out of storage space?
- Did this workload actually behave as expected when run on a new machine?
- How is run X different from run Y?
- If my workload wasn't able to run on this machine, where can I run it?

End users have **no idea** what resources their applications actually need.

and…

Computer systems are **terrible** at describing their capabilities and limits.

and…

They don’t know when to say **NO**.

dV/dt : **Accelerating the Rate of Progress Towards Extreme Scale Collaborative Science**

Miron Livny (UW), Ewa Deelman (USC/ISI), Douglas Thain (ND), Frank Wuerthwein (UCSD), Bill Allcock (ANL)

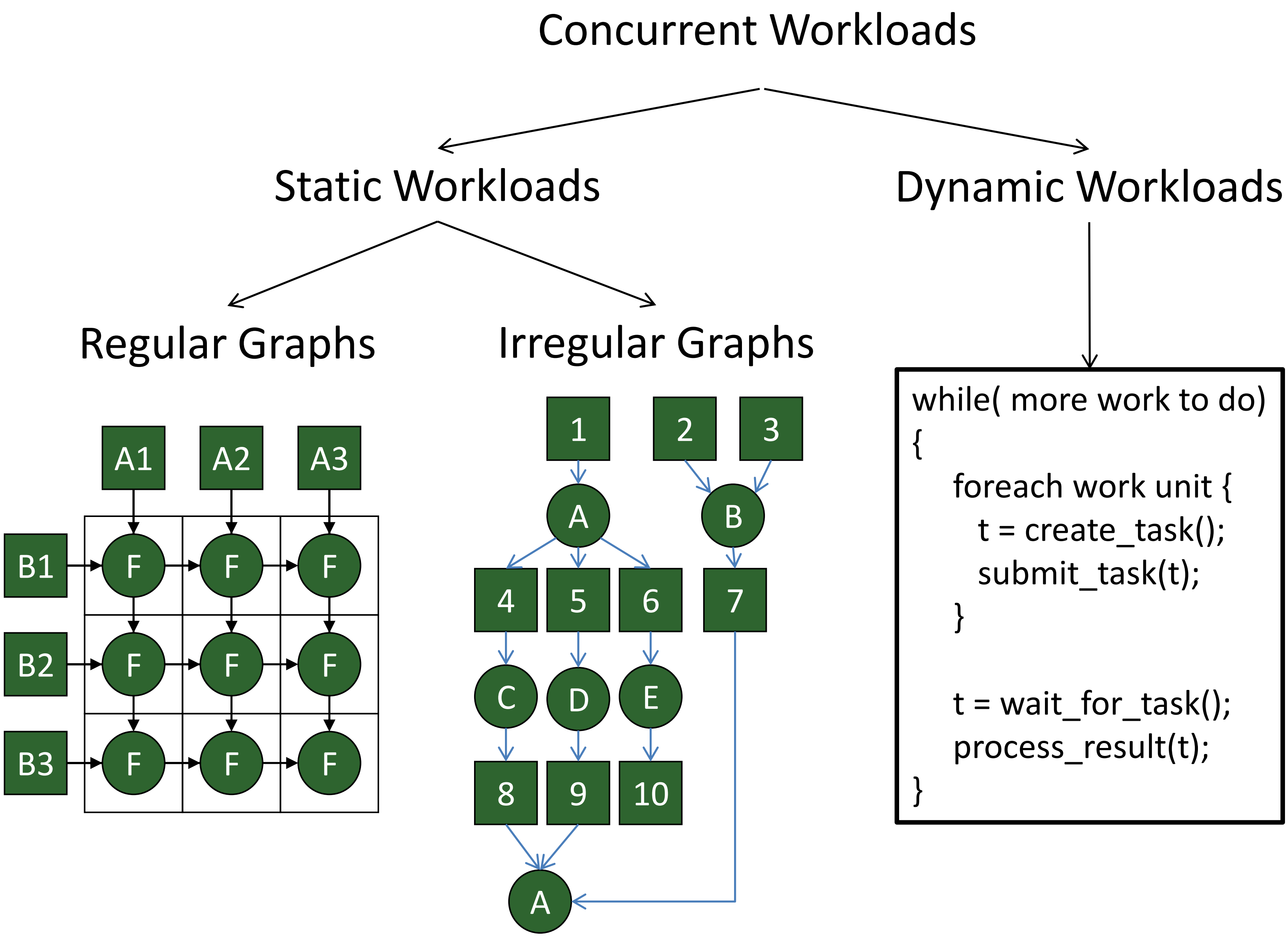
… make it easier for scientists to conduct large-scale computational tasks that use the power of computing resources they do not own to process data they did not collect with applications they did not develop …

Stages of Resource Management

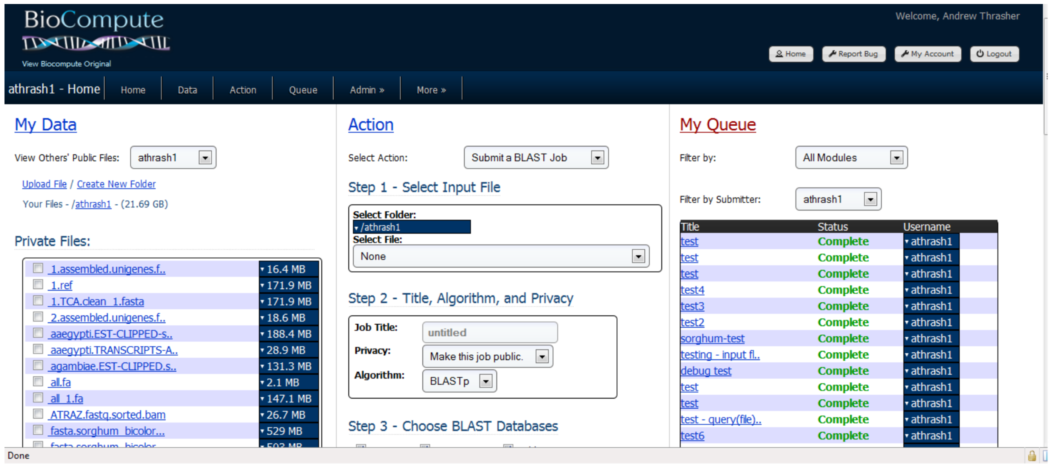
- **Estimate** the application resource needs
- **Find** the appropriate computing resources
- **Acquire** those resources
- **Deploy** applications and data on the resources
- **Manage** applications and resources during run.

- Can we do it for **one task**?
- How about an app composed of **many tasks**?

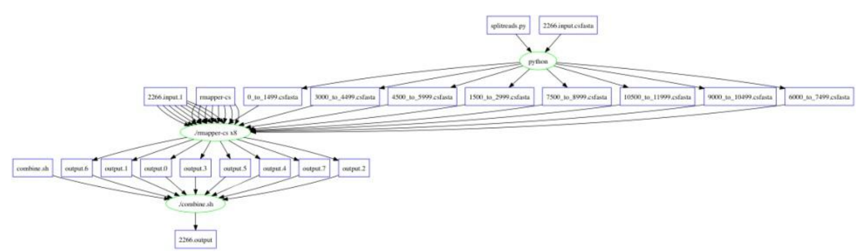
Categories of Applications



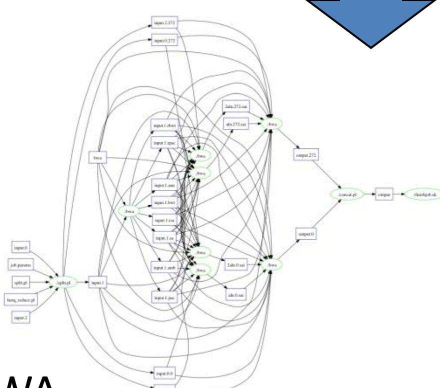
Bioinformatics Portal Generates Workflows for Makeflow



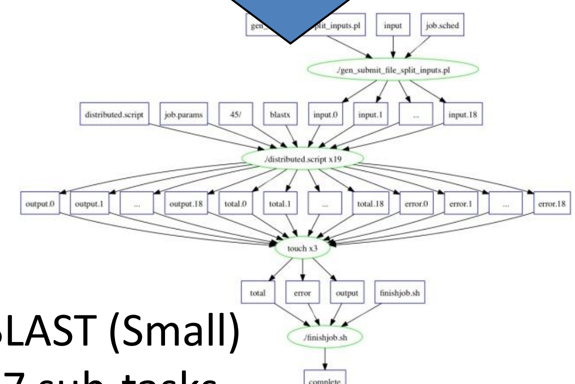
SHRIMP
5080 sub-tasks
~3h on 200 nodes



BWA
825 sub-tasks
~27m on 100 nodes

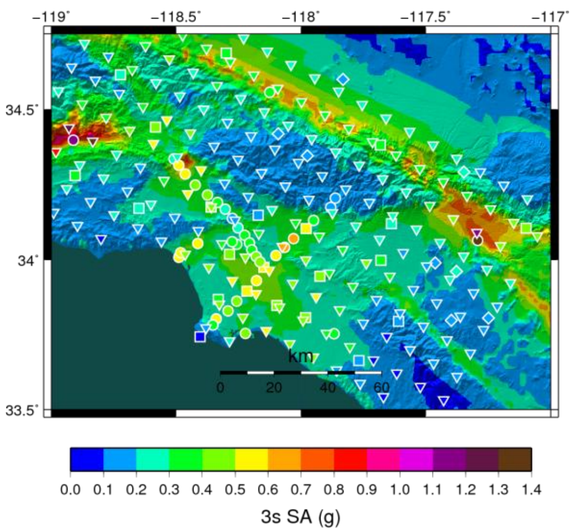


BLAST (Small)
17 sub-tasks
~4h on 17 nodes



Southern California Earthquake Center

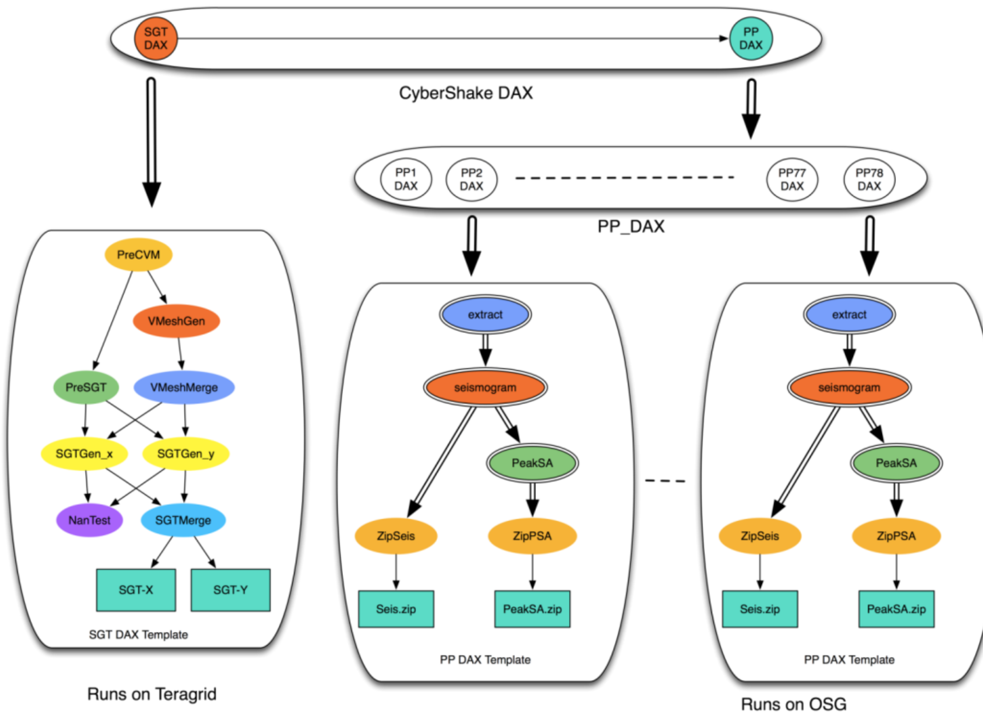
CyberShake PSHA Workflow



❖ **Description**

✧ Builders ask seismologists: "What will the peak ground motion be at my new building in the next 50 years?"

✧ Seismologists answer this question using Probabilistic Seismic Hazard Analysis (PSHA)



239 Workflows

- Each site in the input map corresponds to one workflow
- Each workflow has:

✧ **820,000 tasks**

MPI codes ~ 12,000 CPU hours,
Post Processing 2,000 CPU hours
Data footprint ~ 800GB

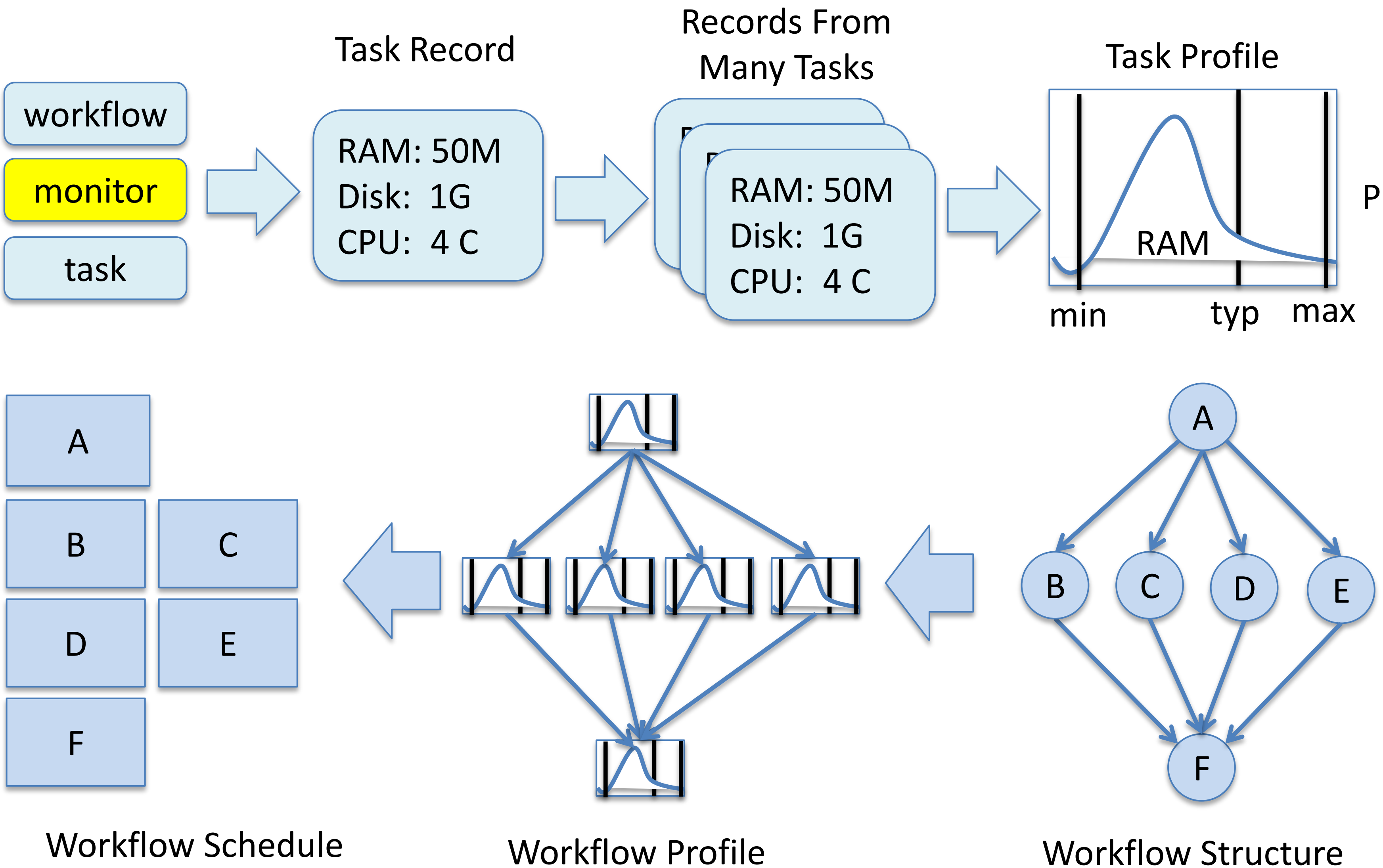
Pegasus managed workflows

Workflow Ensembles

Task Characterization/Execution

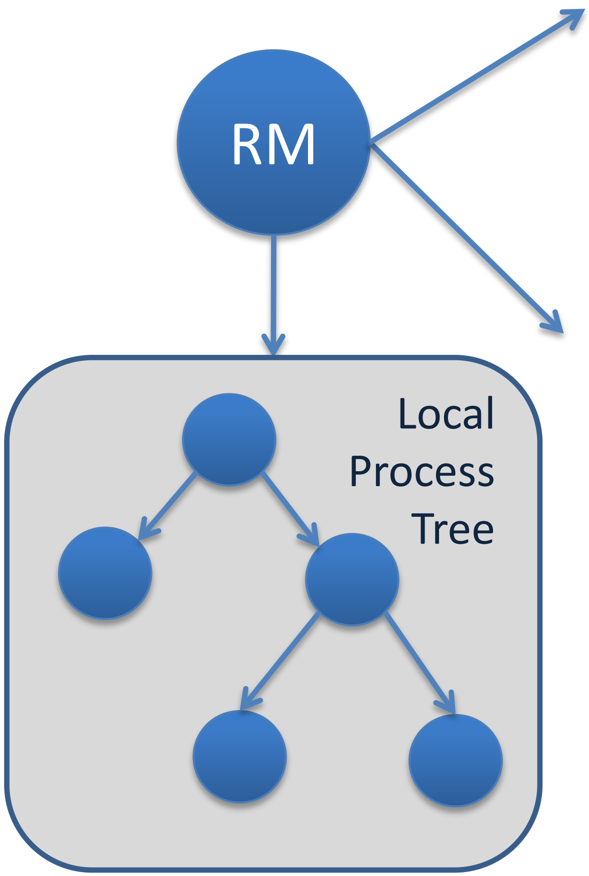
- Understand the resource needs of a task
- Establish expected values and limits for task resource consumption
- Launch tasks on the correct resources
- Monitor task execution and resource consumption, interrupt tasks that reach limits
- Possibly re-launch task on different resources

Data Collection and Modeling



Resource Monitor

% resource_monitor mysim.exe



Log File:

```
#wall_clock(useconds)     concurrent_processes cpu_time(useconds
     virtual_memory(kB)   resident_memory(kB)  swap_memory(kB)
     bytes_read      bytes_written
1  1  0          8700      376        0     385024     0
2  5  20000      326368    6100       0     27381007   1474560
3  6  20000      394412    7468       0     29735839   1503232
4  8  60000      531468    14092      0     36917793   1503232
5  8  100000     532612    16256      0     39285593   1503232
```

Summary File

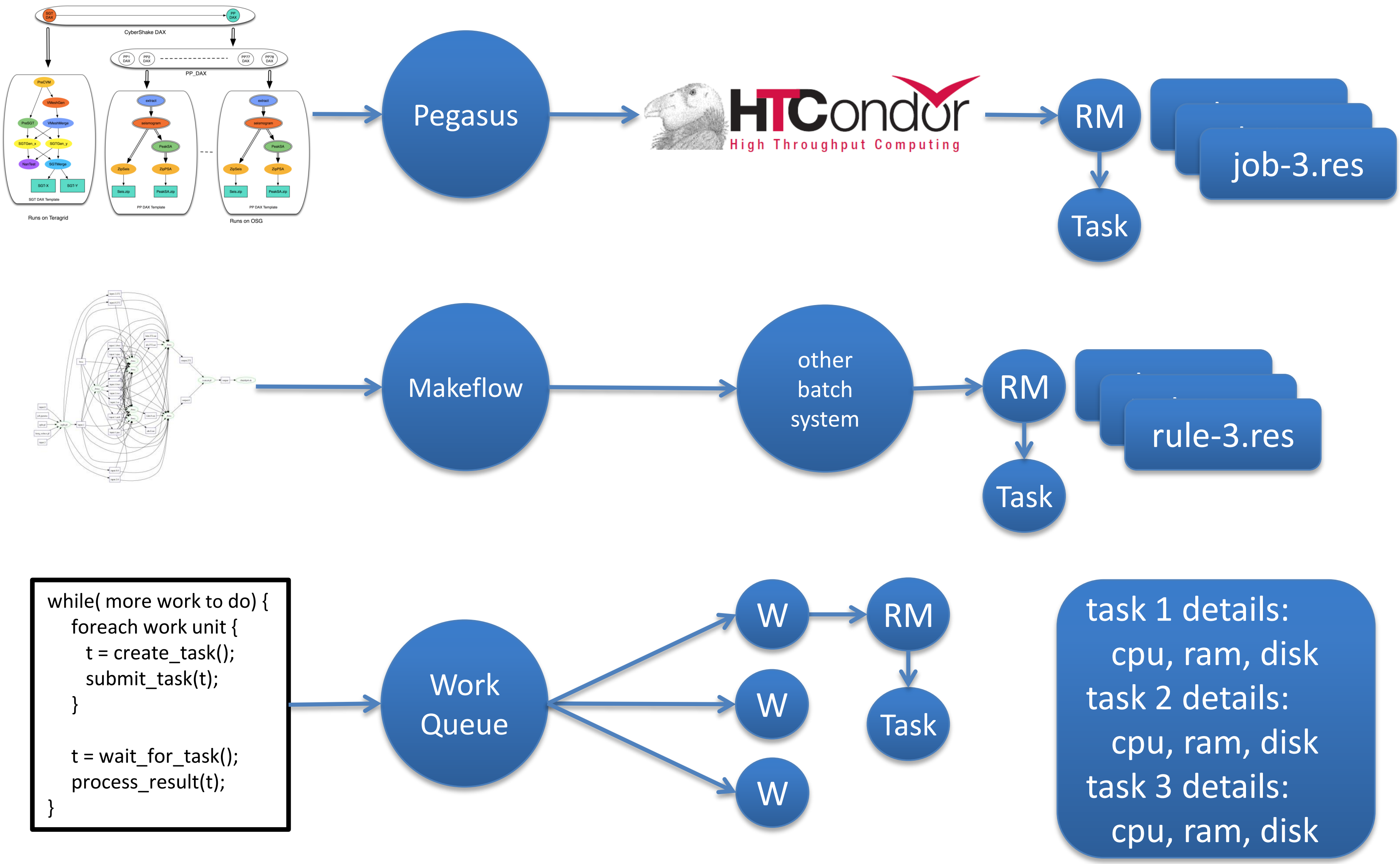
start:	1367424802.676755
end:	1367424881.236612
exit_type:	normal
exit_status:	0
max_concurrent_processes:	16
wall_time:	78.559857
cpu_time:	54.181762
virtual_memory:	1051160
resident_memory:	117604
swap_memory:	0
bytes_read:	4847233552
bytes_written:	256950272

Monitoring Strategies

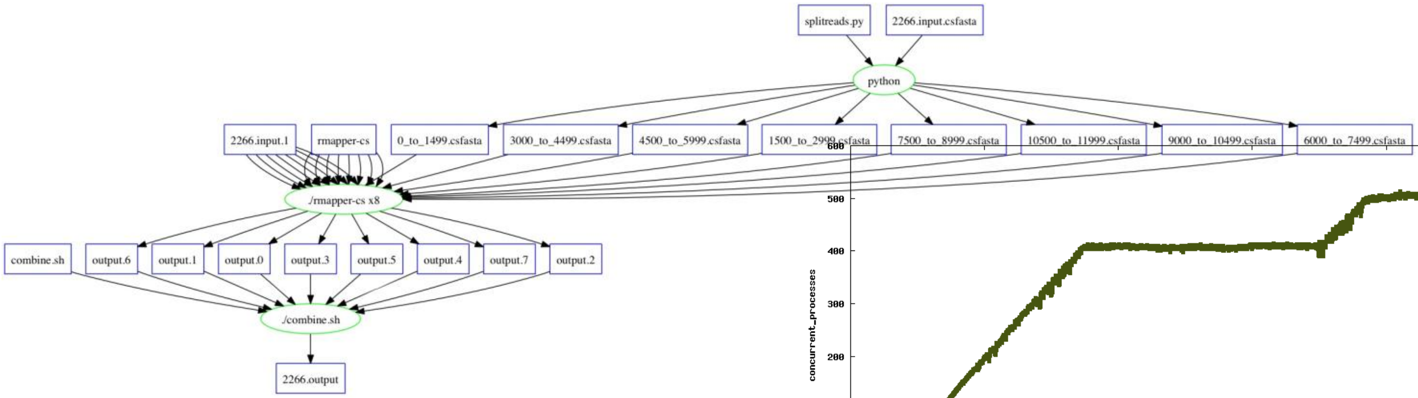
Indirect	Direct
Monitor how the world changes while the process tree is alive.	Monitor what functions, and with which arguments the process tree is calling.

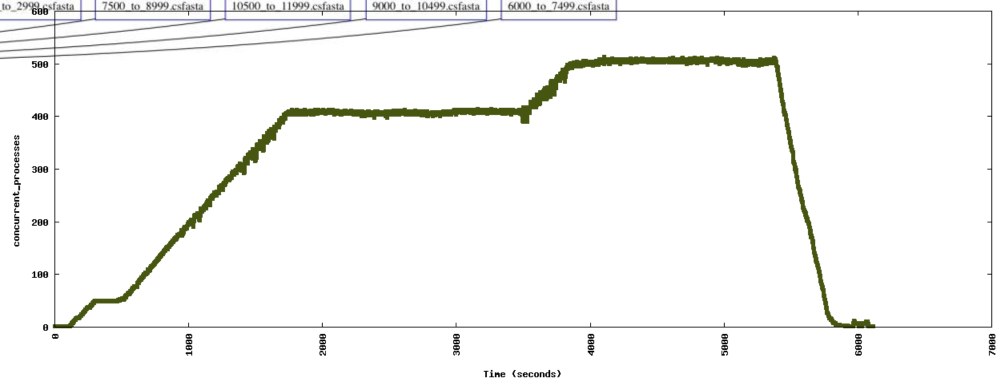
Summaries	Snapshot	Events
getrusage and times	Reading /proc and measuring disk at given intervals.	Linker wrapper to libc
Available only at the end of a process.	Blind while waiting for next interval.	Fragile to modifications of the environment, no statically linked processes.

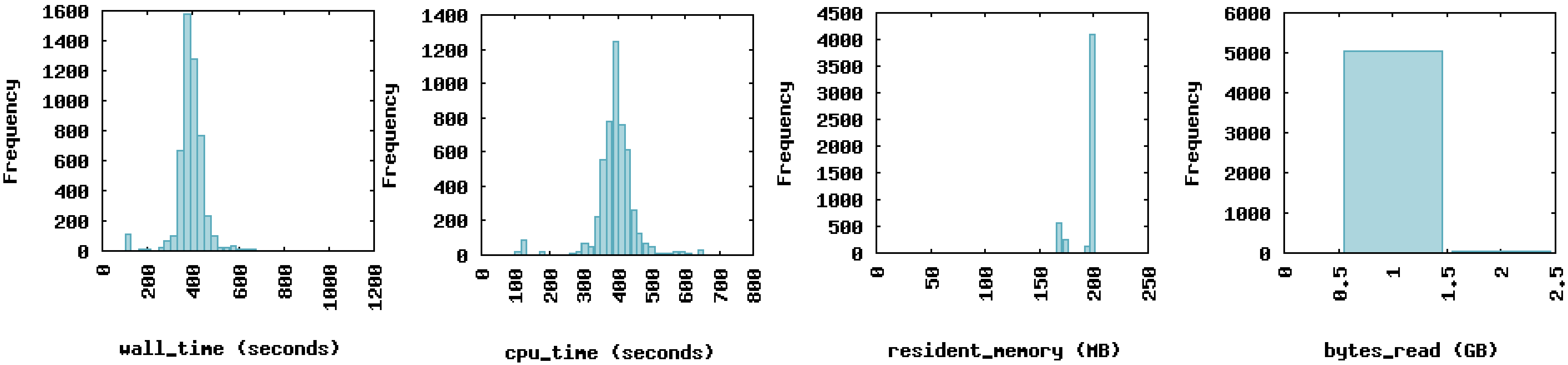
Portable Resource Management



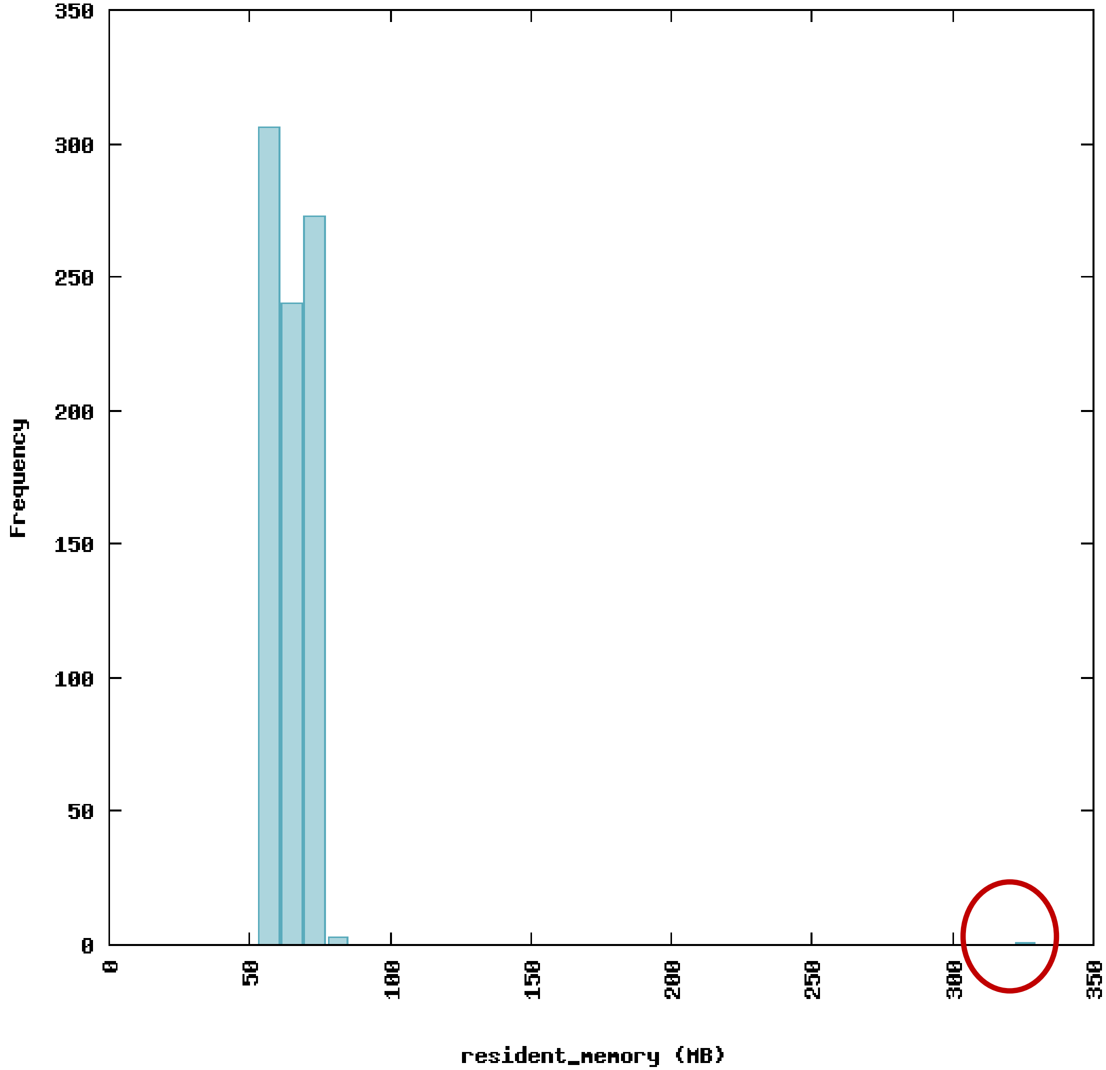
Resource Visualization of SHRiMP

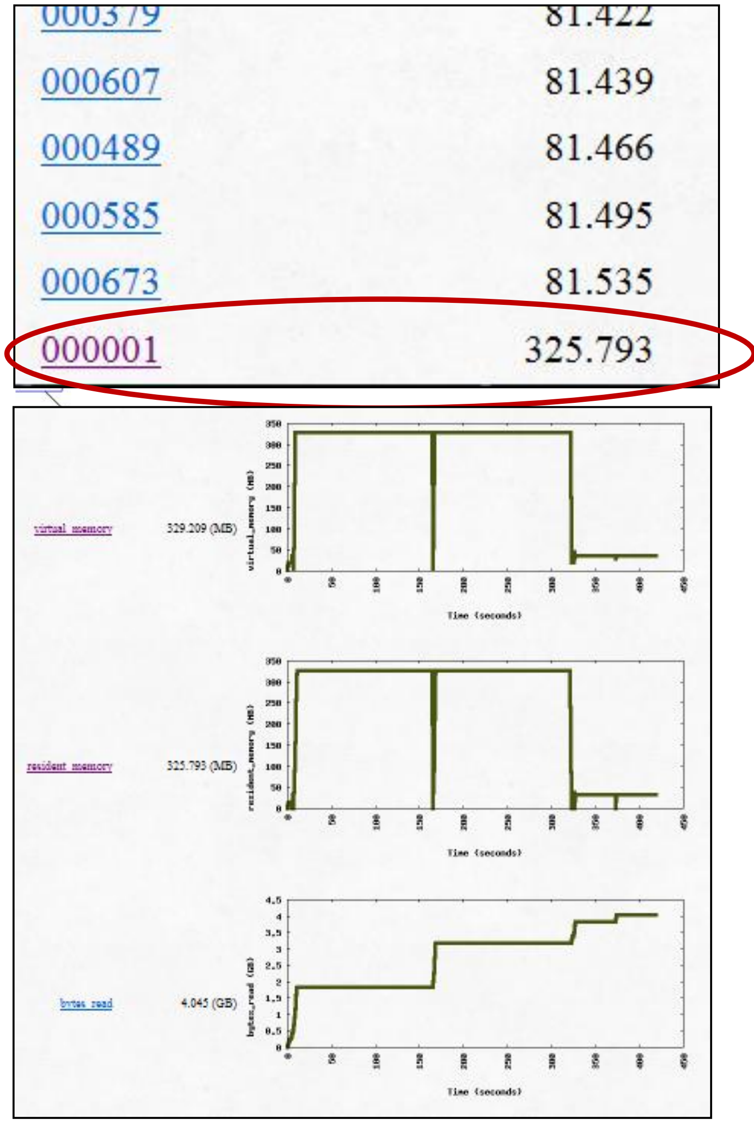




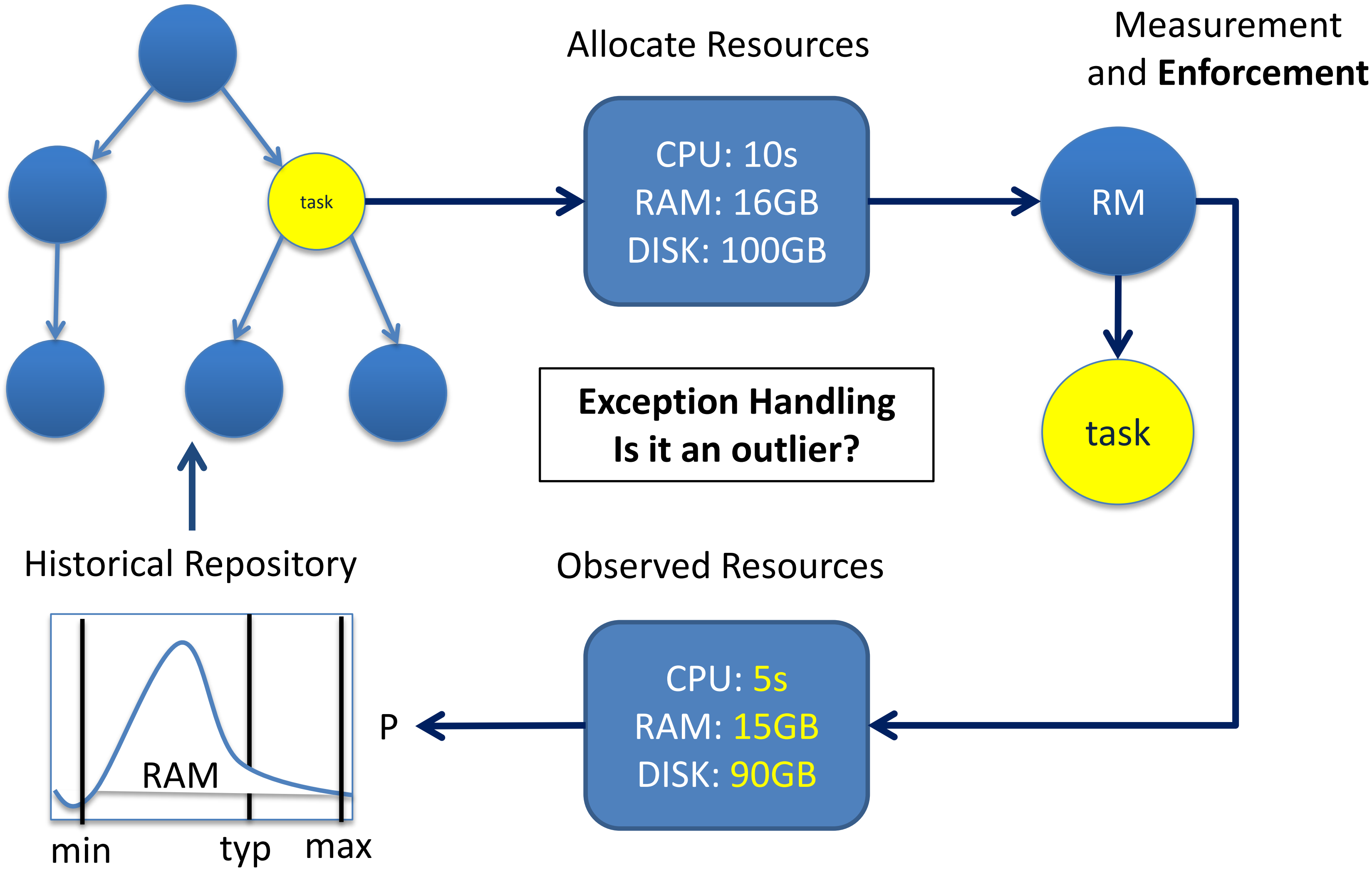


Outliers Happen: BWA Example

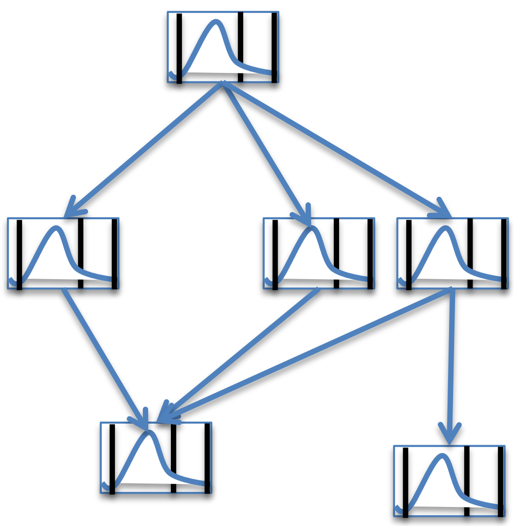




Completing the Cycle



Complete Workload Characterization



128 GB 32 cores X 1	16 GB 4 cores X 10	12 hours 500 Gb/s I/O
128 GB 32 cores X 1	16 GB 4 cores X 100	1 hour 5 Tb/s I/O

X 1000

We can approach the question:

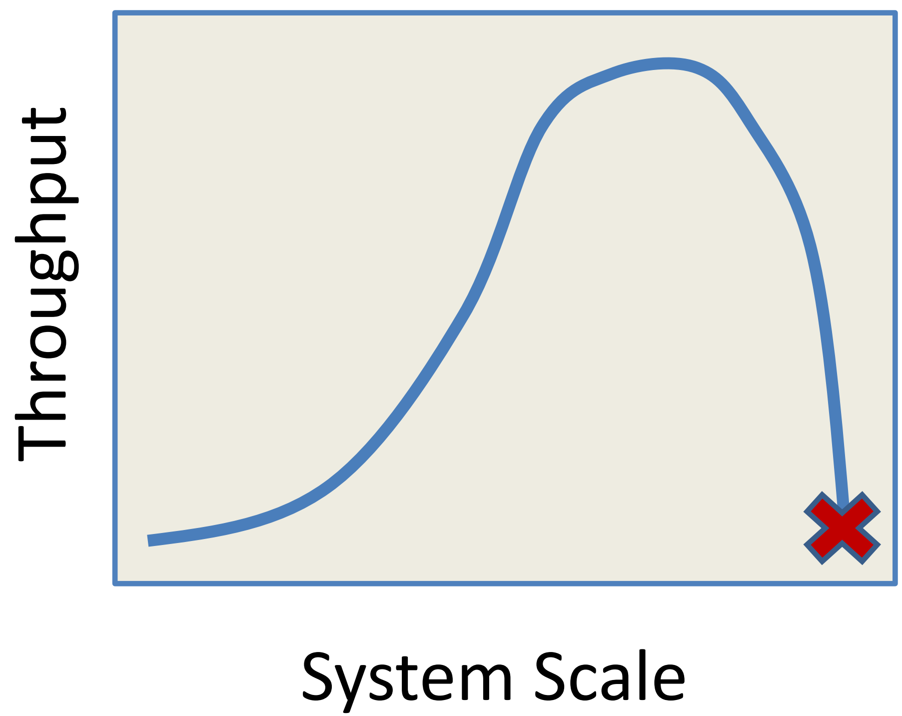
Can it run on this particular machine?

What machines could it run on?

Two jokes about
computer scientists.

How do you tell the difference between a ***computer scientist*** and a ***real scientist?***

What's the difference between a ***computer scientist*** and an ***engineer***?



Posters Preview

- Hierarchical Resource Management
  - Michael Albrecht
- Workflow Dependency Management
  - Casey Robinson
- Application Assembly Technologies
  - Peter Sempolinski

Acknowledgements

dV/dT Project PIs

- Bill Allcock (ALCF)
- Ewa Deelman (USC)
- Miron Livny (UW)
- Frank Weurthwein (UCSD)

CCL Staff

- Ben Tovar

CCL Graduate Students:

- Michael Albrecht
- Patrick Donnelly
- Dinesh Rajan
- Casey Robinson
- Peter Sempolinski
- Li Yu

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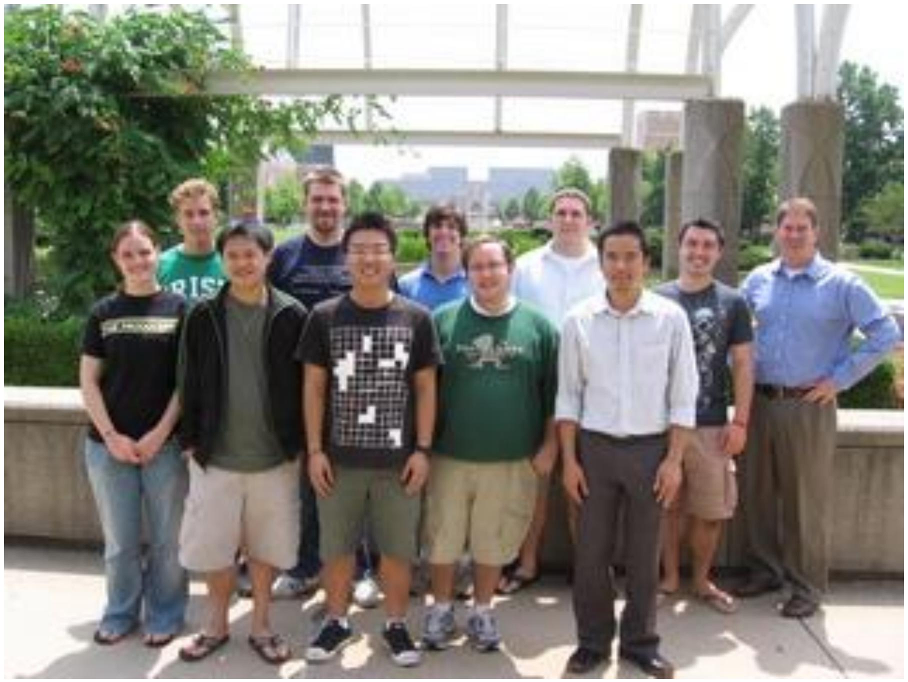

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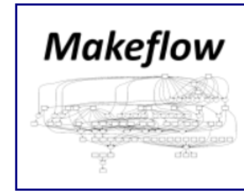

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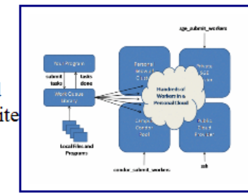

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