Creating Custom Work Queue Applications

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Makeflow vs. Work Queue

• Makeflow
  – Directed Acyclic Graph programming model.
  – Static structure known in advance.
  – All communication through files on disk.

• Work Queue
  – Submit-Wait programming model.
  – Dynamic structure decided at run-time.
  – Communicate through buffers or files.
  – More detailed knowledge of how tasks ran.
Work Queue API

```c
#include "work_queue.h"

queue = work_queue_create();

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
}
```

http://ccl.cse.nd.edu/software/workqueue
Work Queue Applications

Nanoreactor MD Simulations

Scalable Assembler at Notre Dame

Lobster HEP

ForceBalance

Adaptive Weighted Ensemble
Replica Exchange

Simplified Algorithm:
• Submit N short simulations at different temps.
• Wait for all to complete.
• Select two simulations to swap.
• Continue all of the simulations.

Dinesh Rajan, Anthony Canino, Jesus A Izaguirre, and Douglas Thain,
 Genome Assembly

Using WQ, we could assemble a human genome in 2.5 hours on a collection of clusters, clouds, and grids with a speedup of 952X.

Christopher Moretti, Andrew Thrasher, Li Yu, Michael Olson, Scott Emrich, and Douglas Thain, A Framework for Scalable Genome Assembly on Clusters, Clouds, and Grids, IEEE Transactions on Parallel and Distributed Systems, 2012
Adaptive Weighted Ensemble

Proteins fold into a number of distinctive states, each of which affects its function in the organism.

How common is each state?
How does the protein transition between states?
How common are those transitions?
AWE on Clusters, Clouds, and Grids
Work Queue Architecture

Application

Submit Task1(A,B)
Submit Task2(A,C)

Master Library

Send files
Send tasks

Worker Process

4-core machine

Local Files and Programs

A B C

Submit
Wait

Task.1
Sandbox
2-core task
Cache Dir

Task.2
Sandbox
2-core task

Submit Task1(A,B)
Submit Task2(A,C)
Basic Queue Operations

#include "work_queue.h"
struct work_queue *queue;
struct work_queue_task *task;

// Creates a new queue listening on a port, use zero to pick any port.
queue = work_queue_create( port );
// Submits a task into a queue. (non-blocking)
work_queue_submit( queue, task );
// Waits for a task to complete, returns the complete task.
task = work_queue_wait( queue, timeout );
// Returns true if there are no tasks left in the queue.
work_queue_empty( queue );
// Returns true if the queue is hungry for more tasks.
work_queue_hungry( queue );
Basic Task Operations

#include "work_queue.h"
struct work_queue_task *task;

// Create a task that will run a given Unix command.
task = work_queue_task_create( command );

// Indicate an input or output file needed by the task.
work_queue_task_specify_file( task, name, remote_name, type, flags );

// Indicate an input buffer needed by the task.
work_queue_task_specify_buffer( task, data, length, remote_name, flags );

// Destroy the task object.
work_queue_task_delete( task );
Run One Task in C

```c
#include "work_queue.h"

struct work_queue *queue;
struct work_queue_task *task;

queue = work_queue_create( 0 );
work_queueSpecify name( "myproject" );

task = work_queue_task_create("sim.exe -p 50 in.dat >out.txt");
/// Missing: Specify files needed by the task.
work_queue_submit( queue, task );

while(!work_queue_empty(queue)) {
    task = work_queue_wait( queue, 60 );
    if(task) work_queue_task_delete( task );
}
```
use work_queue;

$queue = work_queue_create( 0 );

work_queue_specify_name( "myproject" );

$task = work_queue_task_create("sim.exe -p 50 in.dat >out.txt");

### Missing: Specify files needed by the task.

work_queue_submit( $queue, $task );

while(!work_queue_empty($queue)) {
    $task = work_queue_wait( $queue, 60 );
    if($task) work_queue_task_delete( $task );
}

CCTools
from work_queue import *

queue = WorkQueue( port = 0 )

queue.specify_name( "myproject" );

task = Task("sim.exe -p 50 in.dat >out.txt")

### Missing: Specify files needed by the task.
queue.submit( task )

While not queue.empty():
    task = queue.wait(60)
C: Specify Files for a Task

```
work_queue_taskSpecifyFile( $task,"in.dat","in.dat", $WORK_QUEUE_INPUT, $WORK_QUEUE_NOCACHE );

work_queue_taskSpecifyFile($task,"calib.dat","calib.dat", $WORK_QUEUE_INPUT, $WORK_QUEUE_NOCACHE );

work_queue_taskSpecifyFile( $task,"out.txt","out.txt", $WORK_QUEUE_OUTPUT, $WORK_QUEUE_NOCACHE );

work_queue_taskSpecifyFile( $task,"sim.exe","sim.exe", $WORK_QUEUE_INPUT, $WORK_QUEUE_CACHE );
```
Perl: Specify Files for a Task

work_queue_taskSpecify_file( $task,"in.dat","in.dat", $WORK_QUEUE_INPUT, $WORK_QUEUE_NOCACHE );

work_queue_taskSpecify_file($task,"calib.dat","calib.dat", $WORK_QUEUE_INPUT, $WORK_QUEUE_NOCACHE );

work_queue_taskSpecify_file( $task,"out.txt","out.txt", $WORK_QUEUE_OUTPUT, $WORK_QUEUE_NOCACHE );

work_queue_taskSpecify_file( $task,"sim.exe","sim.exe", $WORK_QUEUE_INPUT, $WORK_QUEUE_CACHE );
Python: Specify Files for a Task

```python
import task

task.specify_file( "in.dat", "in.dat",
    WORK_QUEUE_INPUT, cache = False )

task.specify_file( "calib.dat", "calib.dat",
    WORK_QUEUE_INPUT, cache = False )

task.specify_file( "out.txt", "out.txt",
    WORK_QUEUE_OUTPUT, cache = False )

task.specify_file( "sim.exe", "sim.exe",
    WORK_QUEUE_INPUT, cache = True )
```

sim.exe in.dat –p 50 > out.txt
You must state all the files needed by the command.
Running a Work Queue Program

gcc work_queue_example.c -o work_queue_example
  -I $HOME/cctools/include/cctools
  -L $HOME/cctools/lib
  -lwork_queue -ldttools -lm

./work_queue_example
Listening on port 8374 ...

In another window:
./work_queue_worker master.host.name.org 8374
setenv PERL5LIB ${PERL5LIB}: (no line break)
    ${HOME}/cctools/lib/perl5/site_perl

./work_queue_example.pl
Listening on port 8374 ...

In another window:
./work_queue_worker  master.host.name.org  8374
... for Python

setenv PYTHONPATH ${PYTHONPATH}:
    ${HOME}/cctools/lib/python2.6/site-package

./work_queue_example.py
Listening on port 8374 ...

In another window:
./work_queue_worker master.host.name.org 8374
Start Workers Everywhere

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
Use Project Names

work_queue_worker
-N myproject

Worker

Catalog

Work Queue (port 9037)

connect to india:9037

advertise

query

query

“myproject” is at india:9037

work_queue_status

CCTools

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Specify Project Names in Work Queue

Specify Project Name for Work Queue master:

C:

```c
work_queue Specify name (q, "myproject");
```

Perl:

```perl
work_queue Specify name ($q, "myproject");
```

Python:

```python
q.specify_name ("myproject")
```
Start Workers with Project Names

Start one worker:

$ work_queue_worker -N myproject

Start many workers:

$ sge_submit_workers -N myproject 5
$ condor_submit_workers -N myproject 5
$ torque_submit_workers -N myproject 5
Advanced Features (in the docs)

- Submit / remove tasks by tag / name.
- Auto reschedule tasks that take too long.
- Send in-memory data as a file.
- Log and graph system performance
- Much more!
Managing Your Workforce

Master A

Master B

Master C

Condor Pool

Concurrent Pool

WQ Pool 200

work_queue_factory –T condor 200

WQ Pool 100

work_queue_factory –T sge 100

Submits new workers.
Restarts failed workers.
Removes unneeded workers.
Using Foremen

Approx X1000 at each fanout.

work_queue_worker
--foreman $MASTER $PORT
Multi-Slot Workers

Master

Worker

Worker

1 core task
1 core task
1 core task
1 core task
1 core task

4 cores
512 MB

specify_cores(4);
specify_memory(512);

work_queue_worker
(implies 1 task, 1 core)

work_queue_worker
--cores 8
--memory 1024