Creating Custom Work Queue Applications

Nicholas Hazekamp

CCTools

UNIVERSITY OF NOTRE DAME

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.

CCTools

UNIVERSITY OF NOTRE DAME

Work Queue API

```
#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
}
```

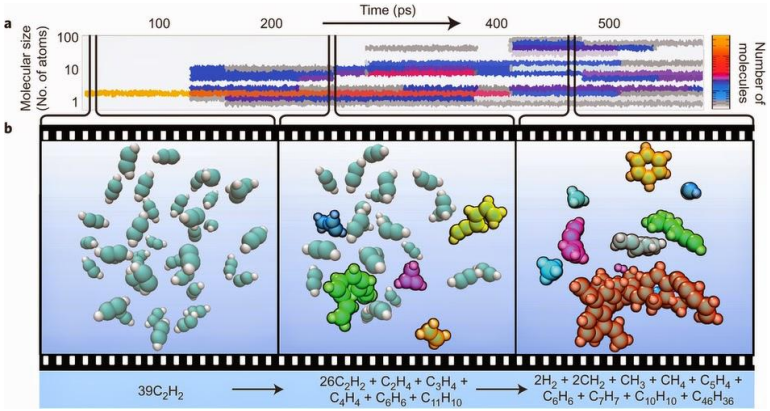
http://ccl.cse.nd.edu/software/workqueue

CCTools

UNIVERSITY OF NOTRE DAME

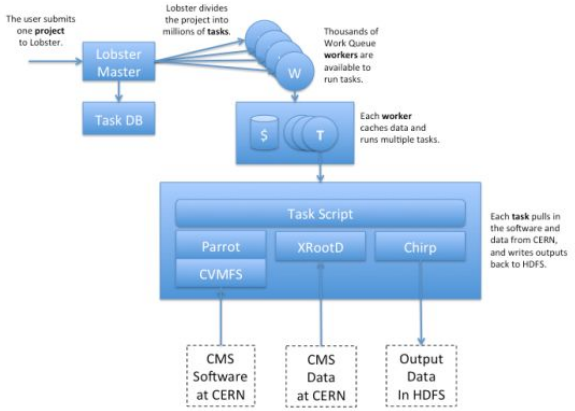
Work Queue Applications

Nanoreactor MD Simulations

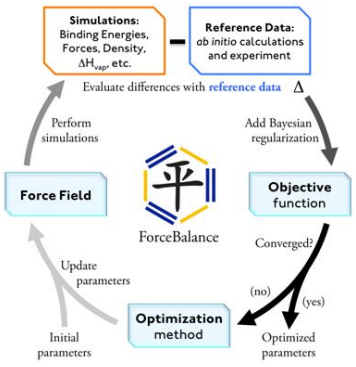


Scalable Assembler at Notre Dame

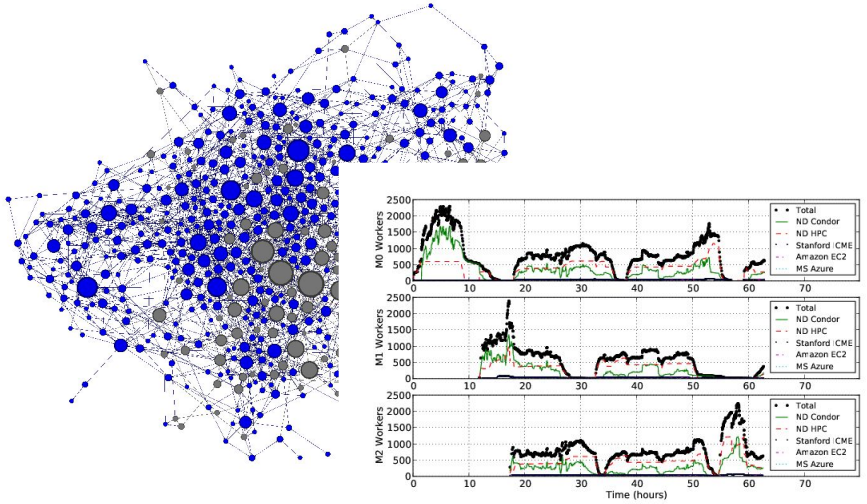
Lobster HEP



ForceBalance



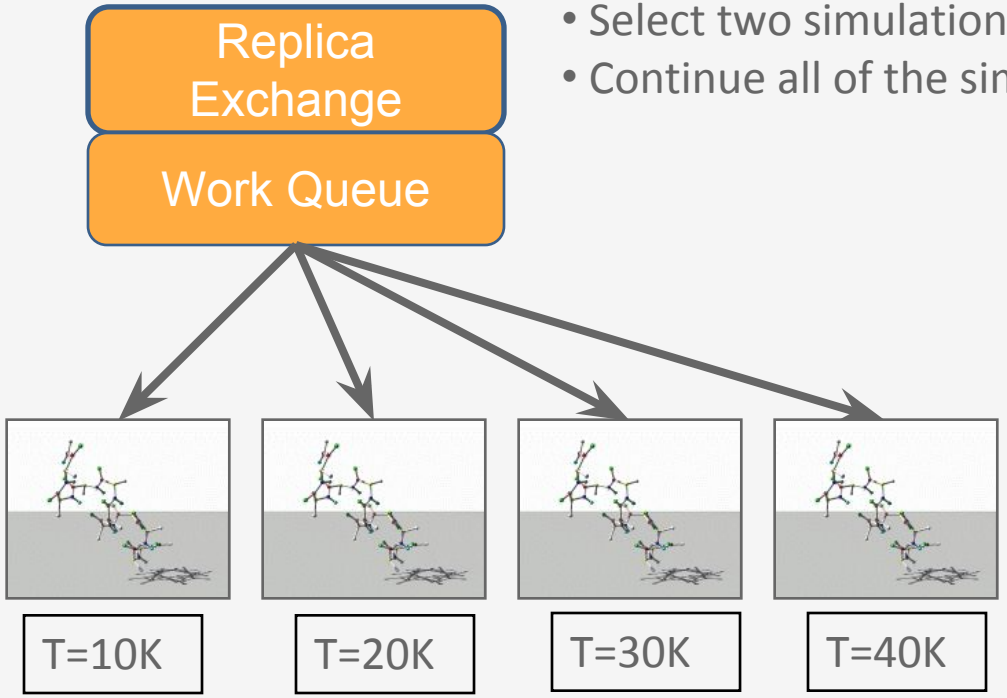
Adaptive Weighted Ensemble

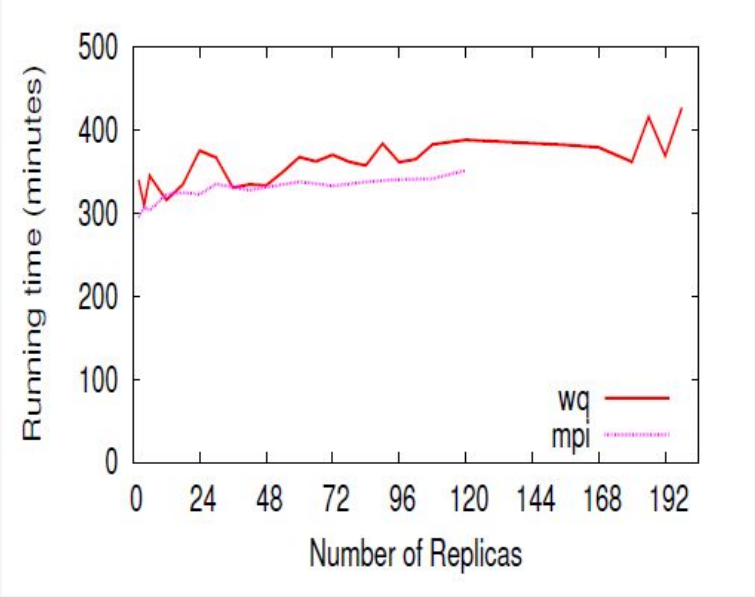


Replica Exchange

Simplified Algorithm:

- Submit N short simulations at different temps.
- Wait for all to complete.
- Select two simulations to swap.
- Continue all of the simulations.



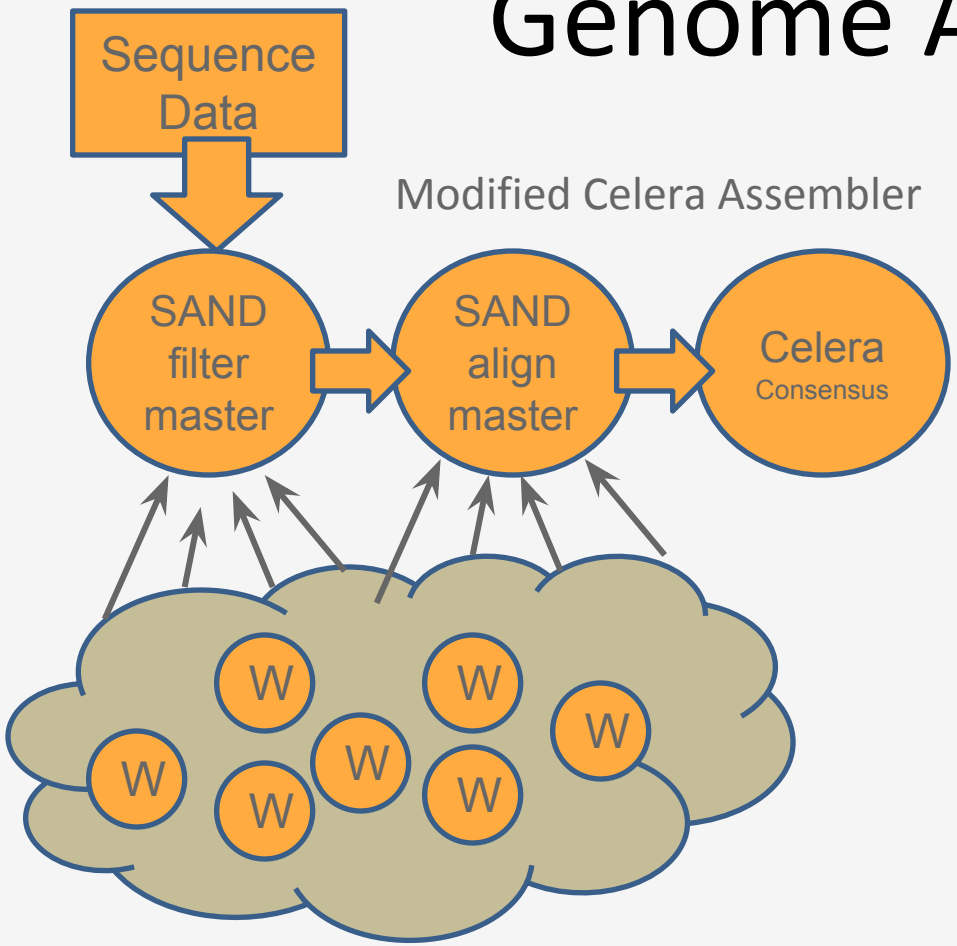


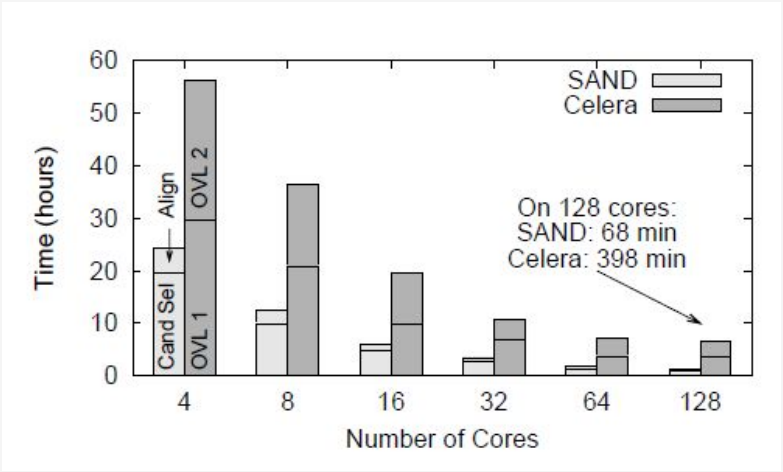
Dinesh Rajan, Anthony Canino, Jesus A Izaguirre, and Douglas Thain,
Converting A High Performance Application to an Elastic Cloud Application, Cloud Com 2011.

CCTools

UNIVERSITY OF NOTRE DAME

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.

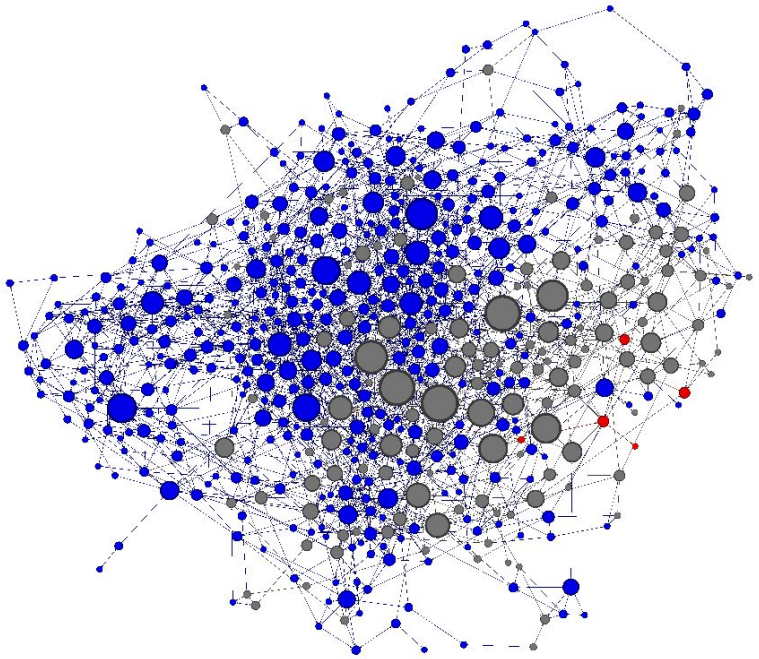
Christopher Moretti, Andrew Thrasher, Li Yu, Michael Olson, Scott Emrich, and Douglas Thain,
A Framework for Scalable Genome Assembly on Clusters, Clouds, and Grids,
IEEE Transactions on Parallel and Distributed Systems, **2012**

CCTools

UNIVERSITY OF NOTRE DAME

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?

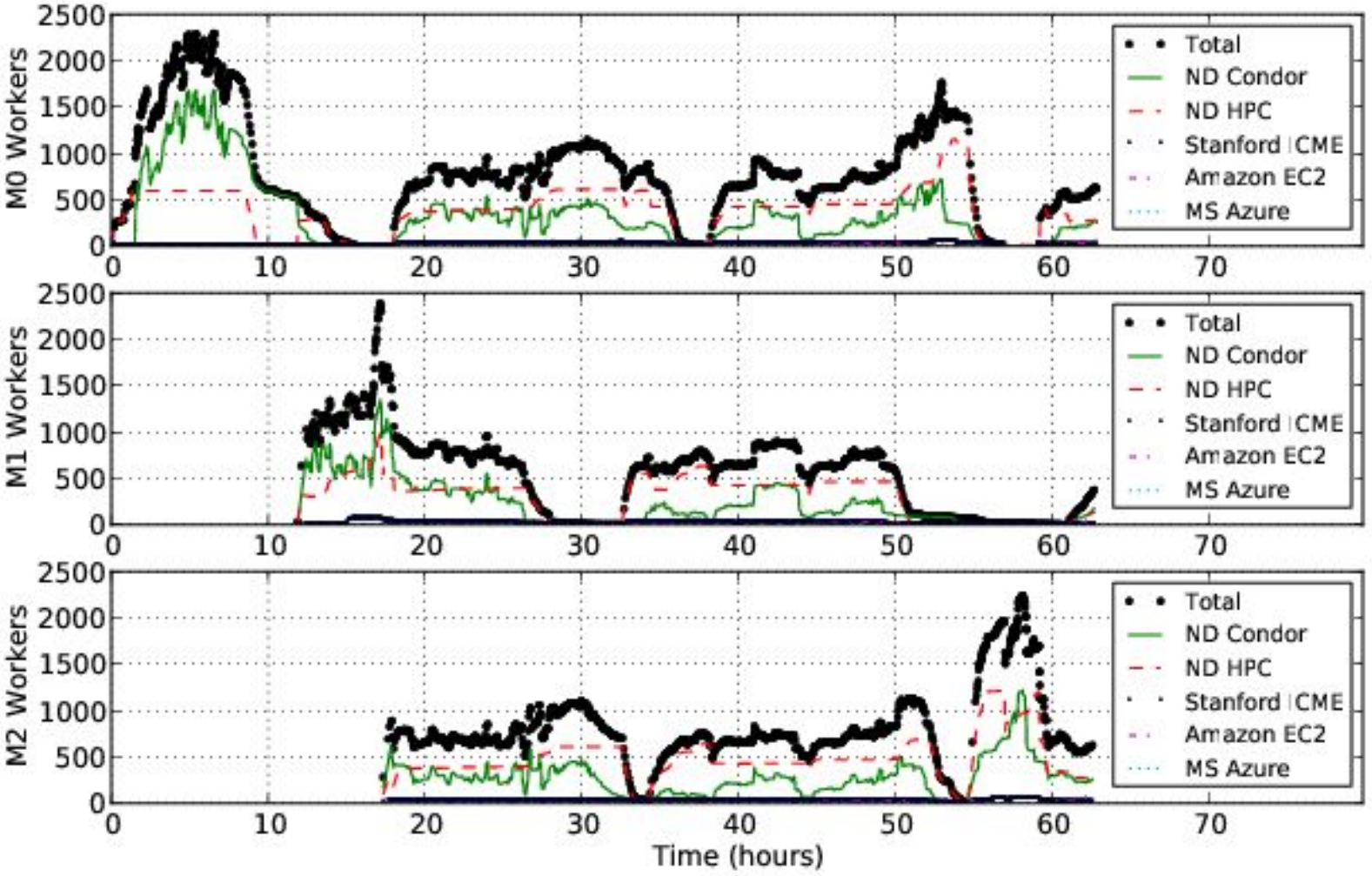
How does the protein transition between states?

How common are those transitions?

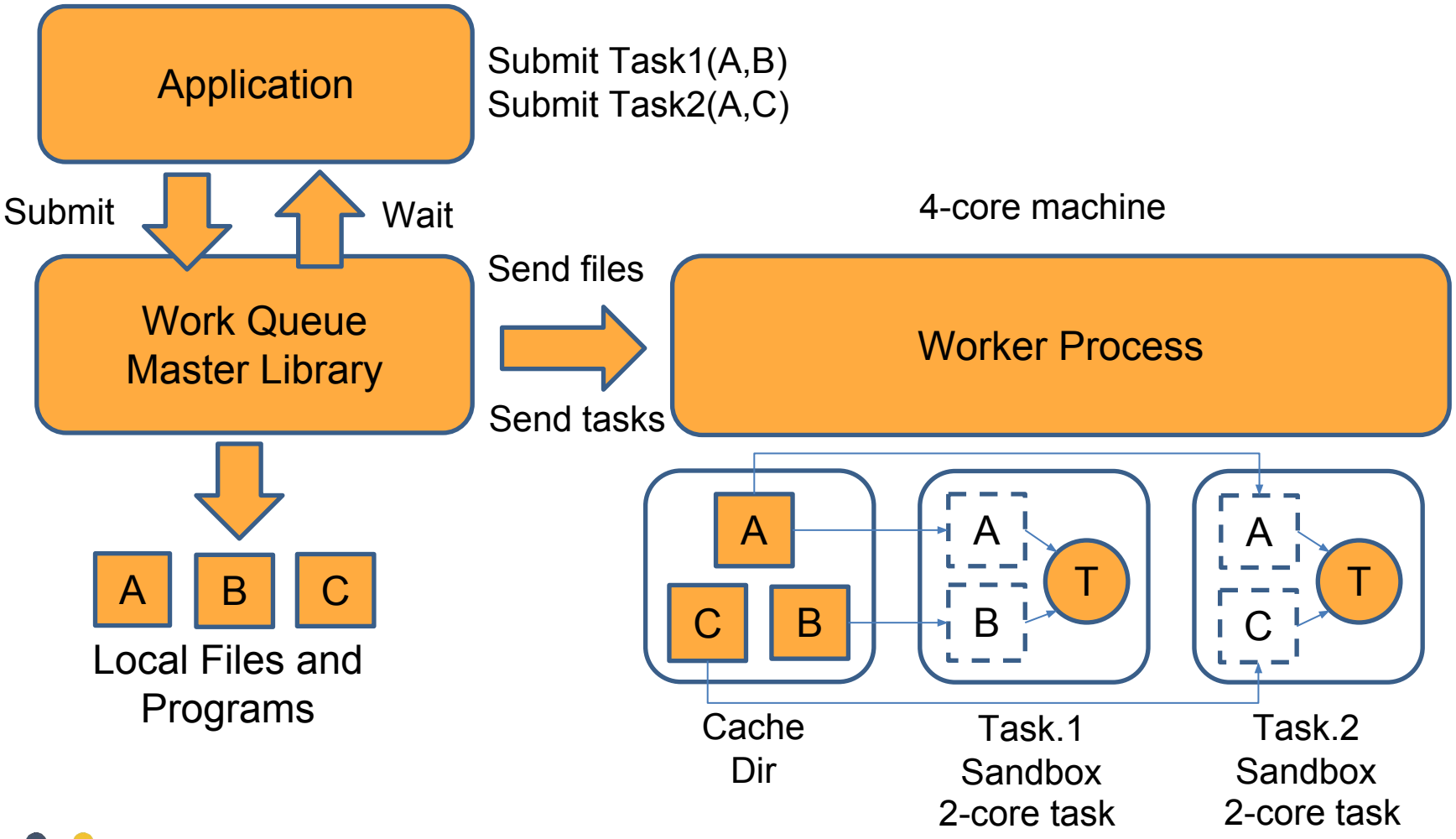
CCTools

UNIVERSITY OF NOTRE DAME

AWE on Clusters, Clouds, and Grids



Work Queue Architecture



CCTools

UNIVERSITY OF NOTRE DAME

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 );
```

CCTools

UNIVERSITY OF NOTRE DAME

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 );
```

CCTools

UNIVERSITY OF NOTRE DAME

Run One Task in C

```
#include “work_queue.h”

struct work_queue *queue;
struct work_queue_task *task;

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

UNIVERSITY OF NOTRE DAME

Run One Task in Perl

```
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

UNIVERSITY OF NOTRE DAME

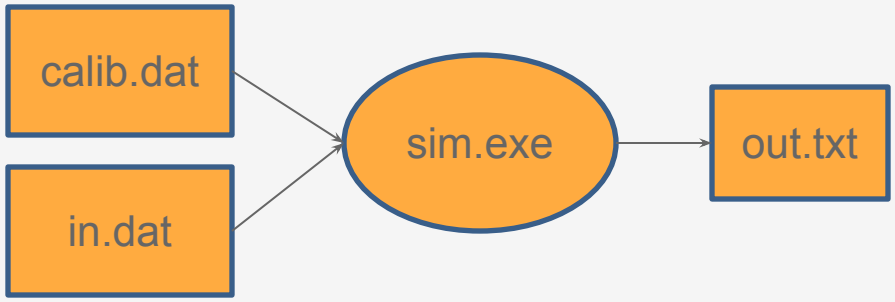
Run One Task in Python

```
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)
```

CCTools

UNIVERSITY OF NOTRE DAME

C: Specify Files for a Task



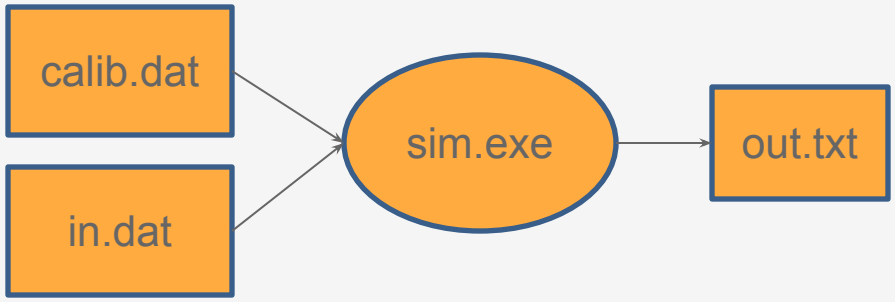
sim.exe in.dat –p 50 > out.txt

```
work_queue_task_specify_file( task,“in.dat”,”in.dat”,
            WORK_QUEUE_INPUT, WORK_QUEUE_NOCACHE );

work_queue_task_specify_file(task,“calib.dat”,”calib.dat”,
           WORK_QUEUE_INPUT, WORK_QUEUE_NOCACHE );

work_queue_task_specify_file( task,“out.txt”,”out.txt”,
           WORK_QUEUE_OUTPUT, WORK_QUEUE_NOCACHE );

work_queue_task_specify_file( task,“sim.exe”,”sim.exe”,
            WORK_QUEUE_INPUT, WORK_QUEUE_CACHE );
```

CCTools

UNIVERSITY OF NOTRE DAME

Perl: Specify Files for a Task



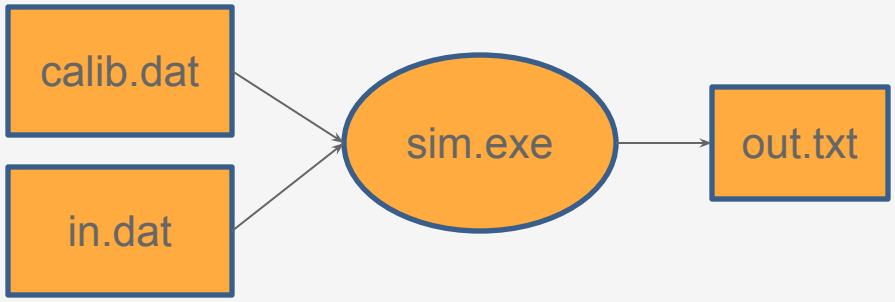
sim.exe in.dat –p 50 > out.txt

```
work_queue_task_specify_file( $task,“in.dat”,”in.dat”,
            $WORK_QUEUE_INPUT, $WORK_QUEUE_NOCACHE );

work_queue_task_specify_file($task,“calib.dat”,”calib.dat”,
           $WORK_QUEUE_INPUT, $WORK_QUEUE_NOCACHE );

work_queue_task_specify_file( $task,“out.txt”,”out.txt”,
           $WORK_QUEUE_OUTPUT, $WORK_QUEUE_NOCACHE );

work_queue_task_specify_file( $task,“sim.exe”,”sim.exe”,
            $WORK_QUEUE_INPUT, $WORK_QUEUE_CACHE );
```

CCTools

UNIVERSITY OF NOTRE DAME

Python: Specify Files for a Task



sim.exe in.dat –p 50 > out.txt

```
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 )
```

CCTools

UNIVERSITY OF NOTRE DAME

CCTools

UNIVERSITY OF NOTRE DAME

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
```

CCTools

UNIVERSITY OF NOTRE DAME

… for Perl

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

CCTools

UNIVERSITY OF NOTRE DAME

… for Python

setenv PYTHONPATH ${PYTHONPATH}: (no line break)
    ${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

CCTools

UNIVERSITY OF NOTRE DAME

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:

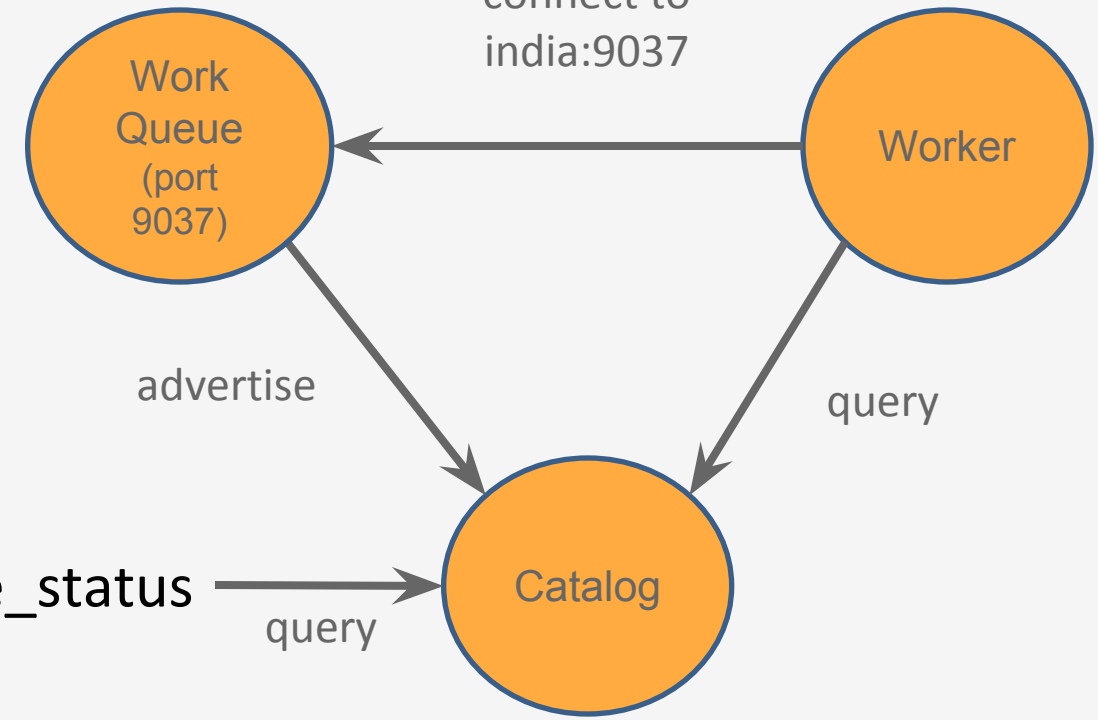
```
torque_submit_workers  master.hostname.org 8374 25
```

CCTools

UNIVERSITY OF NOTRE DAME

Use Project Names

work_queue_worker
–N myproject



CCTools

UNIVERSITY OF NOTRE DAME

Specify Project Names in Work Queue

Specify Project Name for Work Queue master:

C:

```
work_queue_specify_name (q, “myproject”);
```

Perl:

```
work_queue_specify_name ($q, “myproject”);
```

Python:

```
q.specify_name (“myproject”)
```

CCTools

UNIVERSITY OF NOTRE DAME

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
```

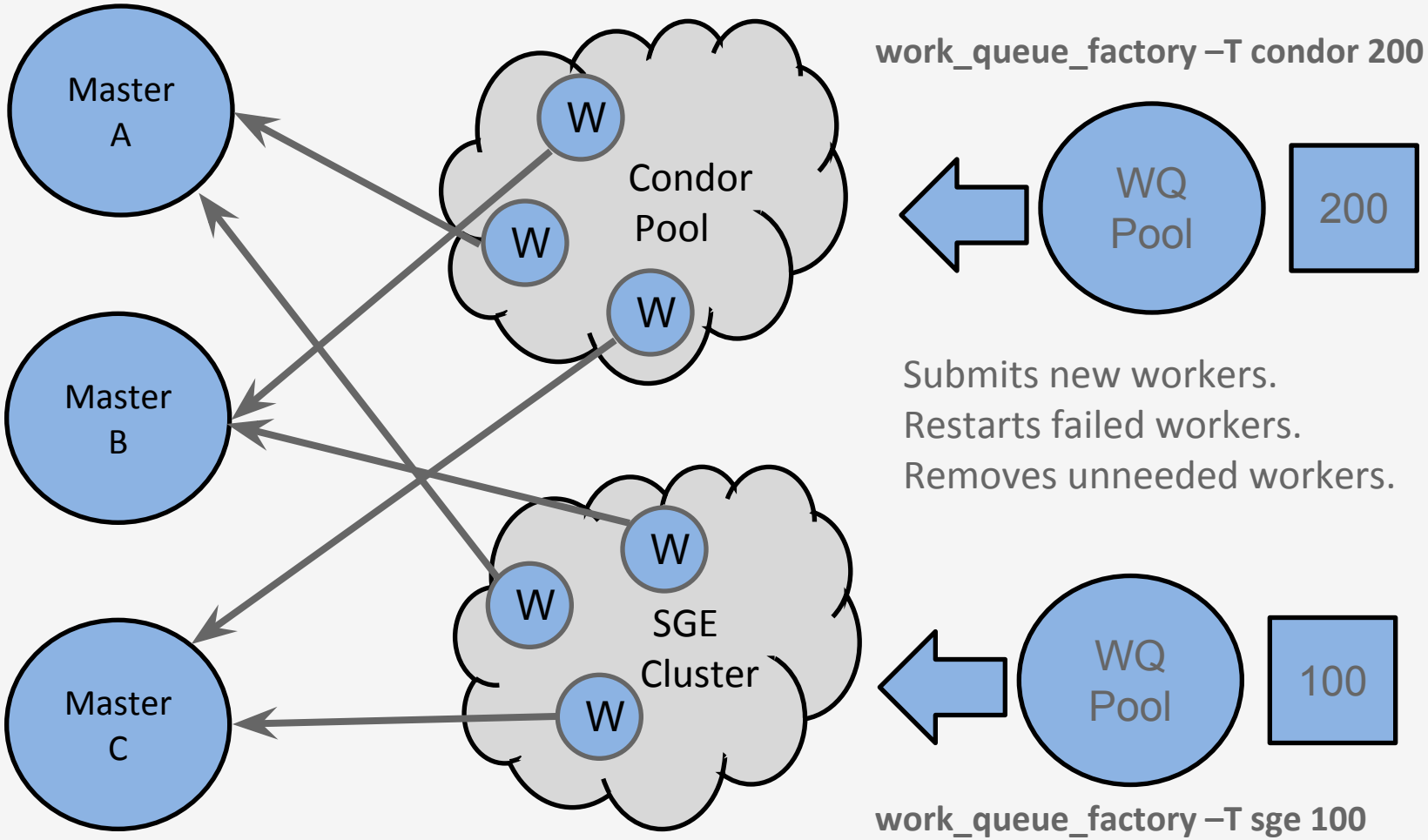
CCTools

UNIVERSITY OF NOTRE DAME

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!

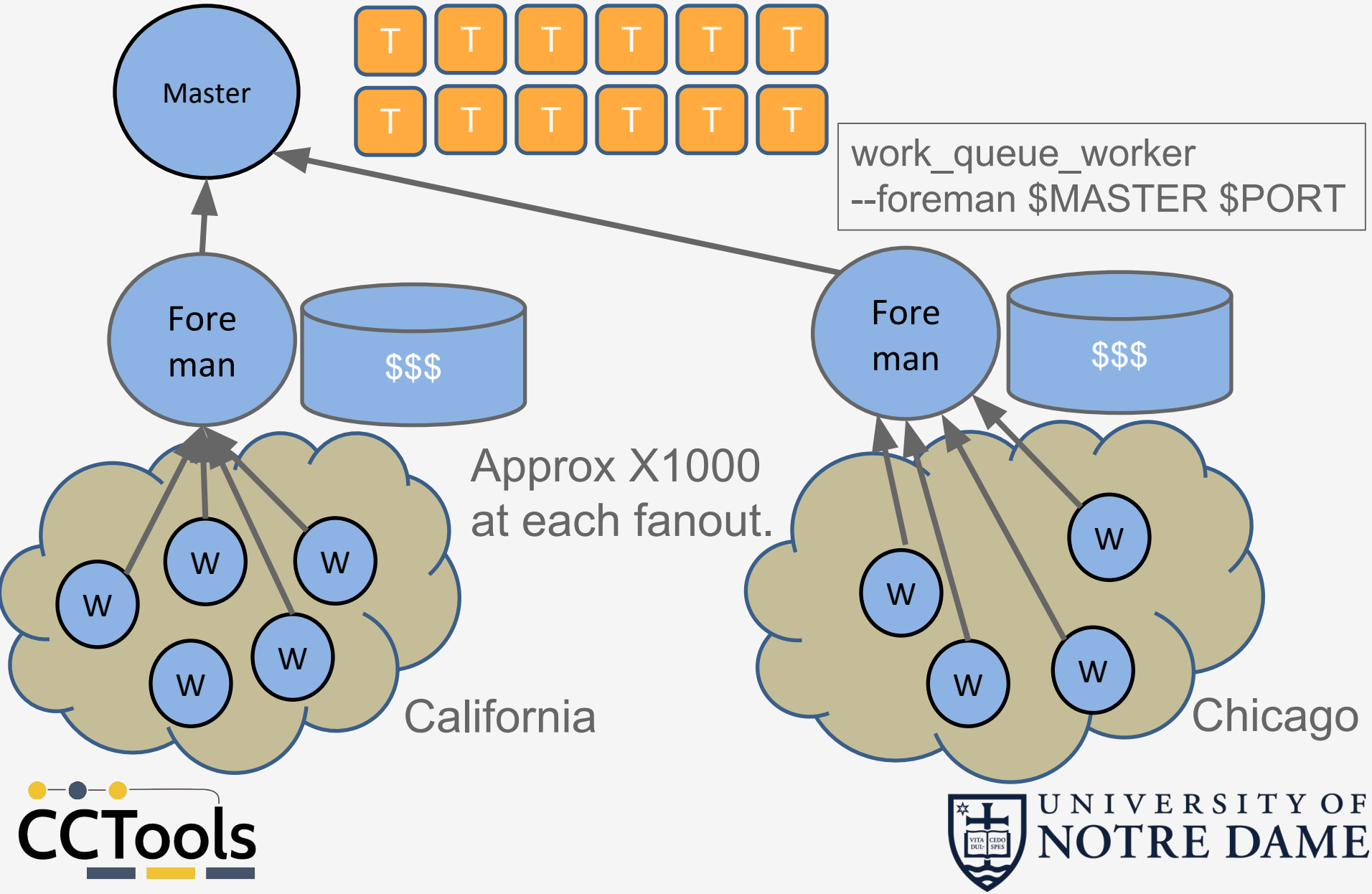
Managing Your Workforce



CCTools

UNIVERSITY OF NOTRE DAME

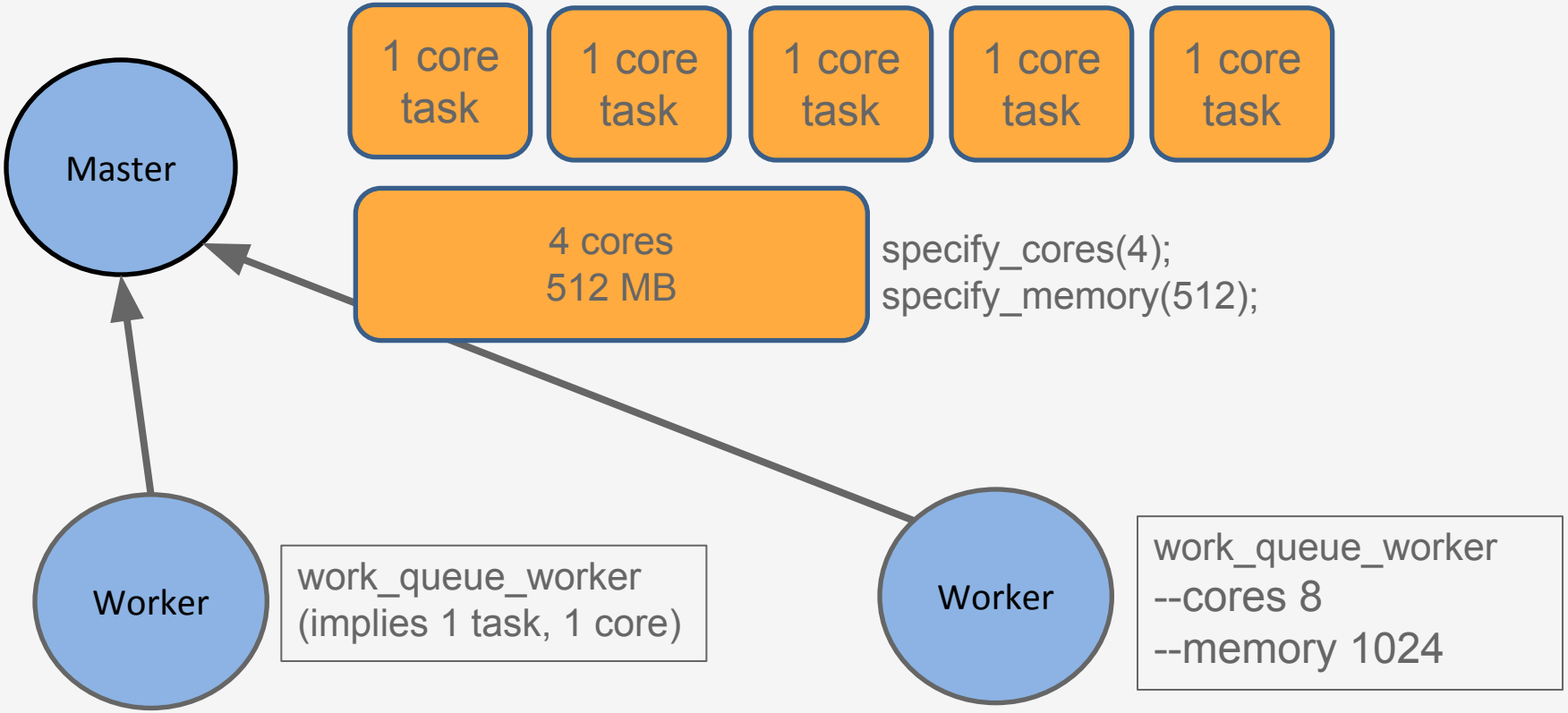
Using Foremen



CCTools

UNIVERSITY OF NOTRE DAME

Multi-Slot Workers



CCTools

UNIVERSITY OF NOTRE DAME