Introduction to Makeflow and Work Queue

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Go to http://ccl.cse.nd.edu and Click on ACIC Tutorial

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 that enables new discoveries through computing in fields such as physics, chemistry, bioinformatics, biometrics, and data mining.

CCL News and Blog

- Automatic job sizing for maximum throughput (26 Oct 2017)
- Makeflow Feature: IX Representation (18 Oct 2017)
- Announcement: CCTools 6.2.0 released (09 Oct 2017)
- 2017 DISC Summer REU Conclusion (30 Aug 2017)
- Announcement: CCTools 6.1.6 released (29 Aug 2017)
- Talk at ScienceCloud Workshop (27 Jun 2017)
- Congratulations to Ph.D. Graduates (22 May 2017)
- Announcement: CCTools 6.1.0 released (17 May 2017)
- Makeflow and Mesos Paper at CCGrid 2017 (05 May 2017)
- More news

Community Highlight

Lifemapper is a high-throughput, webservice-based, single- and multi-species modeling and analysis system designed at the Biodiversity Institute and Natural History Museum, University of Kansas. Lifemapper was created to compute and web publish, species distribution models using available online species occurrence data. Using the Lifemapper platform, known species localities georeferenced from museum specimens are combined with climate models to predict a species’ " niches" or potential habitat availability, under current day and future climate change scenarios. By assembling large numbers of known or predicted species distributions, along with phylogenetic and biogeographic data, Lifemapper can analyze biodiversity, species communities, and evolutionary influences at the landscape level.

Lifemapper has had difficulty scaling recently as our projects and analyses are growing exponentially. For a large proof-of-concept project we deployed on the XSEDE resource Stampede at TACC, we integrated Makeflow and Work Queue into the job workflow. Makeflow simplified job dependency management and reduced job scheduling overhead, while Work Queue scaled our computation capacity from hundreds of simultaneous CPU cores to thousands. This allowed us to perform a sweep of computations with various parameters and high-resolution inputs producing a plethora of outputs to be analyzed and compared. The experiment worked so well that we are now integrating Makeflow and Work Queue into our core infrastructure. Lifemapper benefits not only from the increased speed and efficiency of computations, but the reduced complexity of the data management code, allowing developers to focus on new analyses and leaving the logistics of job dependencies and resource allocation to these tools.

Information from C.J. Grady, Biodiversity Institute and Natural History Museum, University of Kansas.
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 **develop open source software** for large scale distributed computing.

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Tuesday, Nov 14th
- Thinking Opportunistically
- Overview of the Cooperative Computing Tools
- Makeflow
- Makeflow + Work Queue
- Hands-On Tutorial

Thursday, Nov 16th
- Makeflow Features
  - Resource Management
  - Containers
- Work Queue API
- Hands-On Tutorial
Thinking Opportunistically
Much of scientific computing is done in conventional computing centers with a fixed operating environment with professional sysadmins.

But, there exists a large amount of computing power available to end users that is not prepared or tailored to your specific application:

- National HPC facility
- Campus-level cluster and batch system.
- Volunteer computing systems: Condor, BOINC, etc.
- Cloud services.

Can we effectively use these systems for “long tail” scientific computing?
Opportunistic Challenges

- When borrowing someone else’s machines, you cannot change the OS distribution, update RPMs, patch kernels, run as root...
- This often puts important technology just out of reach of the end user, e.g.:
  - FUSE might be installed, but without setuid binary.
  - Docker might be available, but you aren’t a member of the required Unix group.
- The resource management policies of the hosting system may work against you:
  - Preemption due to submission by higher priority users.
  - Limitations on execution time and disk space.
  - Firewalls only allow certain kinds of network connections.
Backfilling HPC with Condor at Notre Dame
Users of Opportunistic Cycles
I can get as many machines on the cloud/grid as I want!

How do I organize my application to run on those machines?
Cooperative Computing Tools
Our Philosophy

- Harness all available resources: desktops, clusters, clouds, and grids.
- Make it easy to scale up from one desktop to national scale infrastructure.
- Provide familiar interfaces that make it easy to connect existing apps together.
- Allow portability across operating systems, storage systems, middleware...
- Make simple things easy, and complex things possible.
- **No special privileges required.**
A Quick Tour of the CCTools

- Open source, GNU General Public License.
- Compiles in 1-2 minutes, installs in $HOME.
- Runs on Linux, Solaris, MacOS, FreeBSD, ...
- Interoperates with many distributed computing systems.
  - Condor, SGE, Torque, Globus, iRODS, Hadoop...
- Components:
  - Makeflow – A portable workflow manager.
  - Work Queue – A lightweight distributed execution system.
  - Parrot – A personal user-level virtual file system.
  - Chirp – A user-level distributed filesystem.

http://ccl.cse.nd.edu/software
MAKEFLOW (MAKE + WORKFLOW)

- Provides portability across batch systems.
- Enable parallelism (but not too much!)
- Fault tolerance at multiple scales.
- Data and resource management.

http://ccl.cse.nd.edu/software/makeflow
#include "work_queue.h"
while( not done ) {
    while (more work ready) {
        task = work_queue_task_create();
        // add some details to the task
        work_queue_submit(queue, task);
    }
    task = work_queue_wait(queue);
    // process the completed task
}
Parrot Virtual File System

Custom Namespace

/home = /chirp/server/myhome
/software = /cvmfs/cms.cern.ch/cmssoft

File Access Tracing
Sandboxing
User ID Mapping

http://ccl.cse.nd.edu/software/parrot
makeflow(1)

NAME
makeflow - workflow engine for executing distributed workflows

SYNOPSIS
makeflow [options] <dagfile>

DESCRIPTION
Makeflow is a workflow engine for distributed computing. It accepts a specification of a large amount of work to be performed, and runs it on remote machines in parallel where possible. In addition, Makeflow is fault-tolerant, so you can use it to coordinate very large tasks that may run for days or weeks in the face of failures. Makeflow is designed to be similar to Make, so if you can write a Makefile, then you can write a Makeflow.

You can run a Makeflow on your local machine to test it out. If you have a multi-core machine, then you can run multiple tasks simultaneously. If you have a Condor pool or a Sun Grid Engine batch system, then you can send your jobs there to run. If you don’t already have a batch system, Makeflow comes with a system called Work Queue that will let you distribute the load across any collection of machines, large or small.

OPTIONS
When makeflow is run without arguments, it will attempt to execute the workflow specified by the Makeflow dagfile using the local execution engine.

Commands
- `--clean` Clean up: remove logfile and all targets.
- `--summary-log <file>` Write summary of workflow to file.

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Makeflow

A Portable Workflow System
MAKEFLOW (MAKE + WORKFLOW)

- Provides portability across batch systems.
- Enable parallelism (but not too much!)
- Trickle out work to batch system
- Fault tolerance at multiple scales.
- Data and resource management.
MAKEFLOW (MAKE + WORKFLOW)
BASED OFF AN OLD IDEA: MAKEFILES

```
part1 part2 part3: input.data split.py
  .split.py input.data

out1: part1 mysim.exe
  .mysim.exe part1 >out1

out2: part2 mysim.exe
  .mysim.exe part2 >out2

out3: part3 mysim.exe
  .mysim.exe part3 >out3

result: out1 out2 out3 join.py
  .join.py out1 out2 out3 > result
```
Makeflow Syntax

[output files] : [input files]

[command to run]

One Rule

out.txt : in.dat \texttt{calib.dat sim.exe}

\texttt{sim.exe in.dat \textasciitilde p 50 > out.txt}

\texttt{sim.exe in.data \textasciitilde p 50 > out.txt}
out.10 : in.dat calib.dat sim.exe
    sim.exe –p 10 in.data > out.10

out.20 : in.dat calib.dat sim.exe
    sim.exe –p 20 in.data > out.20

out.30 : in.dat calib.dat sim.exe
    sim.exe –p 30 in.data > out.30
How to run a Makeflow

• Run a workflow locally (multicore?)
  – makeflow -T local sims.mf
• Clean up the workflow outputs:
  – makeflow --c sims.mf
• Run the workflow on Torque:
  – makeflow --T torque sims.mf
• Run the workflow on Condor:
  – makeflow --T condor sims.mf
Visualization with DOT

- `makeflow_viz -D example.mf > example.dot`
- `dot -T gif < example.dot > example.gif`

DOT and related tools:
http://www.graphviz.org
Makeflow Shapes a Workflow

- Millions of Tasks
- Precise Cleanup
- Transaction Log
- Concurrency Control
- Performance Monitoring
- Thousands of Nodes
- Batch System

Precise Cleanup
Performance Monitoring
Example: Biocompute Portal

Generate Makeflow

Makeflow

Run Makeflow

Transaction Log

Update Status

Progress Bar

BLAST
SSAHA
SHRIMP
EST MAKER
…

Condor Pool

T

T

T

T
- Bioinformatics
- Biometrics
- High Energy Physics
Makeflow + Work Queue

A Portable Workflow System
**MAKEFLOW**

- Makefile
- Makeflow
- Local Files and Programs

- XSEDE Torque Cluster
  - `makeflow -T torque`
- Campus Condor Pool
  - `makeflow -T condor`
- Private Cluster
- Public Cloud Provider
MAKEFLOW + WORK QUEUE

Makefile

Makeflow

submit tasks

Local Files and Programs

Thousands of Workers in a Personal Cloud

XSEDE Torque Cluster

Campus Condor Pool

Private Cluster

Public Cloud Provider
Thousands of Workers in a Personal Cloud
Advantages of Work Queue

- Harness multiple resources simultaneously.
- Hold on to cluster nodes to execute multiple tasks rapidly.
  - (ms/task instead of min/task)
- Scale resources up and down as needed.
- Better management of data, with local caching for data intensive tasks.
- Matching of tasks to nodes with data.
Makeflow and Work Queue

To start the Makeflow

% makeflow -T wq  sims.mf

Could not create work queue on port 9123.

% makeflow -T wq -p 0 sims.mf

Listening for workers on port 8374...

To start one worker:

% work_queue_worker  master.hostname.org 8374
Start 25 Workers in Batch System

Submit workers to Condor:

```
condor_submit_workers master.hostname.org 8374 25
```

Submit workers to SGE:

```
sge_submit_workers master.hostname.org 8374 25
```

Submit workers to Torque:

```
torque_submit_workers master.hostname.org 8374 25
```
Keeping track of port numbers gets old fast...
**Project Names**

- **Master Port 4057**
  - `makeflow ... -N myproject`
  - Connect to chameleon:4057

- **Worker**
  - `work_queue_worker -N myproject`
  - Query

- **Catalog**
  - `work_queue_status`
  - Query
  - Query
  - "myproject" is at chameleon:4057
Project Names

Start Makeflow with a project name:
% makeflow -T wq -N myproject sims.mf
Listening for workers on port XYZ...

Start one worker:
% work_queue_worker -N myproject

Start many workers:
% torque_submit_workers -N myproject 5
<table>
<thead>
<tr>
<th>PROJECT</th>
<th>NAME</th>
<th>PORT</th>
<th>WAITING</th>
<th>BUSY</th>
<th>COMPLETE</th>
<th>WORKERS</th>
</tr>
</thead>
<tbody>
<tr>
<td>awe-fip35</td>
<td>fahnd04.crc.nd.edu</td>
<td>1024</td>
<td>719</td>
<td>1882</td>
<td>1206967</td>
<td>1882</td>
</tr>
<tr>
<td>hfeng-gromacs-10ps</td>
<td>lclsstor01.crc.nd.edu</td>
<td>1024</td>
<td>4980</td>
<td>0</td>
<td>1280240</td>
<td>111</td>
</tr>
<tr>
<td>hfeng2-ala5</td>
<td>lclsstor01.crc.nd.edu</td>
<td>1025</td>
<td>2404</td>
<td>140</td>
<td>1234514</td>
<td>140</td>
</tr>
<tr>
<td>forcebalance</td>
<td>leeping.Stanford.EDU</td>
<td>5817</td>
<td>1082</td>
<td>26</td>
<td>822</td>
<td>26</td>
</tr>
<tr>
<td>forcebalance</td>
<td>leeping.Stanford.EDU</td>
<td>9230</td>
<td>0</td>
<td>3</td>
<td>147</td>
<td>3</td>
</tr>
<tr>
<td>fg-tutorial</td>
<td>login1.futuregrid.tacc</td>
<td>1024</td>
<td>3</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>
Advantages of Work Queue

- MF +WQ is fault tolerant in many different ways:
  - If Makeflow crashes (or is killed) at any point, it will recover by reading the transaction log and continue where it left off.
  - Makeflow keeps statistics on both network and task performance, so that excessively bad workers are avoided.
  - If a worker crashes, the master detects failure and restarts the task elsewhere.
  - Workers can be added and removed at any time during workflow execution.
  - Multiple masters with the same project name can be added and removed while the workers remain.
  - If the worker sits idle for too long (default 15m) it will exit, so as not to hold resources idle.
Alternative Makeflow Formats

Utilizing JSON/JX for easier scripting
Makeflow JSON Syntax

- Verbose flexible structure
- Familiar structure
- Consists of four items:
  - "categories": Object<Category>
  - "default_category": String
  - "environment": Object<String>
  - "rules": Array<Rule>
```json
{
    "outputs": [{"path": "out.txt"}],
    "inputs": [{"path": "in.dat"}, {"path": "calib.dat"}, {"path": "sim.exe"}],
    "command": "sim.exe –p 50 in.dat > out.txt",
}
```
{  
  "outputs": [{"path": "out_10.txt"}],
  "inputs": [ {"path": "in.dat"}, {"path": "calib.dat"}, {"path": "sim.exe"}]
  "command": "sim.exe –p 10 in.data > out_10.txt",
},

{  
  "outputs": [{"path": "out_20.txt"}],
  "inputs": [ {"path": "in.dat"}, {"path": "calib.dat"}, {"path": "sim.exe"}]
  "command": "sim.exe –p 20 in.data > out_20.txt",
},....
- "inputs": Array<File>
- "outputs": Array<File>
- "command": String
- "local_job": Boolean
- "category": String
- "resources": Resources
- "allocation": String
- "environment": Object<String>
Makeflow JX Syntax

- Allows for more compact makeflows.
  - Provides functions for expanding tasks: range, variables, etc...
- Can be used as templates in conjunction with an arguments file.
- Useful for consistently structure data and different data.

Args.jx
Args.jx
Args.jx

Makeflow

Batch System
{  
    "outputs": [{"path": format("out_%d.txt", i)}],  
    "inputs": [ {"path": "in.dat"}, {"path": "calib.dat"}, {"path": "sim.exe"} ]  
    "command": format("sim.exe –p %d in.data > out_%d.txt", i),  
} for i in range(10, 30, 10),
How to run a Makeflow

• Run a workflow from json
  – makeflow --json sims.json

• Clean up the workflow outputs:
  – makeflow --c --json sims.json

• Run the workflow from jx:
  – makeflow --jx sims.jx

• Run the workflow with jx and args:
  – makeflow --jx sims.jx --jx-args args.jx
Tuesday Tutorial

http://ccl.cse.nd.edu
Resource Management

Allowing tasks to share resources
Why Manage Resource?

- More accurate accounting and provisioning.
- Allows for multi-tenant situations.
- Provides consistent resources to tasks.
  - Prevents slower execution.
  - Mitigate failures from under provisioning.
Diagram of Conflicting Resource Usage
Anecdote of BWA failure from limited memory
Makeflow Resource Specification

- Category
  - Cores
  - Memory
  - Disk

```
... CATEGORY=analysis
DISK=1024
MEMORY=1024
CORES=1

out1: part1 mysim.exe
    ./mysim.exe part1 >out1

out2: part2 mysim.exe
    ./mysim.exe part2 >out2

...```

Makeflow Resource Specification

- Category
  - Cores
  - Memory
  - Disk

```makefile
... CATEGORY=analysis
DISK=1024
MEMORY=1024
CORES=1

out1: part1 mysim.exe
    ./mysim.exe part1 > out1

...

... CATEGORY=join
DISK=2048
MEMORY=2048
CORES=2

result: out1 out2 out3 join.py
    ./join.py out1 out2 out3 > result
```
Work Queue Workers

Worker

Makeflow

Task C:1

Cache

Cores

Task C:1
Work Queue Multi-tenant Workers

Same a regular worker!

Makeflow

Task C:1

Task C:1

Task C:1

Task C:1

Cache

Cores
Work Queue Multi-tenant Workers

Same a regular worker!

Makeflow

Cache

Cores

Task C:2

Task C:1

Task C:1

Task C:2
Container Integration

Providing consistent environments
Containers Create Precise Execution Environments

docker run ubuntu-38.23 mysim.exe
Approaches to Containers with Makeflow

- **Approach 1:**
  - Create containers for starting MF and WQ, then let them run as normal.
  - You are responsible for moving container images responsibly.

- **Approach 2:**
  - Let MF create containers as needed for each task.
  - Provides more control over moving container images.
Approach 1: Container for MF/WQ

- `docker run ubuntu makeflow`

Tasks → Makeflow → Worker

- `docker run ubuntu work_queue_worker`
Approach 2: Container for Each Task

Docker Image: ubuntu-38.23

Tasks

Makeflow

Batch System

makeflow --docker ubuntu-38.23 –T sge . . .
Container Technology is Evolving

**Docker Technology**
- `docker run` command executes a container
- Docker runs as a child process, still needs setuid tool

**Singularity Technology**
- `singularity exec` command executes a container
- Singularity runs directly as a child process, still needs setuid tool

Sources:
- [Docker](https://docker.io)
- [Singularity](https://singularity.lbl.gov)
Approach 2 using Singularity

Singularity mage: ubuntu.img

makeflow --singularity ubuntu.img –T sge . . .
Cloud Operation

Methods to Deploying
Approaches to Cloud Provisioning with Makeflow

- **Approach 1:**
  - MF creates unique instance for each task.
  - Provides complete isolation between tasks.
  - Requires startup and tear-down time of instances.

- **Approach 2:**
  - Create instances and run WQ Workers on them, submitting to WQ from MF.
  - Relies on WQ for task isolation, but caches shared files.
  - Instance management relies on the user.
Tasks

Singularity mage:
ubuntu.img

makeflow --singularity ubuntu.img –T sge . . .
Tasks

Singularity mage: ubuntu.img

Makeflow

Batch System

makeflow --singularity ubuntu.img –T sge . . .
Questions?

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CCL Home: http://ccl.cse.nd.edu
Tutorial Link: http://ccl.cse.nd.edu/software/tutorials/acic17