Distributed Computing

DSBA 6190-U90 | Colby T. Ford, Ph.D.

Overview

Terms

History of Parallel Computing

Containerization and Kubernetes

Intro to Apache Spark

Terms

High Performance Computing

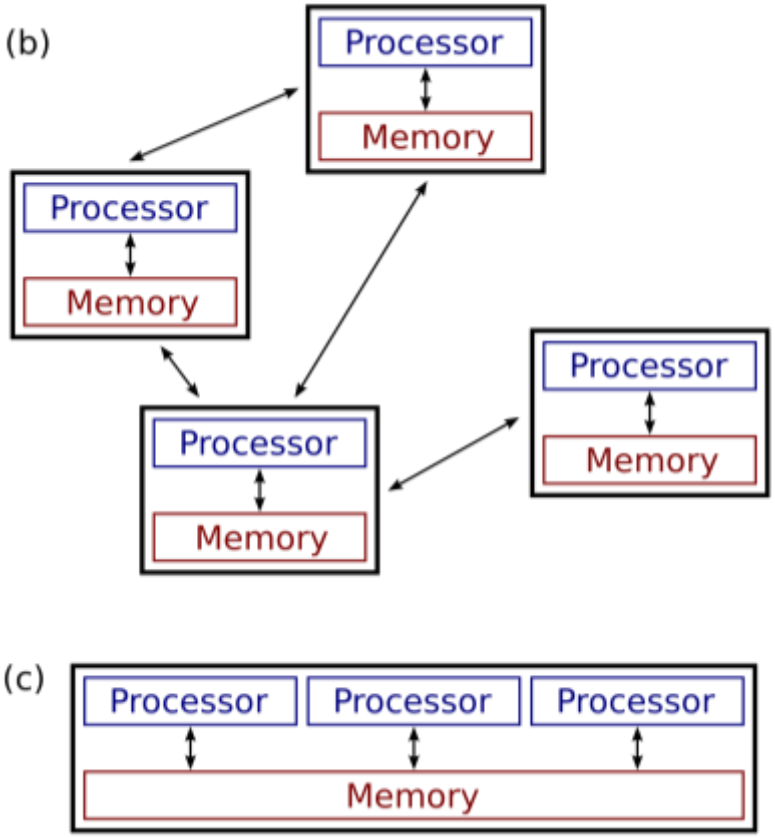
- Using more powerful machines to do computations faster.
- Measured in FLOPS

Parallel Computing (c)

- Using multiple cores to do multiple things at once.
- Measured in degree of parallelism

Distributed Computing (b)

- Using multiple machines to do multiple things at once.
- Measured in degree of distribution and parallelism



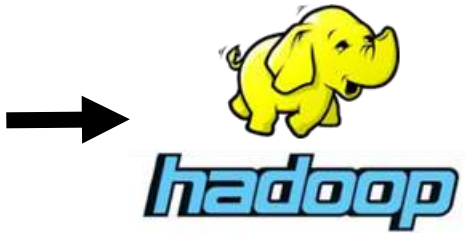
File:Distributed-parallel.svg. (2014, August 28). *Wikimedia Commons, the free media repository*. Retrieved 15:47, October 16, 2019 from https://commons.wikimedia.org/w/index.php?title=File:Distributed-parallel.svg&oldid=132972776.

Technology Pipeline

Multicore

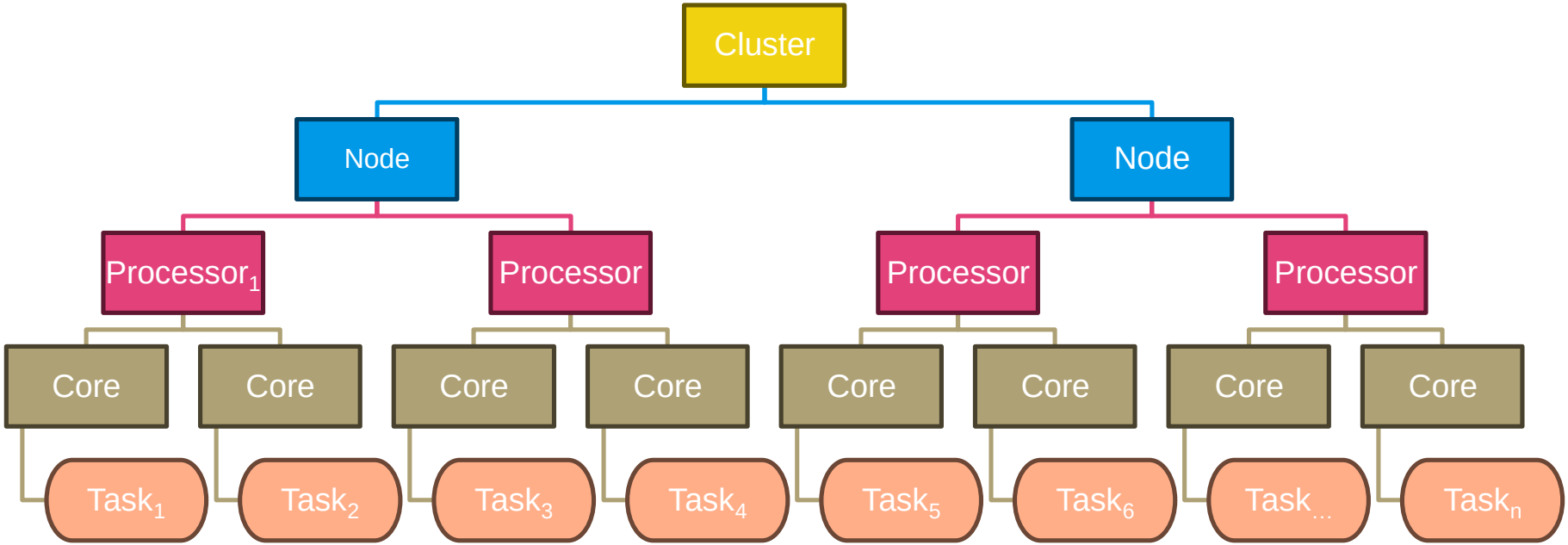
MPI

SNOW



kubernetes

Cluster Architecture



Containerization

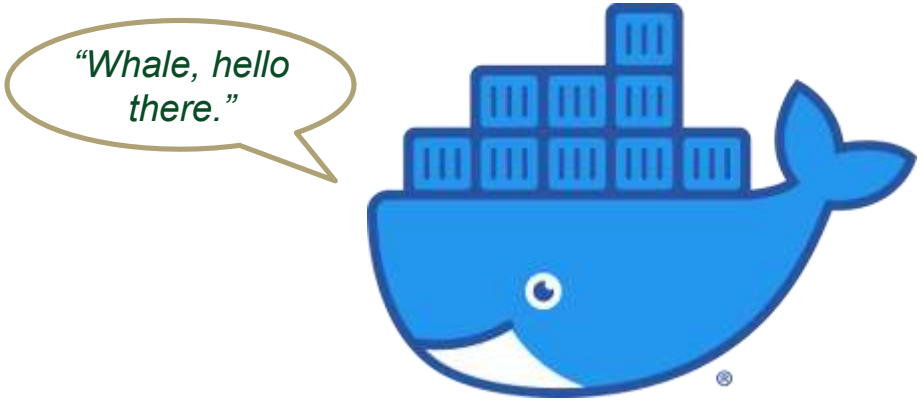
Popular Container Frameworks

Most popular, Full-featured
Requires root
Windows, macOS, and Linux

Less popular, More limited
Daemonless and rootless
Windows, macOS, and Linux

Popular on HPC Clusters
Only for Linux
(formerly “Singularity”)

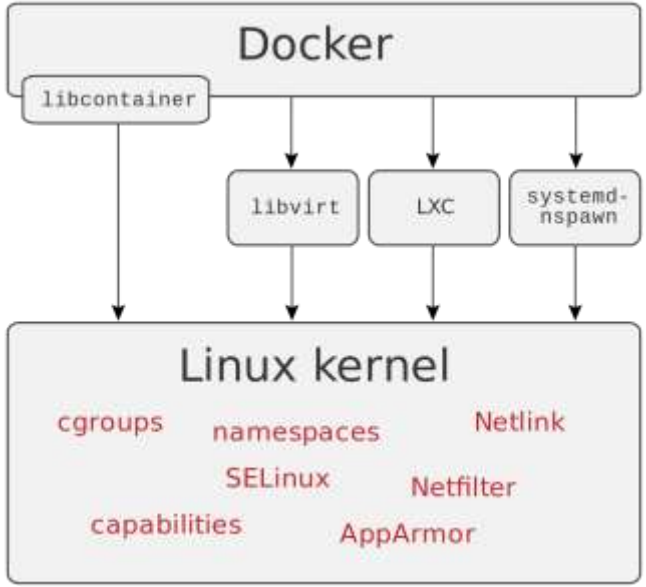
—



Docker

- Support for Linux and Windows Server containers (and now WebAssembly).
- Flexibility to support microservices and traditional app workloads.
- Integrated graphical user interface-based management and operation.
- Granular role-based access control, LDAP, and Azure Active Directory integration.
- Connection to custom networking and volumes (data storage)

- Think of Docker is a trimmed down VM image with sets of packages and settings that are configured for reuse.

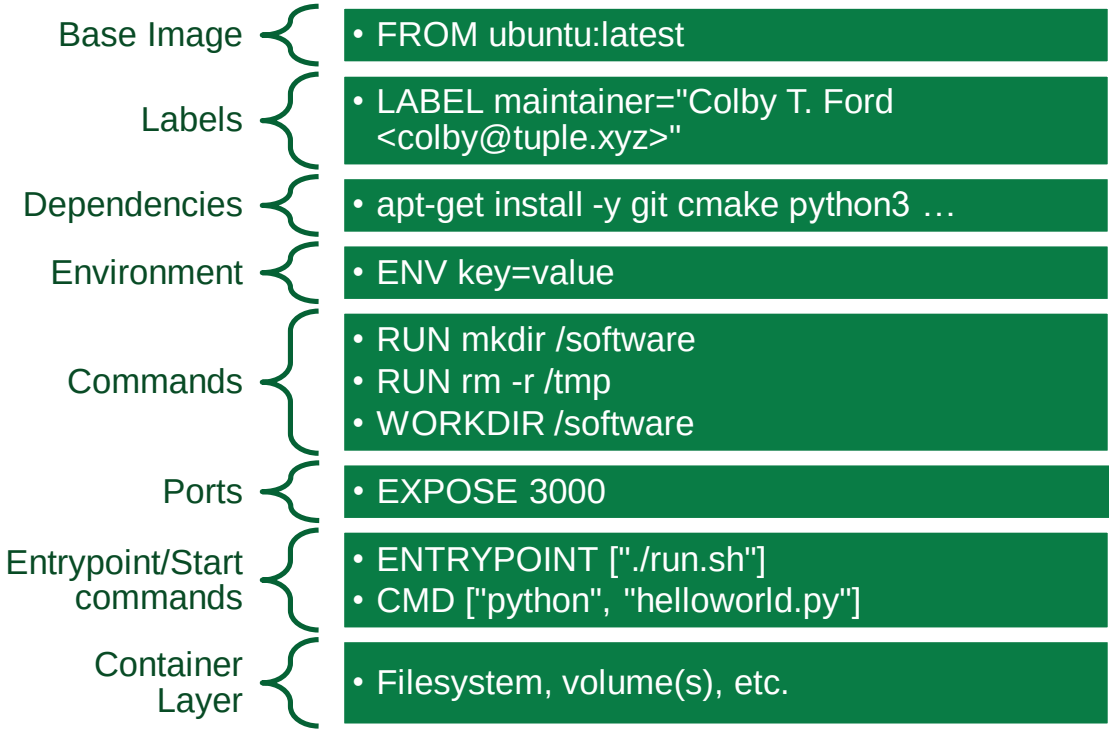


Dockerfile

- Contains layers of instructions for configuring the system and installing libraries and files.
- Specifies a base layer, which is useful for “picking up where someone left off”

Dockerfile Layers

- Docker uses layers to save on image space and on build complexity.
- Each layer contains the information that changes the layer before it.
- When you rebuild, Docker will cache the unchanged layers.



Docker Commands

Get started | Docker Docs

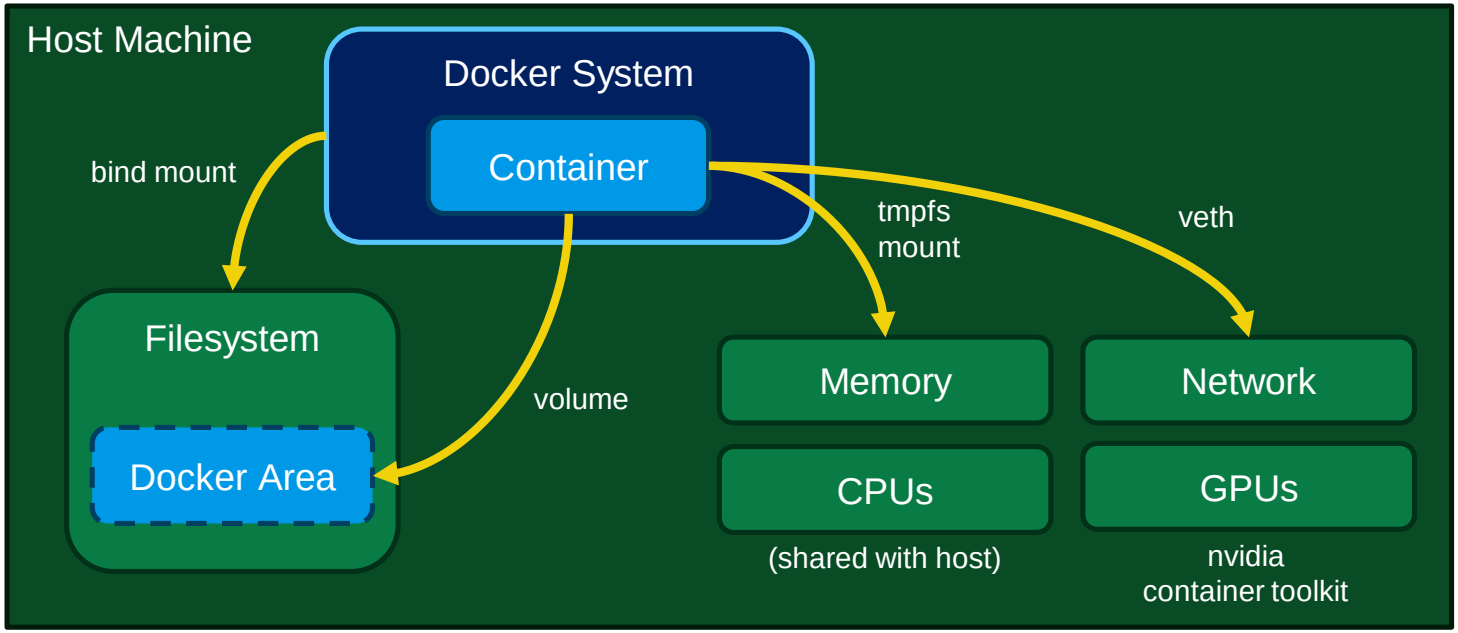
Pull an Image from a Container Registry
- docker pull <url>/<user>/<image>:<tag>
- docker pull nvidia/cuda:12.6.1-cudnn-devel-ubuntu22.04
- docker pull nvcr.io/nvidia/pytorch:22.04-py3

Build an Image Locally
- docker build -t <image tag> .
- docker build -t reactwebapp .

Run a Container Locally
- docker run <image name> <other options>
- docker run -p 8888:8888 -v /data/local:/home/jovyan/work jupyter/base-notebook
- docker run --name cuda_gpu_1 --gpus all -t nvidia/cuda

Execute Command in a Container
- docker run/exec <image name> <commands>
- docker run --name mycontainer1 -it mycontainer /bin/bash
- docker exec -it mycontainer /bin/bash

Volumes (and sharing other resources)



Docker Compose

- Docker Compose allows you to specify multiple images that can communicate with one another.
  - Networking (vNets)
  - Volumes (databases)

- `docker compose up -d`
- `docker compose down`

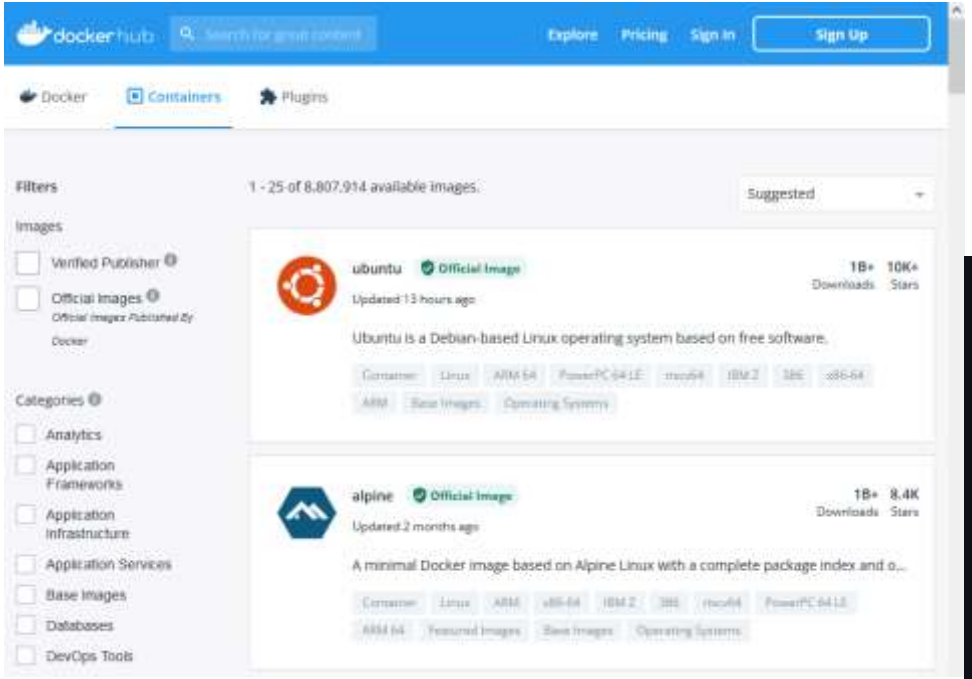
Less used in cloud native environments where PaaS options are more common.

Directory Structure

compose.yaml File

```
services:
  backend:
    build: backend
    ports:
      - 80:80
      - 9229:9229
      - 9230:9230
    ...
  db:
    image: mariadb:10.6.4-focal
    ...
  frontend:
    build: frontend
    ports:
    - 3000:3000
    ...
```

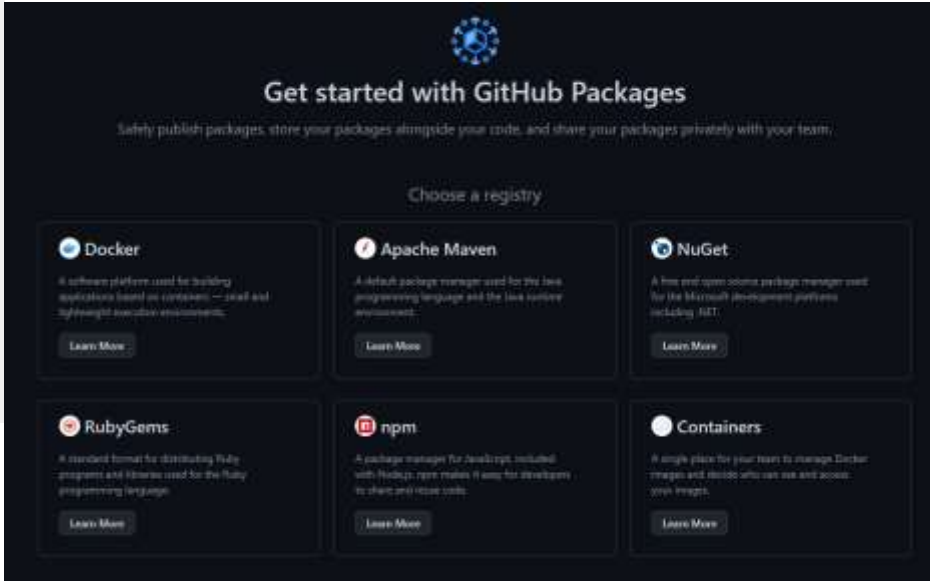
Container Storage



DockerHub

Azure Container Registry

GitHub Packages



Container Usage

- Deploy containerized applications to Azure for quick and scalable use.
- Pick the Runtime Stack (Node, .NET, Python, etc.) and OS (Linux or Windows)
- Pick the size of machine (RAM, CPUs, GPUs)

Azure Web Apps

Azure Container Instances

Azure Kubernetes Service

Container Registry Commands

Login to the Container Registry
- az acr login --name <registry name>
- az acr login --name crdsba6190deveastus001

Tag the Image with the URL, your name, and tag
- docker tag <image name> <registry name>.azurecr.io/<image name>:<tag>
- docker tag instructor_sklearn crdsba6190deveastus001.azurecr.io/instructor_sklearn:latest

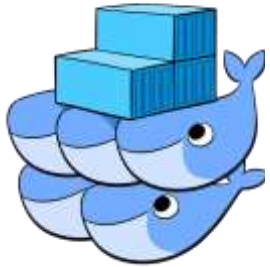
Push the Image to the Container Registry
- docker push <registry name>.azurecr.io/<image name>:<tag>
- docker push crdsba6190deveastus001.azurecr.io/instructor_sklearn:latest

Container Orchestration

- Once containers are created, use container orchestration to organize, coordinate, and schedule their use.
- Useful for scaling containers and making use of distributed environments
- Other capabilities:
  - Security management
  - API Serving
  - Resource Monitoring
  - Load Balancing

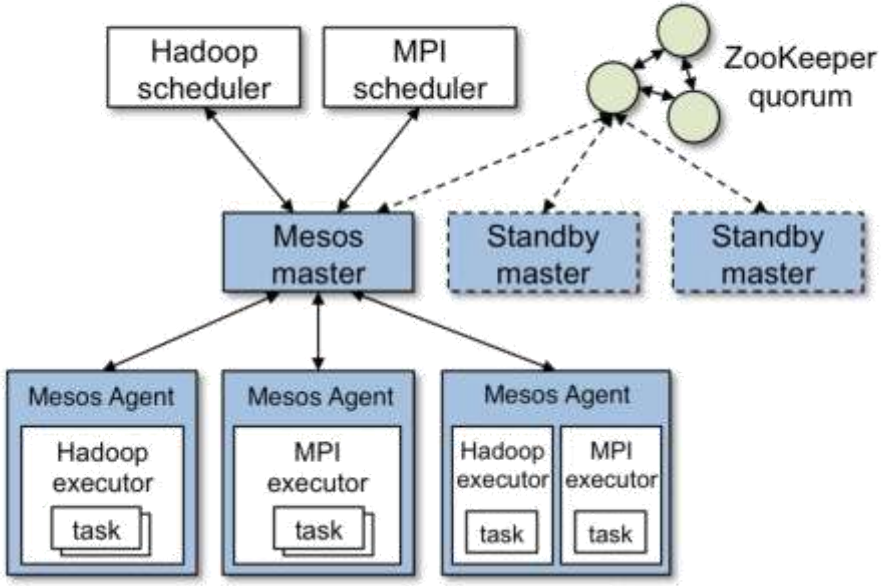
kubernetes

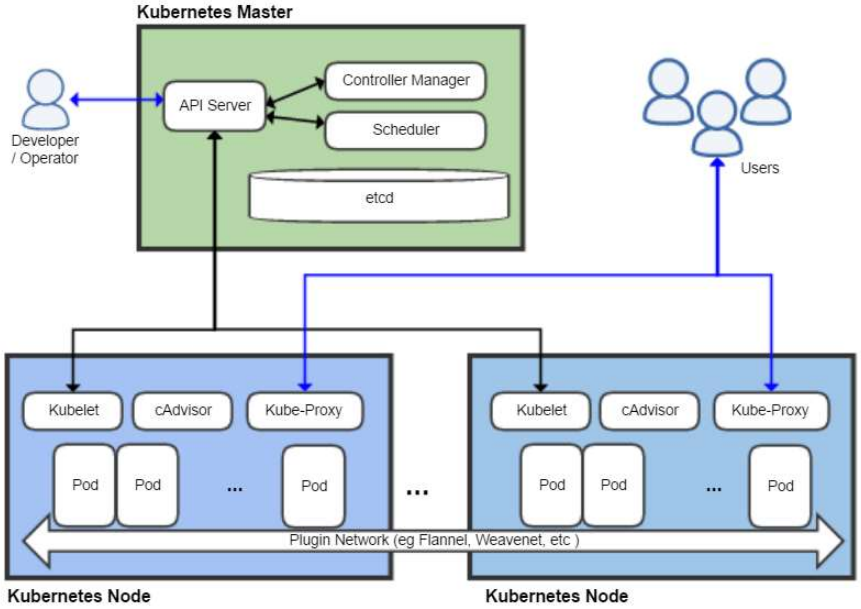
MESOS



https://azure.microsoft.com/en-us/resources/videos/azure-kubernetes-service-overview/

Mesos Architecture





What is / Why Kubernetes?

What is Kubernetes?

Kubernetes (K8s) is an open-source container orchestration system.

Use Docker containers and spin up compute nodes as needed.

Specify different resource needs by node pool.

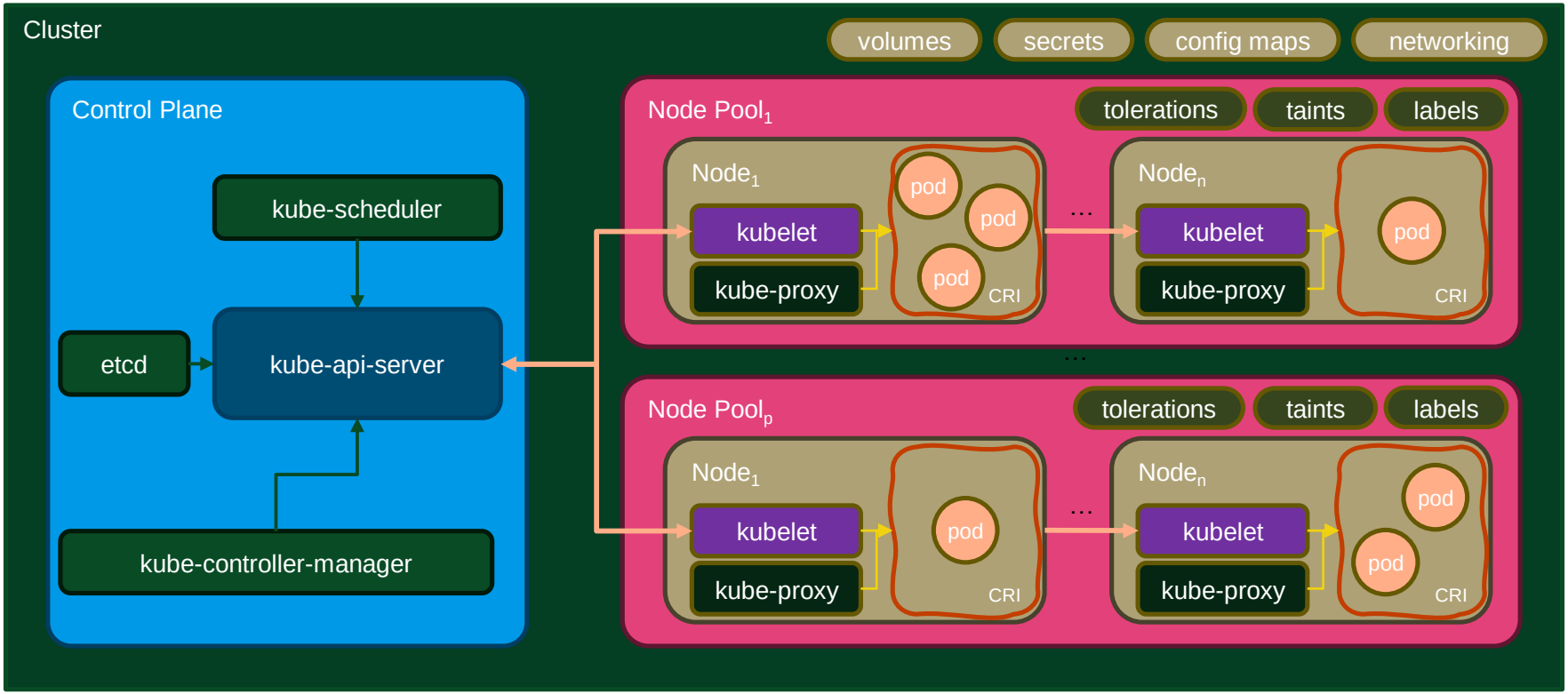
Memory, CPUs, GPUs

Learn more: https://kubernetes.io/

Why (Cloud) Kubernetes?

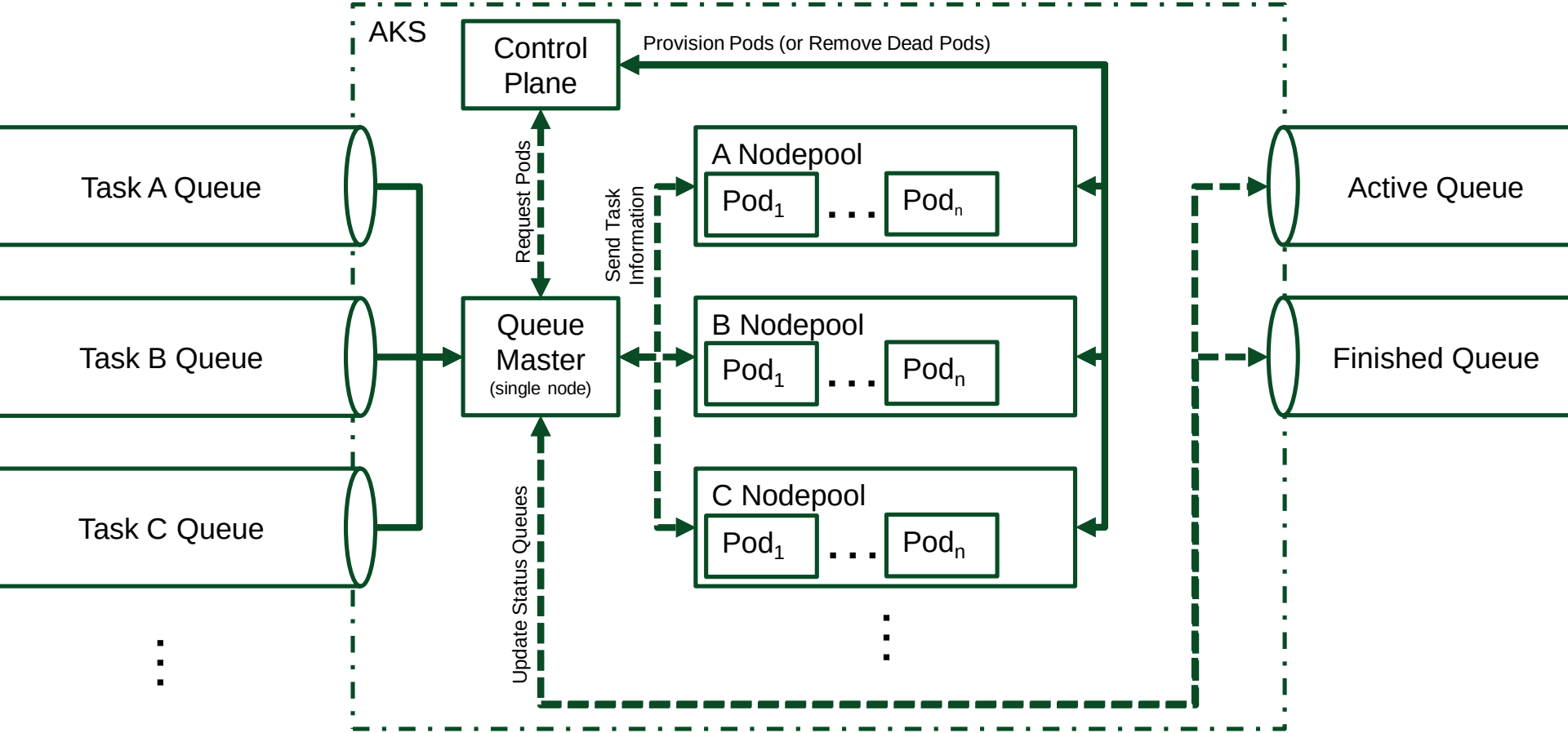
- K8s can be used for everything from microservices to long-running compute tasks
  - Not everything in bioinformatics is a pipeline. (Duct taped shell scripts, anyone?)
  - Not every pipeline has the same needs (GPUs, memory, CPUs, etc.)
- Cloud providers have platform services that are fully compatible with open-source K8s
  - Azure Kubernetes Service (AKS)
  - AWS Elastic Kubernetes Service (EKS)
  - Google Kubernetes Engine (GKE)
- Take advantage of the “limitless” compute capacity of the cloud + networking and security
- Mount your data lake as a Volume in the K8s cluster, making the data available to every container
  - No copying data around
  - Get references and input files from `/mnt`
  - Write results directly back to the data lake

Basic K8s Cluster Architecture



CRI: Container Runtime Interface

Kubernetes + Queue-Based Architecture



Example Pod Specification

- Specifies the name of the pod, its image, and other information.
  - Volumes
  - Commands
  - Secrets
  - Resource Requests
    - CPUs
    - GPUs
    - Memory
  - Tolerations

```yaml
apiVersion: v1
kind: Pod
metadata:
  name: instructor-test-01
spec:
  restartPolicy: Never
  containers:
  - name: instructor-sklearn
    image: crdsba6190deveastus001.azurecr.io/instructor_sklearn:latest
    volumeMounts:
      - name: datalake
        mountPath: "/mnt/datalake/"
        readOnly: false
    # command: ["/bin/bash", "-c"]
    # args: ["./run.py"]
    command: [ "/bin/bash", "-c", "--" ]
    args: [ "while true; do sleep 30; done;" ]
    # resources:
    #   limits:
    #     memory: "2Gi"
    #     cpu: "200m"
  imagePullSecrets:
    - name: acr-secret
  volumes:
    - name: datalake
      persistentVolumeClaim:
        claimName: pvc-datalake-class-blob
```

kubectl Commands

Get Azure Kubernetes Service Credentials

- az aks get-credentials --resource-group rg-ahab-dev-eastus-001 --name kub-ahab-dev-eastus-001 --overwrite-existing

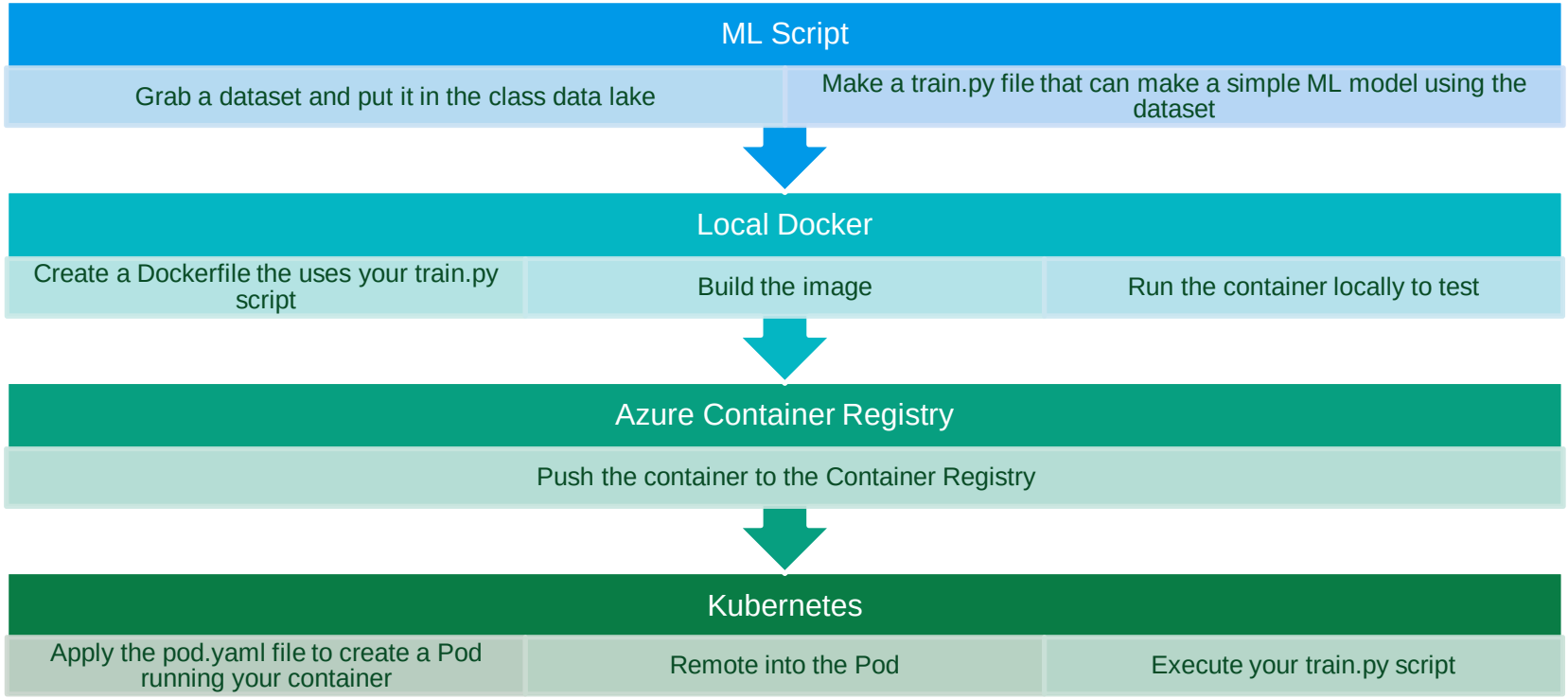
Apply Kubernetes Pod

- kubectl apply -f <pod yaml file>
- kubectl apply -f example_pod.yml

Execute Command in Pod

- kubectl exec -it <pod_name> -- <command>
- kubectl exec -it instructor-test-01 -- /bin/bash

Lab Steps - Kubernetes



Apache Spark + Databricks

Why Spark?

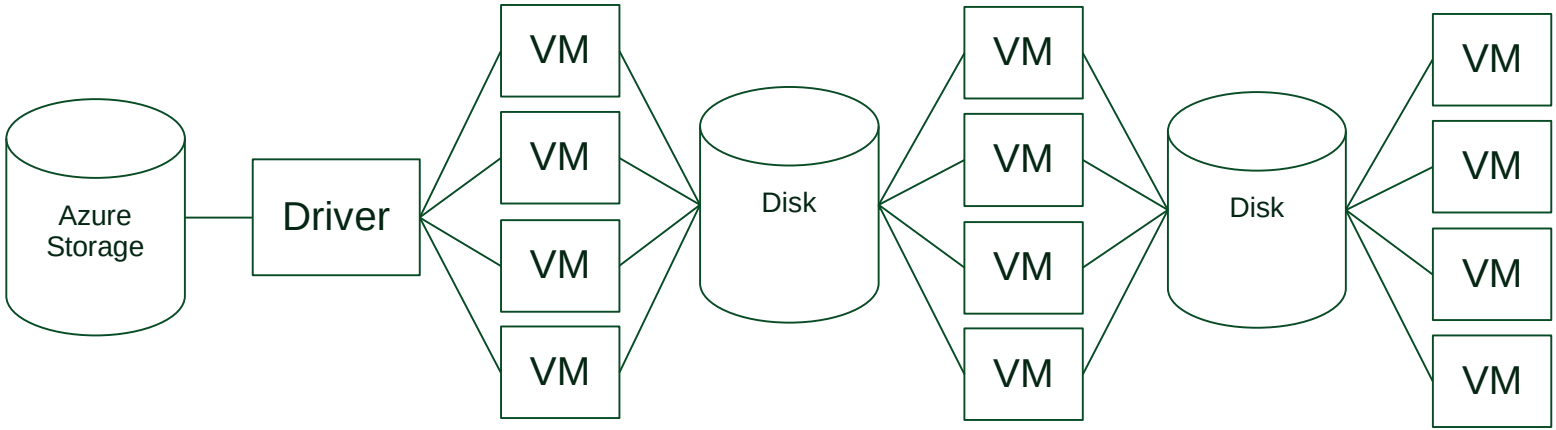
- Open-source data processing engine built around **speed, ease of use, and sophisticated analytics**
- In memory engine that is up to **100 times faster than Hadoop**
- **Largest open-source data project** with 1000+ contributors
- **Highly extensible** with support for Scala, Java and Python alongside Spark SQL, GraphX, Streaming and Machine Learning Library (MLlib)

Why Databricks?

- Databricks is the premium version of Spark available in the market
- Spark founders created Databricks
- Spark is the dominant workload in Hadoop
- **Databricks commits 75% of the code to Open-Source Spark**

Hadoop MapReduce

MapReduce in Hadoop

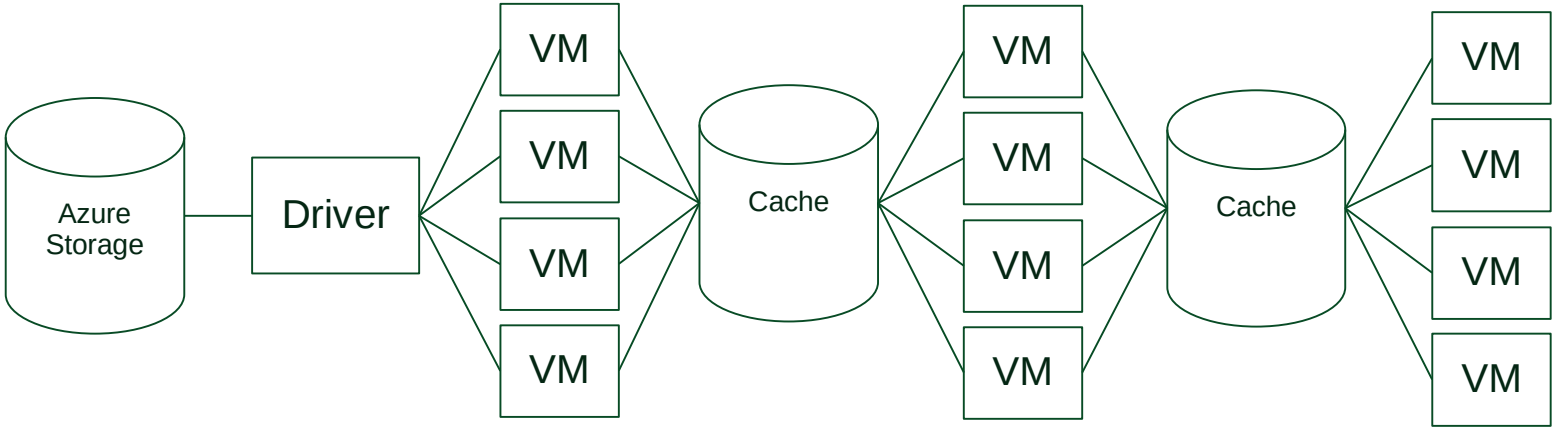


Azure Storage > Driver > VM/Parallelization > write to Disk > VM/Parallelization > write to disk > repeat…

Writing to disk takes time… every time you run this process in MapReduce

What is Azure Databricks?

Apache® Spark™ is FASTER and EASIER than MapReduce in Hadoop

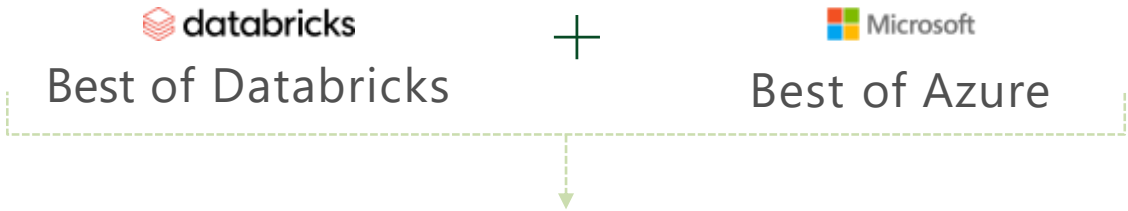


Faster – In Spark data stays in cache this give Spark the speed over MapReduce (writing to disk)

Easier – You can use the language you are most comfortable with in Spark (Python, Scala, R, SQL)

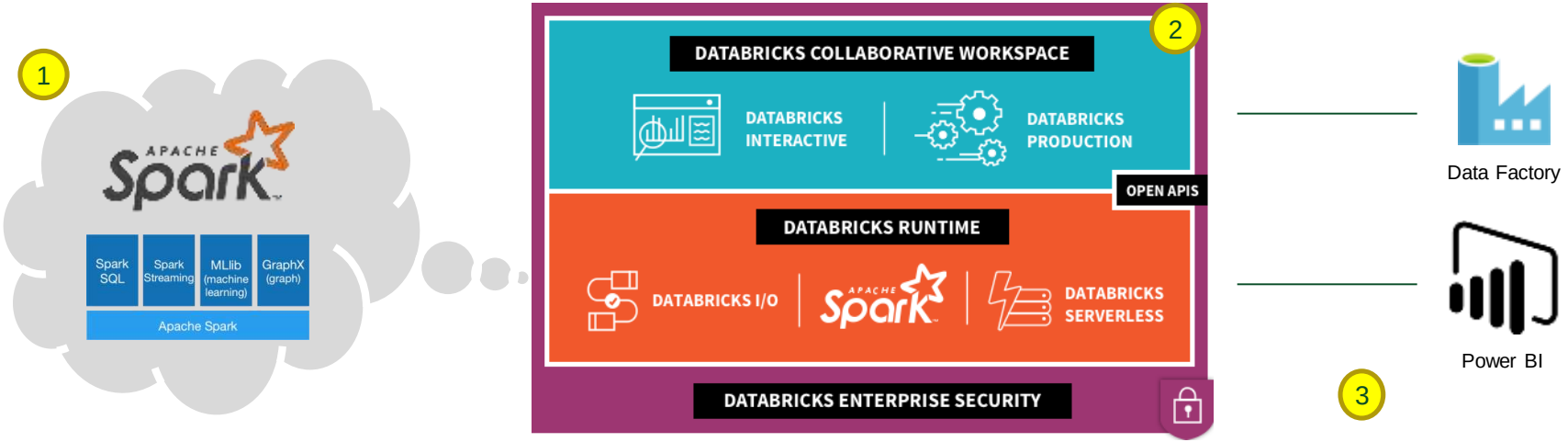
What is Azure Databricks?

A fast, easy and collaborative Apache® Spark™ based analytics platform optimized for Azure

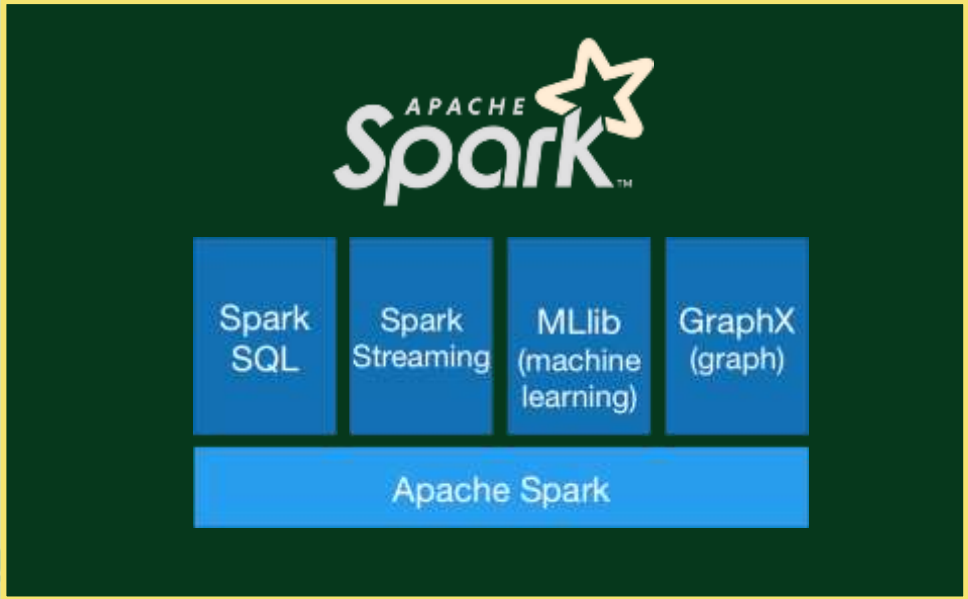


- Designed in collaboration with the founders of Apache Spark
- One-click set up; streamlined workflows
- Interactive workspace that enables collaboration between data scientists, data engineers, and business analysts.
- Native integration with Azure services (Power BI, SQL DW, Cosmos DB, Blob Storage)
- Enterprise-grade Azure security (Active Directory integration, compliance, enterprise-grade SLAs)

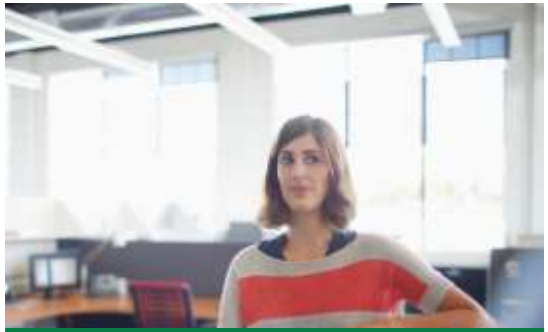
What's Under the Hood?



What's Under the Hood?



Azure Databricks key audiences & benefits



Data scientist

Integrated workspace

Easy data exploration

Collaborative experience

Interactive dashboards

Faster insights

- Best Spark & serverless
- Databricks managed Spark

Data engineer

Improved ETL performance

- Zero management clusters, serverless

Easy to schedule jobs

Automated workflows

Enhanced monitoring & troubleshooting

- Automated alerts & easy access to logs

Zero Management Spark

Cluster democratization (High-concurrency)

CDO, VP of analytics

Fast, collaborative analytics platform accelerating time to market

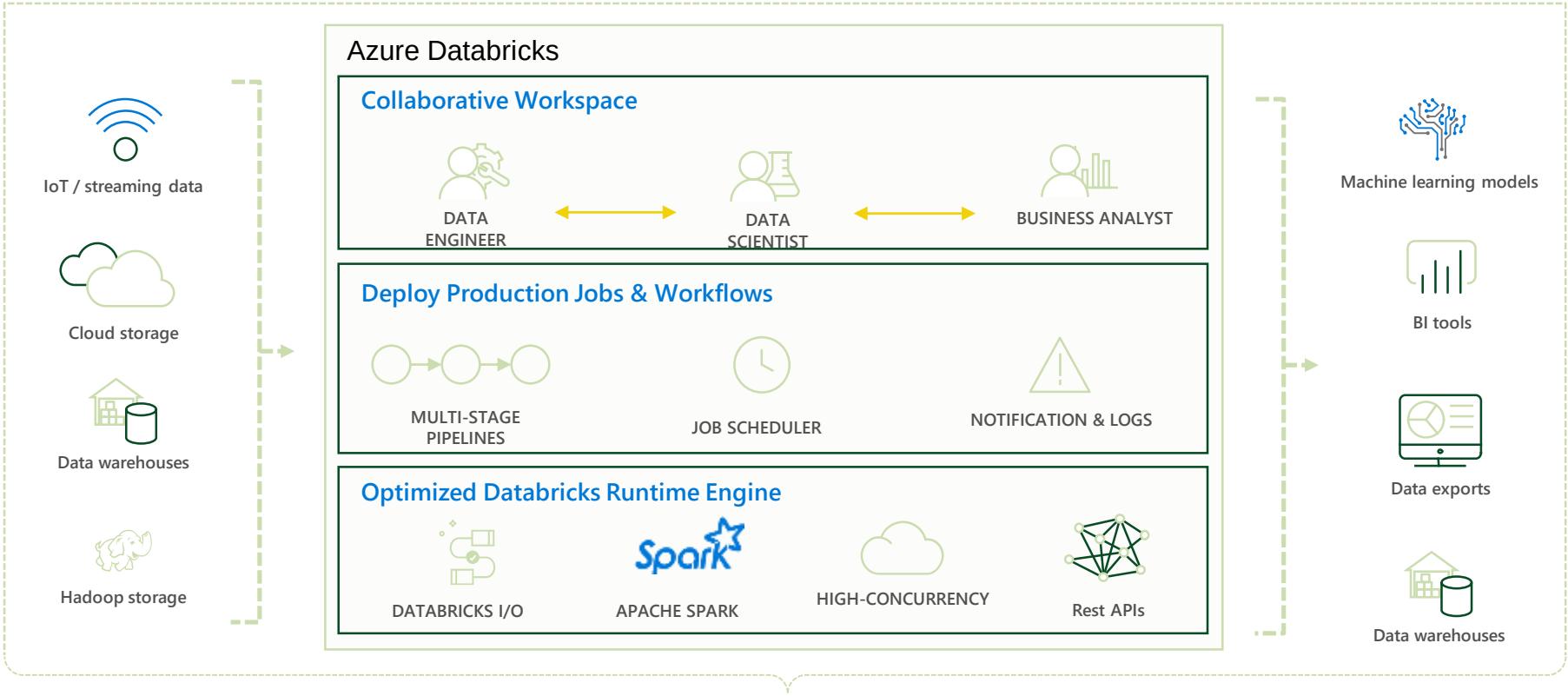
No dev-ops required

Enterprise grade security

- Encryption
- End-to-end auditing
- Role-based control
- Compliance

Unified analytics platform

Azure Databricks



Enhance Productivity

Build on secure & trusted cloud

Scale without limits

Spark is Lazy, but in a Smart Way

When you execute a command, Spark doesn't actually do anything unless it's required to show you something or it has to write something out.

This is the difference between a **Transformation** and an **Action**.

"Lazy Evaluation"

Transformations

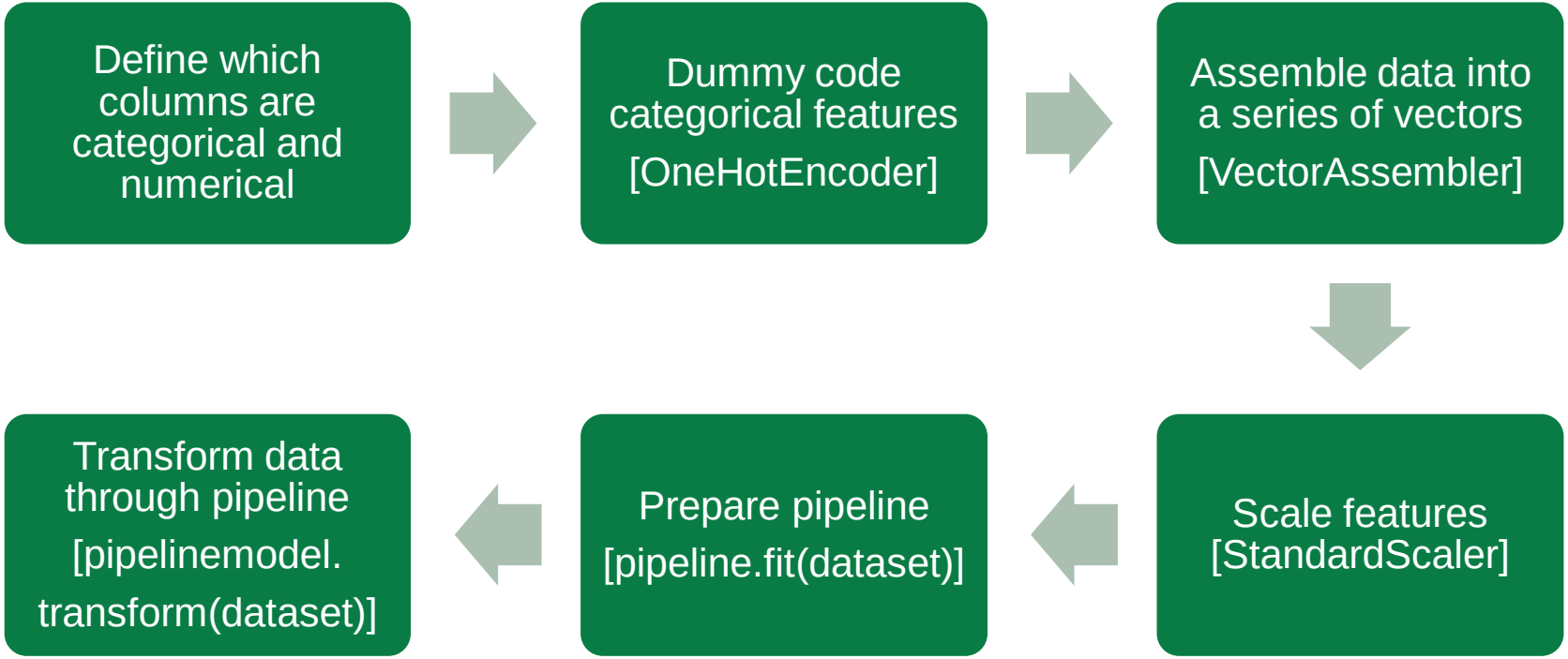
- Lazily evaluated.
- Spark operation that returns a DataFrame (usually).
- Multiple transformations add to the steps of a Spark job, but no data gets processed.
- Examples: select, filter, groupBy, map

Actions

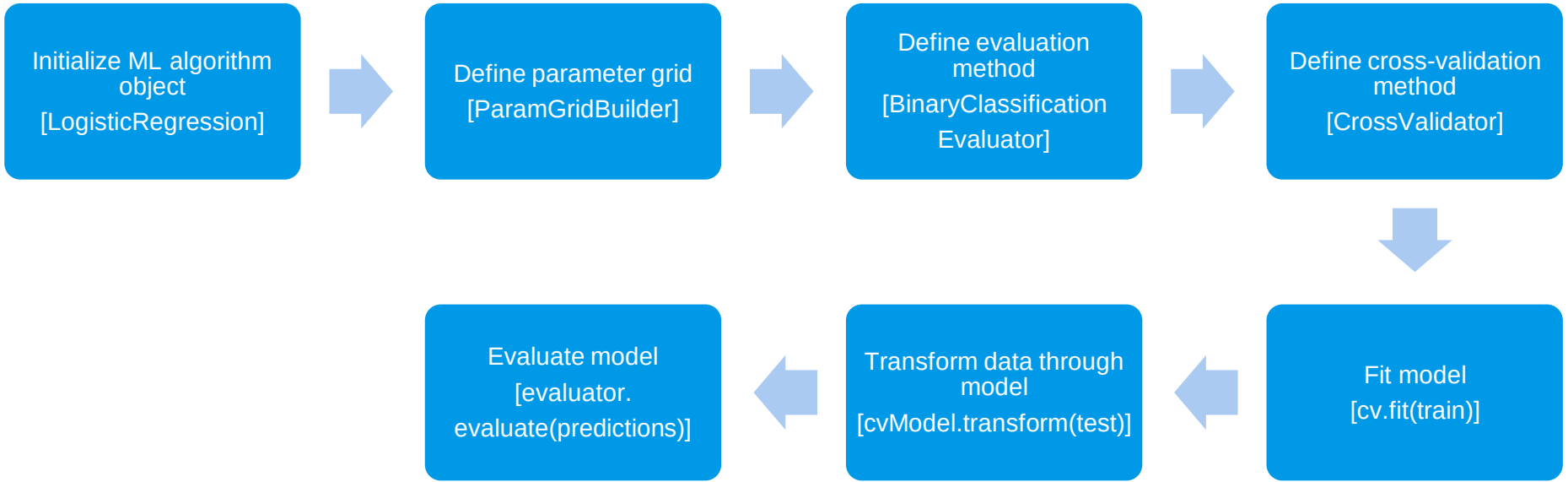
- Not lazily evaluated.
- Returns counts of elements or lists of them (usually)
- Enacts a series of transformations
- Examples: show/display, count, collect, take, write

Spark Pipelines

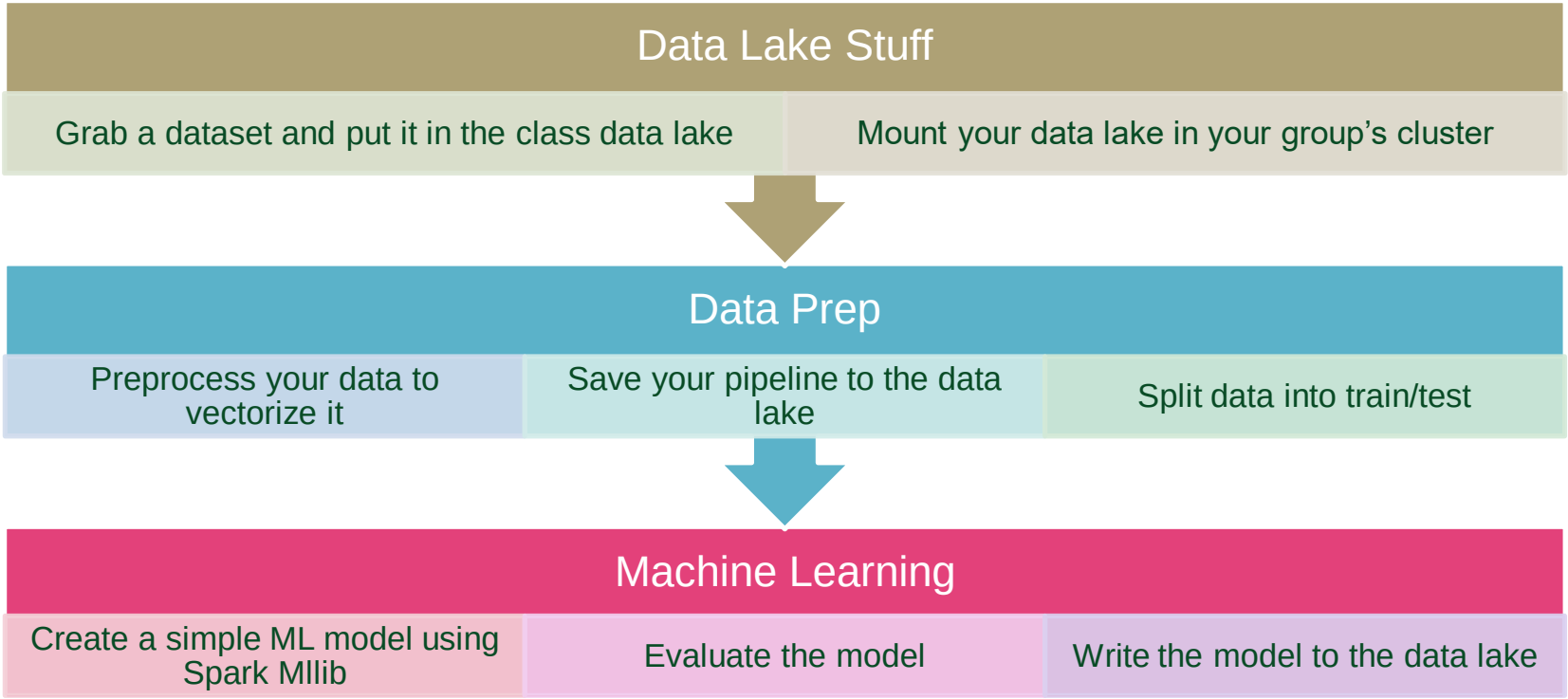
- Can be saved similar to ML models
- Provides stability into the model scoring process



MLlib Models



Lab Steps - Databricks



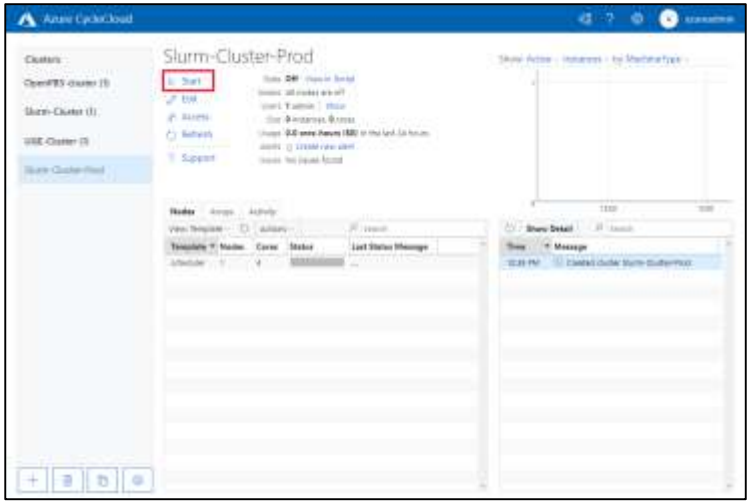
Other HPC Services

Azure Batch

- Dynamically scale to 1,000s of VMs
- Operates in pools with VM sizes, container images, # nodes, etc.
- Operates on “job tasks”

Azure CycleCloud

- Closest to an on-prem HPC cluster
- Operates “templates” that define VM types, # nodes
- Uses various schedulers like SLURM, PBS, etc.




```
az batch pool create \
    --id myPool \
    --image canonical:0001-com-ubuntu-server-focal:20_04-lts \
    --node-agent-sku-id "batch.node.ubuntu 20.04" \
    --target-dedicated-nodes 2 \
    --vm-size Standard_A1_v2
```

```
az batch job create \
    --id myJob \
    --pool-id myPool
```

H- and N-Series VMs

- Fancy/Many Processors
  - Xeon Platium 8000 Series CPUs
    - Largest: 832 vCPUs
- High memory bandwidth
  - 350GB/sec + InfiniBand
- Large memory capacity
  - 10TB+ of Memory
- Multiple Fancy GPUs
  - 8 x H100 94GB GPUs
- High Network I/O
  - 40,000 Mbps

https://learn.microsoft.com/en-us/azure/high-performance-computing/

Azure Limits:

- Azure Kubernetes Service:
  - 5,000 nodes
  - 100 clusters/region
  - 1,000 nodes/pool
  - 100 pools/cluster
- Azure Batch:
  - 2,000 nodes
  - 1,000 active jobs
  - 900-ish cores
  - 500 pools/account
- Azure CycleCloud:
  - Max MPI Job: 36,000 Cores
- Overall:
  - 25,000 VMs/region
  - 75,000-ish cores/region

On-Premise Examples:

- UNCC HPC: https://oneit.charlotte.edu/urc/research-clusters/
- MIT Super Cloud: https://mit-supercloud.github.io/supercloud-docs/systems-and-software/

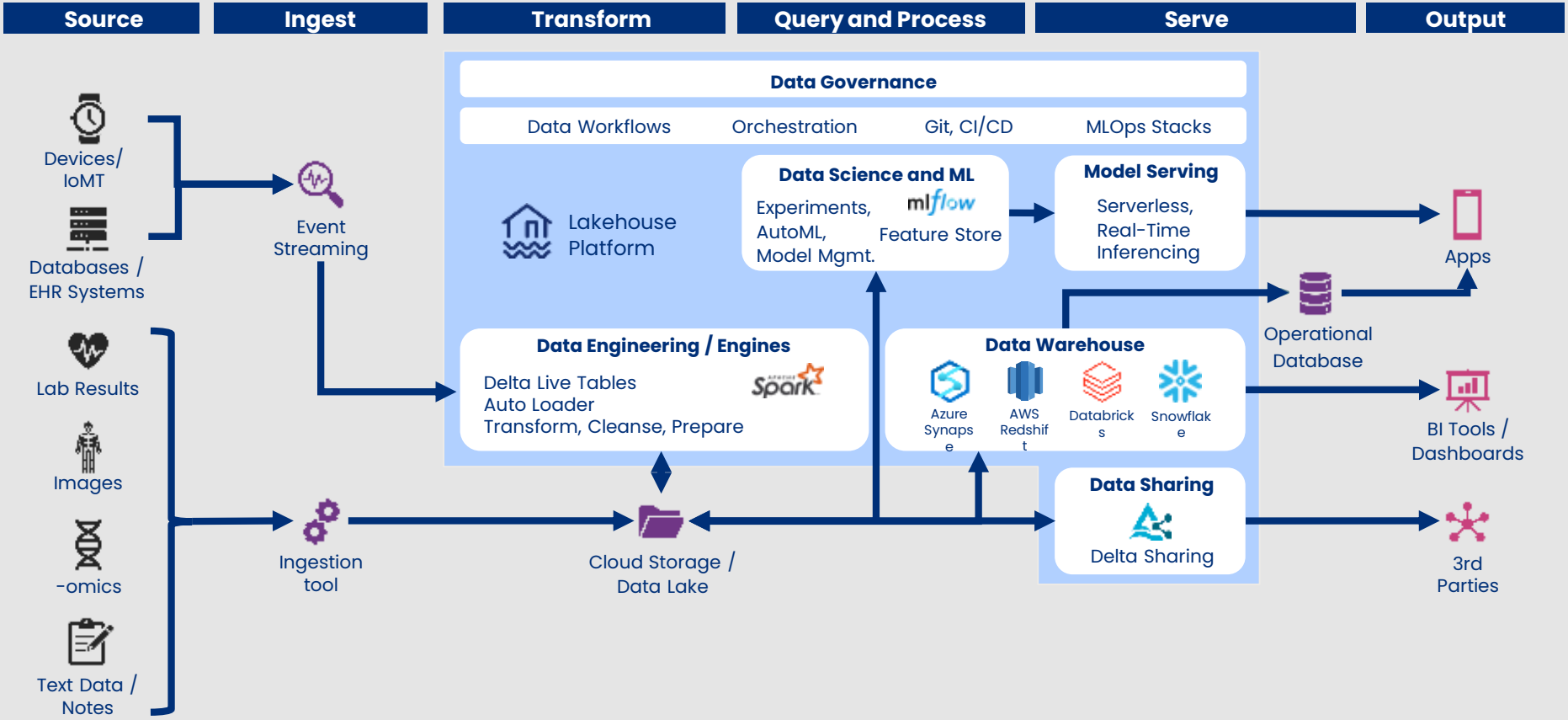
HPC Use Cases

3D Video Rendering	CAD/ Engineering	Genomics
Molecular Modeling	Physics Simulations	Financial Simulations
Geospatial/ Weather Modeling	Large In-Memory Databases	Distributed AI Training

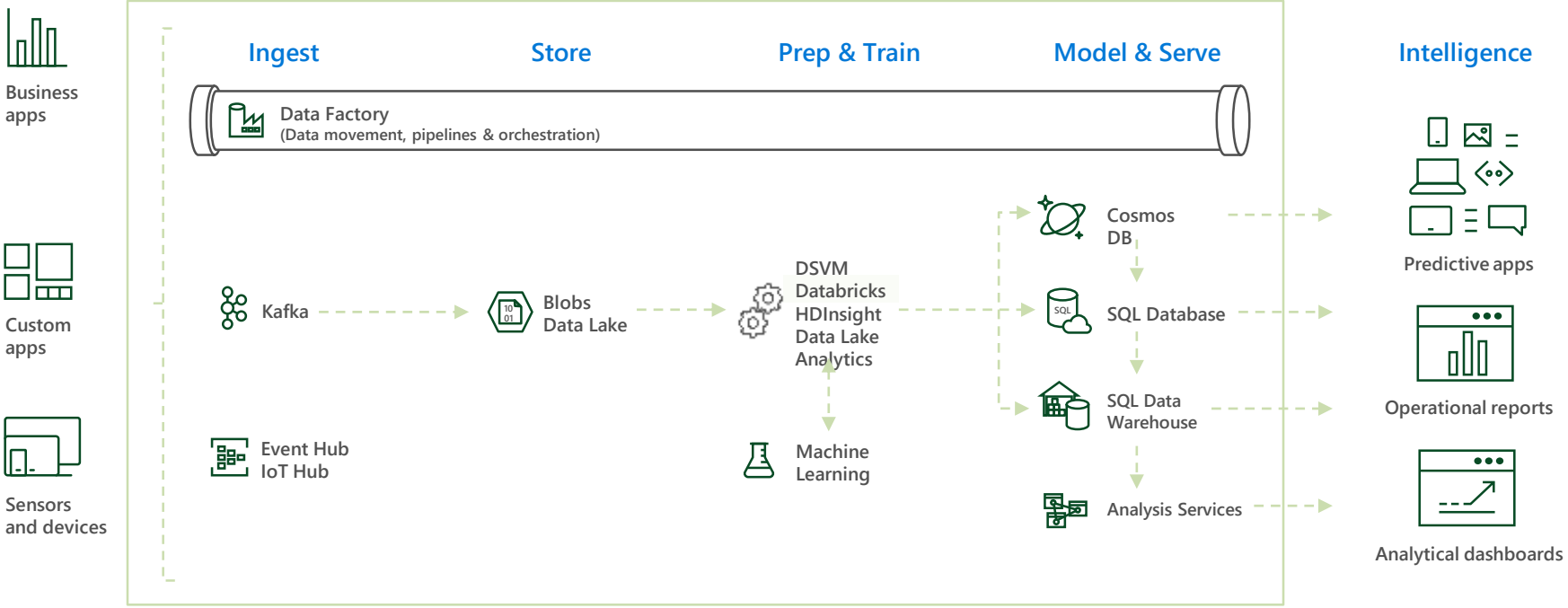
Sample Architectures

https://learn.microsoft.com/en-us/azure/architecture/browse/

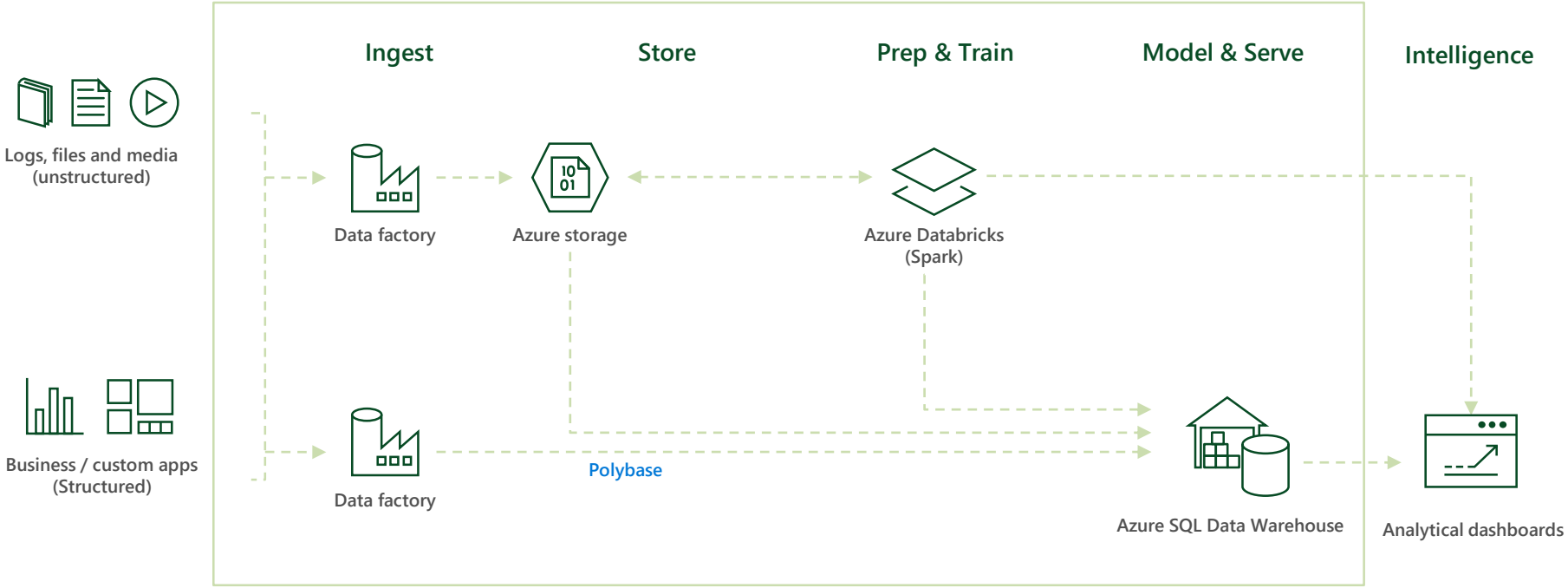
30k Foot View - Architecture



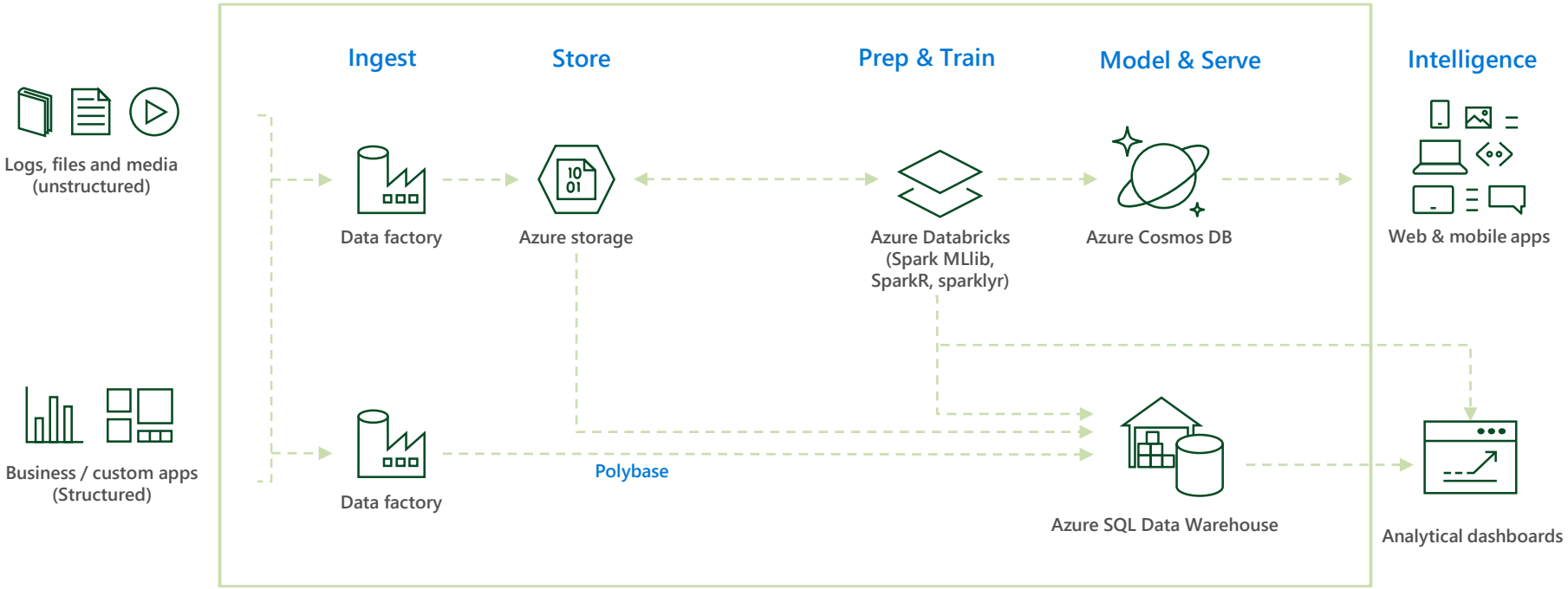
BIG DATA & ADVANCED ANALYTICS AT A GLANCE



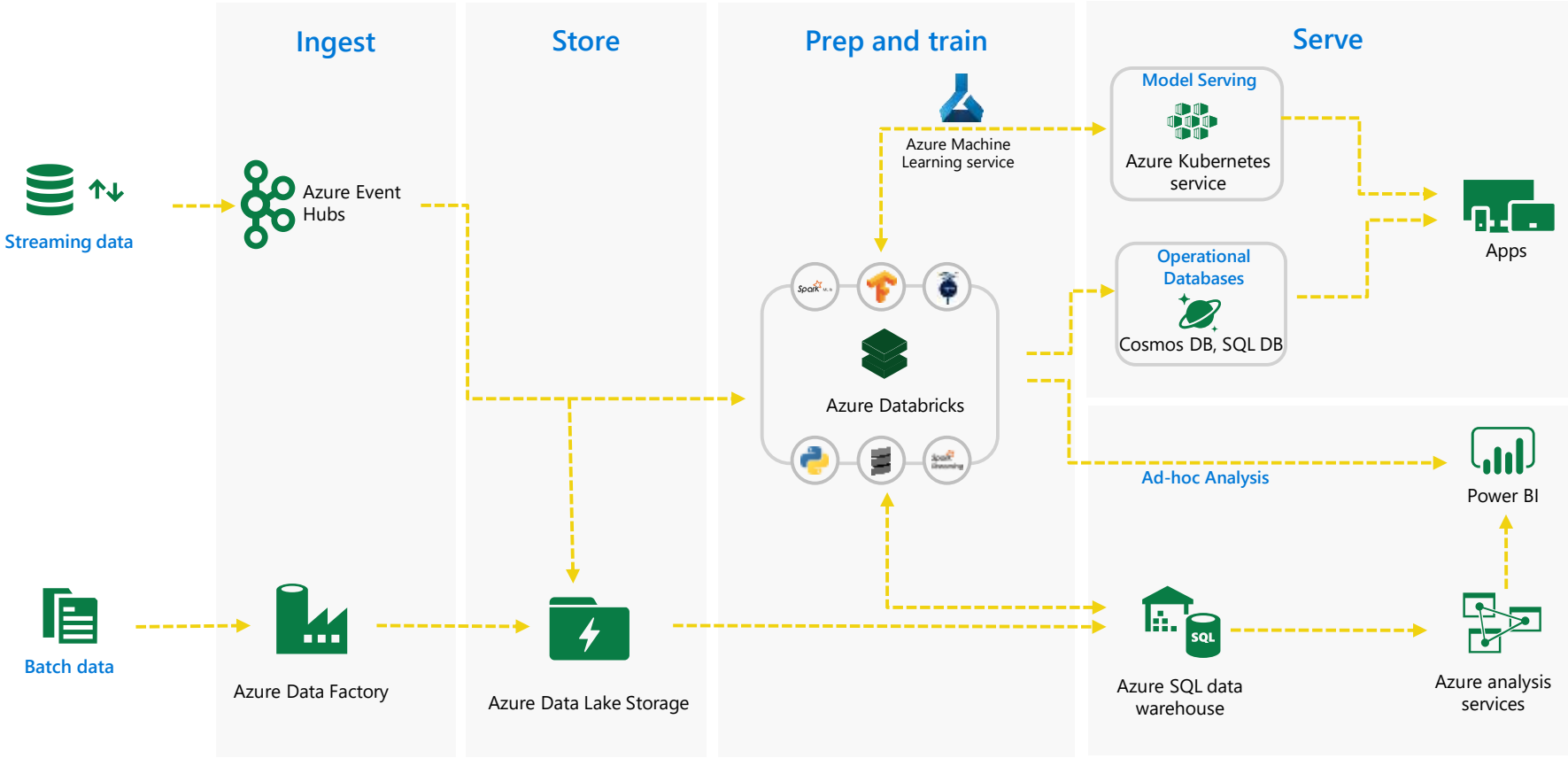
Modern Big Data Warehouse



Advanced Analytics on Big Data



Modern Data Platform with Azure Databricks



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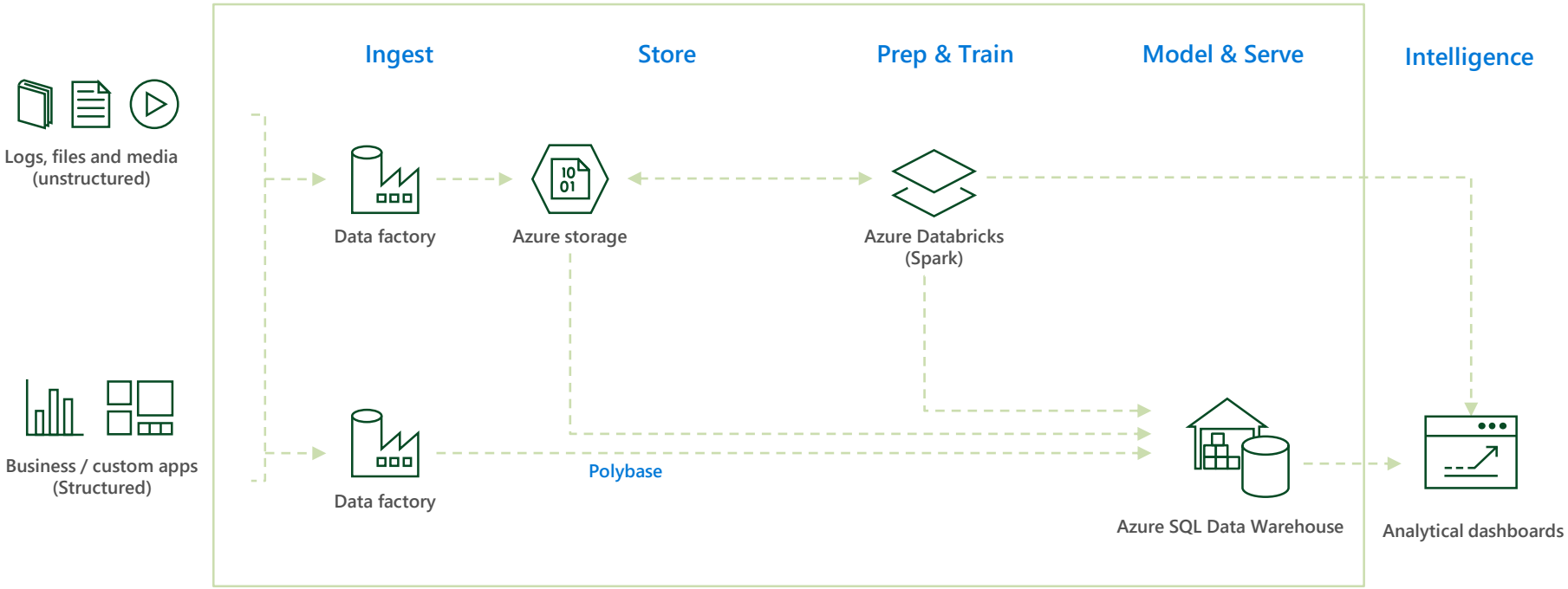
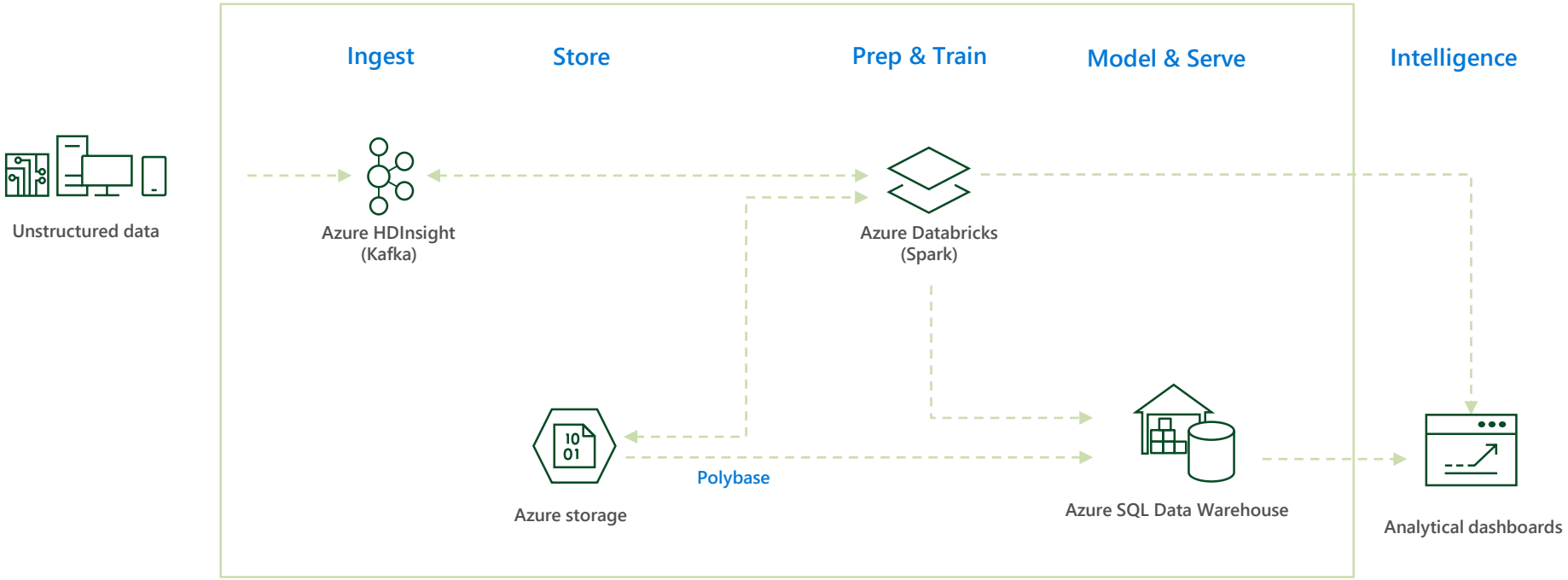
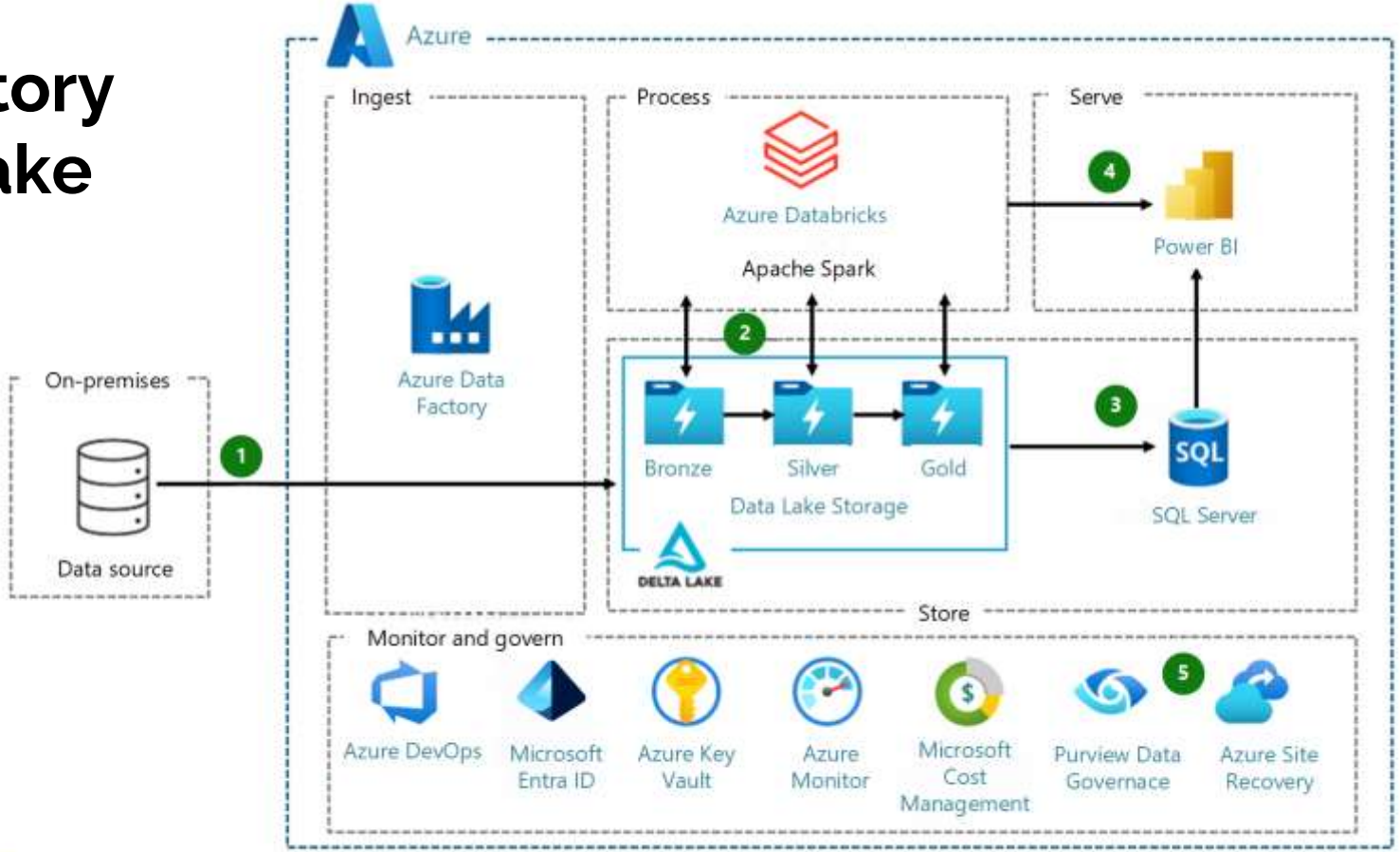


Real-time analytics on Big Data



Data Factory + Data Lake



Microsoft Azure

Computer-Aided Engineering