FORTH
INSTITUTE OF COMPUTER SCIENCE

Challenges and Opportunities in Running Kubernetes Workloads on HPC

5/6/2024 • PASC24

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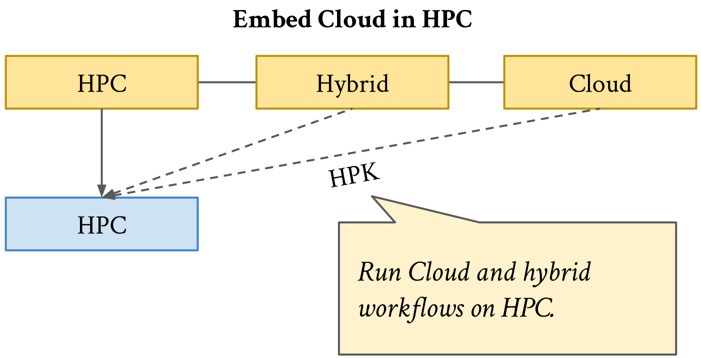
Objectives

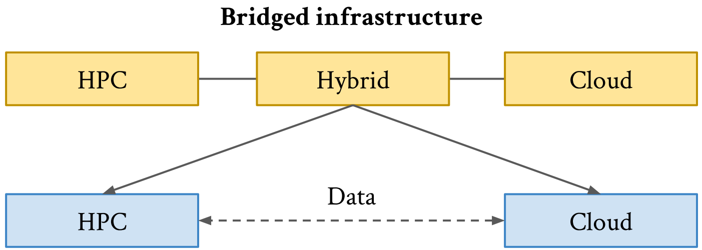
- HPC vs Cloud
  - Tight parallelization vs data distribution
  - Fixed setup vs unlimited resources
  - Low vs. high-level frameworks
  - Run binaries vs. webs of microservices
  - Console access vs interactive GUIs
- Combine best of both worlds using hybrid workflows → run on HPC
  - Provide a way to run Cloud software in HPC
  - Create ephemeral Kubernetes mini-Clouds in HPC

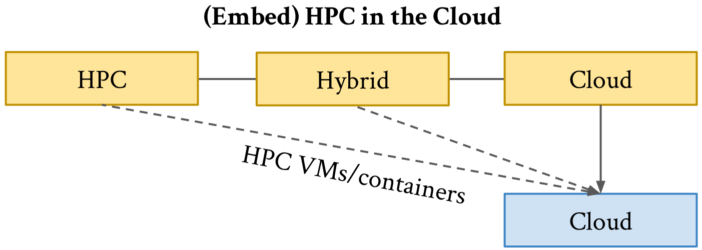


We need to enable portable, reproducible, composite workflows
— Daniel Milroy, LLNL (WOCC'23)

Running hybrid workloads

- Bridge two separate environments
  - Submit HPC jobs from the Cloud side or vice versa[1]
  - Deal with separate data and network contexts, unless running HPC in the Cloud (VM offerings available)
  - Hardware and maintenance costs
- Run in Kubernetes
  - Embed the HPC software stack in containers → Delegate scheduling to Kubernetes[2]
- Install both on the same hardware
  - Inpractical due to interference





[1] KNoC is a Kubernetes node to manage container lifecycle on HPC clusters: https://github.com/CARV-ICS-FORTH/knoc (InteractiveHPC 2022)
[2] Genisys is a Kubernetes scheduler for running HPC jobs inside Virtual Clusters alongside other services: https://github.com/CARV-ICS-FORTH/genisys (VHPC'22)

So... Kubernetes?

Kubernetes is a *container orchestration runtime*

- It manages the container lifecycle
  - Containers are lightweight (vs. VMs) and portable
  - Interface to the container runtime → Docker/containerd
- It is not only a scheduler
  - Handles networking between containers
  - Provides service discovery and load balancing mechanisms
  - Reacts to load (scaling) and failures
- It runs almost everywhere
  - Any scale, most architectures → desktop to Cloud
  - Runs as a system service → Needs "elevated" permissions

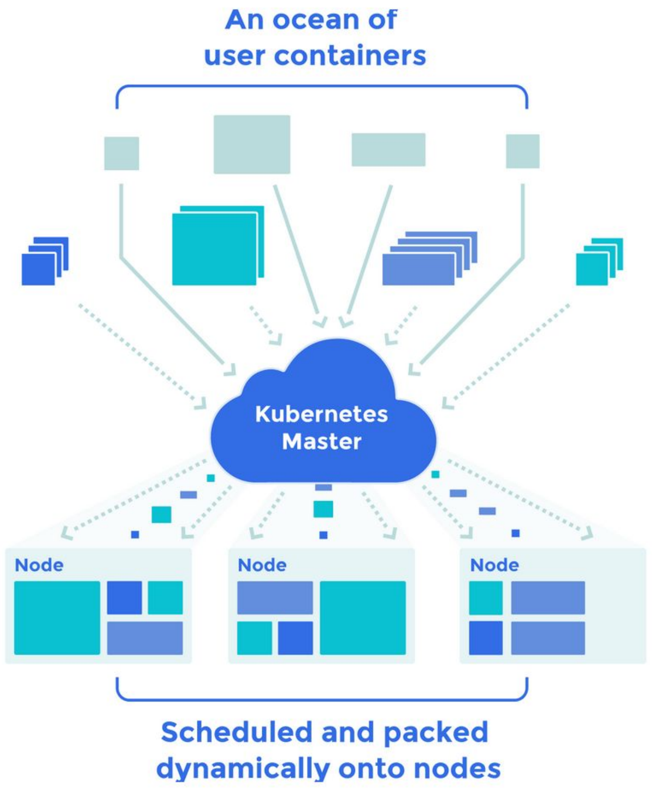
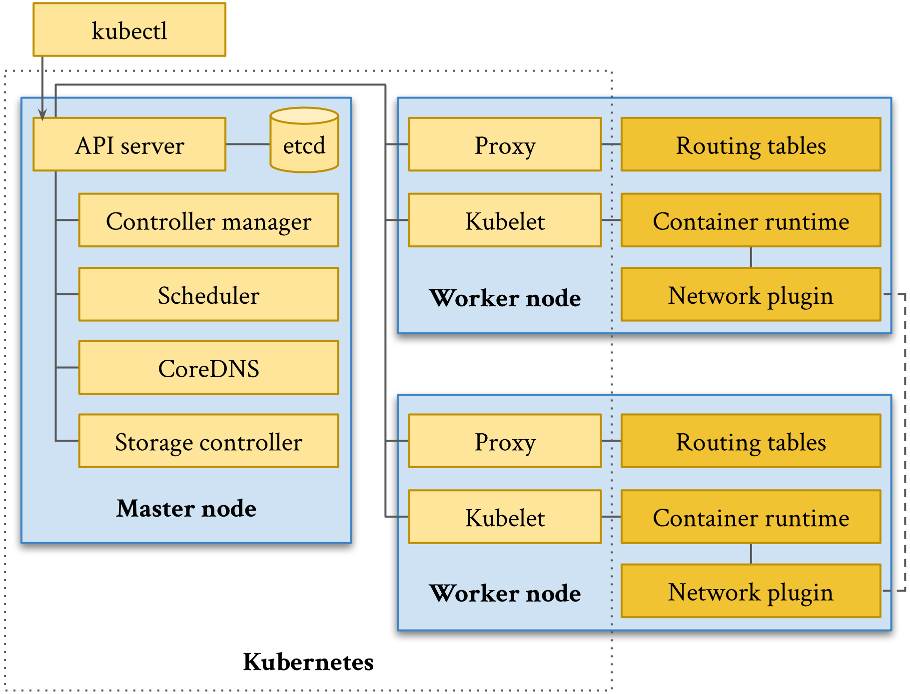


Image source: https://discuss.newrelic.com/t/relic-solution-what-you-need-to-know-about-new-relic-when-deploying-with-docker/52492

Kubernetes concepts

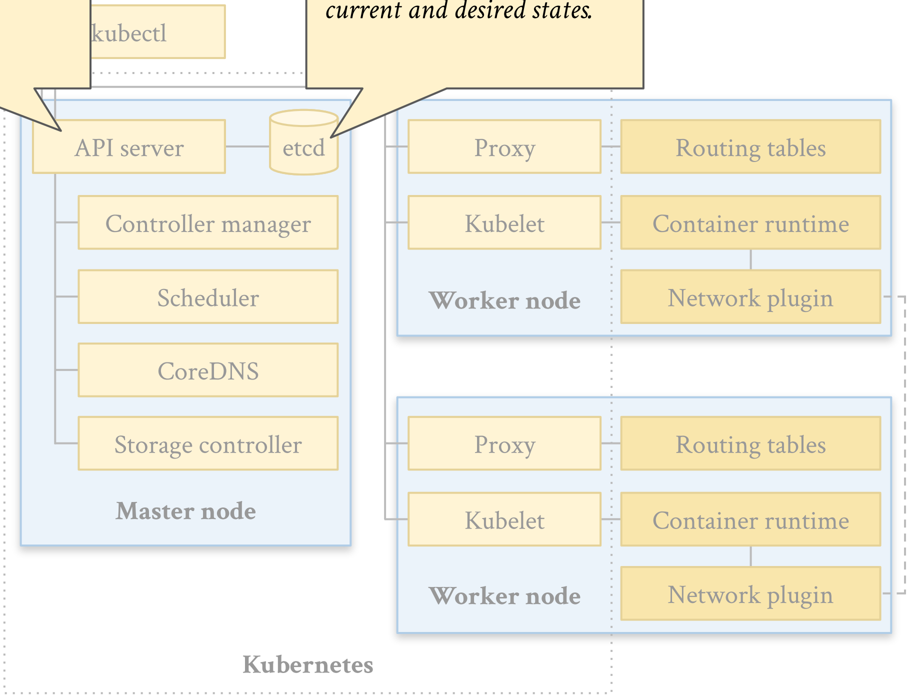
- Declarative vs imperative
- API endpoint & controllers
- Abstractions
  - Pods → Collection of containers
  - Deployments → Replicated pod groups
  - Services → Microservice naming
  - Jobs → Pods that run to completion
  - Volumes → Mountable file collections
  - Labels → Queryable metadata
- DevOps compliant
  - Infrastructure as code
  - Version rollouts, CI/CD workflows
- Typical distributed structure
  - "Control plane" → Scheduling and placement
  - Node agents → Handle execution
  - Monitoring and accounting infrastructure



Kubernetes core components layout

The main entrypoint for all requests to the cluster, the point of sync for all controllers.

A key/value store holding current and desired states.



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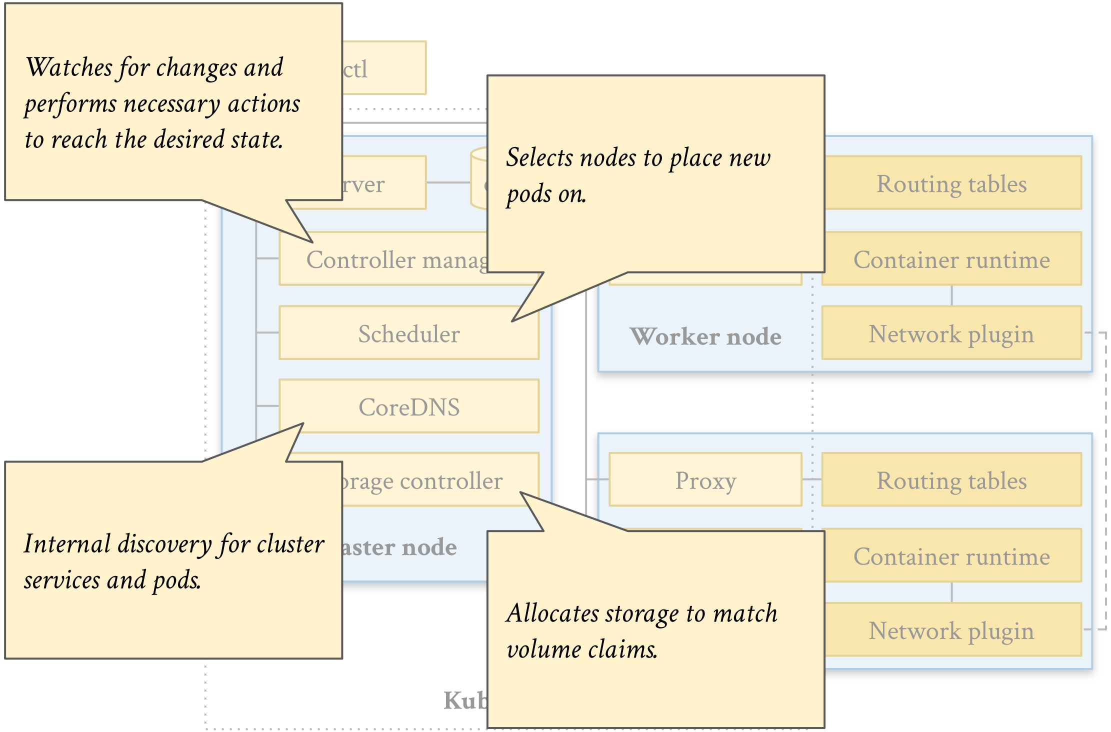

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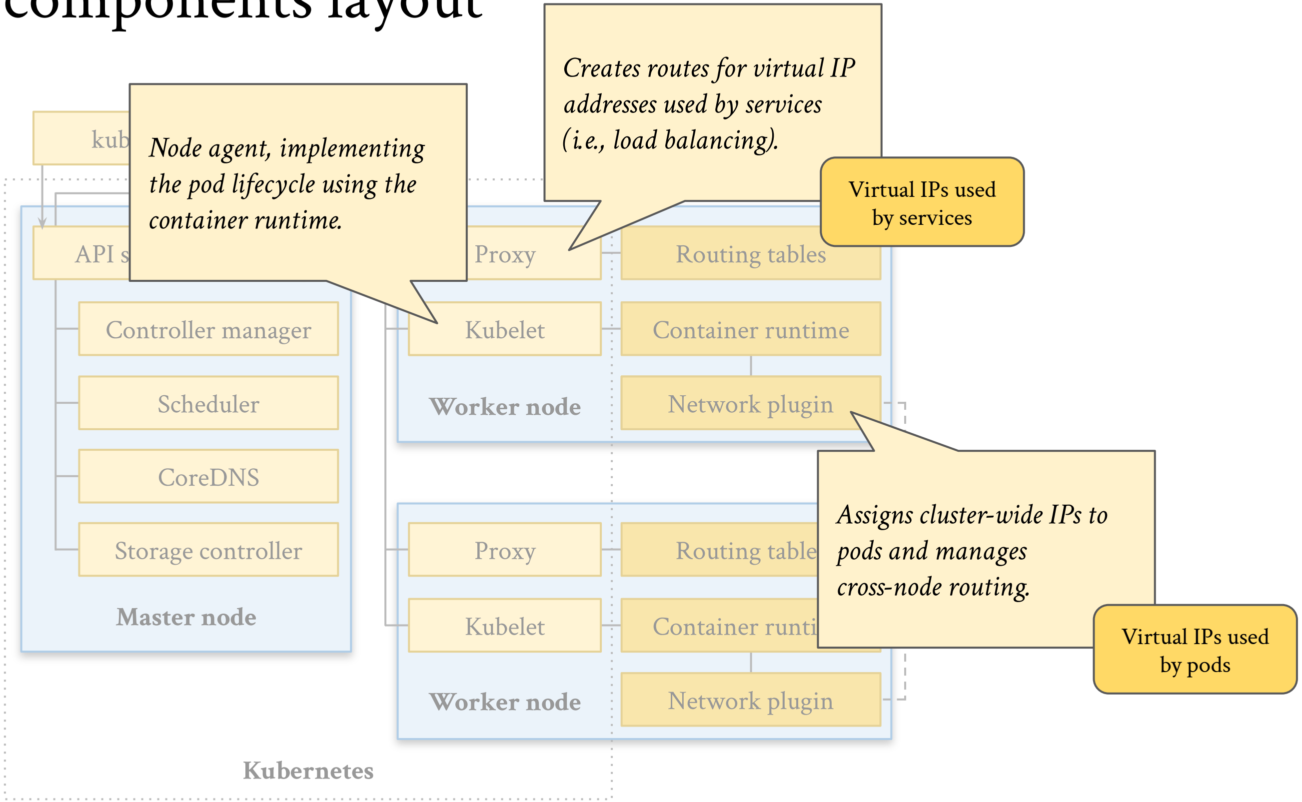

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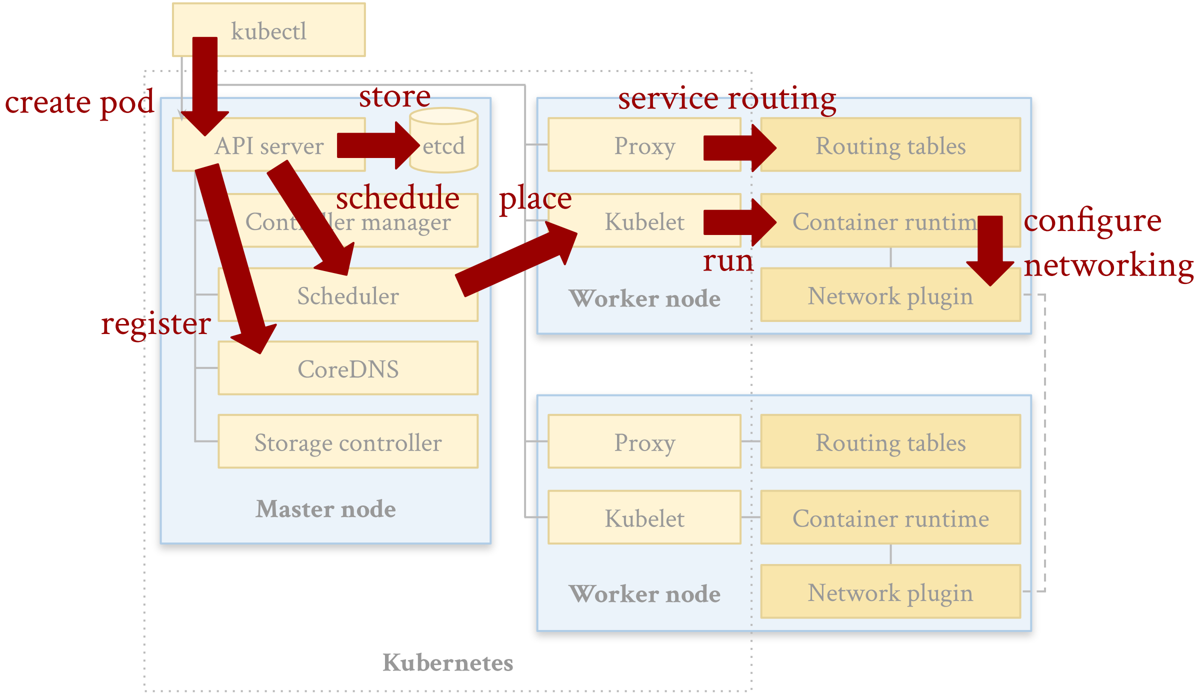


Design goals

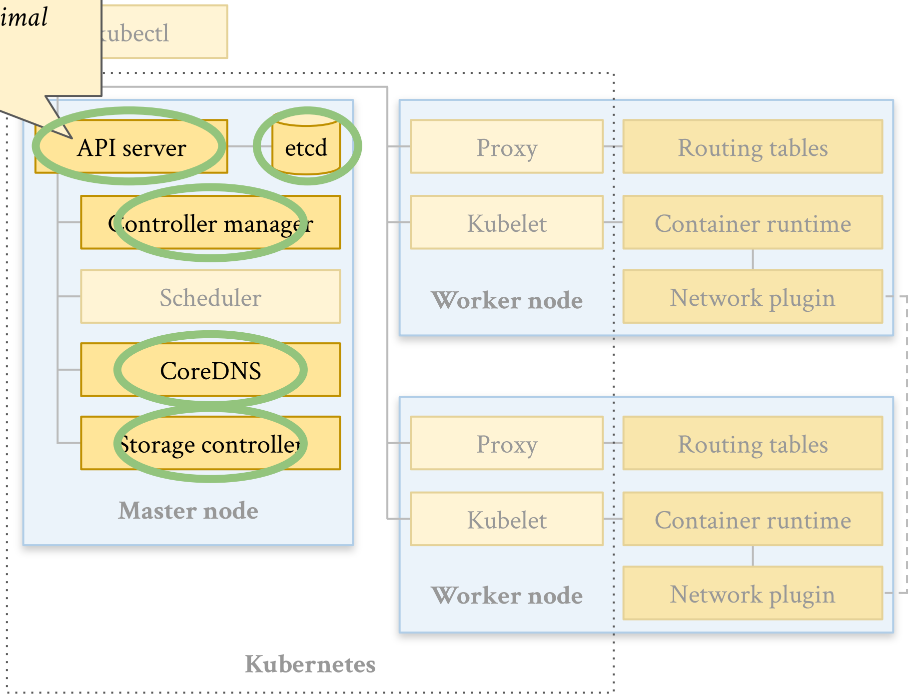
Run *Kubernetes in an HPC environment* as a user → High-Performance Kubernetes (HPK)

Requirements:

- All Kubernetes abstractions should be available and fully functional
    - Except those that affect physical hardware resources (like NodePort services)
    - Private, inter-container network and internal DNS should work as expected
- Delegate resource management to Slurm
    - Respect organization policies
    - Comply with established resource accounting mechanisms
    - Scale across all nodes of the cluster
- Use Singularity as the container runtime
    - Preinstalled in most HPC environments
- Make it easy for HPC administrators
    - No (or little) configuration changes should be required at the host level
    - No reliance on special libraries or binaries that execute with "elevated" permissions
- Make it easy for users
    - All neatly packaged up in one container
    - Simple, one-command deployment via Slurm
    - All relevant configuration and files should be in the user's home folder

Kubernetes components in HPK

Services that run "out of the box", with no special dependencies, or minimal changes.



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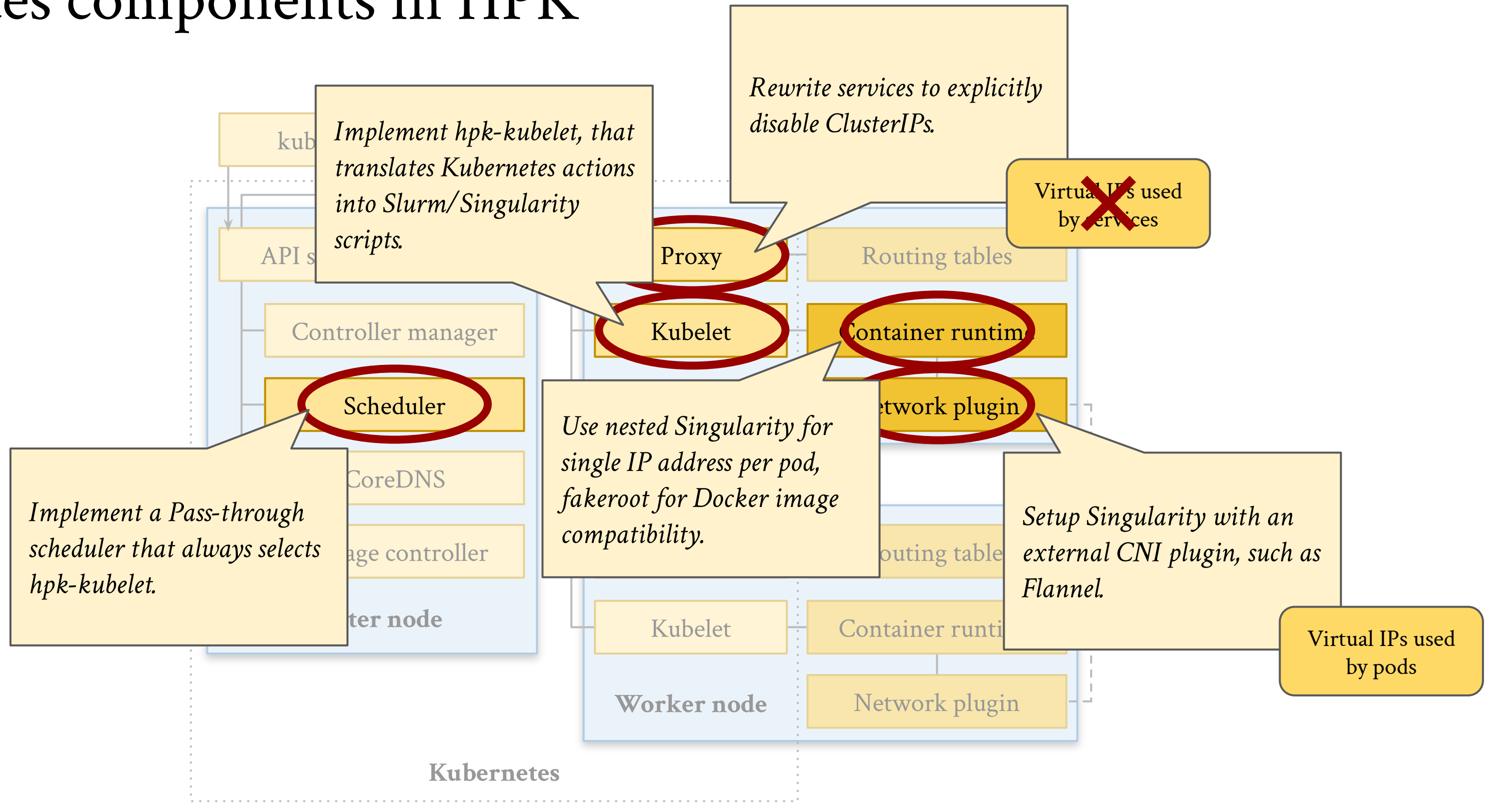
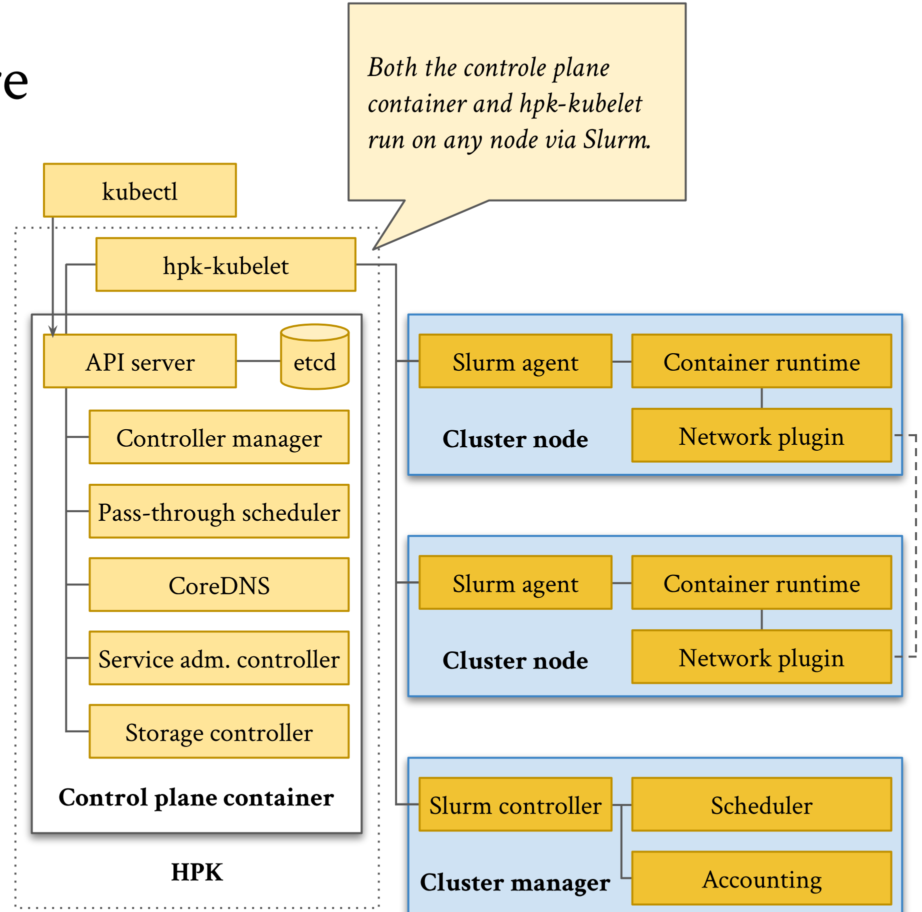


HPK architecture



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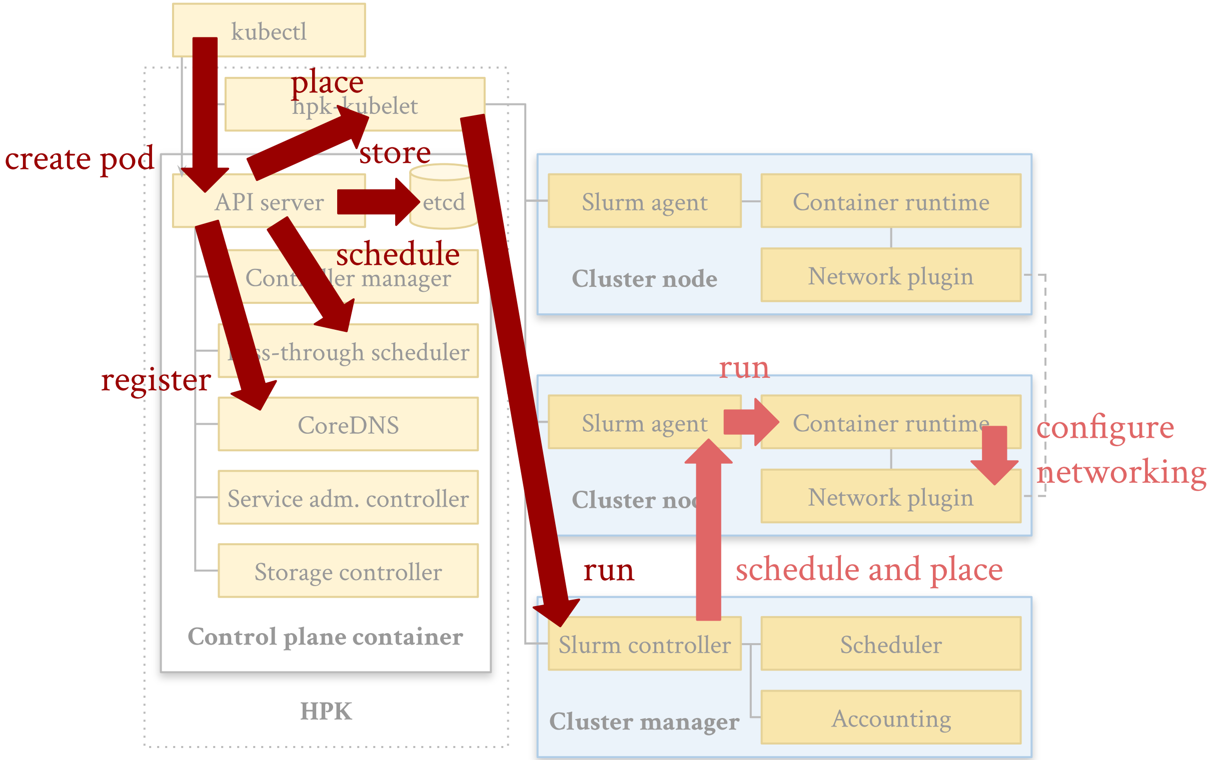
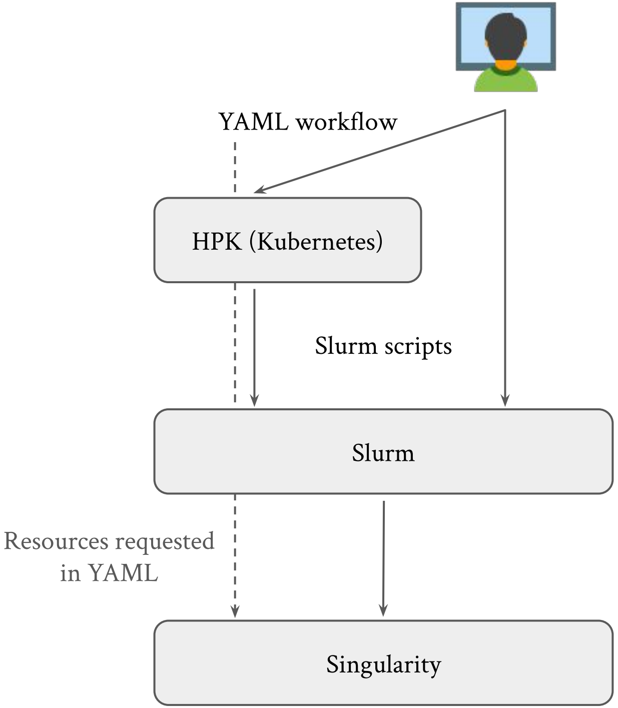


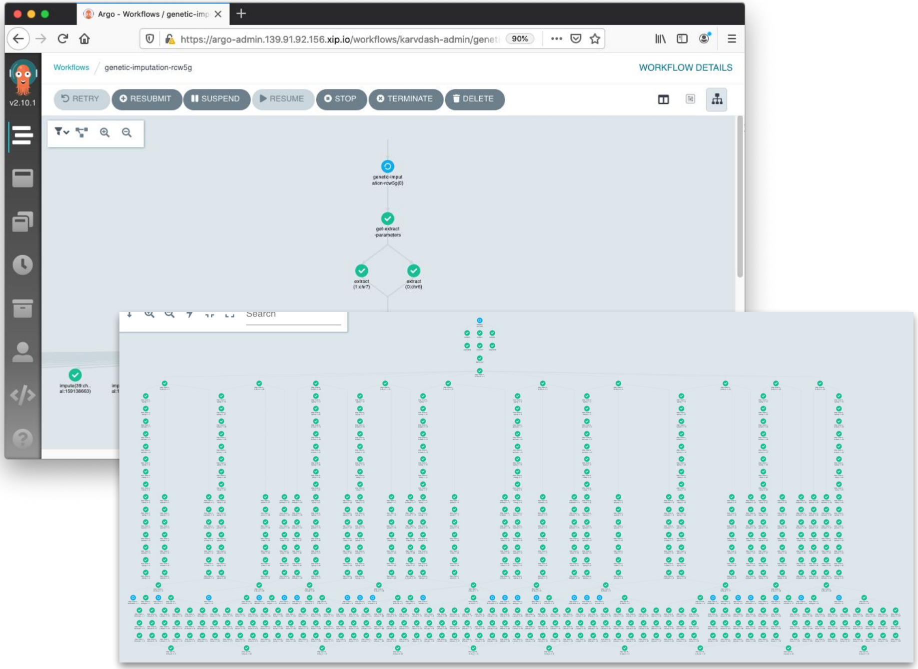
HPK implementation

- HPK translates Kubernetes to Slurm scripts
  - Pods/jobs show enter as YAML through the Kubernetes API, exit as Slurm scripts from hpk-kubelet → Pods show up as Slurm jobs
  - Kubernetes resource requirements end up in Slurm allocation requests → No changes to accounting
- HPK runs as a user process via Slurm
  - User can run both Kubernetes and Slurm workloads at the same time
  - No "special" allocation needed for HPK → 1 CPU, few GBs of RAM should be enough
  - Little support needed by the environment → No Slurm modifications, some Singularity configuration (inc. Flannel or other CNI)



HPK for Cloud-native workflows

- Using Argo Workflows
  - All steps are containers → Containerized code is portable
  - Interactive UI → Monitor, control
- Language features
  - Loops, conditionals
  - High-level parameters (shared across all steps), workflow templates
  - Artifacts → Step I/O
- HPK extensions → Integrate MPI steps
  - Slurm passthrough flags via annotations → Control scalability, allocate GPUs
  - Still need to containerize code



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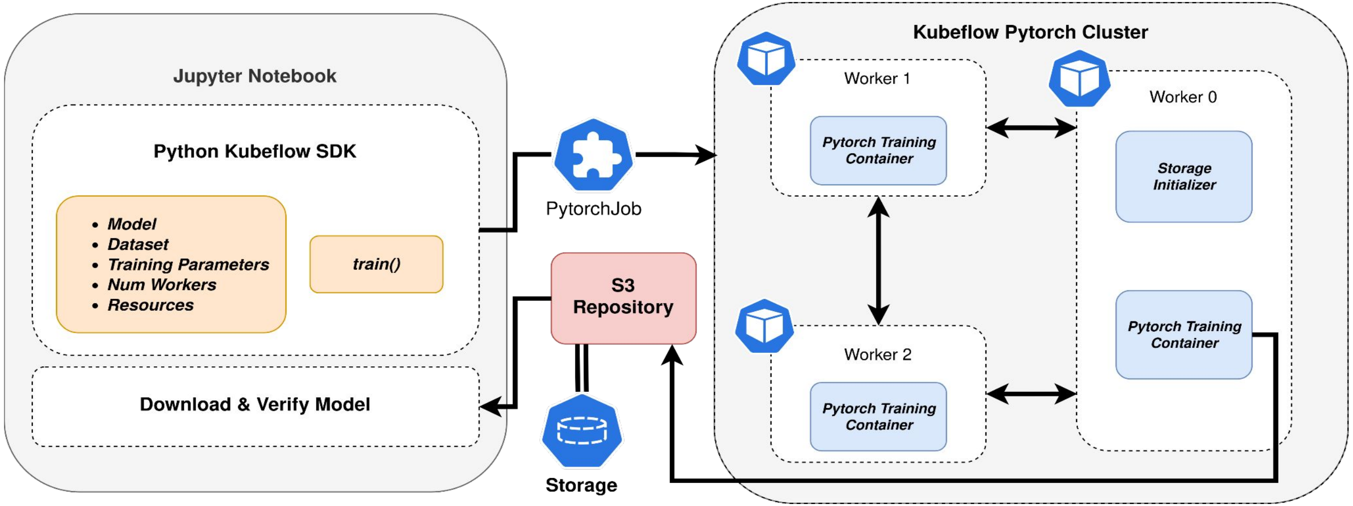
```
kind: Workflow
metadata:
  ...
spec:
  entrypoint: npb-with-mpi
  templates:
  - name: npb-with-mpi
    dag:
      tasks:
      - name: A
        template: npb
        arguments:
          parameters:
          - {name: cpus, value: "{{item}}"}
        withItems:
        - 2
        - 4
        - 8
        - 16
  - name: npb
    metadata:
      annotations:
              slurm-job.hpk.io/flags: "--ntasks={{inputs.parameters.cpus}}"
              slurm-job.hpk.io/mpi-flag : "..."
    inputs: s
      parameters:
      - name: cpus
    container:
      image: mpi-npb:latest
      command: ["ep.A.{{inputs.parameters.cpus}}"]
```

HPK for ML Workflows: Fine-Tune BERT with PyTorch

- Diverse microservices
  - Jupyter notebook → Coordinates tasks (data preprocessing, model fine-tuning, testing)
  - Kubeflow controller → Manages Pytorch jobs
  - MinIO → S3-compatible object store



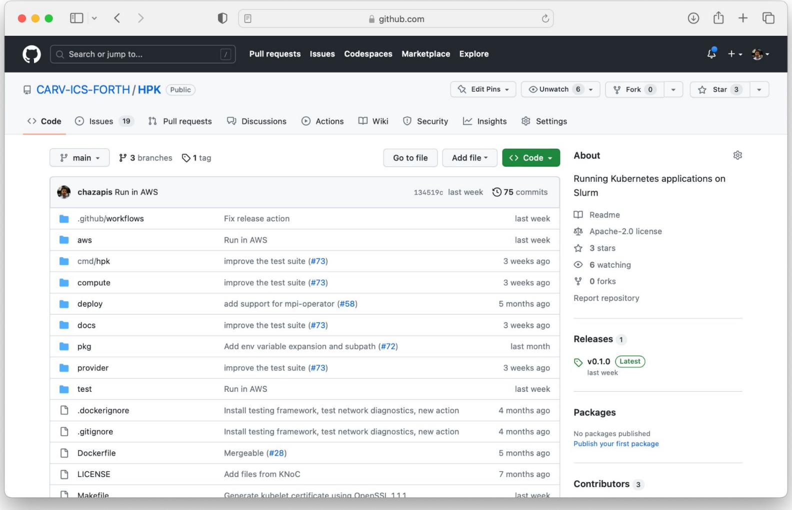
HPK for Spark in HPC

- Evaluated HPK + Spark at Jülich (JSC)
    - TPC-DS benchmark
    - Spark Operator (EKS spark-benchmark) → Manages Spark applications on Kubernetes
    - MinIO → S3-compatible object store
- Challenges
    - Preparation of testbed → Apptainer (fakeroot support), Flannel (deploy on all nodes, configure subnets, requires etcd)
    - Integration with Slurm → Exclusive node policy does not align with container sizes

HPK vision

- Cloud-user PoV → Run on HPC hardware
- HPC-user PoV → Exploit the Cloud software ecosystem
  - Combine HPC codes with backend services (database, queueing systems)
  - Interactive code execution → Jupyter
  - Workflow management → Argo Workflows, Apache Airflow, ...
  - Monitoring utilities → Grafana
  - Frameworks for automatically optimizing and scaling code → Spark, DASK, ...
- HPC centre PoV → Run Cloud workloads on the main HPC partition, attract users
  - The common practice is to have separate partitions for Cloud (analytics) and HPC

HPK is available at https://github.com/CARV-ICS-FORTH/HPK



Acknowledgements

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