Distributed Infrastructures beyond the Grid paradigm

How to choose where to run

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Identify your problem’s features

High throughput

- Efficient execution
- Long execution times
- Large amount of tasks
- Tasks are loosely coupled (sequential)

Example:

- a relatively simple code to analyse a huge amount of experimental data
- each task processes a chunk of the data sample independently

High Performance

- Large amount of computing power
- Short execution times
- Tasks are tightly coupled (parallel)
- Low latency interconnect

Example:

- simulate the atomic motion of a protein in water
- each atom interacts with the others in the system
- communicate data back and forth each sub-task

Image from Gartner (March 2016)

Choose the infrastructure type

Multicore server

Shared memory:

- Single address space
- All processes have access to the pool of shared memory

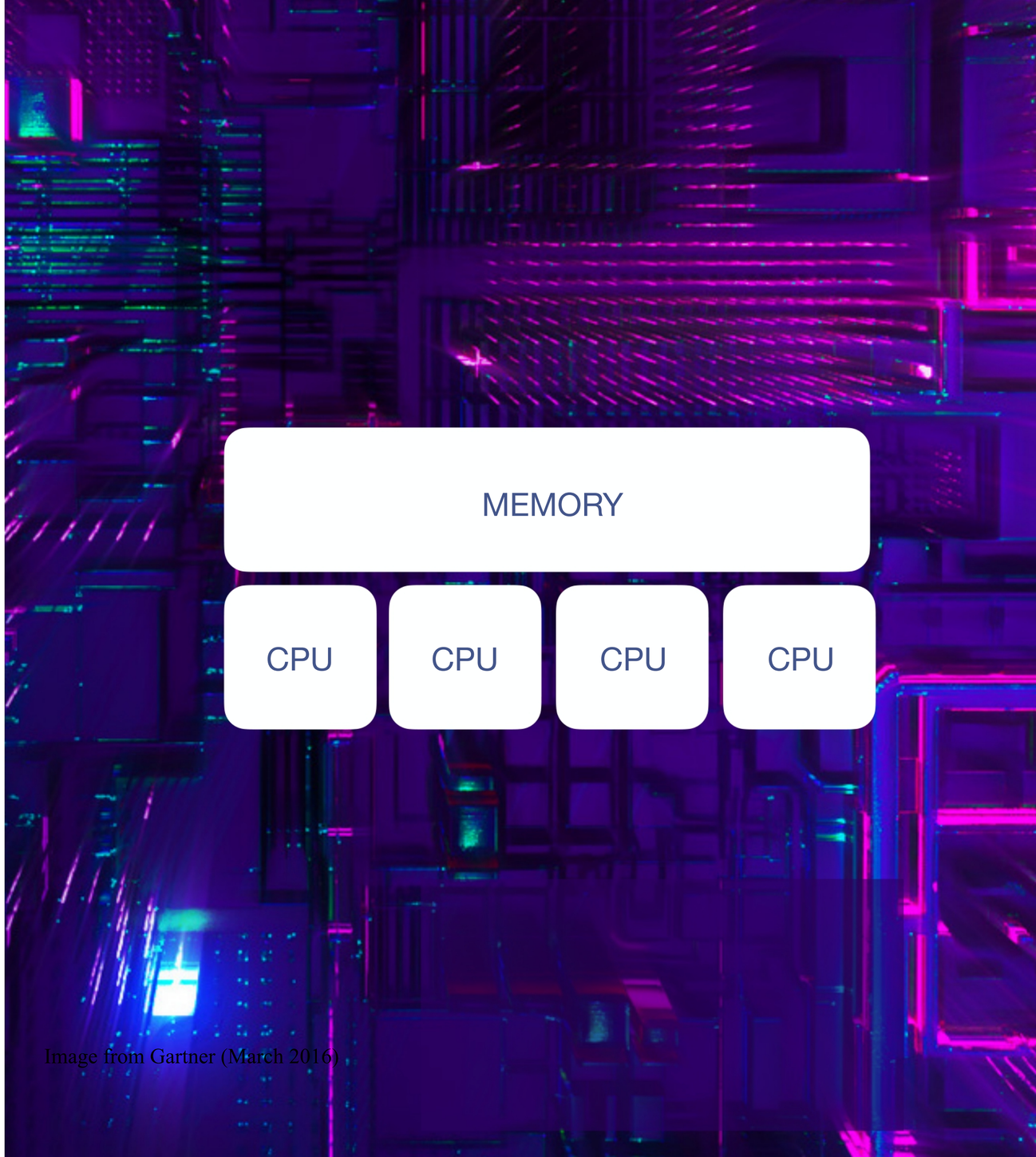


Image from Gartner (March 2016)

Cluster

Distributed memory:

- Each node has its own local memory
- Message passing (mainly) is used to exchange data between processors

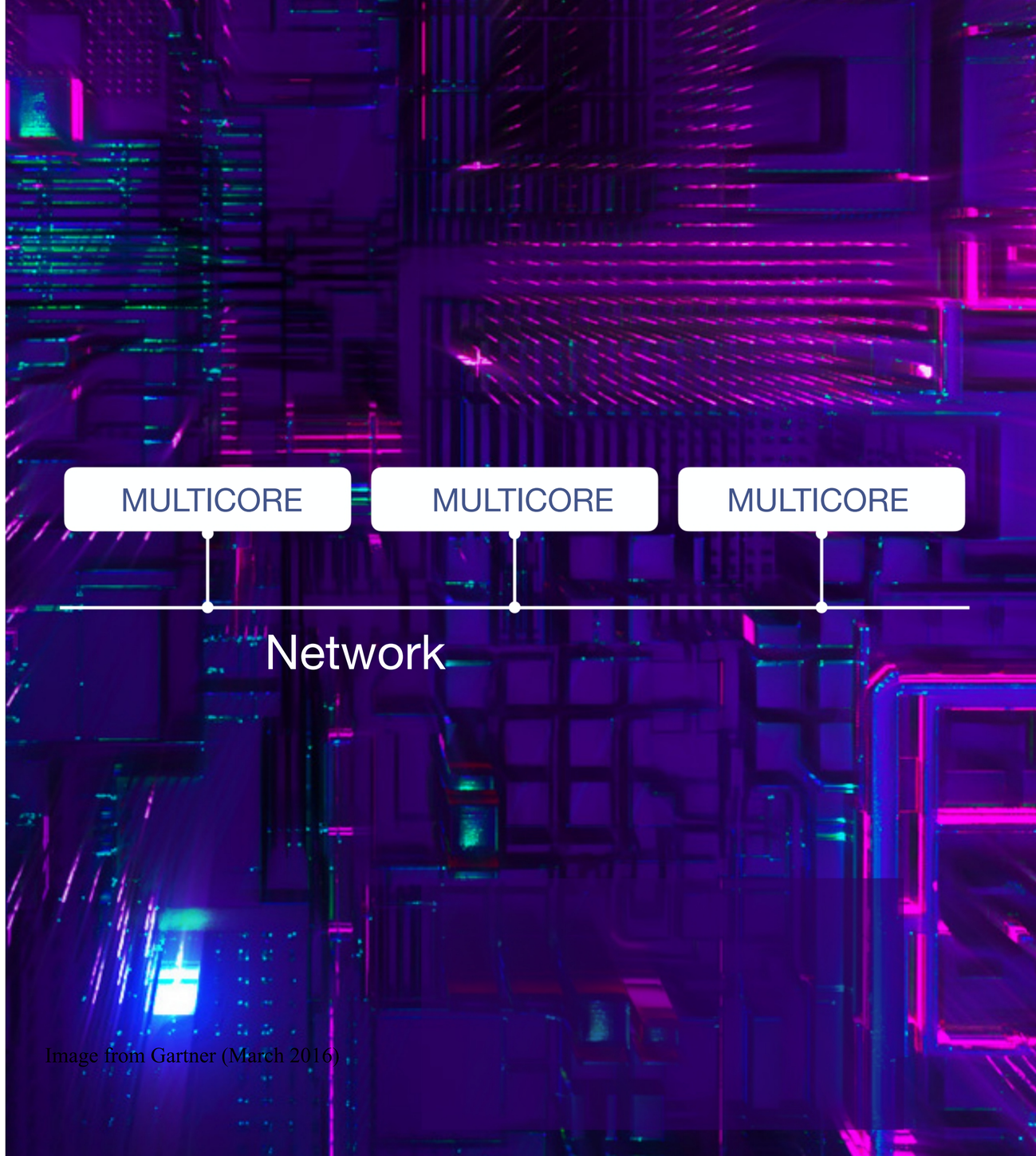


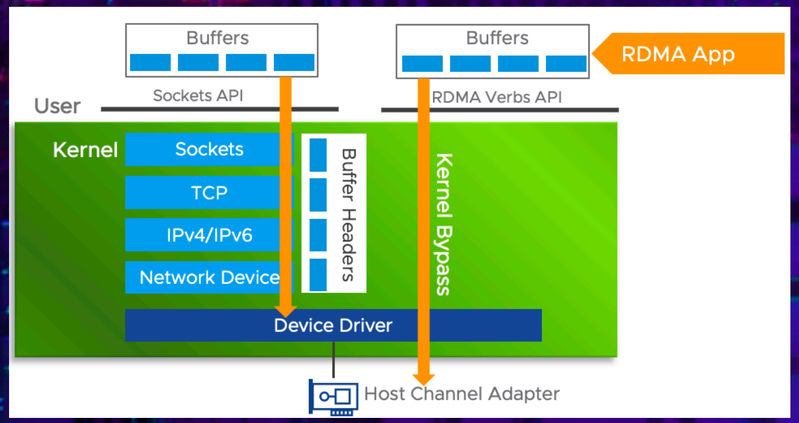
Image from Gartner (March 2016)

HPC Cluster

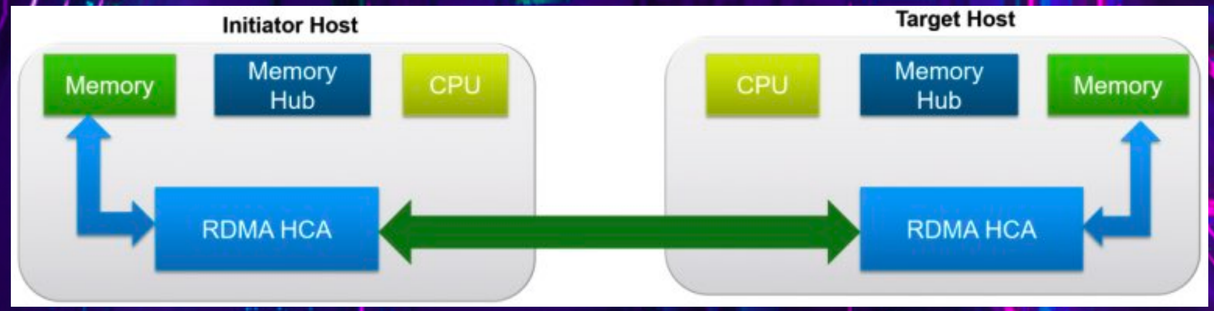
- Performant CPUs (i.e. high clock rate)
- Low latency interconnect:
  - i.e. Mellanox's *InfiniBand* or Intel's *OmniPath*
  - offer an RDMA implementation

Remote Direct Memory Access (RDMA)

- Transfer of memory between different computers
- Direct transfer minimising CPU/Kernel involvement
- Bypassing the Kernel allows high I/O bandwidth and low latency



- Host Channel Adapter (HCA) needed on both source and destination



What about the Cloud?

Cloud computing: a style of computing in which **scalable** and **elastic** IT-enabled capabilities are delivered **as a service** using Internet technologies.

Application

Defined by:

- runtime environment
- resource requirements
- execution model

Virtualisation

- Virtual Machines
- Linux containers

On demand

- Autoscaling

Execution model

VIRTUAL WORKSTATION:

code execution in a single multicore node, possibly with GPU acceleration

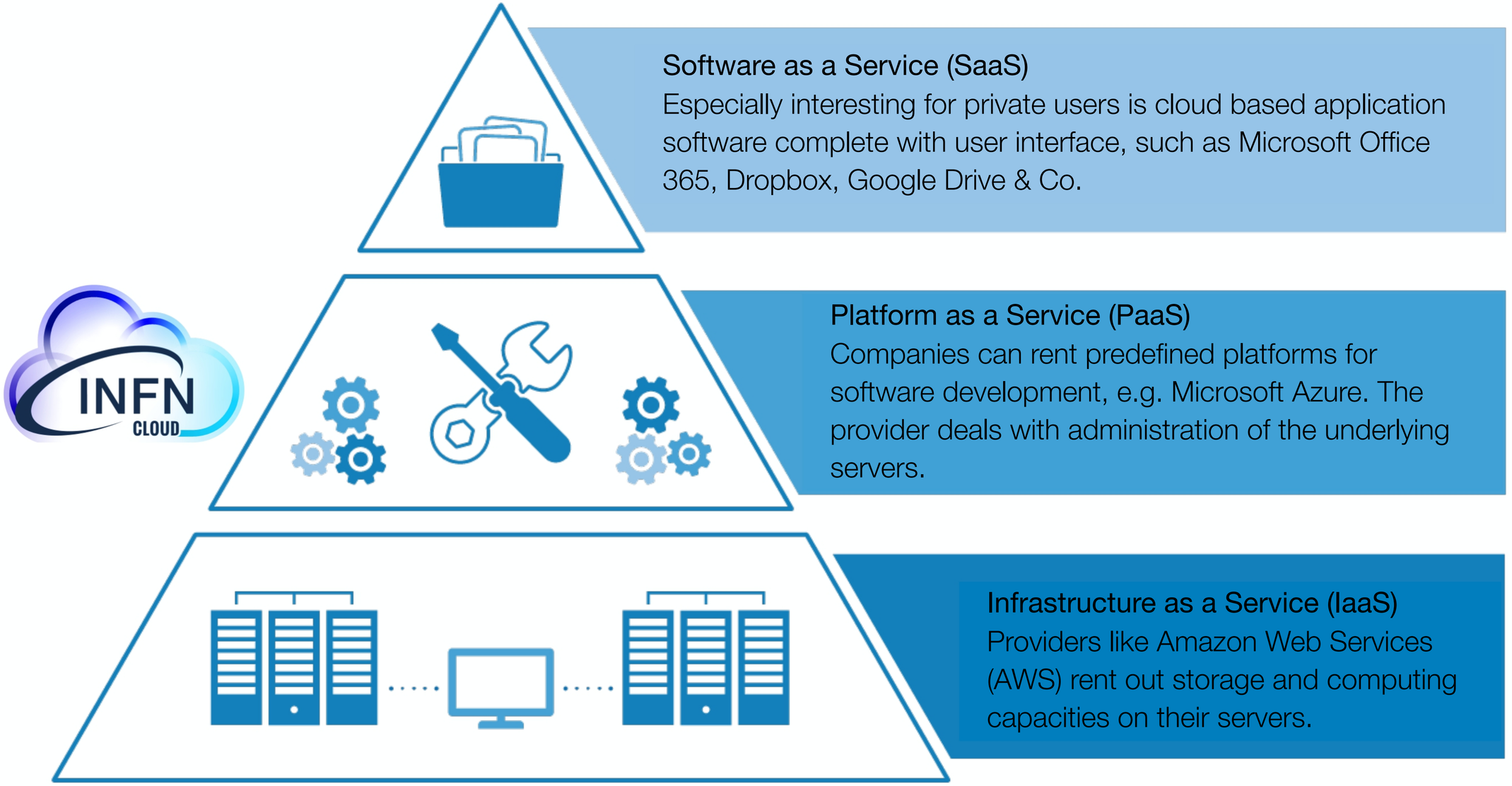
BATCH

multi-node workloads, eventually using MPI and inter-node communication

PIPELINES

multi-step data analysis, possibly requiring high-memory and many cores

The Cloud Pyramid



Software as a Service (SaaS)
Especially interesting for private users is cloud based application software complete with user interface, such as Microsoft Office 365, Dropbox, Google Drive & Co.

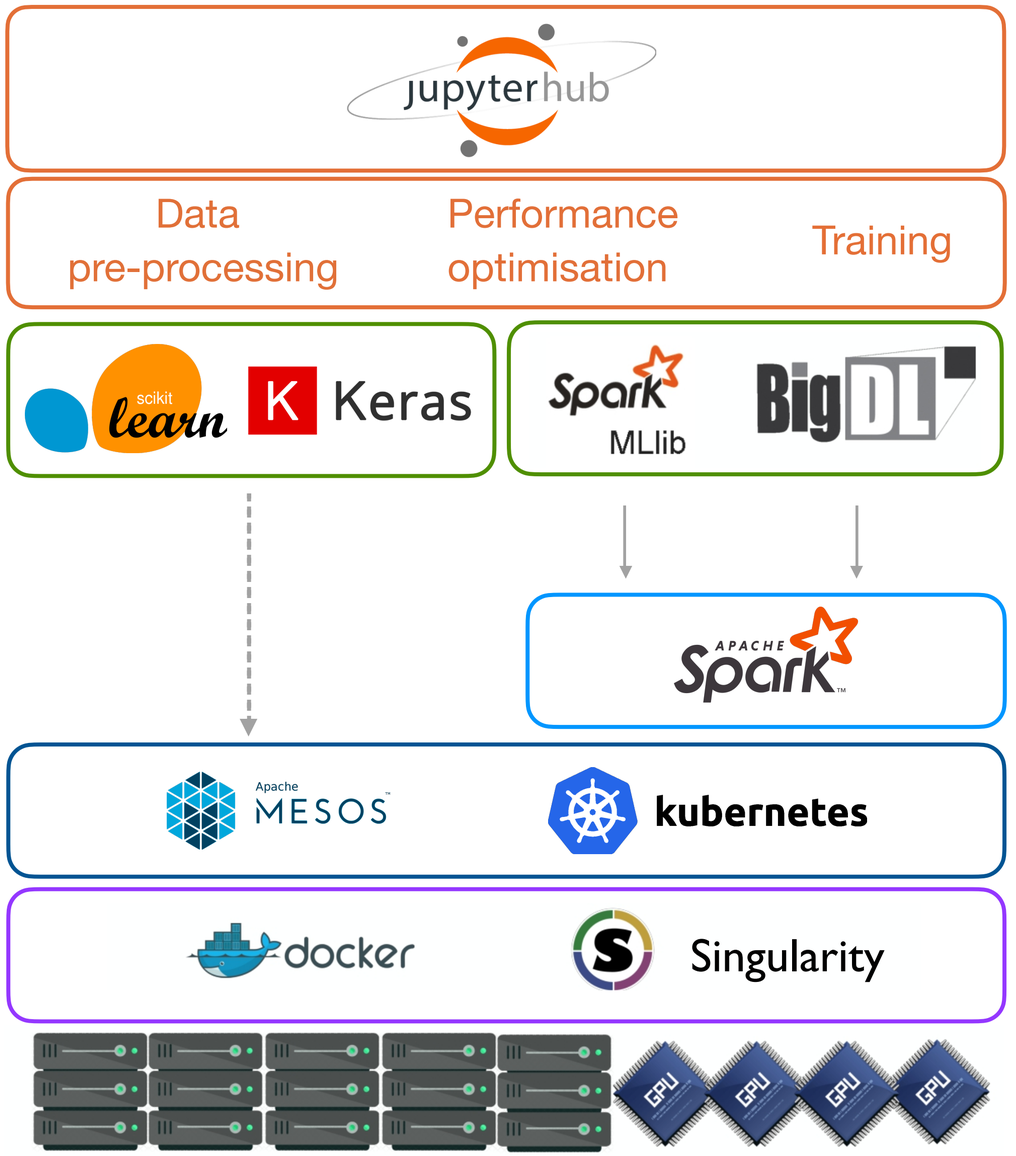
Platform as a Service (PaaS)
Companies can rent predefined platforms for software development, e.g. Microsoft Azure. The provider deals with administration of the underlying servers.

Infrastructure as a Service (IaaS)
Providers like Amazon Web Services (AWS) rent out storage and computing capacities on their servers.

Enabling Machine Learning workflows

ML as a Service

Layers



Frontend:

- Workflow definition
- Process Monitoring
- Authentication

ML libraries

Distributed ML libraries

Cluster framework

(parallelise task)

Orchestrator

(schedule on resources)

Packetisation and virtualisation

Resources:

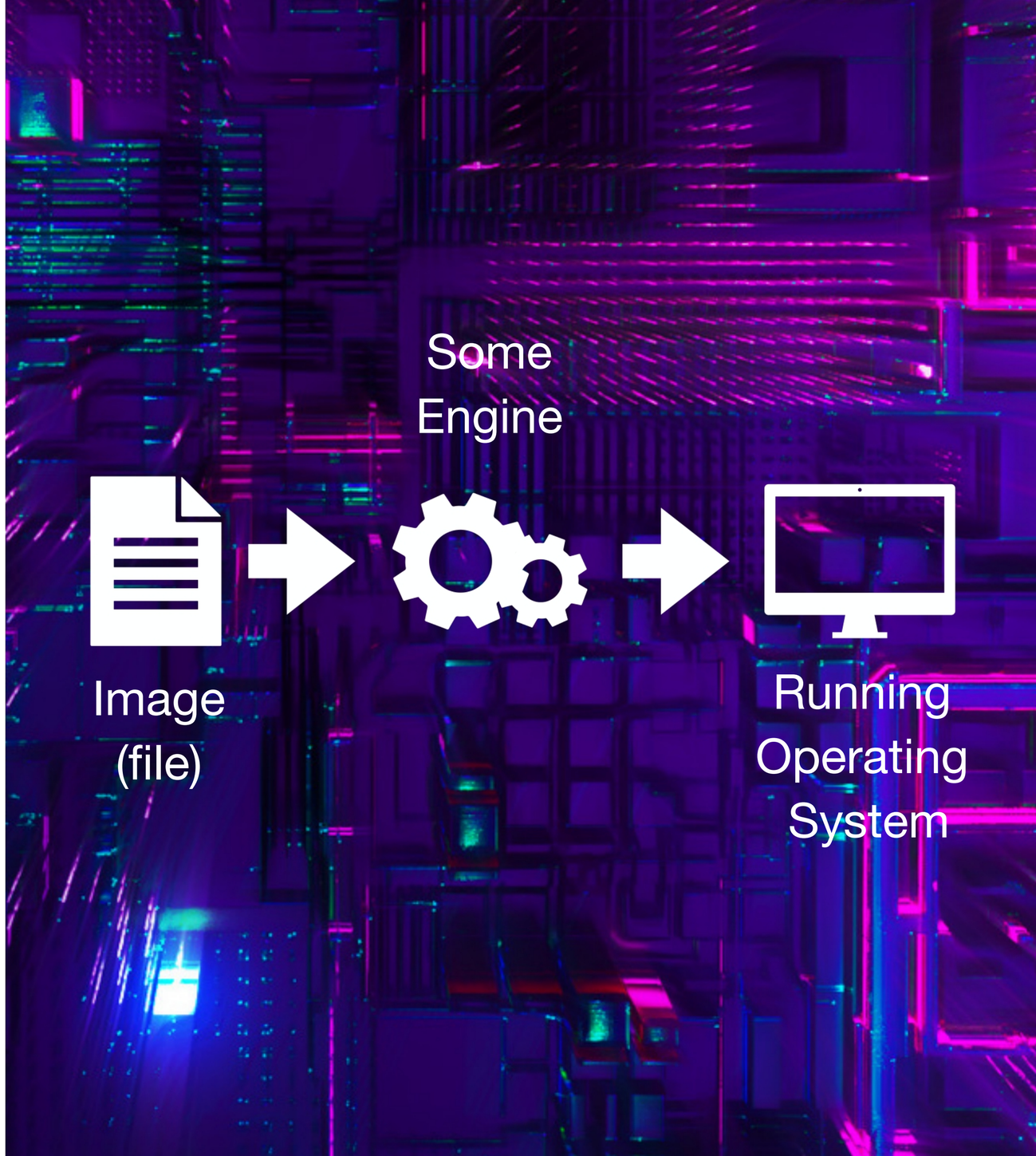
- Bare metal
- IaaS

DATA

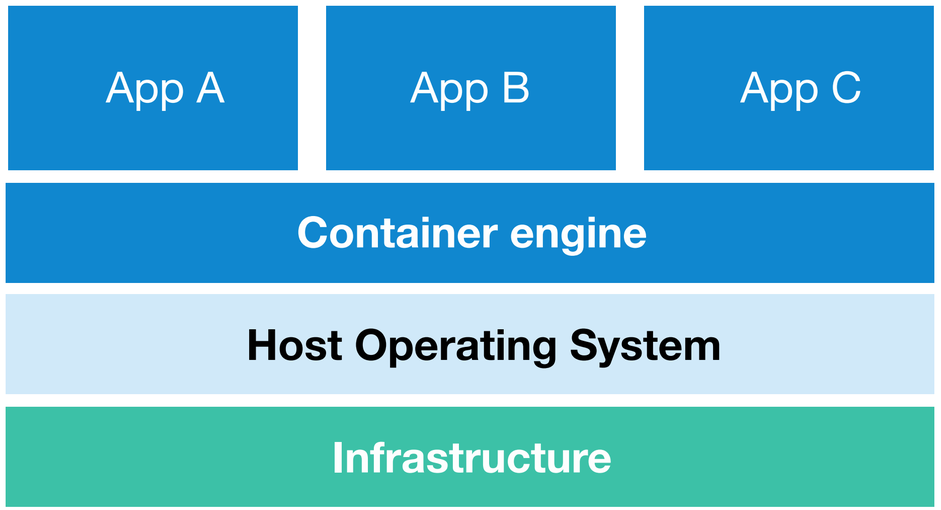
Virtualisation

- Operational definition: a way to provide an isolated environment in which to run an application. The environment is represented as a binary artifact that can be moved between hosts.

- The foundation of **Continuous Delivery**: code changes are automatically built, tested, and packaged for release into production.

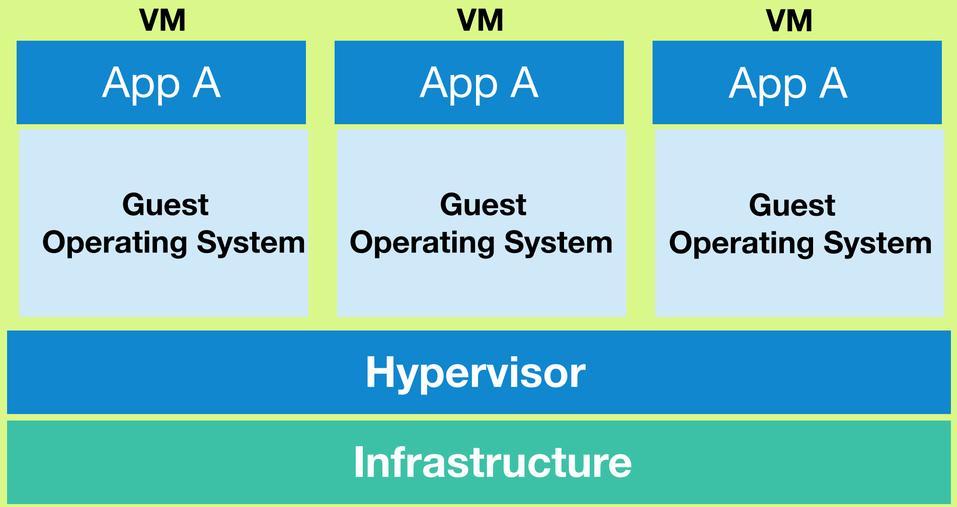


Linux Containers



- Lightweight encapsulation: portable and efficient
- Virtualise the operating system (not hardware)
- Minimal image containing just what is needed

Virtual Machines



- Hardware virtualisation:
  - More isolation
  - But overhead
- Image containing the full operating system

Linux Containers: what about “the engine”?

Docker

- Microservices
- Fancy network set-ups
- Host devices access
- Host storage access
- Requires root privileges (almost)
- Nice ecosystem

Me setting up the Yoga cluster

Microservices

Singularity

- Runs in user-space
- No access to host devices
- No networking

You running on a HPC facility

User Application

Orchestration

Container orchestration refers to the process of organising the work of individual (loosely coupled) containerized components and application layers, that need to work together to allow a given app to function as designed.

Image from Gartner (March 2016)

kubernetes

- Builds upon 15 years of experience of running production workloads at Google
- Integrates ideas and practices from the community
- A widely used tool for Continuous Deployment: every validated change in the application is automatically released to users.

Some nice features

- Service discovery and load balancing
- Storage orchestration
- Automatically places containers based on their resource requirements and other constraints (bin packing)
- Self-healing
- Automated rollouts and rollbacks
- Horizontal scaling

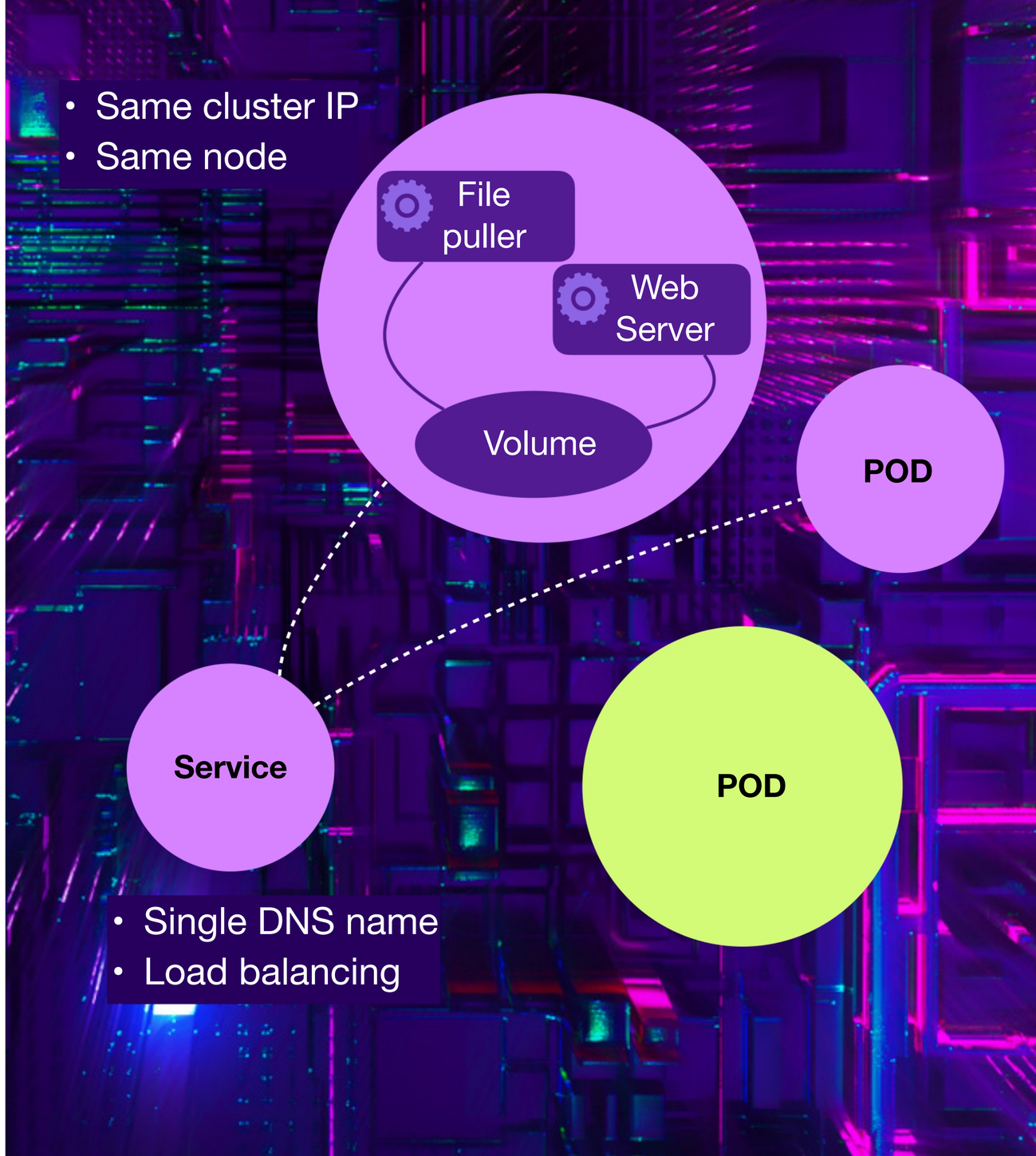
Kubernetes concepts

OBJECTS are abstractions that represent your system's state.

Basic objects include:

- Pod
- Service
- Volume
- Namespace

Plus higher-level abstractions that rely on **Controllers** to build upon the basic objects (i.e. Deployments).



The declarative model

IMPERATIVE: define the exact steps to be executed to achieve the desired final state.

DECLARATIVE: describe your desired final state. Let the system decide how to achieve the goal.

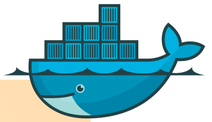
- write local configuration files (yaml)
- use the Kubernetes CLI to apply it
- create, update, and delete operations are automatically detected per-object

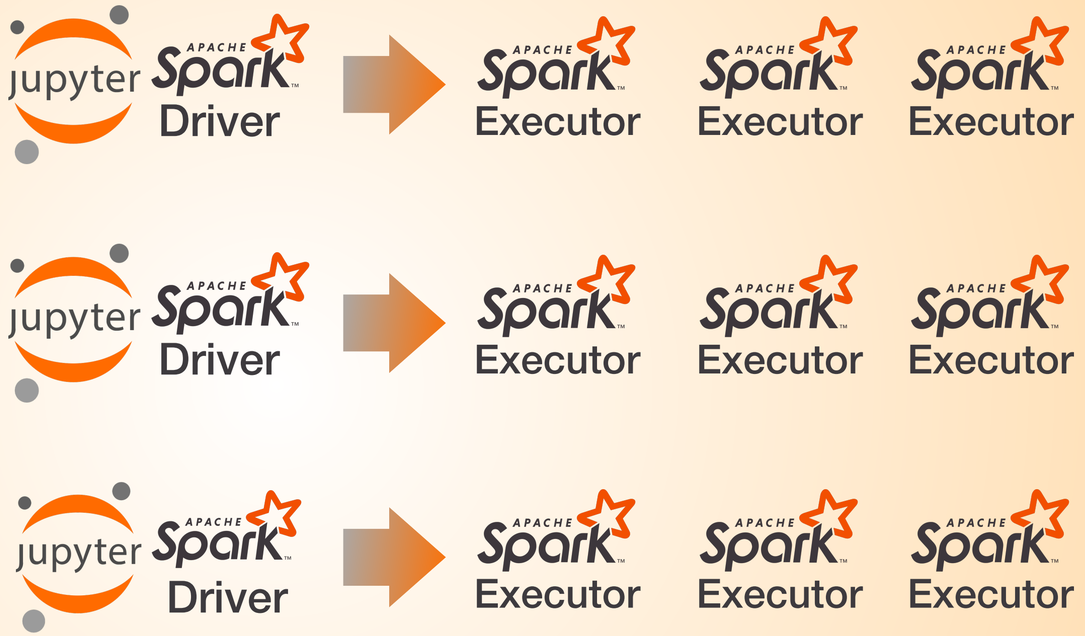
my_service_configuration.yaml

```
apiVersion: v1
kind: Service
metadata:
  name: my-service
spec:
  selector:
    app: MyApp
  ports:
    - protocol: TCP
      port: 80
      targetPort: 9376
```

POD

The Yoga cluster





HDFS (for datasets)

API access

K8s control-plane

K8s workers

Gluster (for home directories)

POSIX access

To take home

- Understand your problem's features: is it embarrassingly parallel or not?
- Choose the right type of infrastructure to execute your task:
- Multi-core
- HTC cluster
- Grid
- HPC cluster
- Any of those over a Cloud (maybe not HPC)





Wrap-up

No BigData/MachineLearning expert is such if she cannot compute a **real-size problem** (scale-out/scale-up)

We introduced several concepts and tools which are at the basis of **modern computing strategies**, now you know how to place them in the right context.

We hope this will help you in your daily work.