Colmena: Parsl for Intelligent Workflows on Exascale HPC

Cleared for public release

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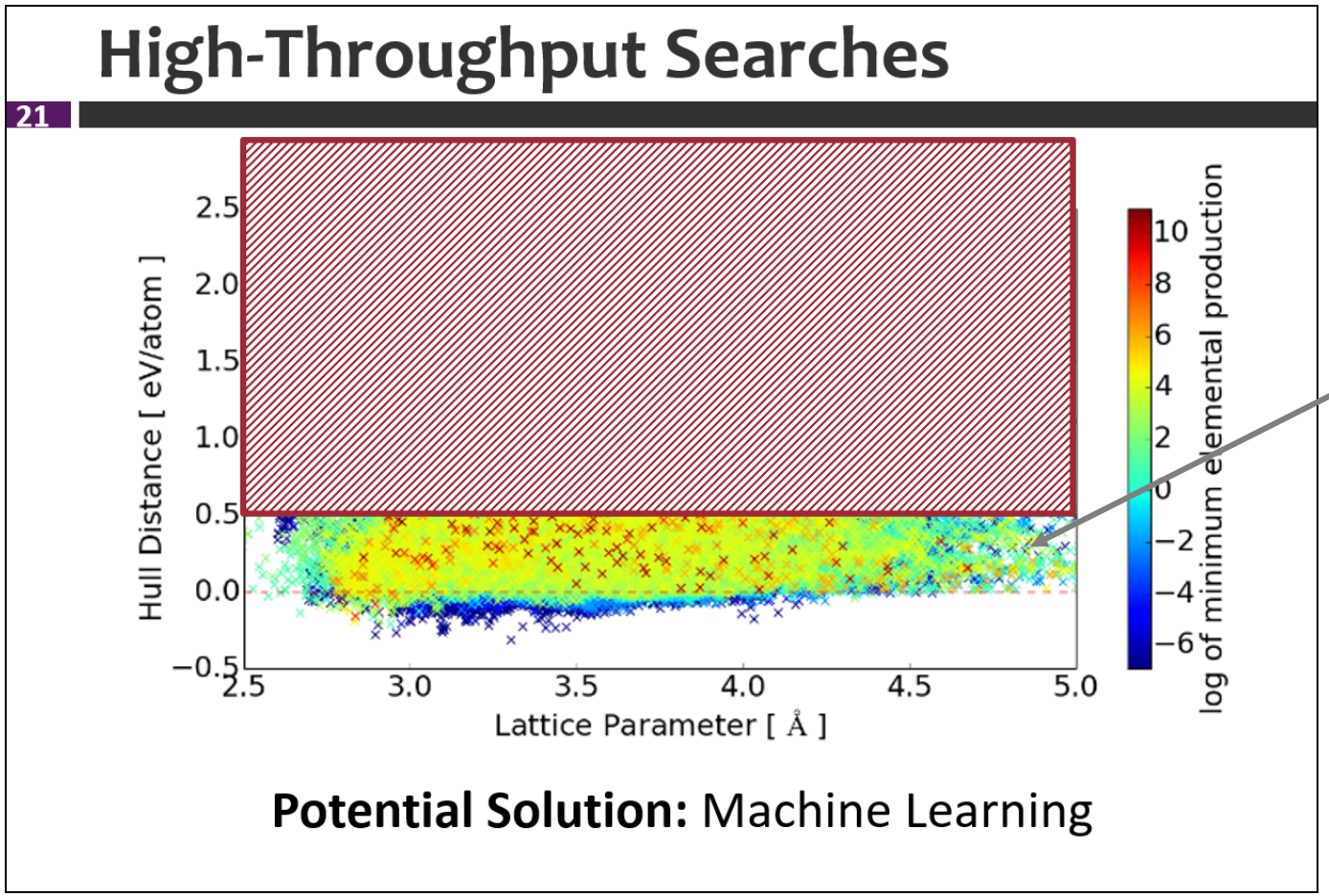
I've been bothered by high-throughput searches for a decade



Each point is ~5 CPU-hr
(~2.5 kW-hr, ~500g coal burned*)

There are few reasons we should be running brute-force

Figure: Kirklin et al. Acta Mat (2016)

*Assuming 500W node, US EPA Greenhouse Gas Calculator

There are easy opportunities for adding intelligence

The Application	The Data Flow Kernel	The Worker

`futures = [`
`  do_science(task)`
`  for task in everything`
`]`
`results = [`
`  task.result()`
`  for task in futures`
`]`
`report_findings(results)`
	Parsl Magic ✨	Science Effort ⚛

Doing Nothing 🙂

Hard at work 😭

Today's Talk: How can we make "The Application" smarter?

Getting More from Your HPC with Colmena

Active Learning is a better plan, and not my idea at all

See also: Bayesian Optimization, Surrogate Optimization, Optimal Experimental Design…

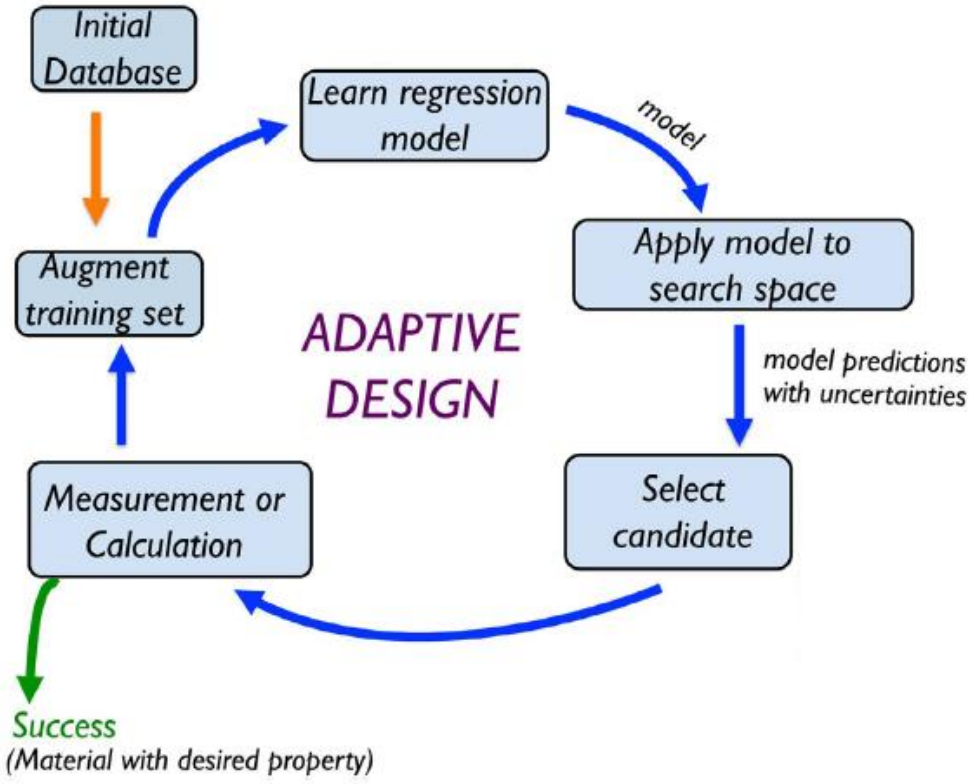
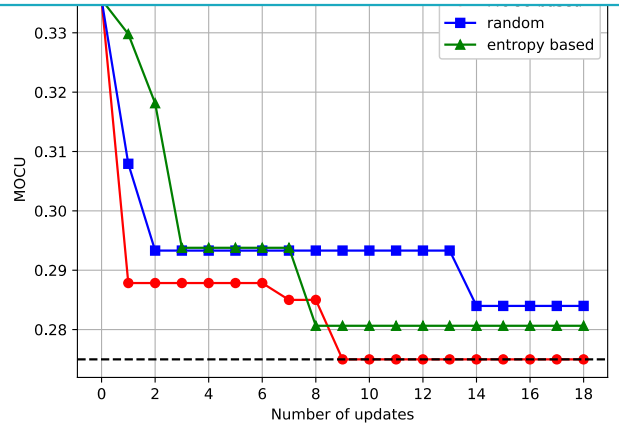


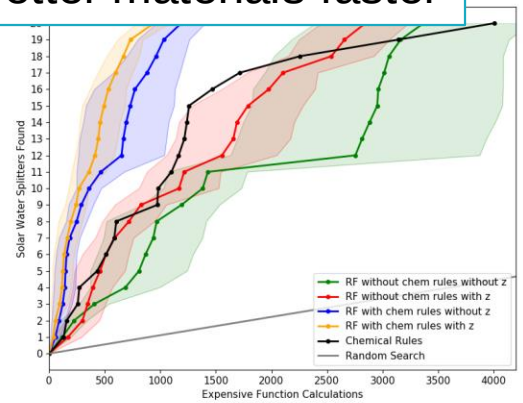
Figure: Balachandran *et al*. Sci. Rep. (2016), 19660.

Fit models with fewer simulations



Courtesy of: Byung-Jun Yoon

Find better materials faster



https://hackingmaterials.lbl.gov/rocketsled/

How would be integrate these concepts into our application?

How can I do this with Parsl?

Inside the Workflow: `join_app`

General Idea: Tasks which make new tasks

Advantages:

- DFK handles all effort
- Simple instructions -> simple functions

Challenges:

- *How should(!?) join_app tasks share state?*

Outside the Workflow: Events, Threads

General Idea: Steering logic from “main.py”

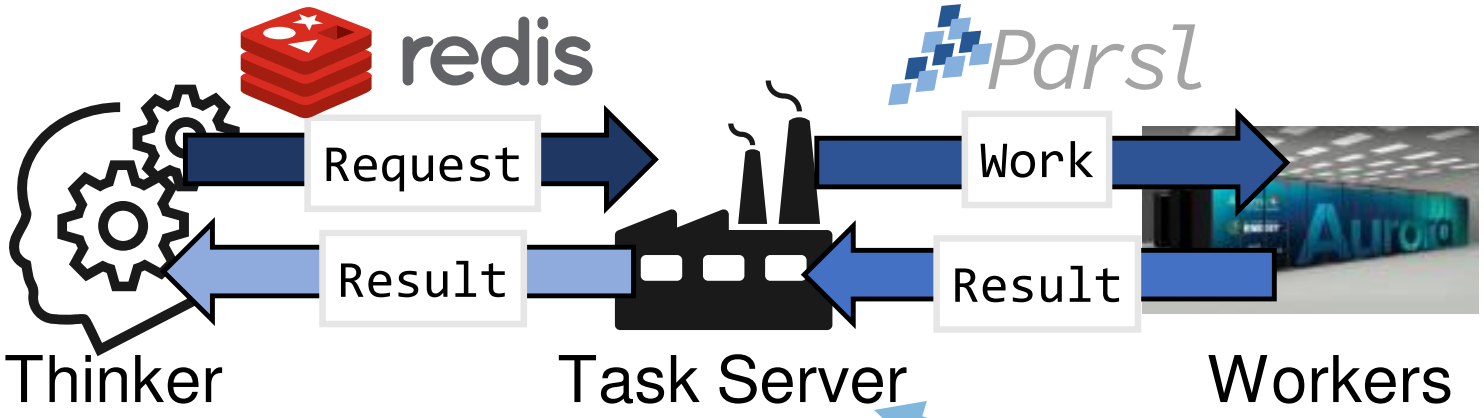
Advantages:

- Clearer control over concurrency
- Explicit control over shared state
- Respond to events besides “task complete”

Challenges:

- ***How would one write such a thing?***

Colmena is a wrapper over Exascale Workflow tools



Programming Model: Task Queues

```
# Primitive Units
queue.send_inputs(1)
result = queue.get_result()
```

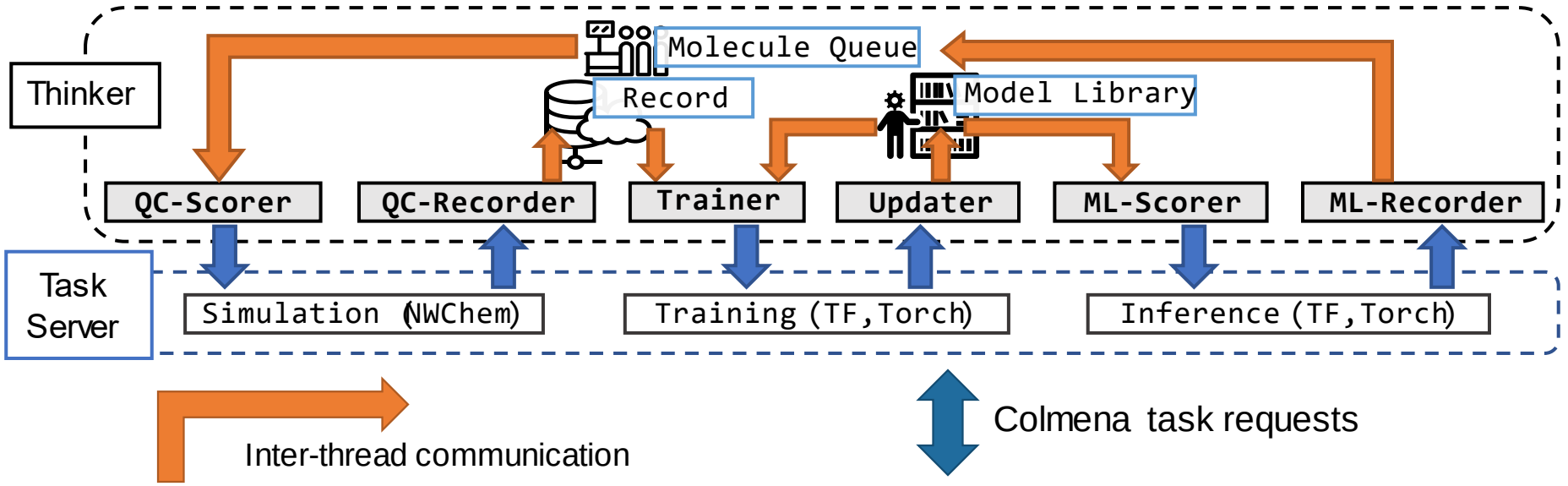
Programming Model: Agents

```
class Thinker(BaseThinker):
 @agent
 def make_work(self):
  self.queue.send_inputs(1)
```

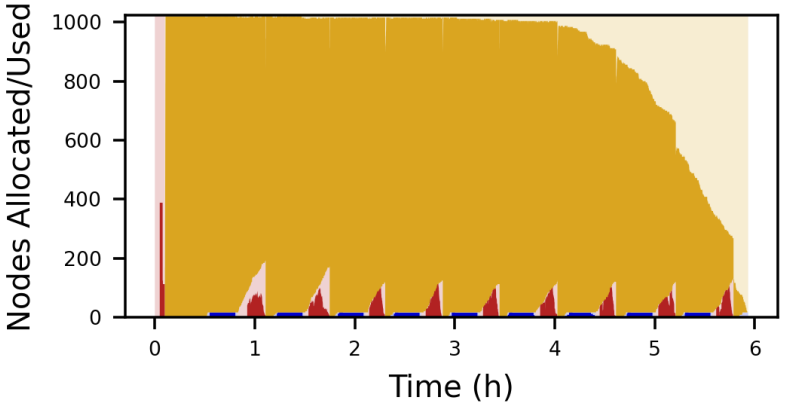
Task Server:
- Dispatches work requests to compute
- Communicates results back to thinker

Backend:
- Supports most HPC and cloud services
- Easily configure multiple worker types, multi-site workflows
- Limited support for ensembles of MPI applications
- *Future:* Balsam, FuncX, RCT

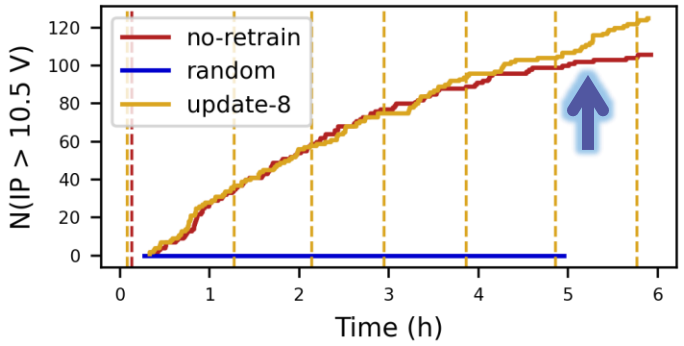
Example application: “Interleaved,” AI-in-the-loop optimizer



Retasking nodes between jobs…



…yields more science per compute-hour.



Details: Ward et al. ML4HPC, SC21.

Tutorial: colmena.rtfd.io/en/latest/examples.html#tutorials

So, what's new in '23?

Building more apps, learning more requirements!

ExaMol: An attempt at user-friendly Colmena

Please, don't look at v0-v4 our molecular design applications

Step 1: Write a spec

```
recipe = RedoxEnergy(charge=1,
                     compute_config='xtb')
spec = ExaMolSpecification(
    database='training-data.json',
    recipe=[recipe],
    search_space='search_space.smi',
    selector=GreedySelector(n_to_select=8),
    simulator=ASESimulator(scratch_dir='/tmp'),
    scorer=RDKitScorer(recipe),
    models=[[KNeighborsRegressor()]],
    num_to_run=8,
    thinker=SingleStepThinker,
    compute_config=config,
    run_dir='run'
)
```

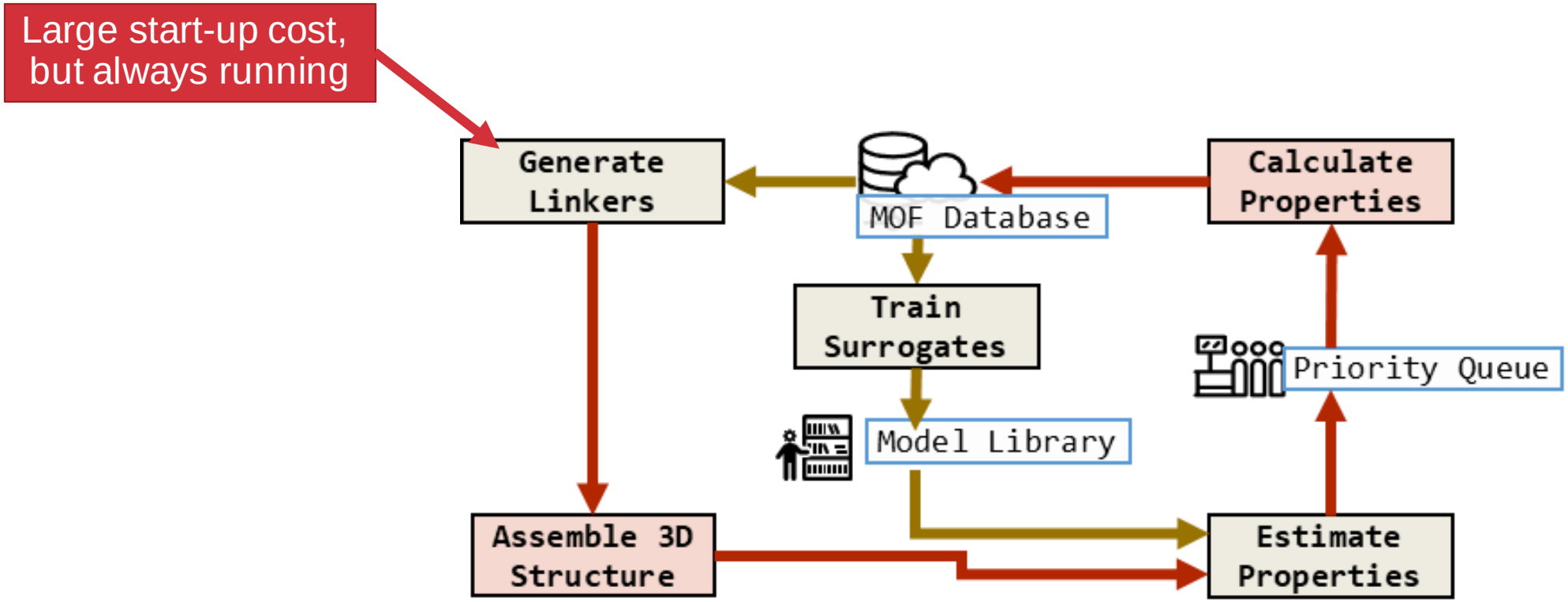
Step 2: Execute

```
examol run spec.py:spec
```

https://exalearn.github.io/ExaMol/

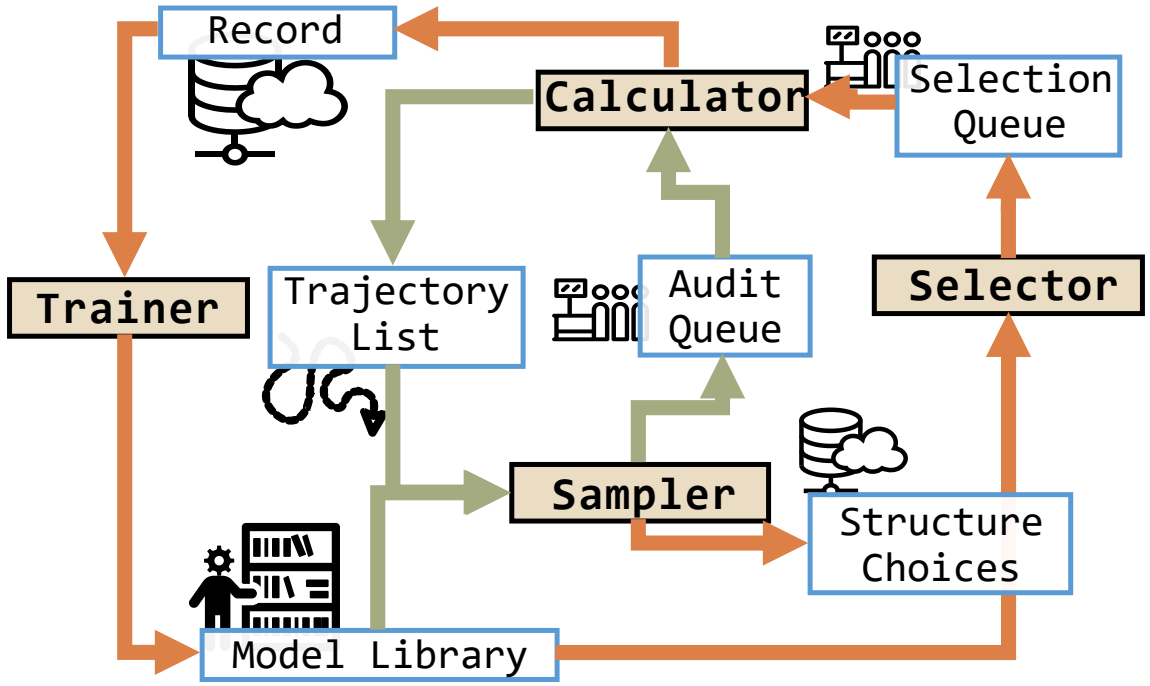
Disclosure: I watch to see how Alex Brace does things 🤨

MOFA: Persistent workers would save time

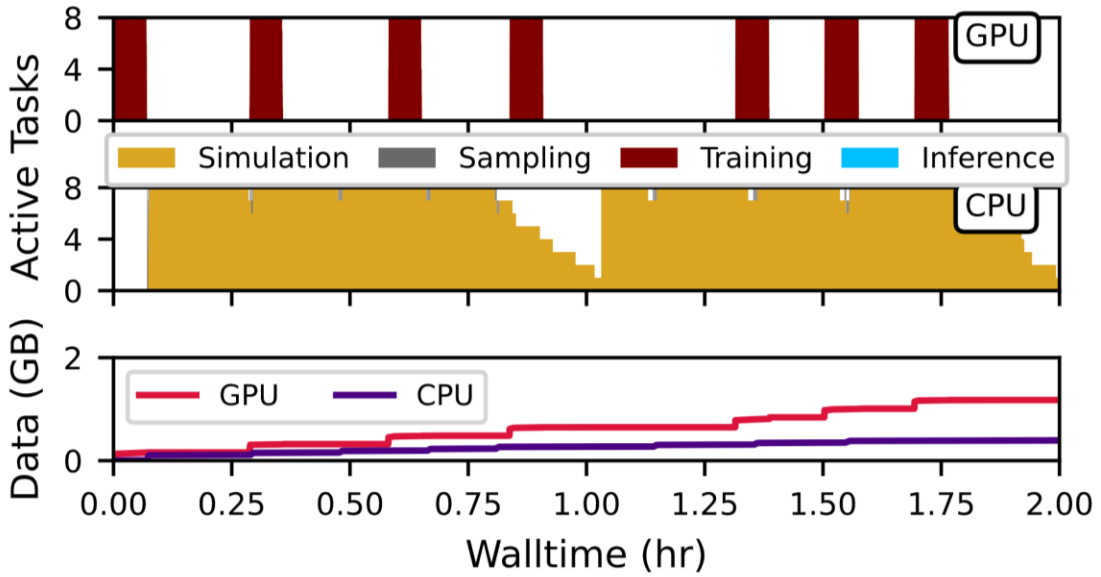


https://github.com/globus-labs/mof-generation-at-scale

FFF: Could I schedule tasks based on worker availability?



Success: We can run on two systems easily



Ugly Secret: We only do this if GPUs available quickly
Why? Training sets would grow stale in queues

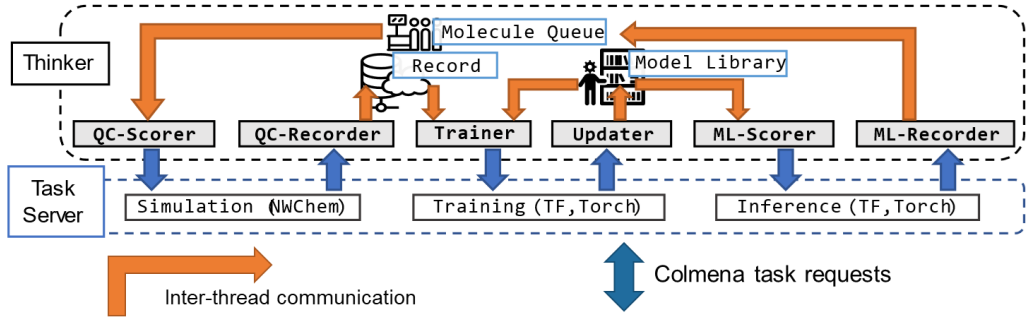
https://github.com/exalearn/fast-finetuned-forcefields*

*I want to merge this with PsiFlow!

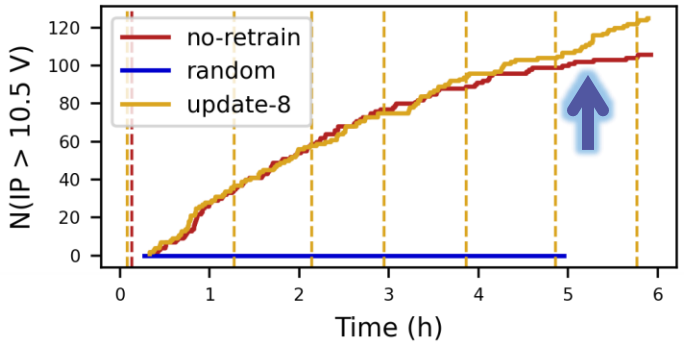
Conclusions and Future for Colmena

What did we build?

Colmena lets you build complex steering policies



… that get more out of your HPC



What to watch for next year?

- More Colmena applications
  - PsiFlow: If Sander agrees 😀
  - ExaMol: Maybe with some Real Chemist users
  - MOFA: A target for many AI apps on ExaScale
  - Jitterbug: GH/globus-labs/faster-molecular-hessians/
- Continued integration with Parsl/Globus Compute
  - Demonstrating Yadu's MPI support?
  - Apps that produce intermediate results?
  - Events and Hooks from Providers?

Acknowledgements: The (growing!) team

Argonne: ExaLearn – Using AI with HPC
Yadu Babuji, Ben Blaiszik, Ryan Chard, Kyle Chard, Ian Foster, Greg Pauloski, Ganesh Sivaraman, Rajeev Thakur

Argonne: JCESR – Molecular modeling for batteries
Rajeev Assary, Larry Curtiss, Naveen Dandu, Paul Redfern

MolSSI – Workflows for quantum chemistry
Lori A. Burns, Daniel Smith, Matt Welborn, *many other open-source contributors*

PNNL: ExaLearn – Graph algorithms for learning
Sutanay Choudhury, Jenna Pope

Argonne ALCF – AI, Data and Simulation on HPC
Murali Emani, Alvaro Vazquez-Mayagoitia, Venkat Vishnawath

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ExaWorks – Interfacing to HPC
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FuncX – Seamless multisite deployment
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