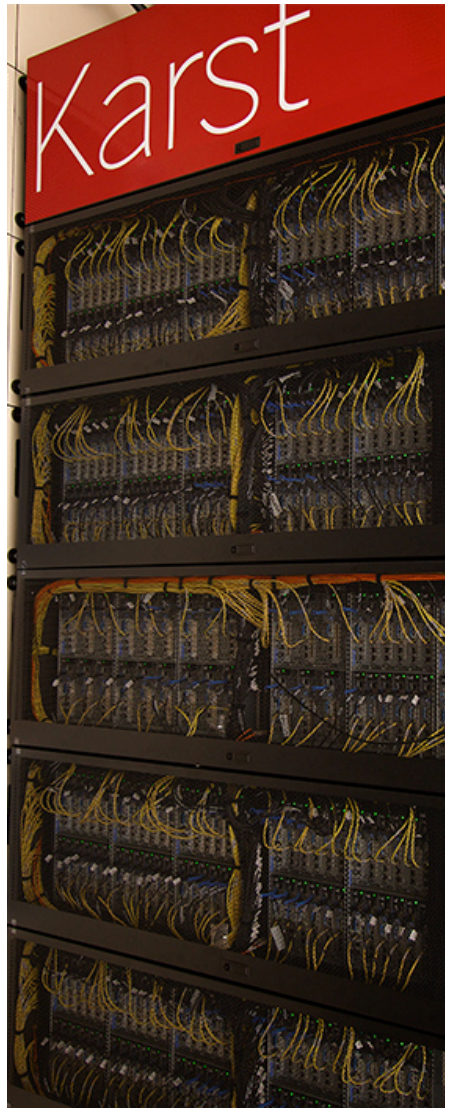
Classic Cluster Scheduling and Queuing

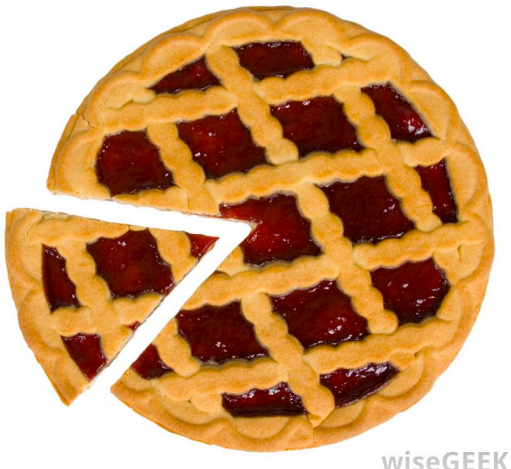
The Karst Cluster at IU

- High-throughput rather than high performance
- Aggregate peak theoretical capability of 91.5 teraflops
- Aggregate RAM of 11 TB.
- Karst consists of 275 nodes total.
  - Red Hat Enterprise Linux 6.x
  - 2 Intel Xeon E5-2650 v2 8-core processors (so 16 cores/node)
  - 32 GB RAM
- 10-gigabit Ethernet interconnect.
- 450 TB of local spinning disk storage.
- See https://kb.iu.edu/d/bezu



Using Karst

- Karst is a resource shared with all other approved users.
- There are many users using part of the system at any given time.
- Problem: how do you get a portion of Karst to run your application?
- Solution: scheduling and resource management.



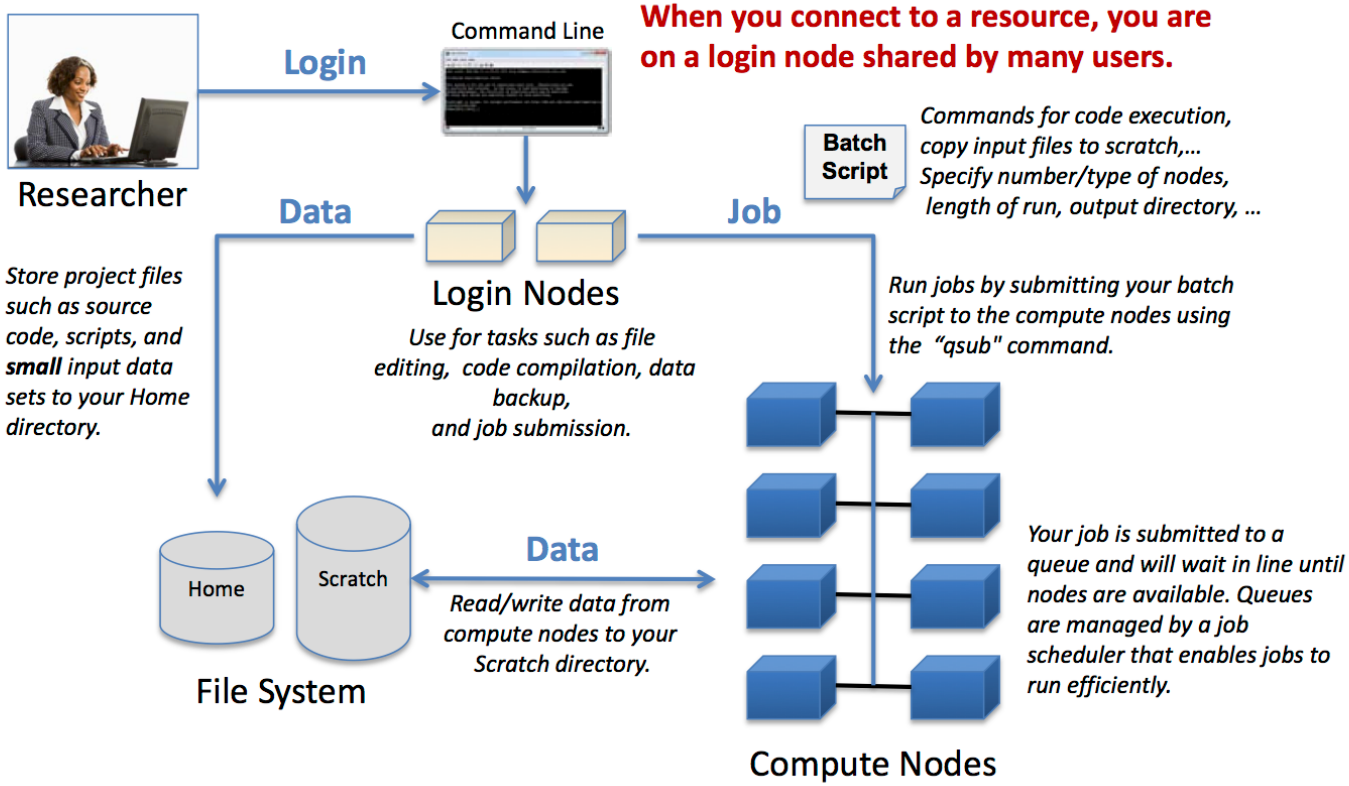
Classic Scheduling and Resource Management

- Scheduling
  - Determines which jobs to run based on resource requests versus availability.
  - Implement policies
    - Fair share: the more you use a resource, the lower your priority.
    - Large versus small requests
    - Important users
    - Reservations
- Resource Management
  - Manages the actual execution of the request on the resource
  - Monitors the health of nodes.
  - Supports fault tolerant execution.
  - Extendable to support different schedulers

A Few Words about Using Karst

https://kb.iu.edu/d/bezu

Running Jobs Overview



https://**bluewaters**.ncsa.illinois.edu/running-your-jobs

Logging In

- You log into Karst with SSH
  - ssh *username*@karst.uits.iu.edu
  - Type your password at the prompt
- karst.uits.iu.edu resolves to 1 of 4 publically accessible head nodes.
  - Most nodes are not reachable directly from outside
- You can and should set up public/private key authentication.
  - See https://kb.iu.edu/d/aews
  - Two-factor authentication: something you have (private key) and something you know (the key's passphrase).

Set Up Your Environment

- Karst administrators maintain many scientific applications, libraries, and tools for compiling codes.
- These can have complicated and conflicting libraries and other dependencies.
- Karst uses the “module” command to help users set up their environments for particular applications.

LAMMPS on Karst: Modules

```
# Run these commands
# Option 1
module load gcc
module load  openmpi/gnu
module load lammps
```

```
#Option 2
module load intel
module load openmpi/intel
module load lammps
```

Create a Job Script

- Job scripts are just scripts but have special directives at the beginning for the scheduler.
  - #PBS for PBS-based schedulers
- Use these directives to specify
  - Number of nodes you want
  - Processors per node
  - Walltime
  - Job name (-N)
  - Notification options (-m)

```
#/bin/bash
#PBS -l nodes=2:ppn=8,walltime=2:30:00
#PBS -m bae
#PBS -N job_myprog

#Move to your working dir
cd $PBS_O_WORKDIR

# Run a parallel job
mpirun -np 16 lmp_openmpi -suffix omp
< in.cmdfile
```

Submit and Monitor Your Job Script

- Submit:
  - qsub ~/work_directory/my_job_script.pbs
- Monitor:
  - qstat -u *username* (Torque)
  - checkjob *job_id* (Moab)
- Get notified by email
  - Use appropriate job script settings
  - Email when jobs begin, end, or abort
- Schedulers/queuers track and log more states than these.
  - Useful to science gateways

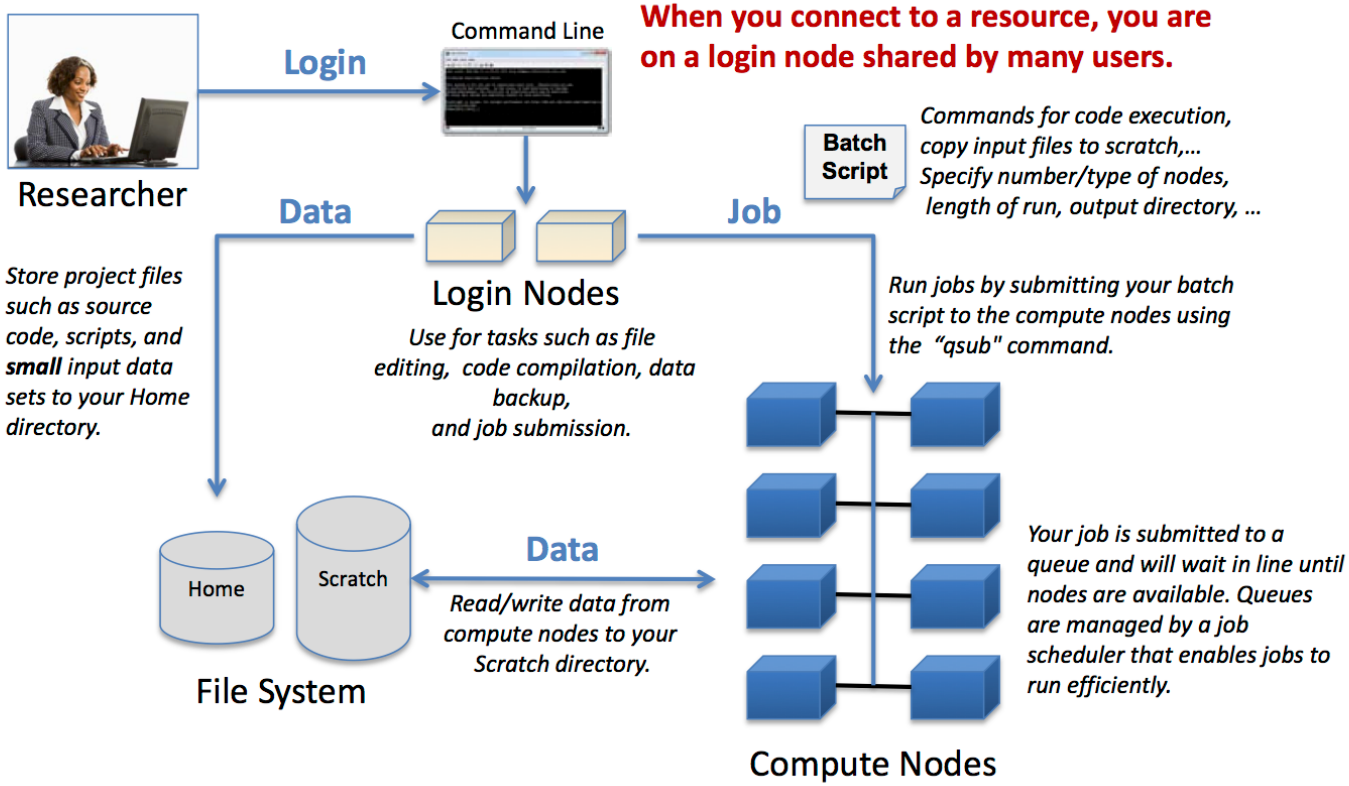
Congratulations!

You've seen now how to run 1 application on 1 cluster at 1 university. There are many applications on many clusters at many universities. Each is its own special snowflake.

Science gateways hide these complexities while enabling more powerful usage.

More on Scheduling and Resource Management

Running Jobs Overview



https://**bluewaters**.ncsa.illinois.edu/running-your-jobs

A Classic Configuration

- A Torque cluster consists of one head node and many compute nodes.
- The head node runs the pbs_server daemon and
- The compute nodes run the pbs_mom daemon.
- The pbs_server process must by high availability.
- The pbs_mom processes can be less so (elastic).

http://docs.adaptivecomputing.com/torque/6-0-0/help.htm

The Job Runs

- Users submit jobs to **pbs_server** using the qsub command.
- The **pbs_server** informs the **scheduler**.
  - Maui, MOAB, FIFO
- When the **scheduler** finds nodes for the job, it sends instructions to run the job with the node list to **pbs_server**.
- Then, **pbs_server** sends the new job to the first node in the node list and instructs it to launch the job.
- This node is designated the execution host and is called ***Mother Superior***.
- Other nodes in a job are called ***sister MOMs***.

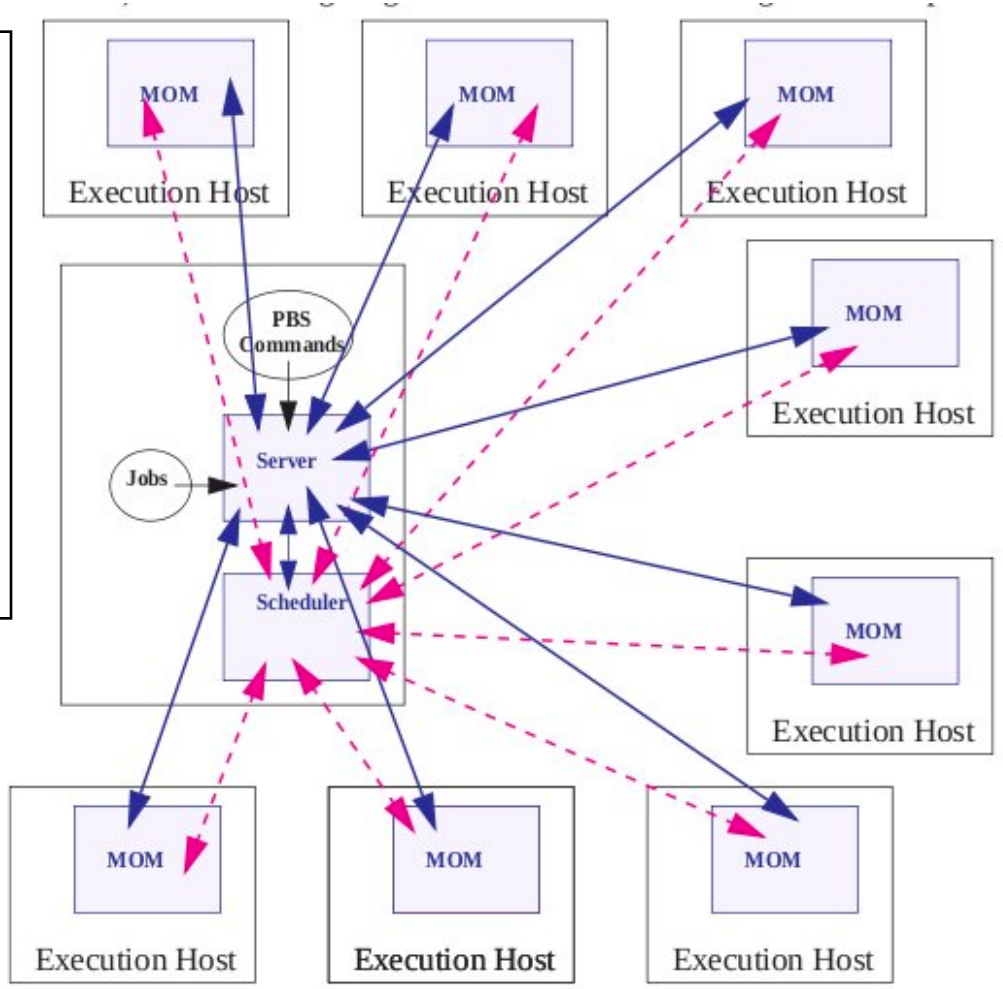
Scheduling

- The head node also runs a scheduler daemon.
- The scheduler interacts with pbs_server to make local policy decisions for resource usage and allocate nodes to jobs.
- A simple FIFO scheduler, and code to construct more advanced schedulers, is provided in the Torque source distribution.
- Most Torque users choose to use a packaged, advanced scheduler such as Maui or Moab.

http://docs.adaptivecomputing.com/torque/6-0-0/help.htm

Basic Torque Cluster Deployment

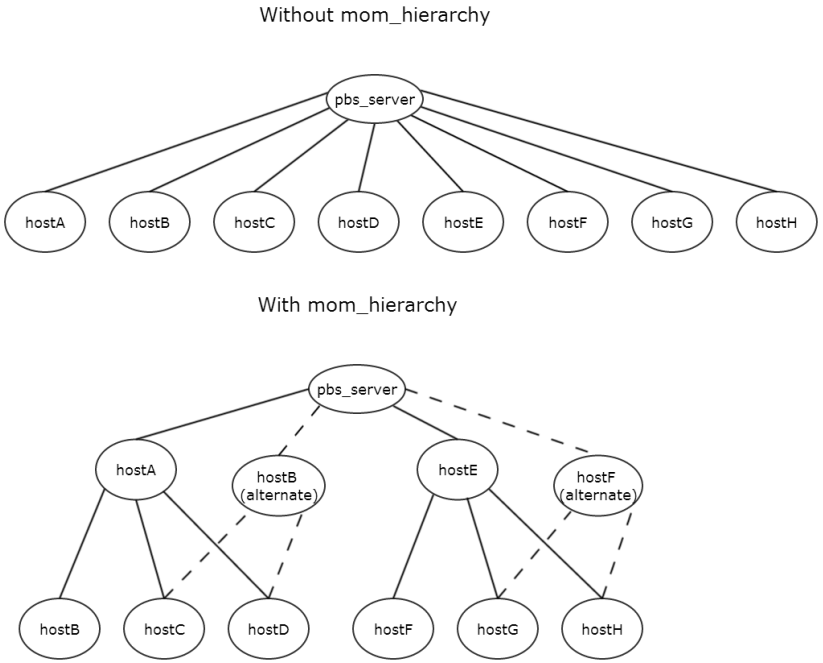
- User submits jobs to server
- Server contacts scheduler
- Scheduler decides when things run.
- Resource managers run applications when told by the scheduler.



What are some problems with this layout?

MOM Hierarchy for Scaling

- Override the compute nodes' default behavior of reporting status updates directly to the pbs_server.
- Each node sends its status update information to another compute node.
- The compute nodes pass the information up a tree or hierarchy until eventually the information reaches a node that will pass the information directly to pbs_server.
- This can significantly reduce network traffic and ease the load on the pbs_server in a large system.



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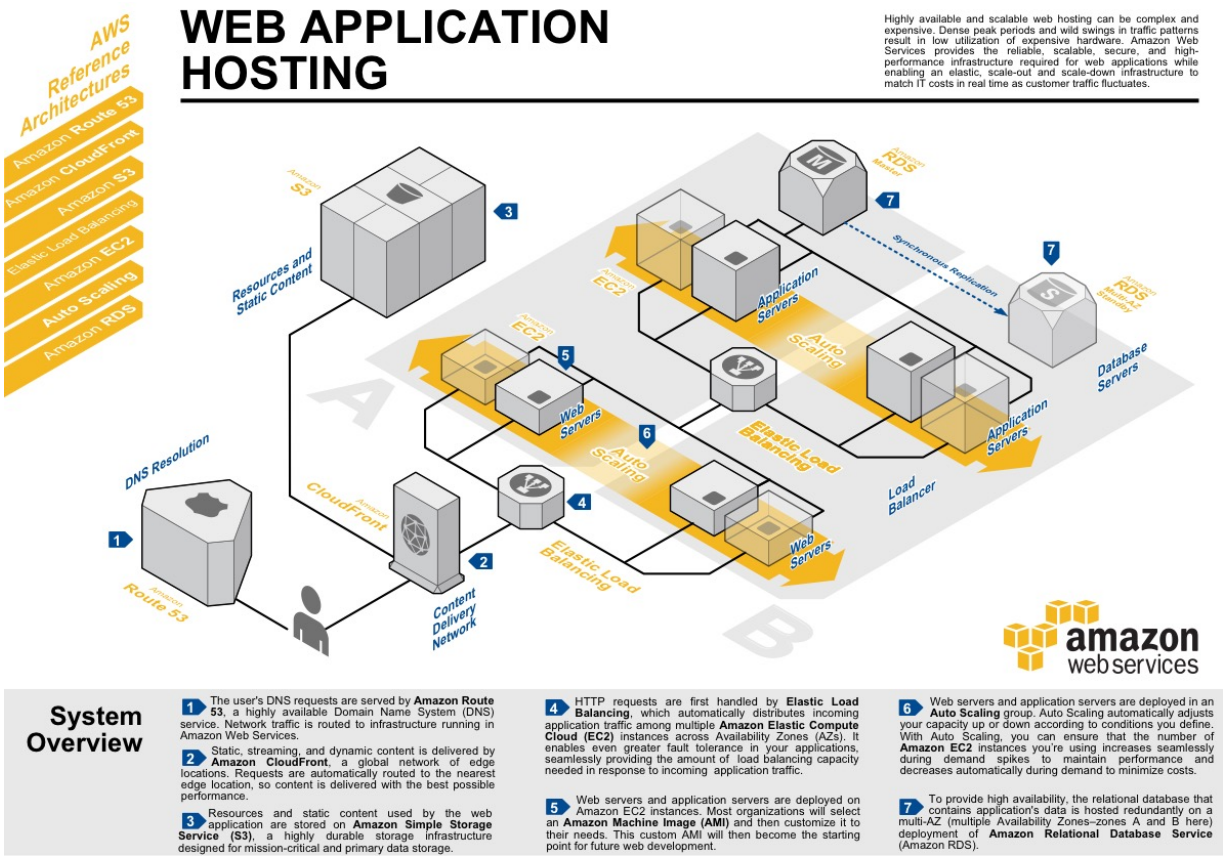
Compare and Contrast

- The manager-worker pattern and its improvements are common in many schedulers.
  - Manager knows the **state**
  - Workers are **stateless**
- Mixture of high availability and fail-able, elastic components.
- Reliable communication needed.
  - But not for everything
- Ephemeral components need to be easily configurable
- These patterns have found their way into other places ->



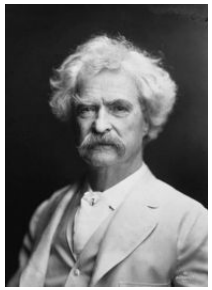
https://aws.amazon.com/architecture

Basic Science Gateway Ideas

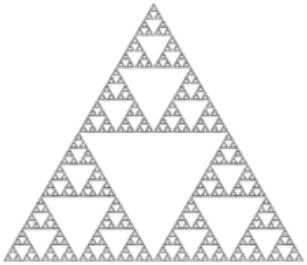
- Hide all those complicated details for submitting and monitor jobs.
- Provide programmatic access to clusters and supercomputers by wrapping command lines, generating scripts, etc
  - Eliminate user errors
- Scale the number of users of scientific applications on clusters.
  - There will always be power users
- Do all of this for multiple applications on multiple resources.
- Provide better user environments

Life Lessons for Gateway Builders

- Every cluster and supercomputer is different
  - Custom built
  - Commodity or custom hardware
- There are multiple scheduling and queuing systems that one can choose.
- Even if two clusters use the same scheduler, the local installation will be different
  - Hardware is different, scheduling policies are different, etc.
- Each application runs in a different way on each machine
  - LAMMPS requires different module recipes on different machines

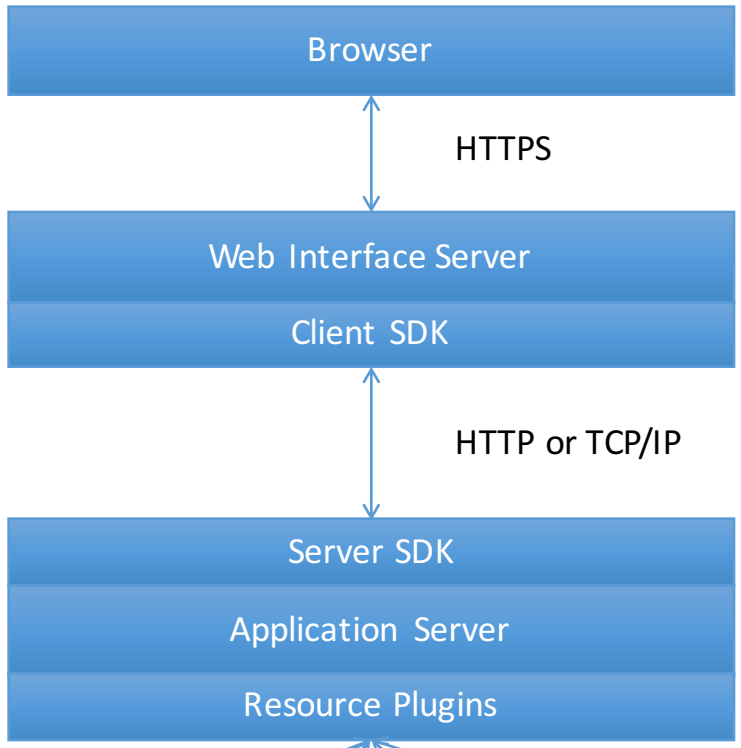


Distributed Computing Rhymes and Fractals



- Schedulers and Resource Managers are sophisticated and powerful software.
  - Scheduling is a classic computer science problem.
  - Provisioning and monitoring resources and running applications at scale is a challenging distributed computing problem.
  - Many task computing, job chaining and other sophisticated execution patterns
    - Who needs Hadoop?
    - But some people also run schedulers inside schedulers: ”Glide-In”, ”Pilot Jobs”
- Gateways operate at a level above but have much to learn and borrow
  - Meta-scheduling
  - Scaling
  - Fault tolerance: what’s high availability and what’s not?
  - Security
  - Messaging
  - State management and recovery

Recall the Gateway Octopus Diagram



In micro-service arch, these also need scheduling

"Super" Scheduling and Resource Management

Different archs, schedulers, admin domains, …