# Colmena: Seamless Computational Campaigns across Multiple Computing Clusters with Parsl/FuncX and Object Proxies

Cleared for public release

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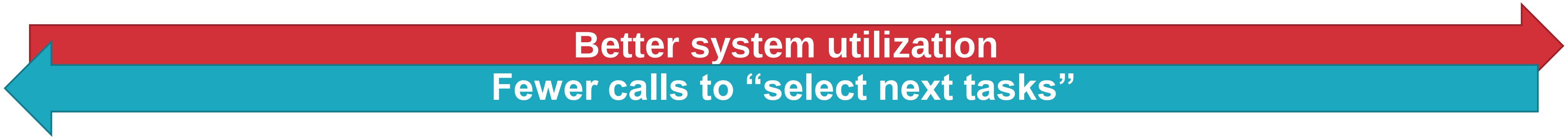
# Strategies for steering computational campaigns are complicated

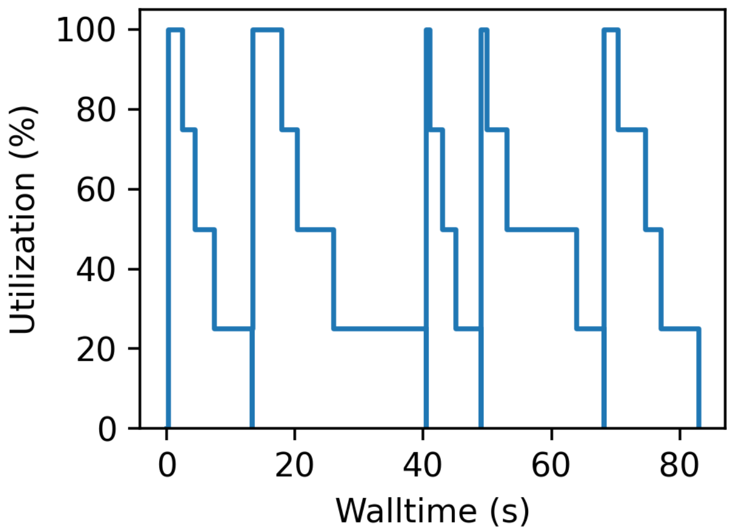
*Parallel Optimizers: A “simple” example with no optimal strategy*



**Better system utilization**

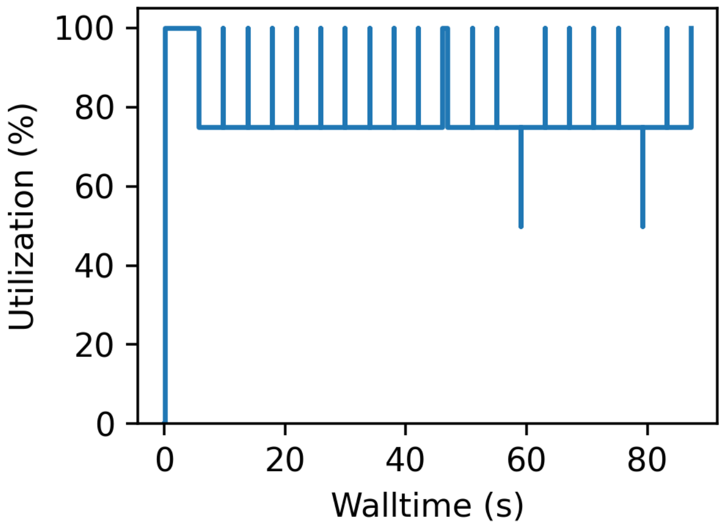
**Fewer calls to “select next tasks”**

## Batch Optimizer



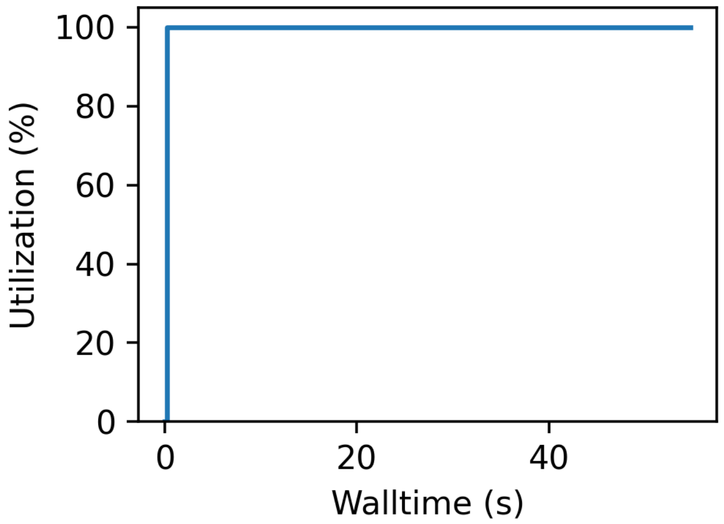
*Wait for N tasks to complete, then pick next batch*

## Streaming Optimizer



*Pick new tasks as soon as one completes*

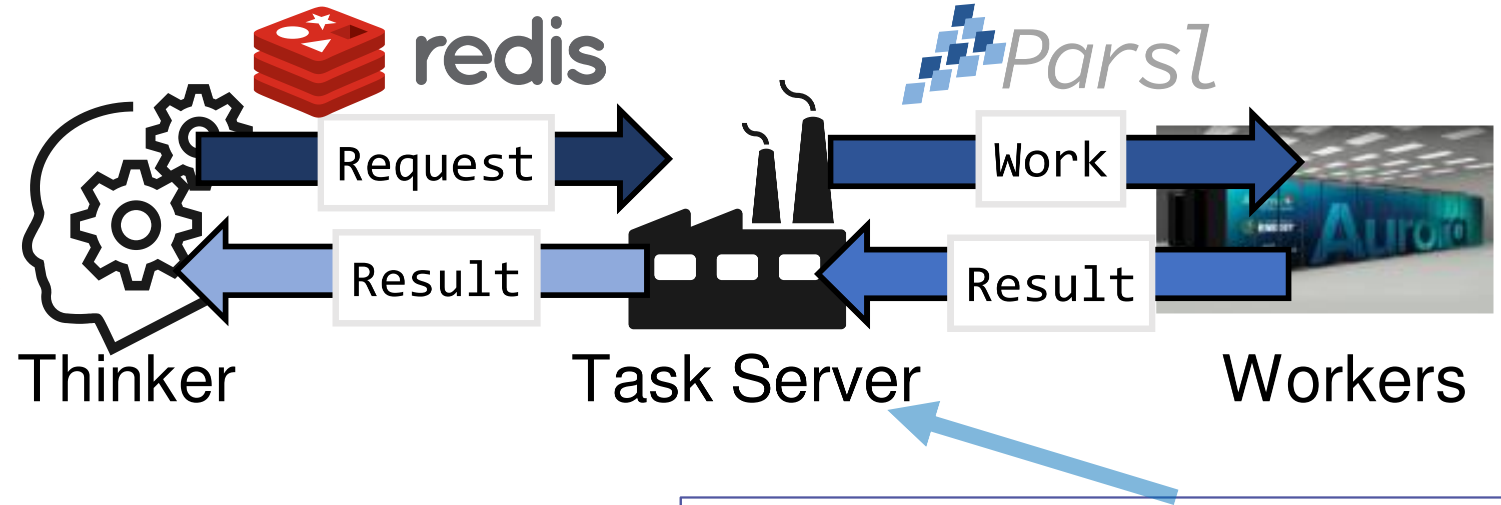
## Interleaved Optimizer



*Maintain a task queue*

Colmena provides simplifies expressing steering strategies

# **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:**

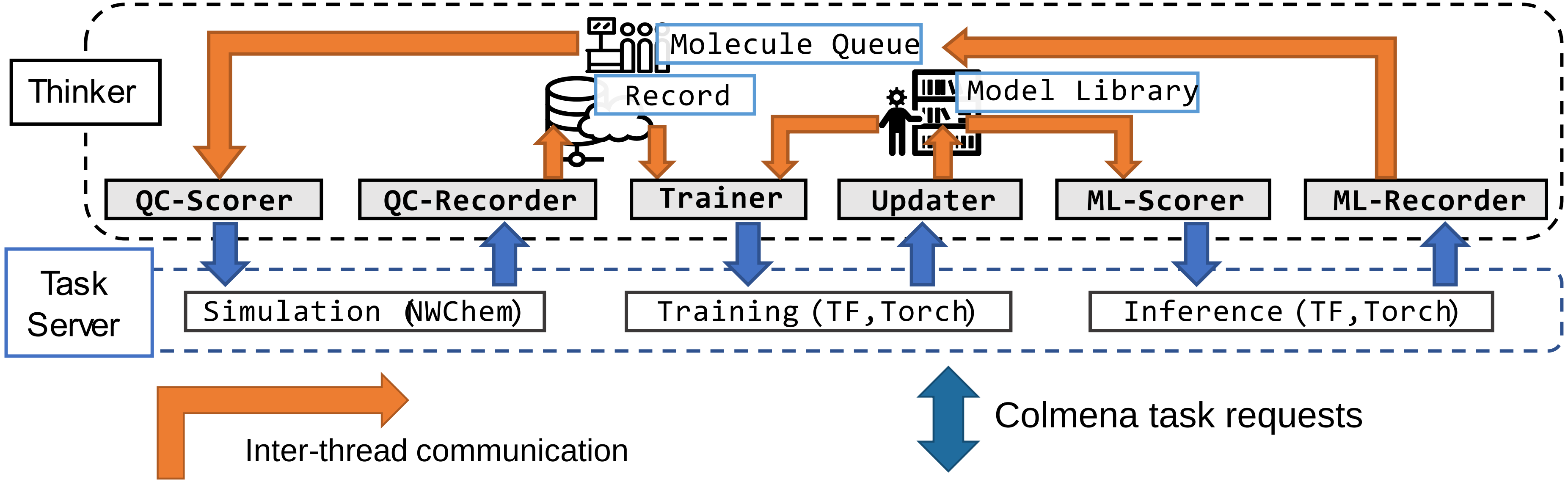
- Dispatches work requests to compute
- Communicates results back to thinker

**Backend:**

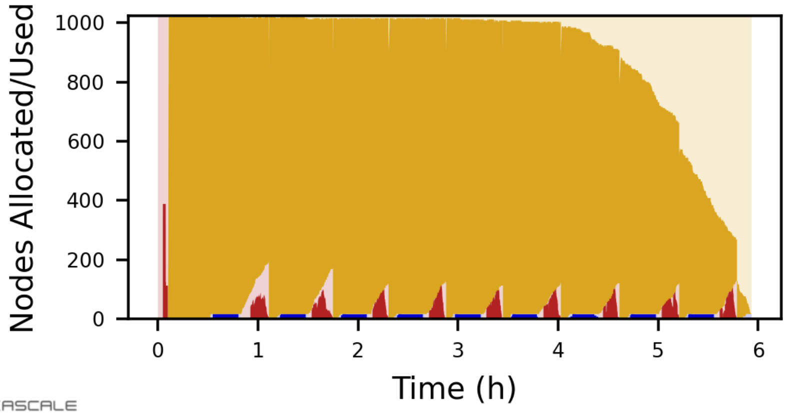
- Supports most HPC and cloud services
- Easily configure multiple worker types, multi-site workflows
- Limited support for ensembles of MPI applications
- *Future:* Balsam, FuncX, RCT

EXASCALE COMPUTING PROJECT

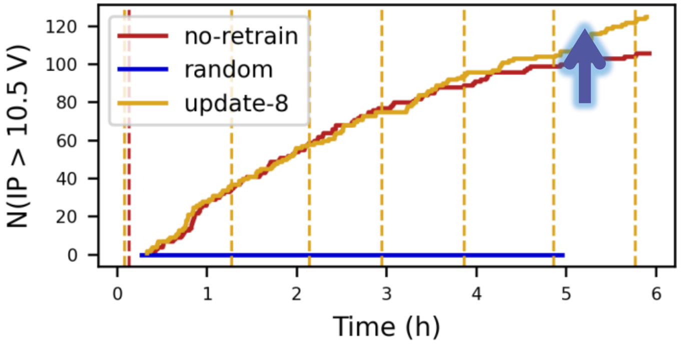
# Example application: "Interleaved," AI-in-the-loop optimizer



**Retasking nodes between jobs…**



**…yields more science per compute-hour.**



Details: Ward et al. ML4HPC, SC21.

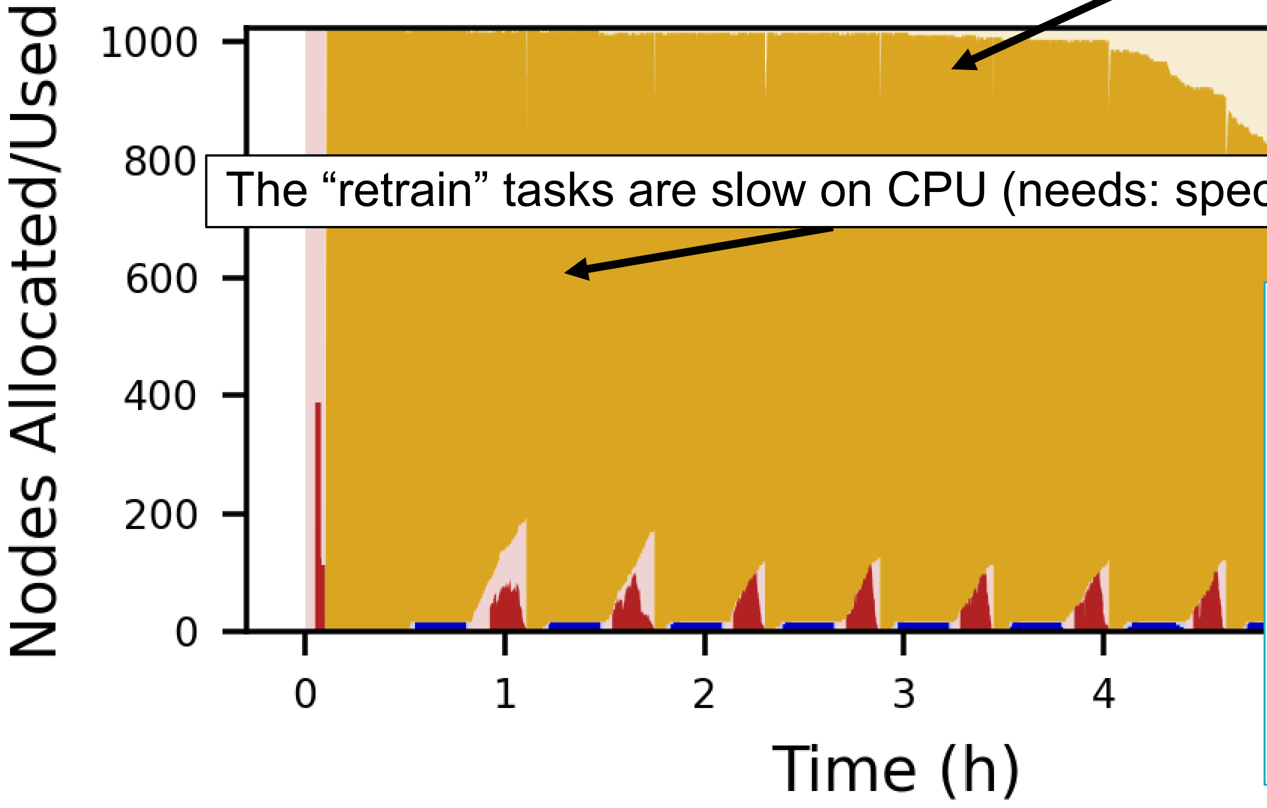
## So, what’s new in ‘22?

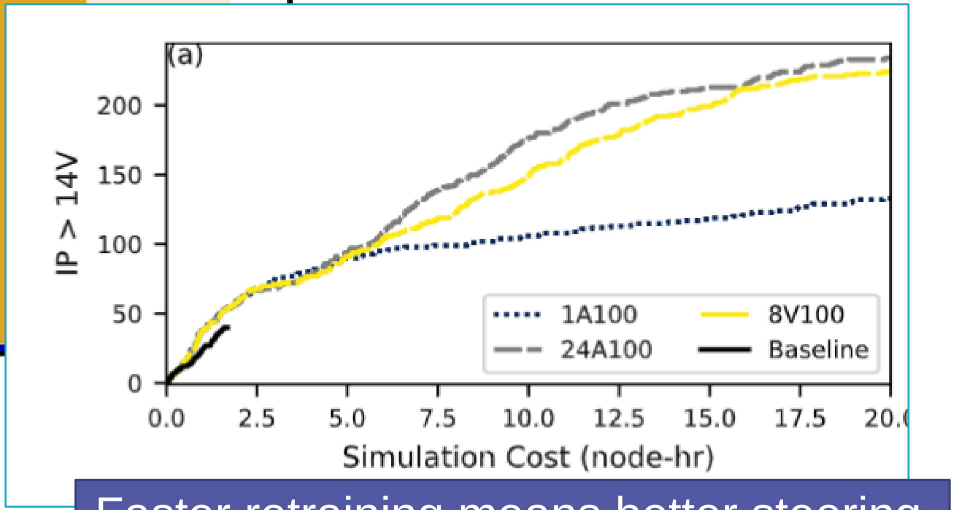
*Multi-site Campaigns!*

# **Why multi-site?** *Moving compute onto best hardware*

Most of our work is CPU-only (needs: many, cheap)

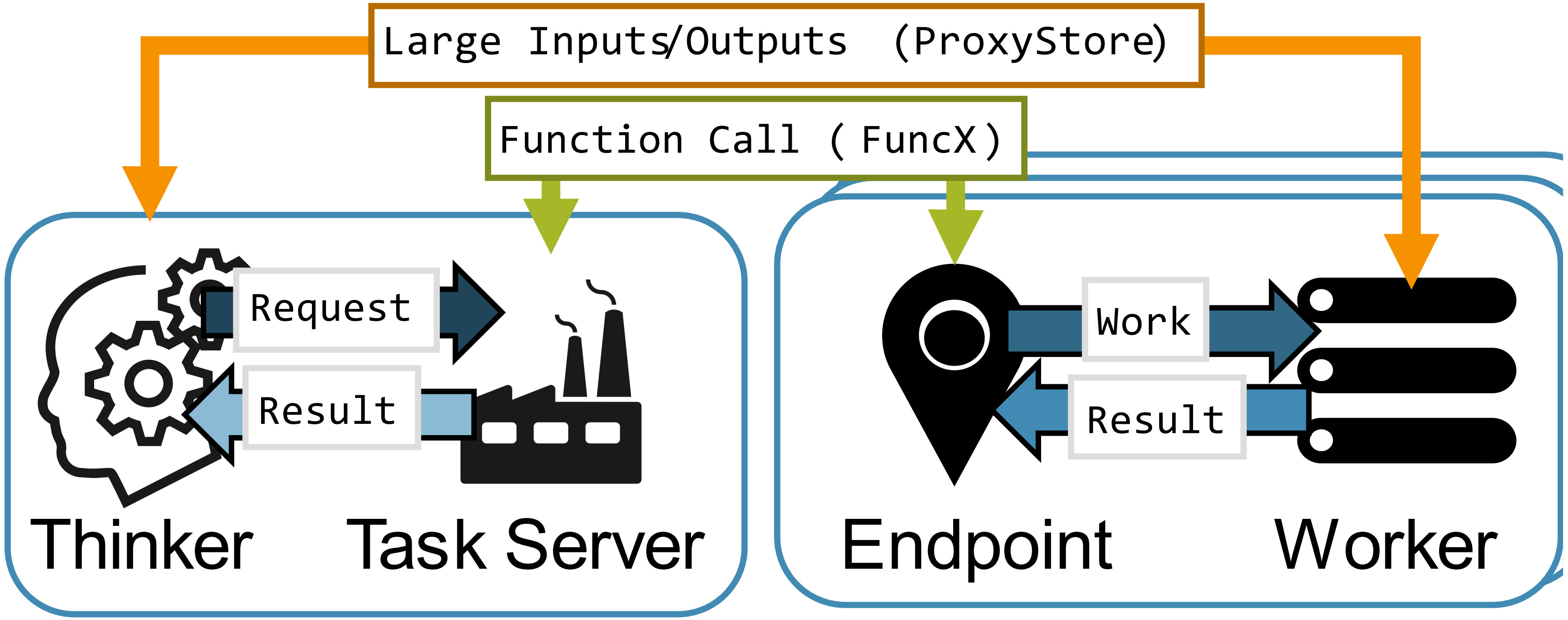
The “retrain” tasks are slow on CPU (needs: specialized)





Faster retraining means better steering

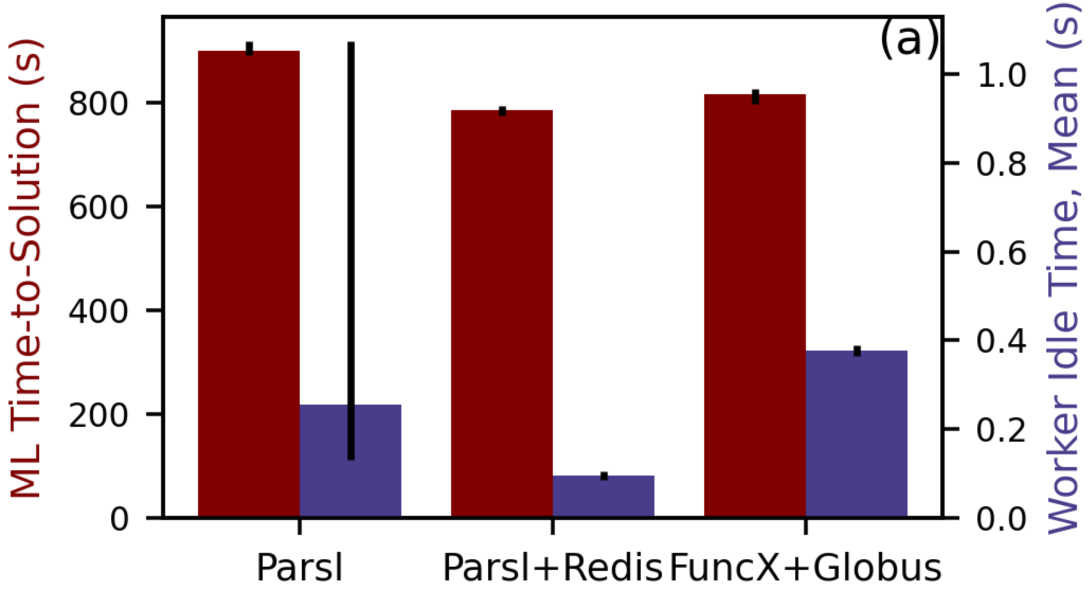
# How multi-site? *FuncX*



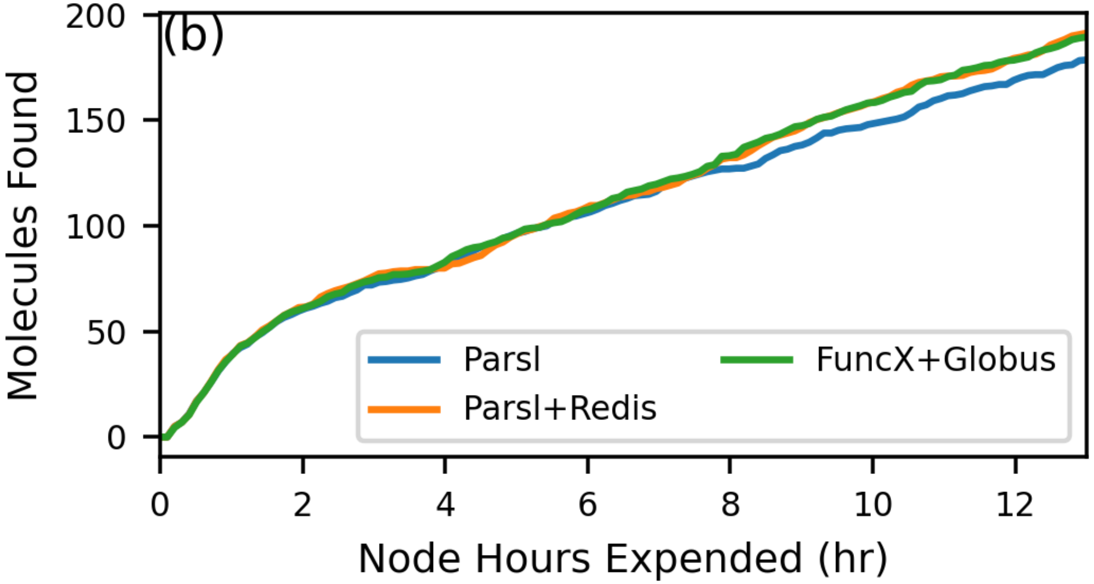
It’s just FuncX. We use the “FuncXExecutor,” so it acts like Parsl

# How good multi-site? *Same performance, less port headache*

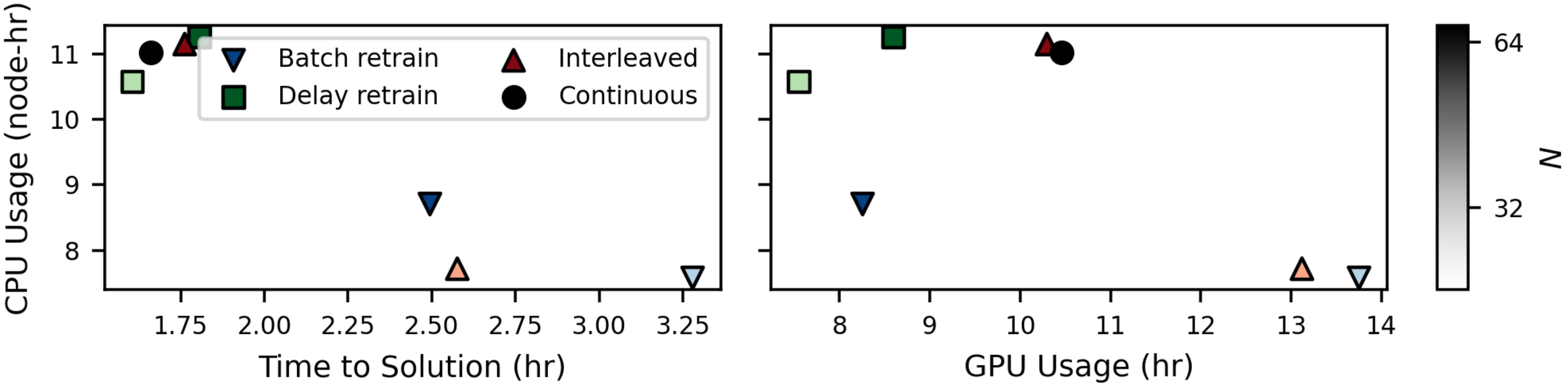
Machine learning tasks take only 3% longer than best-effort with SSH tunnels



Scientific outcomes are identical



# Colmena lets you explore computational cost tradeoffs

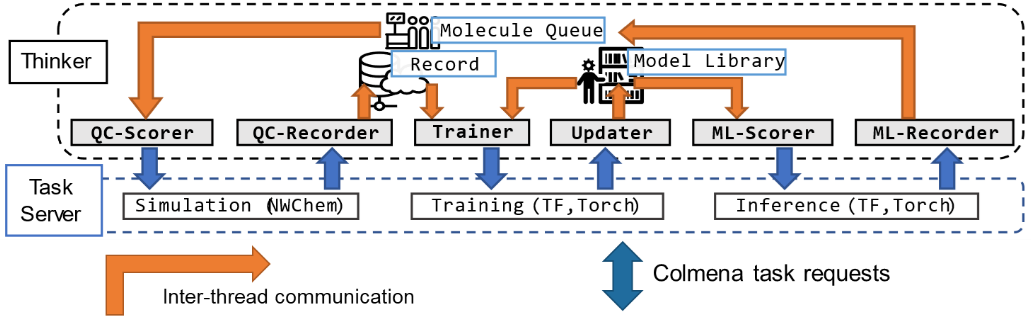


Steering policies tradeoff between time to solution, GPU time, and CPU time

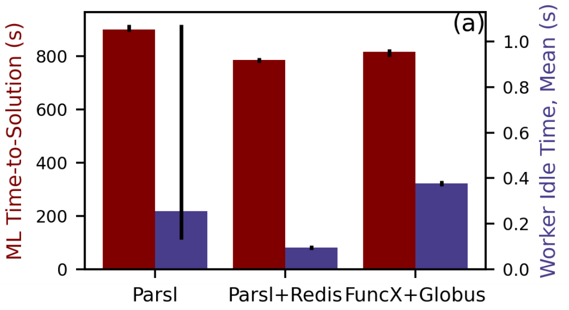
# Conclusions and Future for Colmena

## What did we cover today?

- Colmena lets you build complex steering policies



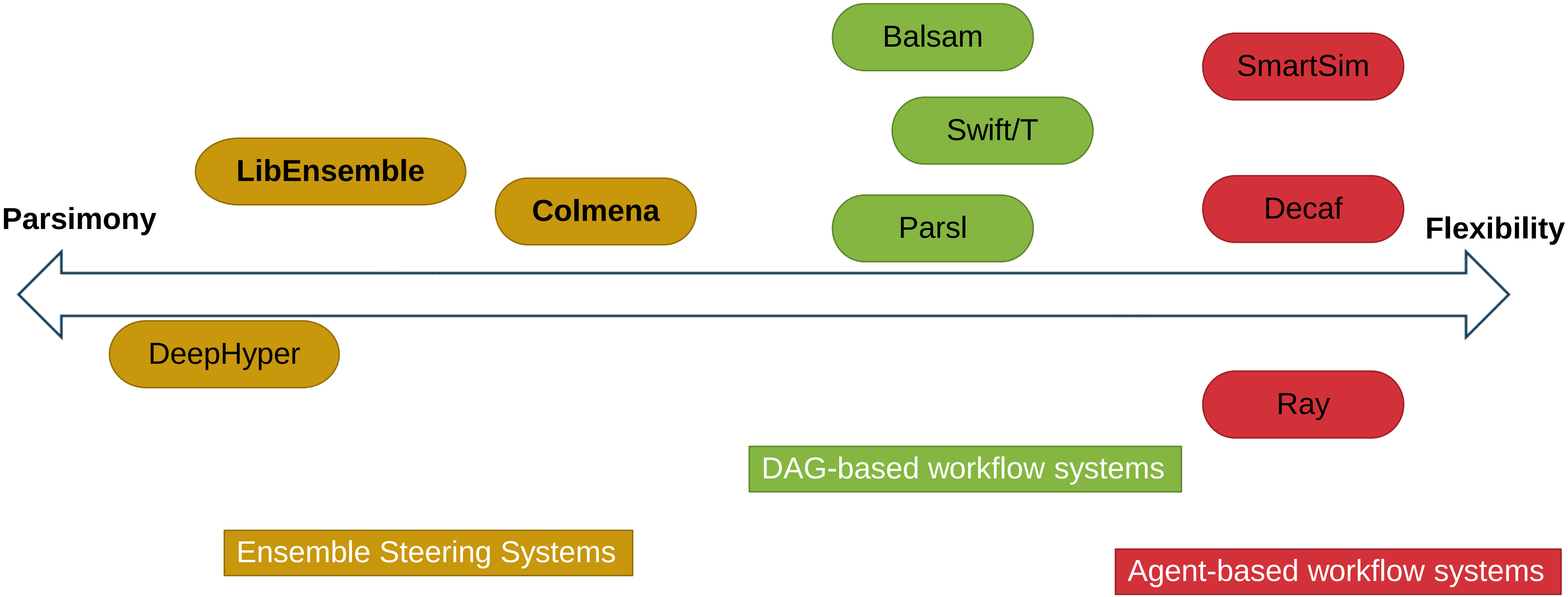
- FuncX lets policies span compute systems



## What to watch for next year?

- This work published (at least on ArXiV!)
- A perspective on ensemble steering toolkits
  - “How are libE and
- More Colmena applications
  - Fitting machine-learned surrogates for simulations
  - Coordinating simulation self-driving laboratories
  - Rapid screening of HPC
- Integration with more workflow engines (e.g., RCT!)

# Got opinions about what Colmena is? Join our interest group



Parsimony

Flexibility

**LibEnsemble**

**Colmena**

DeepHyper

Ensemble Steering Systems

Balsam

Swift/T

Parsl

DAG-based workflow systems

SmartSim

Decaf

Ray

Agent-based workflow systems

Email me (lward@anl.gov) if you want to join the conversation!

# Acknowledgements: The (growing!) team

**Argonne: ExaLearn** – Using AI with HPC
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**MolSSI** – Workflows for quantum chemistry
Lori A. Burns, Daniel Smith, Matt Welborn, *many other open-source contributors*

**BNL: ExaLearn –** Optimal experimental design
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**FuncX** – Seamless multisite deployment
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**Argonne: JCESR** – Molecular modeling for batteries
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**PNNL: ExaLearn** – Graph algorithms for learning
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**Argonne ALCF** – AI, Data and Simulation on HPC
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**ExaWorks** – Interfacing to HPC
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**Ensemble Group** – Defining ensemble needs
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