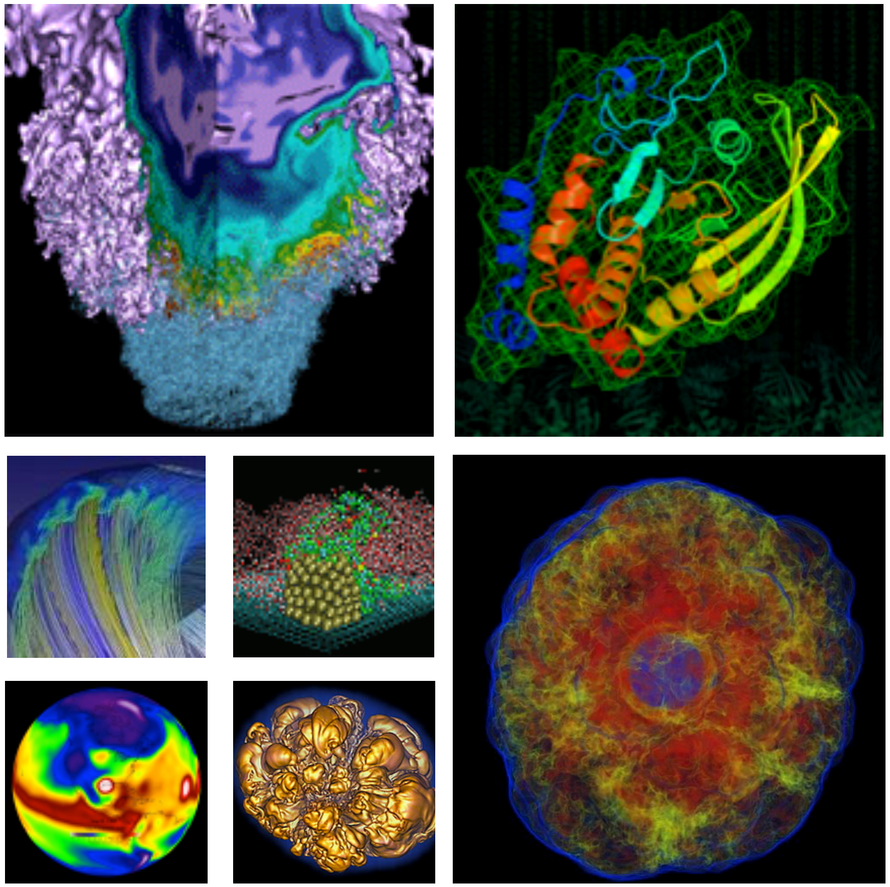
Workflow Tools at NERSC



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NERSC User Meeting
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What Does Workflow Software Do?

- **Automate connection of applications**
  - Chain together different steps in a job pipeline.
  - Automate provenance tracking -> enable ability to reproduce results.
  - Assist with data movement.
  - Monitor running processes and handle errors.
  - Data processing of streaming experimental data (including near-realtime processing).
- **Workflows help work with (around?) batch scheduler and queue policies.**

Workflows are Personal

- Many tools exist in the workflow space
  - Google: “Scientific Workflow Software”
- It seems like each domain has its own workflow solution to handle domain-specific quirks
- No single tool solves every single problem

- Fireworks
- qdo
- Tigres
- Galaxy
- Swift
- BigPanda
- Pegasus
- Taverna
- Airavata
- …….

Workflows Working Group

- **Last year Workflows working group investigated breadth of technologies**
- **We 'support' 2 tools at NERSC**
  - **FireWorks**
  - **Swift**
  - this doesn't mean other tools won't be used/supported at NERSC, only that DAS has specific expertise in these.
- **Create an ecosystem to enable self-supported WF tools**
  - Databases, User defined software modules, AMQP services etc.

http://www.nersc.gov/users/data-analytics/workflow-tools/

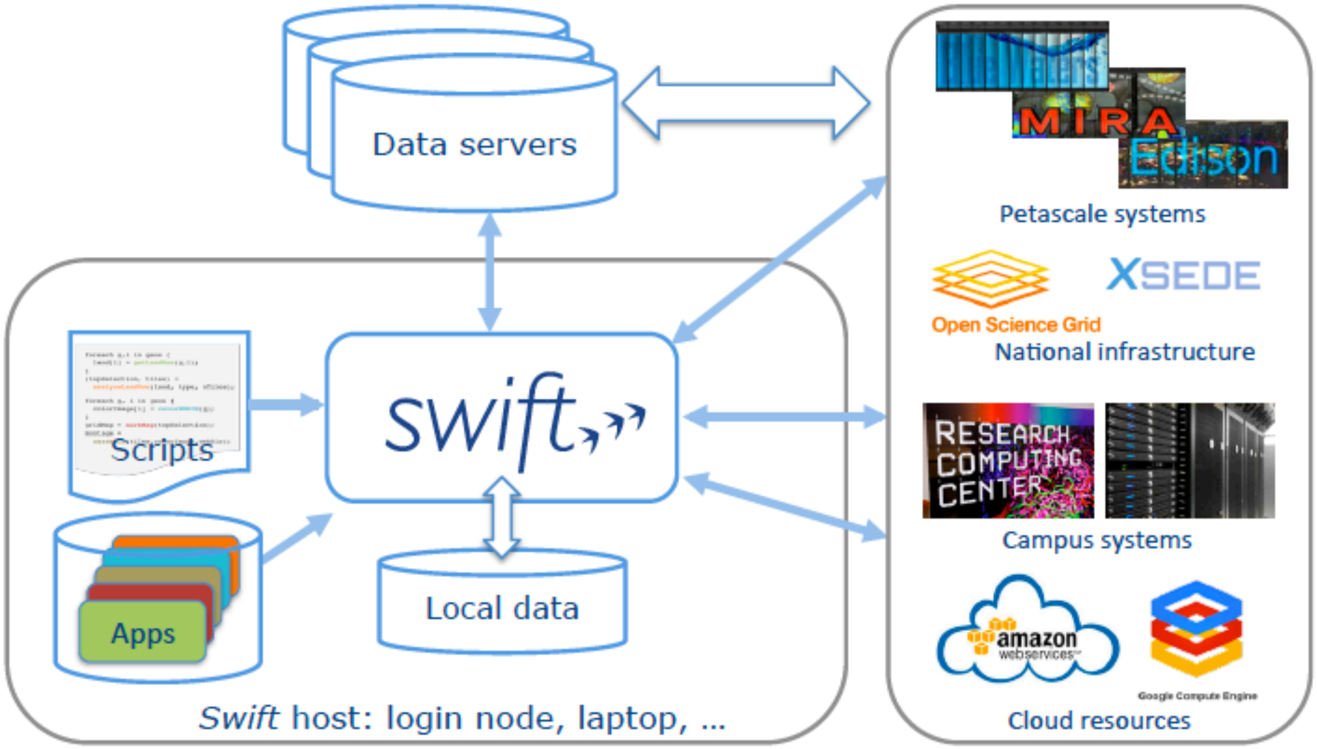
Existing Workflow Ecosystem @ NERSC

- **Science Gateways**
- **Databases**
  - Mongo, Postgres, MySQL, SQLite, SciDB
- **Workflow tools (self-supported)**
  - Fireworks, swift, Tigres, qdo, Galaxy
- **High throughput batch queues**
- **NEWT REST API**
- **Globus / Data Transfer Nodes**
- **Many task frameworks**
  - MySGE, Taskfarmer
- **Other web based tools for interactive use cases**
  - iPython, R Studio, NX
- **MapReduce frameworks**
  - Spark, Hadoop

Workflow tools exist in and interact with a rich environment of NERSC capabilities and services.

Use Case: Swift

- Enables execution over multiple compute resources
- Swift language "encapsulates" application, easing distribution, parallelisation and provenance capture



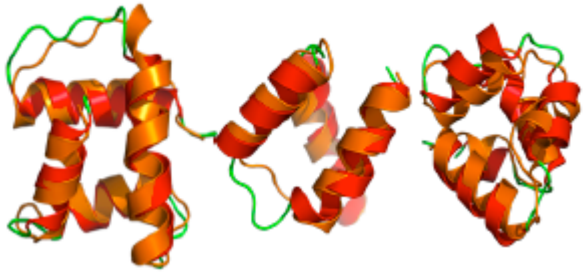
Use Case: Swift (Biosciences)

- **Functional language: powerful parallel loops**
- **Example: protein simulation for drug screening**

```
Sweep(Protein pSet[ ])
{
  int nSim = 1000;
  int maxRounds = 3;
  float startTemp[ ] = [ 100.0, 200.0 ];
  float delT[ ] = [ 1.0, 1.5, 2.0, 5.0, 10.0 ];
  foreach p, pn in pSet {
    foreach t in startTemp {
      foreach d in delT {
        IterativeFixing(p, nSim, maxRounds, t, d);
      }
    }
  }
}
```

O(10) proteins implicated in a disease

X



10 proteins x 1000 simulations x
3 rounds x 2 temps x 5 deltas
= 300K tasks

https://www.nersc.gov/users/data-analytics/workflow-tools/swift/

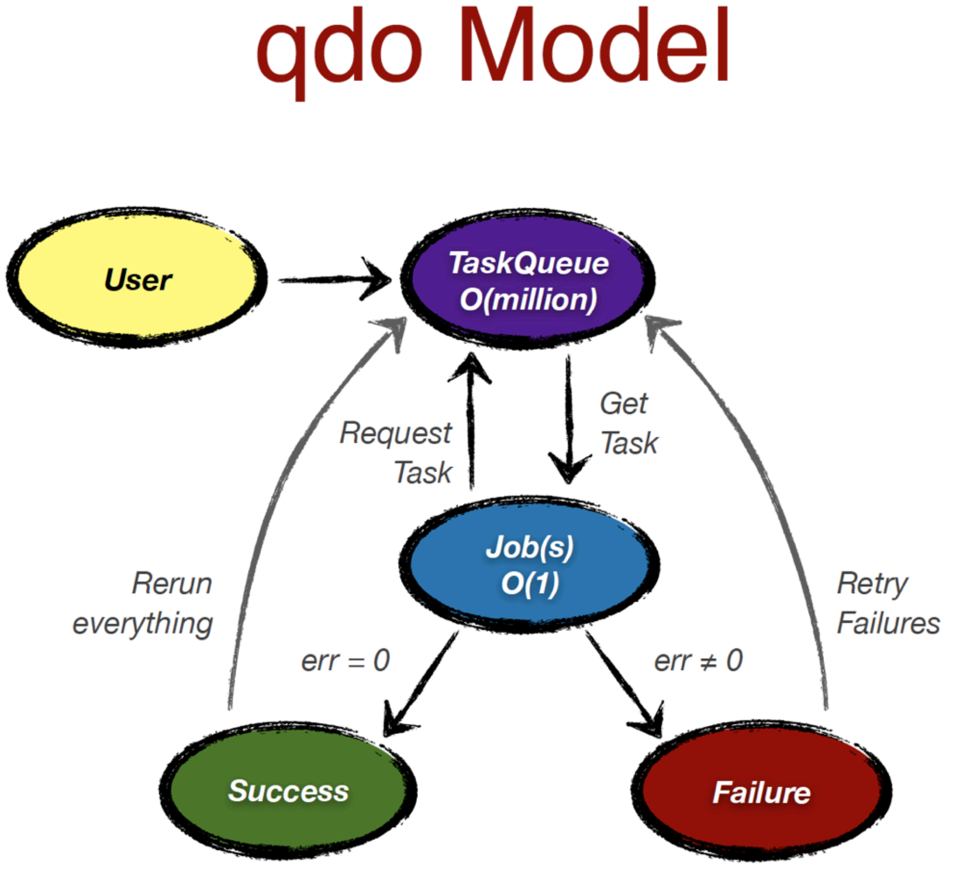
Workflows and Data Intensive Science

- **Data intensive scientific computing may not always fit the traditional HPC paradigm**
  - Large numbers of tasks, low degree of parallelism.
  - Job dependencies and chaining.
  - Need to communicate with external datasources, DBs.
- **Workflow and work orchestration in this context can be thought of as sequences of compute and data-centric operations.**

High Throughput "Bag of Tasks"

- **Often need to process large numbers of smallish tasks repeatedly.**
- **Typical queue policies work against you**
  – a lot of time lost waiting.
  – Batch system not set up for lots of little tasks.
- **Instead use a workflow system**
  – to queue up tasks.
  – to launch long running workers to consume these tasks.

Use Case: qdo (cosmology)



- qdo is specifically designed to package up multiple small tasks into one batch job.

http://www.nersc.gov/users/data-analytics/workflow-tools/other-workflow-tools/qdo/

qdo examples

```
#- Command line
qdo load Blat commands.txt     #- loads file with commands
qdo launch Blat 24 --pack      #- 1 batch job; 24 mpi workers
```

```
#- Python
import qdo
q = qdo.create(“Blat”)
for i in range(1000):
   q.add(“analyze blat{}.dat”.format(i))

q.launch(24, pack=True)
```

```
#- Python load 1M tasks
commands = list()
for x in range(1000):
    for y in range(1000):
        commands.append(“analyze -x {} -y {}”.format(x, y))

q.add_multiple(commands)   #- takes ~2 minutes
q.launch(1024, pack=True)
```

Many-task frameworks

- Repeatedly perform tasks on a large dataset
- Map => perform an operation across a large set i.e. map a task across the dataset
- Reduce => collect and reduce the results from map operation
- Split the data across nodes and run task on each node
- Typically does not require much cross node communication
- Frameworks at NERSC
  - Spark
  - Hadoop

  - MySGE
  - Taskfarmer

Batch Queues

- **NERSC has queues suited to jobs that need less than one compute core**
  - –Cori Shared queue designed specifically for these use cases.
- **Reservations available for special needs.**
- **Consider using job packing options in various workflow tools to optimize for HPC queue infrastructure**
  - –also for packing single-core jobs into a multi-core node.

Use Case: TaskFarmer

- **Simple NERSC-developed utility that farms single-core tasks onto a multi-core compute node, tracks job success**

1) Write a wrapper that defines one task to run

```
cd $SCRATCH/myDir
python myScript.py $1 $2 $3
```

2) Make list of tasks to run, with options to pass to your wrapper

```
wrapper.sh 0 0 1
wrapper.sh 0 1 0
wrapper.sh 0 1 1
```

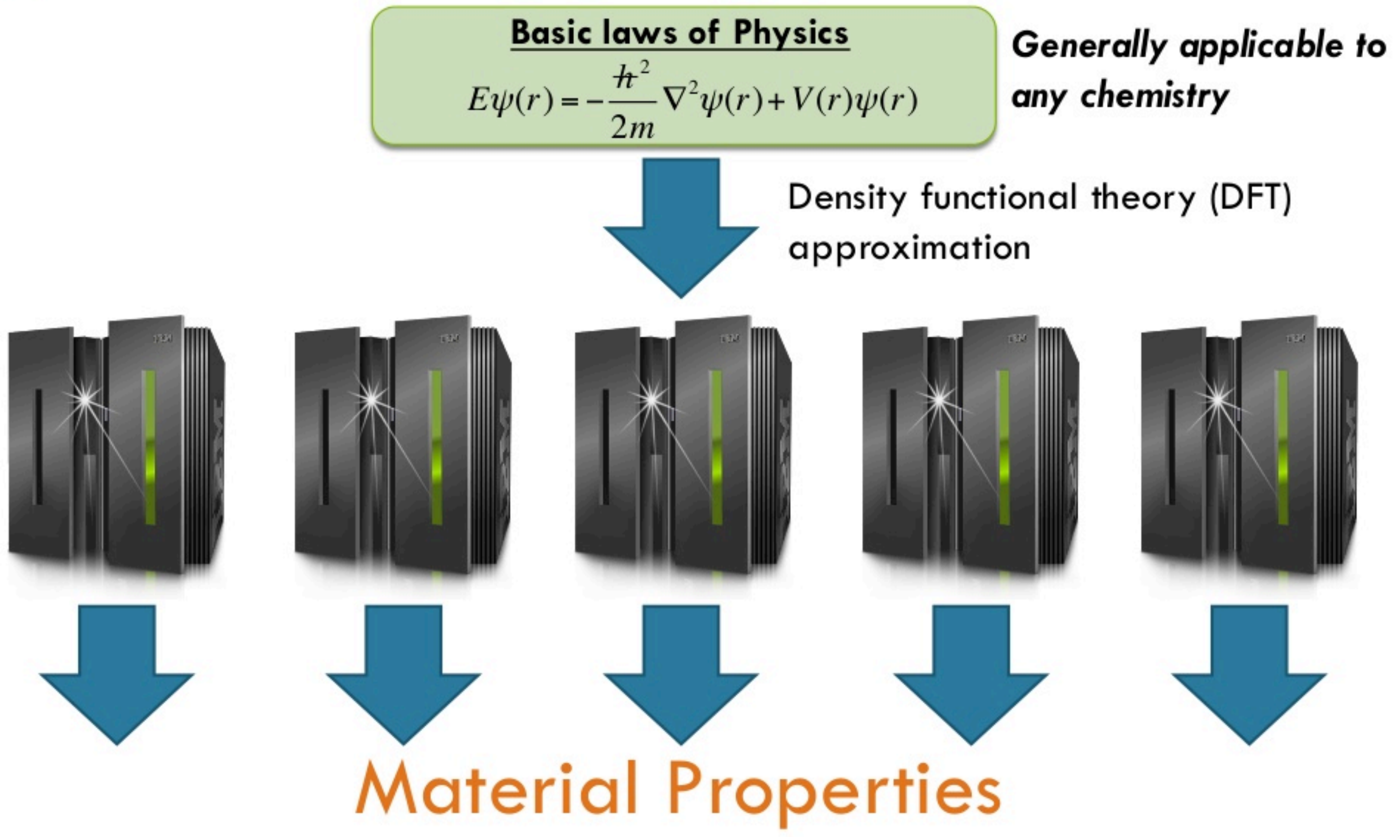
3) Write a batch script that will run your tasks on compute nodes

```
#!/bin/sh
#SBATCH -N 2 -c 32
#SBATCH -p debug
#SBATCH -t 00:05:00
cd $SCRATCH/myDir
export THREADS=32
runcommands.sh tasks.txt
```

http://www.nersc.gov/users/data-analytics/workflow-tools/taskfarmer/

Putting it all together: Materials Project

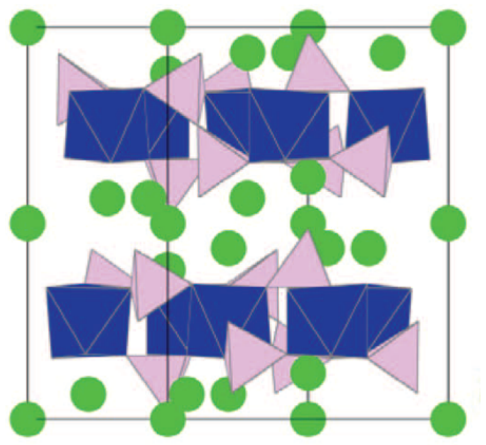
- **Simulate properties of all possible materials.**



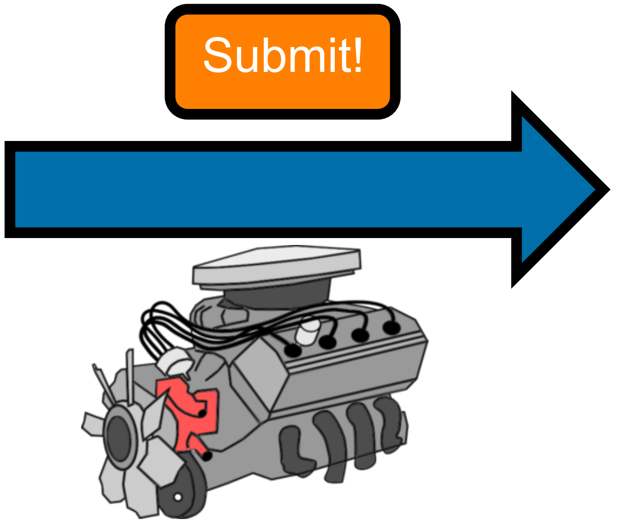
Basic laws of Physics
$$E\psi(r) = -\frac{\hbar^2}{2m}\nabla^2\psi(r) + V(r)\psi(r)$$
Generally applicable to any chemistry
Density functional theory (DFT) approximation
Material Properties

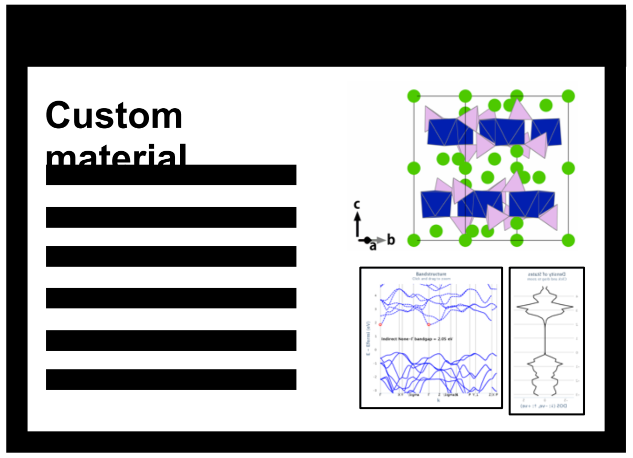
https://www.materialsproject.org/

Materials Project Workflow



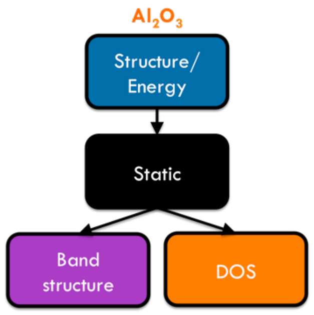
input: A cool material !!





output: Lots of information about cool material !!

Input generation (parameter choice)



Workflow mapping

Supercomputer submission / monitoring

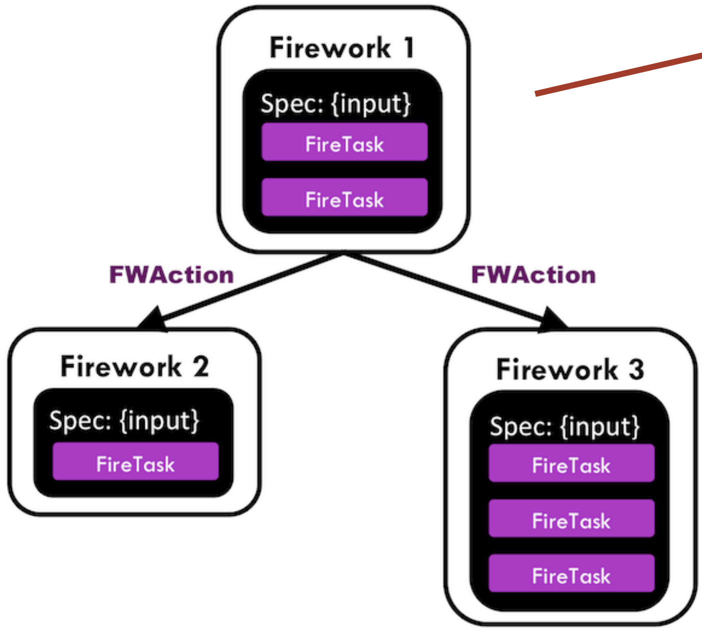
Error handling

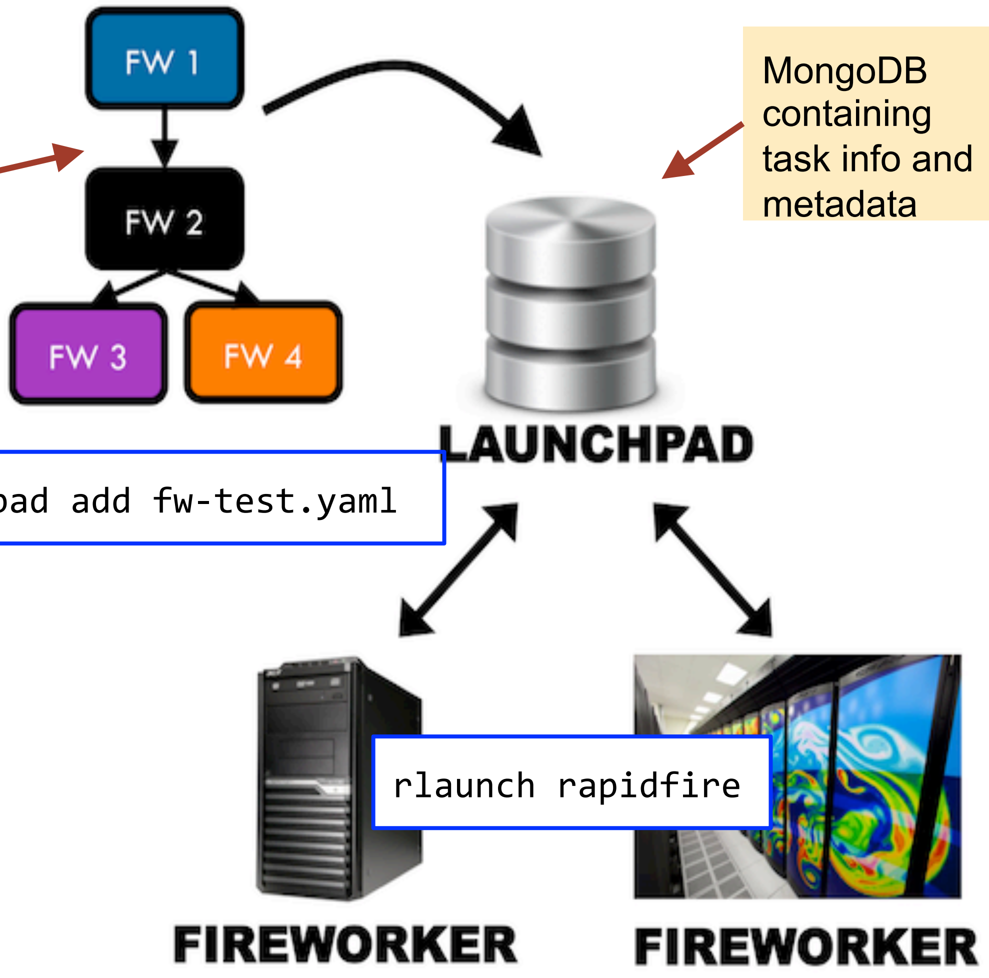
File Transfer

File Parsing / DB insertion

Use Case: Materials Project

- **Fireworks used to organise simulation and data workflow**





MongoDB containing task info and metadata

```
lpad add fw-test.yaml
```

```
rlaunch rapidfire
```

```
spec:
    _tasks:
    - fw_name: ScriptTask
    script: echo "hello" >> hello.txt
```

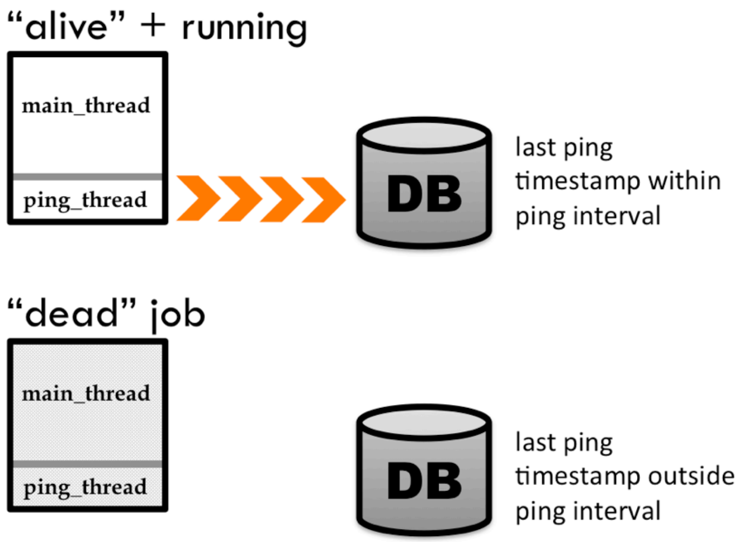
https://www.nersc.gov/users/data-analytics/workflow-tools/fireworks/

Use Case: Materials Project

- **Tasks submitted to Fireworks MongoDB via API/ python script etc.**
- **MongoDB keeps track of all tasks**
- **Fireworks submits workers to NERSC queues.**
- **Workers pull jobs from MongoDB.**
- **Fireworks manages job orchestration**
  - Retry on failure
  - File transfer
  - Job Dependencies
  - Flow control for subsequent jobs
  - Duplicate management

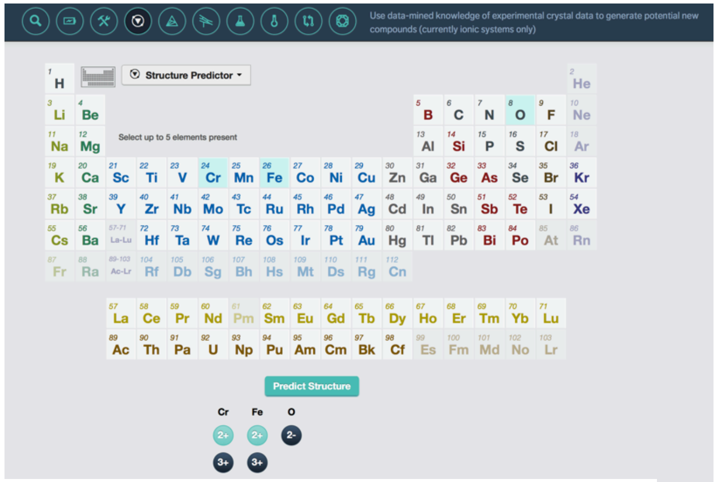
Fireworks: Error Handling and Dynamic Workflows

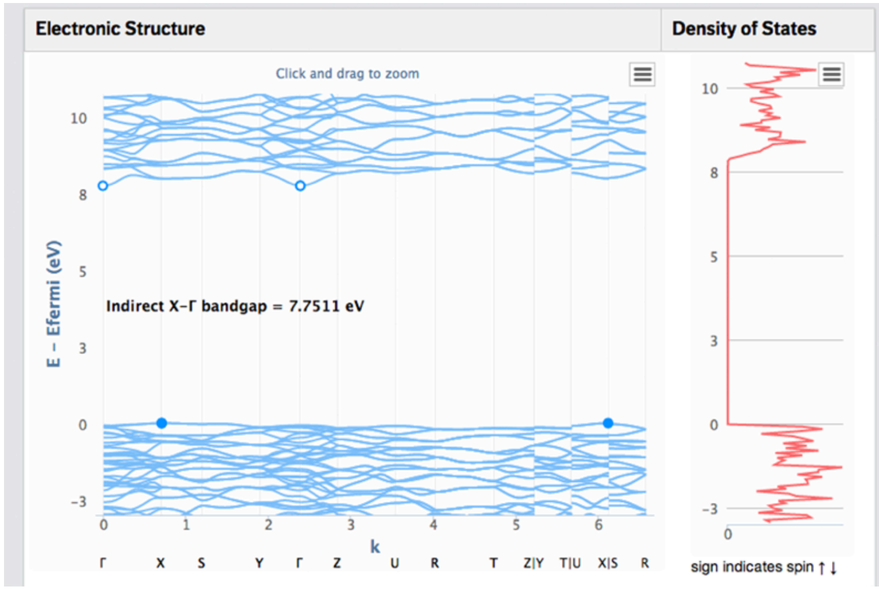
- Can change next step of workflow, based on outcome of previous step
- Can specify action based on soft failures, hard failures, human errors
  - "lpad rerun –s FIZZLED"
  - "lpad detect_lostruns –rerun"

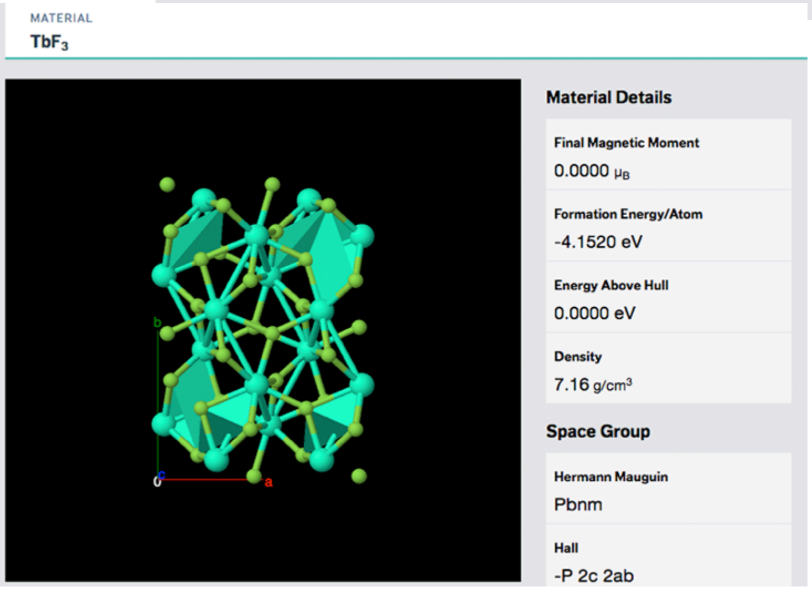

"alive" + running
main_thread
ping_thread
DB
last ping timestamp within ping interval
"dead" job
main_thread
ping_thread
DB
last ping timestamp outside ping interval

I DON'T ALWAYS MAKE A CATACLYSMIC MISTAKE
BUT WHEN I DO, I JUST GO BACK IN TIME AND FIX IT
Signs of the Timms

Materials Project Gateway


Use data-mined knowledge of experimental crystal data to generate potential new compounds (currently ionic systems only)
Structure Predictor
Select up to 5 elements present
Predict Structure
Cr
Fe
O
2+
2+
2-
3+
3+





MATERIAL

TbF_3

Material Details

Final Magnetic Moment	0.0000 μ_B
Formation Energy/Atom	-4.1520 eV
Energy Above Hull	0.0000 eV
Density	7.16 g/cm^3

Space Group

Hermann Mauguin	Pbnm
Hall	-P 2c 2ab

Finding the Right Hammer

- Workflow tools have lots of features but there is no one size-fits-all
- NERSC is building expertise in classes of workflow tools and will help guide you towards the right tool for your job
- Consider stitching together a couple of different tools to make it all work for you.

Thank you.