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KubeFlux: an HPC Scheduler Plugin for Kubernetes

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Wednesday, May 18, 2022

KubeFlux: an HPC Scheduler Plugin for Kubernetes

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LLNL-PRES-834303

What is a supercomputer?

- High performance: LLNL El Capitan to achieve > 2 exaFLOPs (projected world's fastest in 2023)
- High power requirements: less than 40 MW
- High density, typically liquid cooled
- High utilization: typically 99%
- High bandwidth: 200Gb/s per link
- Low latency: sub-μs switching
- Heterogeneous co-processors

El Capitan will feature integration of cloud technology

Computing achieves High Performance (HPC) through efficiency, proximity, and shape.

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- HPC applications strive for high parallel efficiency (scalability)
- Many HPC apps are tightly coupled
  - problem subdivided across processors
  - *neighbor* communication
- A major way to achieve HP is through placement:
  - topology (connectivity; shape): NUMA nodes, L1-3 cache, network
  - distance (link length; speed of light can be limiting factor)

Cloud is a dominant market force influencing HPC.

- Public cloud revenue forecast: $500B by 2022, $600B by 2023 (Gartner)
  - HPC spending 2022: $32B (Hyperion Research, 2020)
- KubeCon + Cloud Native Con is very popular
  - K8s has a huge user, open-source developer community
  - HPC shouldn't become a technology island
- Containers in HPC and CANOPIE (SC) workshops (among many others): increasing interest from HPC community
- *HPC scheduling in K8s is not fully realized*

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Strategically important LLNL workflows like AMPL exhibit the need for HPC+cloud converged computing.

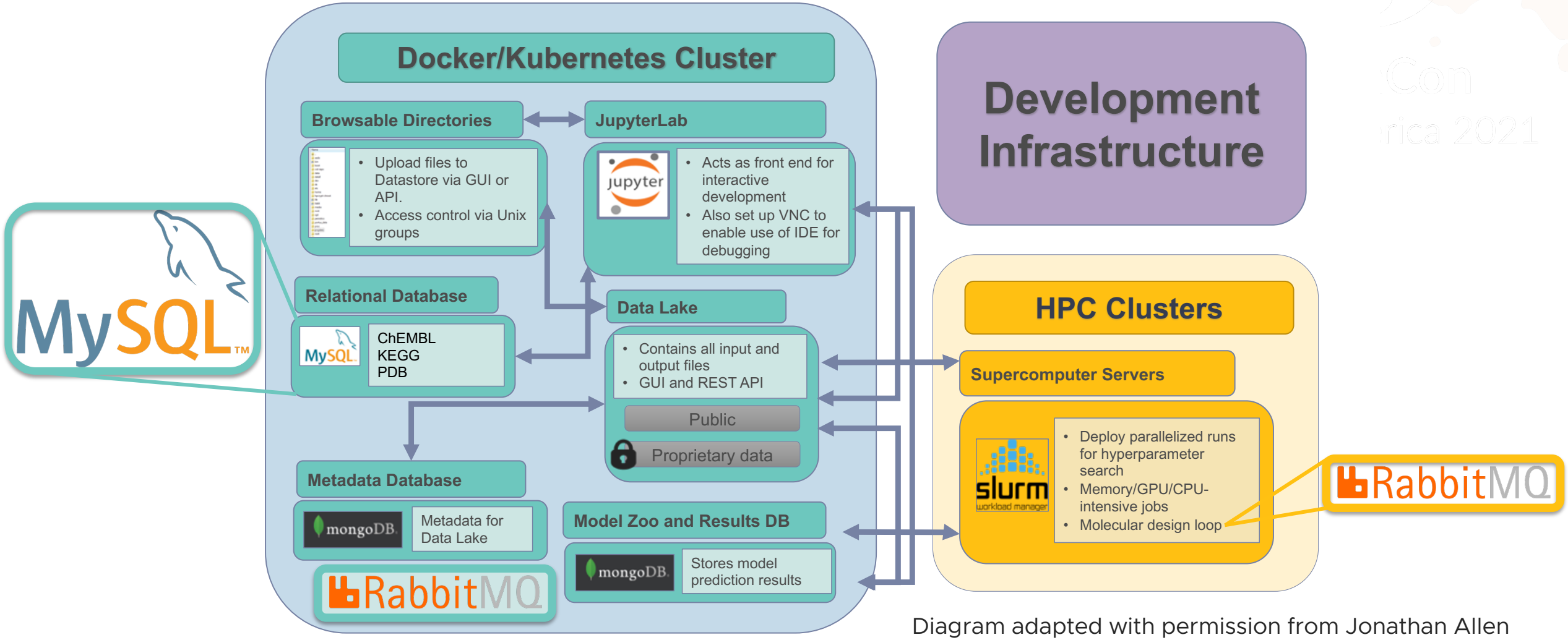

Diagram adapted with permission from Jonathan Allen

Other LLNL workflows are demanding cloud technologies in HPC, and the demand will increase.

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- American Heart Association Molecule Screening (AHA MoleS) workflow
- Rapid COVID-19 small molecule drug design workflow (based on 2020 ACM Gordon Bell Special Prize finalist)
- Autonomous MultiScale project
- Rutgers-LLNL: RADICAL-Pilot for COVID-19 research

The 2020 LLNL HPC Application Survey determined <10% of apps are currently using cloud… but 73% may adopt cloud in the future

HPC schedulers and K8s are complementary technologies

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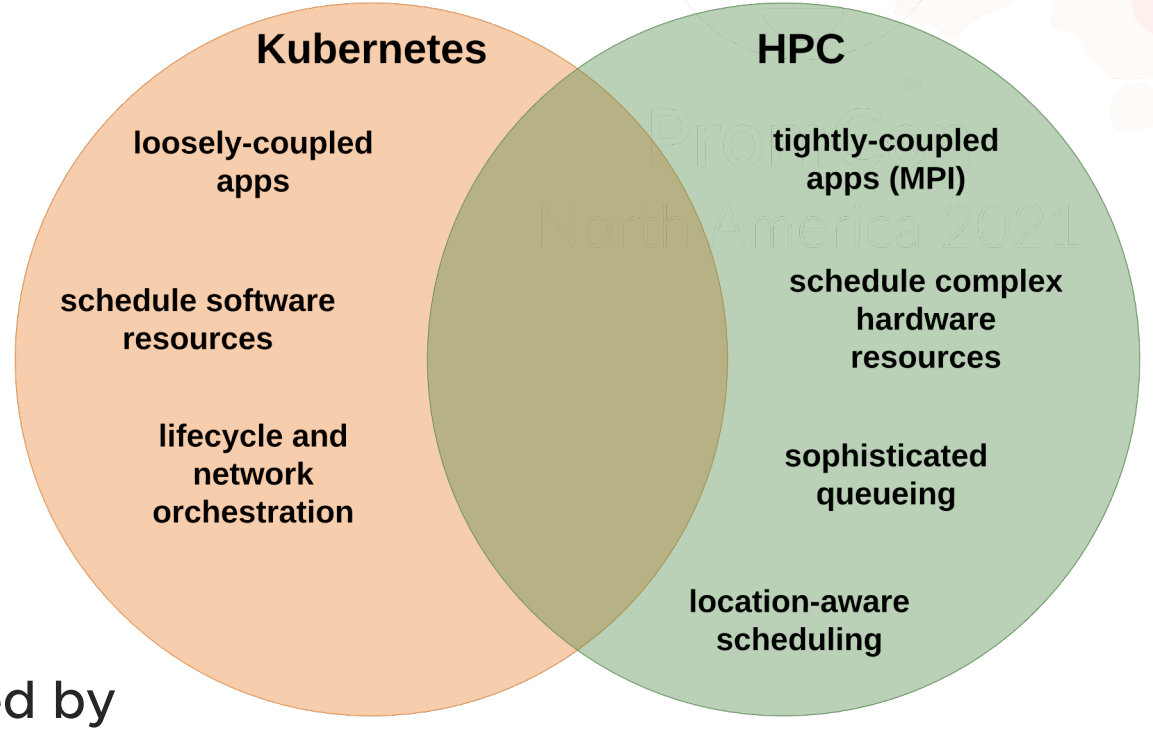
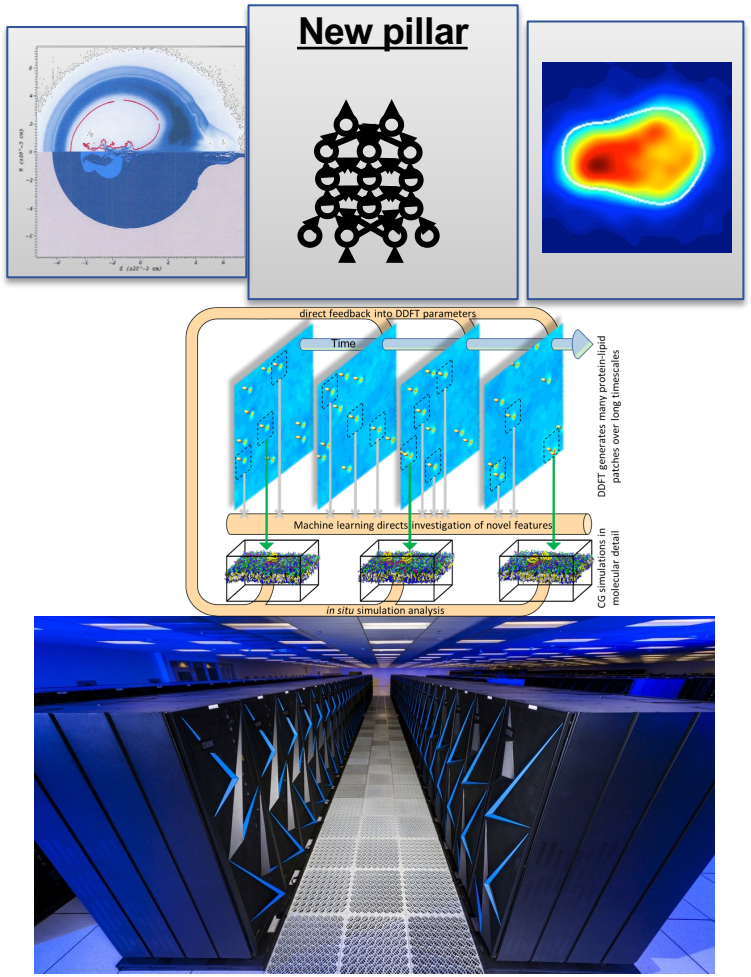
- HPC disadvantages:
  - can't orchestrate container lifecycle and networking
  - not designed for elasticity
- K8s disadvantages for converged computing:
  - designed for loosely coupled apps
  - kube-scheduler is limited
  - limited resource expression for HPC, mitigated by Node Feature Discovery (NFD)



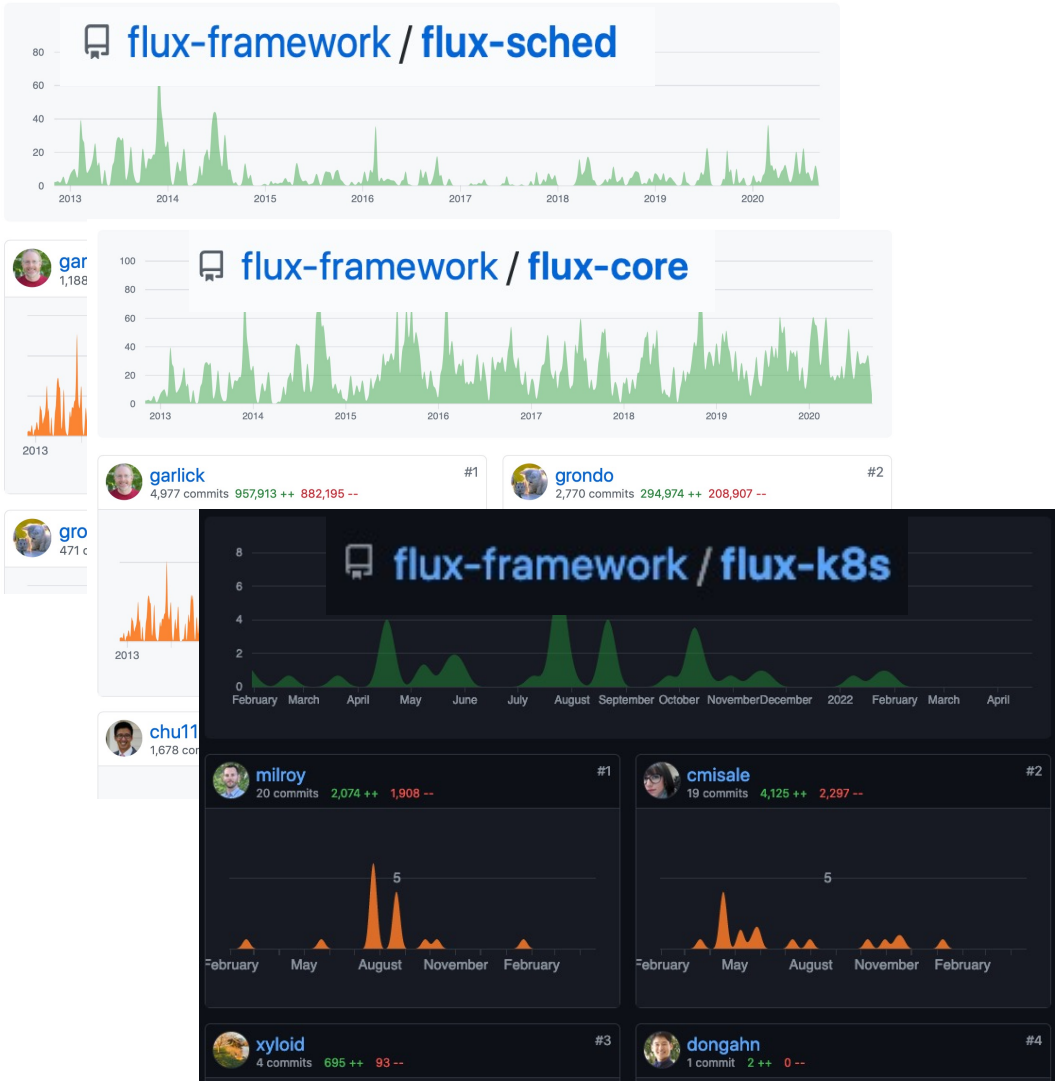
Fully-featured HPC scheduling in K8s has not been achieved.

Trends towards complex workflows, extreme resource heterogeneity, and converged computing render traditional workload managers increasingly ineffective.



- Co-scheduling
- Job throughput
- Job communication/coordination
- Portability
- Extremely heterogenous resources

Flux framework solves the key technical problems that emerge from these trends.



- Open-source, active flux-framework GitHub org.
  - flux-core, -sched, -security, ***-k8s***, etc.
  - over 15 contributors including some of the principal engineers behind SLURM
- Single-user and multi-user modes
  - single-user mode in production for ~4 years
  - multi-user mode debuts on LLNL Linux clusters
- Plan of record for El Capitan

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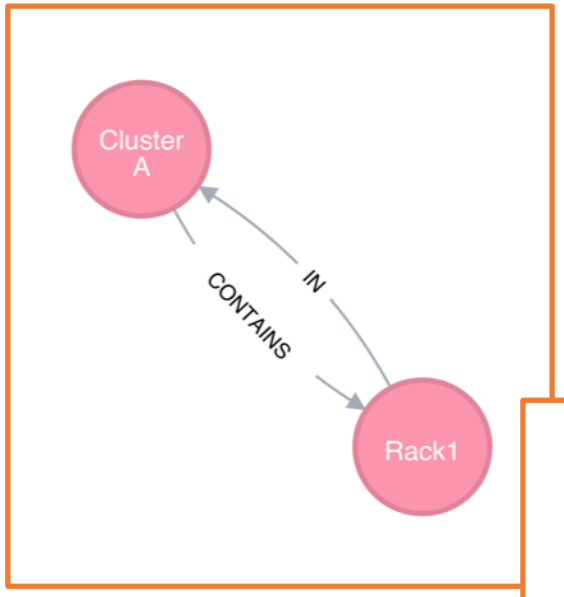
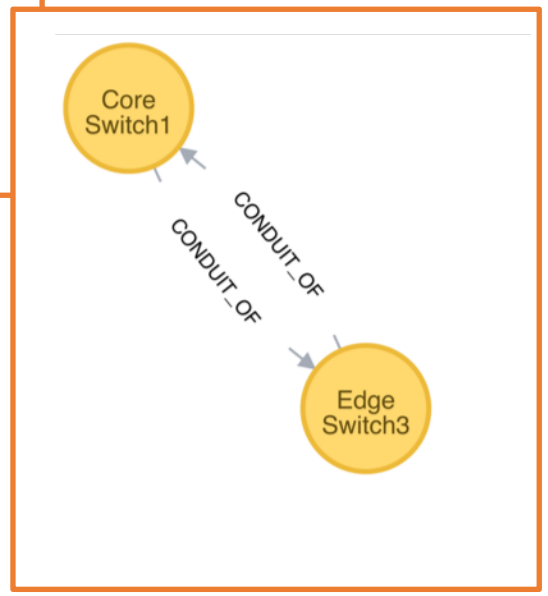
Flux pioneers graph-based scheduling to manage complex combinations of extremely heterogenous resources.

- Traditional resource data models are largely ineffective for resource heterogeneity
  - designed when systems were simpler
  - node-centric models are monogenous
- Elevate resource relationships (***edges***) to an equal footing with resources (***vertices***)
- Complex scheduling can be expressed without changing the scheduler code
- Rich and well-defined API for graph traversal and allocation

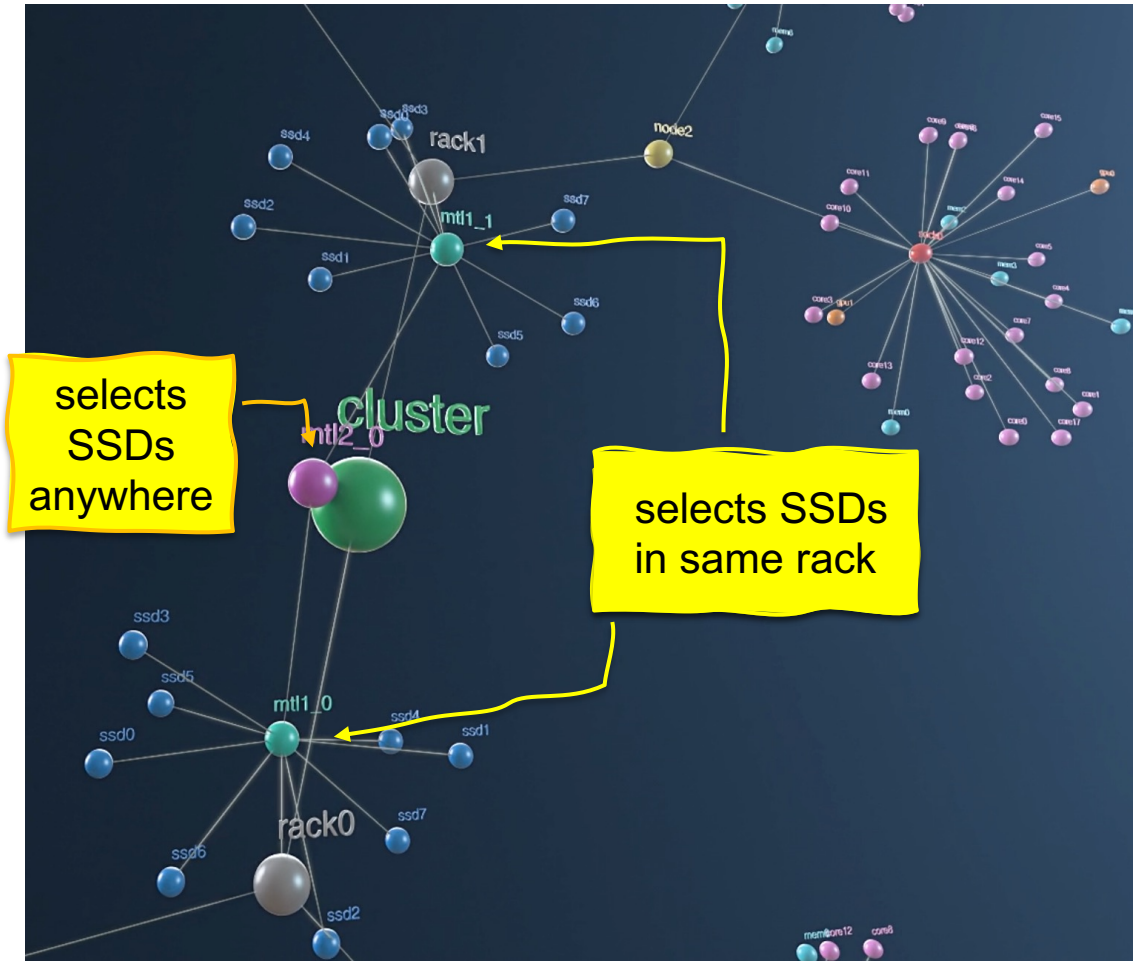


Containment subsystem



Network connectivity subsystem

Our graph approach solves the critical scheduling need for El Capitan's Rabbit multi-tired storage.



- Schedule SSDs in each rack
  - mount as node-local storage to compute in same rack
  - used to build ephemeral Lustre
  - deemed too difficult for traditional schedulers
- Easily enabled by Fluxion; no code change
- End-to-end job state transition
  - DataWarp/Rabbit mock service containers by HPE
  - Kubernetes CRD

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Requirements for HPC on K8s, KubeFlux Internals

Claudia Misale

Run HPC on Kubernetes

Requirements:

1. Batch/group scheduling
2. Topology awareness
3. Optimized placement for multiple workloads
4. Choose among placement algorithms

..possibly combine all of the above

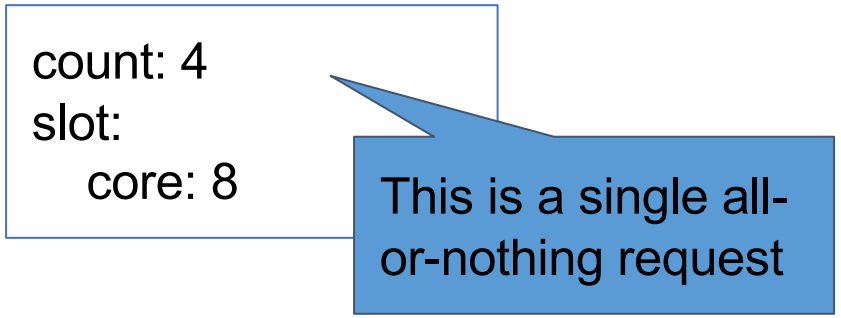
Batch/Group Scheduling

Upstream Kubernetes:
PodGroup CRD and Coscheduling[1] scheduler plugin implement group scheduling

KubeFlux uses PodGroup to create the groups

- Fluxion is a batch scheduler -> group placement done right and for free

Example: MPIJob, 4 worker nodes, 8 cores



[1]https://github.com/kubernetes-sigs/scheduler-plugins/blob/master/pkg/coscheduling/README.md

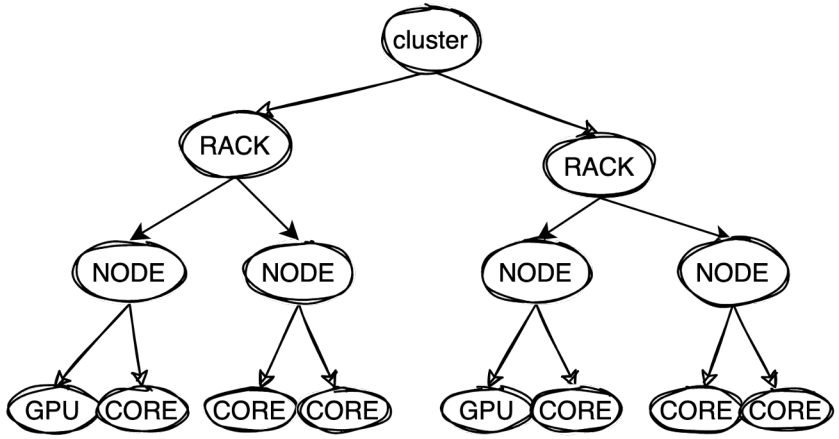
Topology Awareness

Upstream Kubernetes:

- NodeResourceTopology CRD and Topology[1] Aware scheduler plugin (NUMA)
  - Topology at node level
- Use of labels, (anti-)affinity, taint/toleration
  - Not scalable

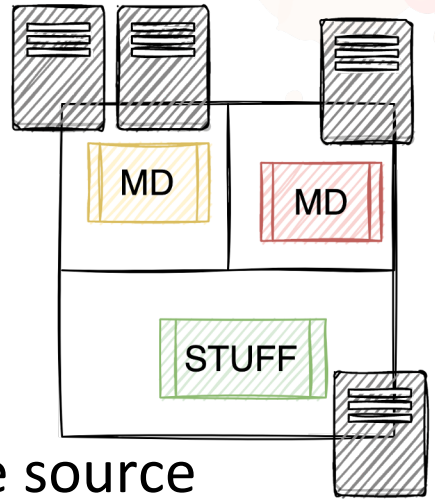
KubeFlux resource model is graph based

- Topology at cluster level
- Job spec converted to graph for matching



[1]https://github.com/kubernetes-sigs/scheduler-plugins/blob/master/pkg/noderesourcetopology/README.md

Optimized Placement for Multiple Workloads



Upstream Kubernetes:

- Use labels, taints/tolerations, (anti-) affinity, not scalable solution
- Trimaran load-aware scheduler plugin
    - Learns from running workloads, does not solve the problem at the source

KubeFlux provides exclusive usage of resources at any level of the topology

- Avoid noisy neighbors
- Oversubscription possible but not preferable for HPC

[1]https://github.com/kubernetes-sigs/scheduler-plugins/blob/master/pkg/trimaran/README.md

Different Placement Algorithms

Upstream Kubernetes:

- Add multiple profiles to the scheduler. Facilitated by Scheduler Framework
- Can force placement with affinity/taint up to a certain level
- Cannot spread with anti-affinity

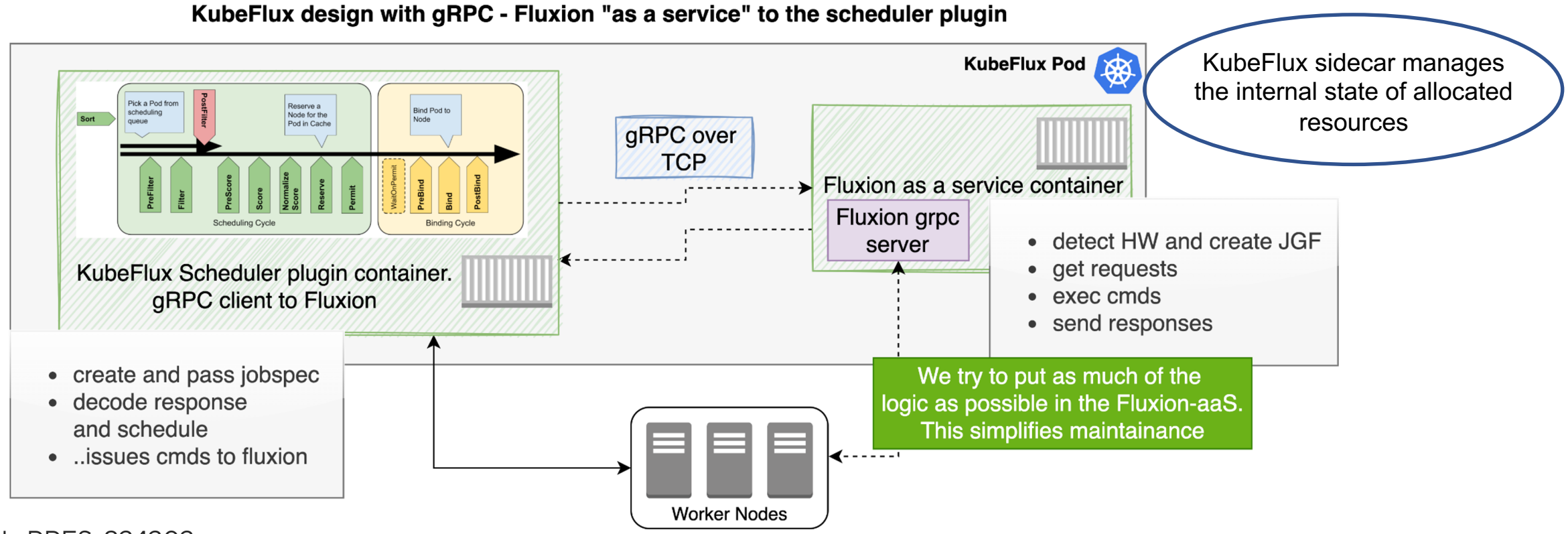
KubeFlux:

- Can decide between different flavors of packing and spreading
    - compute intensive vs network intensive workloads
- High- and low-level constraints captured in a jobspec also create different placement (i.e., shared vs exclusive use)

KubeFlux Plugin Description

Based on **Fluxion**, the scheduler component in **Flux Framework**

- Used in KubeFlux as sidecar container

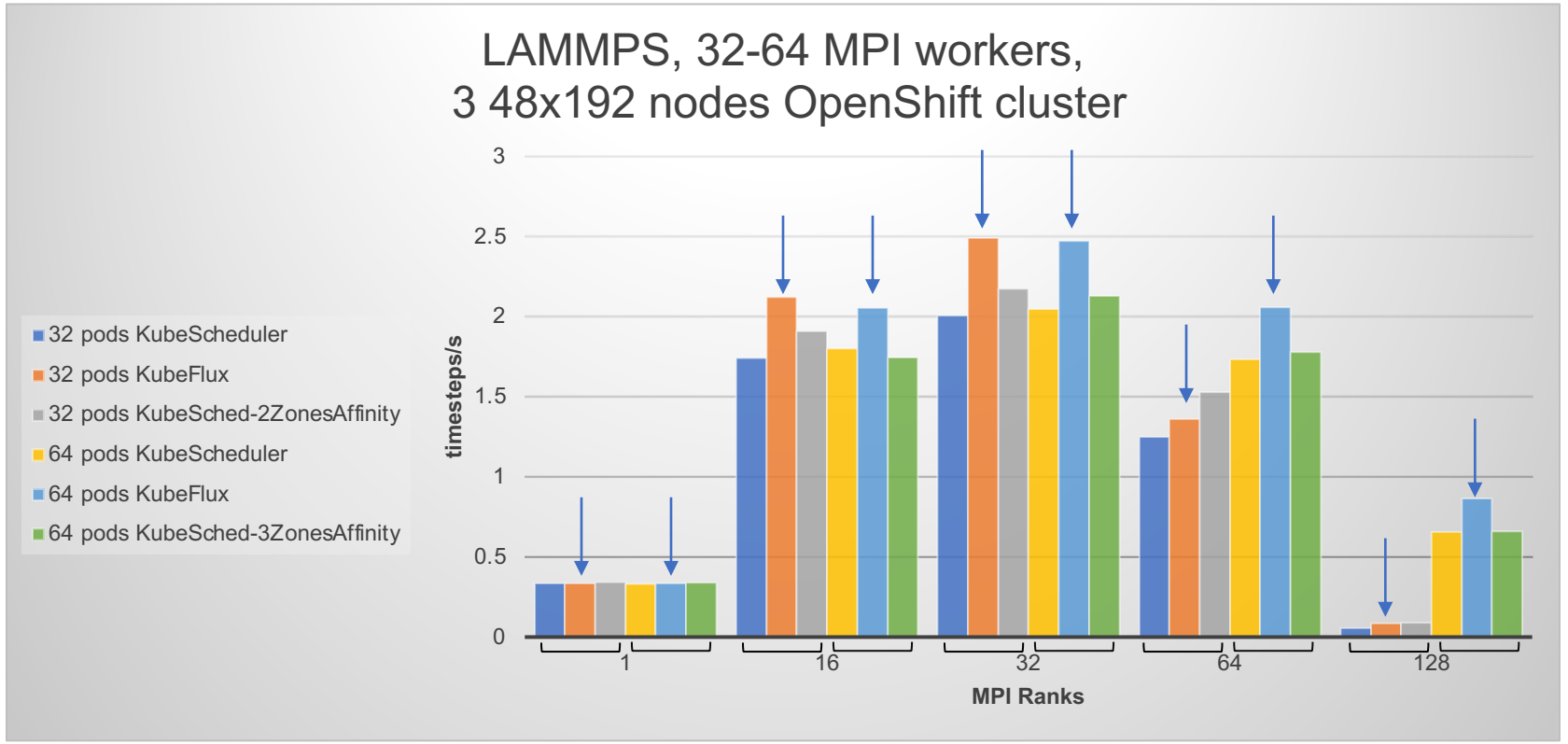


Use Case: Traditional HPC (LAMMPS)

MPI-based molecular dynamics application that models ensembles of particles in a liquid, solid, or gaseous state

KubeFlux:
- pack match policy

KubeScheduler:
- Default
- Zone affinity to force a limited packing

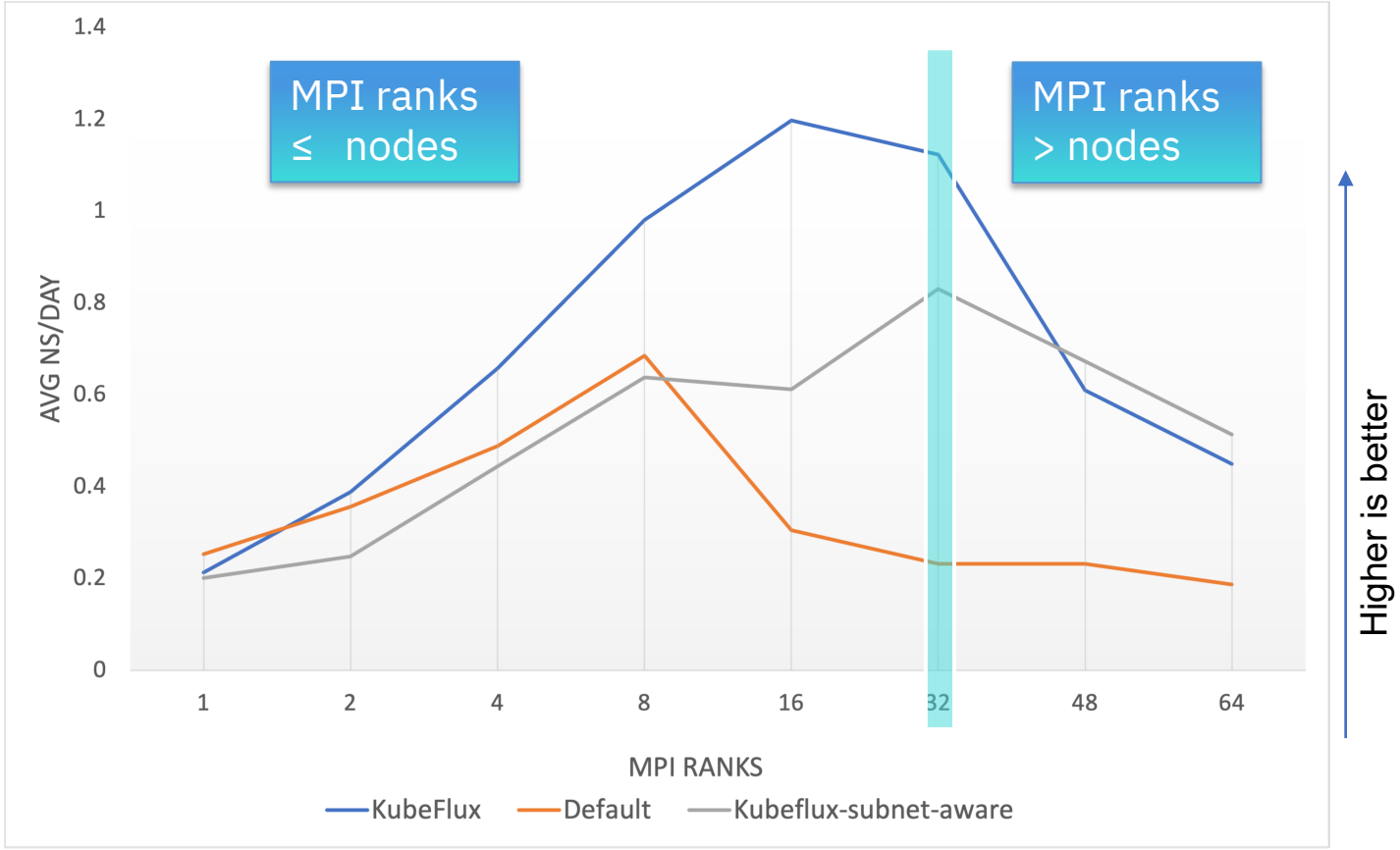


Use Case: Traditional HPC (GROMACS)

MPI-based large-scale simulations of molecular dynamics – benchmark: water molecules

KubeFlux:
- Vanilla spread match policy
- AZ aware spread match policy

KubeScheduler:
- Default



Published at SC'21 CANOPIE Workshop (to appear)
It's a Scheduling Affair: GROMACS in the Cloud with the KubeFlux Scheduler

There is a significant gap between K8s and HPC RJMS. KubeFlux is the first step to closing it.

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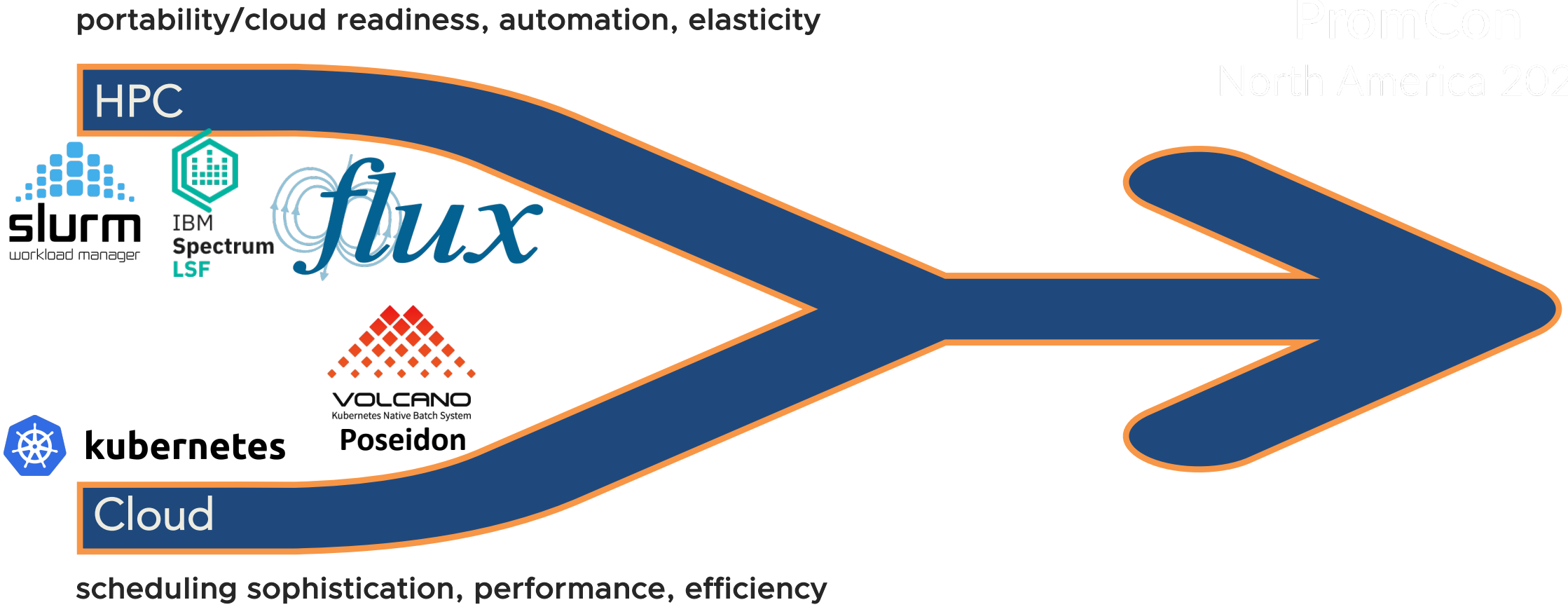

Thanks!

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git@github.com:cmisale/scheduler-plugins.git

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