Day 12: Scripting Workflows I

Parameter Sweeps

Turn In Homework

Homework Review

Scripting Workflows

The Need for Scripting

- Since Condor runs jobs and manages workflows, why do we even need to script anything?
- Jobs are usually part of much larger workflow
  - Instruments → data → ***jobs*** → results → papers → funds!
  - Human tasks: Design experiments, interpret results, …
  - Scripting can assist in these steps
- But even for the jobs…
  - Beforehand: Prepare workflow, jobs, data
  - Afterward: Handle data, clean up

Example

- Queue simulator! Say, for the UW Credit Union
- Vary:
  - Number of tellers:1–3
  - Arrival rate: 1–60 per hour
  - Allow departures or not
- 360 combinations
  - Each combination is one set of command-line args.
  - 360 **`arguments`** and **`queue`** statements
- Do ***you*** want to set up and submit jobs manually?

Parameter Sweeps

Parameter Sweeps Defined

- **Run same code for a range of input values**
- Combinations of multiple ranges (***n*** dimensions)

- Defining ranges
  - ***Start - stop - step***
    - Are boundaries included?
    - E.g.: 1 to 1000 2–256, evens **[**40.0, 80.0**)** by 0.25
  - ***Start - stop - count***
    - Are boundaries included?
    - E.g.: 1000 runs from 40.0 up to 60.0
  - ***Start - count - step***
    - E.g.: 1000 trials starting at 1200 counting by 10s

Parameter Sweep in One Dimension

- Enumerating all values of a numeric range is easy
- Convert to ***start-stop-step*** and use **`xrange()`**
  - Arguments are integers, can convert to float in loop
  - Range stops before ***`stop`***
  - ***`start`*** defaults to 0; ***`step`*** defaults to 1, can be < 0

```
for i in xrange(start, stop, step):
    # Calculate real value, if needed
    # Do something with value
```

- Non-numeric ranges use sequences: **`list`**, **`file`**, …

```
for i in list_of_values:
```

Parameter Sweep in Many Dimensions

- Use nested loops:

```
for i in parameter_1:
    for j in parameter_2:
        for k in parameter_3:
            # Calculate real value(s)
            # Do something with values
```

- Bank queue example:

```
for tellers in xrange(1, 4):
    for rate in xrange(2, 120):
        real_rate = rate / 2.0
        run_queue_sim(tellers, real_rate)
```

Data-Driven Code

- Writing loops is easy
- But what happens when you change your design?

- Consider writing generic parameter sweep code
- Actual parameter ranges come from file
- Changing parameters = changing a text file

- This is an example of ***data-driven*** code:
  - Write general purpose code
  - Vary behavior from outside (files, arguments)
  - Spend less time changing code to use
  - But… make only as general as you need now!

Data-Driven Parameter Sweeps I

- First, design format of parameters in file

```
# Very simple: Bank queue parameters
tellers, 1, 4, 1
rates, 1.0, 60.0, 0.5
```

- Getting fancier:
  - Different types of parameters
  - More human-friendly syntax

```
# Way more complex
site: "Site Code" = {ABC, DEF, GHI, JKL}
power: "Power Factor" = [0.0, 1.0) x 0.05
gain: "Gain" = 1-4 ((10 ** _))
```

Data-Driven Parameter Sweeps II

- Write code to read and parse parameter file
- Create sequences for each parameter

```
params = []
for line in param_file:
    parts = re.split(r'\s*,\s*', line)
    start = int(parts[1])
    stop = int(parts[2])
    step = int(parts[3])
    p_range = xrange(start, stop, step)
    params.append((parts[0], p_range))
```

Data-Driven Parameter Sweeps III

- Use iterator function to visit every combination: **`itertools.product()`** (Python ≥ 2.6), else:

```
def product(*args):
    pools = map(tuple, args)
    result = [[]]
    for pool in pools:
        result = [x + [y] for x in result for y in pool]
    for prod in result:
        yield tuple(prod)
```

```
# pN is parameter range in sequence type
for t in itertools.product(p1, p2, p3):
    # t is tuple of parameter values
    # Do stuff with this combination
```

Condor

Overview of Approaches

Assuming that we want to run a Condor job for each combination of parameter values, …

1. Separate submits
2. One submit, many **`arguments`** & **`queue`** statements
3. One submit, many directories

Separate Submit Files

- How it works:
  - For each combination of parameter values:
  - Write a Condor submit file with all necessary lines
  - Parameter values: **`arguments`** statement or input file
- Disadvantages
  - Must submit each job separately
  - Extra overhead
  - Leaves many submit files around

Parameters in Arguments I

- Overview
  - Script creates one huge submit file
  - Each parameter combo gets **`arguments`** & **`queue`** lines
  - Input, output, error, and log files:
    - All in same directory; files named with **`$(process)`**
    - Each in separate directory per **`$(process)`**

```
...
arguments "1 20"
queue
arguments "1 21"
queue
...
```

Parameters in Arguments II

- Put all of the common submit statements in a file:

```
# submit-prefix.txt
executable = sweep.py
universe = vanilla
output = sweep-out/sweep-$(PROCESS).out
error  = sweep-err/sweep-$(PROCESS).err
log    = sweep-log/sweep-$(PROCESS).log

should_transfer_files = YES
when_to_transfer_output = ON_EXIT
```

Parameters in Arguments III

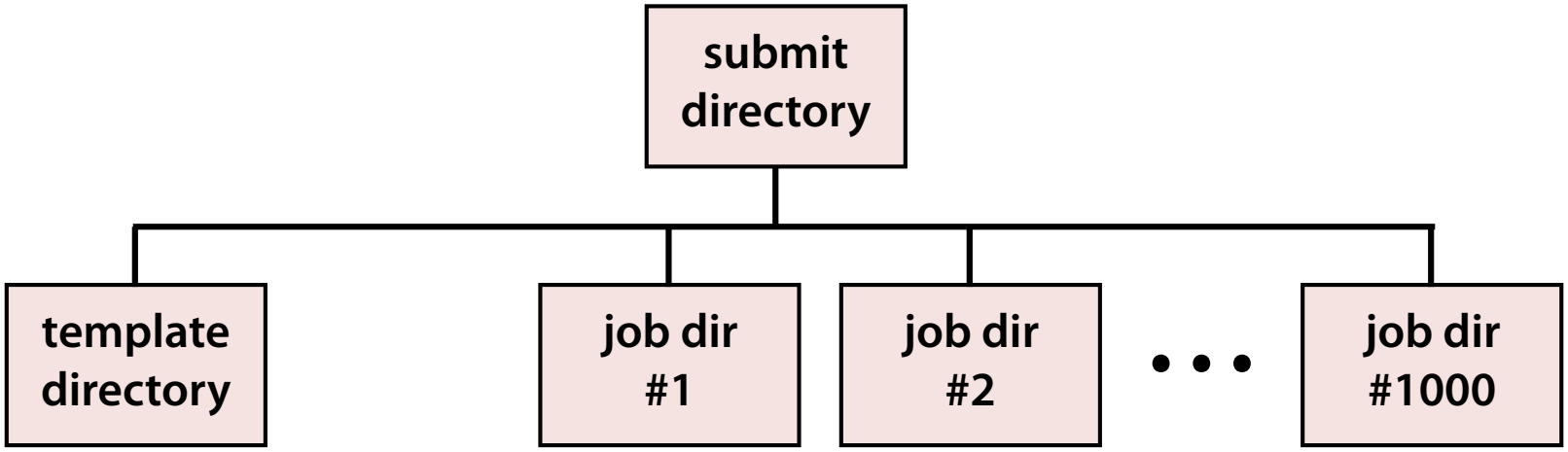
```
# Sketch of main script to make submit file

header = read_submit_prefix()    # string
submit = open(filename, 'w')
submit.write(header)

params = read_parameters_file()  # from earlier
for t in product(*params):
    args = ' '.join(t)
    submit.write('arguments = "%s"\n' % args)
    submit.write('queue\n')
submit.close()

if options.submit:
    print 'Submitting job...'
    os.system('condor_submit ' + filename)
```

Arguments vs. Files

- Parameters via ***command-line arguments***
  - When you must, because of the program
  - For few and/or simple parameters
- Parameters via ***input files***
  - When you must, because of the program
  - For complex parameters
  - When you must use input files for other reasons

Parameters in Files I

- How it works:
  - Manually write one submit file (details on next slide)
  - For each combination of parameter values, script:
    - Creates a numbered subdirectory
    - Writes template files, possibly modified, into directory
    - Like homework assignment #6



Parameters in Files II

- Write one submit file for all jobs
- Use **initialdir** with **$(PROCESS)** for job subdirs
- Put **queue *N*** at end (script should modify ***N***)

```
executable = file-sweep.py
universe = vanilla
initialdir = sweep-$(PROCESS)
output = sweep.out
error  = sweep.err
log    = sweep.log
should_transfer_files = YES
when_to_transfer_output = ON_EXIT
transfer_input_files = params.txt, ...
queue 1000
```

Parameters in Files III

- Need good function to write modified template file
- Pick parameter placeholder text to avoid conflicts

```
# Outline of a template writer function
# params: (('p1', 42), ('p1', 43), ...)
def write_template(text, target_name, params):
    for p in params:
        p_name, p_value = p
        p_src = '{:%s:}' % p_name
        text = text.replace(p_src, p_value)
    output_file = open(target_name, 'w')
    output_file.write(text)
    output_file.close()
```

Parameters in Files IV

- Read files from template dir into, say, dictionary
- Then, make all directories and files for run

```
# Outline of code to prepare a template run
# sources: dict from filename to contents
def write_job_dirs(sources, count, params):
  for i in xrange(count):  # [0, count)
    dirname = 'sweep-' + str(i)
    os.mkdir(dirname)
    pfile = os.path.join(dirname, 'params.txt')
    write_parameters(params, pfile)
    for filename in sources:
      text = sources[filename]
      target = os.path.join(dirname, filename)
      write_template(text, target, params)
```

Parameters in Files V

- Top-level plan: Read data, write directories and files
- Could also submit Condor job

```
# Outline of main script

opts, args = parse_command_line()

params = read_parameters(args['param_path'])
sources = read_sources(args['template_dir'])

update_queue_n(params)
write_job_dirs(sources, count, params)

if opts.submit:
    os.system('condor_submit sweep.sub')
```

Output

Harvesting Output

- Need a post-script to gather or consolidate output?
- Without DAGMan, no post-script in job per se
- If this is significant work, use a separate job!

```
# Assumes all interesting output is from stdout
for outfile in glob.glob('sweep-*/sweep.out'):
    handle_output(outfile)
```

```
outfiles = ('sweep.out', 'out1.txt', 'out2.csv')
regexp = r'sweep-\d+$'
for d in os.listdir('.'):
  if (os.path.isdir(d) and re.match(regexp, d)):
    for outfile in outfiles:
      handle_output(d, outfile)
```

Consolidating Output

- Combine all output files into one
- Prefix each line with parameter info
- Need way to recover parameters for each run (maybe write to file when creating run directory?)

```
combo = open(combined_output_filename, 'w')
for d in run_directories:
    d_params = read_run_params(d)
    d_output = read_run_output(d)
    for line in d_output:
        combo.write('\t'.join(d_params) + '\t')
        combo.write(line)
combo.close()
```

Cleaning Up

- If running many times, clean up after each run

```
# Just a sketch of some possibilities

def handle_output(dir, file):
    out_path = os.path.join(dir, file)
    n = re.match(r'sweep-(\d+)$', dir)[1]
    new_file = 'output-%d.txt' % (n)
    new_path = os.path.join('output', new_file)
    shutil.move(out_path, new_path)

for run_dir in run_directories:
    handle_output(run_dir, 'sweep.out')
    shutil.rmtree(run_dir)
```

Homework

Homework

- Make a pretty picture!
- Instead of one long job, break into several smaller jobs… by "tile"
- Lots of background info, read carefully to understand
- For now, stitch resulting image files together manually