

# Empowering GPU Workloads:

## Our journey to enabling ML with K8S

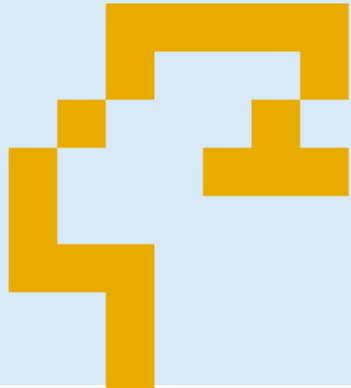
Gustav RASMUSSEN

Marius TANAWA TSAMO



# Agenda

- **Introduction**
  - The Story: Why AI in Novo Nordisk?
- **Technical Foundations**
  - Why Use Very Large Container- and Model Images?
  - Data Plane
- **Infrastructure and Tools**
  - Gefion: The Nvidia DGX SuperPOD
  - Enabling GPU workloads scheduling with the NVIDIA Operator and Volcano
- **Challenges and Solutions**
  - Challenges Encountered in Setting Up the Platform
  - Solutions and Best Practices
- **Future Directions**
  - Roadmap for Further Enhancements
  - Open Discussion and Q&A

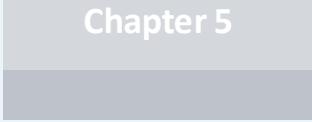
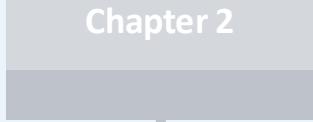
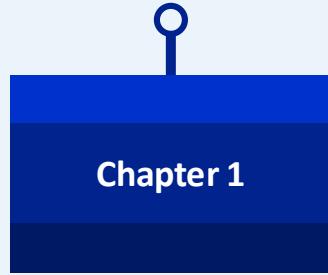
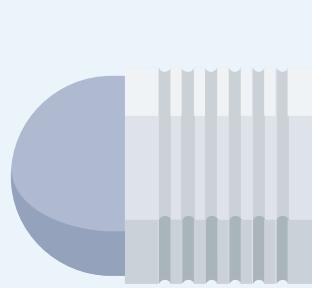


# Introduction



## Introduction

The Story: Why AI in Novo Nordisk



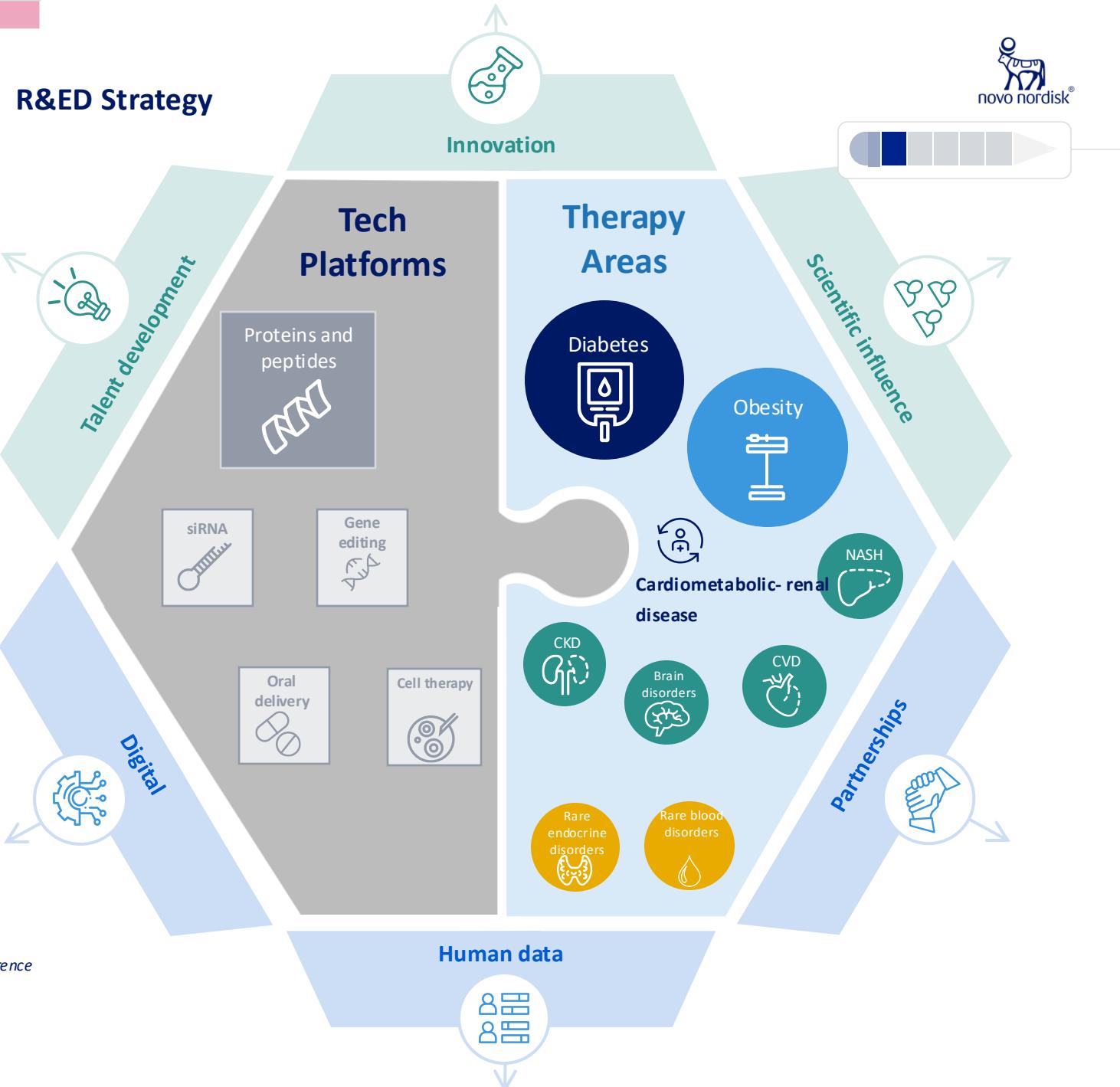
## Infrastructure and Tools

## Future Directions

## Technical Foundations

## Challenges and Solutions

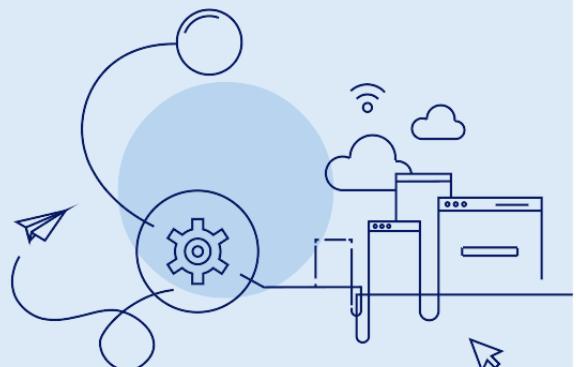
Building on our core capabilities, a range of opportunities for expansion have materialised



# R&ED is one global organisation with knowledge & opportunities across the value chain



# Capability Delivery Model



	Targets & Translational					Modalities & Pharmacology				Non-Clinical		
	CoApps	Genomics	Genetics Suite	BrainIN/NewRON	Cohorts & Omics	Target Discovery Data Platform	LabDroid Enablement	Entity Registration	ELN	GADS	OpenPKAI	Molecular Design AI
Lab Operations	Applications Services and Product Support (ASAPs) - DK											
	IIDP – Raw Data Capture											
	IMS – Sample Inventory Management											
	Lab Data Insights											
	Oxonium											
	“Research Lab Solution” - DK											
	.scicorm											
ML & Infrastructure	Hybrid Storage & Compute											
	Research High performance Computing Platforms (HPC)											
	Cloud Infrastructure											
	Scientific Applications Operations											
	ML Infrastructure											
	Containerization & Container Orchestration											
Data Enabler	Imaging Solutions											
	Research Collaboration Platform (RCP)											
	Data Asset Discovery											
	Data Management Delivery Team											
	Computational Science Platforms											
	Data Platform & Data Product Enabling											



## Shared Services

Agile Delivery & Compliance

DSI Local LACE

Organization Change Management (OCM)

Project Management Office (PMO)



Pending strategy



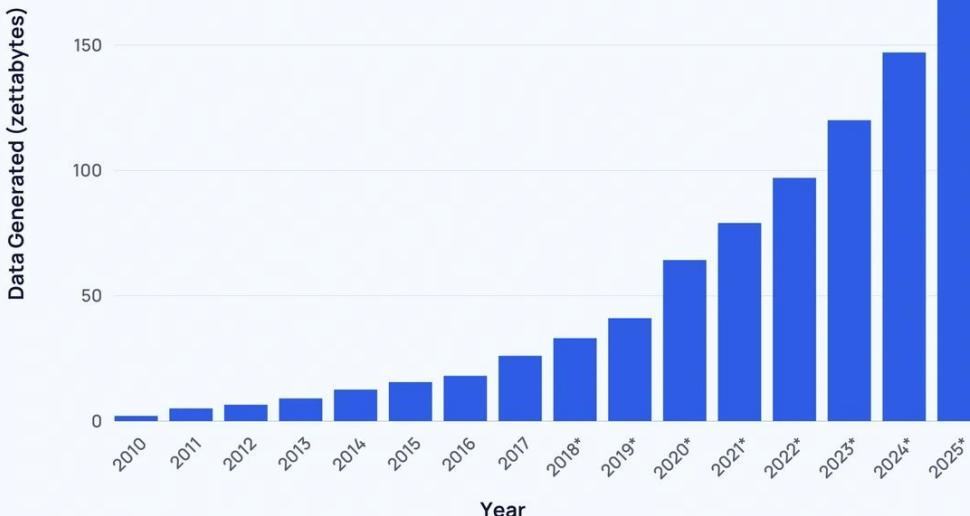
# Existing Technologies and Tools in Research NN

							
<b>Data Ingestion</b>	<b>Data Catalog</b>	<b>API Gateway</b>	<b>Data Storage</b>	<b>ETL &amp; Explorative Analysis</b>	<b>Data Viz</b>	<b>Observability</b>	<b>Orchestration</b>
AWS DataSync	Purview	AWS API Gateway	NNEDH/NNEDL (Lakeformation)	Databricks	BI products (Spotfire, Power BI, Tableau)	Splunk	Apache Airflow
AWS DMS	ESL	Mulesoft	CEPH RDBMS Snowflake	AWS Glue HPC Platform Snowflake Domino Datalab Research Datalab	Streamlit Shiny apps	Grafana Puppet Prometheus	Azure pipelines Gitlab pipelines GitHub Actions
							
<b>Scientific data capture</b>	<b>Key research databases</b>	<b>Scientific APIs</b>	<b>Research platforms</b>				
IIDP/TetraScience OMS IMS	NNCD ELN GADS	Biolink/.sciworm Biopages BraiNN AssayWeb	SevenBridges Imaging Platform JIRA RCP				

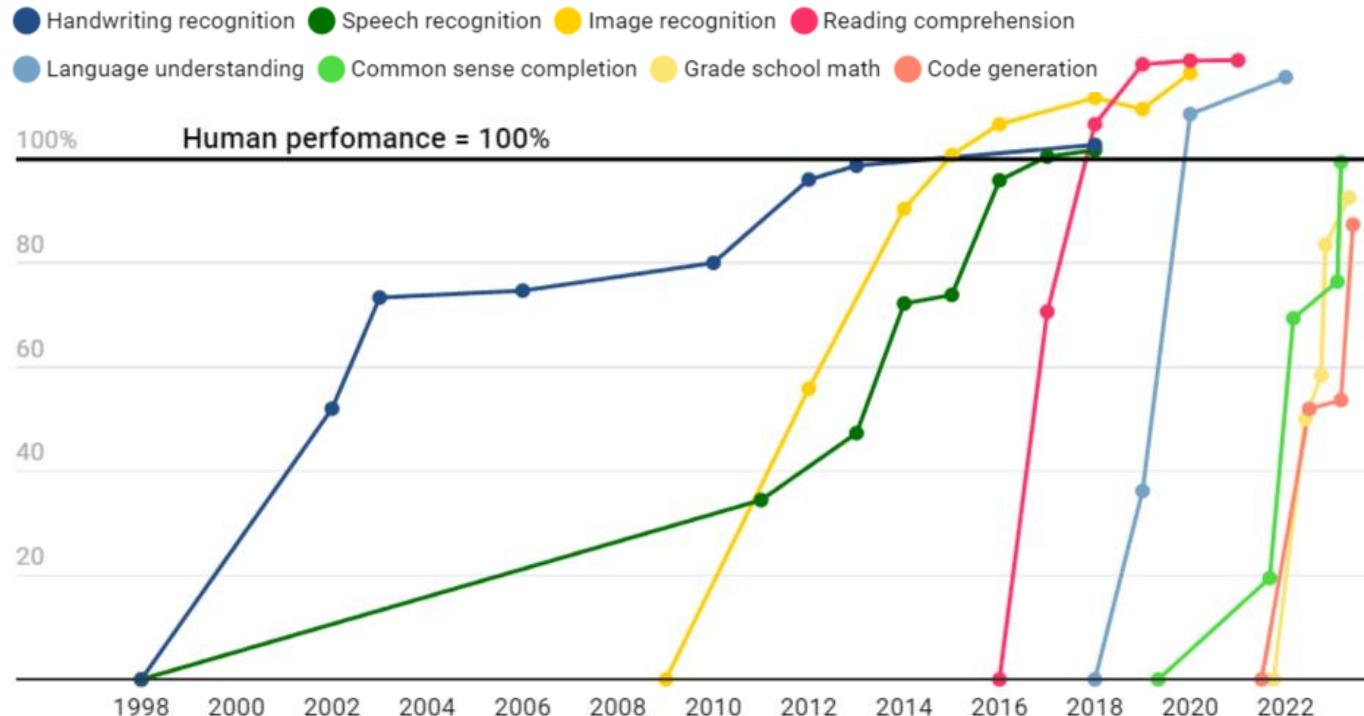
# Why do we need AI in Novo Nordisk?



## Global Data Generated Annually



## State-of-the-art AI performance on benchmark, relative to human performance



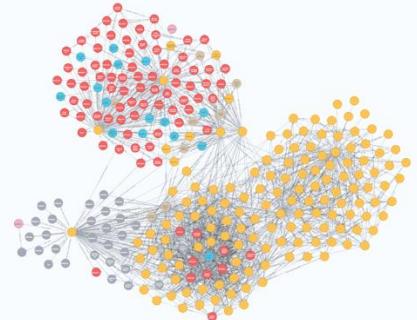
Need to ensure that Novo Nordisk adopt AI technology across the organization following best practices

This is a Must-Win battle for Novo Nordisk

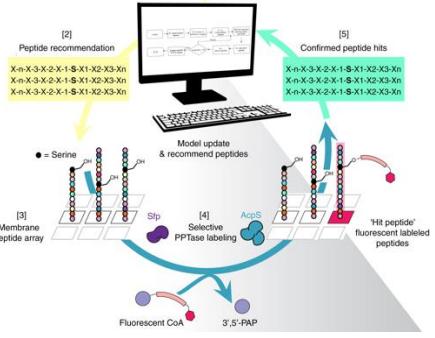
# AI as a competitive differentiator or AI for all?



## Bespoke AI | Competitive differentiator



Knowledge Graphs



Diabetes Target Discovery



Generative AI Agents

## Citizen AI | AI for everyone



NN ChatGPT



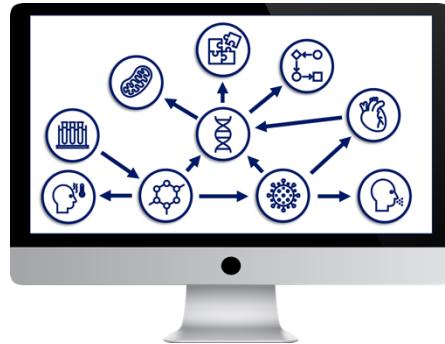
Microsoft Copilot



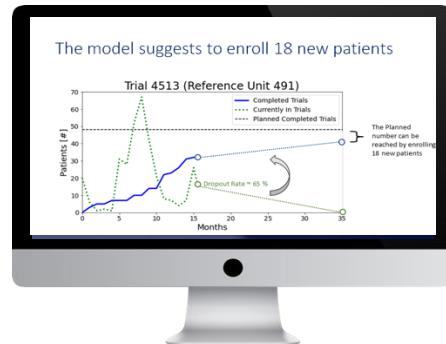
Github Copilot

Prerequisites | Cloud, Compute, Data

# AI Across the Value Chain



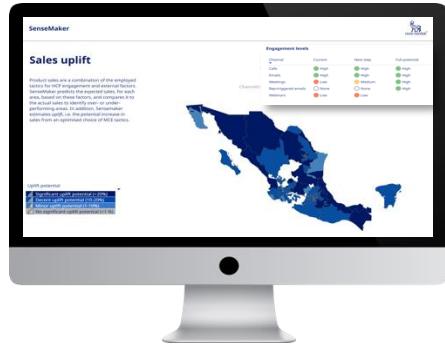
Molecule graph analytics



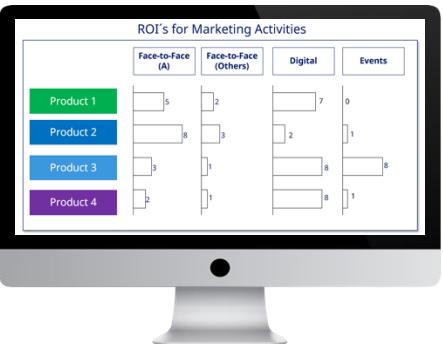
Trial dropout PoC



AI-based visual inspection

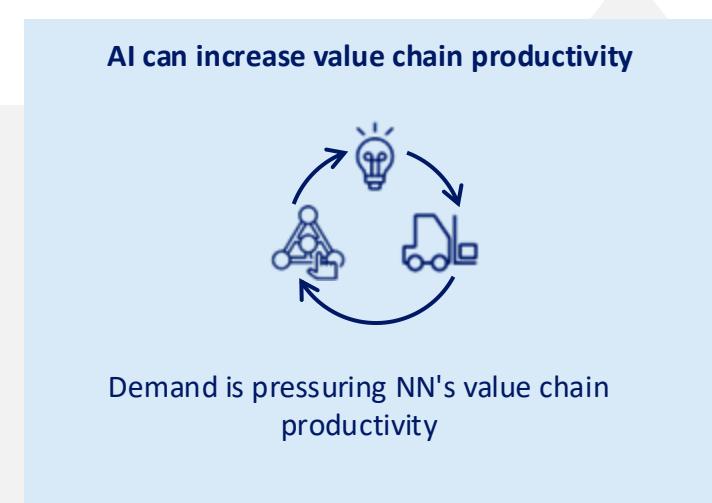
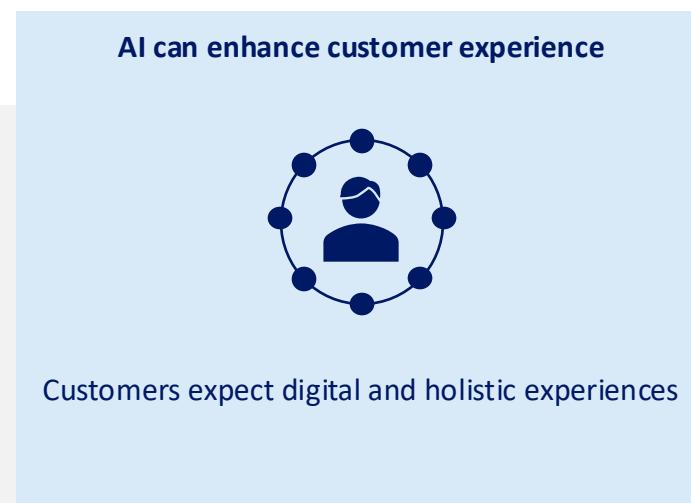


Sales uplift modelling



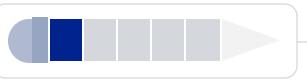
Marketing Mix Modelling

# AI has immense potential to revolutionalise Novo Nordisks patient journey and value chain



\*Expected AI healthcare market valuation in 2030

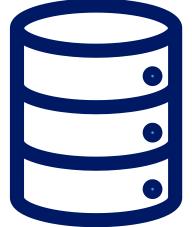
1: 2023, Statista, [link](#); 2: OECD, The Lancet, Strategy & analysis



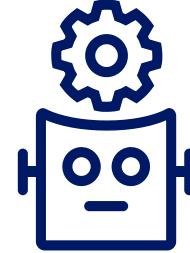
# The Equation of Scaled AI



People



FAIR Data



Technology



Business  
Value

*X-functional  
Ethics & Compliance*

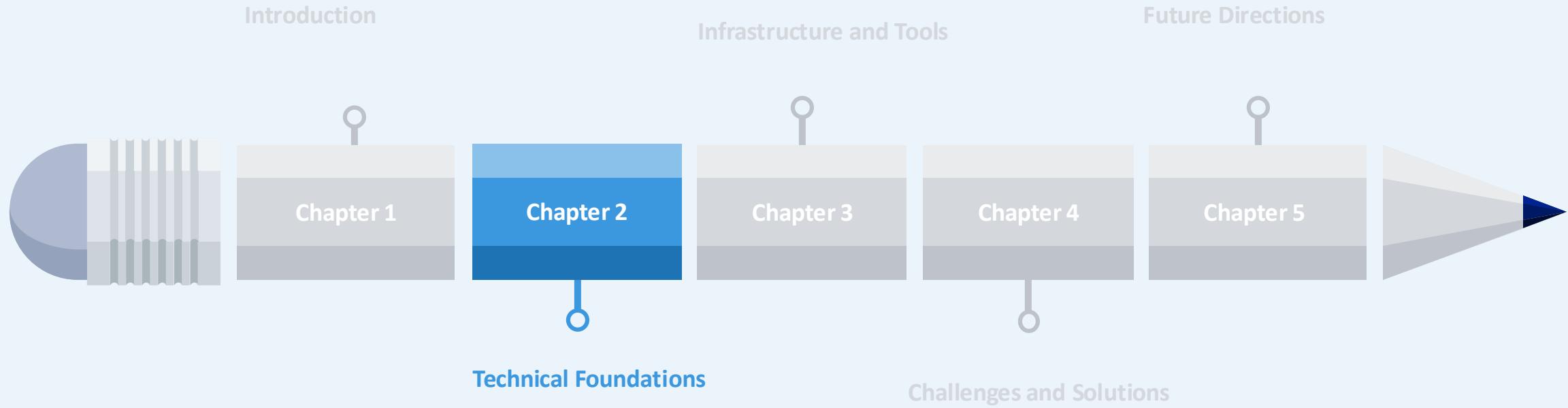
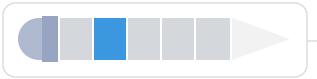
*Reusable  
Data products*

*MLOPS  
Reusable Tech*

*Fail Fast.  
Learn. Iterate.*

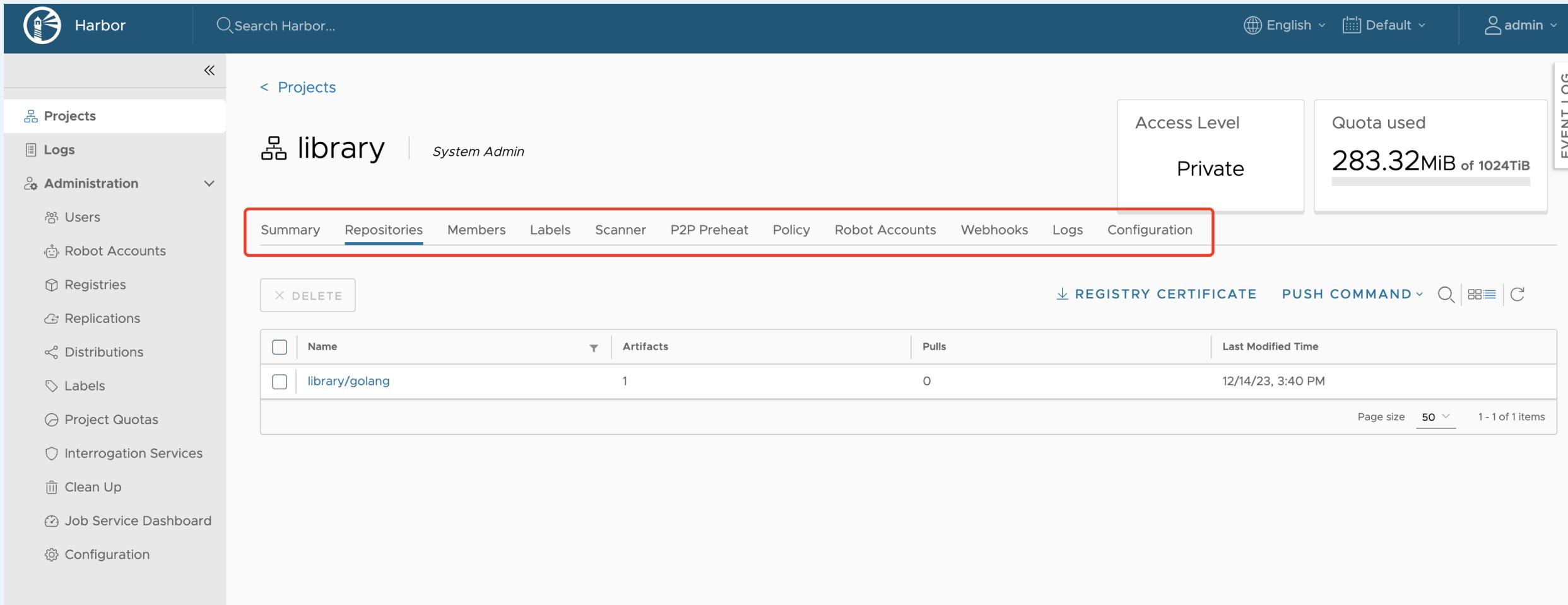
FAIR: Findable, Accessible, Interoperable, Reproducible

# Technical Foundations



- Container Registry
- Data plane

# Harbor UI



Harbor

Search Harbor...

English Default admin

Projects

Logs

Administration

Users

Robot Accounts

Registries

Replications

Distributions

Labels

Project Quotas

Interrogation Services

Clean Up

Job Service Dashboard

Configuration

< Projects

library | System Admin

Access Level  
Private

Quota used  
283.32MiB of 1024TiB

EVENT LOG

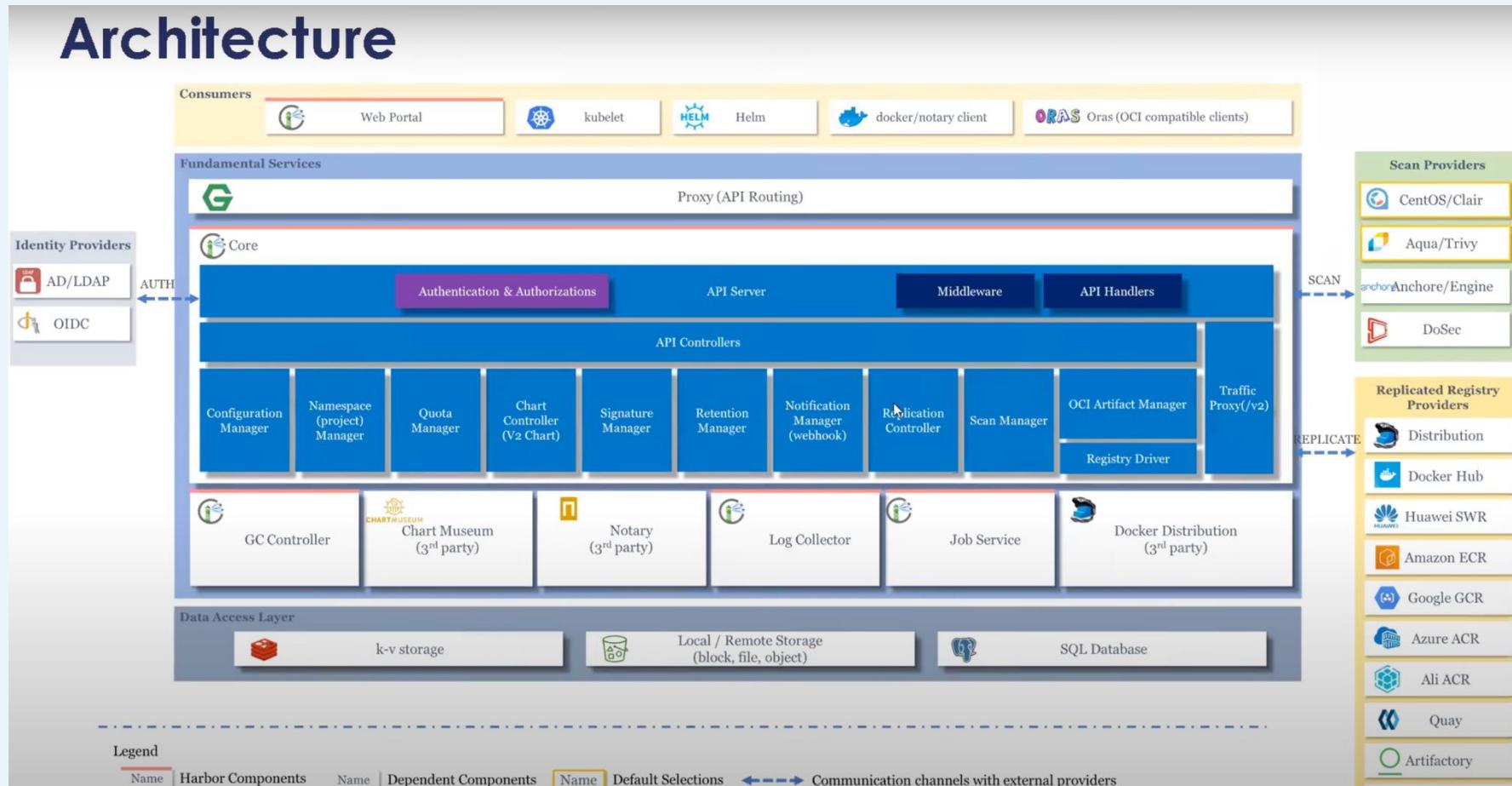
Summary Repositories Members Labels Scanner P2P Preheat Policy Robot Accounts Webhooks Logs Configuration

X DELETE REGISTRY CERTIFICATE PUSH COMMAND Q C

Name	Artifacts	Pulls	Last Modified Time
library/golang	1	0	12/14/23, 3:40 PM

Page size 50 1 - 1 of 1 items

# Harbor Architecture





# Serving ML Containers

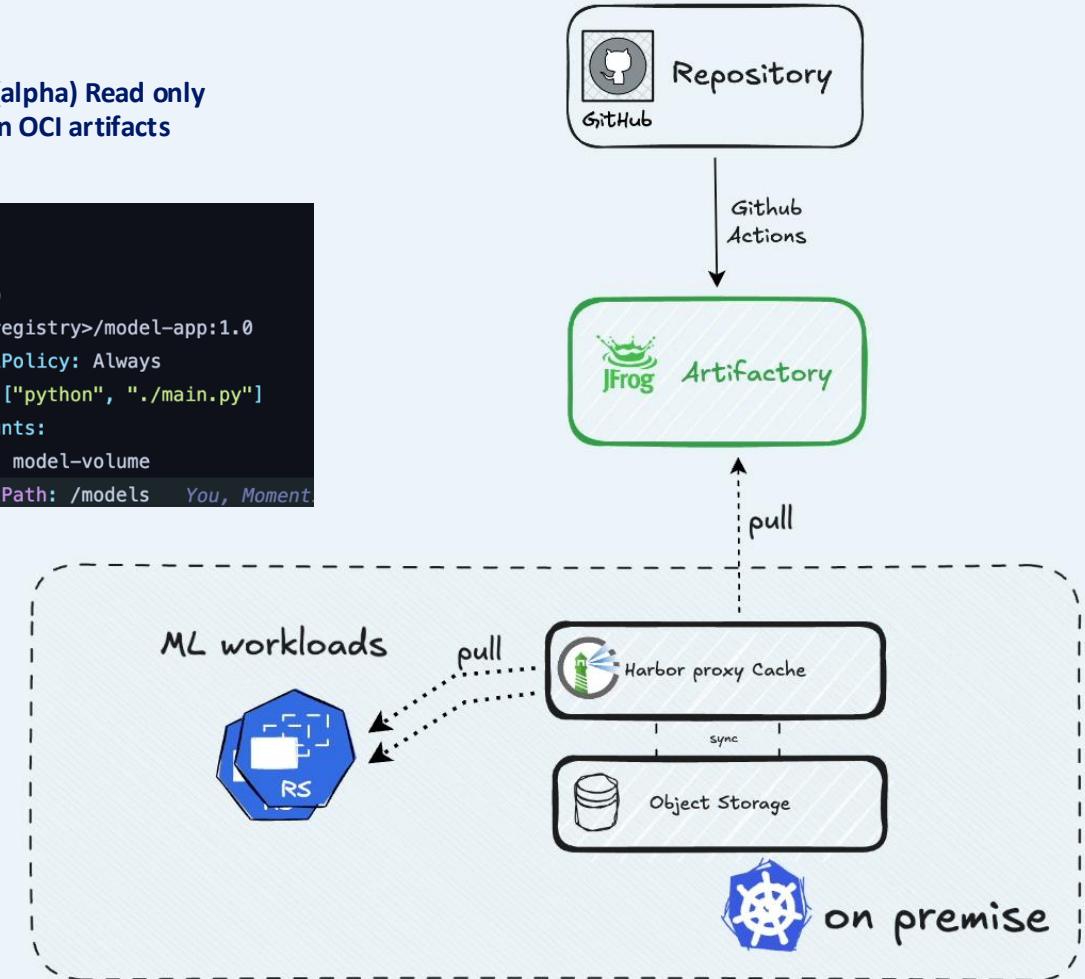
- ML container images are **LAAARGE**

```
initContainers:
  - name: model-init
    image: <registry>/model-data:1.0
    imagePullPolicy: Always
    command: ["/bin/sh"]
    args: ["-c", "cp /usr/src/model-data/* /models"]
    volumeMounts:
      - name: model-volume
        mountPath: "/models"
```



```
containers:
  - name: app
    image: <registry>/model-app:1.0
    imagePullPolicy: Always
    command: ["python", "./main.py"]
    volumeMounts:
      - name: model-volume
        mountPath: /models
```

Kubernetes 1.31(alpha) Read only volumes based on OCI artifacts



# Data Quality



If you torture the data long enough,  
it will confess.

Ronald Coase



onlinebehavior.com

Forbes

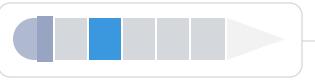
Google's AI Recommended Adding Glue To Pizza And Other Misinformation—What Caused The Viral Blunders?

Jack Kelly Senior Contributor 

*Jack Kelly covers career growth, job market and workplace trends.*

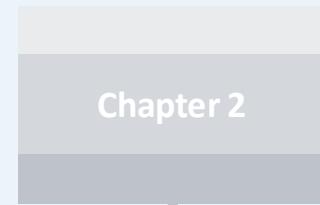
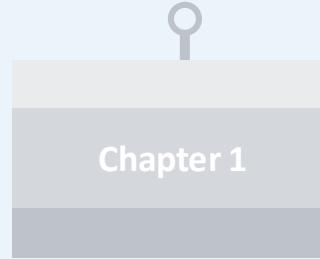
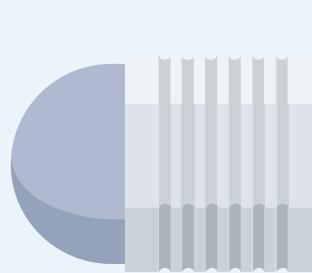
Follow

# Data Gravity





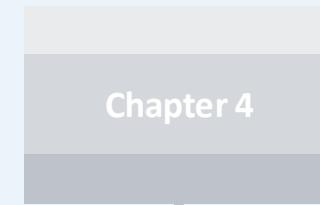
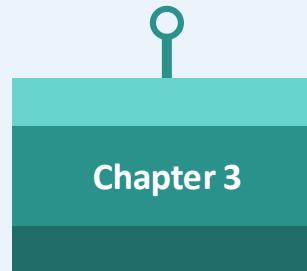
## Introduction



Technical Foundations

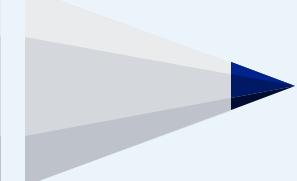
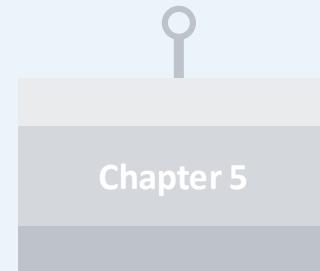
## Infrastructure and Tools

- Gefion - Nvidia DGX SuperPOD
- GPU scheduling (Nvidia/volcano)



Challenges and Solutions

## Future Directions



# Gefion: The Nvidia DGX SuperPOD



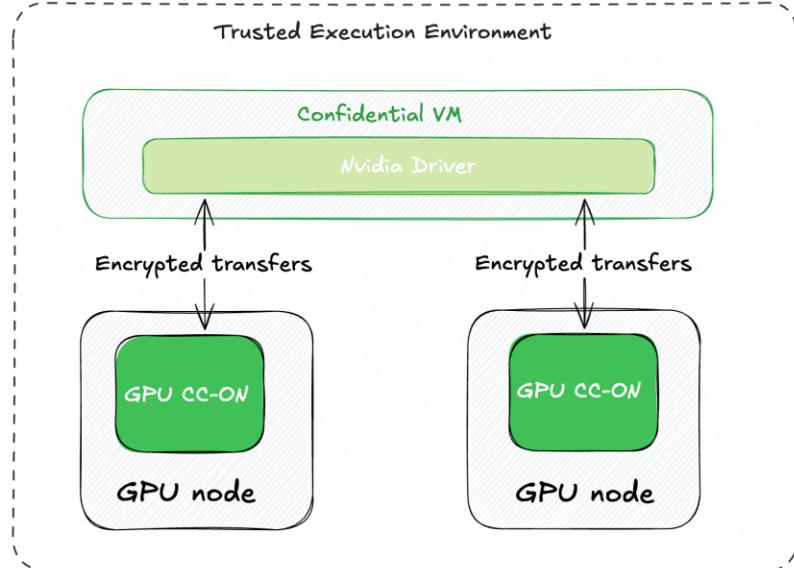
- 191 NVIDIA DGX H100
- 1528 NVIDIA H100
- NVIDIA Quantum-2 InfiniBand



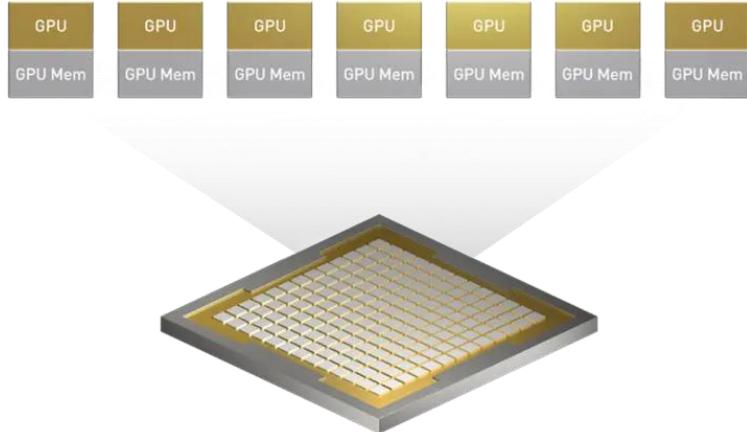
# Specifics about the Hopper architecture



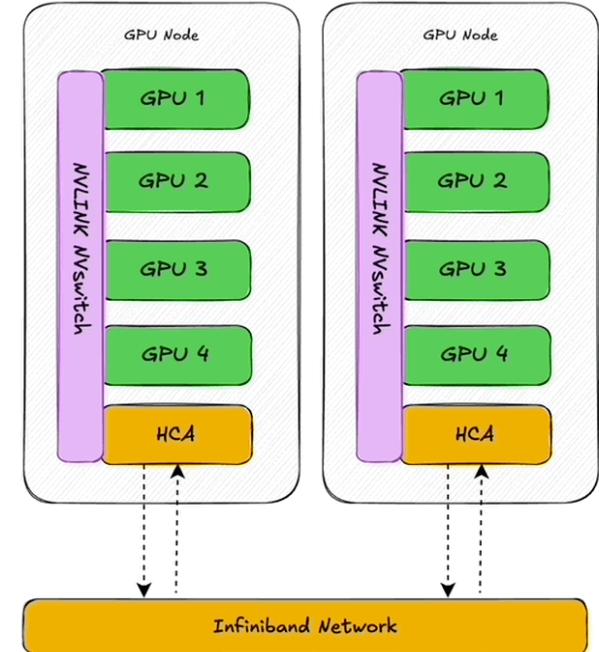
## Confidential Computing



## Multi-Instance GPU

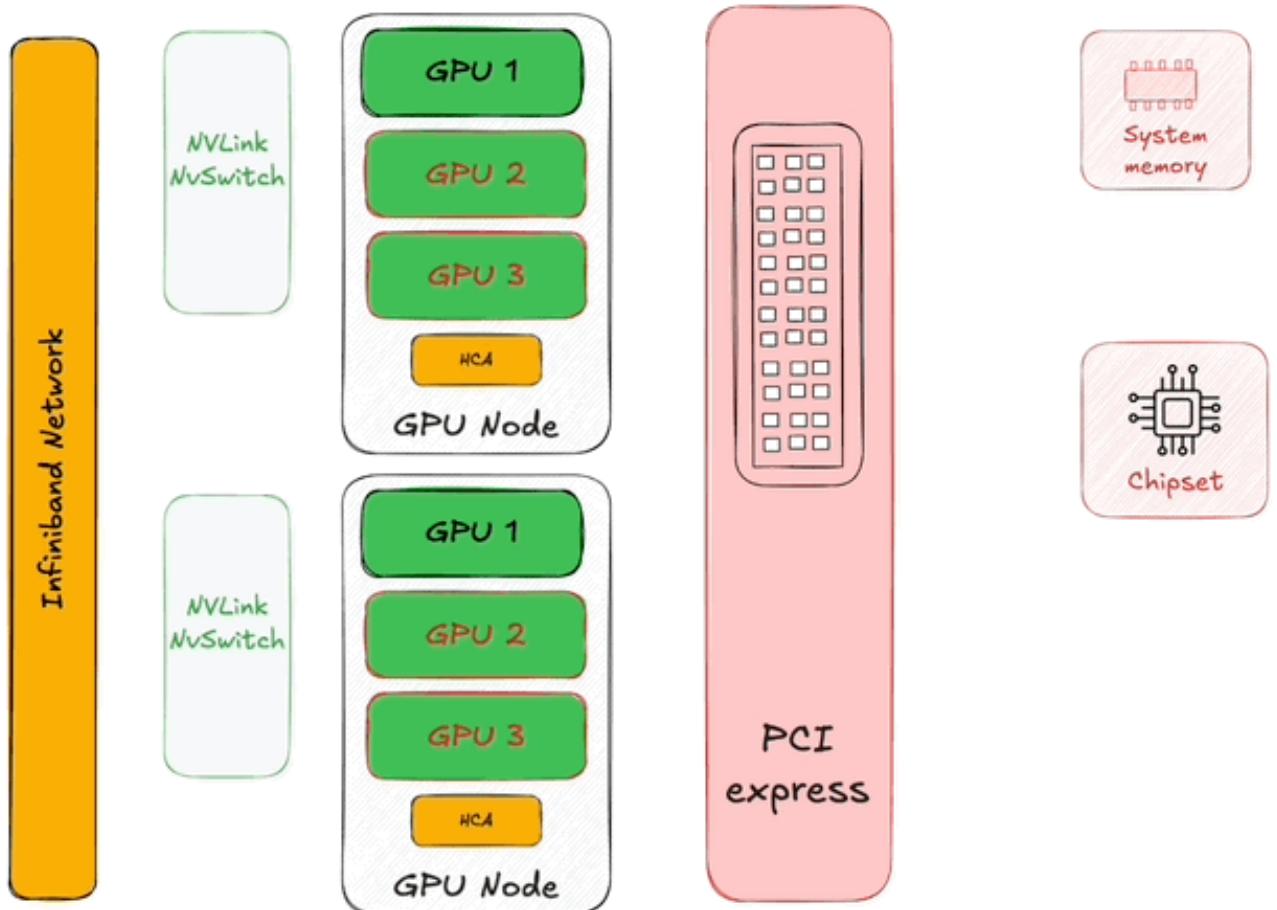


## Scalable interconnects



# Networking is crucial for scaling

GPU – GPU ( Infiniband peer to peer)



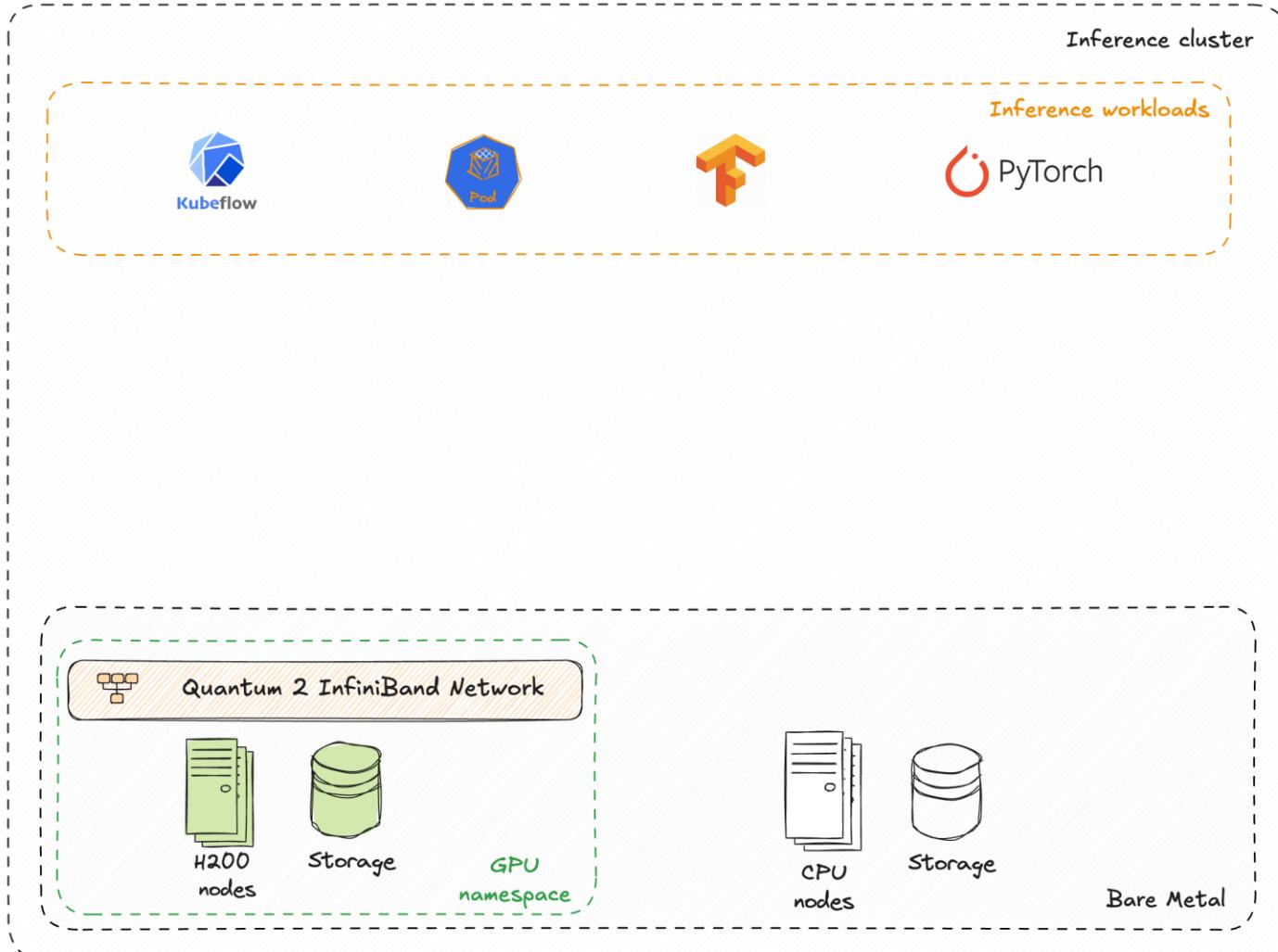
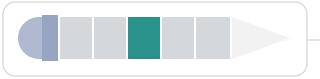
...even more crucial  
for Drug Discovery  
(Molecular Dynamics)

PCIe max speed:  
~63GB/s

Nvlink min speed:  
300 GB/s

# Our Team contribution within the department

## Building an Inference Cluster



## Multiturn user interactions

# Shortening the access to the GPU



A k8s cluster with heterogeneous nodes



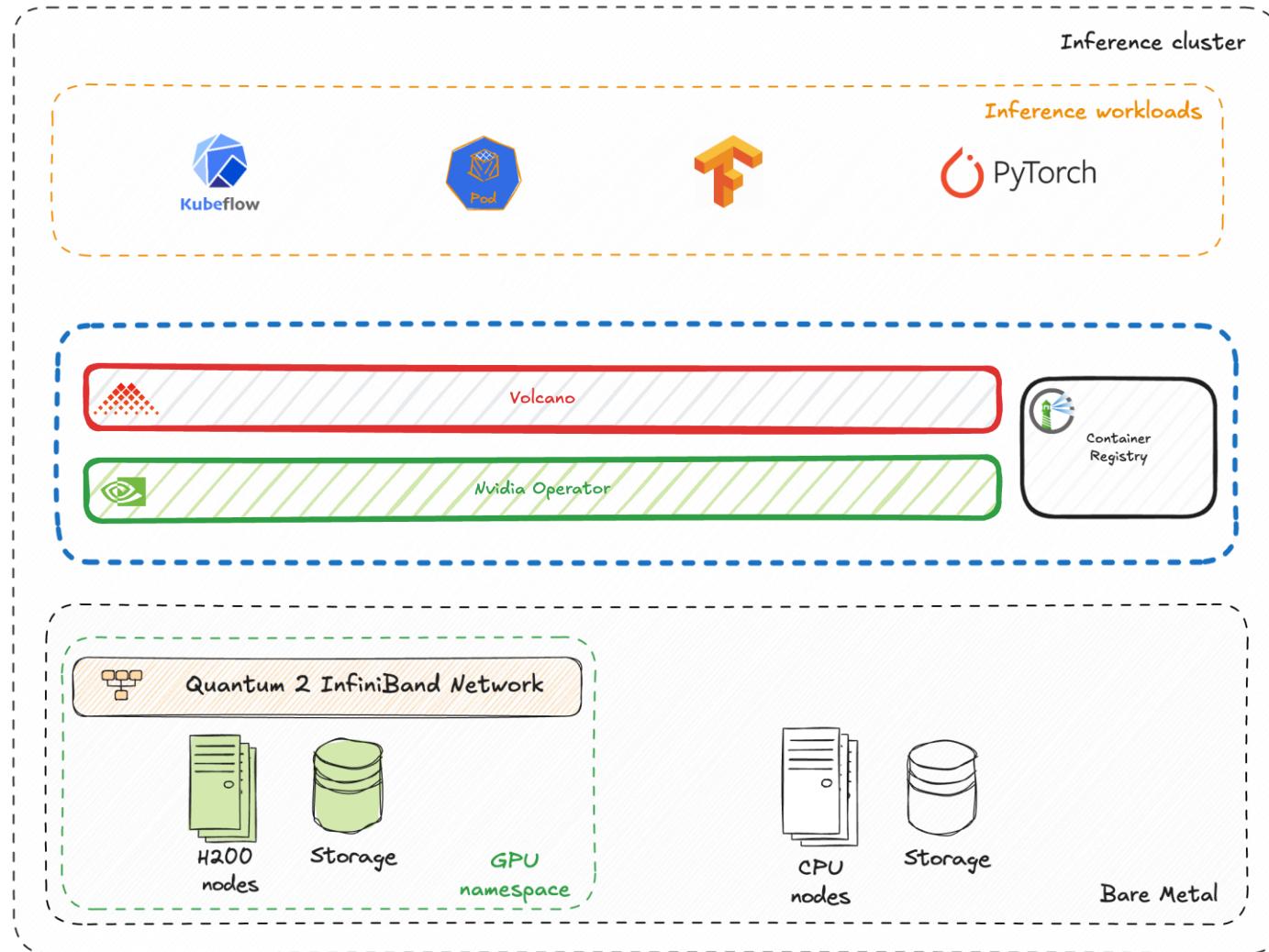
Optimize the scheduling system/experience



Contribution with the other SMEs



\* SME: Subject Matter Experts



# Volcano and Nvidia Operator



Cons
Poor documentation
Community and Ecosystem

Pros
Batch Scheduling
Dynamic resource sharing CPU
Mainstream computing frameworks



Cons
Compatibility and Versioning
Learning curve

Pros
GPU Sharing Strategies
Simplified Deployment
Multiple GPU Types

# Demo – Scheduling with Nvidia Operator

```
>> asciinema play /var/folders/6j/fwyl_cwd09zcmnw6zpcm_63r0000gp/T/tmp6edw49ew-ascii.cast
Starting .zshrc initialization
Finished .zshrc initialization
apple ~ %
> az aks nodepool list --resource-group rg-volcano-cco --cluster-name volcano-poc-cco -o table
```



# Demo – Scheduling with Nvidia Operator

```

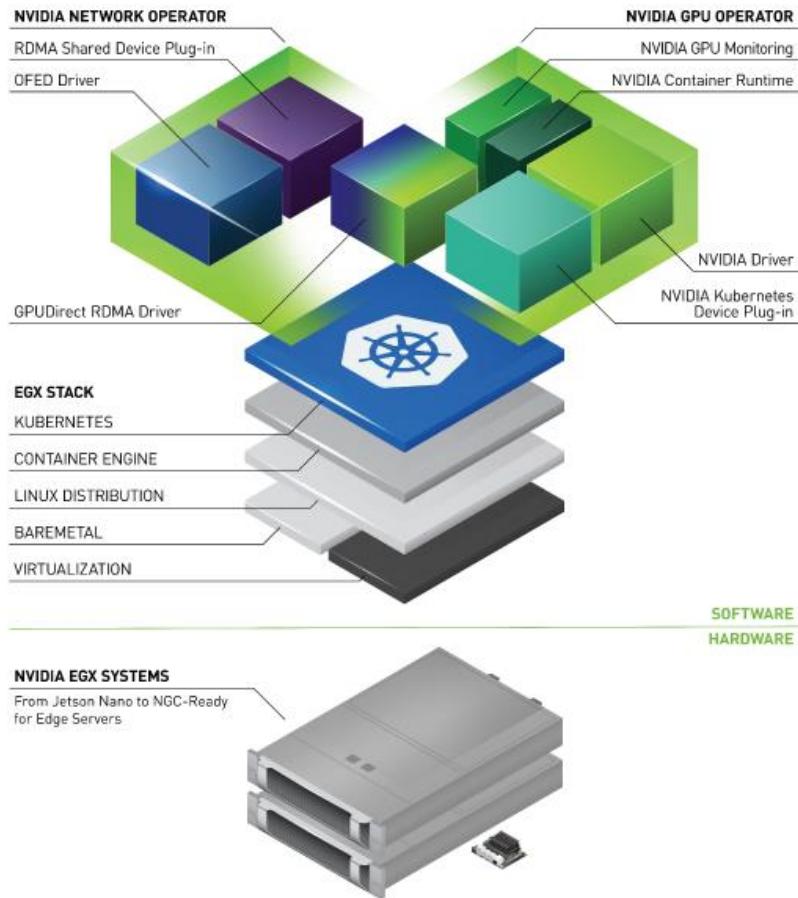
❯ k get no -o wide
NAME          STATUS  ROLES   AGE    VERSION  INTERNAL-IP  EXTERNAL-IP  OS-IMAGE           KERNEL-VERSION      CONTAINER-RUNTIME
aks-a10-13210892-vmss000000  Ready   <none>  11h   v1.29.7  10.224.0.11  <none>       Ubuntu 22.04.5 LTS  5.15.0-1073-azure  containerd://1.7.22-1
aks-a10-13210892-vmss000001  Ready   <none>  11h   v1.29.7  10.224.0.7   <none>       Ubuntu 22.04.5 LTS  5.15.0-1073-azure  containerd://1.7.22-1
aks-ib-48715644-vmss000000  Ready   <none>  16d   v1.29.7  10.224.0.10  <none>       Ubuntu 22.04.5 LTS  5.15.0-1073-azure  containerd://1.7.22-1
aks-nodepool1-19569833-vmss000000  Ready   <none>  16d   v1.29.7  10.224.0.4   <none>       Ubuntu 22.04.5 LTS  5.15.0-1073-azure  containerd://1.7.22-1
aks-nodepool1-19569833-vmss000001  Ready   <none>  16d   v1.29.7  10.224.0.5   <none>       Ubuntu 22.04.5 LTS  5.15.0-1073-azure  containerd://1.7.22-1
aks-nodepool1-19569833-vmss000002  Ready   <none>  16d   v1.29.7  10.224.0.6   <none>       Ubuntu 22.04.5 LTS  5.15.0-1073-azure  containerd://1.7.22-1
❯ helm list -n gpu-operator
NAME        NAMESPACE  REVISION  UPDATED             STATUS      CHART          APP VERSION
gpu-operator-1731312306  gpu-operator  5          2024-11-11 19:34:02.528394 +0100 CET  deployed  gpu-operator-v24.9.0  v24.9.0
❯ k get po -n gpu-operator
NAME                           READY  STATUS   RESTARTS  AGE
gpu-feature-discovery-47z44    1/1    Running  0          10h
gpu-feature-discovery-jtjvl    1/1    Running  0          10h
gpu-operator-1731312306-node-feature-discovery-gc-6778f8bf7brvk  1/1    Running  0          10h
gpu-operator-1731312306-node-feature-discovery-master-7b5dkr4sf   1/1    Running  0          10h
gpu-operator-1731312306-node-feature-discovery-worker-2vbj8     1/1    Running  0          10h
gpu-operator-1731312306-node-feature-discovery-worker-5hrzk     1/1    Running  0          10h
gpu-operator-1731312306-node-feature-discovery-worker-6lmkv     1/1    Running  0          10h
gpu-operator-1731312306-node-feature-discovery-worker-crs7d     1/1    Running  0          10h
gpu-operator-1731312306-node-feature-discovery-worker-f9vxg     1/1    Running  0          10h
gpu-operator-1731312306-node-feature-discovery-worker-t9hjl     1/1    Running  0          10h
gpu-operator-6b68cc6654-nbpg9  1/1    Running  0          10h
nvidia-container-toolkit-daemonset-n25h9  1/1    Running  0          10h
nvidia-container-toolkit-daemonset-nwpt7  1/1    Running  0          10h
nvidia-cuda-validator-6tmt5   0/1    Completed 0          10h
nvidia-cuda-validator-s5dw9   0/1    Completed 0          10h
nvidia-dcgm-exporter-8x5fk   1/1    Running  0          10h
nvidia-dcgm-exporter-n4lxt   1/1    Running  0          10h
nvidia-device-plugin-daemonset-8cr6v  1/1    Running  0          20m
nvidia-device-plugin-daemonset-sq24s  0/1    Init:0/1  0          20m
nvidia-operator-validator-dz52c  0/1    Init:1/5  0          20m
nvidia-operator-validator-ttdj2  0/1    Init:1/5  0          19m
❯ helm list -n ollama
NAME        NAMESPACE  REVISION  UPDATED             STATUS      CHART          APP VERSION
ollama      ollama     1          2024-11-11 17:55:22.785464 +0100 CET  deployed  ollama-0.65.0  0.4.1
❯ k get po -n ollama
NAME                           READY  STATUS   RESTARTS  AGE
ollama-68895b6f66-vs5xl    1/1    Running  0          120m
❯ k get po -n ollama -o yaml | yq e '.items[].spec.containers[].resources'
limits:
  nvidia.com/gpu: "1"
requests:
  nvidia.com/gpu: "1"

```

system 19:55:50



# Unlocking the full potential



- **Kubernetes Device Plugins**
- **DRA over CDI for GPU requests**

```
apiVersion: v1
kind: Pod
metadata:
  name: gpu-example
spec:
  containers:
  - name: ctr
    image: nvidia/cuda
    command: ["nvidia-smi", "-L"]
    resources:
      limits:
        nvidia.com/gpu: 2
      requests:
        nvidia.com/gpu: 2
```

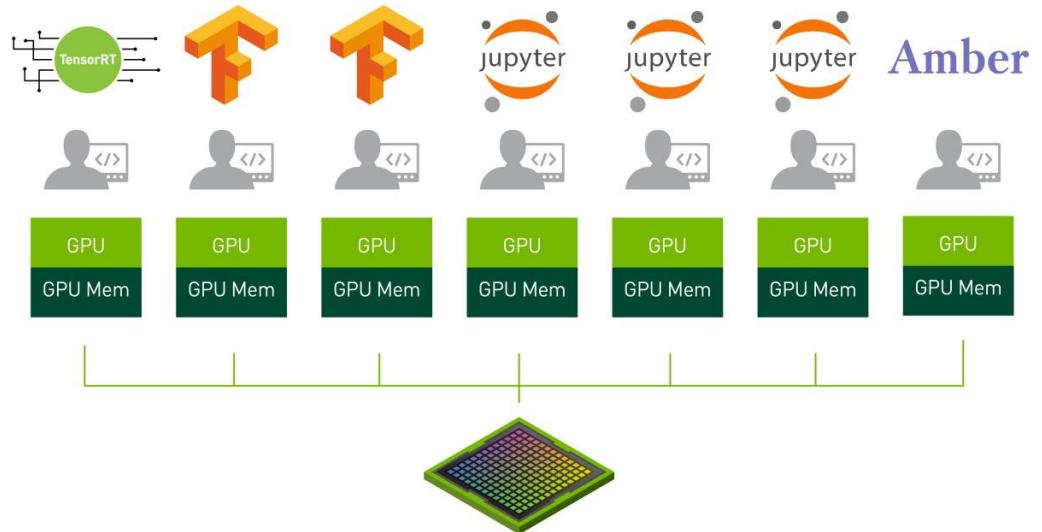


```
apiVersion: v1
kind: Pod
metadata:
  name: gpu-example
spec:
  containers:
  - name: ctr
    image: nvidia/cuda
    command: ["nvidia-smi", "-L"]
    resources:
      limits:
        nvidia.com/gpu: 2
      requests:
        nvidia.com/gpu: 2
```

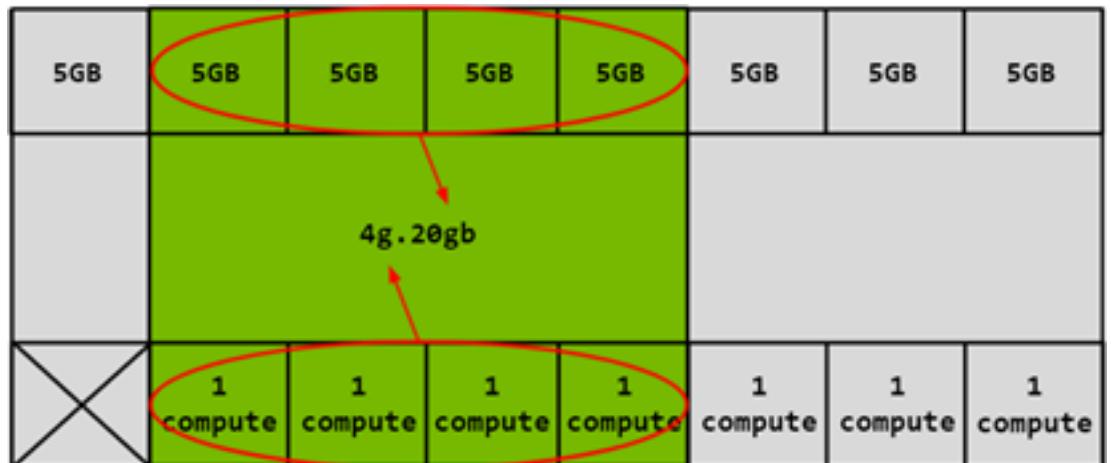
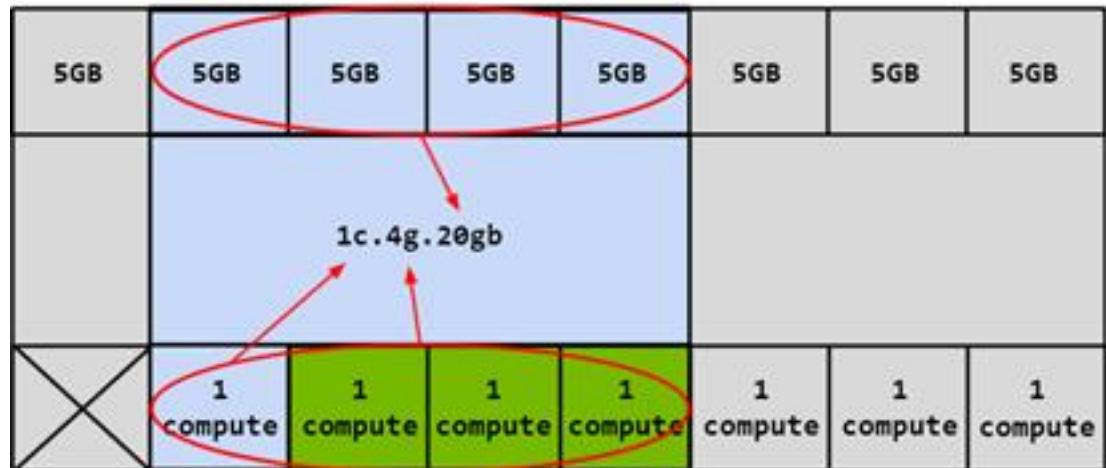
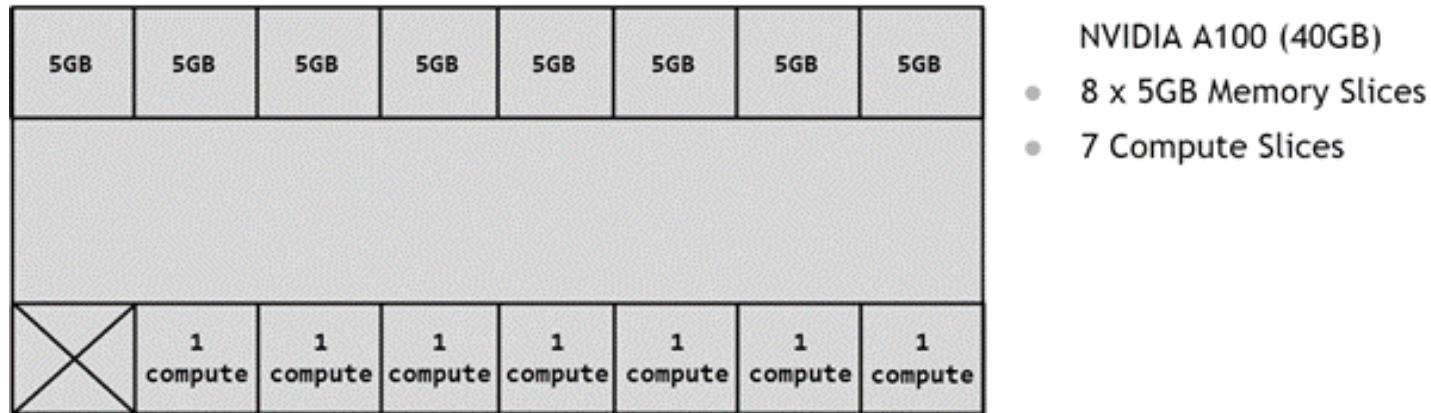
```
apiVersion: resource.k8s.io/v1alpha2
kind: ResourceClaimTemplate
metadata:
  name: gpu-template
spec:
  spec:
    resourceClassName: gpu.nvidia.com
```

\* DRA: Dynamic Resource Allocation  
 \* CDI: Container Driver Interface

# Sharing GPUs with MiG



Amber

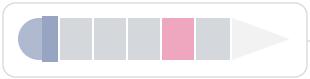


# Batch Scheduling on Kubernetes

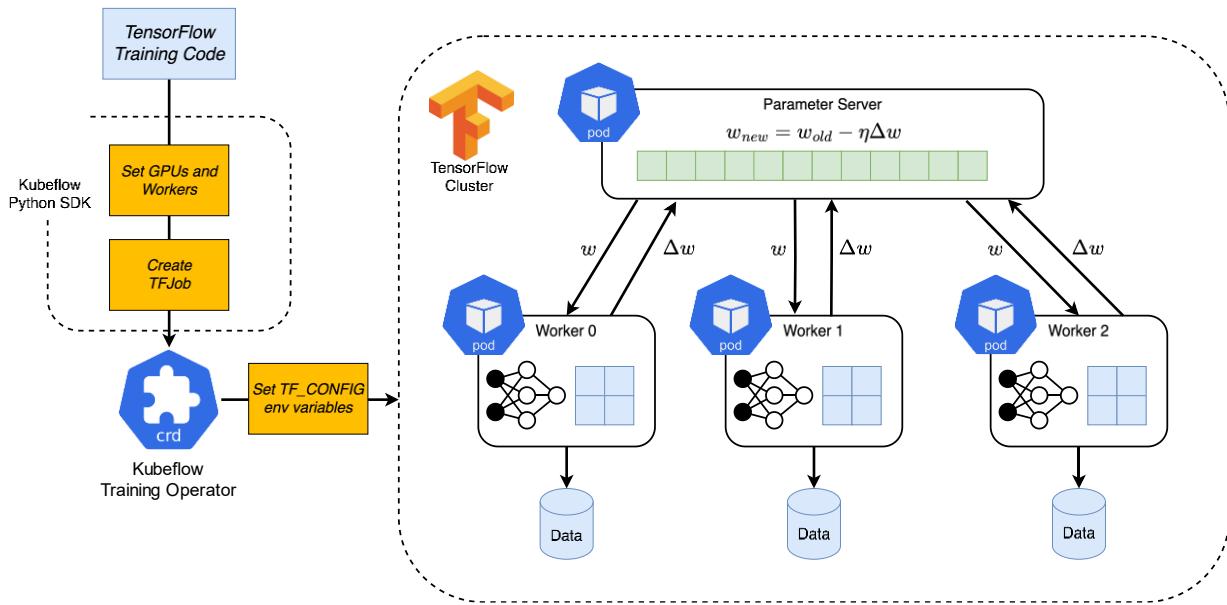
- Queue concept
- Gang Scheduling
- ML frameworks compatible



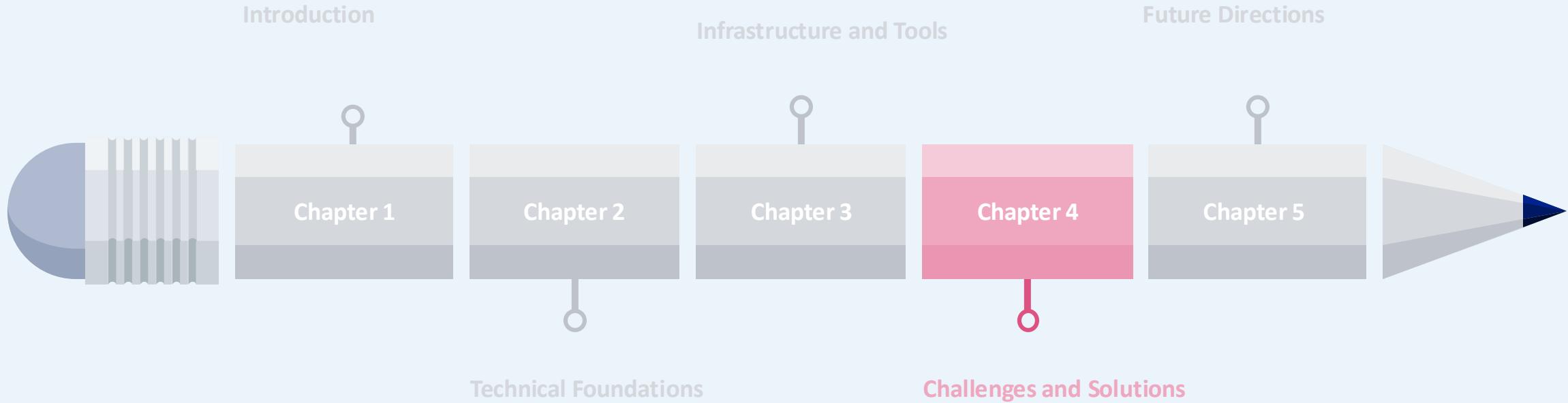
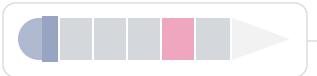
# Batch Scheduling on Kubernetes



```
apiVersion: kubeflow.org/v1
kind: TFJob
metadata:
  generateName: tfjob
  namespace: your-user-namespace
spec:
  tfReplicaSpecs:
    PS:
      replicas: 1
      restartPolicy: OnFailure
      template:
        metadata:
          annotations:
            sidecar.istio.io/inject: "false"
        spec:
          containers:
            - name: tensorflow
              image: gcr.io/your-project/your-image
              command:
                - python
                - -m
                - trainer.task
                - --batch_size=32
                - --training_steps=1000
    Worker:
      replicas: 3
      restartPolicy: OnFailure
      template:
        metadata:
          annotations:
            sidecar.istio.io/inject: "false"
        spec:
          containers:
            - name: tensorflow
              image: gcr.io/your-project/your-image
              command:
                - python
                - -m
                - trainer.task
                - --batch_size=32
                - --training_steps=1000
```



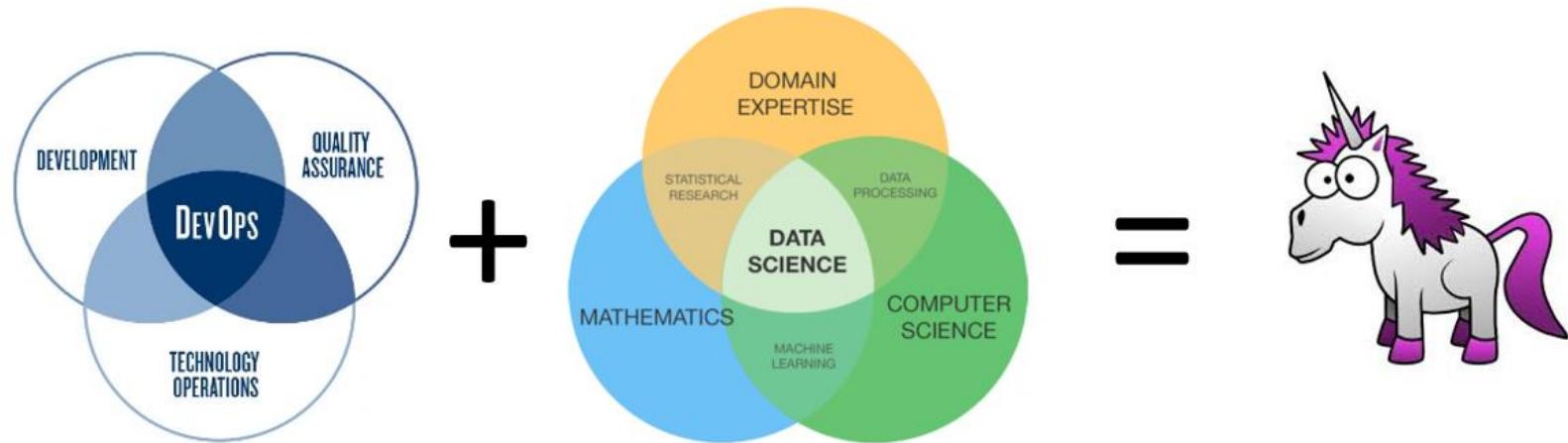
# Challenges and potential solutions



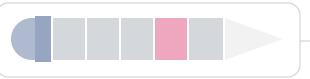
# Stay Focused



- Contribute Drug Discovery
- ML Engineers and Data Scientists are not **Platform/DevOps** Engineers

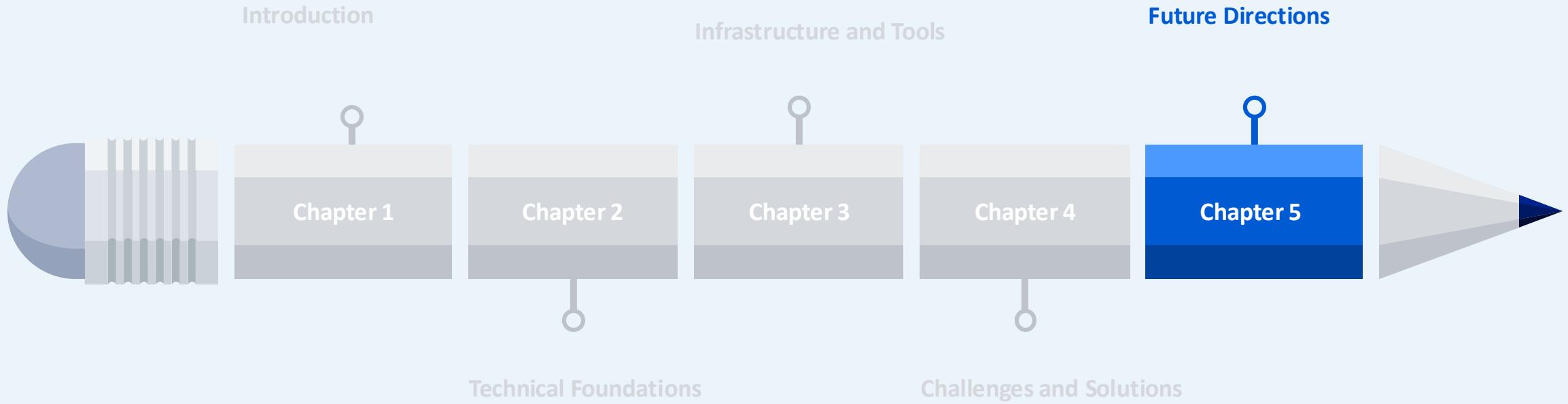
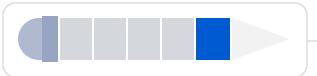


# ...while keeping the expertise

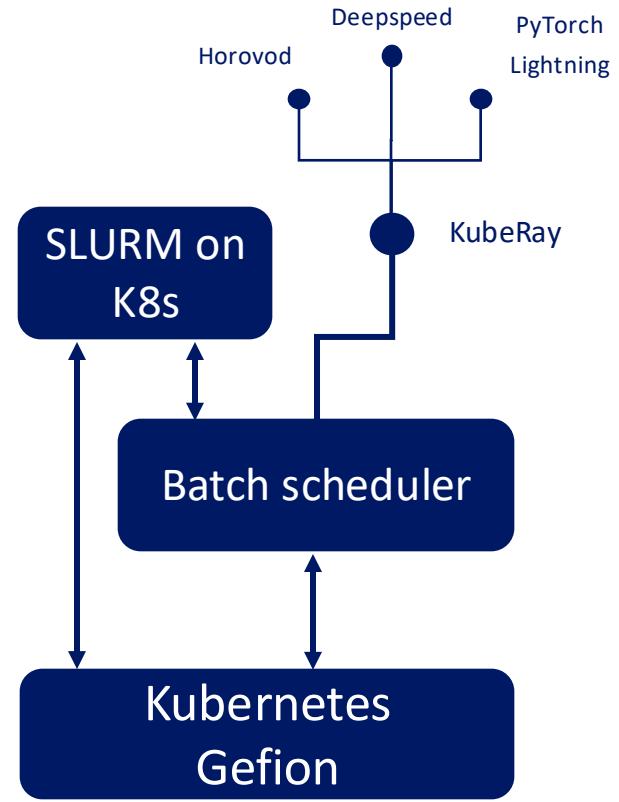
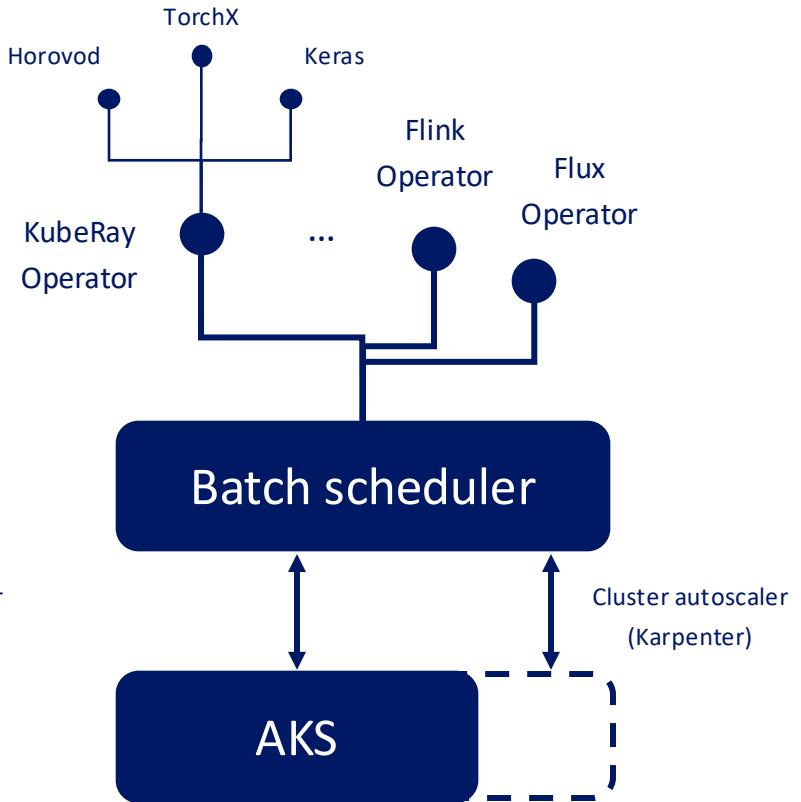
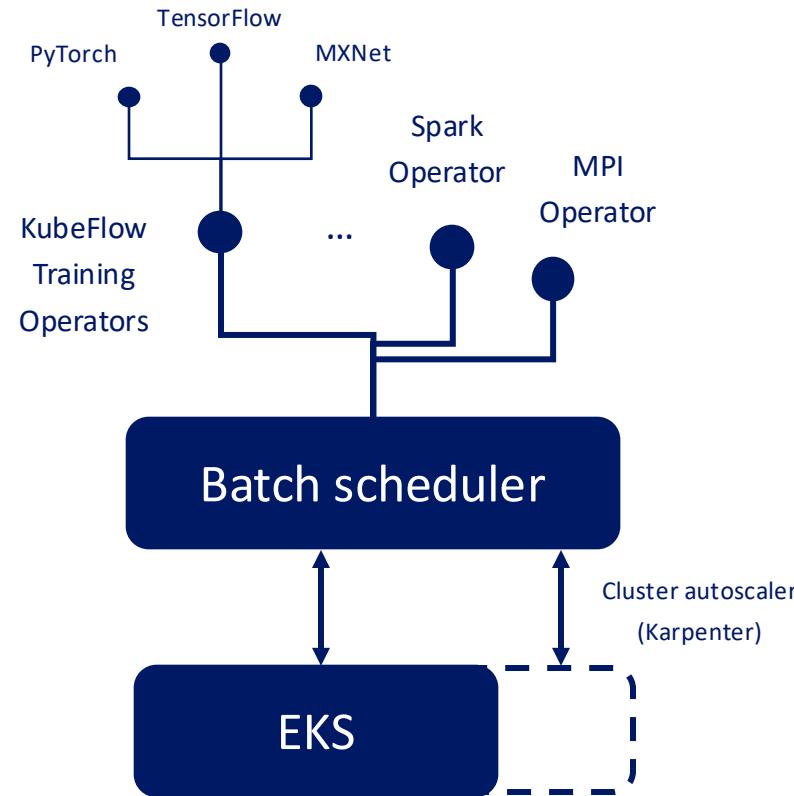


- Battle Royale Workshops
- Keep information decomplexified and flat as possible

# Future Directions



# Possible future landscape (examples)



# Thank you!

