Hosted Science:
Managing Computational Workflows in the Cloud

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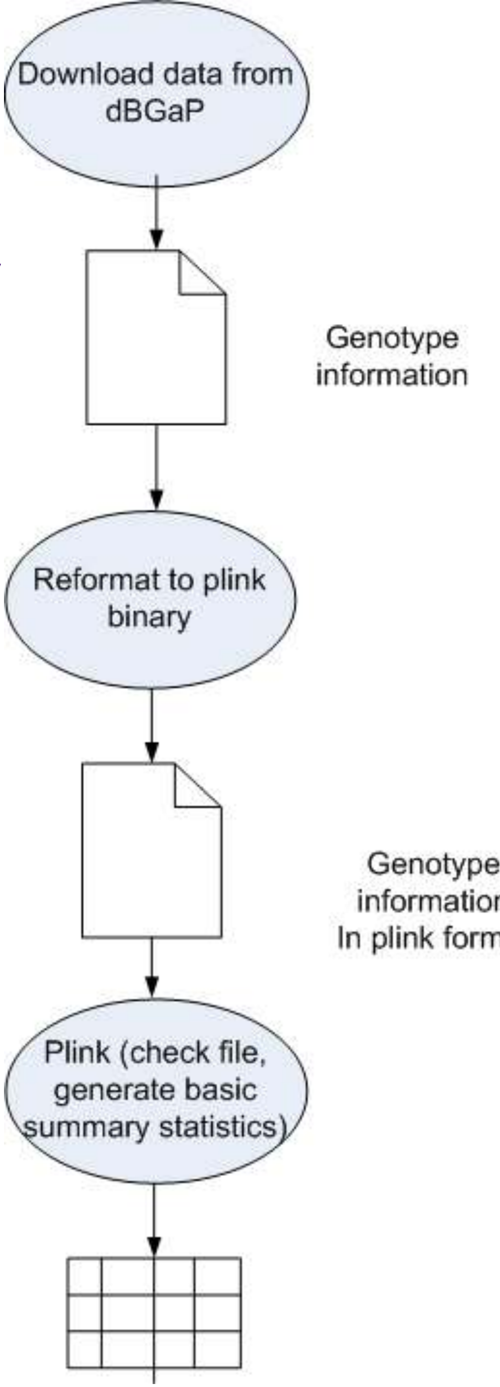
The Problem

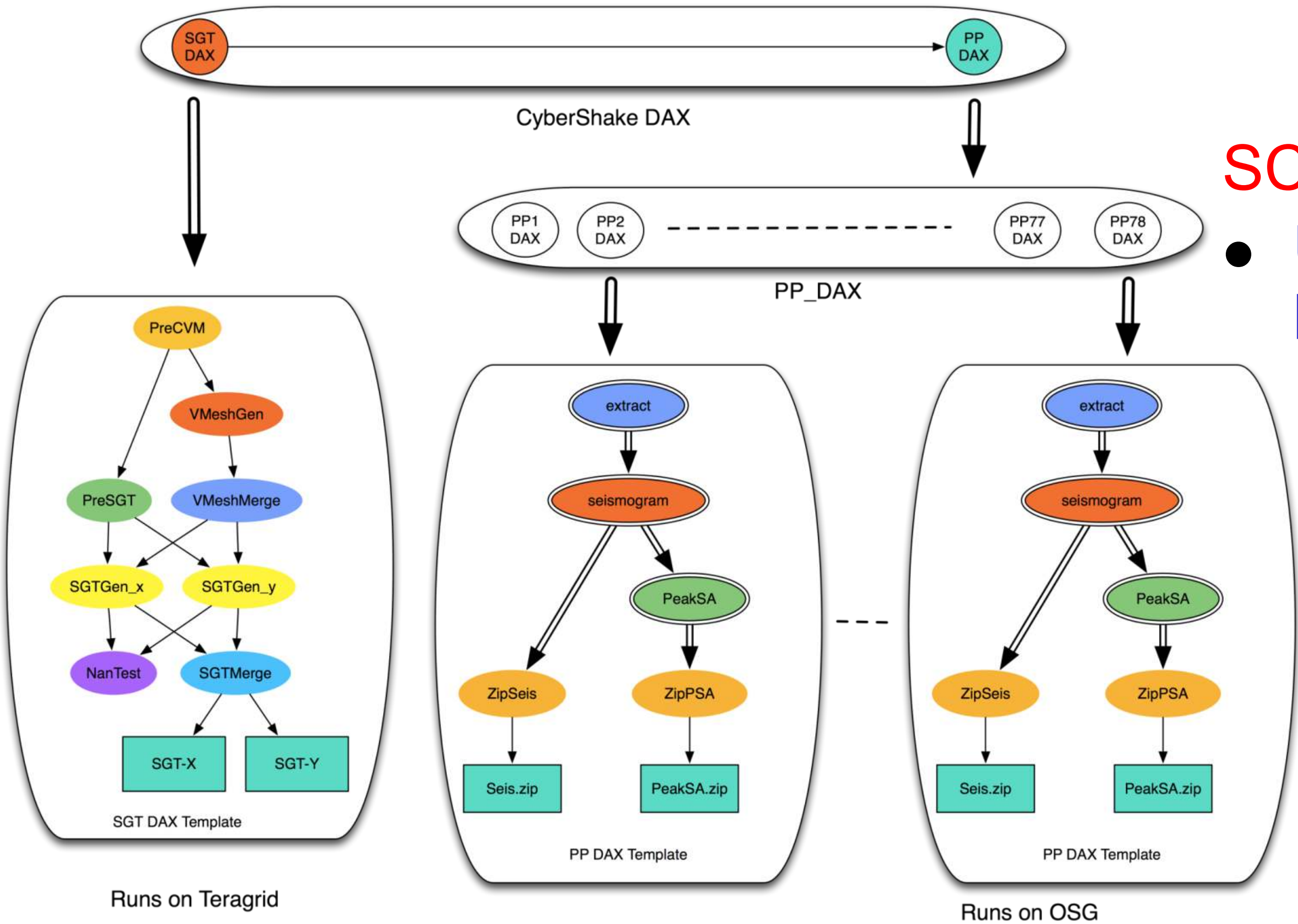
- Scientific data is being collected at an ever increasing rate
  - The “old days” -- big, focused experiments– LHC
  - Today “cheap” DNA sequencers – and an increasing number of them
- The complexity of the computational problems is ever increasing
- Local compute resources are often not enough (too small, limited availability)
- The computing infrastructure keeps changing
  - Hardware, software, but also computational models

Computational workflows --managing application complexity

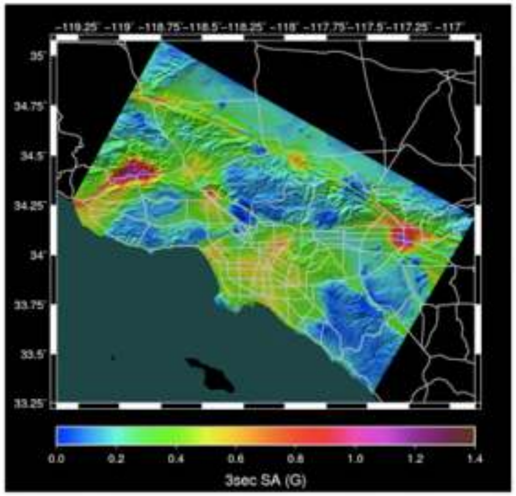
- Help express multi-step computations in a declarative way
- Can support automation, minimize human involvement
  - Makes analyses easier to run
- Can be high-level and portable across execution platforms
- Keep track of provenance to support reproducibility
- Foster collaboration—code and data sharing



So far applications have been running on local/campus clusters or grids



~ 850,000 tasks

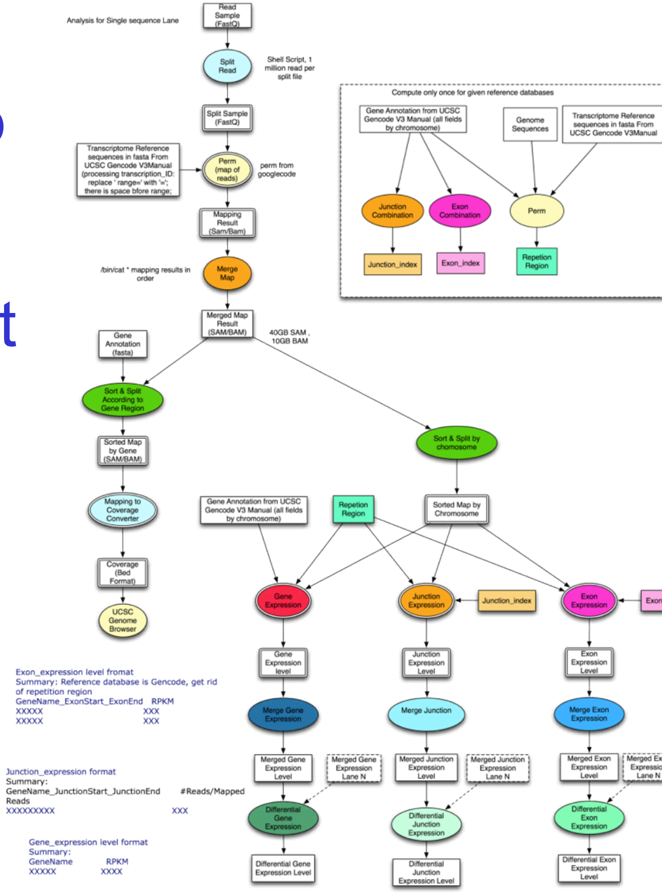


SCEC CyberShake

- Uses physics-based approach
  - 3-D ground motion simulation with anelastic wave propagation
  - Considers ~415,000 earthquakes per site
    - <200 km from site of interest
    - Magnitude >6.5

DNA sequencing, a new breed of data-intensive applications

- Data collected at a sequencers
  - Needs to be filtered for noisy data
  - Needs to be aligned
  - Needs to be collected into a single map
- Vendors provide some basic tools
  - you may want to try the latest alignment algorithm
  - you may want to use a remote cluster
- Challenges:
  - automation of analysis, reproducibility
  - Portability
  - provenance USERS!



Outline

- Role of hosted environments
- Workflows on the Cloud
  - Challenges in running workflows on the cloud
  - Data management aspects
- Hosted Science
  - Managing workflow ensembles on the cloud
  - Within user-defined constraints
- Conclusions

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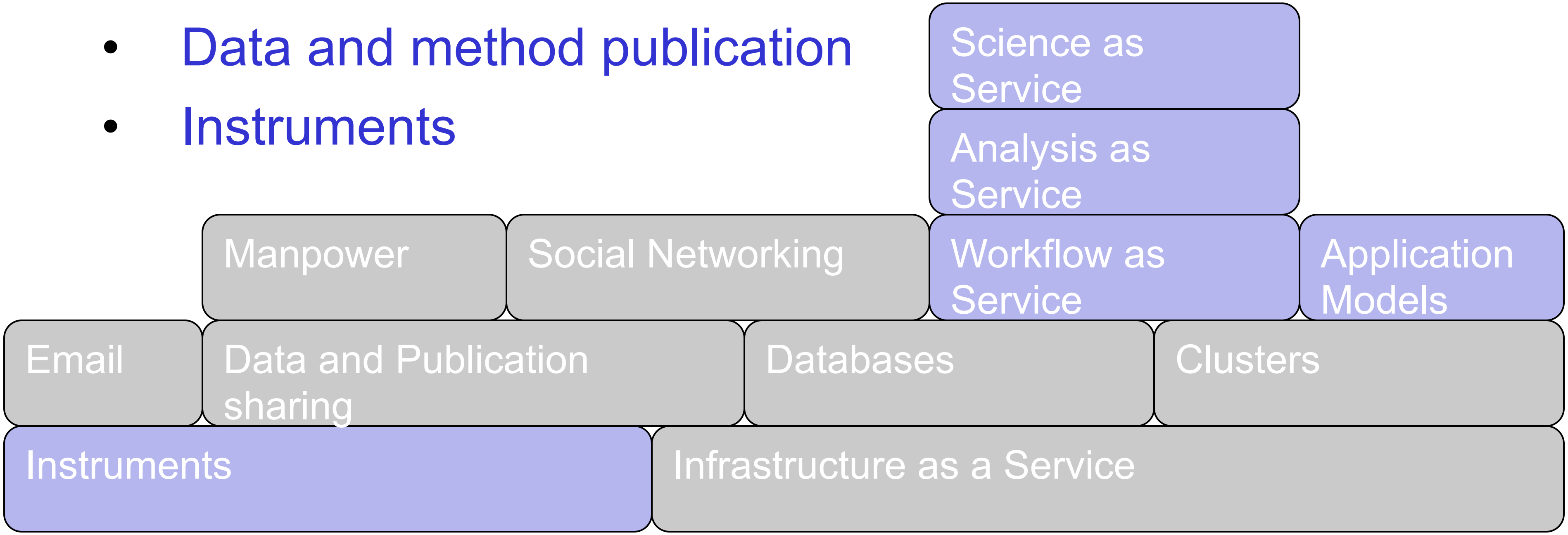
New applications are looking towards Clouds

- Originated in the business domain
- Outsourcing services to the Cloud (successful for business)
- Pay for what you use, elasticity of resources
- Provided by data centers that are built on compute and storage virtualization technologies
- Scientific applications often have different requirements
  - MPI
  - Shared file system
  - Support for many dependent jobs

Google's Container-based Data Center in Belgium
http://www.datacenterknowledge.com/

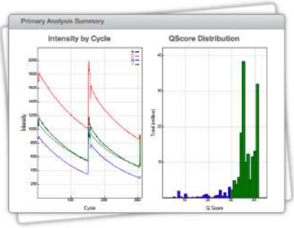
Hosted Science

- Today applications are using the cloud as a resource provider (storage, computing, social networking)
- In the future more services will be migrating to the cloud (more integration)
  - Hosted end-to-end analysis
  - Data and method publication
  - Instruments



The Future is Now Illumnia's BaseSpace

Data Analysis



BaseSpace now performs one alignment and variant detection for free on all Illumina data! To learn more about what's included, click here.

BaseSpace makes data analysis easy. Push-button tools let researchers easily leverage all types of analysis applications and seamlessly view their results. Our flexible "app store" environment is being developed to bring the industry's best tools to your fingertips, with new tools added constantly.

Currently, BaseSpace can perform the following analyses on your data:

RESEQUENCING ALIGNMENT
Sequencing of an enriched portion of the human genome, or of a small genome (such as e.coli). Reads are aligned against the reference, and variants are noted.

AMPLICON SEQUENCING
Sequencing of PCR amplicons from probes targeting particular genome positions (up to ~384 loci from up to ~96 samples).

DE NOVO ASSEMBLY
Assembly of small (< 20MB) genome from 16S ribosomal RNA reads without the use of a genomic reference.

SMALL RNA ANALYSIS
Resequencing workflow applied to microRNAs.

LIBRARY QC
Fast resequencing of a reference genome to QC the DNA library

METAGENOMICS
The 16S metagenomics workflow is used to classify organisms from a metagenomic sample by amplifying specific regions in the 16S ribosomal RNA. The main output of this workflow is a classification of reads at several taxonomic levels (kingdom, phylum, class, order, family, genus)

Prep
15 minutes hands-on
1.5
HOURS

Sequence
20 minutes hands-on
4
HOURS

Analyze
fully automated
3
HOURS

Share
secure and store
BaseSpace®

Workflow times include dual surface scanning and v2 kits.

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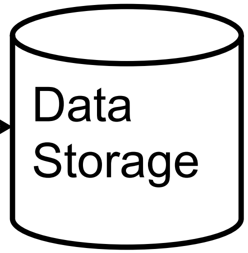
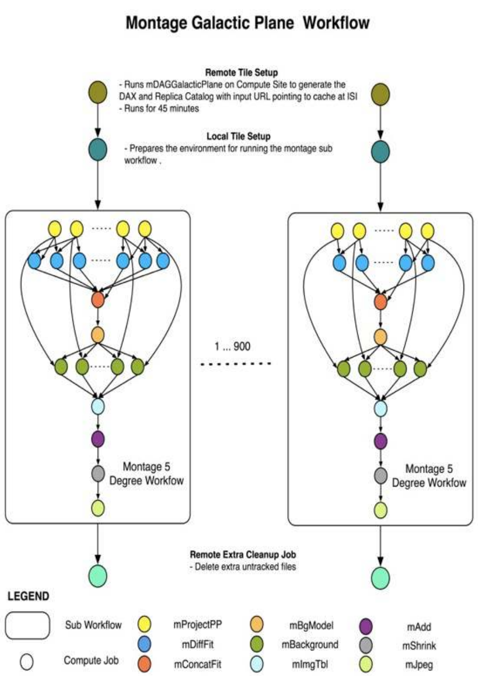
Issues

- It is difficult to manage cost
  - How much would it cost to analyze one sample?
  - How much would it cost to analyze a set of samples?
  - The analyses may be complex and multi-step (*workflows*)
- It is difficult to manage deadlines
  - "I would like all the results to be done in a week"
  - "I would like the most important analyses done in a week"
  - "I have a week to get the most important results and $500 to do it"

Scientific Environment
How to manage complex workloads?





Work definition

Local Resource

Campus Cluster

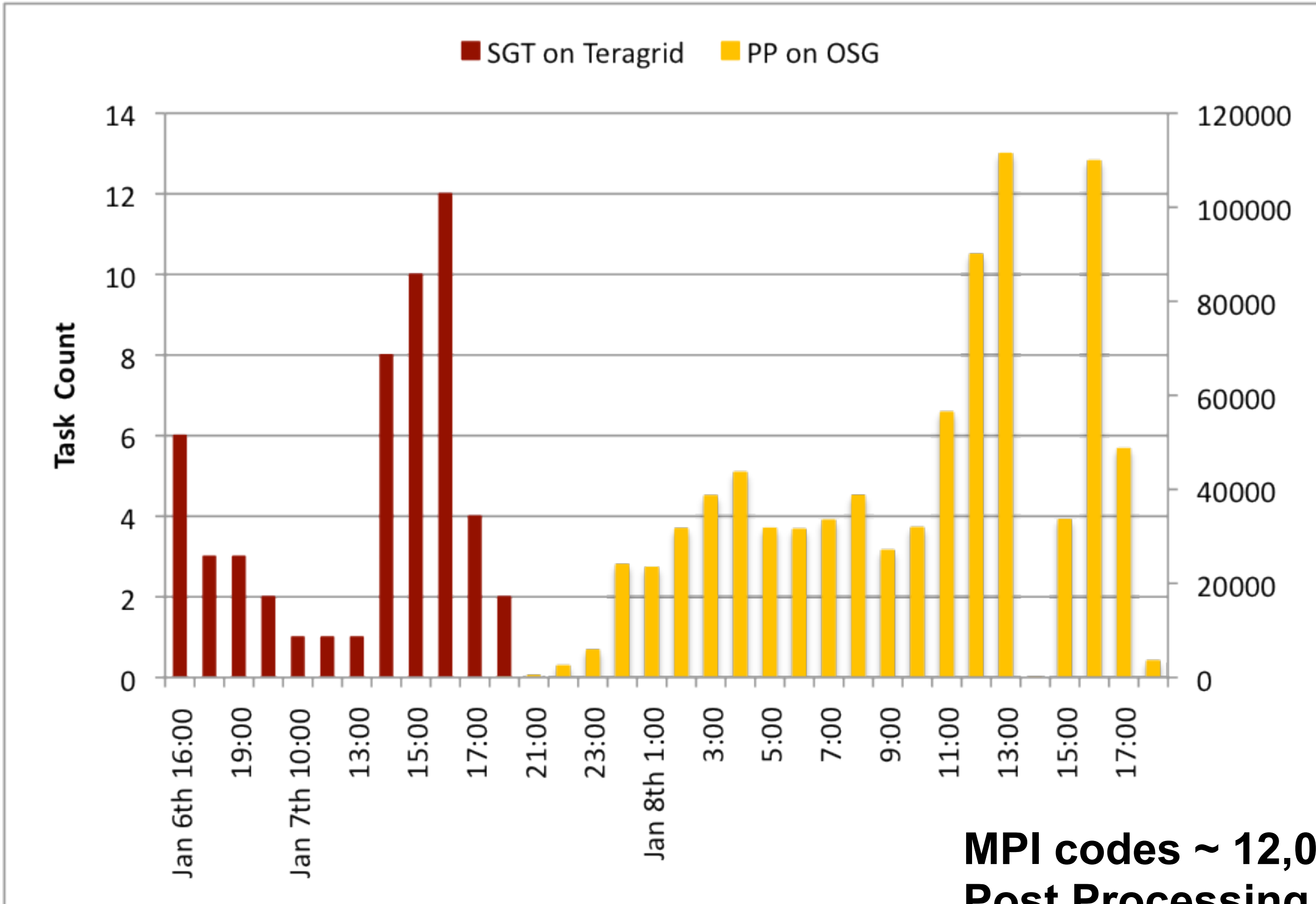
EGI

TeraGrid/XSEDE

Open Science Grid

Amazon Cloud

Workflows have different computational needs --need systems to manage their execution



SoCal Map needs 239 of those

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

Peak # of cores on OSG 1,600
Walltime on OSG 20 hours, could be done in 4 hours on 800 cores

Workflow Management

You may want to use different resources within a workflow or over time

- Need a high-level workflow specification
- Need a planning capability to map from high-level to executable workflow
- Need to manage the task dependencies
- Need to manage the execution of tasks on the remote resources

- Need to provide scalability, performance, reliability

Our Approach

- Analysis Representation
  - Support a declarative representation for the workflow (dataflow)
  - Represent the workflow structure as a Directed Acyclic Graph (DAG)
  - Use recursion to achieve scalability
- System (Plan for the resources, Execute the Plan, Manage tasks)
  - Layered architecture, each layer is responsible for a particular function
  - Mask errors at different levels of the system
  - Modular, composed of well-defined components, where different components can be swapped in
  - Use and adapt existing graph and other relevant algorithms

Use the given Resources

Data
Storage

data

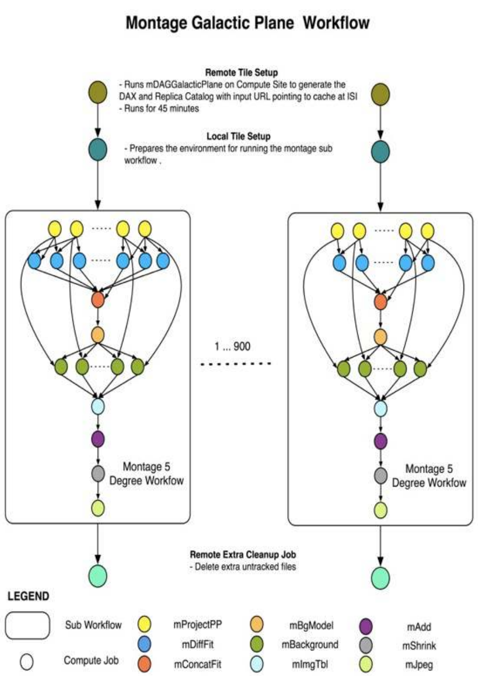
Campus Cluster

EGI

TeraGrid/XSEDE

Open Science Grid

Amazon Cloud



Work definition
As a WORKFLOW

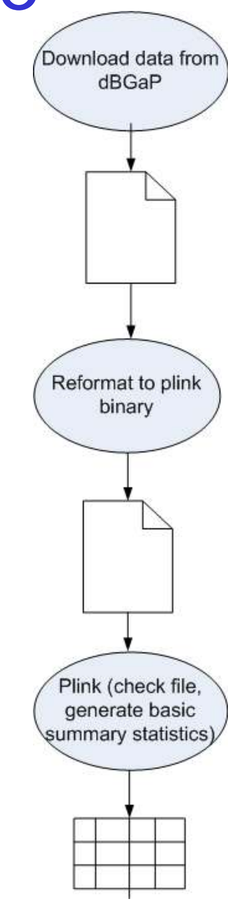
Workflow
Management
System

Local Resource

work

Challenges of running workflows on the cloud

- Clouds provide resources, but the software is up to the user
- Running on multiple nodes may require cluster services (e.g. scheduler)
- Dynamically configuring such systems is not easy
  - Manual setup is error-prone and not scalable
  - Scripts work to a point, but break down for complex deployments
- Some tools are available
- Workflows need to communicate data—often through files, need filesystems
- Data is an important aspect of running on the cloud



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Workflow Data In the Cloud

Executables
- Transfer into cloud
- Store in VM image

Input Data
- Transfer into cloud
- Store in cloud

Intermediate Data
- Use local disk (single node only)
- Use distributed storage system

Output Data
- Transfer out of cloud
- Store in cloud

Amazon Web Services (AWS)

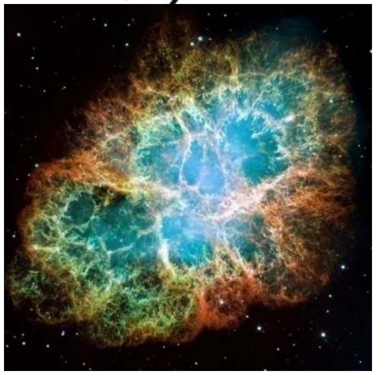
IaaS Cloud, Services

- Elastic Compute Cloud (EC2)
  - Provision virtual machine instances
- Simple Storage Service (S3)
  - Object-based storage system
  - Put/Get files from a global repository
- Elastic Block Store (EBS)
  - Block-based storage system
  - Unshared, SAN-like volumes
- Others (queue, RDBMS, MapReduce, Mechanical Turk etc.)

We want to explore data management issues for workflows on Amazon

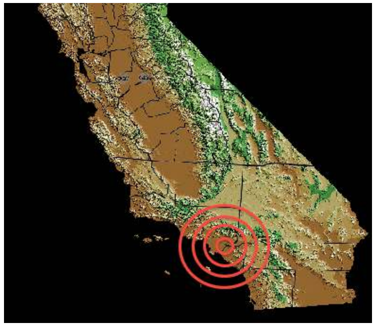
Applications

- Not CyberShake SoCal map (PP) could cost at least $60K for computing and $29K for data storage (for a month) on Amazon (one workflow ~$300)
- Montage (astronomy, provided by IPAC)
  - 10,429 tasks, 4.2GB input, 7.9GB of output
  - I/O: High (95% of time waiting on I/O)
  - Memory: Low, CPU: Low



- Epigenome (bioinformatics, USC Genomics Center)
  - 81 tasks 1.8GB input, 300 MB output
  - I/O: Low, Memory: Medium
  - CPU: High (99% time of time)

- Broadband (earthquake science, SCEC)
  - 320 tasks, 6GB of input, 160 MB output
  - I/O: Medium
  - Memory: High (75% of task time requires > 1GB mem)
  - CPU: Medium



Storage Systems

Local Disk

- RAID0 across available partitions with XFS

NFS: Network file system

- 1 dedicated node (m1.xlarge)

PVFS: Parallel, striped cluster file system

- Workers host PVFS and run tasks

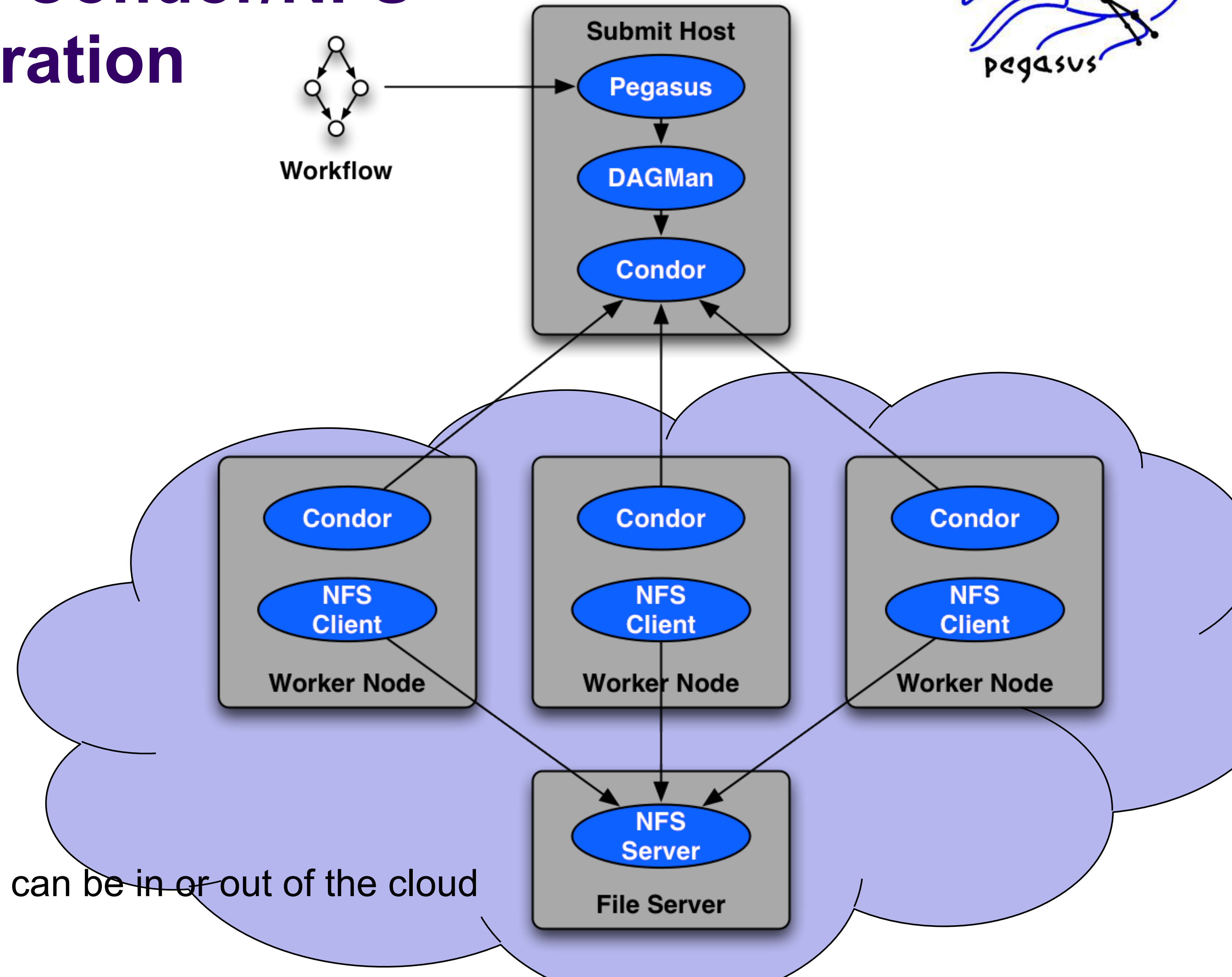
GlusterFS: Distributed file system

- Workers host GlusterFS and run tasks
- NUFA, and Distribute modes

Amazon S3: Object-based storage system

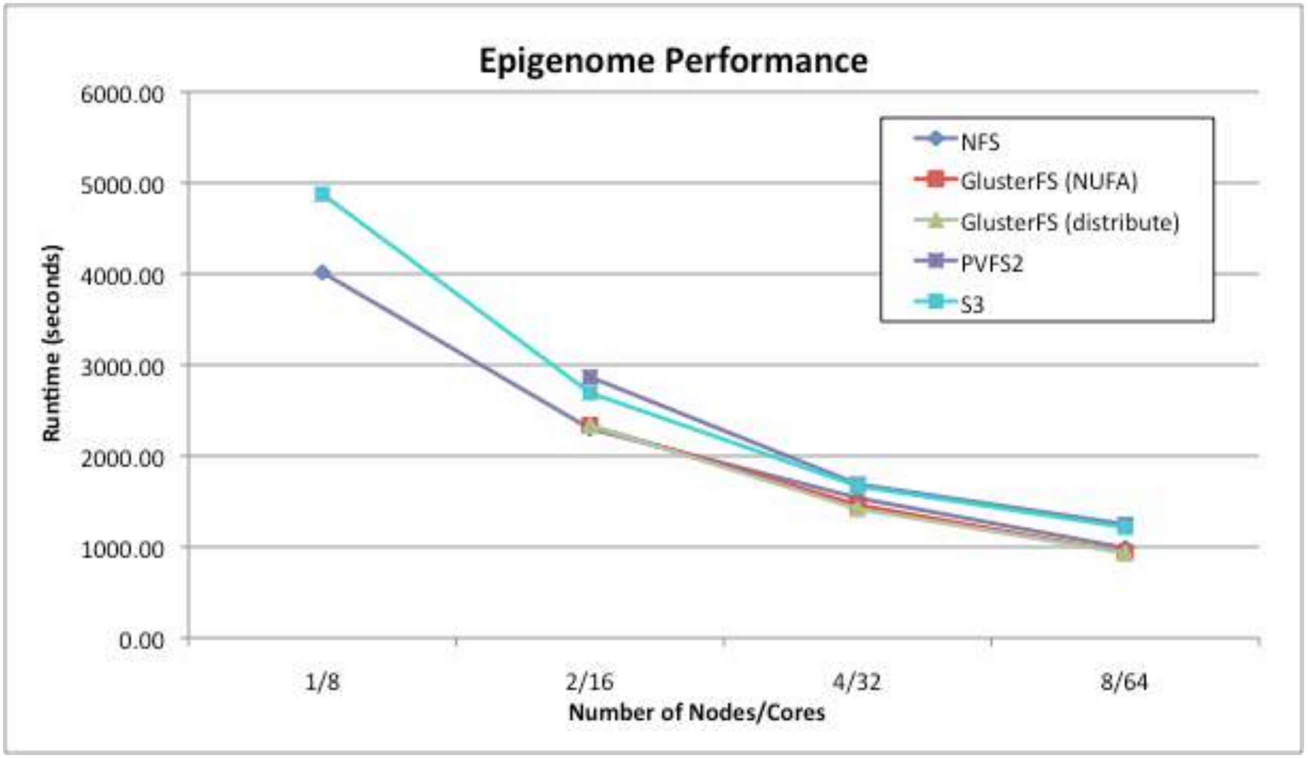
- Non-POSIX interface required changes to Pegasus
- Data is cached on workers

A cloud Condor/NFS configuration

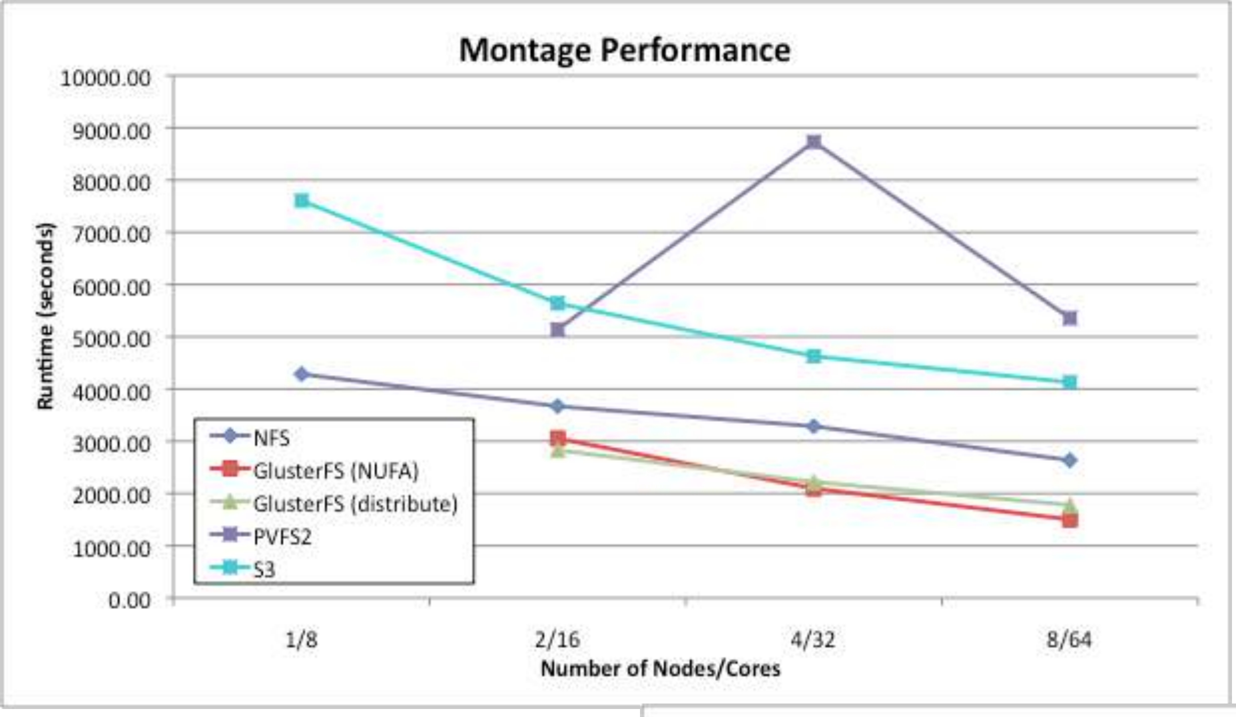


The submit host can be in or out of the cloud

Storage System Performance



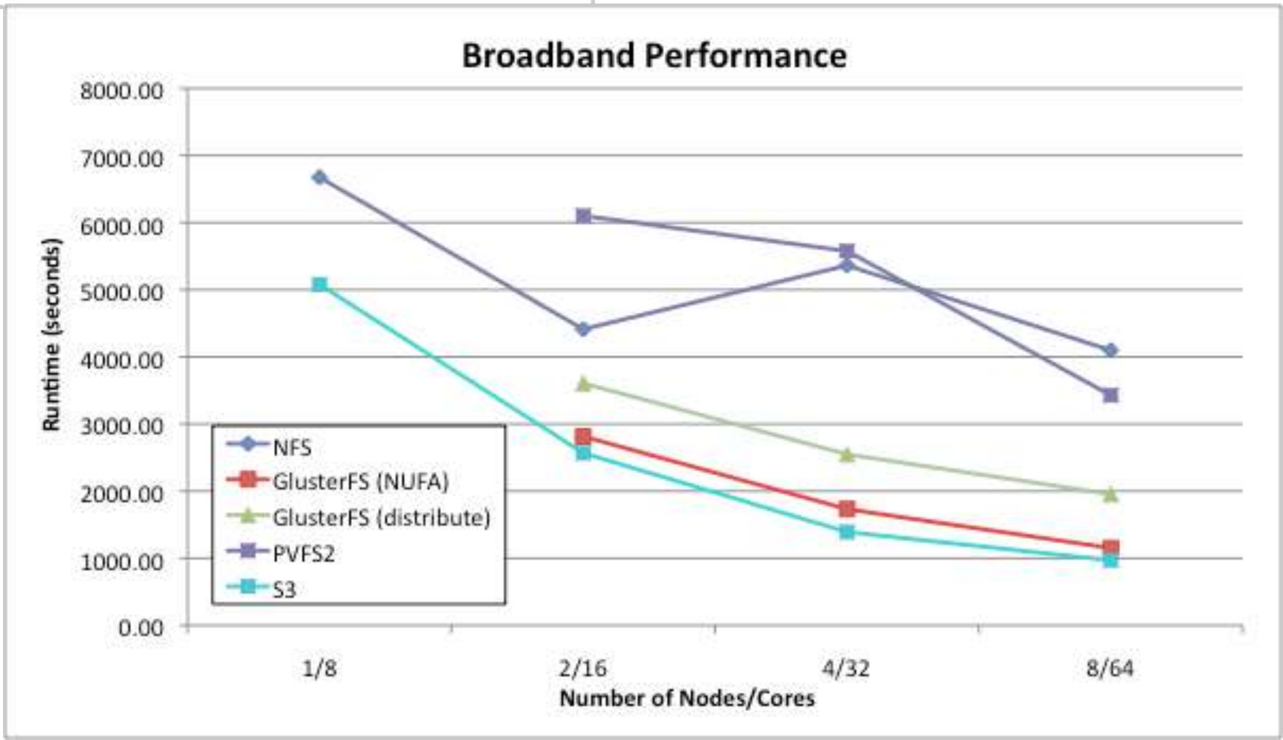
- NFS uses an extra node
- PVFS, GlusterFS use workers to store data, S3 does not
- PVFS, GlusterFS use 2 or more nodes
- We implemented whole file caching for S3



pegasus

Lots of small files

Re-reading the same file



Cost Components

Resource Cost

- Cost for VM instances
- Billed by the hour

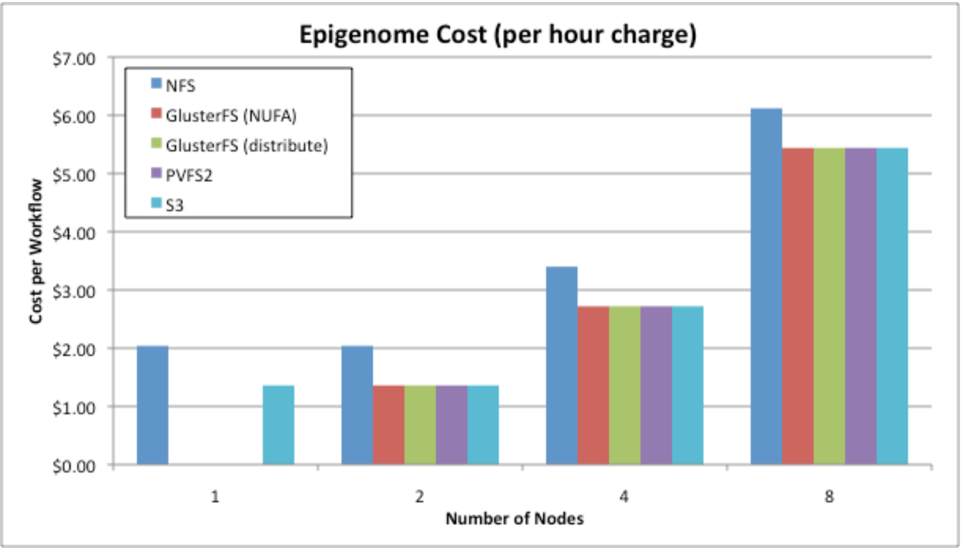
Transfer Cost

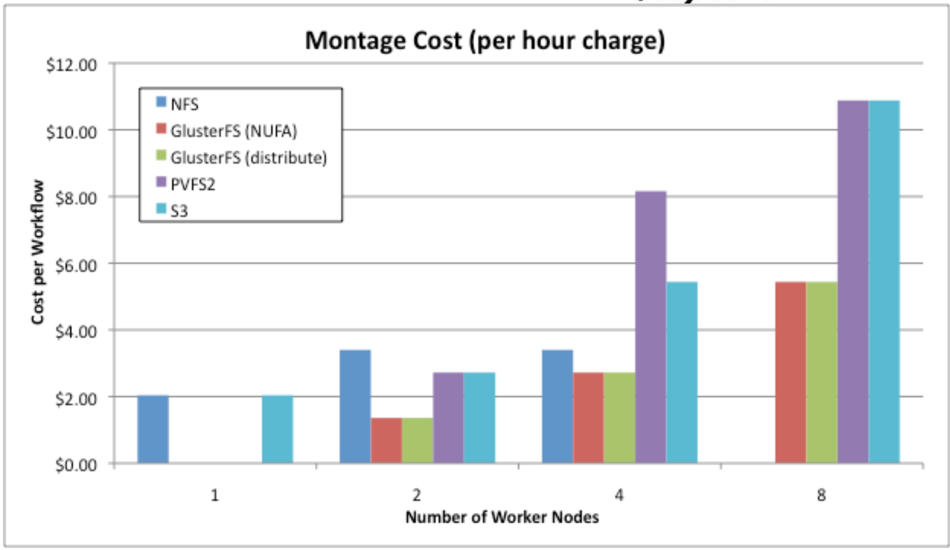
- Cost to copy data to/from cloud over network
- Billed by the GB

Storage Cost

- Cost to store VM images, application data
- Billed by the GB, # of accesses

Resource Cost (by Storage System)

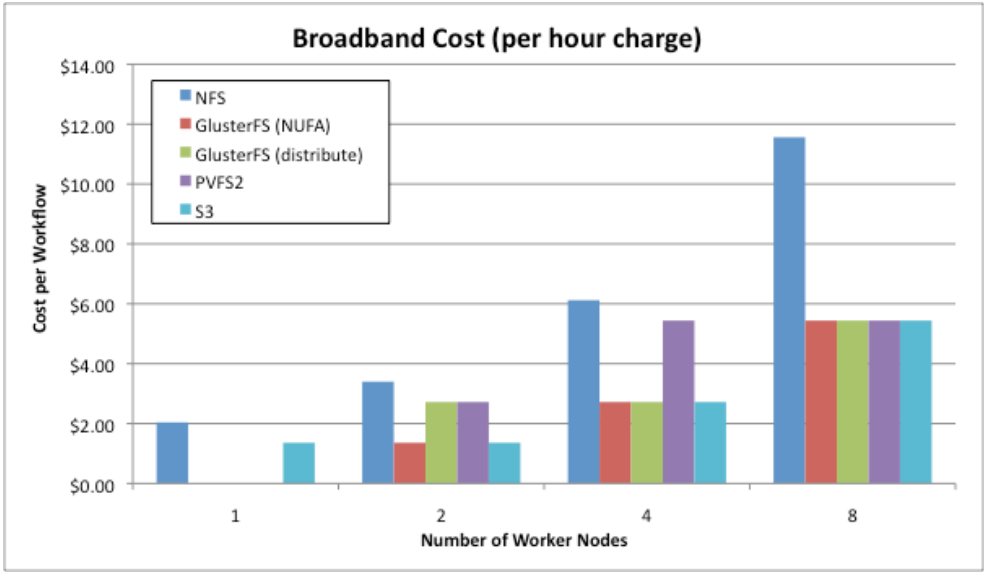




Cost tracks performance

Price not unreasonable

Adding resources does not usually reduce cost



Transfer Cost

Application	Input	Output	Logs
Montage	4291 MB	7970 MB	40 MB
Broadband	4109 MB	159 MB	5.5 MB
Epigenome	1843 MB	299 MB	3.3 MB

Transfer Sizes

Application	Input	Output	Logs	Total
Montage	\$0.42	\$1.32	< \$0.01	\$1.75
Broadband	\$0.40	\$0.03	< \$0.01	\$0.43
Epigenome	\$0.18	\$0.05	< \$0.01	\$0.23

Transfer Costs

- Cost of transferring data to/from cloud
  - Input: \$0.10/GB
  - Output: \$0.17/GB
- Transfer costs are a relatively large
  - For Montage, transferring data costs more than computing it (\$1.75 > \$1.42)
- Costs can be reduced by storing input data in the cloud and using it for multiple workflows

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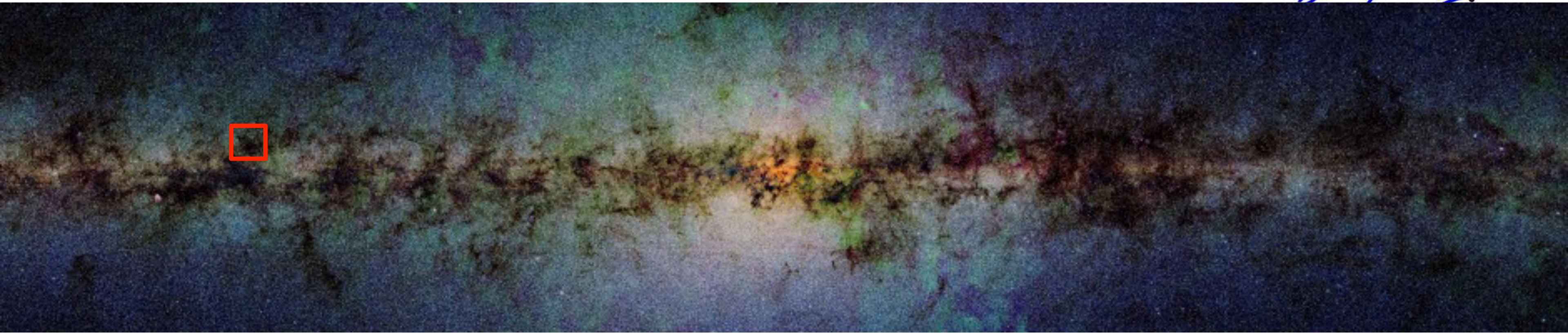
Large-Scale, Data-Intensive Workflows



Montage Galactic Plane Workflow

- 18 million input images (~2.5 TB)
- 900 output images (2.5 GB each, 2.4 TB total)
- 10.5 million tasks (34,000 CPU hours)

× 17

An analysis is composed of a number of related workflows– *an ensemble*

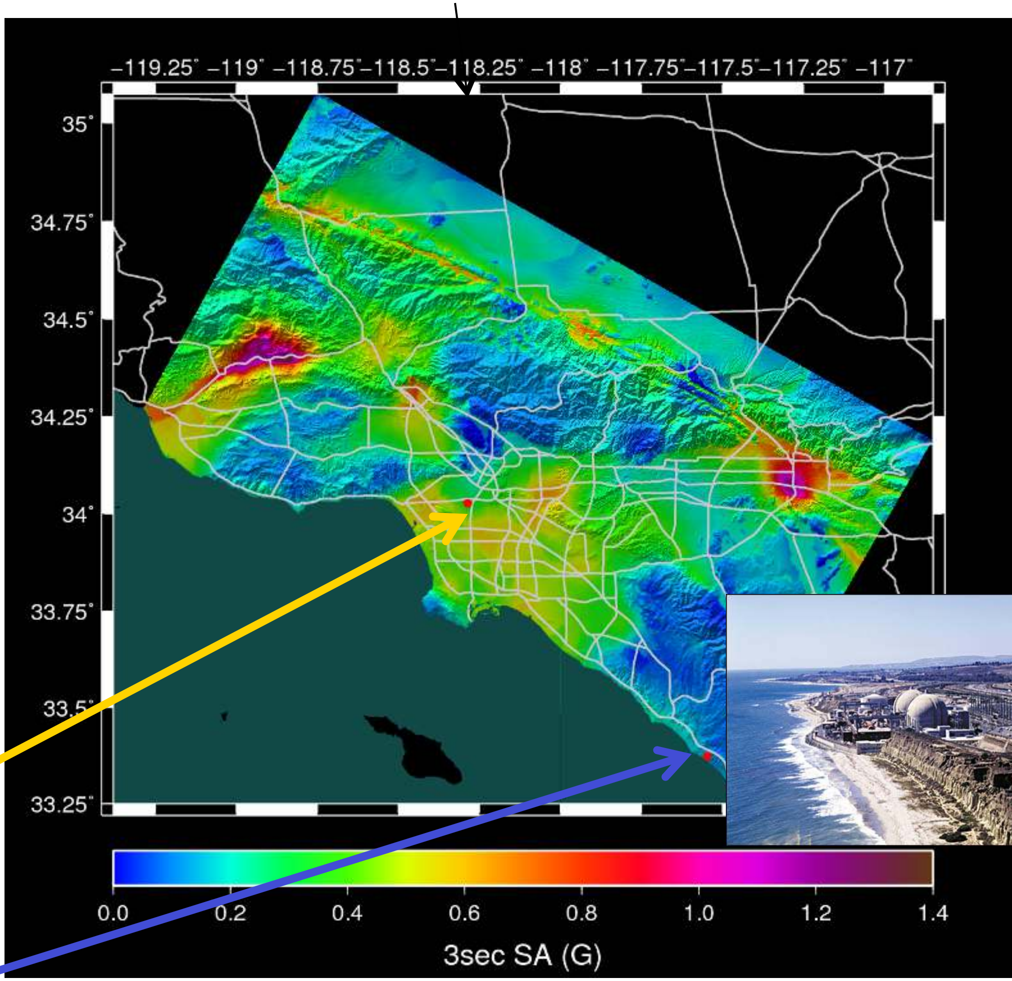
Workflow Ensembles

Set of workflows

- Workflows have different parameters, inputs, etc.

Prioritized

- Priority represents user's utility



USC

San Onofre Nuclear Power Plant

Problem Description

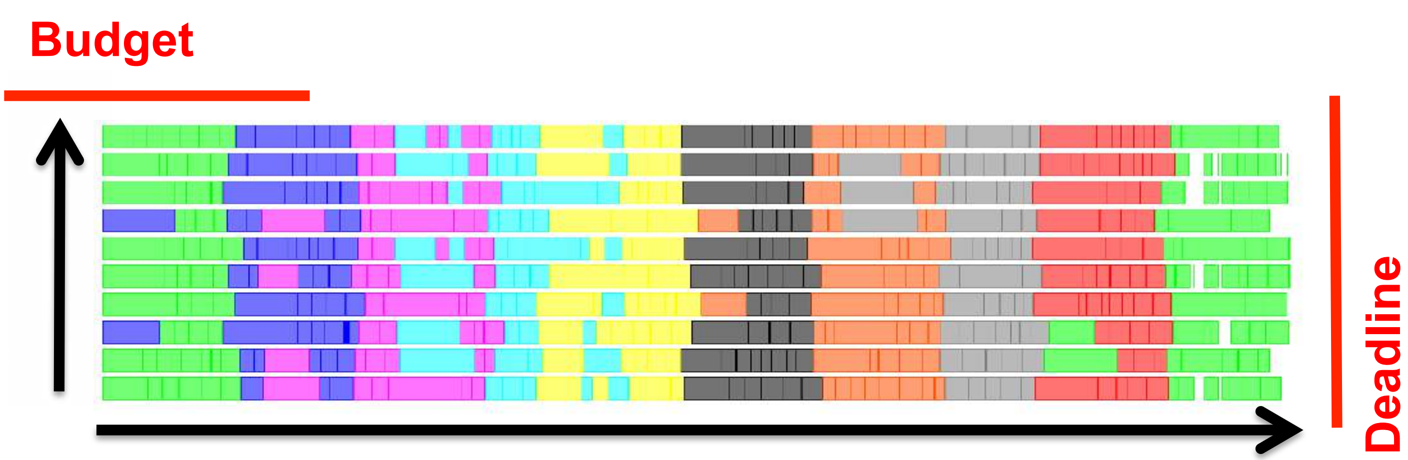
How do you manage ensembles in hosted environments ?

Typical research question:

How much computation can we complete given the limited time and budget of our research project?

Constraints: **Budget** and **Deadline**

Goal: given budget and deadline, maximize the number of prioritized workflows in an ensemble



Explore provisioning and task scheduling decisions

Inputs:

Budget, deadline, prioritized ensemble, and task runtime estimates

Outputs:

Provisioning: Determines # of VMs to use over time

Scheduling: Maps tasks to VMs

Algorithms:

SPSS: Static Provisioning, Static Scheduling

DPDS: Dynamic Provisioning, Dynamic Scheduling

WA-DPDS: Workflow-Aware DPDS

SPSS

- Plans out all provisioning and scheduling decisions ahead of execution (offline algorithm)
- Algorithm:
  - For each workflow in priority order
  - Assign sub-deadlines to each task
  - Find a minimum cost schedule for the workflow such that each task finishes by its deadline
  - If the schedule cost <= the remaining budget: accept the workflow
  - Otherwise: reject the workflow
- Static plan may be disrupted at runtime

DPDS

- Provisioning and scheduling decisions are made at runtime (online algorithm)
- Algorithm:
  - Task priority = workflow priority
  - Tasks are executed in priority order
  - Tasks are mapped to available VMs arbitrarily
  - Resource utilization determines provisioning
- May execute low-priority tasks even when the workflow they belong to will never finish
  - We assume no pre-emption of tasks

WA-DPDS

DPDS with additional workflow admission test:

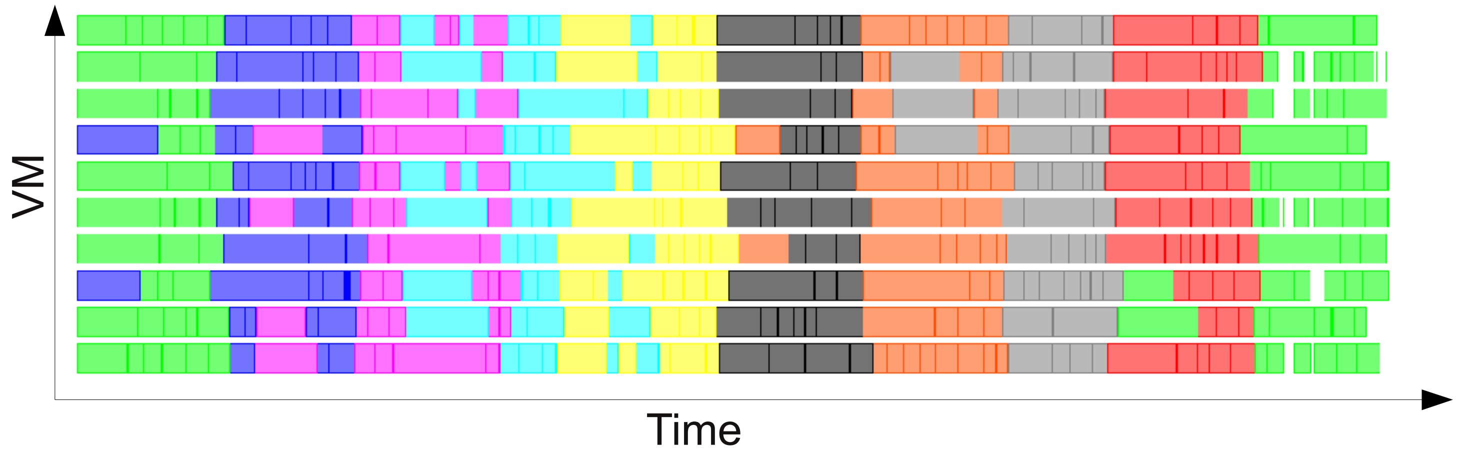
- Each time a workflow starts
- Add up the cost of all the tasks in the workflow
- Determine critical path of workflow
- If there is enough budget: accept workflow
- Otherwise: reject workflow

Other admissions tests are possible

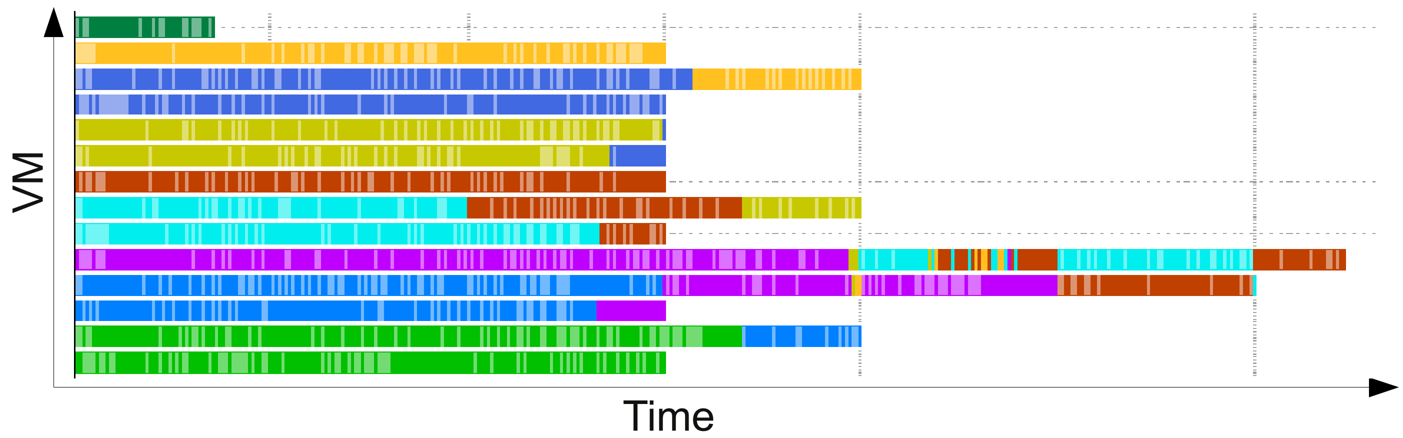
- e.g. Critical path <= time remaining

Dynamic vs. Static
Task execution over time

Dynamic



Static



Evaluation

Simulation

- Enables us to explore a large parameter space
- Simulator uses CloudSim framework

Ensembles

- Use synthetic workflows generated using parameters from real applications
- Randomized using different distributions, priorities

Experiments

- Determine relative performance
- Measure effect of low quality estimates and delays

Ensemble Types

Ensemble size

Number of workflows (50)

Workflow size

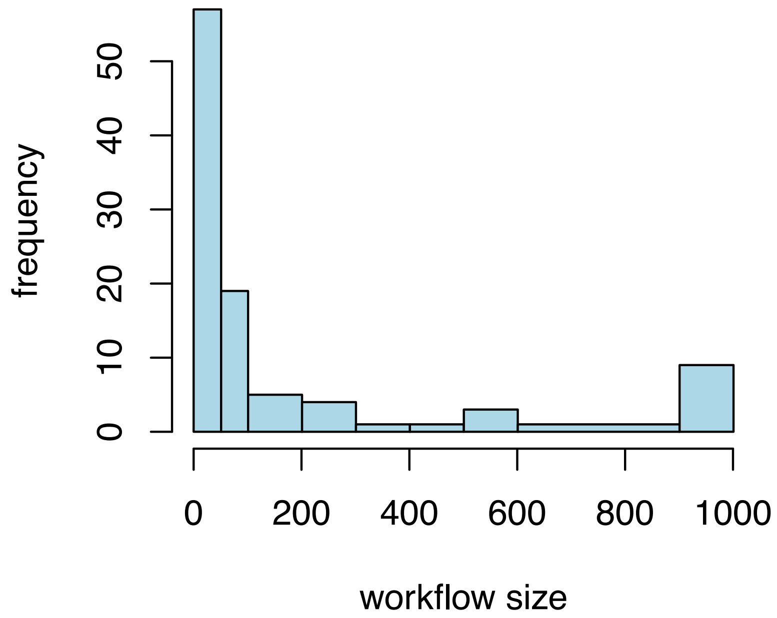
{100, 200, 300, 400,

500, 600, 700, 800, 900, and 1000}

Constant size

Uniform distribution

Pareto distribution



Priorities

Sorted: Priority assigned by size

Unsorted: Priority not correlated with size

Performance Metric

Exponential score:

$$Score(e) = \sum_{w \in Completed(e)} 2^{-Priority(w)}$$

Key: High-priority workflows are more valuable than all lower-priority workflows combined:

$$2^{-p} > \sum_{i = p+1, \ldots} 2^{-i}$$

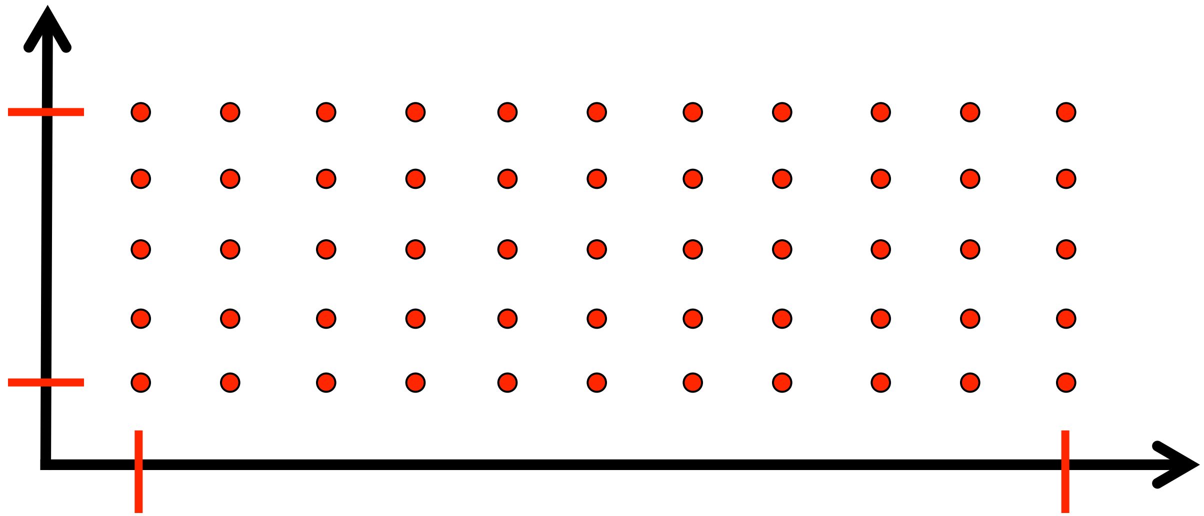
Consistent with problem definition

Budget and Deadline Parameters

Goal: cover space of interesting parameters

$$\left[\min_{w \in e} Cost(w), \sum_{w \in e} Cost(w)\right]$$

$$\left[\min_{w \in e} CriticalPath(w), \sum_{w \in e} CriticalPath(w)\right]$$



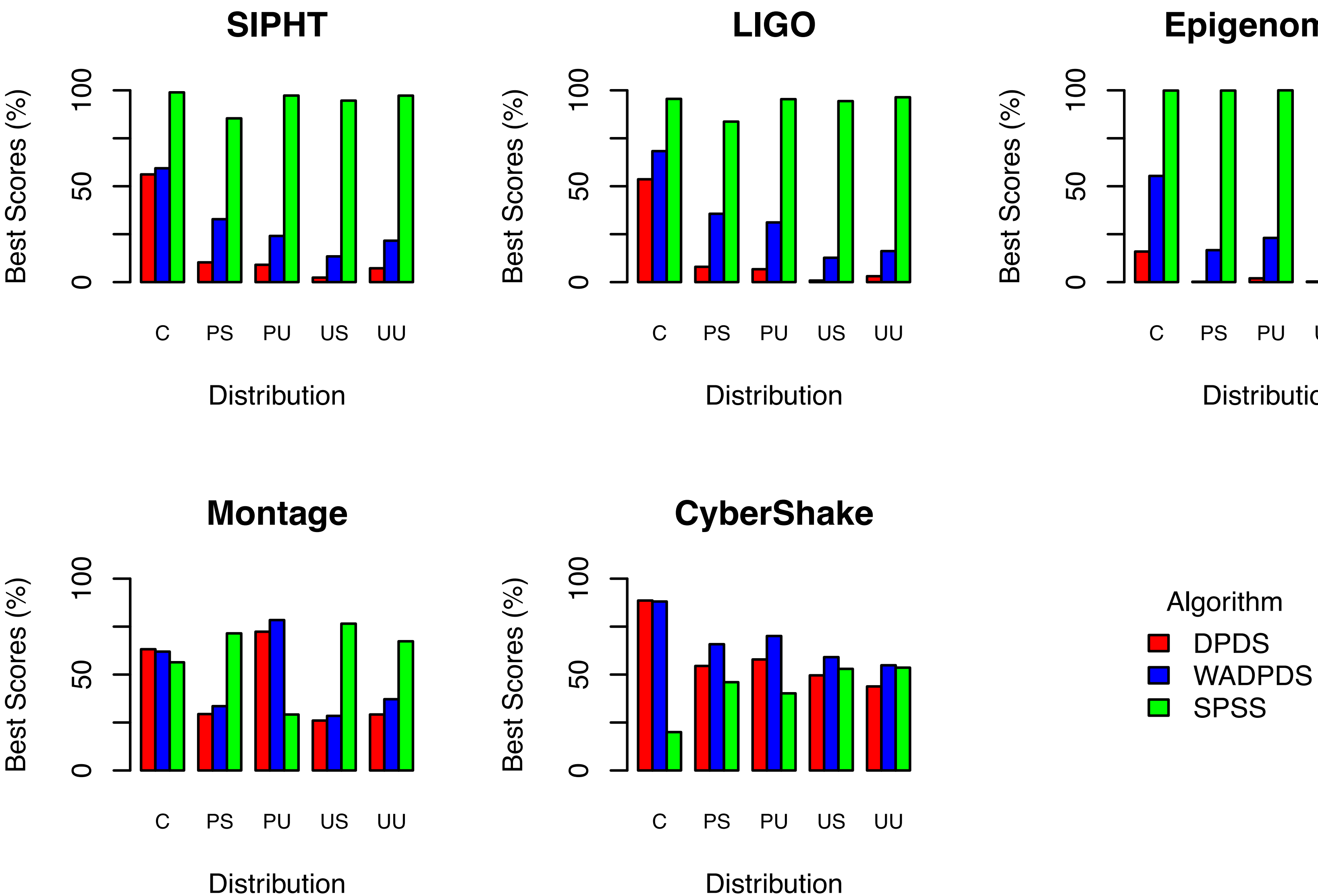
Relative Performance

How do the algorithms perform on different applications and ensemble types?

Experiment:

- Compare relative performance of all 3 algorithms on 5 applications
- 5 applications, 5 ensemble types, 10 random seeds, 10 budgets, 10 deadlines

Goal: Compare % of ensembles for which each algorithm gets the highest score



C = constant, PS = Pareto sorted, PU=Pareto unsorted,
US=uniform sorted, UU=uniform

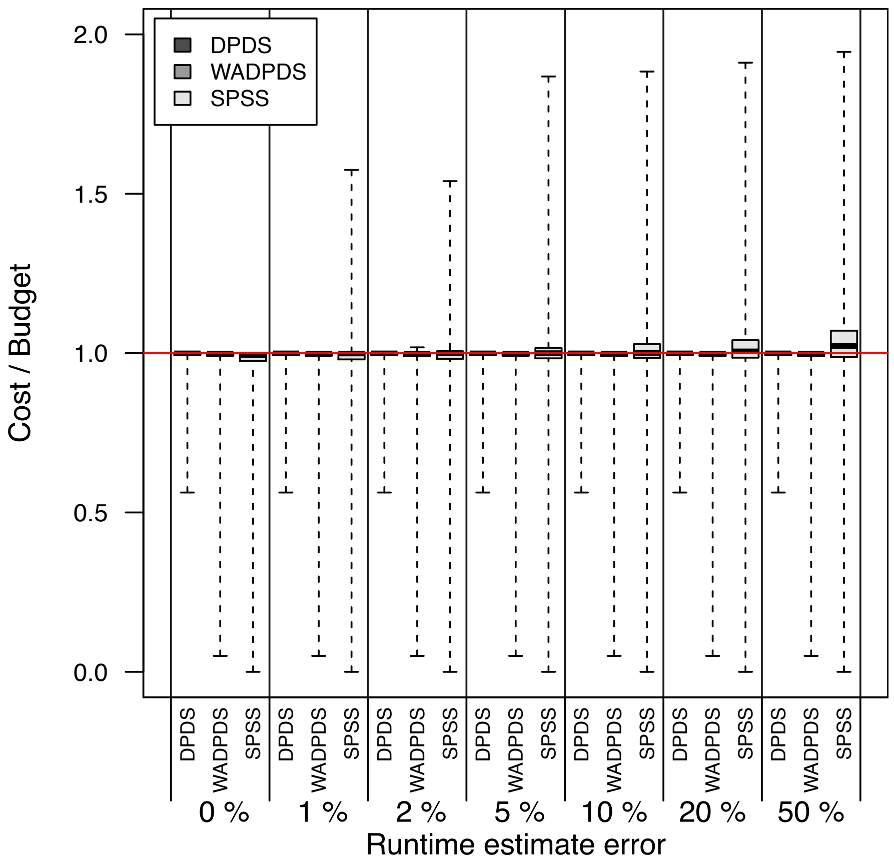
Inaccurate Runtime Estimates

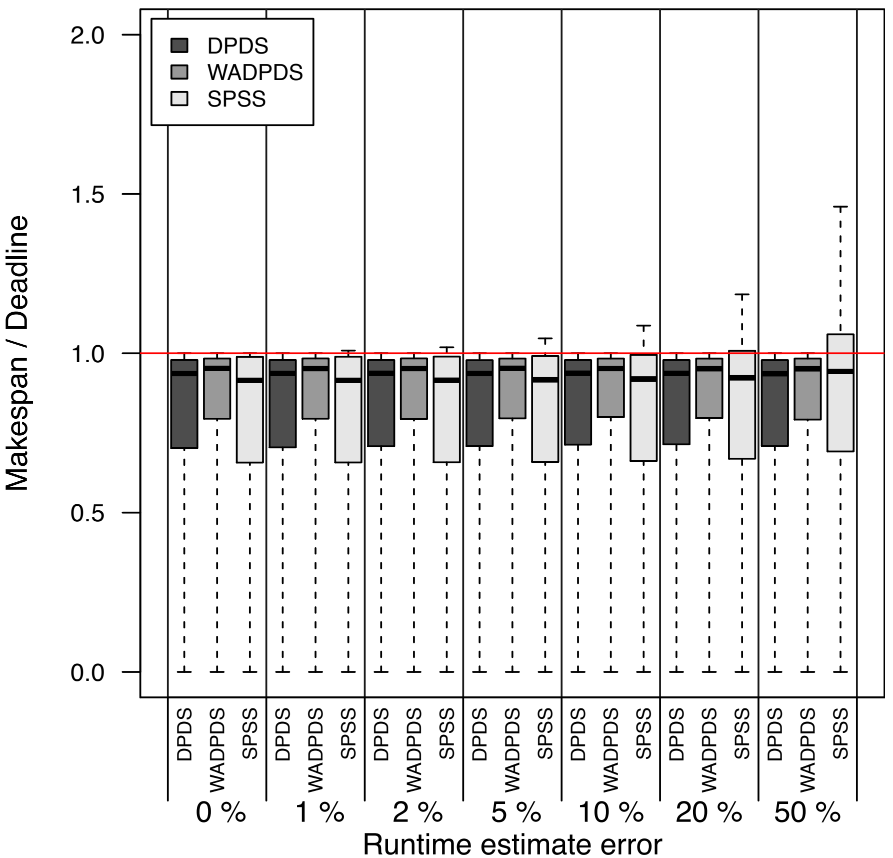
- What happens if the runtime estimates are inaccurate?
- Experiment:
  - Introduce uniform error of ±p% for p from 0 to 50
  - Compare ratios of actual cost/budget and actual makespan/deadline
  - All applications, all distributions, and 10 ensembles, budgets and deadlines each
- **Goal:** See how often each algorithm exceeds budget and deadline

Inaccurate Runtime Estimate Results

Cost / Budget

Makespan / Deadline





Task Failures

Large workflows on distributed systems often have failures

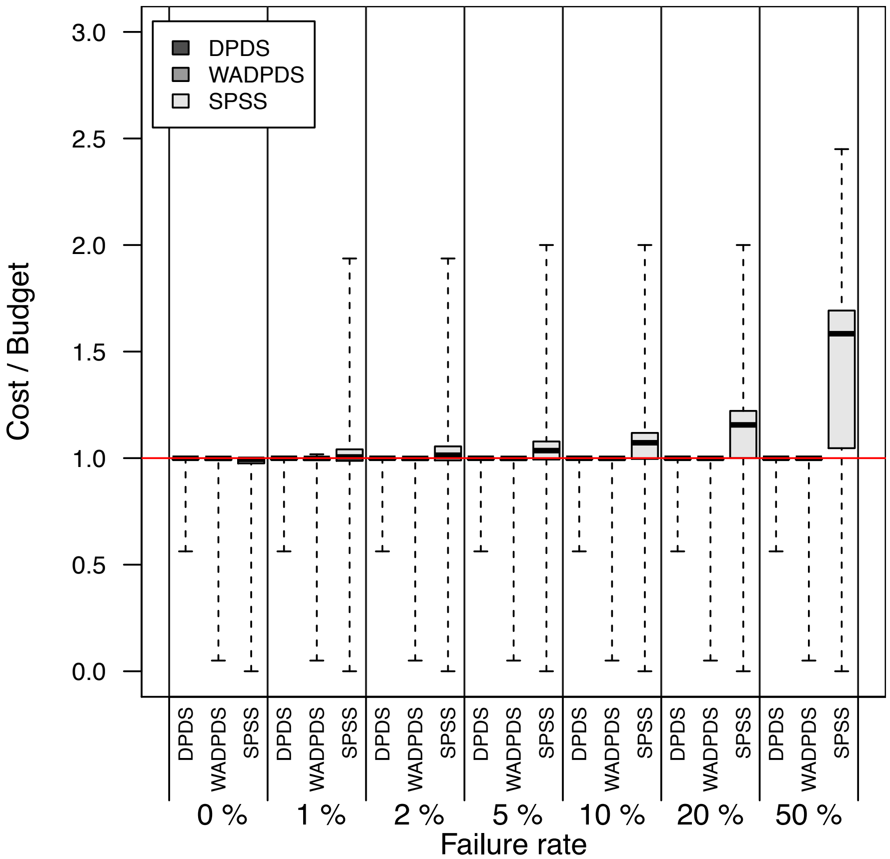
Experiment:

- Introduce a uniform task failure rate between 0% and 50%
- All applications, all distributions, and 10 ensembles, budgets and deadlines

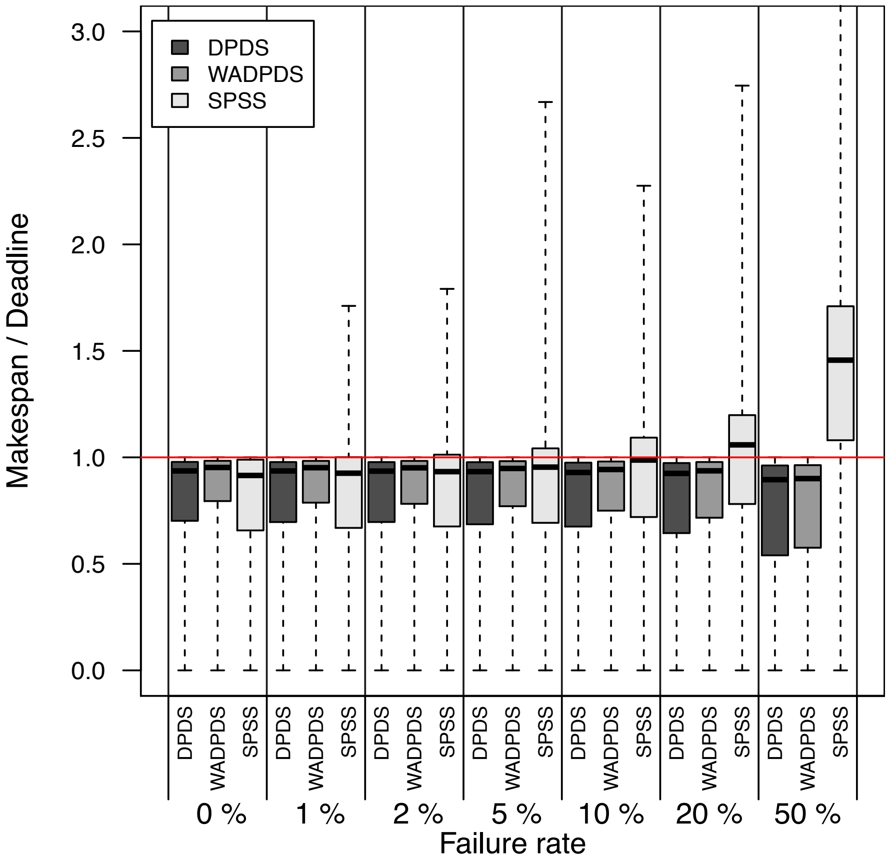
Goal: Determine if high failure rates lead to significant constraint overruns

Task Failure Results

Cost / Budget



Makespan / Deadline



Summary I--observations

- Commercial clouds are usually a reasonable alternative to grids for a number of workflow applications
  - Performance is good
  - Costs are OK for small workflows
  - Data transfer can be costly
  - Storage costs can become high over time
- Clouds require additional configurations to get desired performance
  - In our experiments GlusterFS did well overall
- Need tools to help evaluate costs for entire computational problems (ensembles), not just one workflows
- Need tools to help manage the costs, the applications, and the resources

Summary II—looking into the future

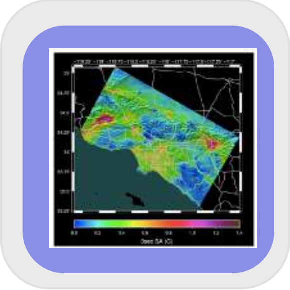
There is a move to hosting more services in the cloud

Hosting science will require

- a number of integrated services
- seamless support for managing resource usage and thus cost and performance
- ease of use---can you do science as an app?

References: **http://pegasus.isi.edu**

Paper on ensembles at SC’12 in Salt Lake City



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