Integrating Containers into Workflows: A Case Study Using Makeflow, Work Queue, and Docker

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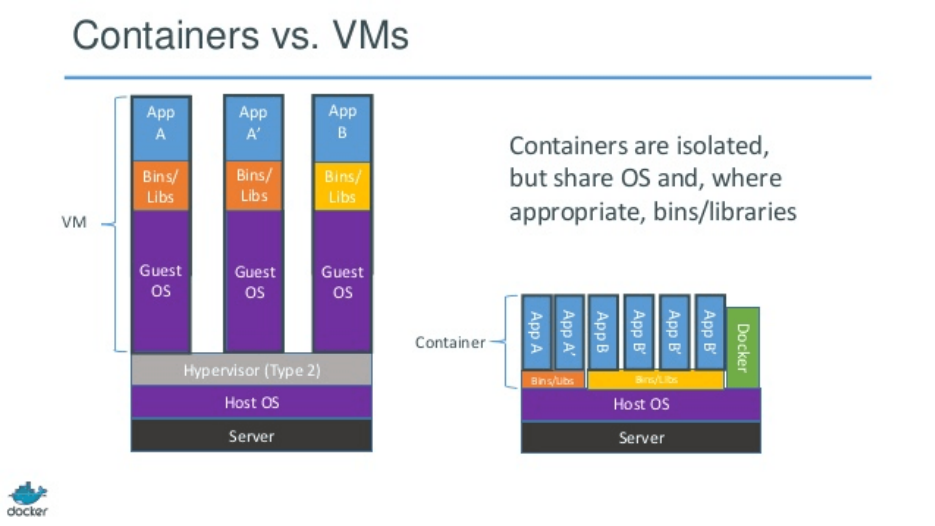
What is a container
and why we want to use it?

- A container is a way of "jailing" an application so that it cannot see other applications.

- Instead of virtualizing hardware, containers rest on top of a single Linux instance, which leaves us with a small, neat capsule containing our application



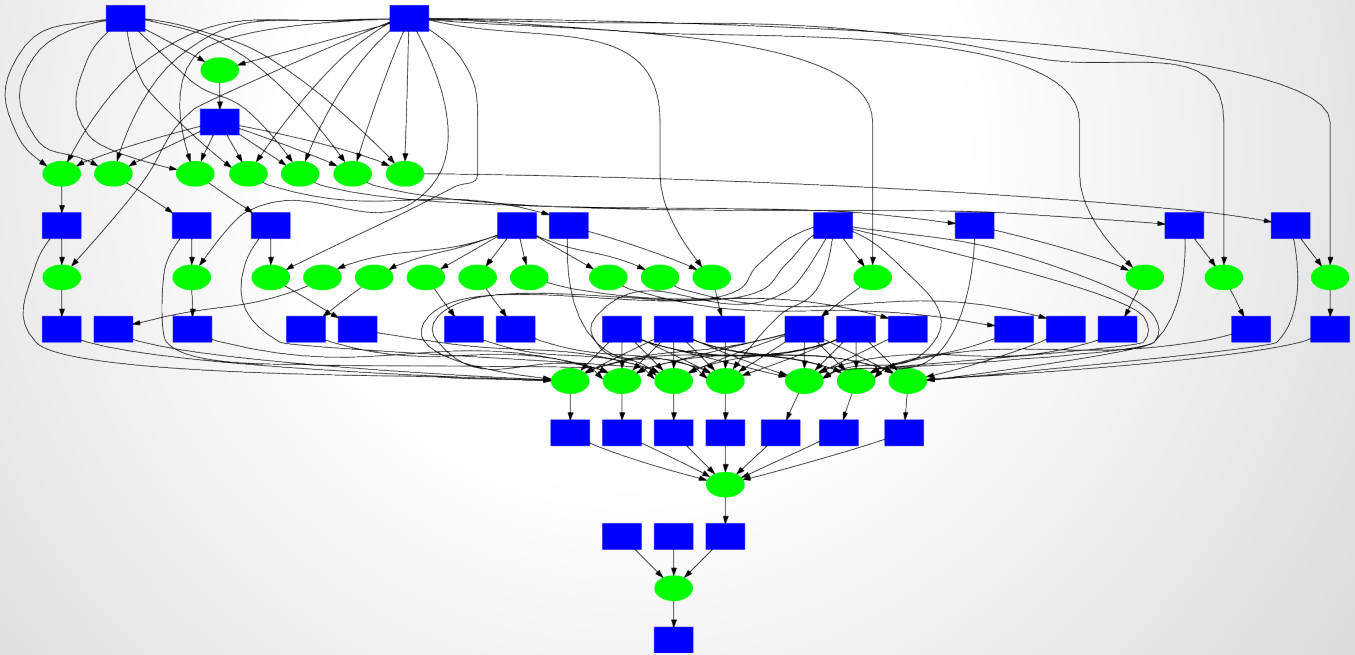
How is it used in the wider world?

- Used as a tooling mechanism to improve resource management, process isolation and security in application virtualization

- Be incorporated into most DevOps applications, including Puppet, Chef and Vagrant

What is workflows?

- A workflow is a form of a workflow management system designed for executing a series of computation and data analysis



What is Makeflow and Work Queue and how they work together?

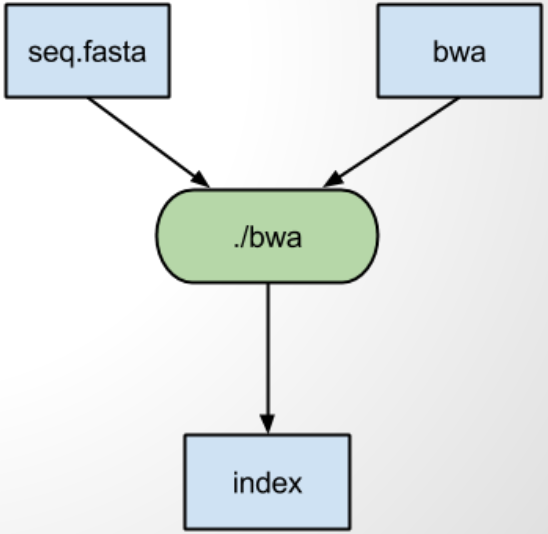
Makeflow

A command line workflow engine using a syntax similar to classic Make

Example:

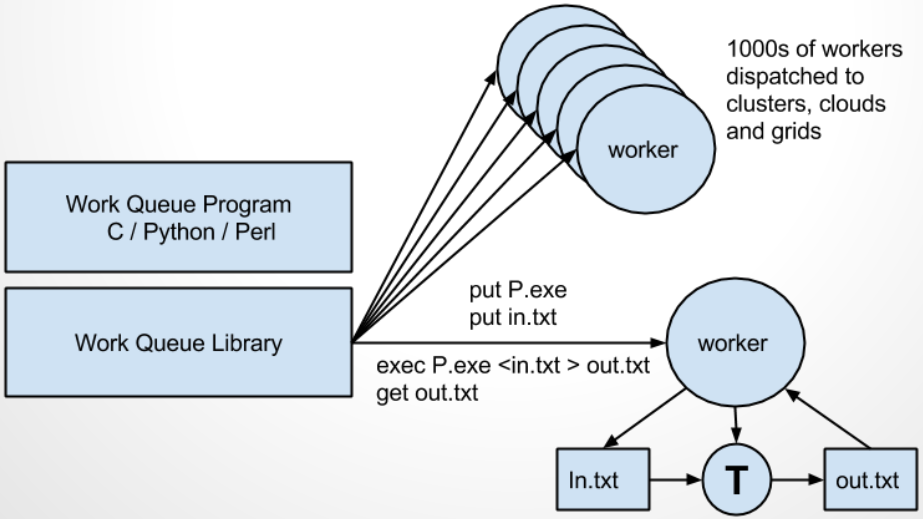
index: seq.fasta bwa

./bwa -index seq.fasta

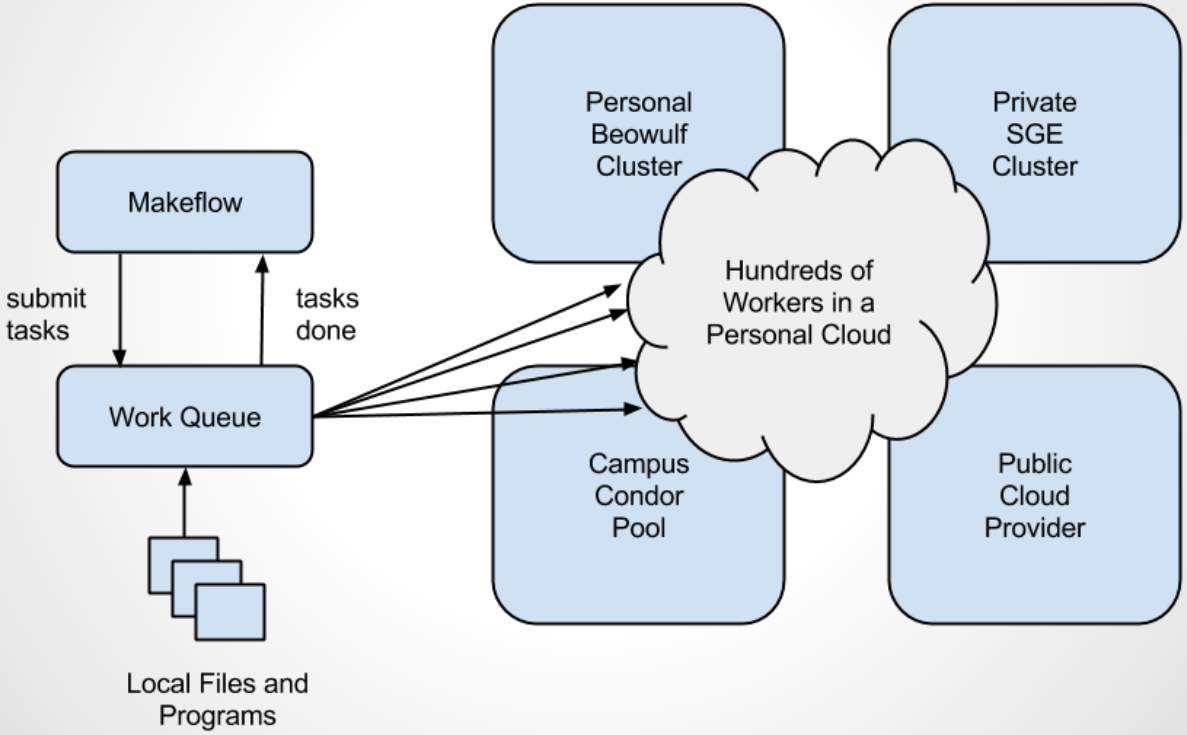


Work Queue

A user-level execution engine, which consists of a master library and many worker processes that deployed across clusters.



Put them together



How to create execution environment for workflow?

- Install desired operating system and applications on all computing nodes
- Create sandbox directories and place all dependencies in the sandbox
- Use virtual machines to define a consistent environment.

The approach we proposed and how we implement it

- Use Lightweight container (Docker) to define the execution environment

- Integrating Docker into different level of Makeflow and Work Queue system

  - Wrapper-script
  - Worker-in-container
  - Container-in-worker
  - Shared-container

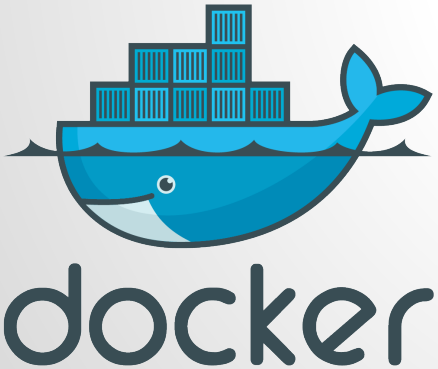
What is Docker and why we chose it?

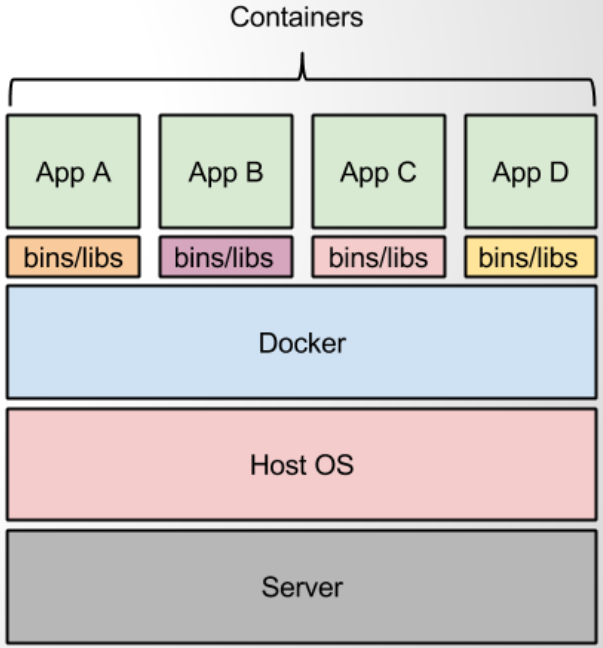
Docker

An operating-system level container technology used for deliver desired execution environment.

Example:

docker run ubuntu bwa -index seq.fasta





- Big user community and well supported
- Global Docker Hub, which is easy to use
- Build once, run anywhere

- New docker related projects
  - Docker Swarm: Turns a pool of Docker hosts into a single, virtual host

    https://docs.docker.com/swarm/
  - Docker Machine: help you easily deploy Docker Engines on cloud providers and in your own data center

    https://docs.docker.com/machine/
  - Docker Compose: help you to define a multi-container application in a single file

    https://docs.docker.com/compose/

The implementation details of four different ways to manage containers

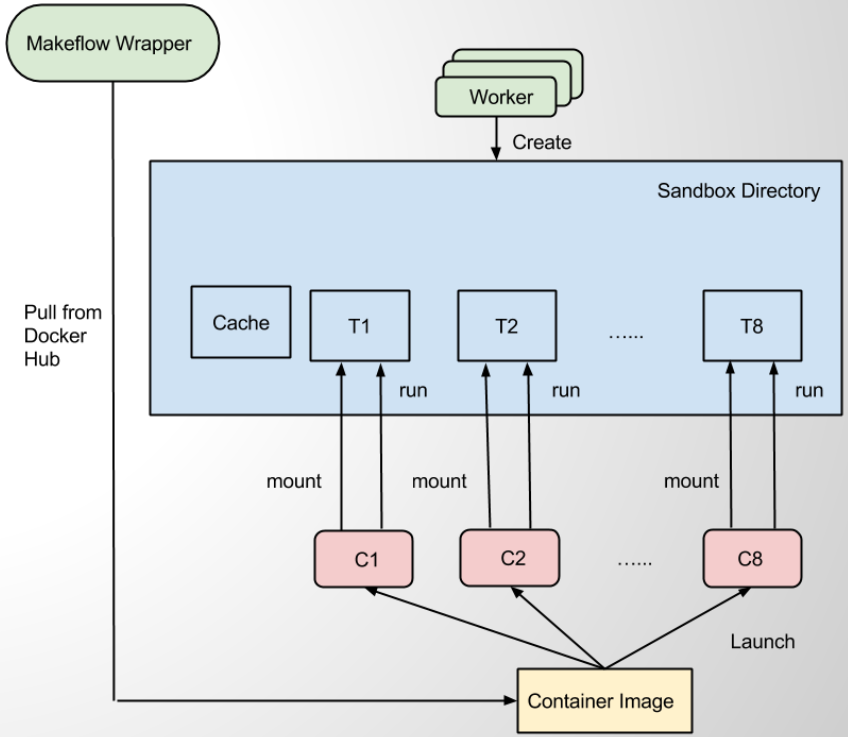
Wrapper-script

Wrapping each task at the workflow level

Example:

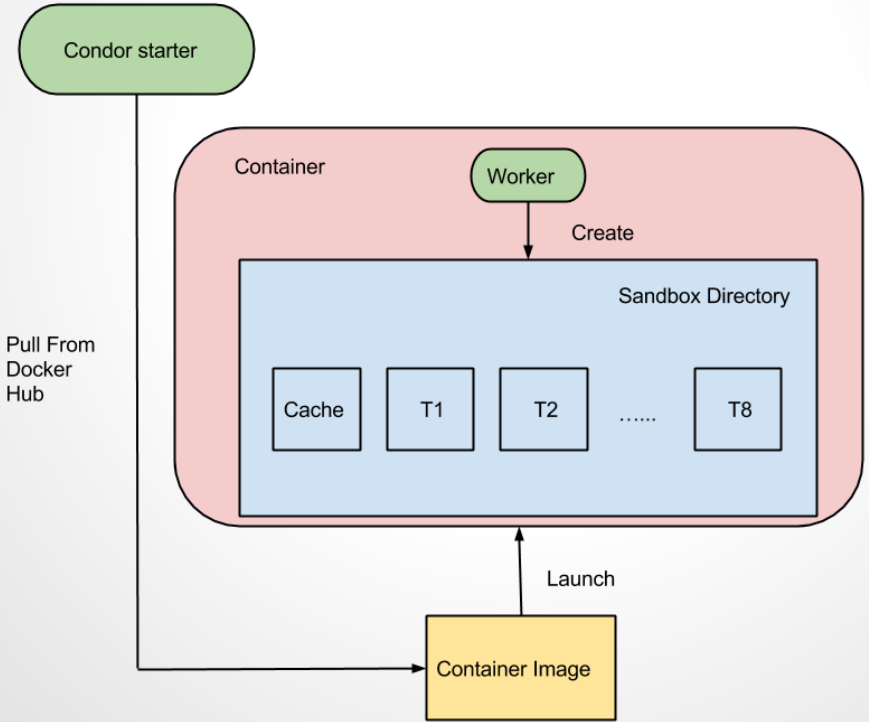
makeflow --docker ccl/debian_cctools

makeflow --docker ccl/debian_cctools
--docker-tar debian_cctools.tar



Worker-in-container

Running each worker inside a container



Container-in-worker

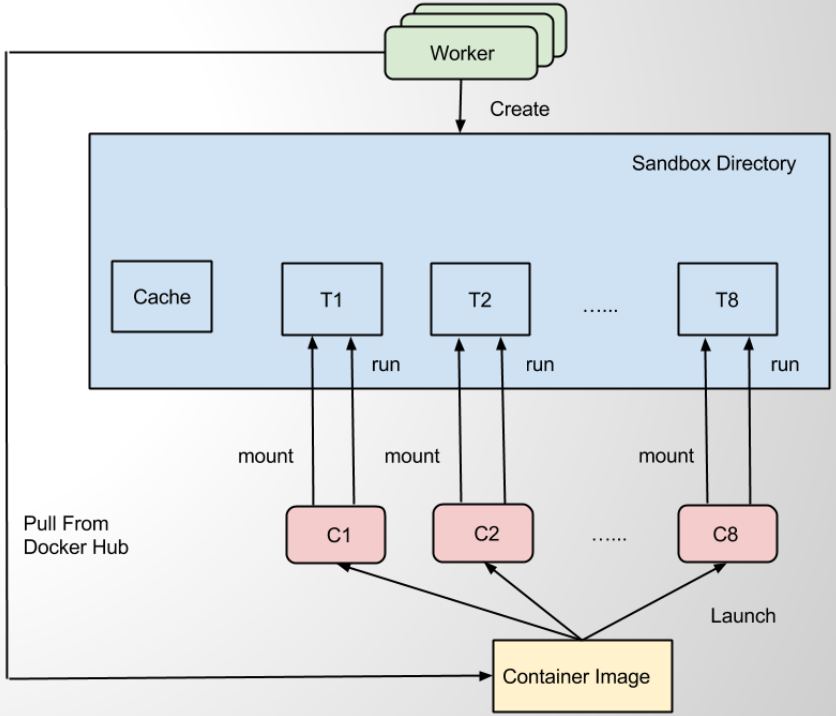
Running each task inside a container

Example:

work_queue_worker

--docker ccl/debian_cctools

localhost 9123



Shared-container

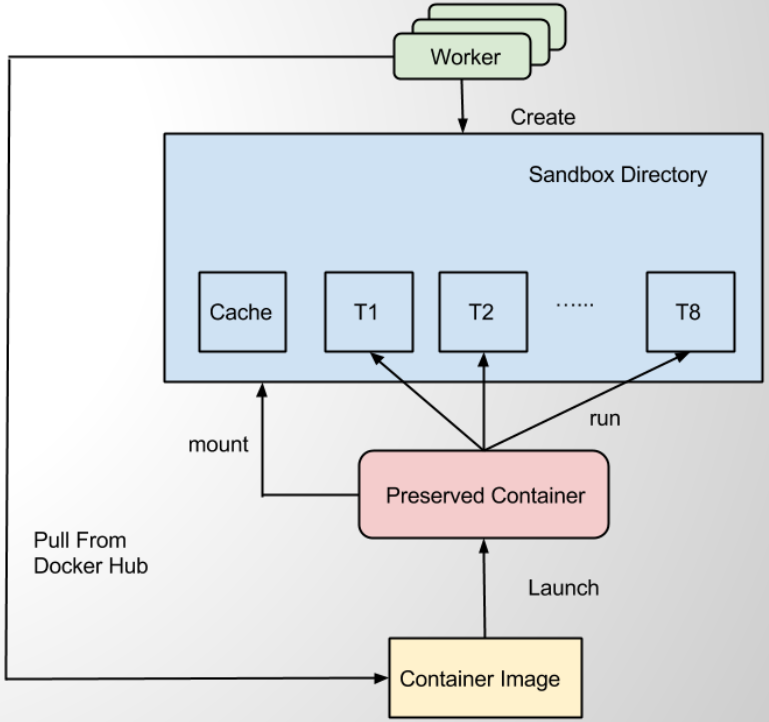
Running multiple compatible tasks inside one container

Example:

work_queue_worker

--docker-preserve ccl/debian_cctools

localhost 9123



Three different ways to manage container images

- **Dockerfile:** Describes the entire procedure of building an image.

- **Tarball:** Encoding and saving a binary image into a tarball and later loading the image from the tarball.

- **Image registry:** Global container image repository, which can be used to store container images.

- **The desired approach:**
  - Workflow manager build image on the submit machine
  - Exported the generated image as a tarball
  - Included it as an input dependency for each task
  - Distribute the tarball across all computing nodes

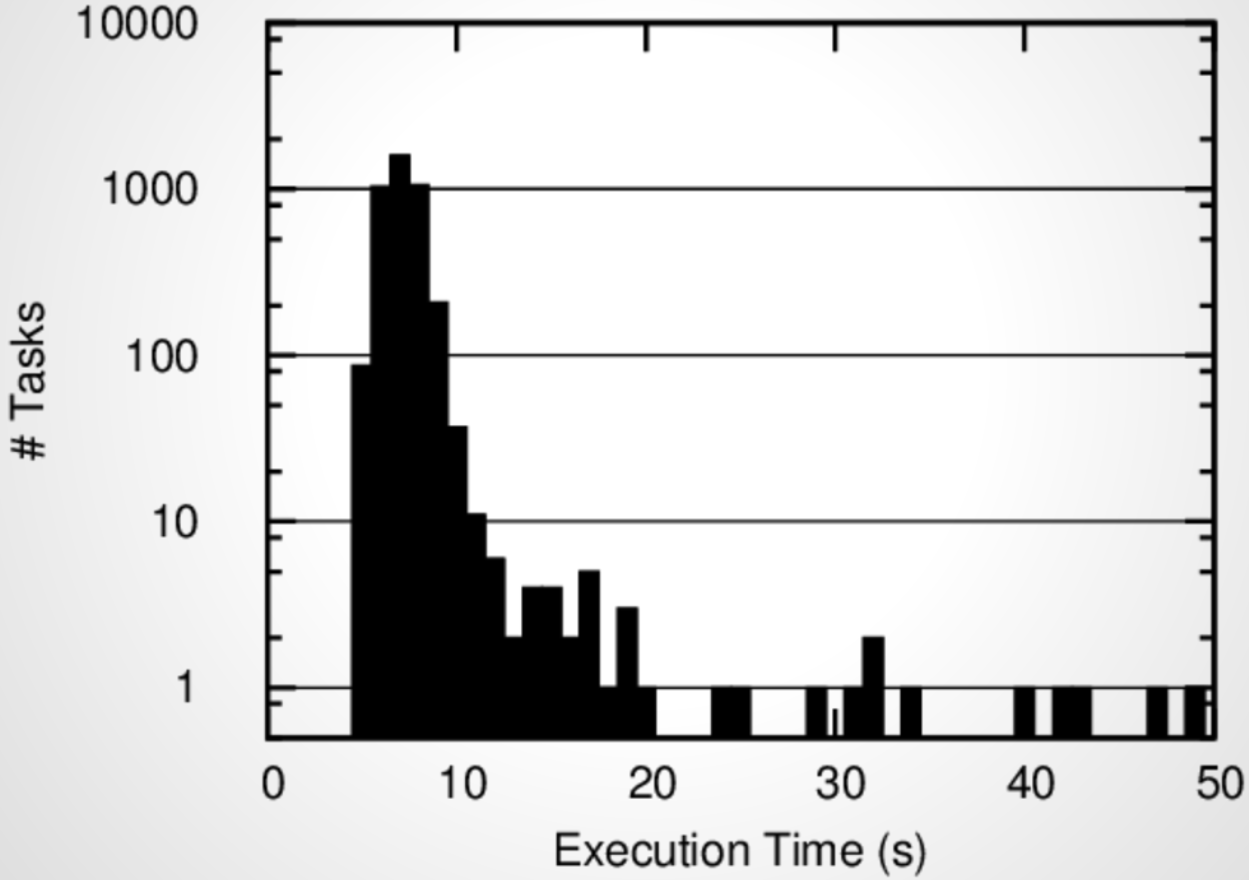
How we evaluate the performance

- **Hardware we used:** Notre Dame Data intensive science cluster(DISC), which consisted of 24 8-core Intel Xeon E5620 CPUs each with 32 GB RAM, 12 2TB disks, 1Gb Ethernet, running Red Hat Enterprise Linux 6.5.

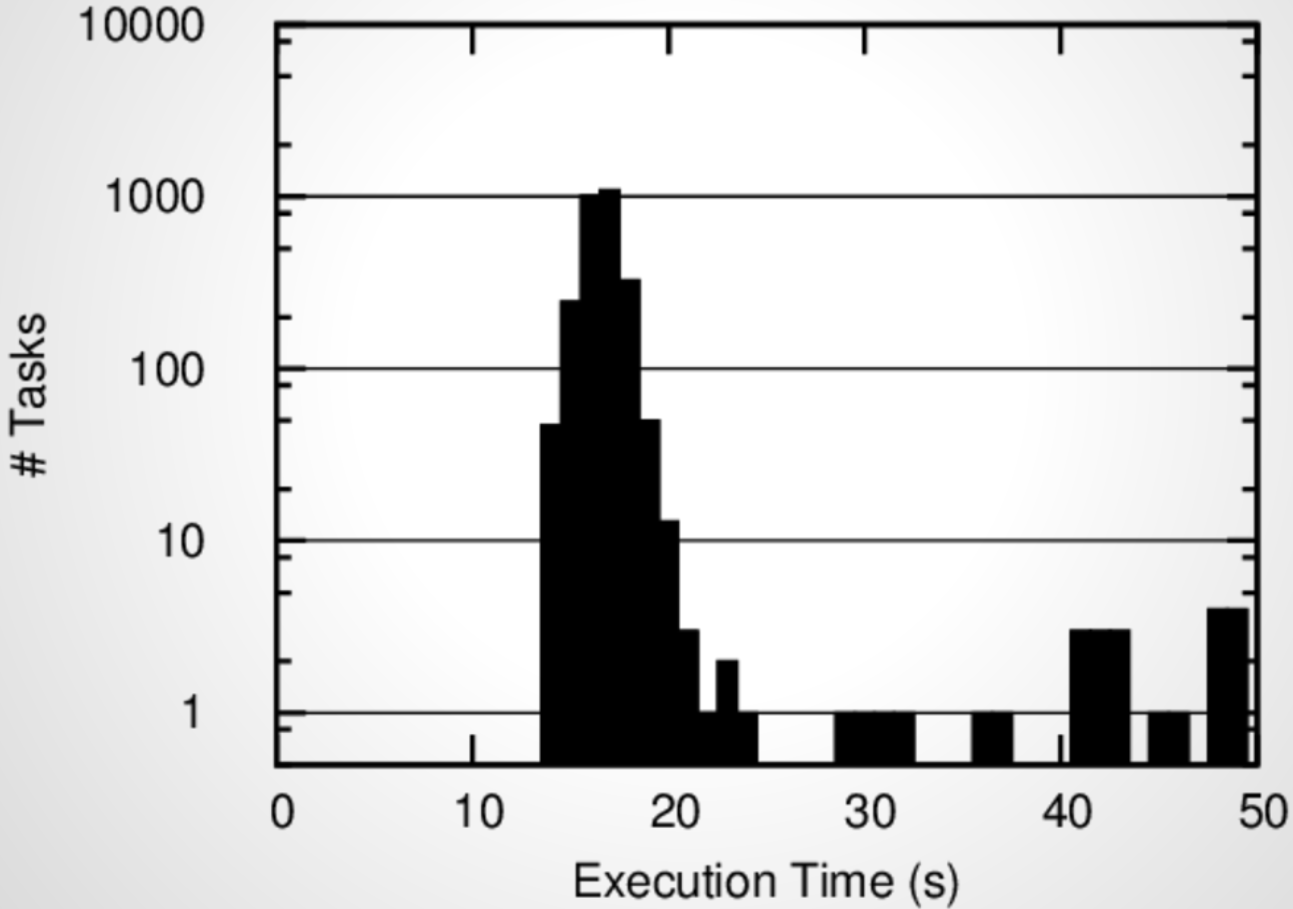
- **Experimental workload**: Burrows-Wheeler Alignment (BWA) bioinformatics workflow, which has 4082 short-running tasks.

The evaluation result we got

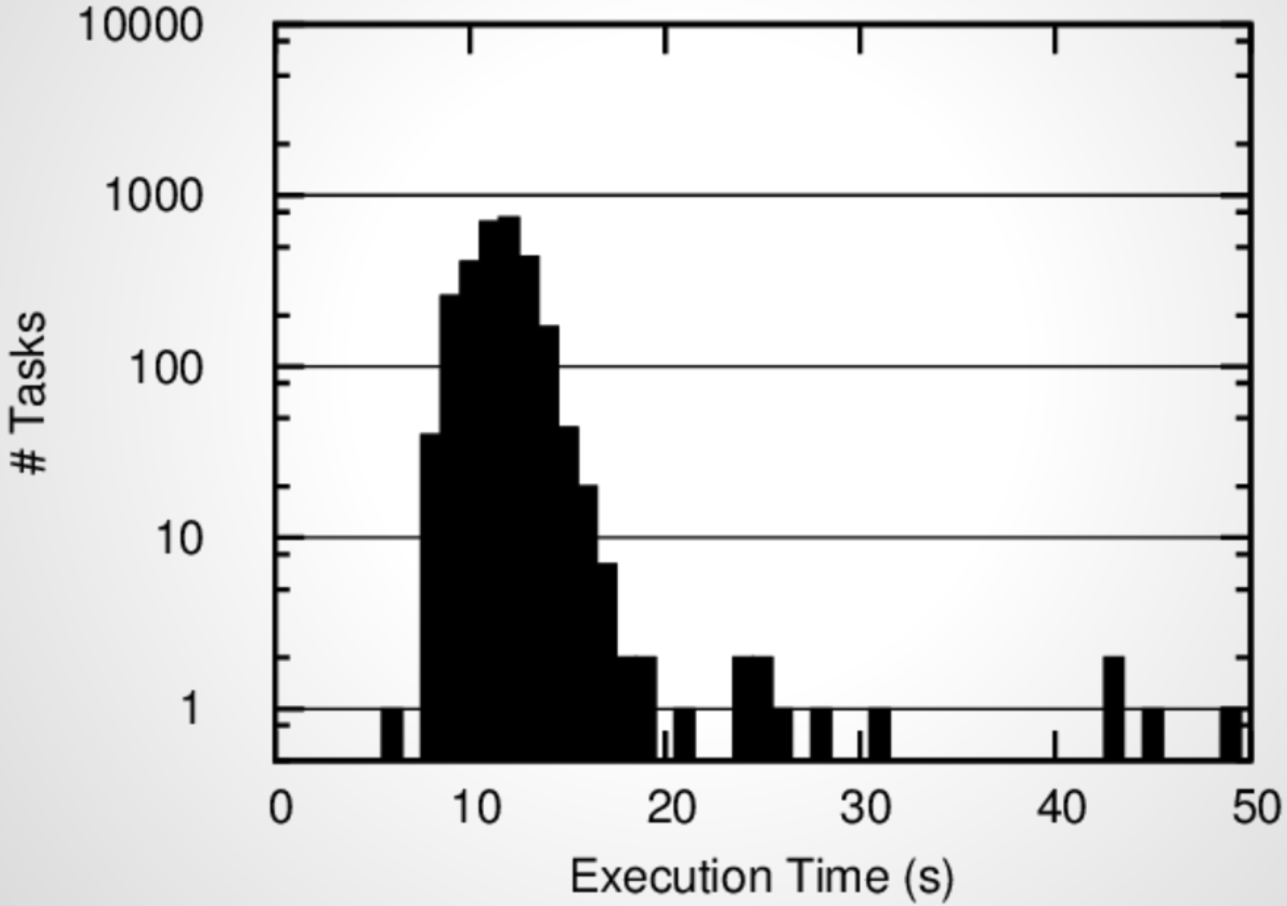
Base architecture



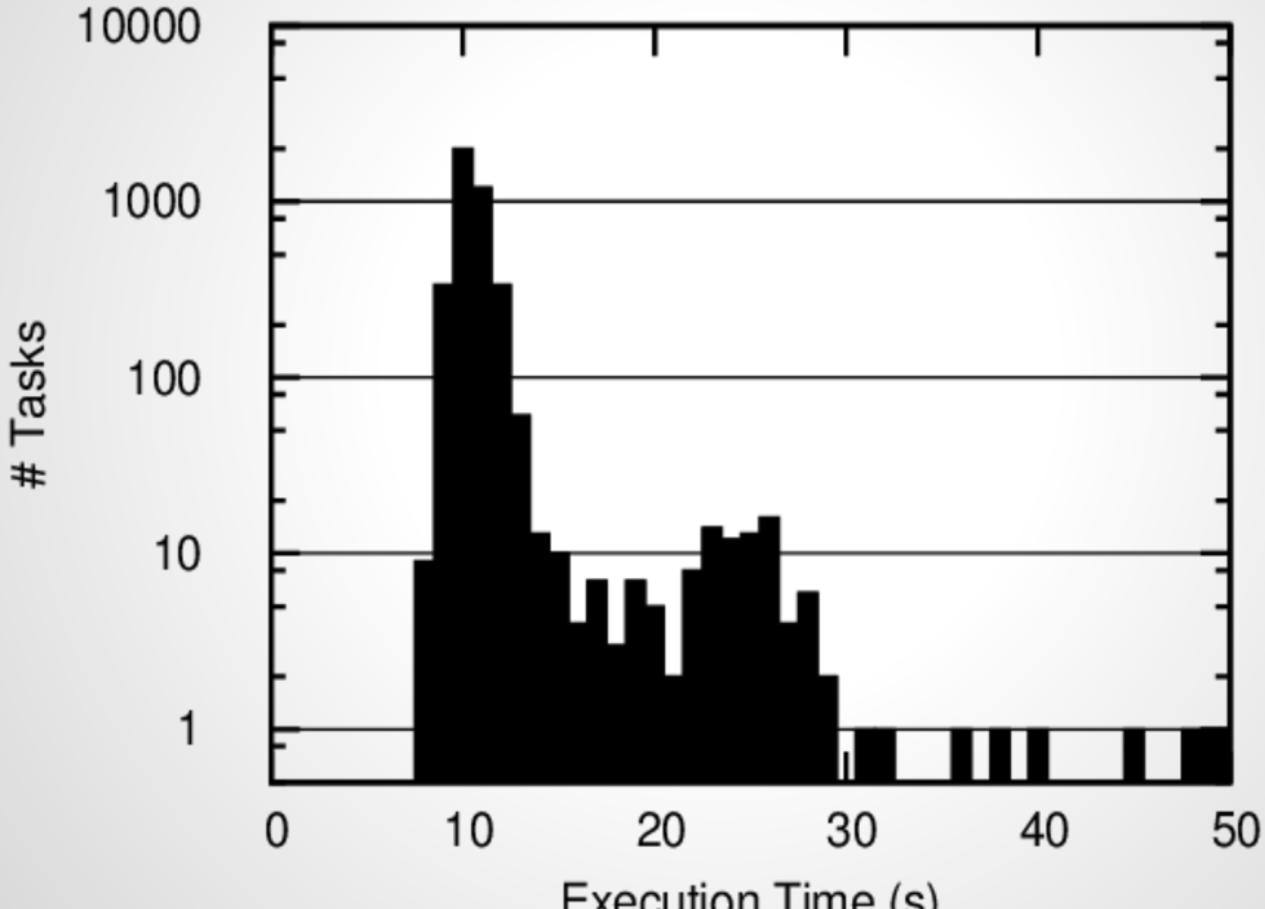
Wrapper-script



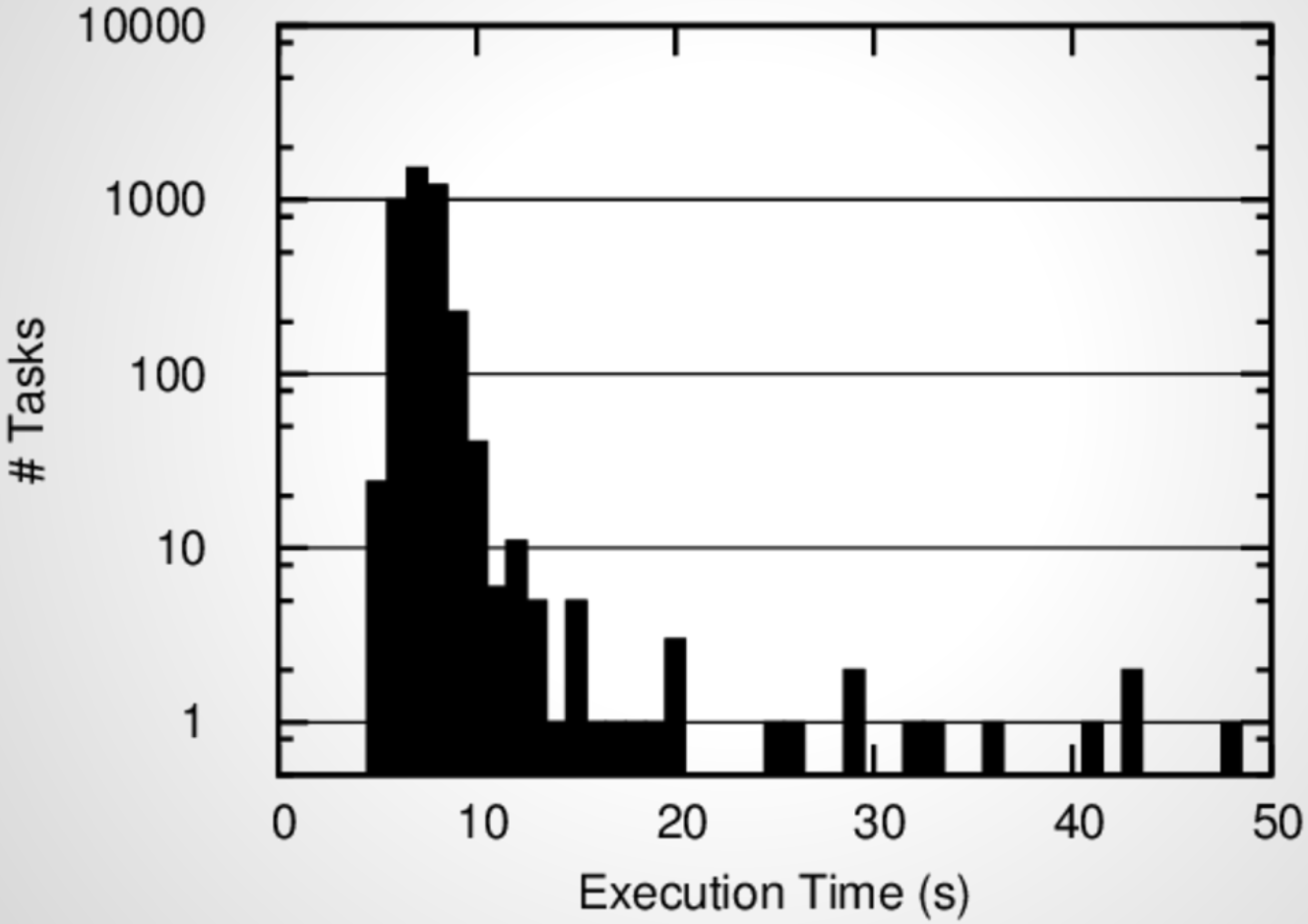
Worker-in-container



Container-in-worker



Shared-container



What we have learned

- There are tradeoffs between performance, isolation and consistency.
  - If most of tasks in the workflow require same execution environment, the Shared-container configuration should be chosen
  - If isolation is required across tasks, the Container-in-worker configuration should be chosen

- The management of containers is better done by distributed system rather than user
  - If we are using both Makeflow and Work Queue, Work Queue should be adopted to manage containers.

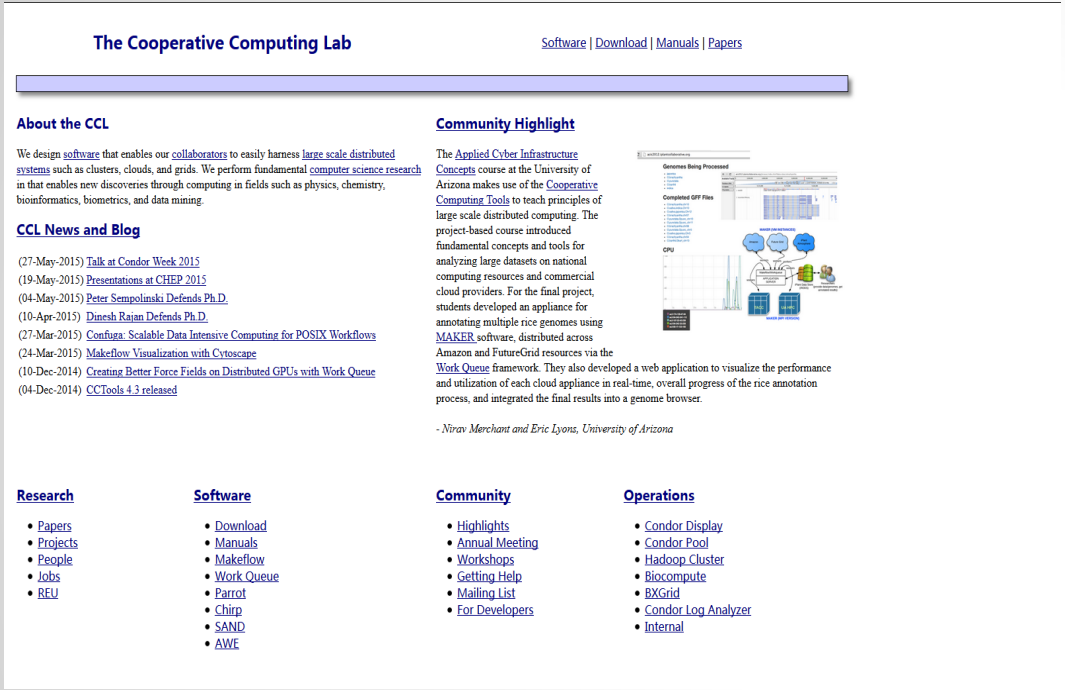
Further thing remain to be done

- Develop an advanced container management mechanism, which aims to control the number of private and shared containers.

- Integrate other container runtime into the Makeflow and Work Queue system, like Rocket.

Where can you get the software

Lab link: http://ccl.cse.nd.edu/



The Cooperative Computing Lab

Software | Download | Manuals | Papers

About the CCL

We design software that enables our collaborators to easily harness large scale distributed systems such as clusters, clouds, and grids. We perform fundamental computer science research in that enables new discoveries through computing in fields such as physics, chemistry, bioinformatics, biometrics, and data mining.

CCL News and Blog

(27-May-2015) Talk at Condor Week 2015
(19-May-2015) Presentations at CHEP 2015
(04-May-2015) Peter Sempolinski Defends Ph.D.
(10-Apr-2015) Dinesh Rajan Defends Ph.D.
(27-Mar-2015) Confuga: Scalable Data Intensive Computing for POSIX Workflows
(24-Mar-2015) Makeflow Visualization with Cytoscape
(10-Dec-2014) Creating Better Force Fields on Distributed GPUs with Work Queue
(04-Dec-2014) CCTools 4.3 released

Community Highlight

The Applied Cyber Infrastructure Concepts course at the University of Arizona makes use of the Cooperative Computing Tools to teach principles of large scale distributed computing. The project-based course introduced fundamental concepts and tools for analyzing large datasets on national computing resources and commercial cloud providers. For the final project, students developed an appliance for annotating multiple rice genomes using MAKER software, distributed across Amazon and FutureGrid resources via the Work Queue framework. They also developed a web application to visualize the performance and utilization of each cloud appliance in real-time, overall progress of the rice annotation process, and integrated the final results into a genome browser.

- Nirav Merchant and Eric Lyons, University of Arizona

Research

- Papers
- Projects
- People
- Jobs
- REU

Software

- Download
- Manuals
- Makeflow
- Work Queue
- Parrot
- Chirp
- SAND
- AWE

Community

- Highlights
- Annual Meeting
- Workshops
- Getting Help
- Mailing List
- For Developers

Operations

- Condor Display
- Condor Pool
- Hadoop Cluster
- Biocompute
- BXGrid
- Condor Log Analyzer
- Internal

Cooperative Computing Tools(cctools) contains: Parrot, Chirp, Makeflow, Work Queue, SAND and other software.

Stable version, 4.4.2

Release version, 4.5.0

- Download a source package from the download page. And

  gnuzip cctools-4.4.2-source.tar.gz

  tar xvf cctools-4.4.2-source.tar

  cd cctools-4.4.2-source

  ./configure

  make

  make install

  export PATH=${HOME}/cctools/bin:$PATH

- Go to the makeflow working directory and run

  makeflow example.makeflow

Contact us

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