The Materials Project: An application of high-throughput computing

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Materials development is a key bottleneck to realizing renewable energy

solar PV

electric vehicles

other:

waste heat recovery (thermoelectrics)

hydrogen storage

catalysts/fuel cells

Example: Everyone hates batteries

PHONES

Why Your Smartphone Battery Sucks

By Megan Geuss, PCWorld May 18, 2011 6:36 PM

If you're hoping your next smartphone will run faster, shine brighter, connect at 4G speed, *and* last longer on one battery charge, you may be in for a rude surprise. The thirst for battery power in new smartphones and tablets is far outpacing improvements in battery technology. Battery makers are trying to wring the last bits of capacity out of 15-year-old lithium ion technology, while device and app makers seem to be just waking up to the seriousness of the problem. There's an equal share of blame for all parties; meanwhile the immense promise of innovation in mobile devices could come to an early halt due to power limitations, and consumer angst over constantly having to "plug in."

Used to be, you could forget your feature phone's charger at home, go on a long weekend vacation, and--as long as you didn't play hours of Snake--still come home with enough battery life to call a cab. Today, though, we're wedded to our chargers, glaring hawkishly at people who've been hogging airport and coffee shop outlets for too long.

Gadgets

When Lithium-ion Batteries Explode

Paul Mah - May 27, 2008 6:47 PM

Print ShareThis New +1 0 20 comment(s) - last by cogito.. on May 29 at 1:55 AM

Lithium-ion batteries are both a blessing and a curse when it comes to mobile electronics

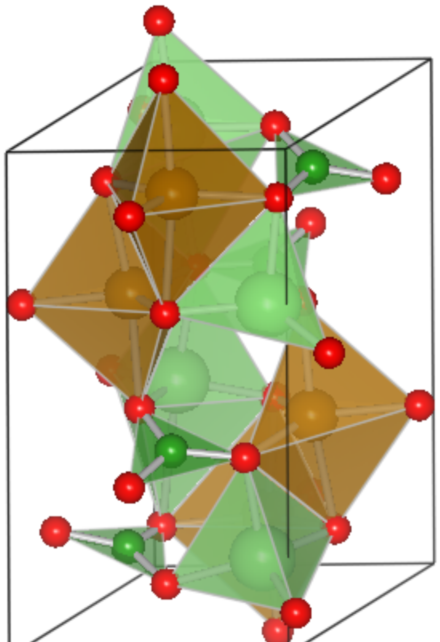
BlackBerry Curve battery: Cells made in Japan, but assembled where? (Source: Paul Mah)

The topic of exploding lithium-ion batteries has been debated to death in the wake of massive battery recalls over the last couple of years. Amidst the deft public relations maneuvering and finger-pointing, however, the question as to why they explode in the first place is still shrouded in mystery for many.

The most important thing to understand here is that lithium-ion technology is considerably more volatile compared to other forms of rechargeable battery technologies. Defects in the insulating membrane can result in a mini-explosion that rips a battery open to release steam in excess of 600 degrees Fahrenheit.

Manufacturers are aware that it is statistically probable for a lithium-ion to fail, though the calculations employed to sideline the risk are sometimes quite suspect. To determine the mean time between failures (MTBF), manufacturers take a sample of say, 1,000 batteries, which are then used until one fails.

Density Functional Theory is a way to generate materials properties



- ~200 CPU-hours per calc.
- 1-5 calcs per material
- moderately finicky calcs.

$;t)$

$$H = \sum_{i=1} \nabla_i + \sum_{i=1} V_{nuclear}(r_i) + \sum_{i=1} V_{effective}(r_i)$$

Examples of real materials design:

G. Hautier, A. Jain, and S.P. Ong,
From the computer to the laboratory: materials discovery and design using first-principles calculations
Journal of Materials Science (2012)

Total energy
Optimized structure
Magnetic ground state
Charge density
Band structure / DOS

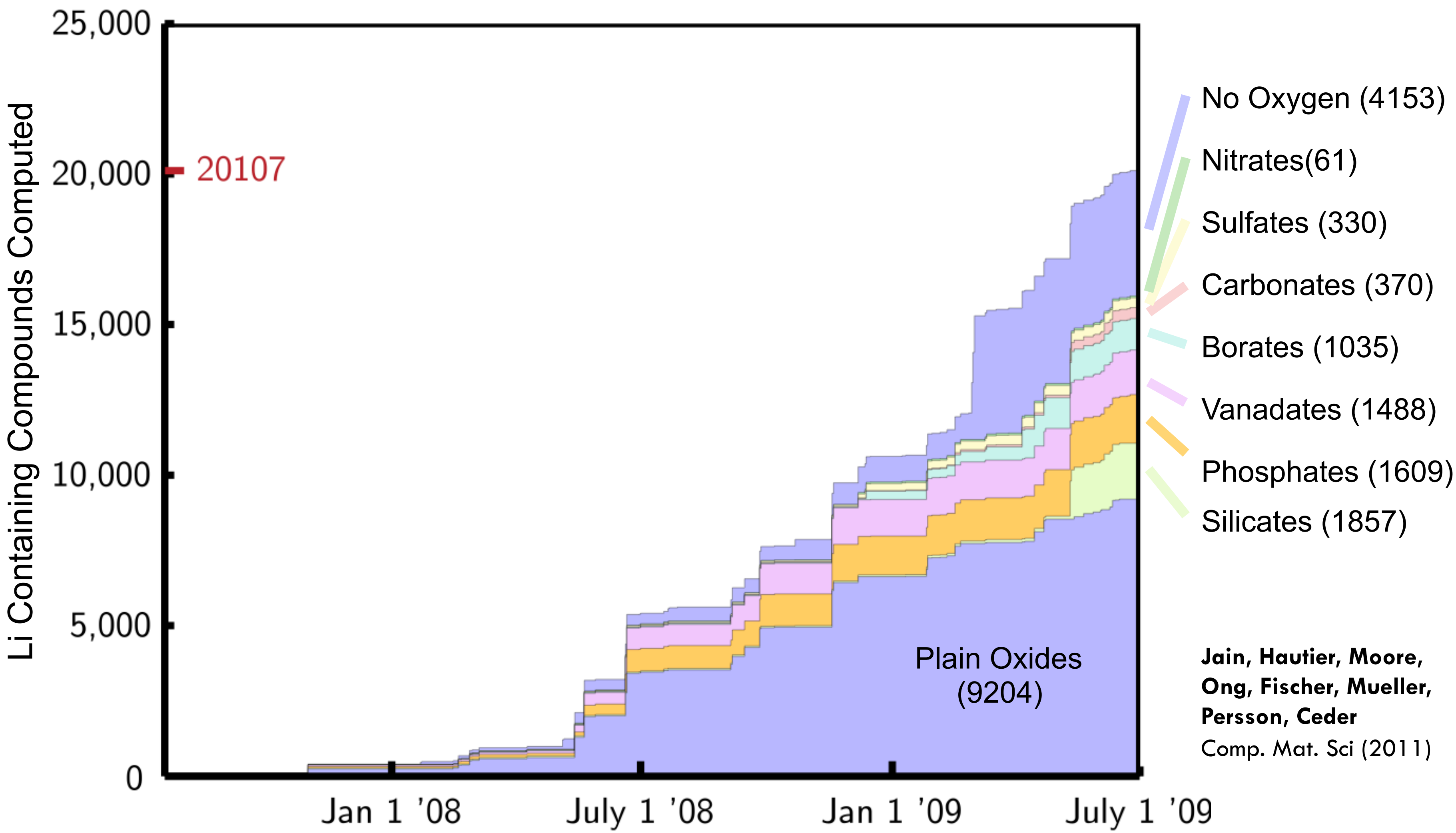
Searching for Li ion battery materials

$$Li_a\ M_b\ (XY_c)_d$$

Li ion source	electron donor / acceptor	structural framework / charge neutrality
	examples: $V^{4+/5+}$, $Fe^{2+/3+}$	examples: O^{2-}, $(PO_4)^{3-}$, $(SiO_4)^{4-}$

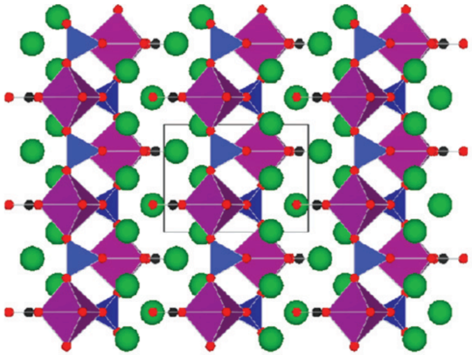
common cathodes: $LiCoO_2$, $LiMn_2O_4$, $LiFePO_4$

Compounds screened over time



Jain, Hautier, Moore, Ong, Fischer, Mueller, Persson, Ceder
Comp. Mat. Sci (2011)

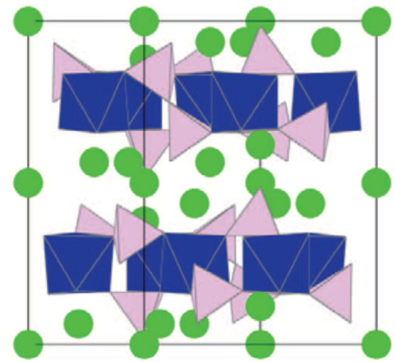
New materials found for Li ion batteries



Li_3 (Fe, Mn) PO_4 CO_3

Hautier, Jain, Moore, Chen, Moore, Ong, Ceder
Journal of Materials Chemistry (2011)
Chen, Hautier, Jain, Moore, Kang, Doe et al.
Chemistry of Materials (2012)

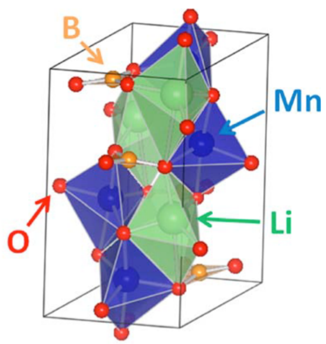
(patent filed)



Li_9 V_3 $(P_2O_7)_3$ $(PO_4)_2$

Jain, Hautier, Moore, Kang, Lee, Chen, Twu, Ceder
Journal of the Electrochemical Society (2011)

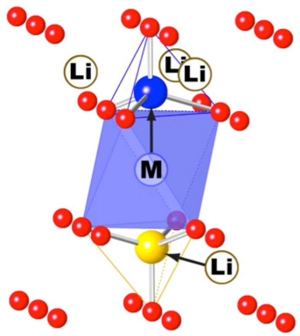
(patent issued allowance)



Li Mn BO_3

(patent filed)

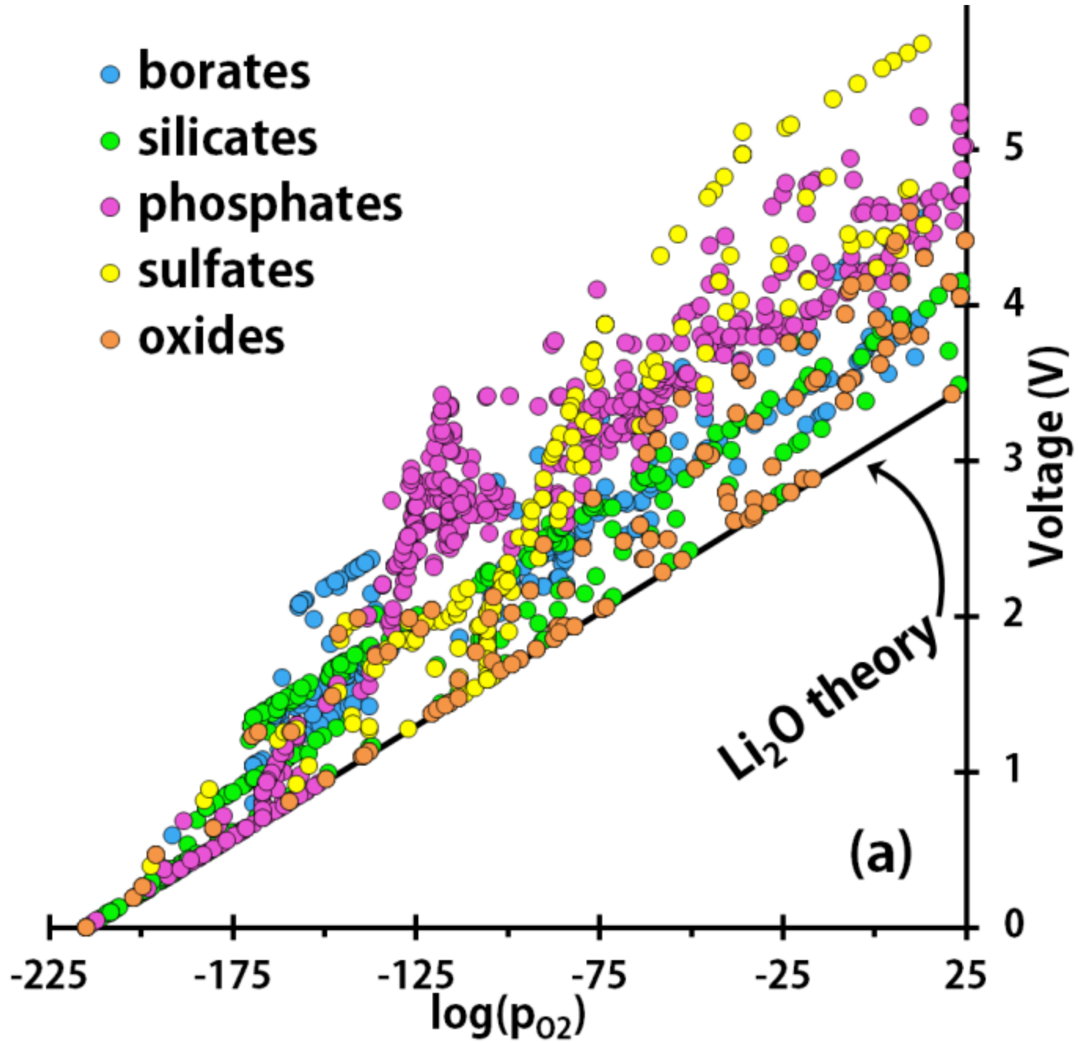
Kim, Moore, Kang, Hautier, Jain, Ceder
Journal of the Electrochemical Society (2011)



Li (V, Cr) O_2

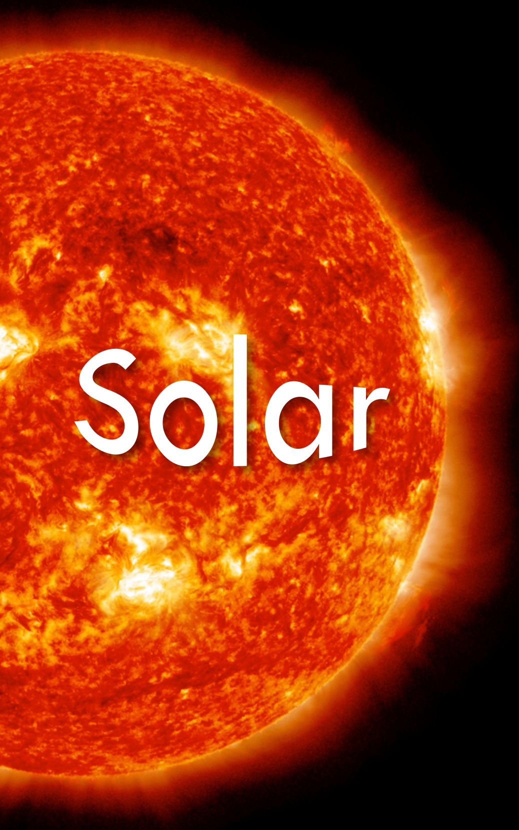
Ma, Hautier, Jain, Ceder
Journal of the Electrochemical Society (submitted)

High voltage materials are less safe: but there is lots of scatter

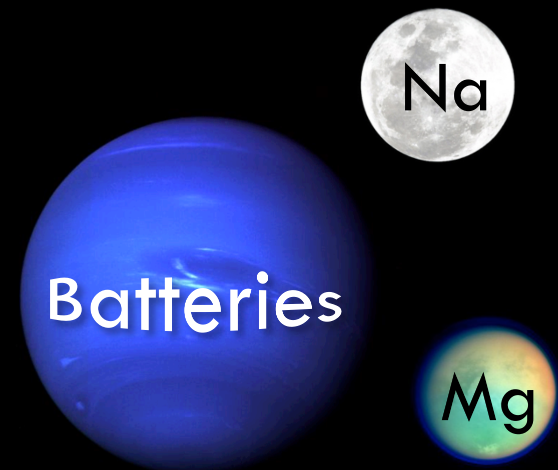


Jain et al.
(in preparation)

Once the army is in place, you can attack more problems



Jain, Reihani, Fischer, Couling, Ceder, Green,
Chemical Engineering Science 65, (2010).

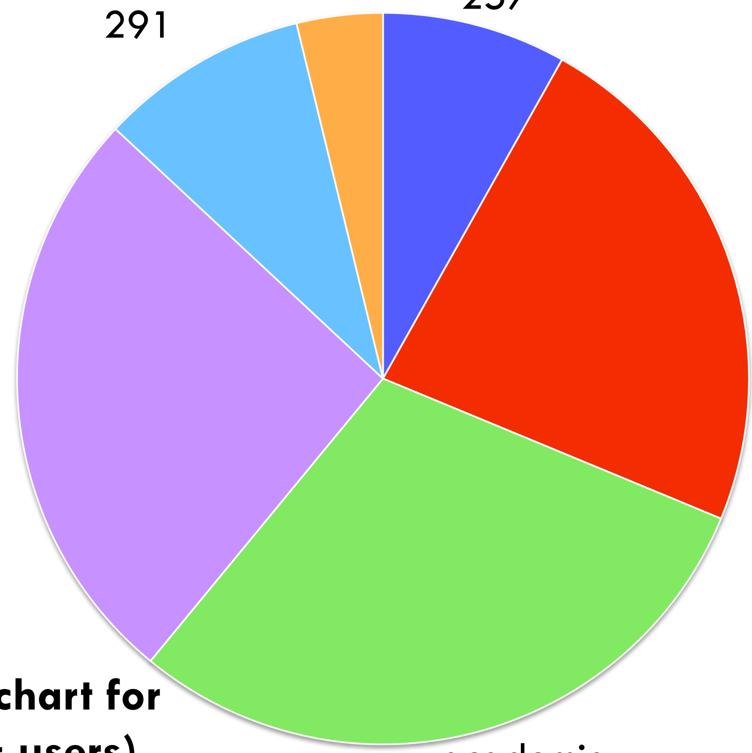


collaboration with Cambridge
another collaboration at LBL

High-throughput diffusion calculations (NEB)
XANES and EXAFS spectra codes
Multiscale modeling / porous materials
Rapid Phase Diagrams
Bulk modulus

www.materialsproject.org

3500 users and growing!



(*Old chart for 3150+ users)

User Papers using Materials Project data

Table III. Observed average voltage (vs Li) and the average voltage at 0 K calculated from the Materials Genome Project[15] for some Li_xM alloys.

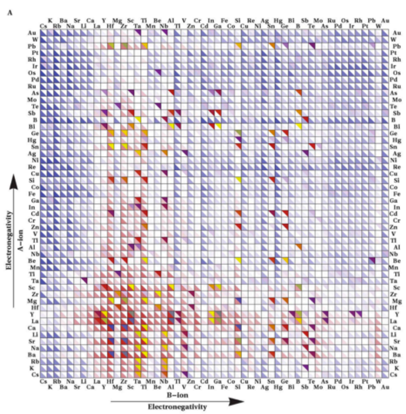
	Average Voltage (V)	
Alloy System	Calculated	Measured
Li_xSi	0.34	0.36
Li_xSn	0.57	0.51
Li_xAl	0.35	0.40

Design of alloy anodes for Li ion batteries

(compared measurements to calculations)

Tran, Obrovac

Journal of the Electrochemical Society (2011)



Computational screening of perovskite metal oxides for optimal solar light capture

(crystal structures for candidate stability screening)

Castelli, Olsen, Datta, Landis, Dahl, Thygesen, Jacobsen

Energy & Environmental Science (2011)

TABLE 16. Energies calculated from the MGP Reaction Calculator vs. measured enthalpies taken from MGP database, and the ratios of these numbers

	$\Delta E^f_{ox}(0)$ kJ/mol	ΔH^f_{ox} kJ/mol	$\Delta E^f_{ox}(0)/\Delta H^f_{ox}$
$MgCO_3$	–81	–117	0.69
$CaCO_3$	–148	–178	0.83
$SrCO_3$	–198	–235	0.84
$BaCO_3$	–238	–276	0.86

DFT Formation Enthalpies of Rare Earth Orthophosphates

(find scaling factor for computed heat of formation)

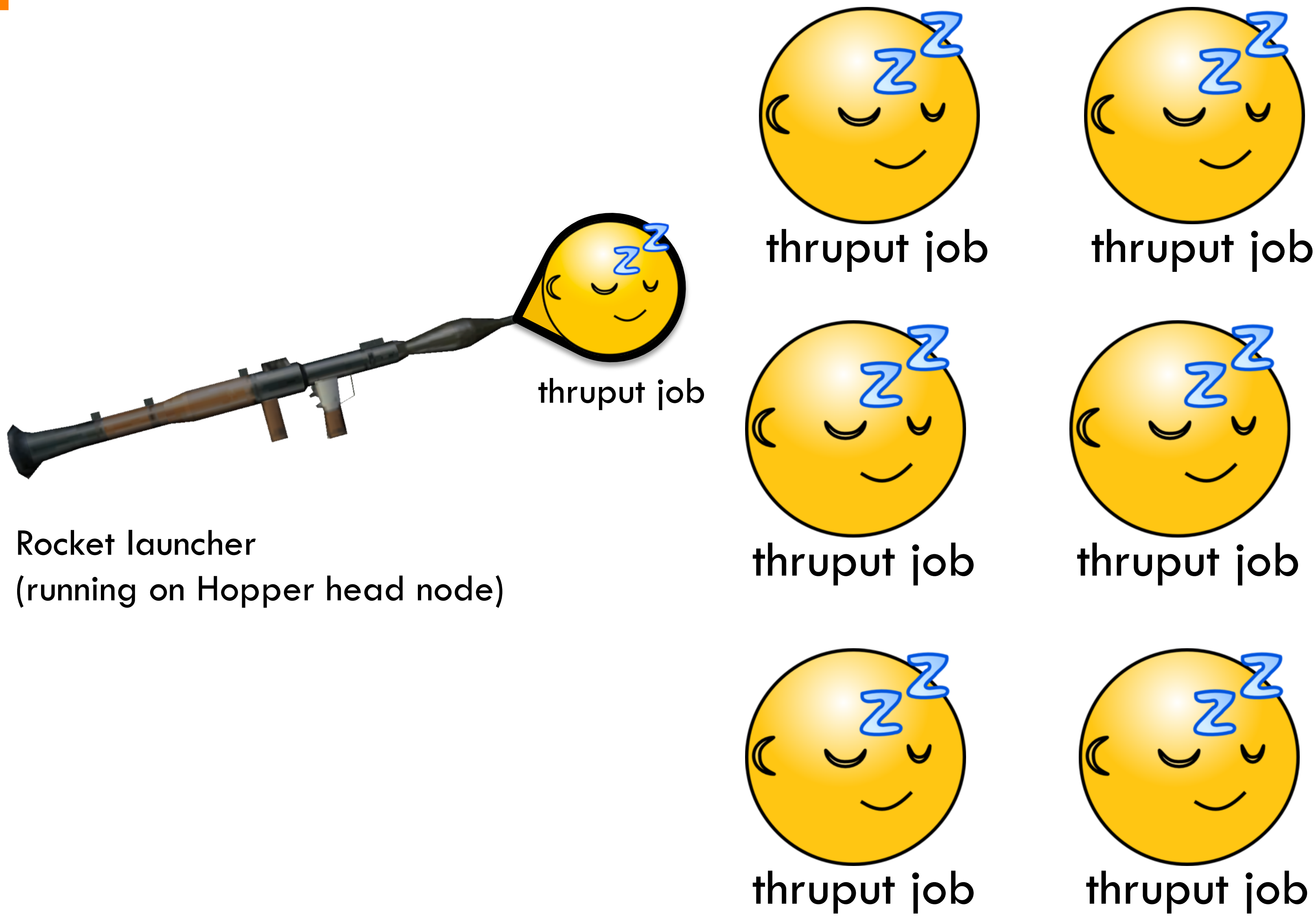
Rustad

American Minerologist (2012)

"Thanks. Your product is astounding. I redid work for a recent paper that took weeks in about 15 minutes! I guess this is truly “transformative” science in the NSF sense!"

"Toruk makto":
How to get Hopper to run high-throughput?

How we set up our NERSC infrastructure



What happens when job starts running?

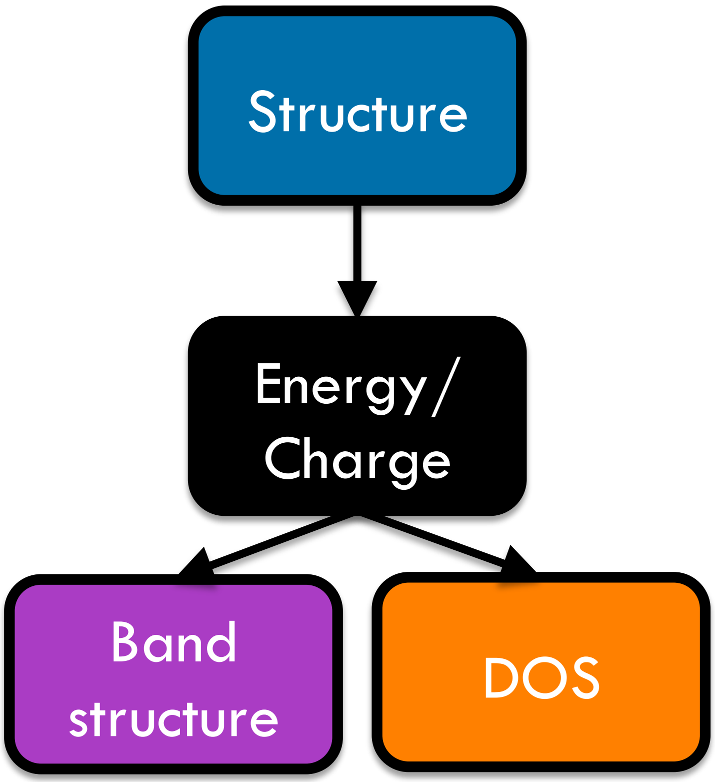
Job wakes up when PBS runs it

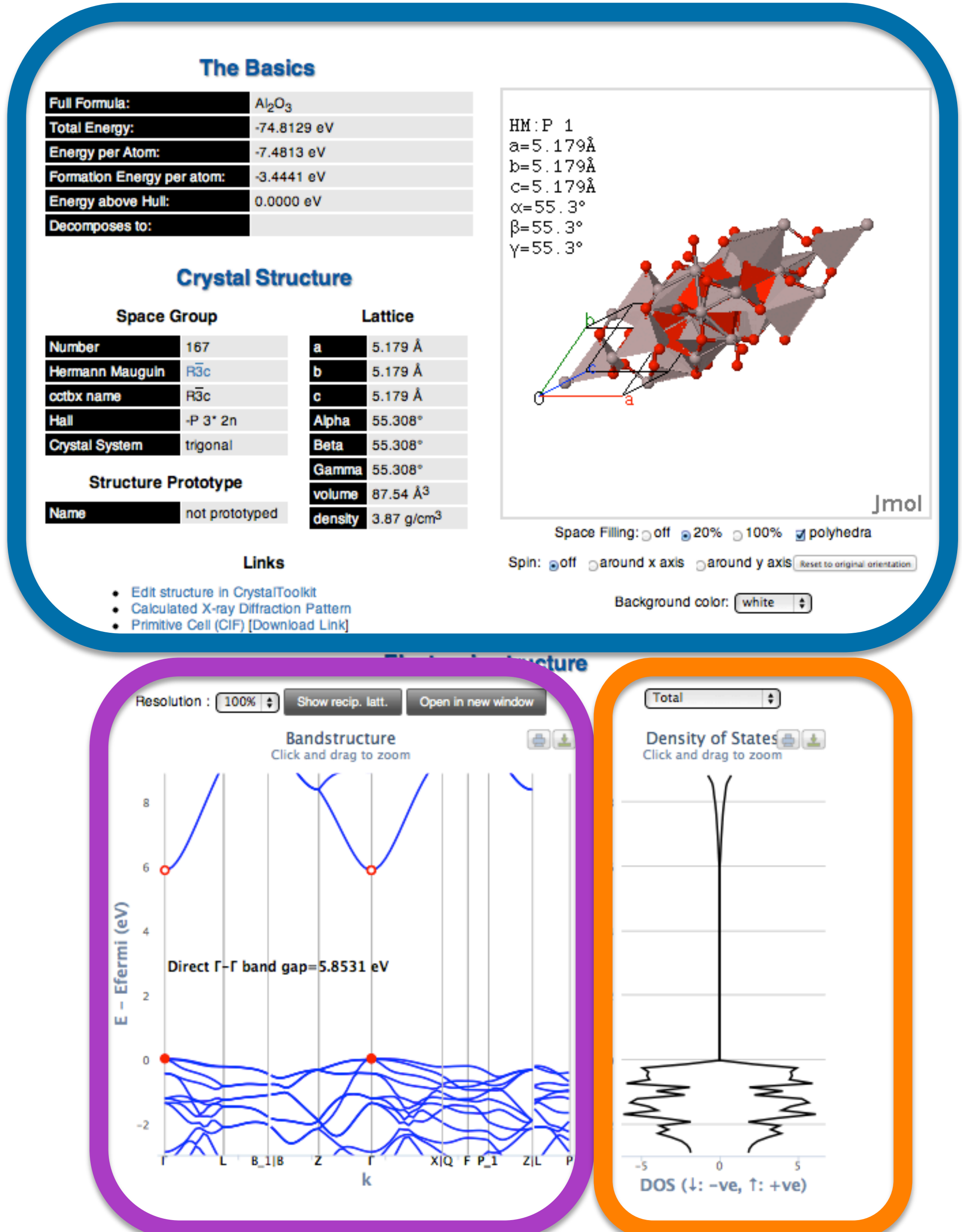
Grabs the latest job description from an external DB

Runs the job based on DB description

Need workflow to get multiple properties

Al_2O_3

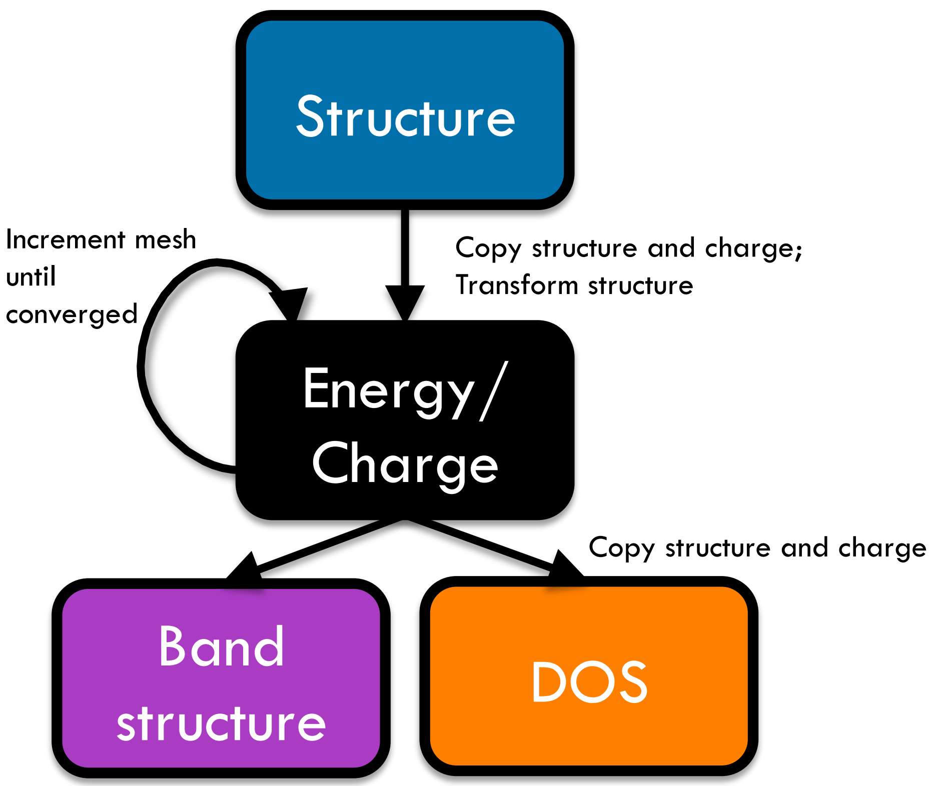




Workflow handles logic and 'Plan B'

CALCULATION PLAN

Al_2O_3

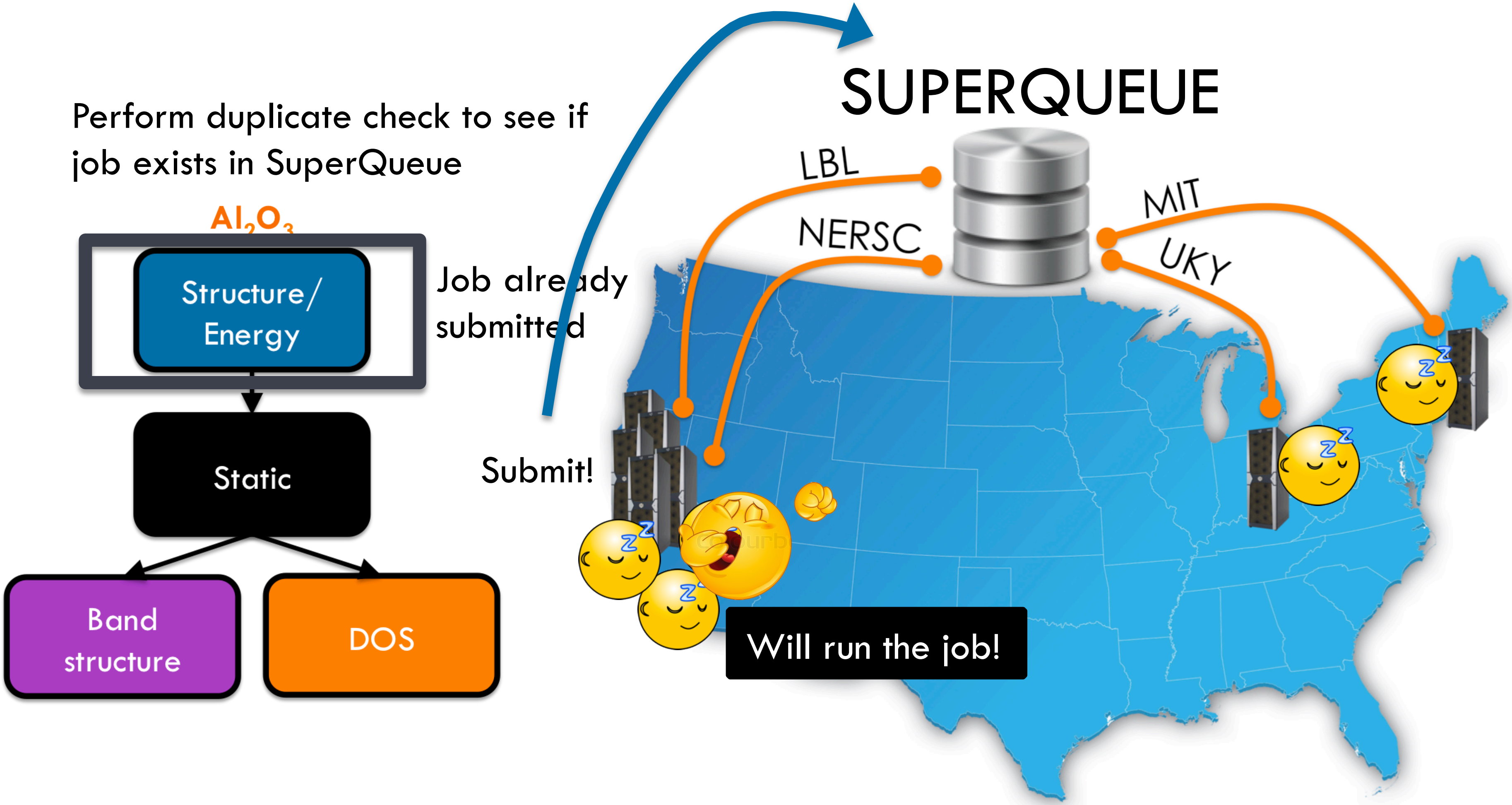


How should the system respond if:

- A node crashes?
- The calculation does not converge?
- Early calculations indicate a materials is more/less interesting?
- We might have already done this calculation?

Specify **DYNAMIC** workflow!

A calculations superqueue distributes jobs over multiple resources



work done with M. Kocher

Which workflow do we use?

Developed our own workflow software based on Mon

opment:

In Pro

FireW

Interested in FireWorks?

http://pypi.python.org/pypi/FireWorks/

or Google 'PyPi FireWorks'

Open-source

The impact of the workflow system

- We completed over ***10 million*** CPU-hours of high-throughput DFT computations in under 6 months at NERSC

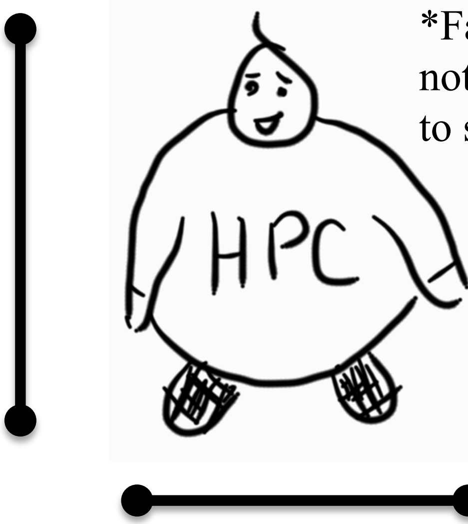
- Used 2300+ CPUs on average, 24/7

- Our army is large!

HPC vs. HT – there's still a mismatch

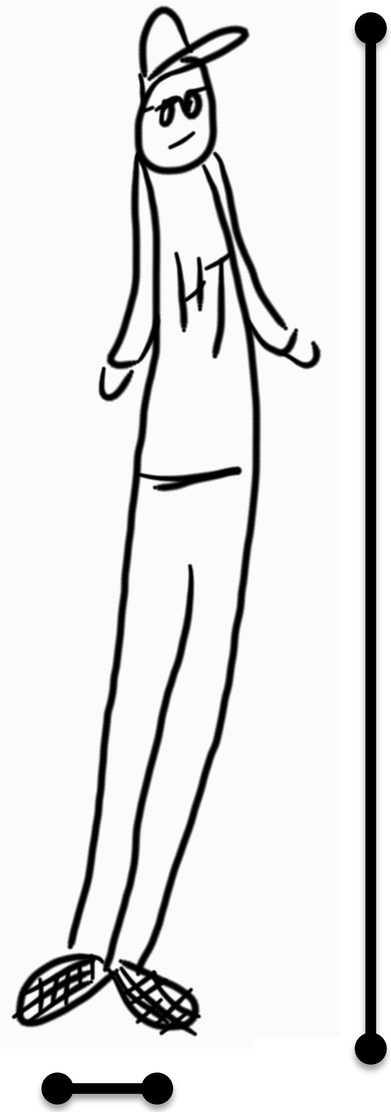
Our jobs need to gain weight (and lose height)!

Short walltime
~hours



*Fatness not drawn to scale

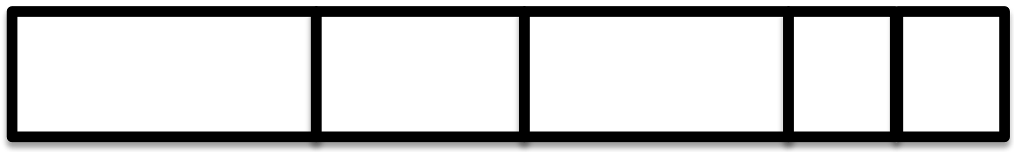
“Fat” concurrency
(16000+ nodes)



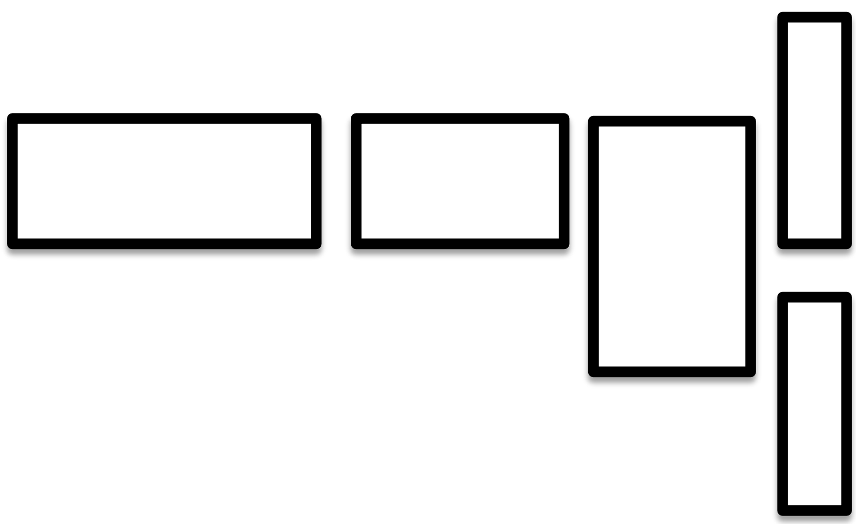
Long walltime
~days

“Thin” concurrency
(1 node)

The height issue – workflows sometimes help



Single script that does multiple tasks in succession

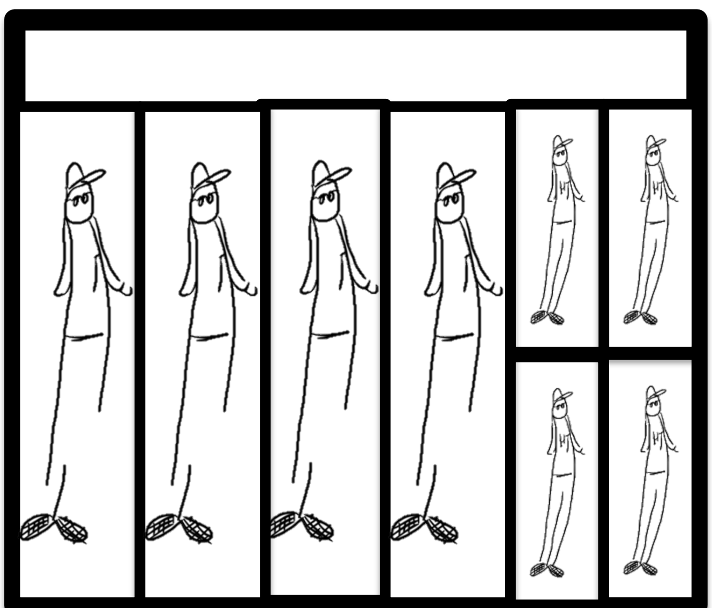


Atomic tasks connected by workflow software

The height issue:
Need to implement checkpoint/restart

From skinny to fat:
PBS autopacking to address concurrency

Need checkpoint/restart to fill leftover time



PBS

~

Trying to build this into FireWorks in the future

Conclusion / Final thoughts on HT

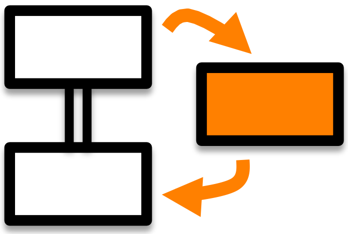
- Materials Project is an example of 'Science Gateway' based on HT-computed data
- At NERSC, viable options for HT already exist
  - We use thruput queue heavily (you may have noticed)
  - new tools under development
- Different groups are developing solutions
  - Will be interesting to know what 'sticks', or if equilibrium will be unique workflow per project
  - Would love to discuss it with you!

Thank you!

- Materials Project
  - Kristin Persson, Gerbrand Ceder, Shyue Ping Ong, Geoffroy Hautier, Michael Kocher, David Skinner, Dan Gunter, Shreyas Cholia, NERSC staff
- Funding
  - DOE, NSF, 2010 LBL LDRD
- Contact:
  - ajain@lbl.gov

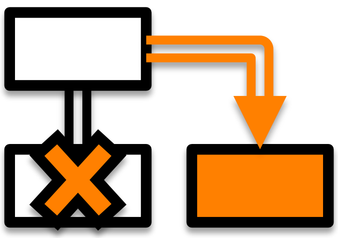
Backup slides

Deviations from a simple linear workflow



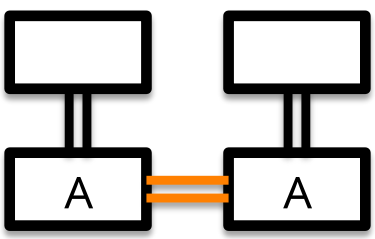
Detours

(about 10-20% of jobs fail and must be rerun with different input parameters)



Branches

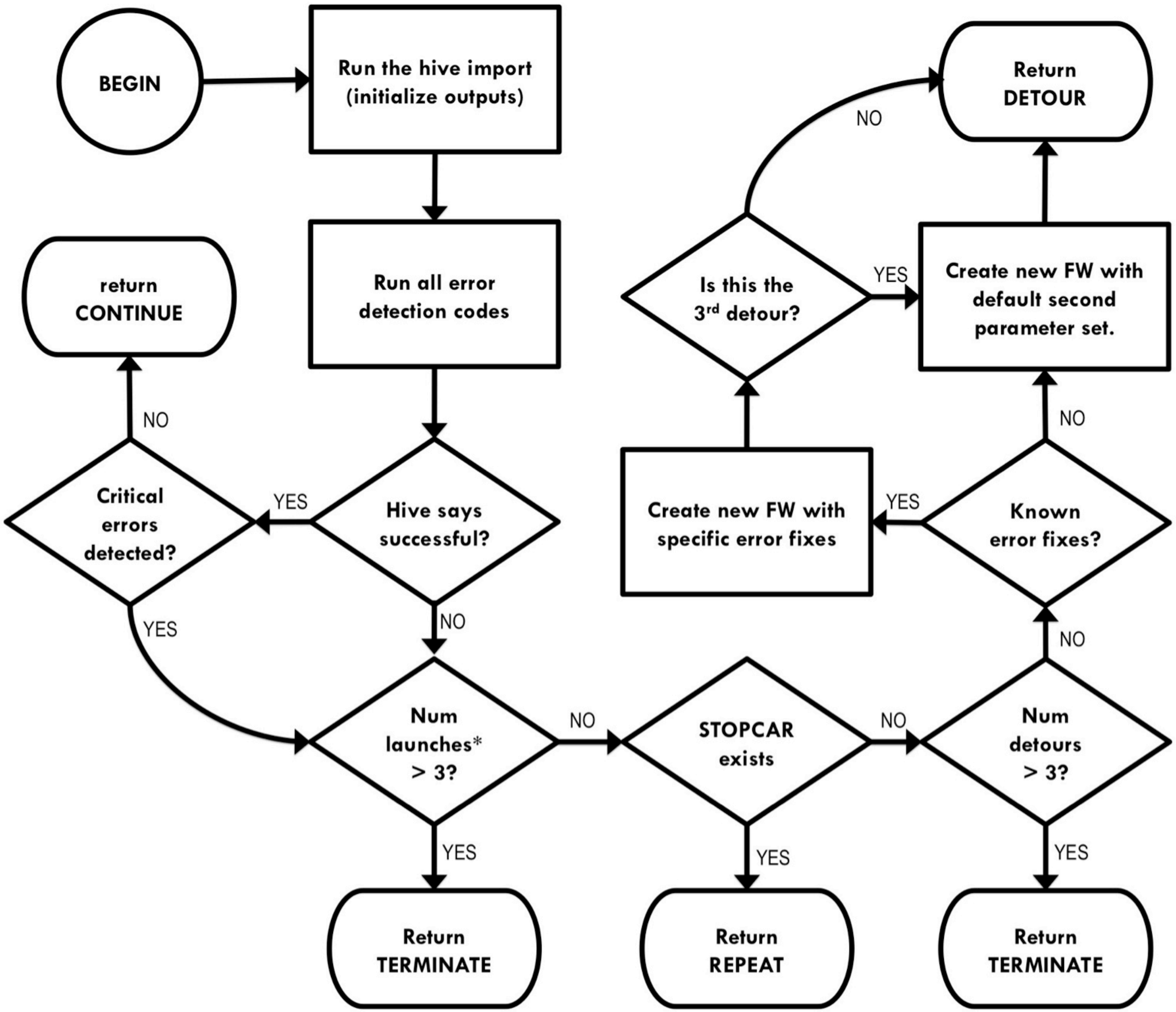
(based on the result of a calculation, the entire workflow might need to be modified)



Duplicate Job detection

(if two workflows contain an identical step, ensure that the step is only run once)

Example: Analyzer object decides how to proceed once a VASP calculation finishes



Examples of high-throughput studies

Application	Researcher	Search space	Candidates	Hit rate
Scintillators	Klintenberg et al.	22,000	136	1/160*
	Curtarolo et al.	11,893	?	?
Topological insulators	Klintenberg et al.	60,000	17	1/3500*
	Curtarolo et al.	15,000	28	1/535*
High T_C superconductors	Klintenberg et al.	60,000	139	1/430*
Thermoelectrics	Curtarolo et al.	2,500	20	1/125*
1-photon water splitting	Jacobsen et al.	19,000	20	1/950*
2-photon water splitting	Jacobsen et al.	19,000	12	1/1585*
Transparent shields	Jacobsen et al.	19,000	8	1/2375*
Hg adsorbers	Bligaard et al.	5,581	14	1/400*
HER catalysts	Greeley et al.	756	1	1/756
Li ion battery cathodes	Ceder et al.	20,000	4	1/5000

Entries marked with * have not experimentally verified all the candidates.
Hit rates are optimistic because the search space is often restricted based on intuition.