The Materials Project, FireWorks, and high-throughput computing at NERSC

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Should big computers run small calculations?

(a) No, because only massively parallel simulations require large computers
(b) No, because massively parallel jobs are more important than smaller jobs
(c) Yes - but small jobs should be second class citizens
(d) Yes, and small jobs should have equal rights!
The Materials Project requires lots of computing, but not massively parallel

- 20+ million CPU-hours so far
  - 200,000+ individual electronic structure calculations
  - more is always needed

- 50+TB disk so far
  - always hitting disk limits

- 5600+ users so far
  - they need more computed data!
We built our own workflow software – why?

http://www3.canisius.edu/~grandem/animalshabitats/animals.jpg
Our workflow computing “habitat”

- Failures are common; search status of every job over the course of years
  - like UPS packages, database is a necessity
- Very dynamic workflows
  - results of a calculation greatly affect workflow, e.g. “self-healing” detours or “metal vs. insulator” flows
- Intelligently handle collisions/duplicates
  - people submitting the same material, perhaps with some calculations in common and some distinct
- Runs on a laptop or a supercomputer
- Can learn it by yourself without help/support
Hierarchical codebases:
FireWorks is our general workflow code
How FireWorks operates

ROCKET LAUNCHER / QUEUE LAUNCHER

Directory 1

Directory 2

FW 1

FW 2

FW 3

FW 4

LAUNCPAD
Workflows are simple JSON/YAML documents that have very little “fluff” (no ugly XML)

(this is YAML, a bit prettier for humans but less pretty for computers)

```yaml
fws:
- fw_id: 1
  spec:
    _tasks:
    - _fw_name: ScriptTask
      script: echo 'To be, or not to be,'
- fw_id: 2
  spec:
    _tasks:
    - _fw_name: ScriptTask
      script: echo 'that is the question:'

links:
  1:
  - 2
metadata: {}"
JSON + MongoDB means you can store workflows directly and make rich queries

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```

Just some of your search options:

- simple matches
- match in array
- greater than/less than
- regular expressions
- match subdocument
- Javascript function
- MapReduce...

All for free, and all on the native workflow format!
Jobs can return objects that modify workflows or future jobs via JSON language.

- Use MongoDB’s dictionary update language to allow for JSON document updates.

Workflows can create new workflows or add to current workflow:
- a recursive workflow
- calculation “detours”
- branches
But wait – there’s more!
JSON duplicate checking simple and automatic

input_array: 1 + 1 → Sum: 2
input_array: 2 + 2 → Sum: 4
input_array: 3 + 4 → Sum: 7
Many execution modes

- Run directly on a node
- Run a single job within a PBS script
  - generic or highly tailored to the job
- Consecutively pull many jobs in a PBS script
- Run via PBS/SGE/SLURM/NEWT
- Distribute jobs over many workers
- Pack jobs and pretend to be a big job without any setup
Examples of successes

- Completed 575000+ PBS jobs worth of computations
- Gracefully recovered from many failures
  - very easy to track down which jobs failed, resubmit them with new code as needed
- Random people can submit the materials they care about and not worry about duplication
- Random people have downloaded and set it up without any outside help
FireWorks is free and open-source

http://pythonhosted.org/FireWorks/

or Google “Python FireWorks”
You may not care about FireWorks, but you might consider open-sourcing your own code

- Real open source on a web site like Github
  - not “email me for code”
Things that have and haven’t happened when going open source … overall very positive

**HAPPENED**

- I was automatically wrote better code and documentation
- Tricky but important bugs identified/fixed by community
- New bugs introduced by newcomers (but quickly fixed)
- Python 3 compatible by volunteer
- Internals became cleaner & user-friendly
- Heated arguments that resulted in improvements
- Learned about management
- Lots of good feature suggestions, some feature implementation by community
- Pace of development greatly accelerated
- Friendly users I had no relation to gradually came out of the woodwork and asked questions

**DID NOT HAPPEN**

- Code went viral
  - the world mostly did not notice…
- Thieves stole the code and didn’t attribute it
  - I think…
- People blamed me for publishing imperfect code

**FW Teammates**
Shyue Ping Ong
Xiaohui Qu
Morgan Hargrove
David Waroquiers
Dan Gunter
Wei Chen
Kristin Persson (very patient funder)