



Autonomous Science Is Inheriting a Workflow Infrastructure Problem

Glenn K. Lockwood, Ph.D.

Principal Technical Strategist

VAST Data

“Please don’t submit too many jobs”

Humans are slow, and Slurm was designed for humans.

Persson Group Handbook

The Cori queue system can be **unreasonably slow when submitting many (e.g., hundreds, thousands) of small (e.g., single node or 2 nodes) jobs**

--Persson Group Handbook

UArizona HPC Documentation

Use Arrays instead of Loops for

Users submitting large numbers (> 100s) of jobs using loops will be contacted and asked to adjust their workflows.

--UArizona HPC Documentation

Yale Center for Research Computing

Need Help?

If you plan to run many similar jobs, use our Dead Simple Queue tool or job arrays - we enforce limits on job submission rates on all clusters.

--Yale CRC

Job arrays in

If you plan to run many similar jobs, use our **Dead Simple C arrays** - we enforce limits on **job submission rates** on all cl

ULHPC Techni

If you plan to submit many small jobs in an array that require the allocation of more than 10 jobs per minute, please use GNU parallel

--ULHPC Technical Documentation

When not to use job arrays

Every job in a job array requires an allocation from the scheduler, which is an expensive operation. If you plan to submit many small jobs in an array that require the allocation of **more than 10 jobs per minute**, please use **GNU parallel** to batch multiple tasks in a single job allocation.

Array and Chain Jo

... whenever you are tempted to write a **shell loop around sbatch** ... **do not do it** - instead, use Slurm's job array feature.

--HPC Wiki

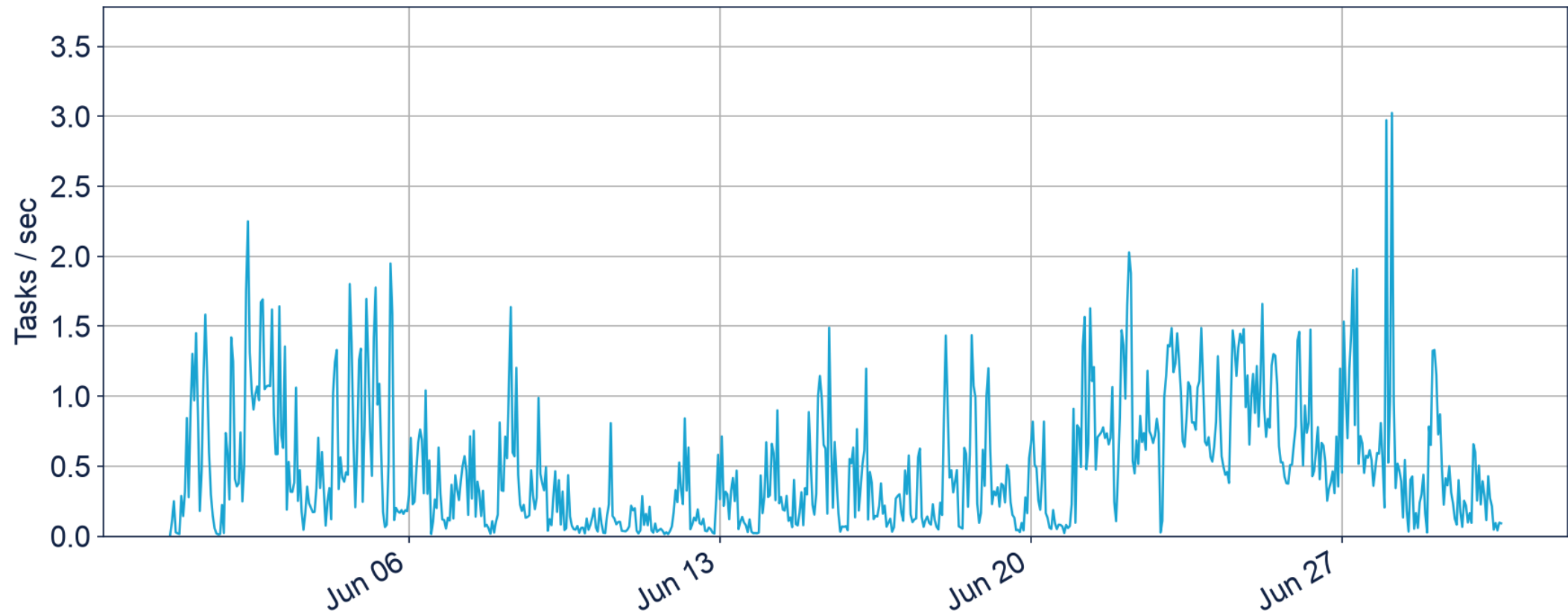
```
for i in {1..1000}
do
sbatch myJobSc
done
```

do not do it - instead, use Slurm's **job array** feature.

Humans issue tasks in human-like ways

R-CCS Fugaku, June 2023 job submission traces (539 humans)

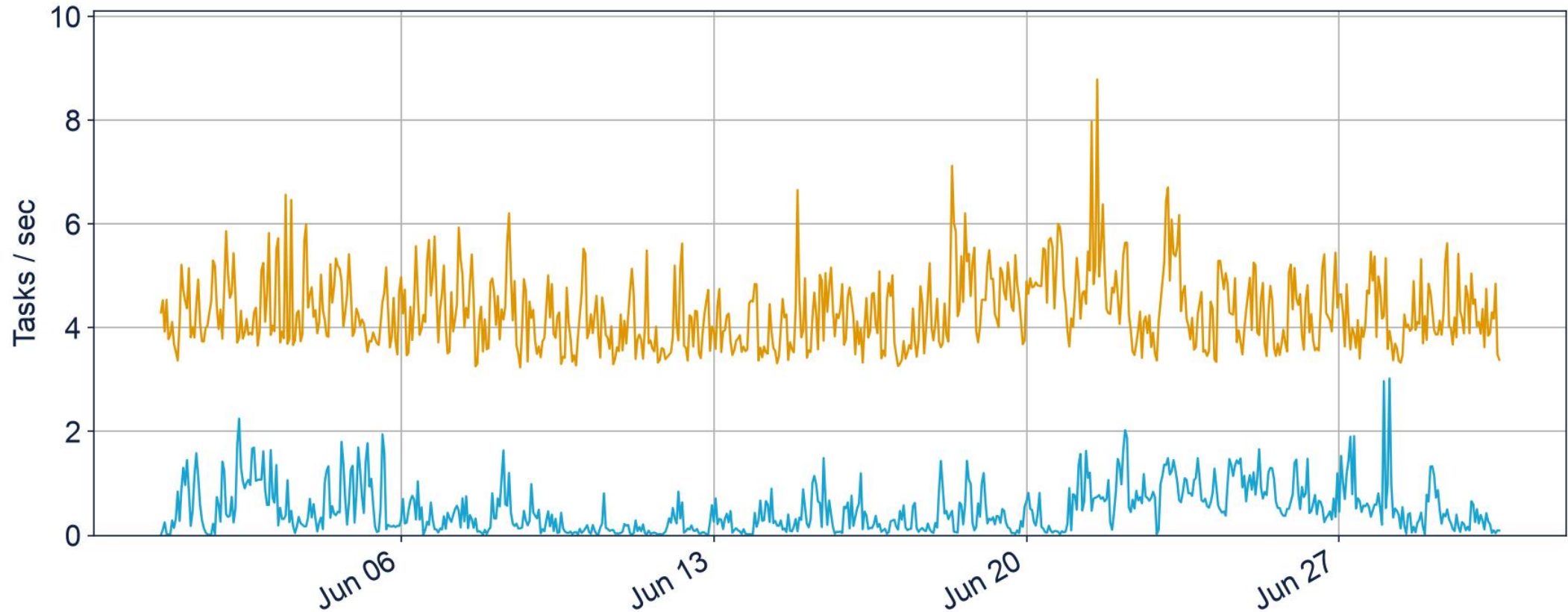
Human-driven (0.504 tasks/sec)



Agents squeeze out human idle time

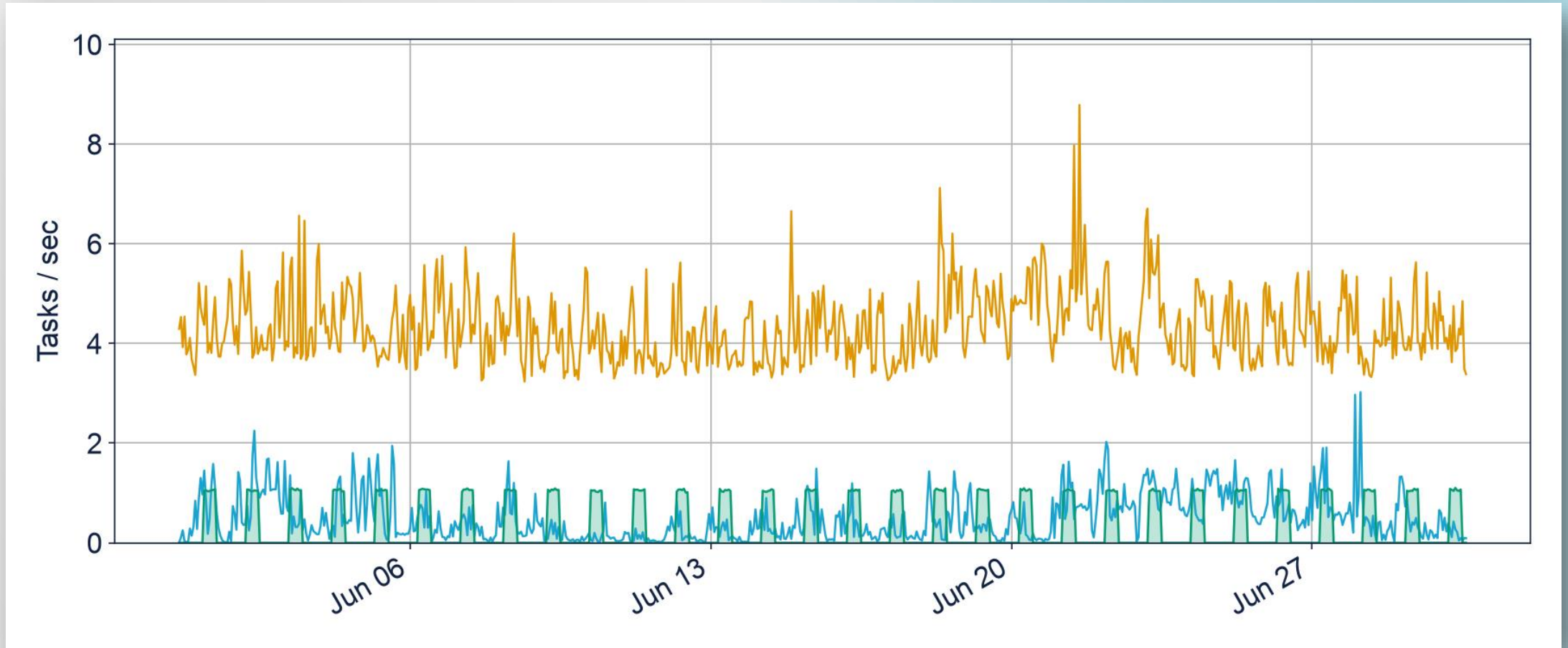
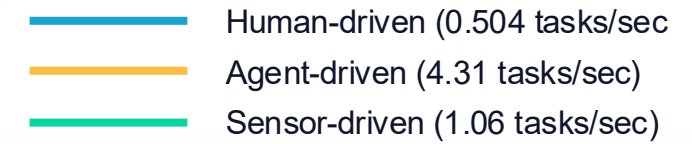
Modeled using Fugaku job submission traces (539 agents)

Human-driven (0.504 tasks/sec)
Agent-driven (4.31 tasks/sec)



Observational data increases baseline

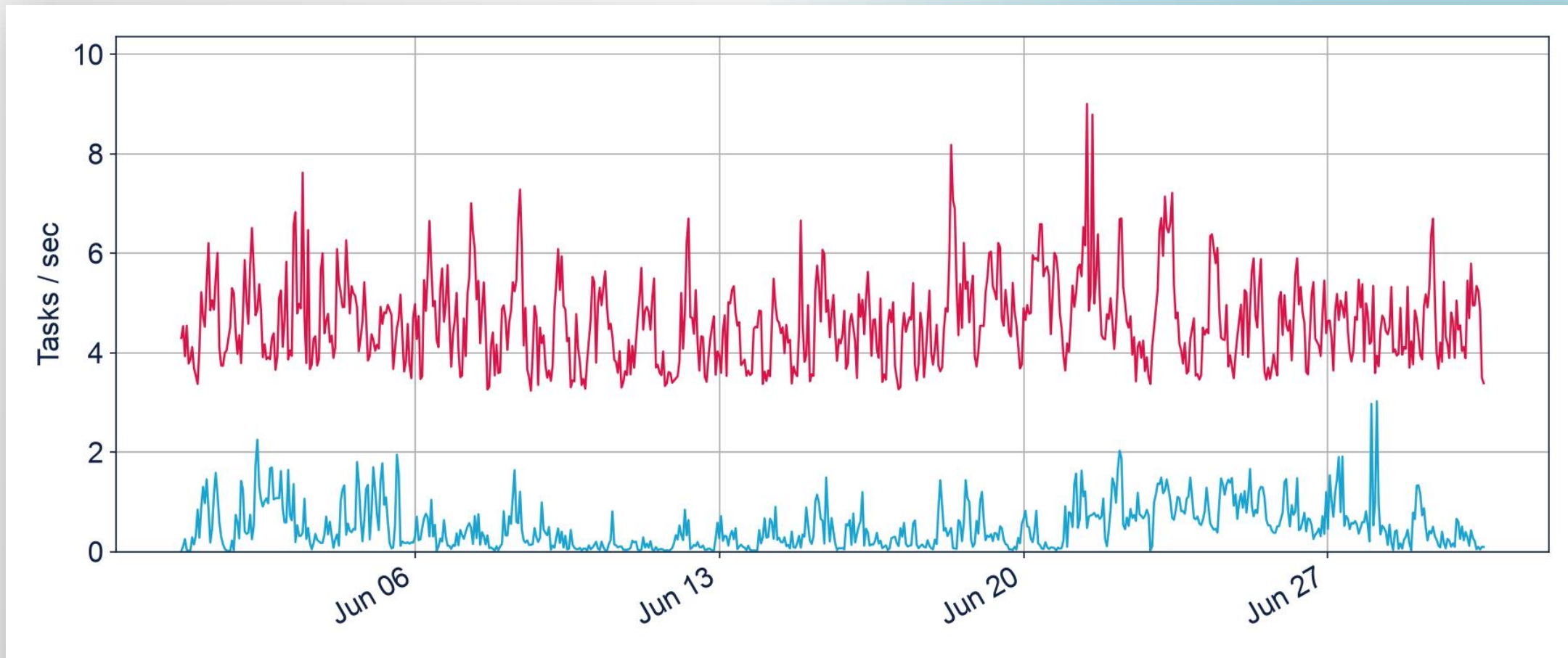
Modeled from Zwicky Transient Factory (one 600 megapixel camera)



Autonomous labs: 9x more tasks than leading HPC centers

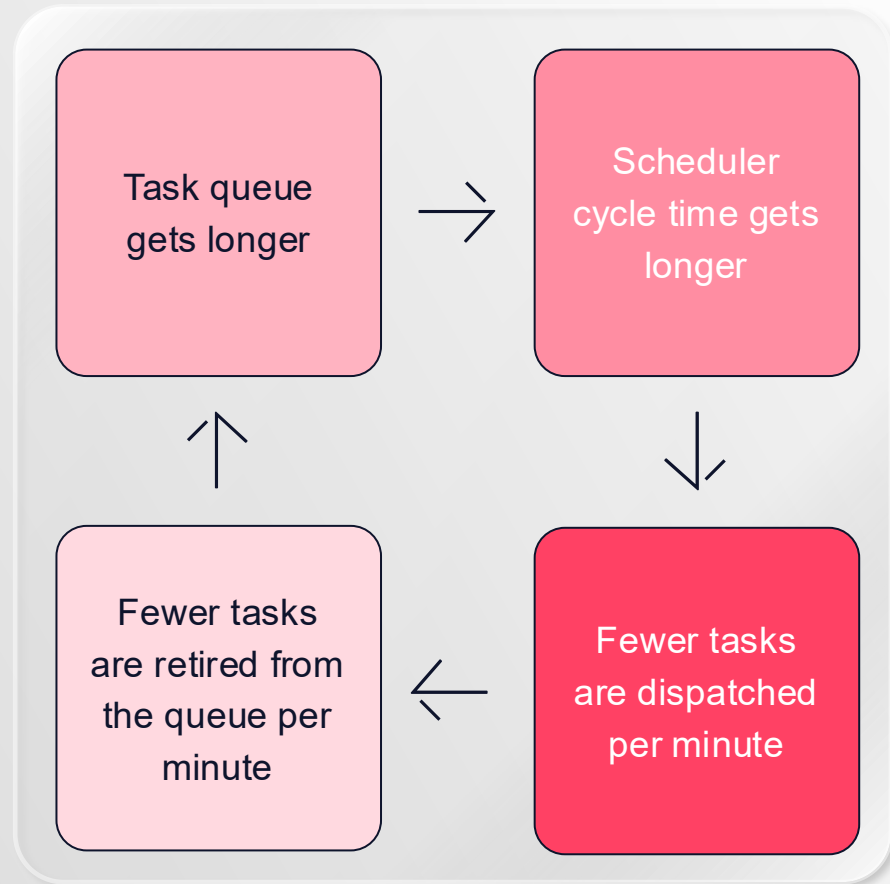
Agents and instruments could average 16,000 job submissions per hour

Human-driven HPC center
Autonomous laboratory

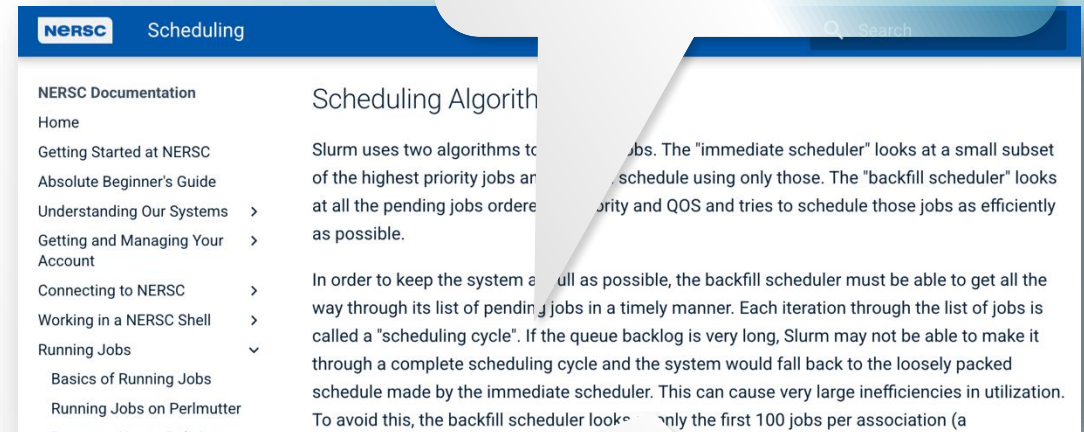


Centralized task orchestration will become the bottleneck

Batch scheduling is at odds with real-time, high-throughput tasking of autonomous systems



"If the queue backlog is very long, **Slurm may not be able to make it** through a complete scheduling cycle ..."

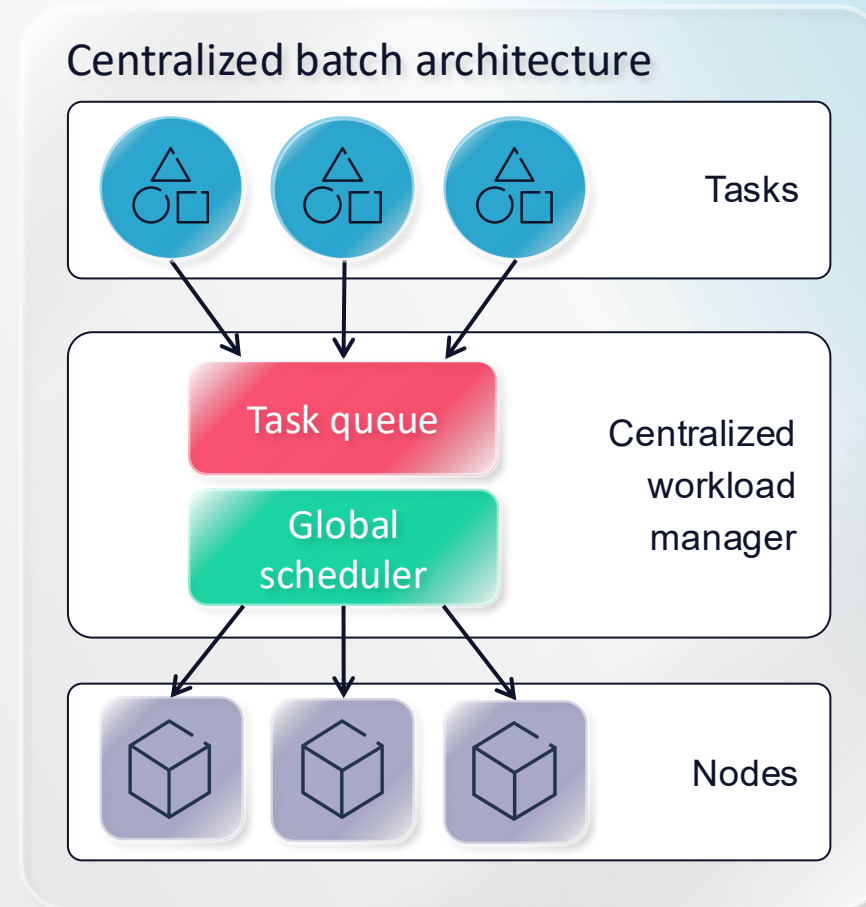


Scheduling - NERSC Documentation.
<https://docs.nersc.gov/jobs/scheduling/>

"This can cause **very large inefficiencies in utilization.**"

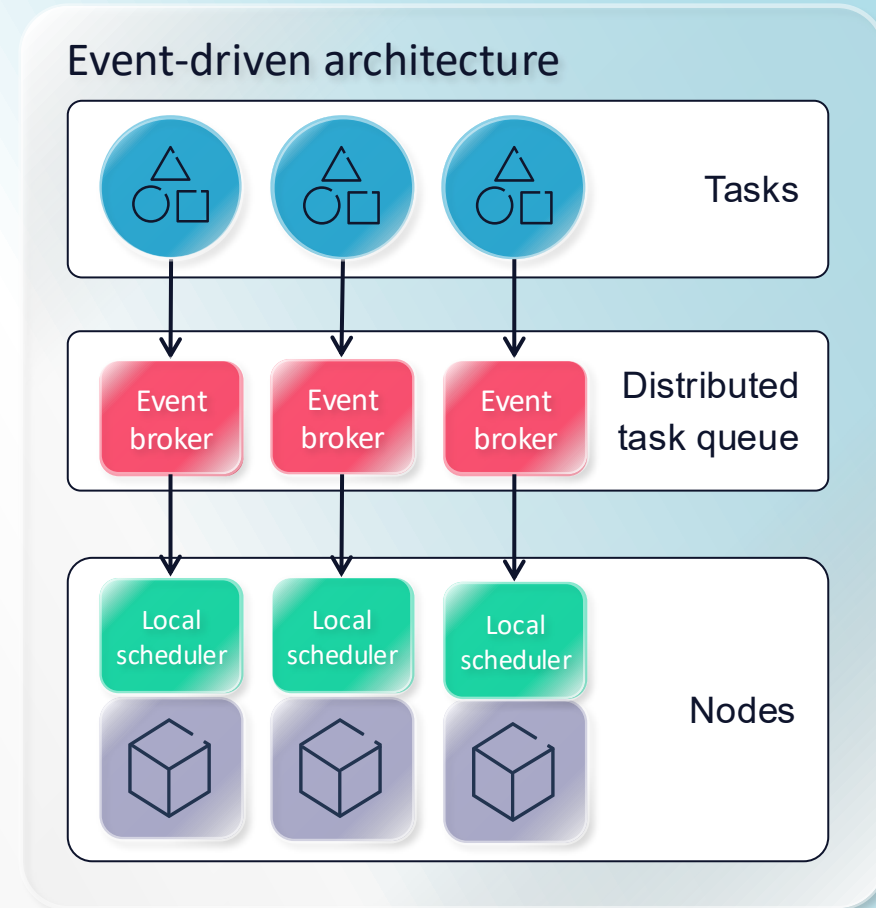
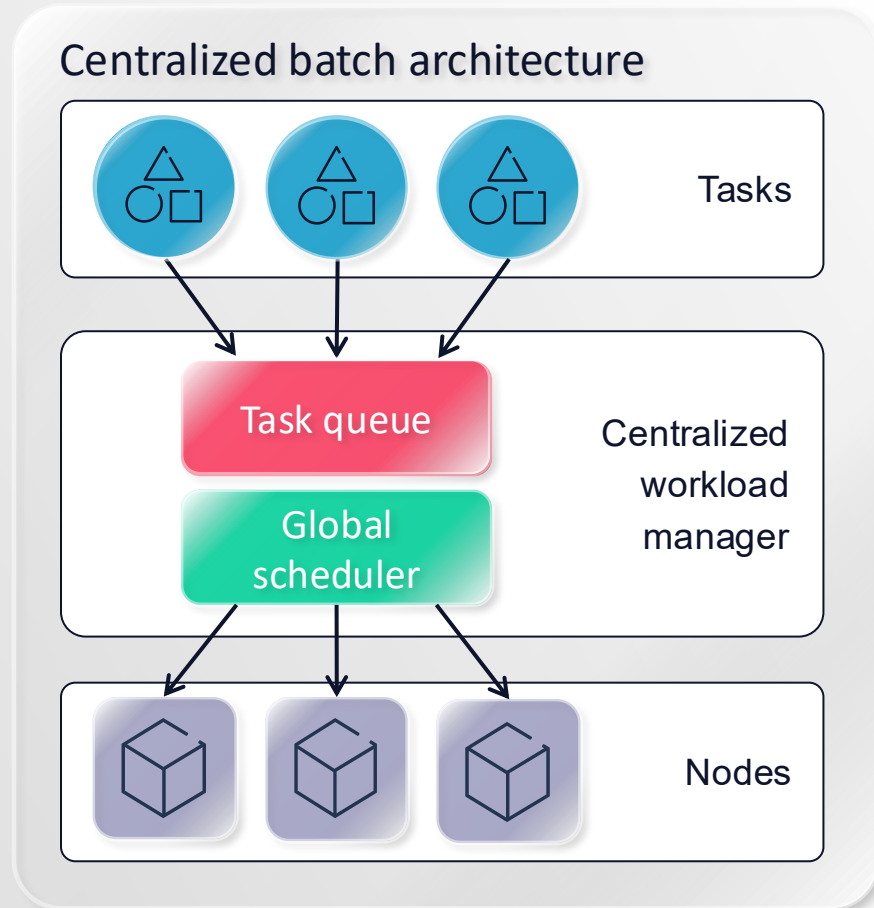
Centralized task orchestration is fundamentally not scalable

Scheduling is NP-hard and gates task ingestion and dispatch



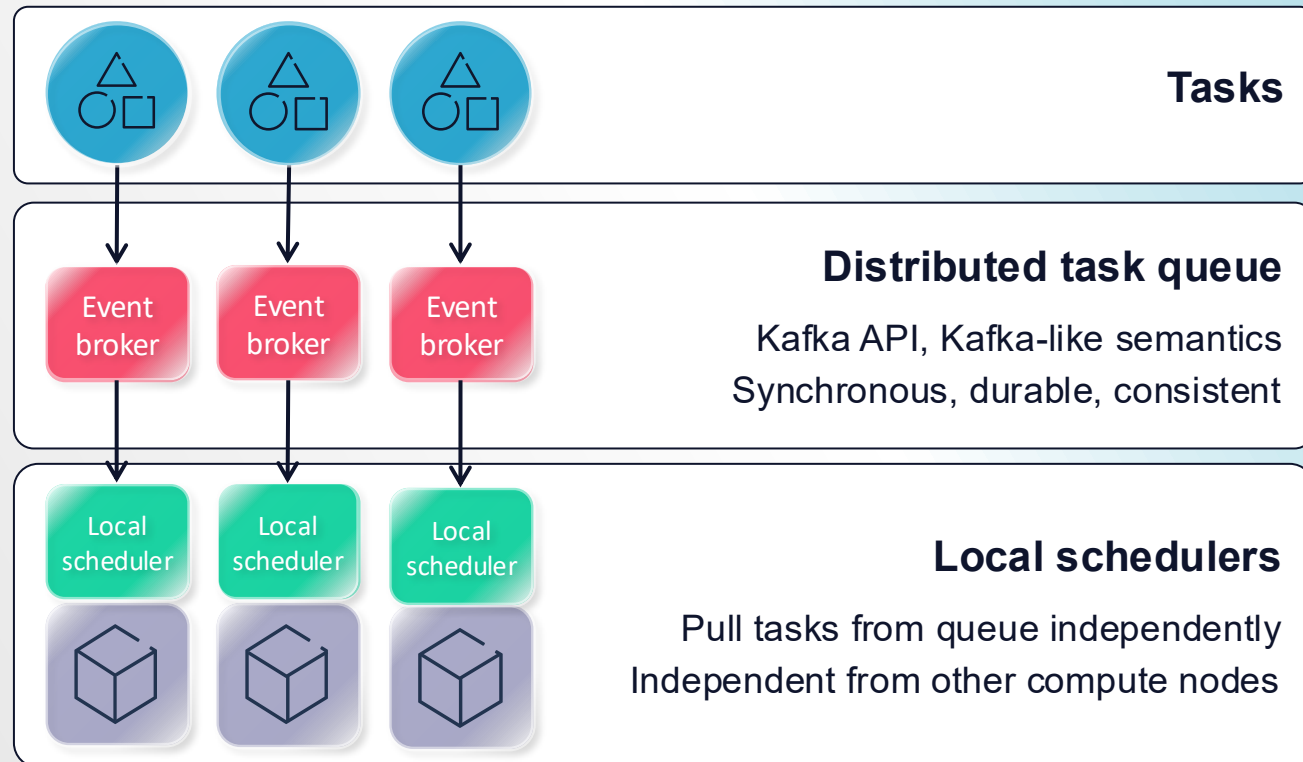
Event-based orchestration is fundamentally scalable

Nodes pull work from a durable queue, separating task ingest from dispatch



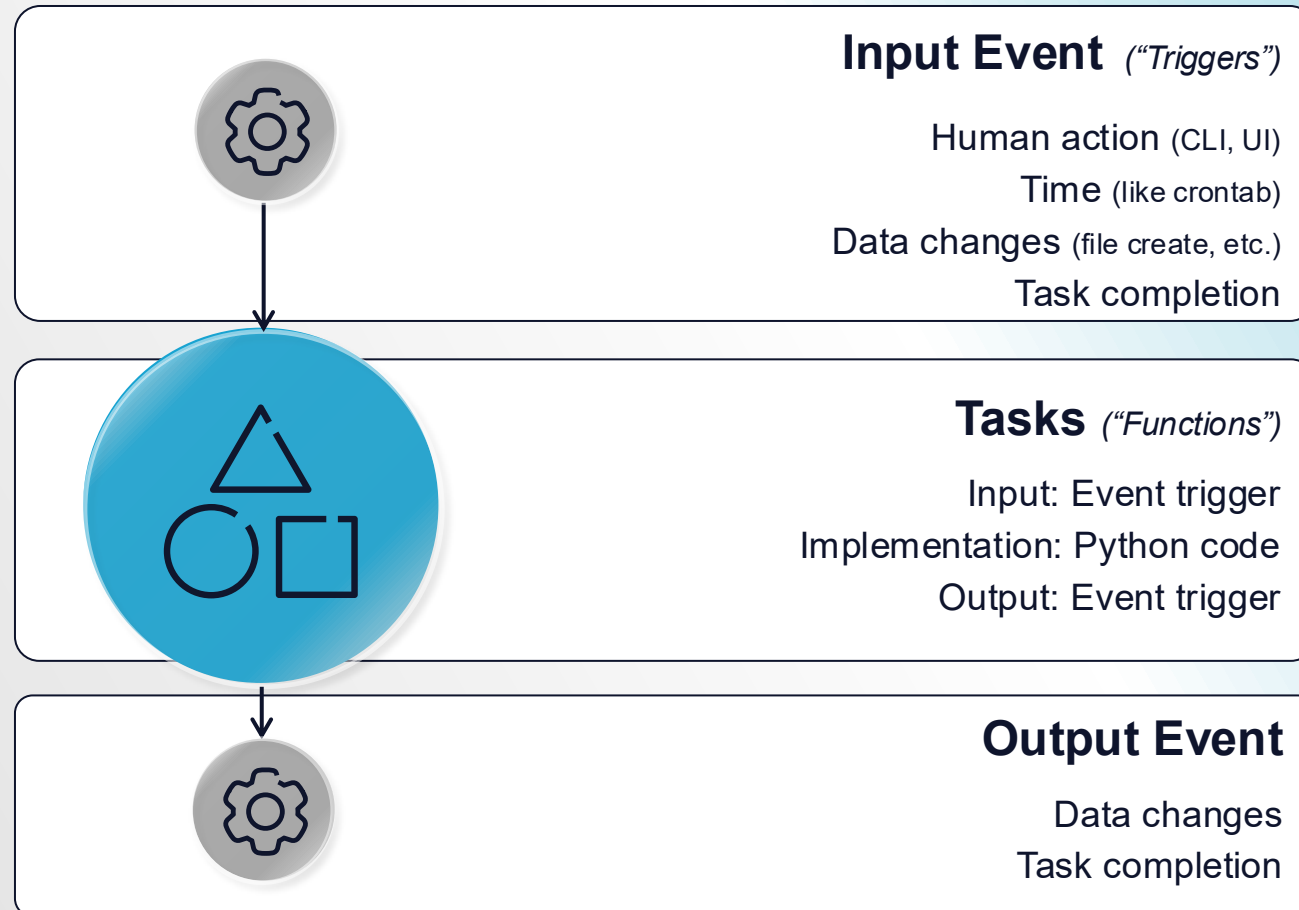
Event-based orchestration is fundamentally scalable

Nodes pull work from a durable queue, separating task ingest from dispatch



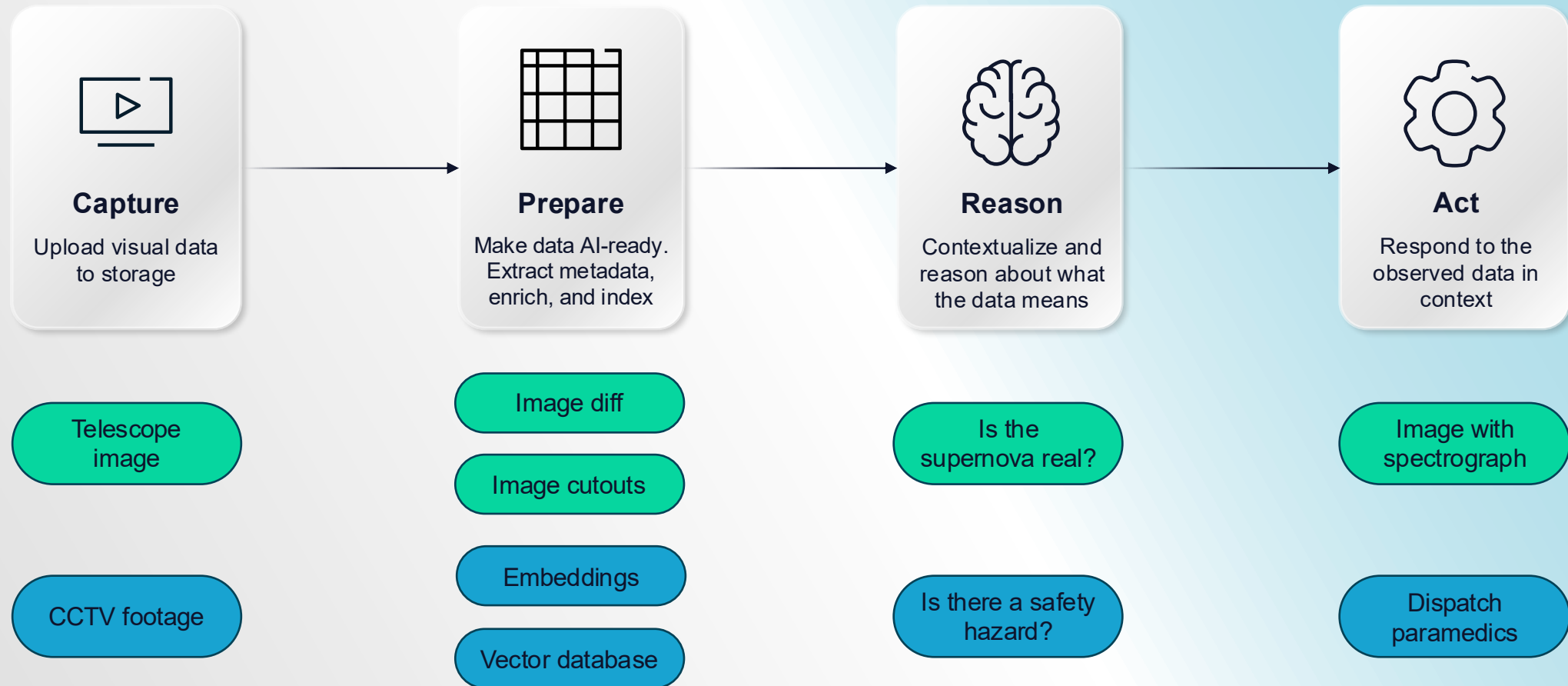
Tasks compose into workflows through triggers

Tasks are created in response to triggers and emit triggers upon completion



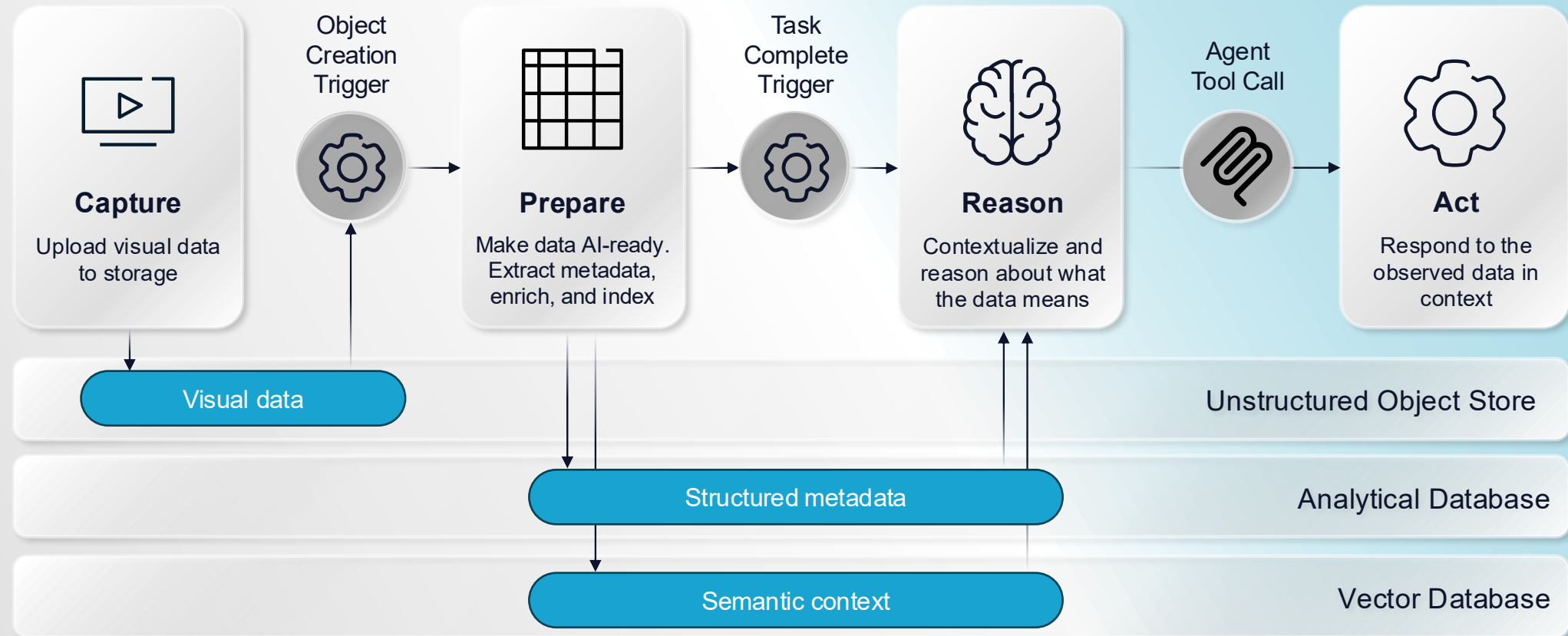
Autonomous visual reasoning follows a common pattern

Astrophysical transient detection and autonomous public safety monitoring are computationally similar



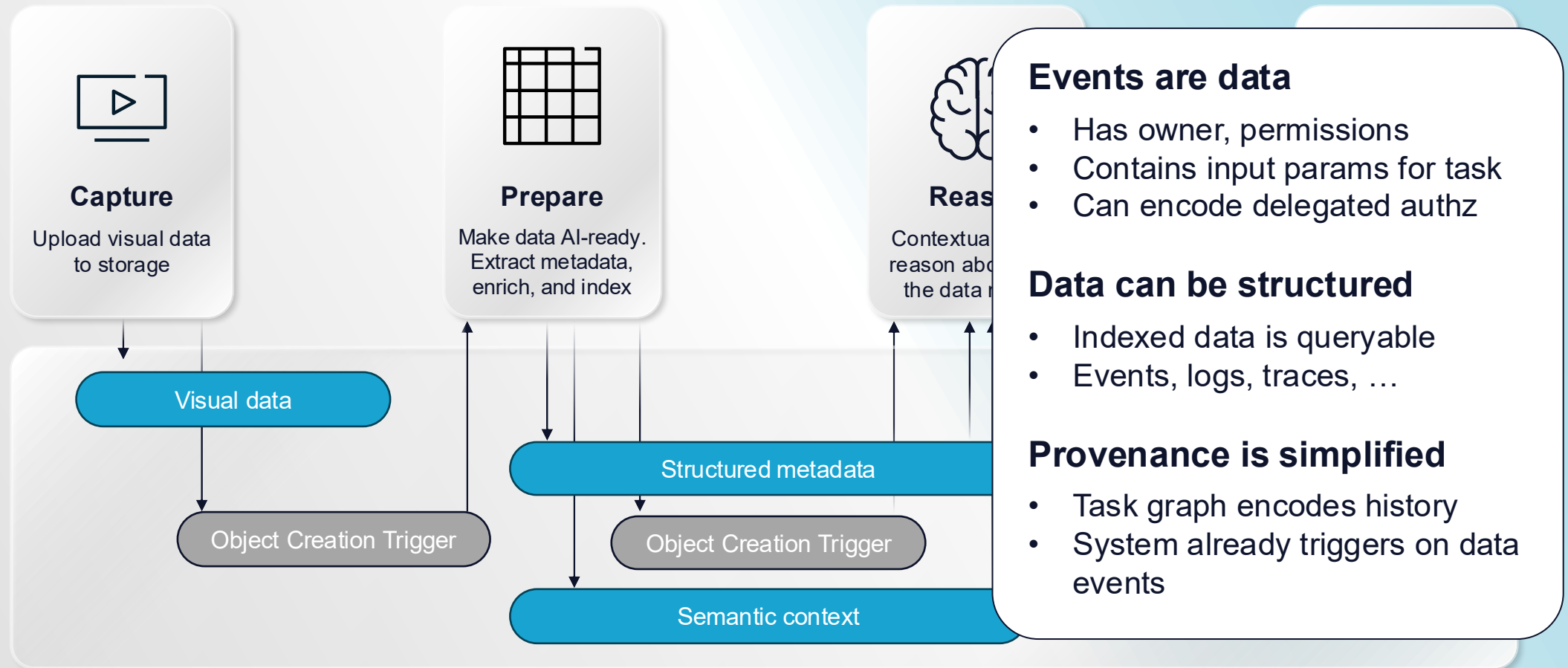
Visual reasoning maps well to event-driven orchestration

Same pipeline and same task code scales from one sensor to tens of thousands



Events are data too

Tasks and events can be treated as data, simplifying observability, provenance, governance



The right tool for the right shape

Event-driven for the majority; centralized scheduling when task geometry demands it

Event-driven architectures map to autonomous systems

- Many small tasks needing real-time responsiveness
- Observability, provenance, and governance automatically inherited by treating workflows as data

But centralized orchestrators aren't bad!

- Multi-node, topology-sensitive task placement
- Long-running, latency-insensitive tasks

The ideal orchestrator combines both

- All tasks are event-driven, but
- Call out to a centralized orchestrator as-needed



