ADAC8

Cray Shasta Orchestration for HPC and Cloud

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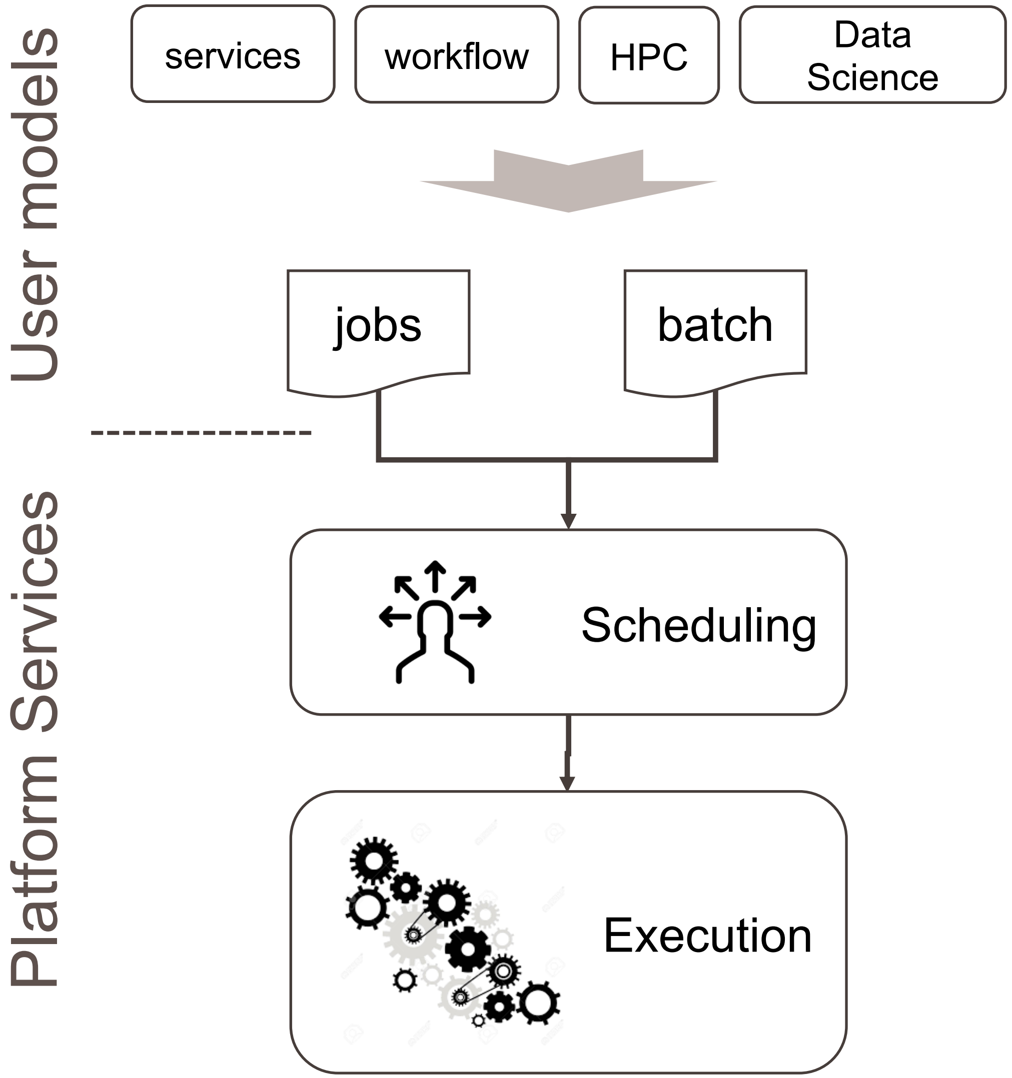
Agenda

- Overview
- Scheduling
  - Traditional HPC
  - Cloud Orchestration
- Emerging Technologies
  - Workflow agents
  - Capsules
- Q&A

Overview

- Objective: execute traditional batch jobs and cloud-native services & workflows
- Fully utilize system resources
- Three components
  - User models
  - Scheduling services
  - Execution services



HPC Orchestration User Cases

- Kubernetes Use Cases (for HPC)
  - Projects need to express their workflows and supporting services in a portable cloud-native way
  - Third-party tools will increasingly assume compatibility with the kubernetes platform
  - Emerging workflow tools assume kubernetes or strongly support it
    - Argo: container native workflow engine for parallel jobs
    - Kube-batch: batch ‘like’ scheduler for kubernetes
    - Others: kubeflow, nextflow, airflow, volcano

SCHEDULING

Scheduler Technologies

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Meta-schedulers
- Mesos, …(GridWay)
- Attributes:
  - Broker resources
  - Global resource view

HPC Schedulers
- WLM: Slurm, PBS, Flux, etc.
- Attributes:
  - Placement
  - Scheduling polices
  - Resource controls

Container Orchestrators
- Kubernetes, Swarm, Nomad, etc.
- Attributes:
  - Lifecycle Management
  - Monitoring
  - Placement

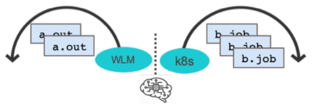
Orchestration and Workload Management

partitioned ← … → converged

Separate environments	Containers via a WLM	Orchestration job scheduling features	Run both natively in shared environment
• Deploy containerized applications separate from HPC applications • Benefit: Avoid disrupting existing environments • Challenge: Siloed partitions	• Use workload manager to instantiate containers • Benefit: Containerized workloads with minimal disruption to their environment. • Challenge: no access to orchestration features	• Use existing scheduling facilities in orchestrator • Benefit: Leverage innovation in orchestration tools • Challenge: Interaction with traditional HPC and relevant schedulers increases complexity and potentially decreases performance	• Orchestration and workload manager co-exist on the same cluster • Benefit: With this approach, WLM acts as a resource manager, making resources available to the Orchestrator. • Challenge: Difficulty of sharing resources

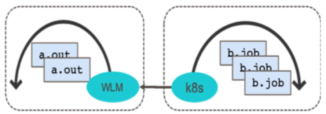
Multi-framework Scheduling Options

- A – **Independent schedulers**



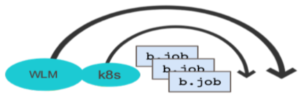
  - Admin manages scheduling domains – fixed allocations
  - Rebalancing requires reboot
  - Inefficient use of system resources

- C – **Master worker scheduler**



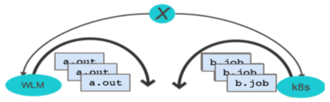
  - Corporative scheduling environment
  - Authoritative scheduling – single system view
  - Requires bridging master and subordinate schedulers

- B – **Subordinate scheduler**



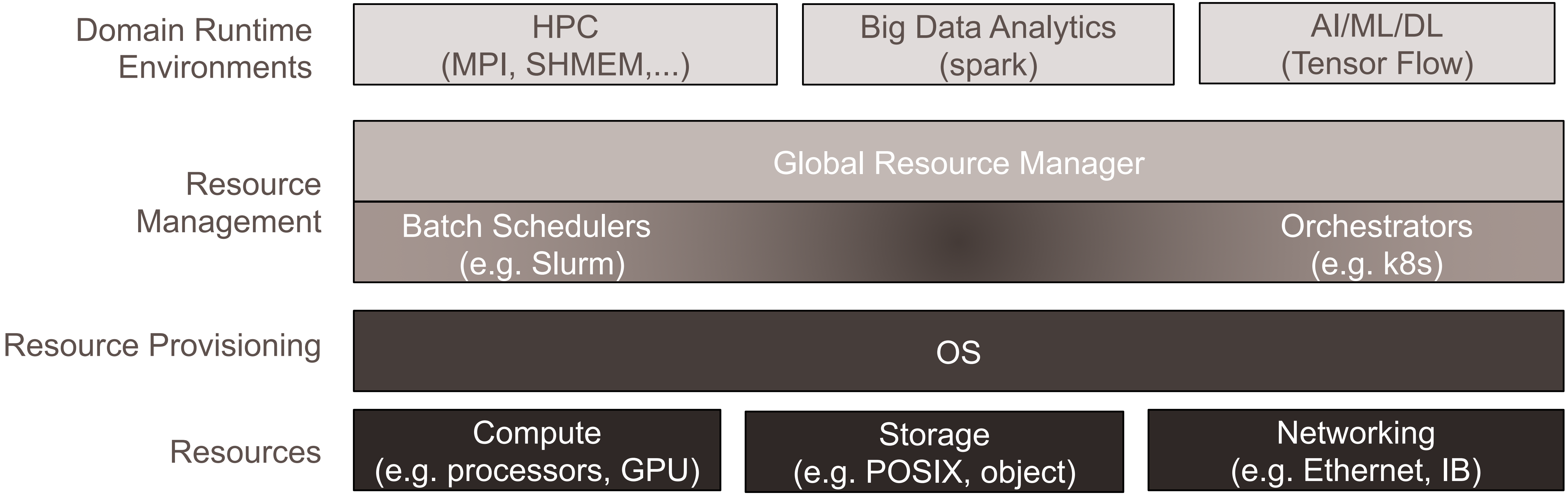
  - User defined framework
  - Outer scheduler owns resources, Inner uses resources
  - Independent/adversarial schedule policies
    - Inefficient use of system resources

- D – **Meta-scheduler environment**



  - Supports multiple workload paradigms
  - Authoritative scheduling – single system view
  - Requires scheduler modifications

Converged System

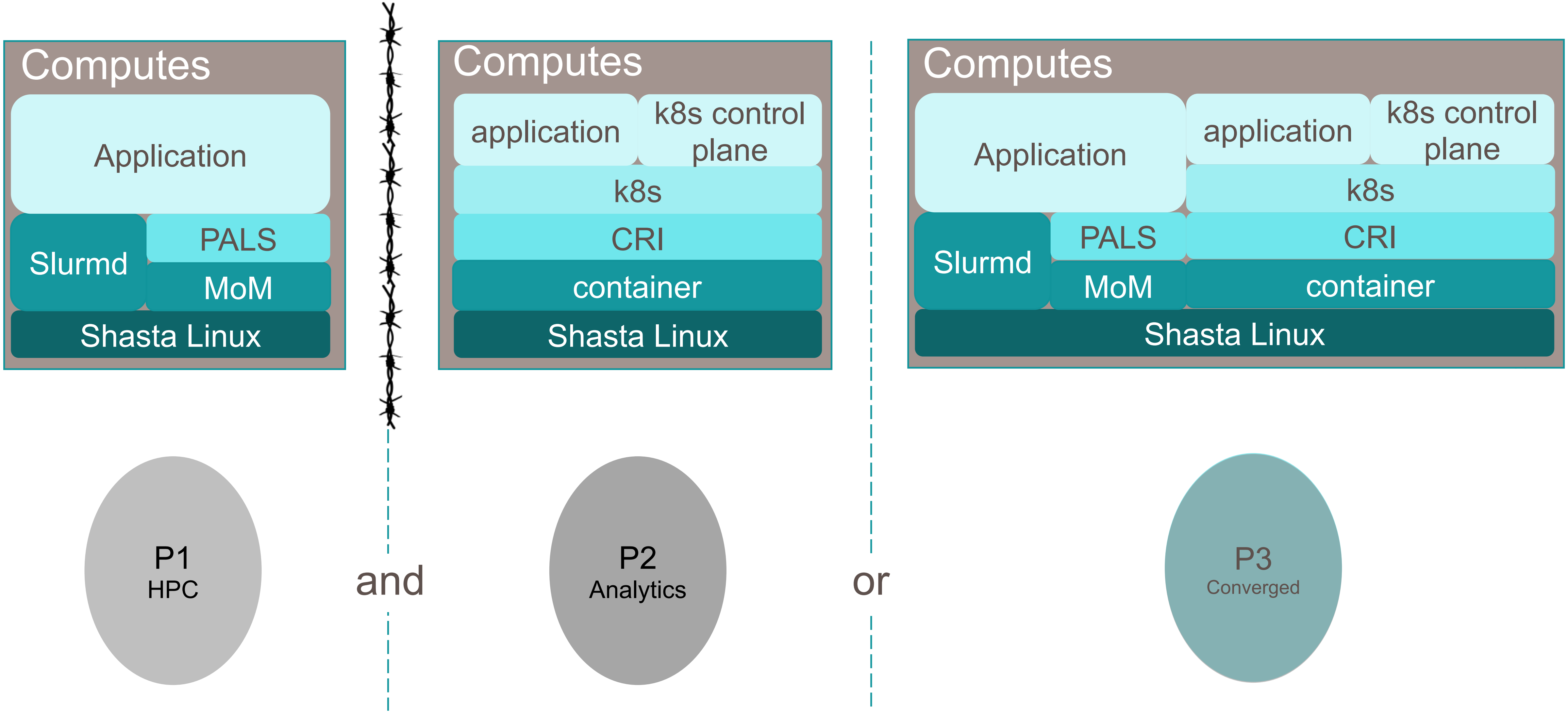


Assumptions in Orchestration Services

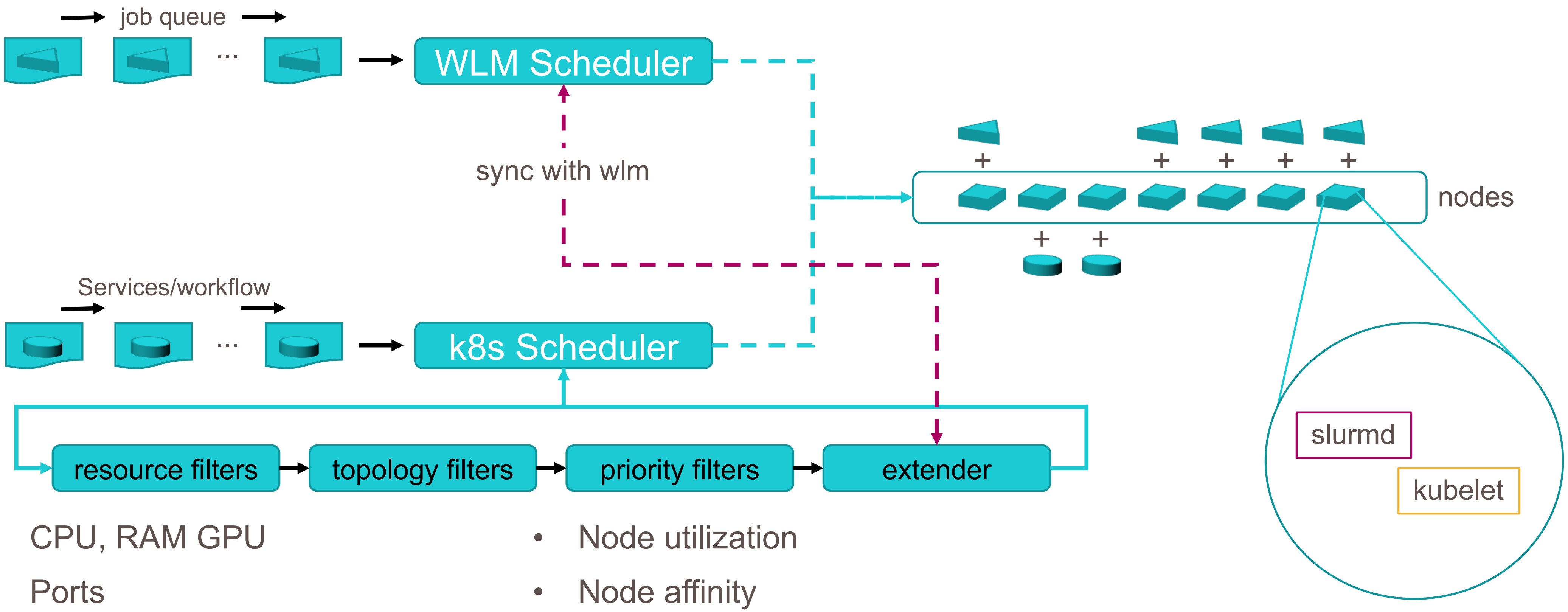
- Typically used in cloud environments – not HPC
- The user “owns” the resources
- Focused on deploying a set of services and keeping them in a good state
  - Tends to assume there is always enough resource (or it can be quickly provisioned – elastic consumption)
  - Persistent, long-running (no walltime)
  - Not HPC application focused[†]
- Definition of a consumable can be extensible

† kube-batch offers some HPC semantics, job priorities, polices

Shasta Provisioned Stacks



K8S – Extension Scheduler



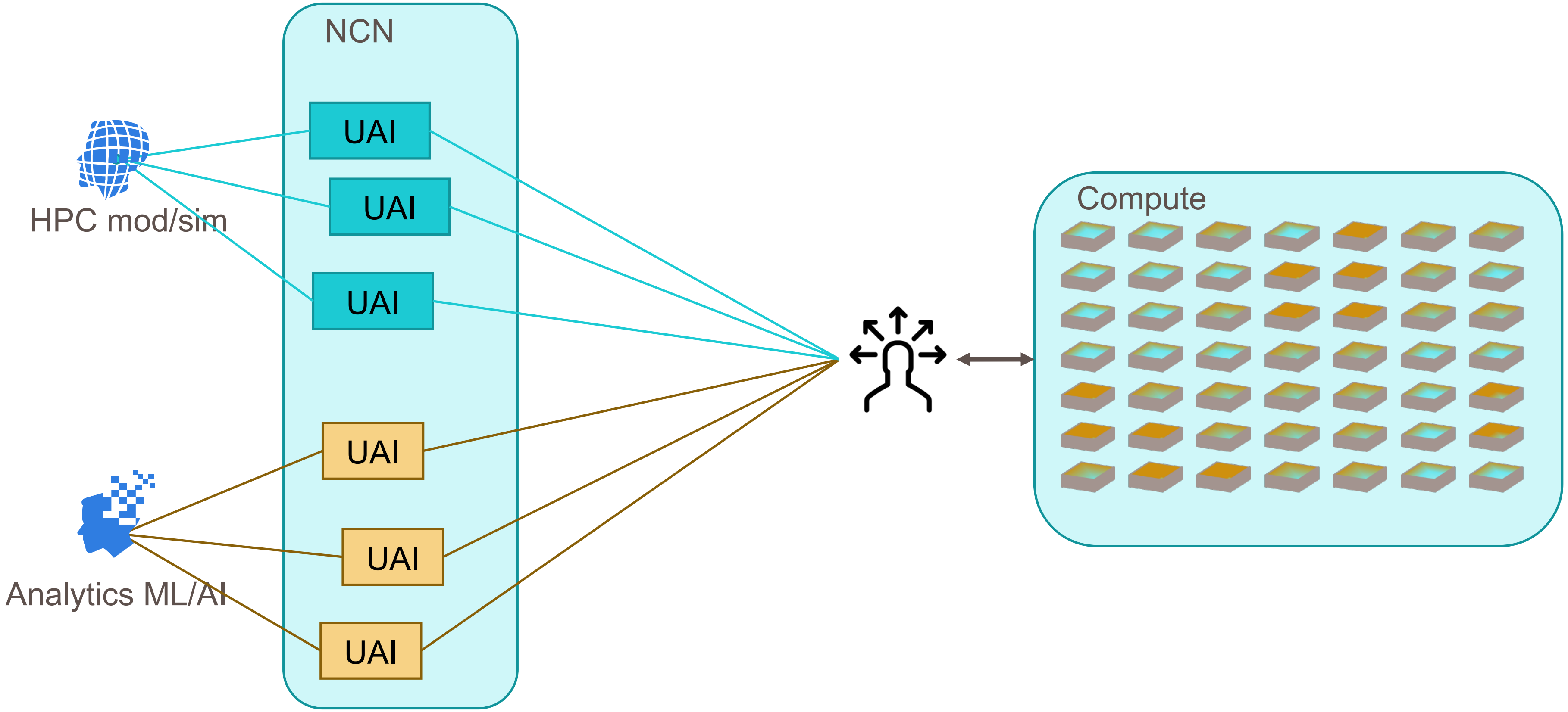
- CPU, RAM GPU
- Ports
- RAM, disk pressure

- Node utilization
- Node affinity
- Taint toleration

- Constraints
- Affinity
- Taints

- WLM decision/reservation

Shasta User View – Hybrid-Scheduling



Scheduling Opportunities and Challenges

- Job Type Characteristics
  - Parallel jobs – gang scheduling (kube-batch)
  - High throughput (million jobs) – scheduler latency
  - Interactive and batch
- Resource Dependencies
  - Accelerators, networks, storage – resource plugins
- Different Scheduling Options
  - On demand vs. queue
  - Workflow agents – argo, kube-flow, nextflow, etc.

CAPSULES

Introduction

What are Capsules

- A Capsule is a declarative specification of a desired runtime environment
- Aims to provide a common abstraction for running a wide variety of workloads
  - Reduce cognitive overheads of running across differing schedulers and orchestrators
    - i.e. don't force end users to be K8S/Slurm/PBS experts
  - Focus has been on enabling interactive supercomputing

Capsules – Design Goals

- Declarative
  - Define what the user wants
  - Capsules handles details of launching that on the underlying platform
- User Friendly
  - Inspired by common tools, such as conda, docker, git
- Portable
  - Define a capsule once, run on any supported hardware/software (within reason)
- Extensible
  - Extensible architecture allows vendor (and customers) to quickly support new functionality

Capsules – Example ML Workflow

```
> capsule create my-workflow
> capsule open my-workflow
> capsule add payload tensorflow
> capsule edit payload add --config name simple-tf
> capsule edit payload set --image default tensorflow/tensorflow
> capsule edit payload remove --args "--user_str1=hello"
> capsule edit payload add --config trainingScript simple.py
> capsule edit payload set --data home `pwd` /home/trainer Directory false all
> capsule close
> capsule launch my-workflow
> … wait for job to complete …
> capsule kill my-workflow
```

- Open a capsule for editing, make changes and close it to save those changes
- Then launch the capsule, wait for results and clean up when done

Capsules – Example HPC Workflow

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```
> capsule create mpi-example
> capsule open mpi-example
> capsule add payload hpc-job
> capsule edit payload add --config command /lus/<username>/a.out
> capsule edit payload add --resource instance nodes 4 \
    --resource instance per-node 4 --resource memory per-node 4G
> capsule close
> capsule launch mpi-example --attach
> … wait for job to complete …
> capsule kill my-workflow
```

- Very similar workflow to previous example, just different config options
- This time using **--attach** to directly attach ourselves to the capsule
  - In this example this will result in monitoring the job output file

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