Colmena:
Steering Ensemble Simulations on HPC

Cleared for public release

EXASCALE COMPUTING PROJECT

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Argonne ALCF – AI, Data and Simulation on HPC
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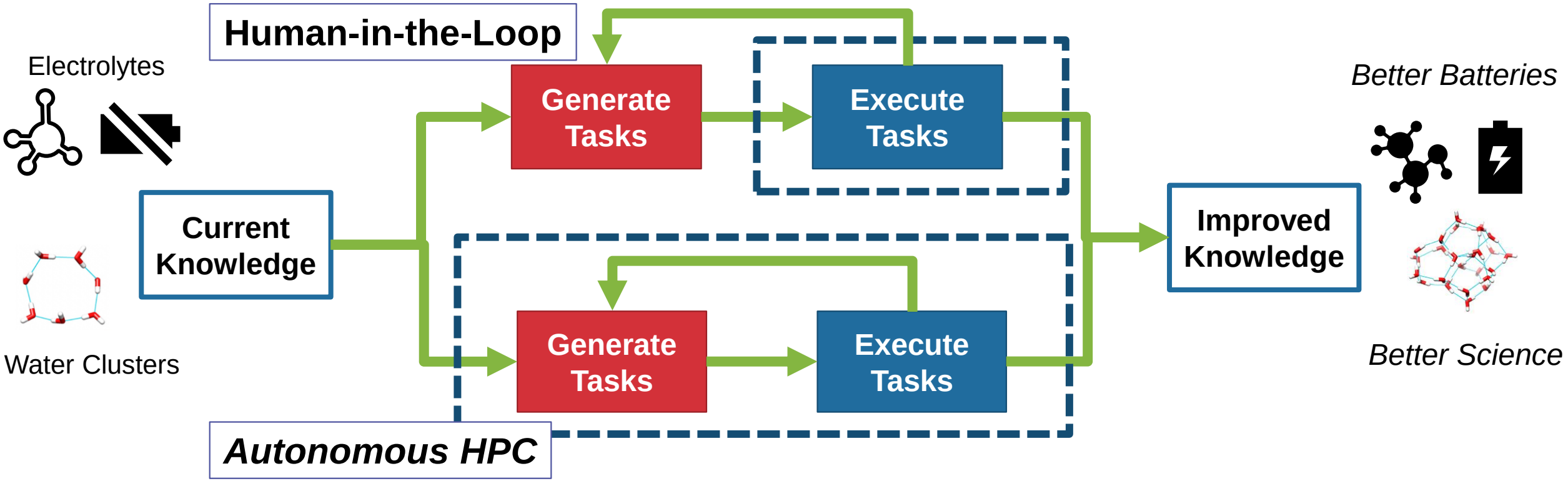
Big Picture: Expanding Computational Campaigns to the ExaScale

Current Model: Humans steer HPC, HPC performs simulations

Current Model Won't Scale. Humans are **slow and not getting any faster**

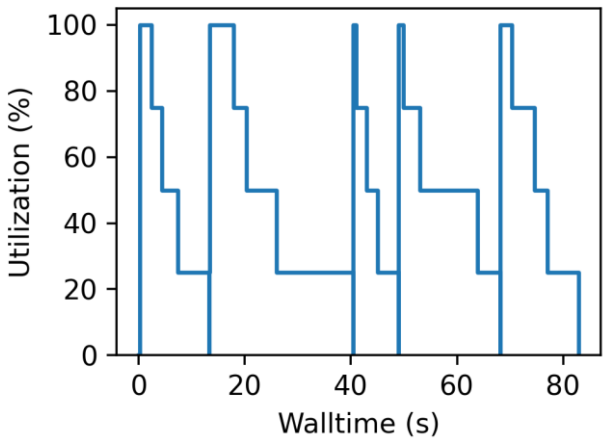


Our goal: HPC steering itself!

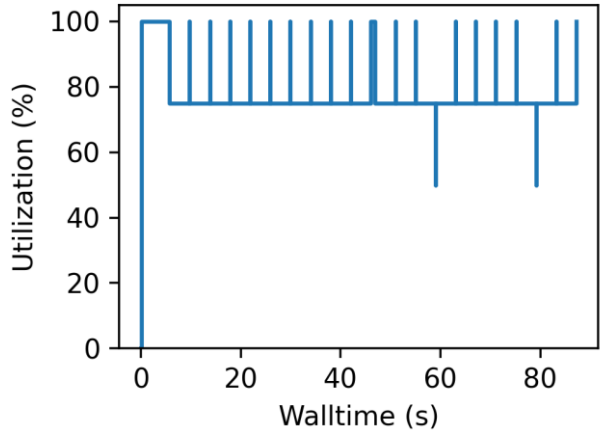
Parallelism makes steering on HPC difficult

Root Problem: Sequential search is impractical, we must run >1 simulation at once

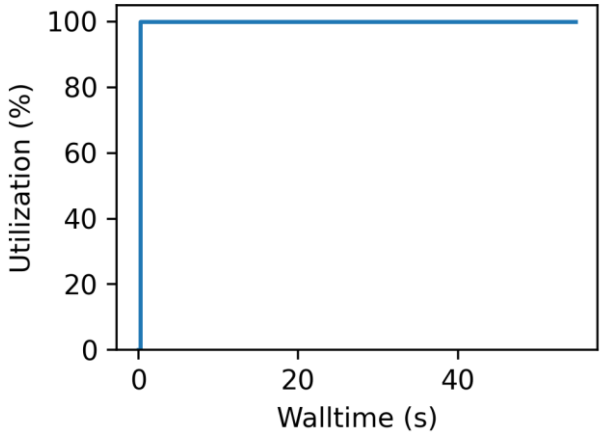
Consider a few parallel strategies…



Wait for N tasks to complete, then pick next batch



Pick new tasks as soon as one completes



Maintain a task queue

↑ Most information per decision
↓ Least utilization

↓ Least information per decision
↑ Greatest utilization

Bottom Line: Active learning on HPC requires intelligent policies

Today's Talk: You can build complicated steering with Colmena
…and that lets you do cool things.

Colmena: An overview

What kind of “intelligence” goes into steering applications

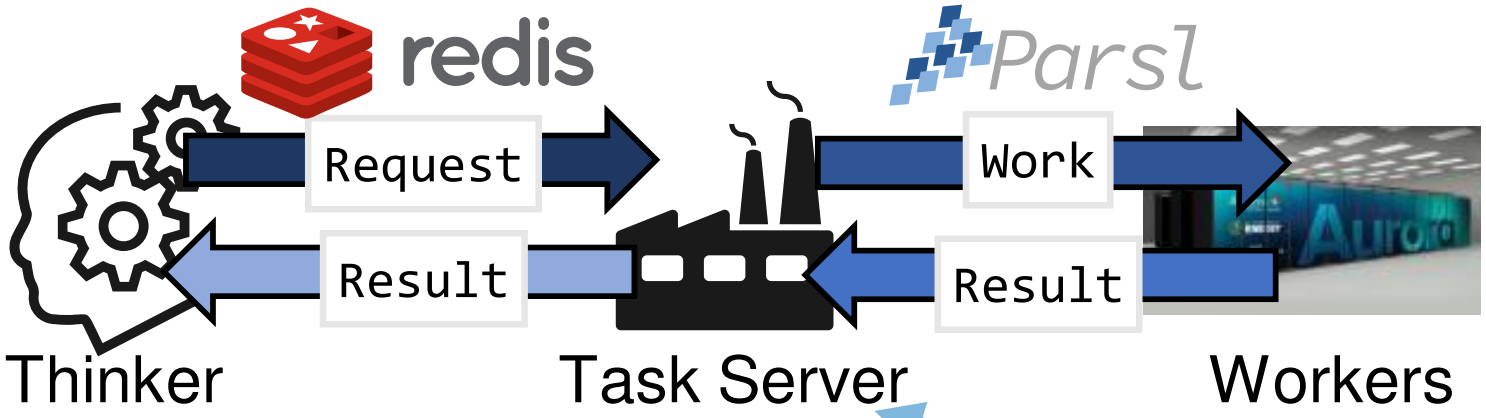
Observation: We have many policy ideas…

- *Submit a new simulation* ***once another completes*** ← Event-triggered
- *Retrain a model* ***after 8 successful computations*** ← Conditional logic
- ***Allocate more nodes to inference*** *after models finish training* ← Resource management

and others are possible.

Solution: We need a way of programming ***agents*** to encode such policies

Colmena is a wrapper over Exascale Workflow tools (e.g. Parsl!)



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: Parsl
- 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

Building a Colmena app: Defining the “tasks” and **“thinker”**

Key points:

1. Subclass the “BaseThinker” abstract class
2. Mark “agent” operations form the policy
3. Communicate with method server via queues
4. Communicate with other via Threading primitives

How does it work:

– “.run()” launches all agents

```
class Thinker(BaseThinker):
  def __init__(self, queue):
    super().__init__(queue)
    self.remaining_guesses = 10
    self.best_guess = None
    self.best_result = inf

  @result_processor(topic='simulate')
  def consumer(self, result):
     # Update the best result, check for termination
     if result.value < self.best_result:
        self.best_result = result.value
        self.best_guess = result.args[0]
     self.remaining_guesses -= 1
     if self.remaining_guesses == 0:
        self.done.set()

  @agent
  def producer(self):
    while not self.done.is_set():
       # Make a new guess
      self.queues.send_inputs(self.best_guess,
           method='task_generator', topic='generate')
      # Get the result, push new task to queue
      result = self.queues.get_result(topic='generate')
```

Main effort: Defining the **“tasks”** and “thinker”

- **Main steps:**
  1. Write methods as Python functions
  2. Specify computational sources
  3. Instantiate method server

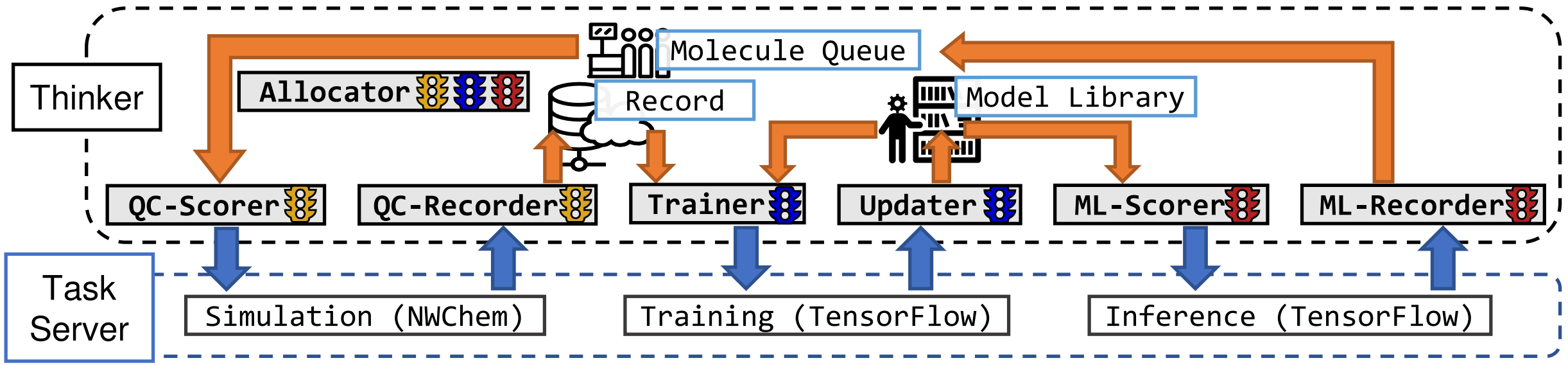
```
def target_function(x: float) -> float: return x ** 2
def task_generator(best_to_date: float) -> float:
    from random import random
    return best_to_date + random() - 0.5

config = Config(executors=[
    HighThroughputExecutor(max_workers=4)])

doer = ParslTaskServer([target_function, task_generator],
        server_queues, config)
```

- **Launching the server:**
  - “.run()” launches server as a second process
  - Main thread reads from queue, launches workflows
  - Workflows end by writing results to queue
  - Parsl distributes work, collects results

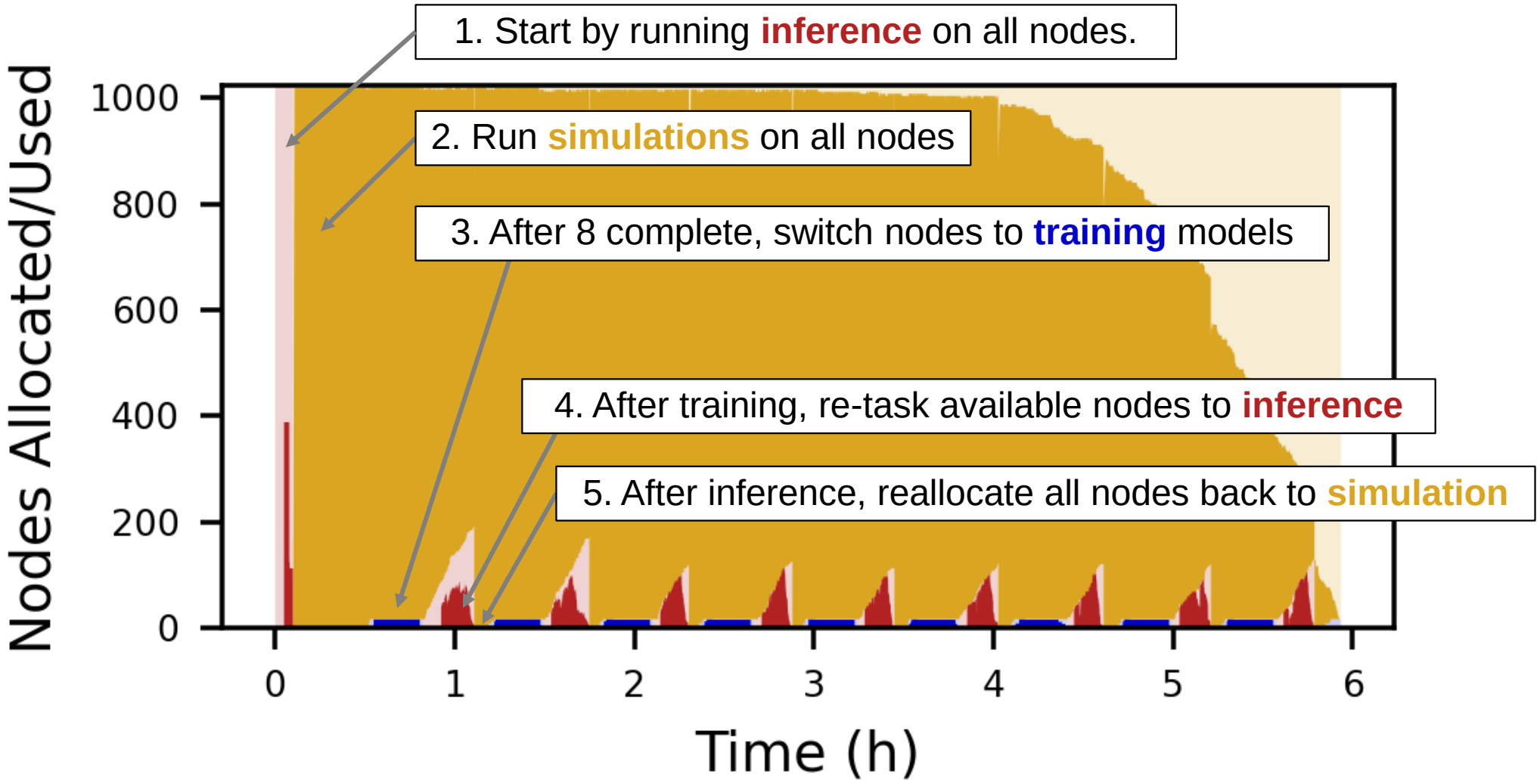
```
doer.start()
```

Colmena and Molecular Design

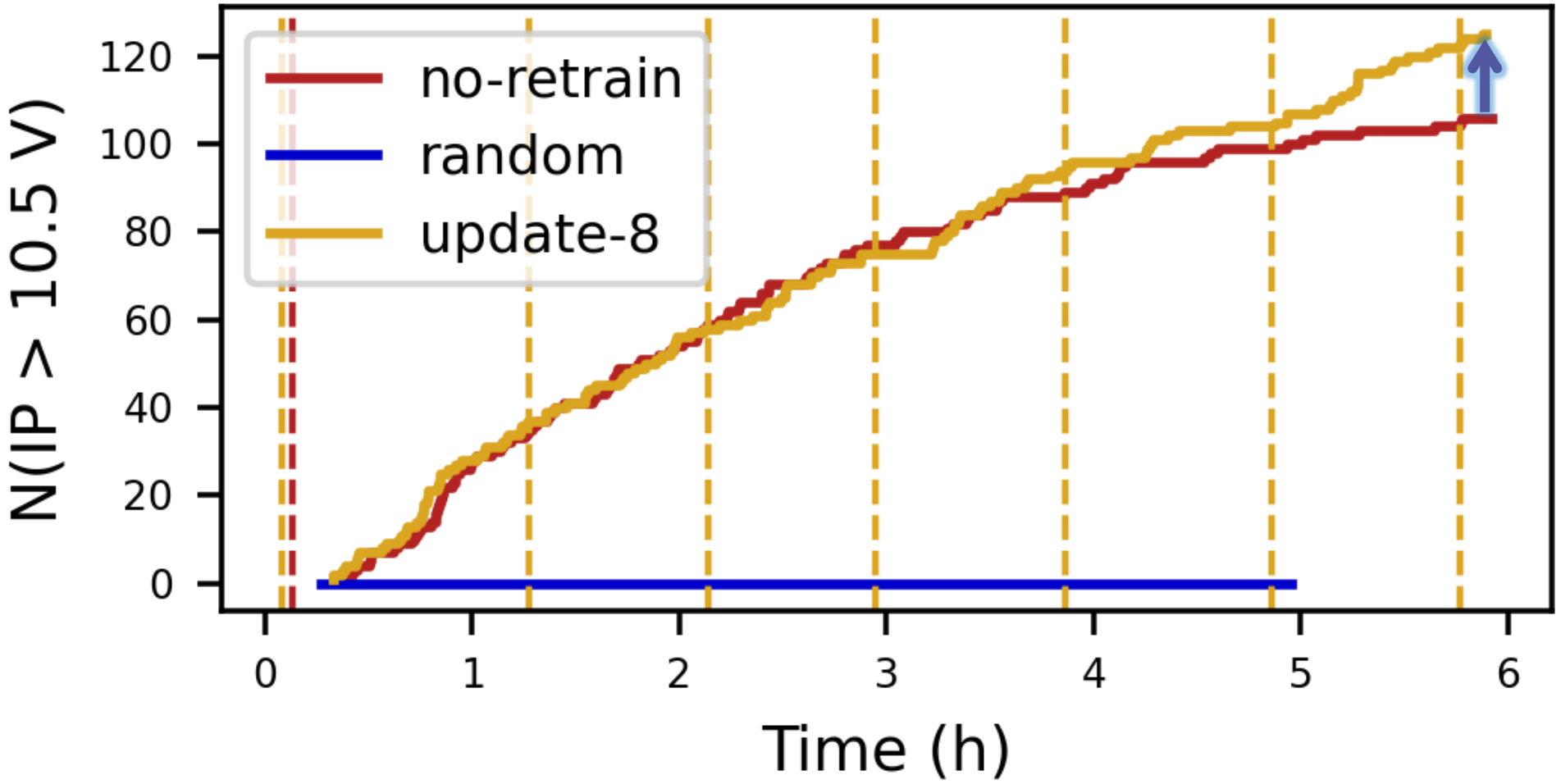
What does our “active learning application” look like



What is the application behavior?



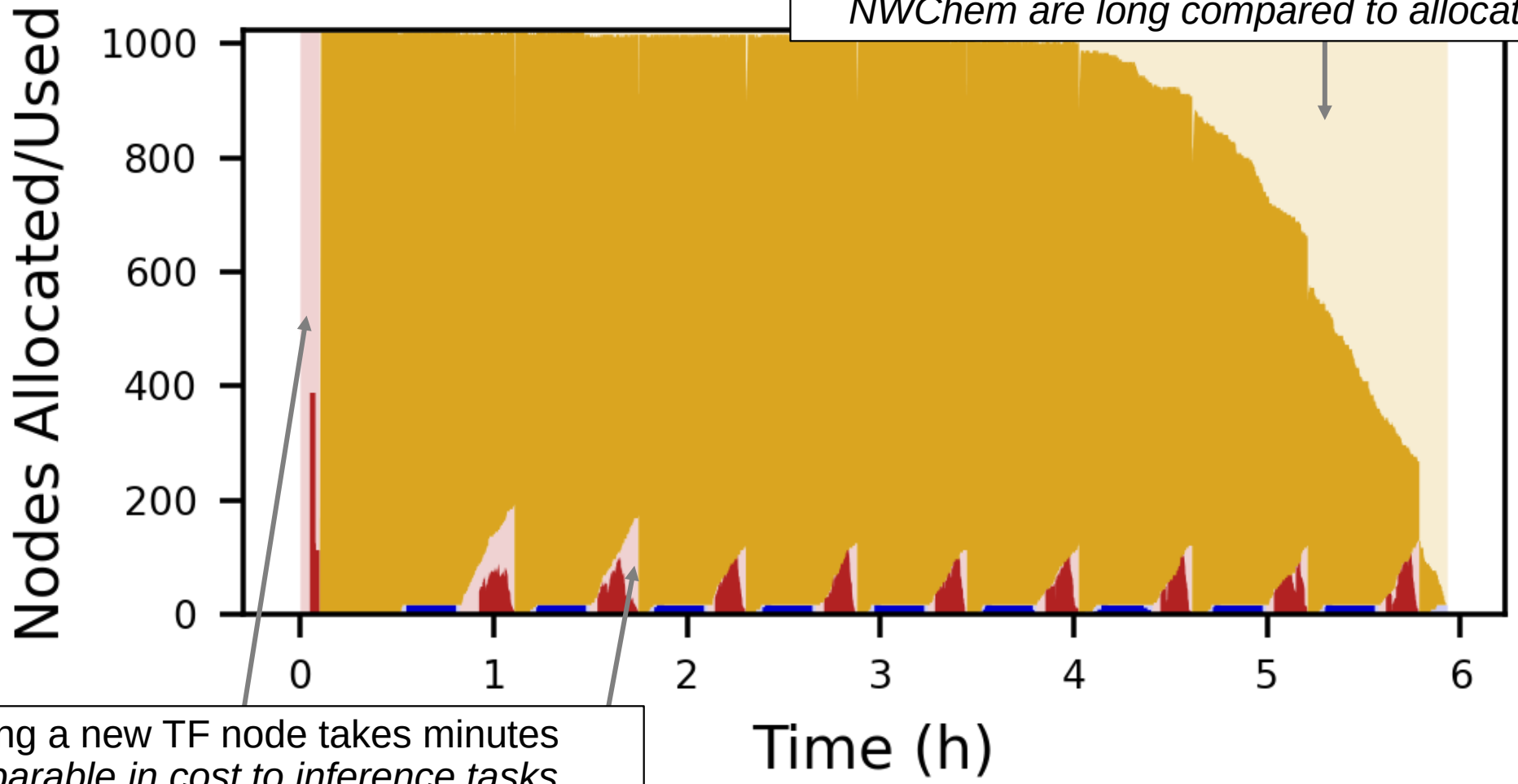
Did the application have good scientific performance? **[Yes]**



Found 10% more high-performing molecules with same allocation size

Where are the sources of underutilization in ours run?

Poor utilization due to long-tail, trailing NWChem tasks
NWChem are long compared to allocation walltime

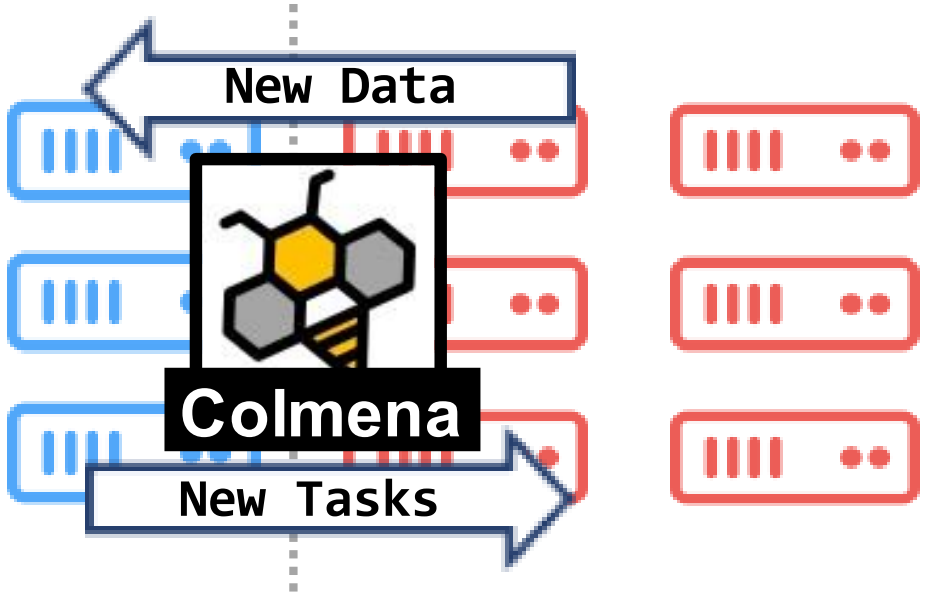


Starting a new TF node takes minutes
Comparable in cost to inference tasks

Summary: Colmena is for deploying AI+Simulation HPC

Key points:

- AI will play an increasing role in **controlling campaigns of simulations**
- Success will require **deploying AI on HPC**
- **Colmena** provides a Python library for building applications to interleave simulation and AI workflows
  - Simple, agent-based programming model
  - Backed by performant workflow engines (Parsl!)



See also: https://colmena.rtfd.io/ , https://github.com/exalearn/colmena