DEEPHEALTH

UNIVERSITÀ DEGLI STUDI DI TORINO

The OpenDeepHealth toolkit

Iacopo Colonnelli (iacopo.colonnelli@unito.it)

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Wednesday, January 26th

The project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 825111.

OpenDeepHealth Platform

UNIVERSITÀ DEGLI STUDI DI TORINO

DEEPHEALTH

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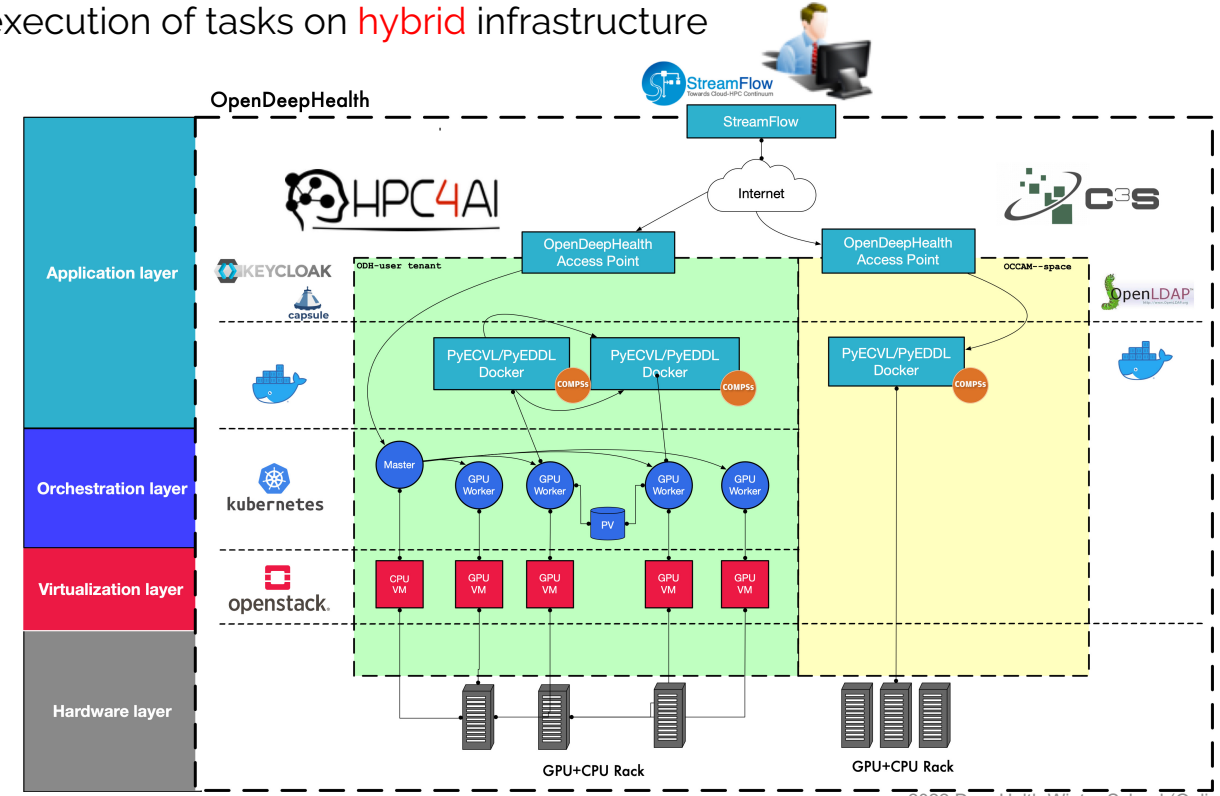
Multi-tenant private Kubernetes for AI training

Literate workflows to write complex distributed pipelines as Jupyter Notebooks



Super Computer cluster providing an elastic virtual farm of containers on bare metal

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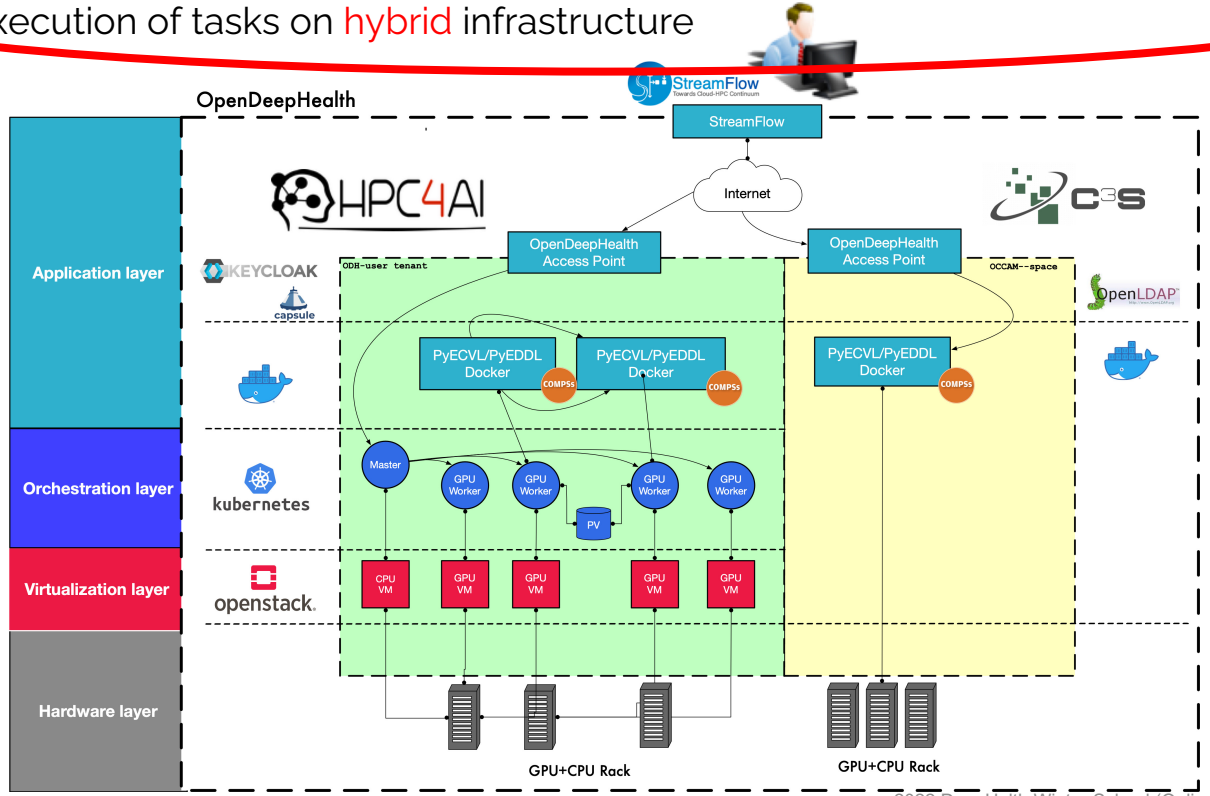

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Designed around two main principles:

- Allowing the execution of tasks in **multi-container environments**, in order to support concurrent execution of multiple communicating tasks in a multi-agent ecosystem

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The StreamFlow WMS

Designed around two main principles:

- Allowing the execution of tasks in **multi-container environments**, in order to support concurrent execution of multiple communicating tasks in a multi-agent ecosystem
- Relaxing the requirement of a single shared data space, in order to allow for **hybrid workflow** executions on top of multi-cloud or hybrid cloud/HPC infrastructures.

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Hybrid workflows

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- Direct communications and data transfers among different locations **may not be allowed**.

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- Knowing the locations topology can lead to better scheduling algorithms, privileging **data locality** and minimising the **data transfer overhead**;
- Delegating data transfers and computation offloading to the Workflow Management System (WMS) brings **additional features OOTB** (e.g. security, fault-tolerance, cross-stack, urgency-based scheduling).

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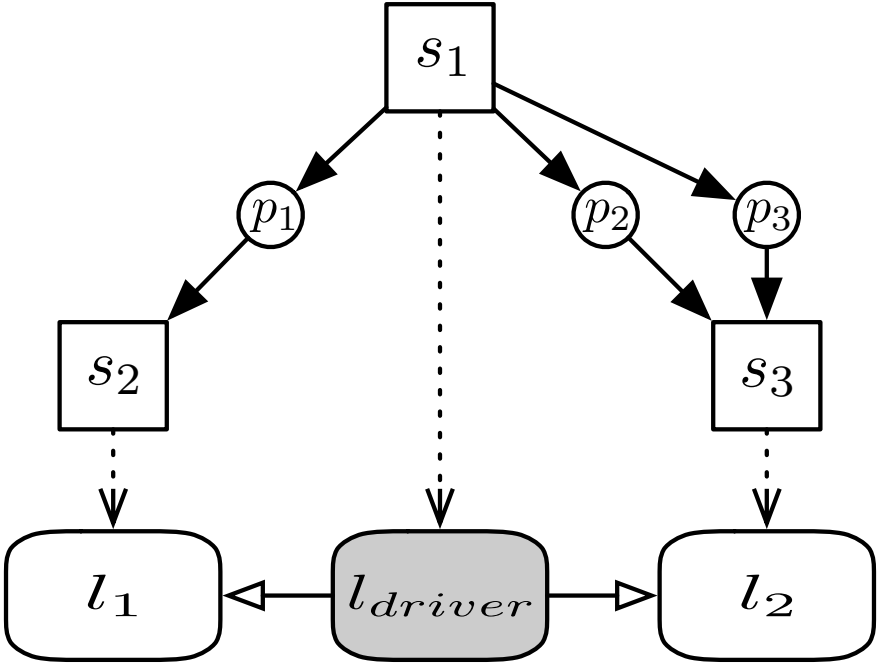
Hybrid workflows



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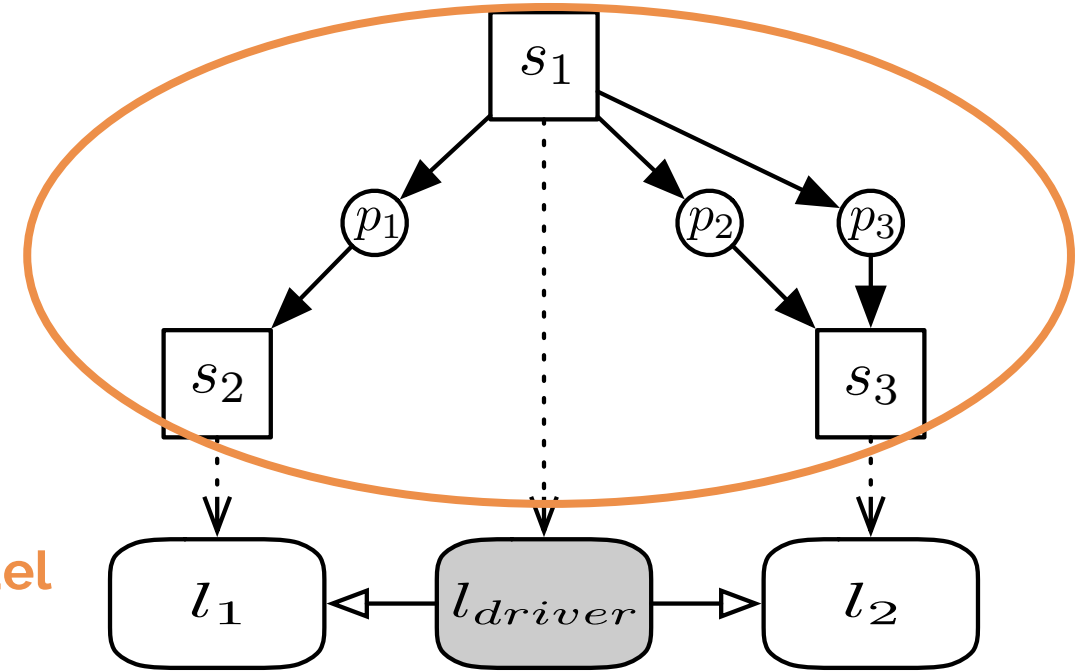

Workflow model

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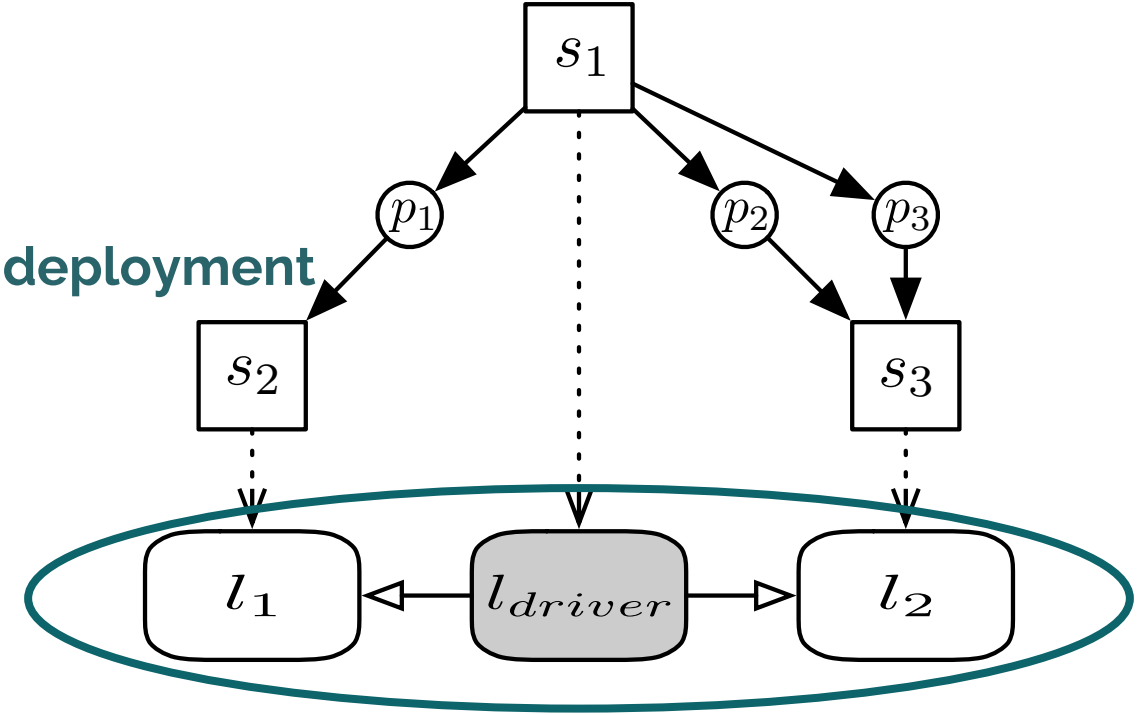
Hybrid workflows

Topology of deployment locations



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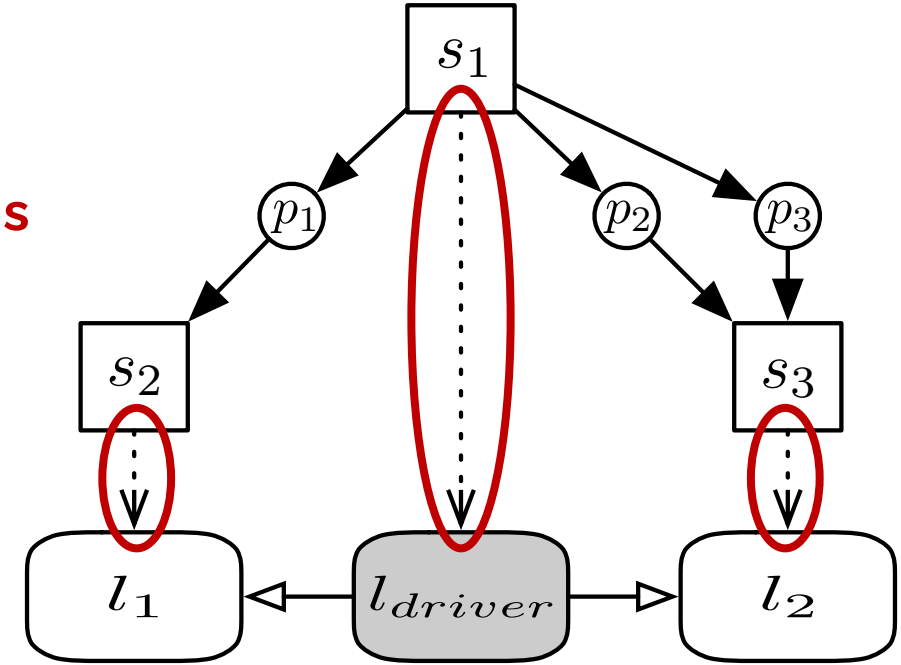
Hybrid workflows

Mapping relations



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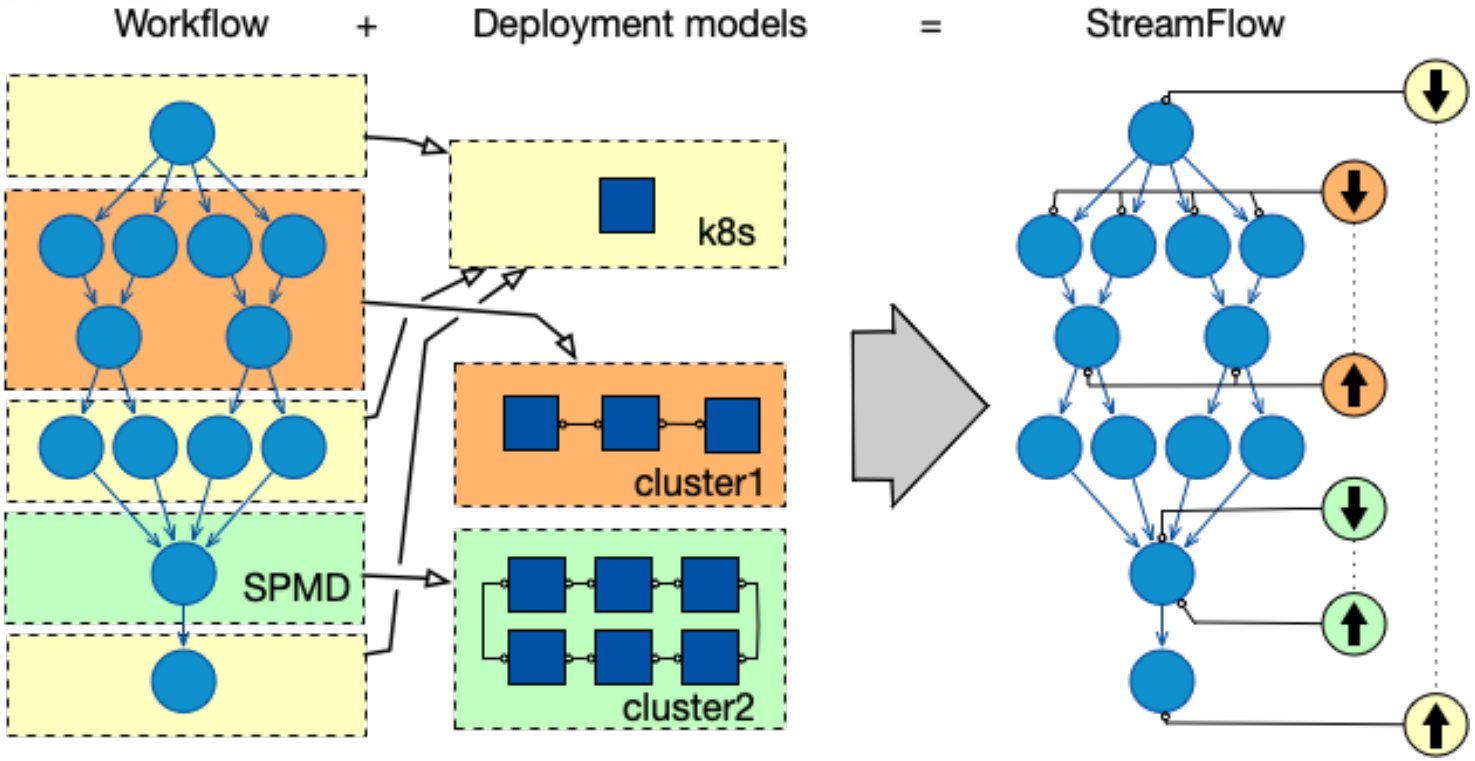

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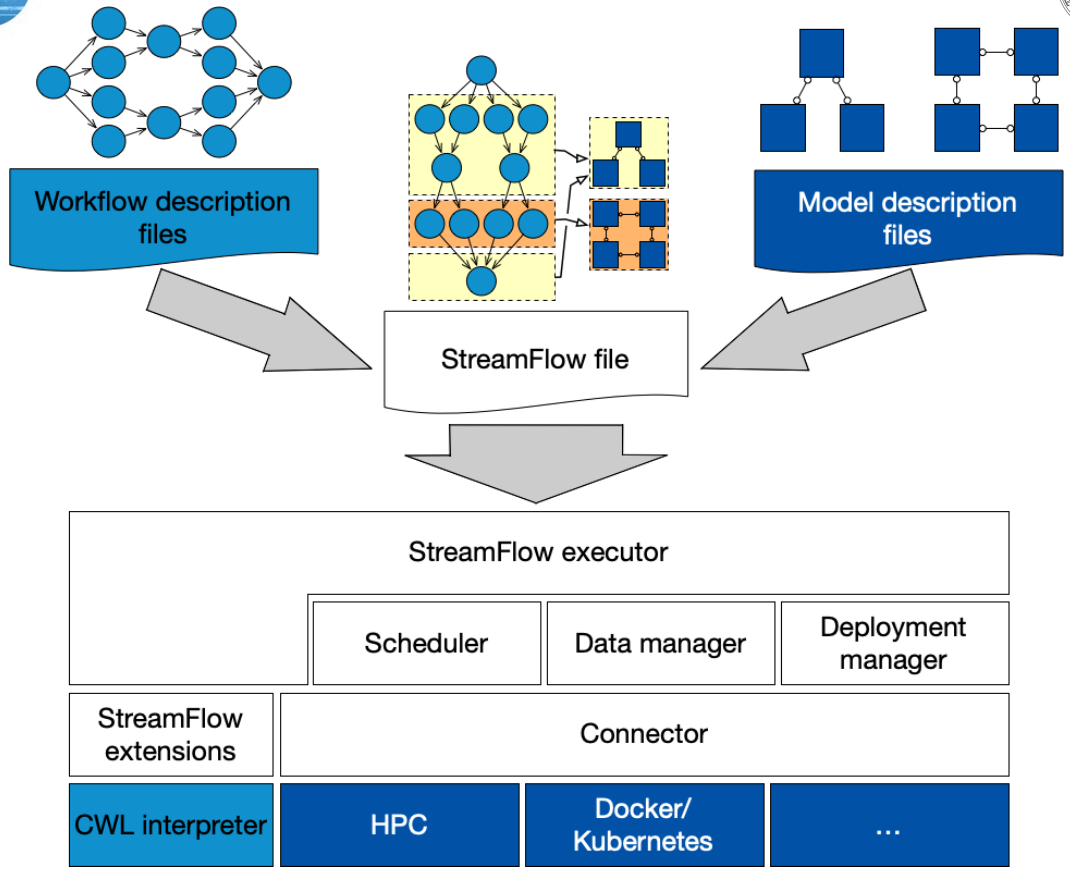

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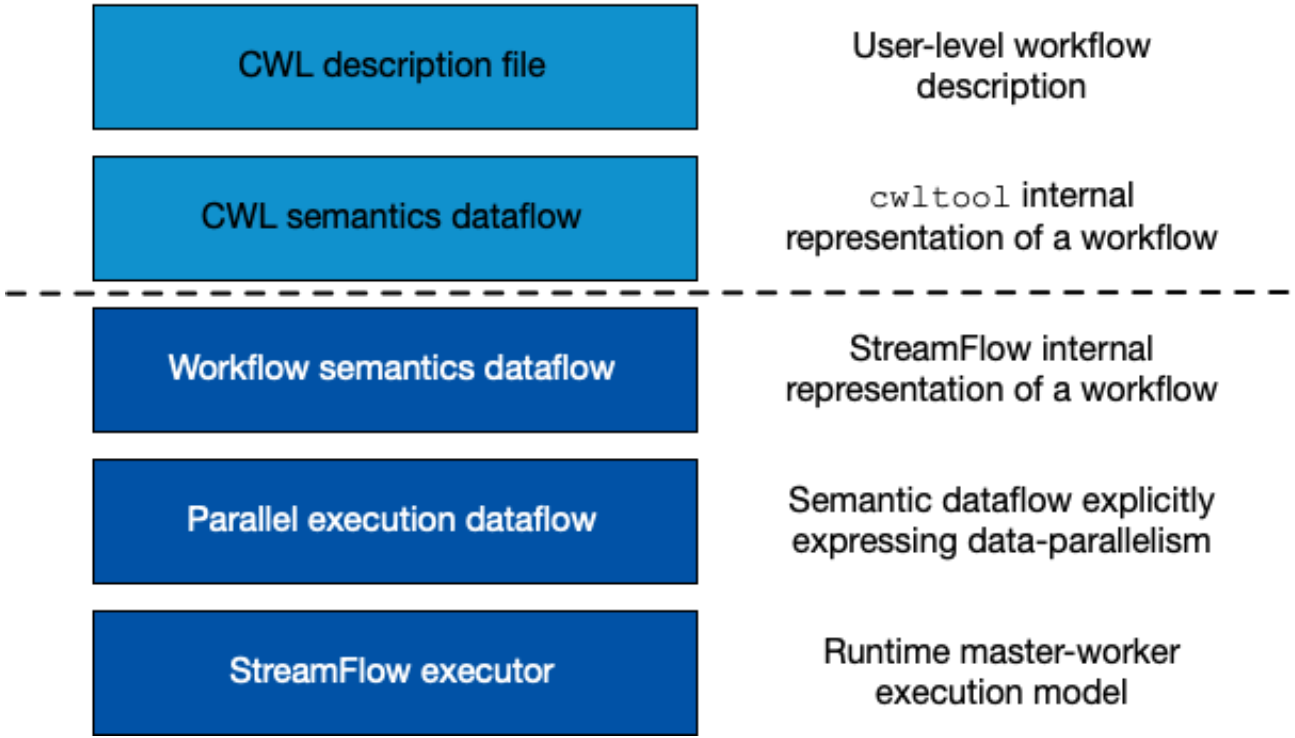

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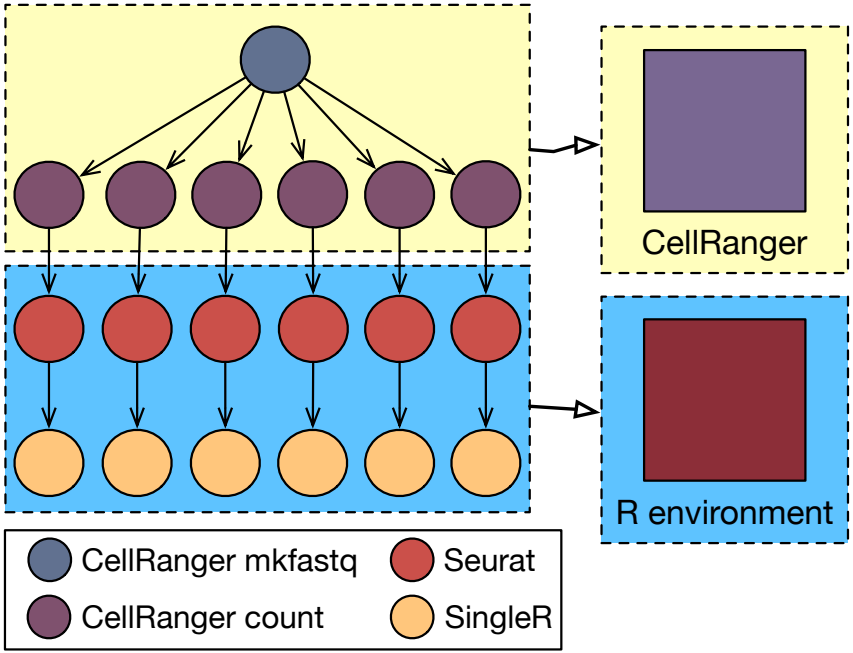
Single-Cell RNA Sequencing Pipeline



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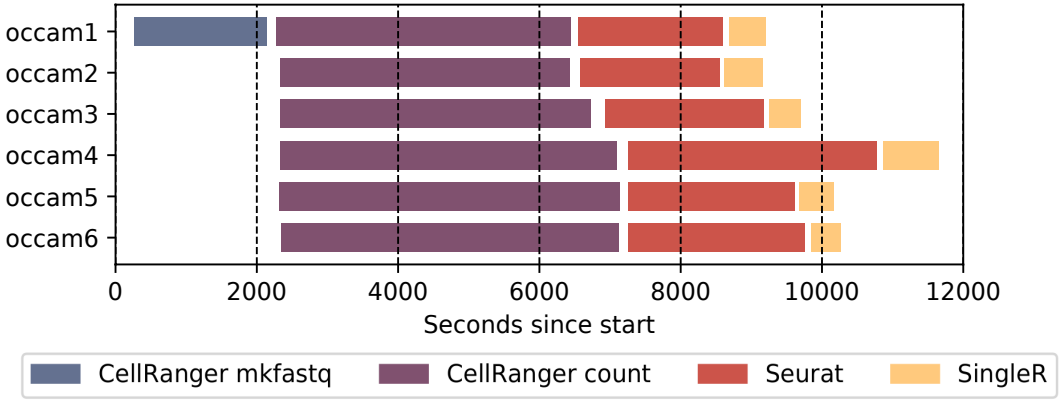

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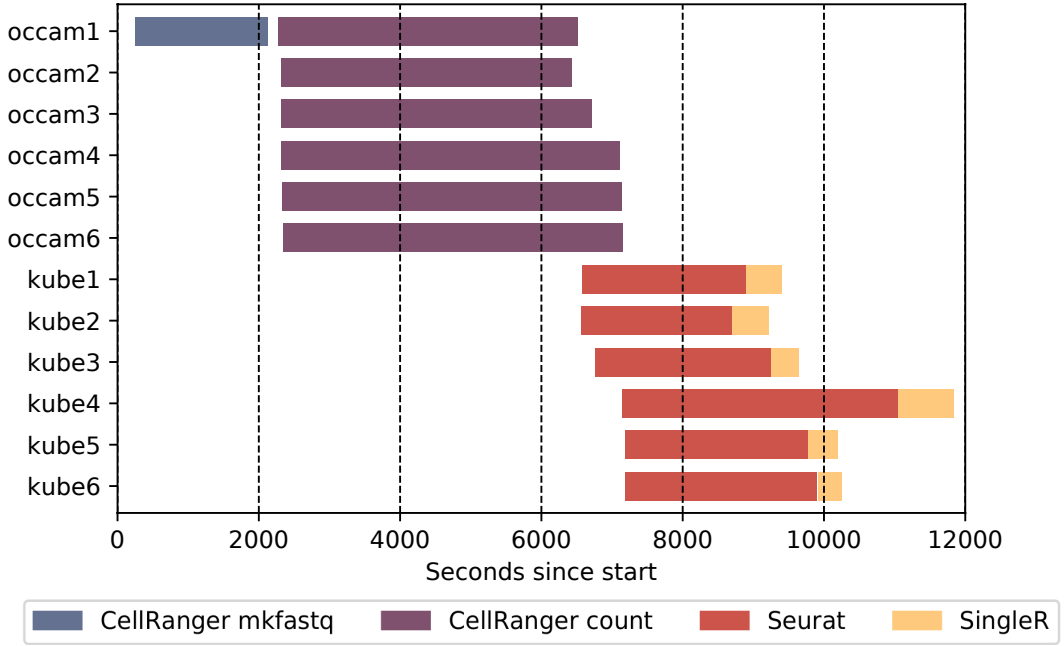

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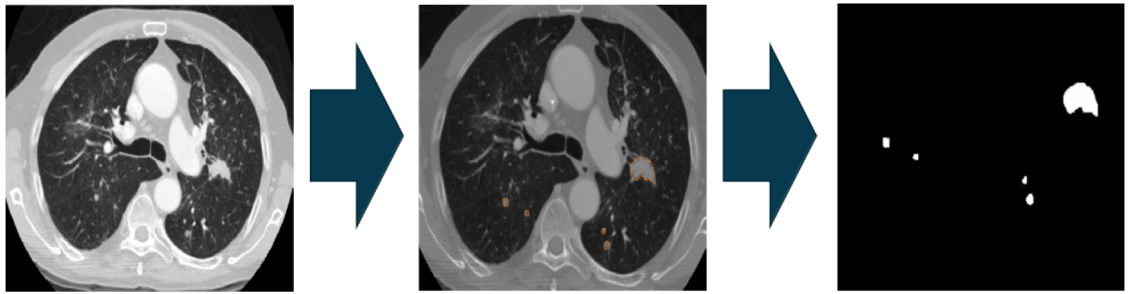
Lung Nodules Segmentation

- **Lung nodules** are quite common incidental findings in **CT** (Computed Tomography) **scans** and can be defined as **small focal lesions** (ranging from 5 to 30 mm) that can be solitary or multiple.
- The **goal** of DeepHealth UC4 is to train **AI systems to recognize lung nodules** using chest CT scans, providing radiologists an efficient tool for daily activity.



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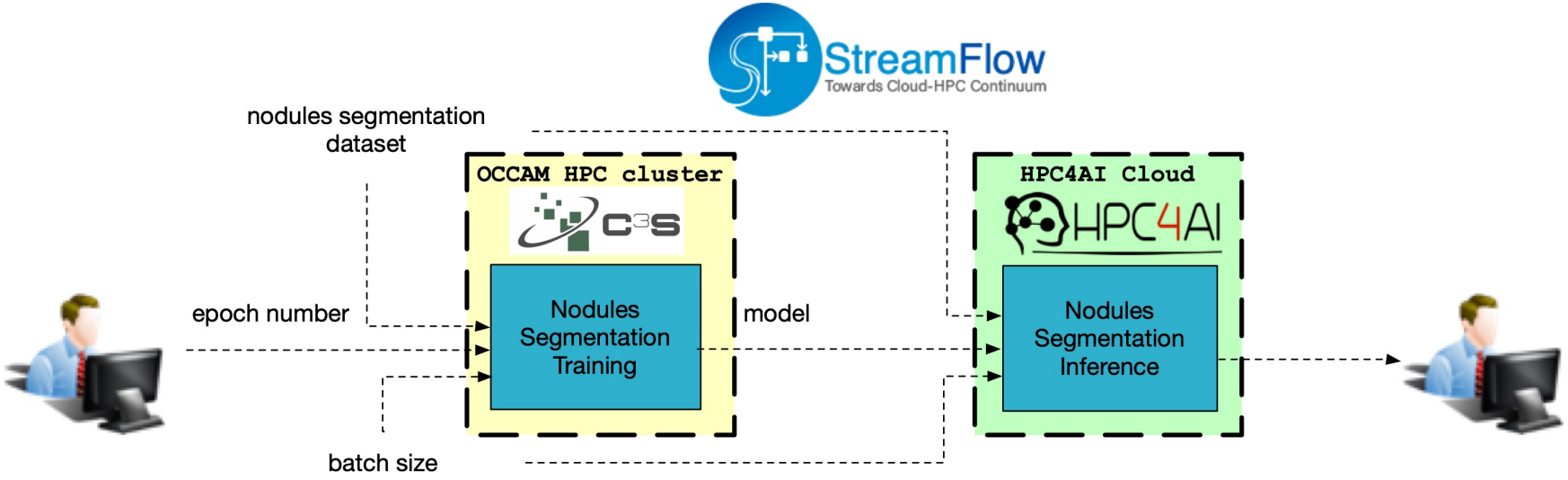

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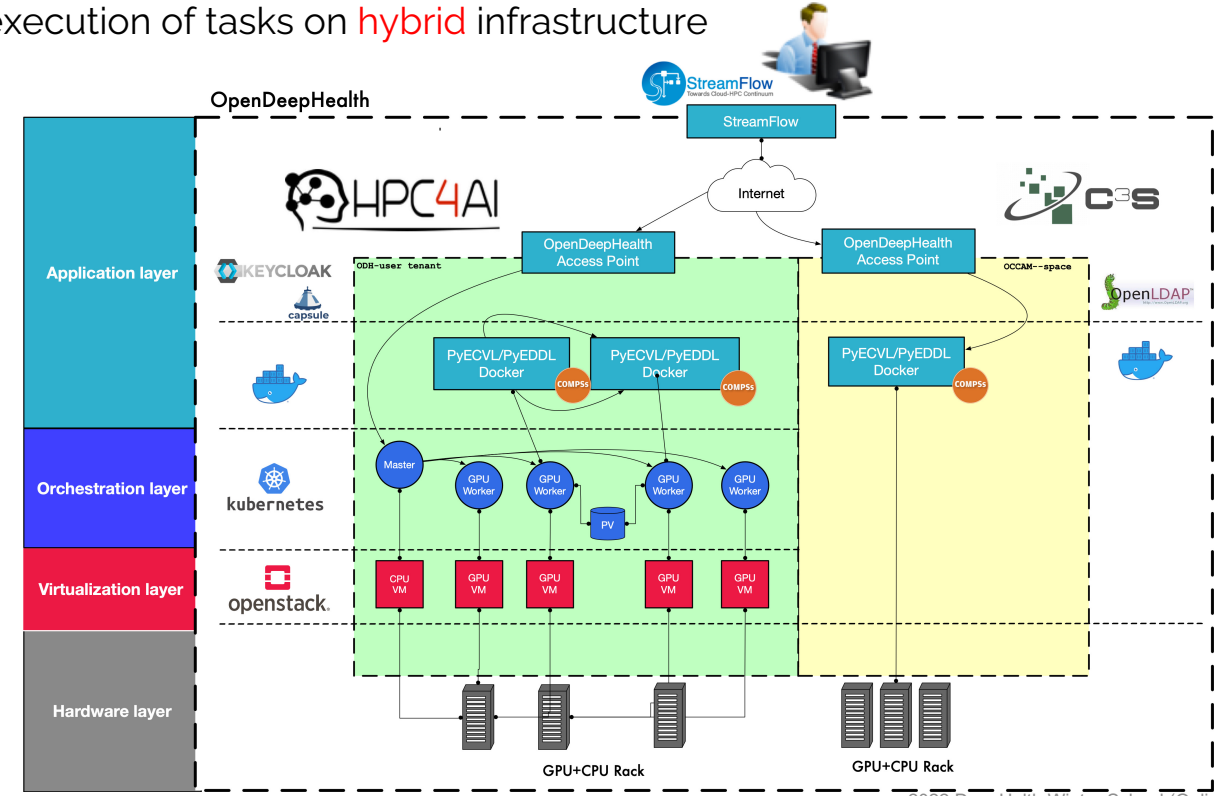

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Notebooks have limits

- Notebooks **are not parallel**: the default execution flow is sequential
- Notebooks **are not distributable**: code is executed in a single backend (kernel)
- Notebooks **are not scalable**: they cannot normally run on HPC environments

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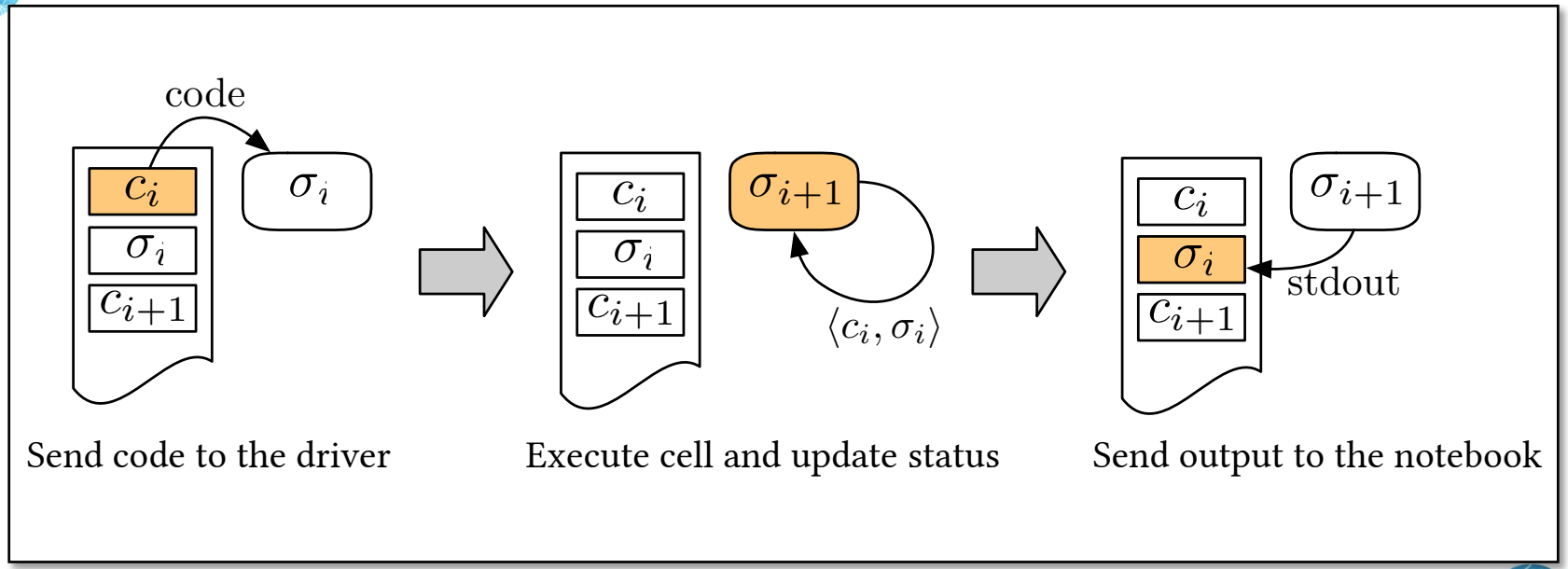

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Solution 1: write scalable code

- Notebooks do not scale, but **user code can scale** (e.g. using parallel libraries as Spark, Tequila, PyCOMPSs, Parsl, Ray, …)

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- Deployment of the parallel environment (e.g. a remote Spark cluster) is commonly **out of the scope of the notebook**, i.e. not documented

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Solution 2: write workflows of notebooks

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- Single notebooks are **not self-contained**: they only make sense in combination with the entire workflow

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Solution 3: write workflows as notebooks

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- Each notebook is **self-contained**: both host and coordination logics are packed in the same format
- Coordination logic is **transparent**: user code can still run sequentially as usual in an environment without workflow metadata interpreters

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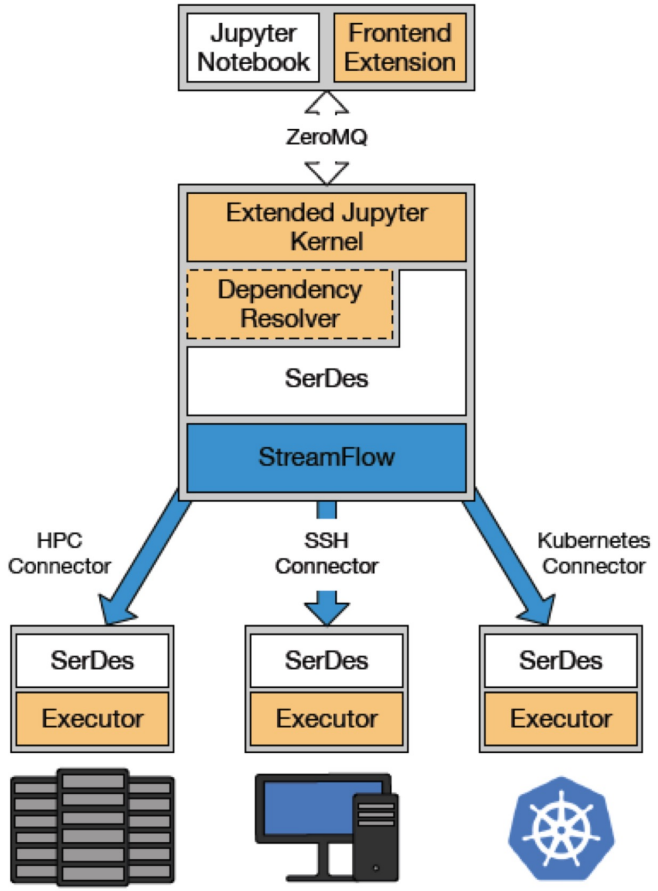
Jupyter-workflow

The **Jupyter-workflow** kernel extends the IPython software stack to support hybrid literate workflows in the Jupyter stack. It consists of three main components:



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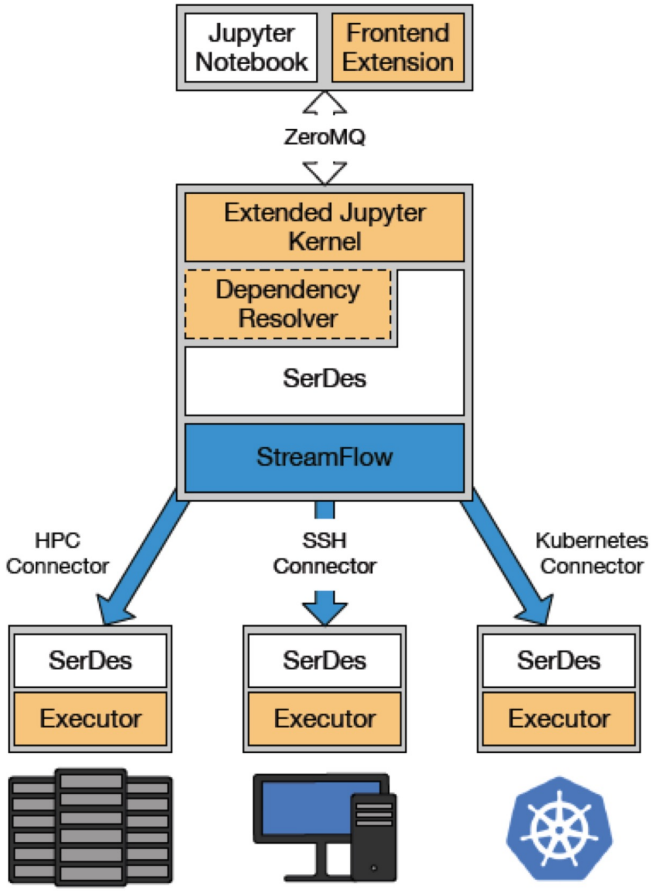

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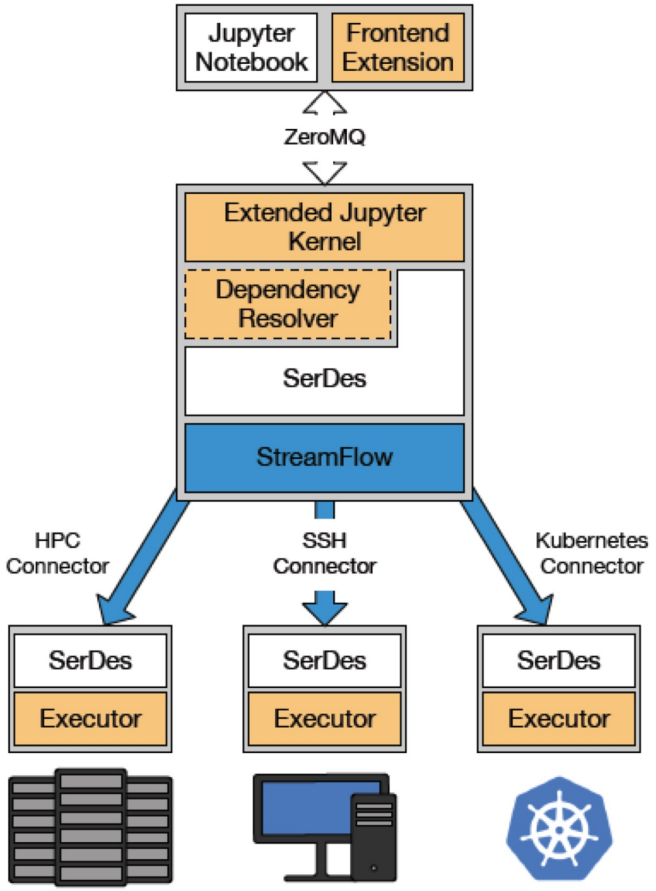

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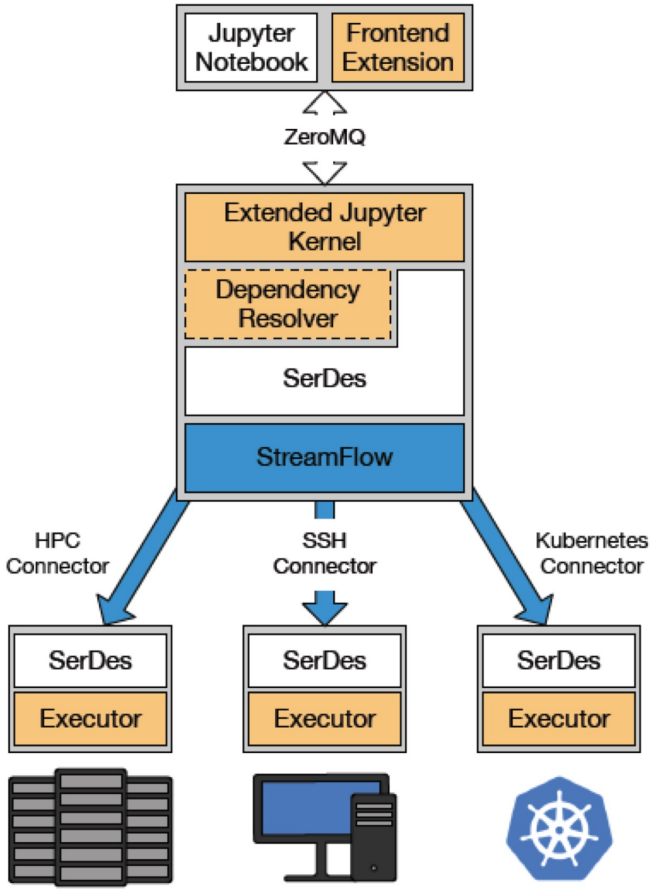
- A **dependency resolver component** to help users identify the input dependencies of each cell;
- A **Jupyter stack extension** to handle coordination metadata, execute cells remotely and manage data transfers (through StreamFlow).



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The workflow metadata format

```
# Workflow metadata
{
    "step": {
        "in": [{   # List the members of In(c_i)
                "type": "name" | "env" | "file" | "control",
                "name": "variable name",
                "scatter": {
                    "size": "token num"
                },
                "serializer": {
                    "predump": "code executed before serialising",
                    "postload": "code executed after serialising"
                },
                "value": "value to assign to the name",
                "valueFrom": "can take value from a different variable"
            }],
        "autoin": True | False, # Resolve In(c_i) automatically
        "out": [   # List the members of Out(c_i)
            ...
        ]
    },
```

Input and output dependencies

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Explicit data-parallel constructs

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Custom object serialization

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```

Automatic dependency retrieval

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The workflow metadata format

Description of remote environments

```
    "target": {# Part of the StreamFlow format
        "model": {# Description of the execution environment
            ...
        },
        "service": "target service inside the model",
        "resources": "number of workers to reserve",
        "workdir": "working directory on the remote resource"
    },
    "version": "v1.0"
}
```


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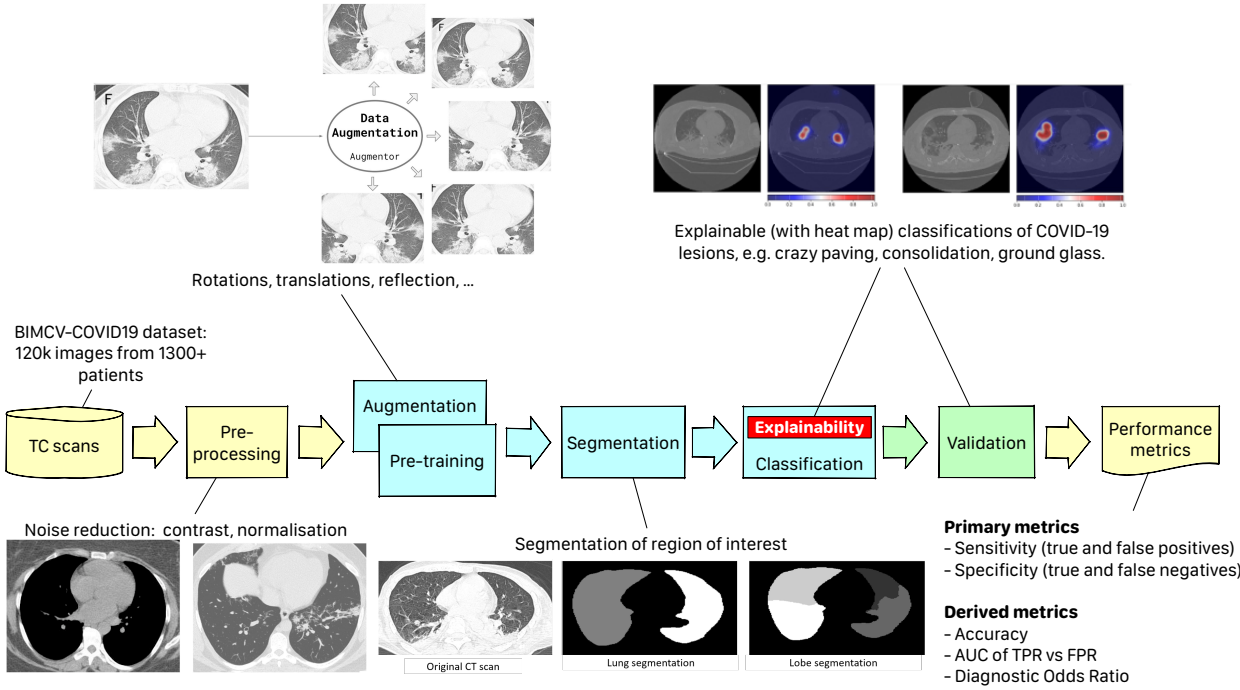
CLAIRE-COVID19 Universal Pipeline



M. Aldinucci, “[Invited Talk] HPC application cloudification: the streamflow toolkit,” in *PARMA-DITAM 2021*

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CLAIRE-COVID19 Universal Pipeline

PreDNN (2 varianti)

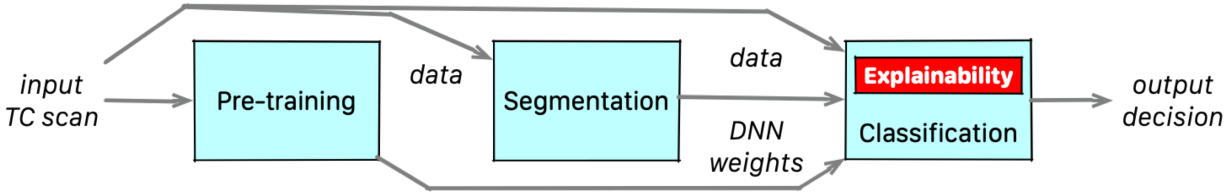
1. Pre-training
2. Self-training

SegDNN (5 varianti)

1. None
2. Fully-convolutional (ResNet)
3. DeepLabV3 (ResNet)
4. U-net
5. Tiramisu

ClassDNN (11 varianti)

1. Inception (3 varianti)
2. ResNet (3 varianti)
3. DenseNet (3 varianti)
4. AlexNet
5. Inception-ResNets



Iper-parametri (9 varianti)

A. Learning rate (3 valori)
B. Weight decay (3 valori)
C. Learning rate decay step (3 valori)

M. Aldinucci, “[Invited Talk] HPC application cloudification: the streamflow toolkit,” in *PARMA-DITAM 2021*

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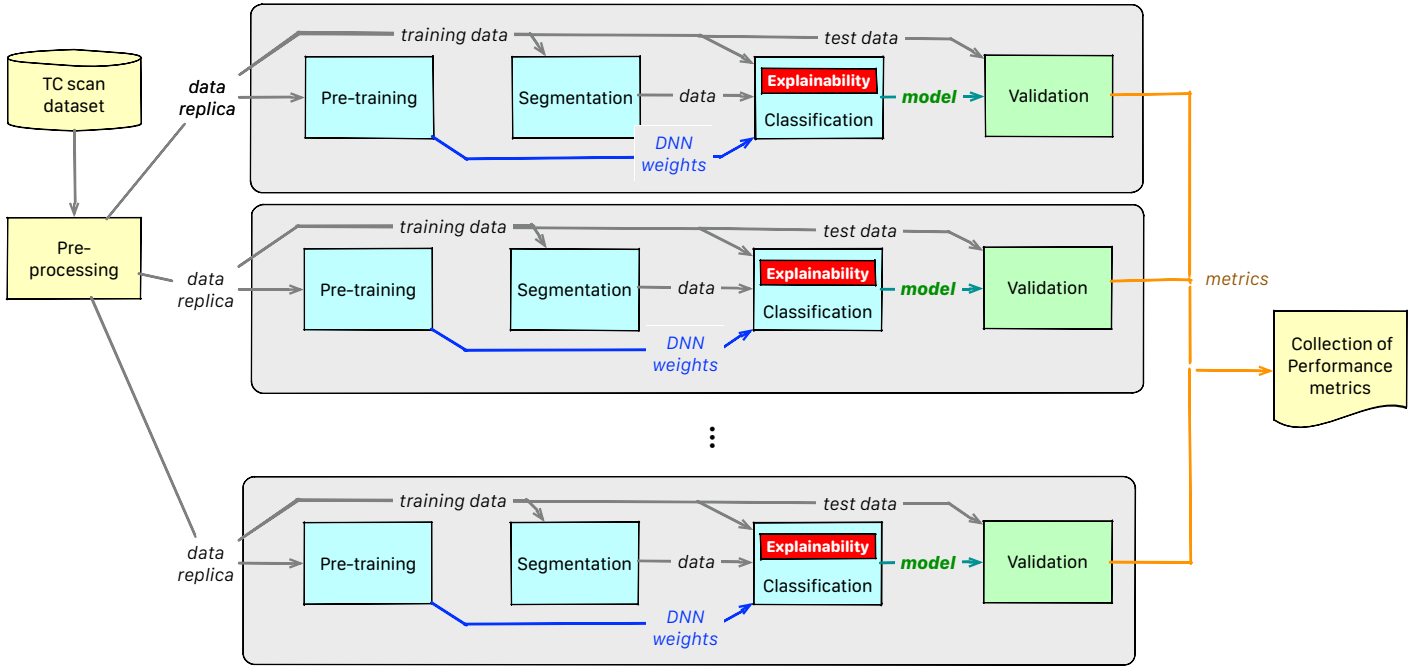
CLAIRE-COVID19 Universal Pipeline



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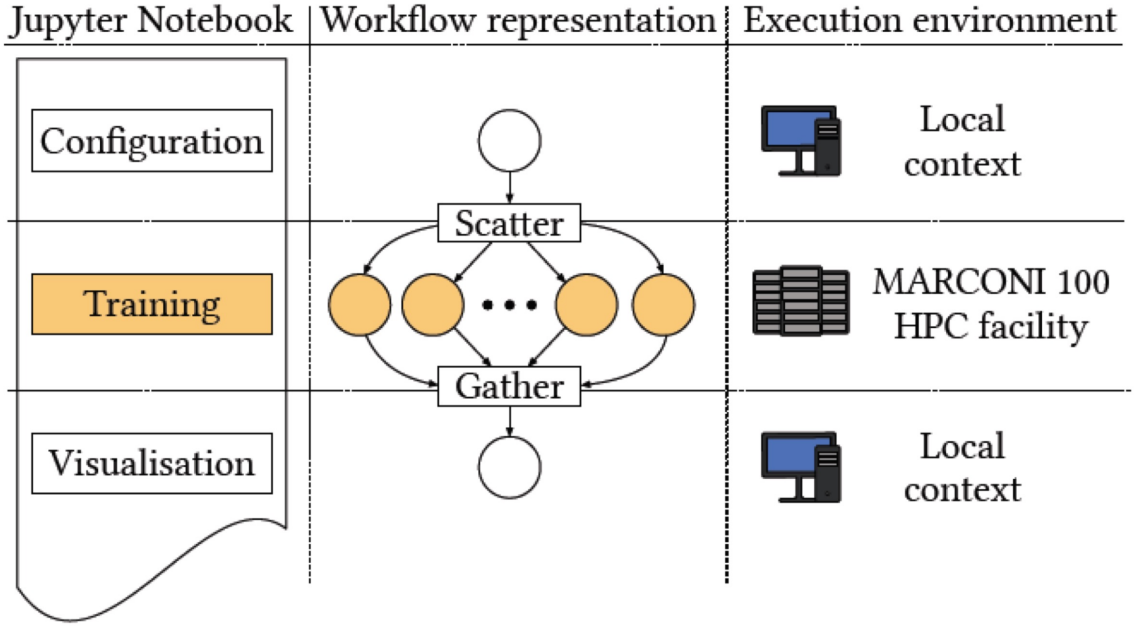

I. Colonnelli et al., ”Distributed workflows with Jupyter,” in *Future Generation Computer Systems*

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CLAIRE-COVID19 Universal Pipeline

Pre-trained DenseNet-121 Fine-tuning with Adam on BIMCV-COVID19

Hyperparameter	Values
Batch size	64
Learning rate (LR)	$[10^{-3}, 10^{-4}, 10^{-5}]$
LR decay step	[10, 15]
LR decay gamma	10^{-1}
Weight decay	$[5 \cdot 10^{-4}, 5 \cdot 10^{-5}]$

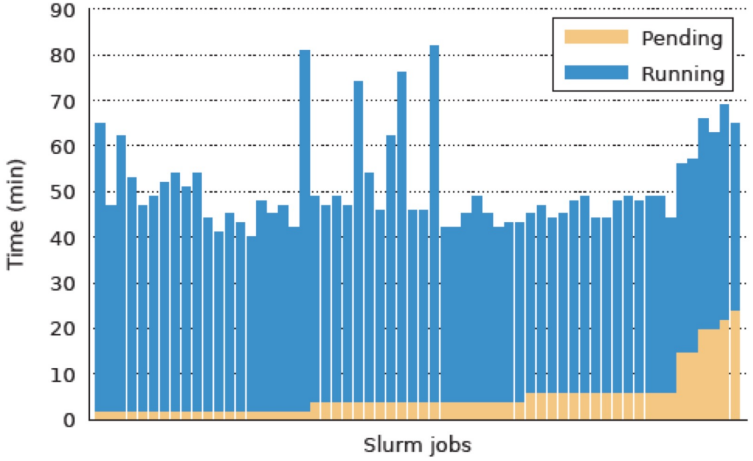

Figure 4: Execution times for the 60 Densenet-121 training experiments running in parallel on 60 GPU-equipped nodes of the CINECA MARCONI 100 facility.

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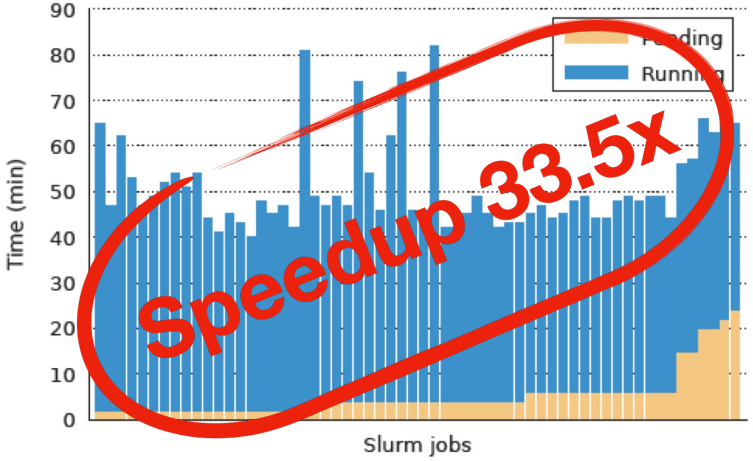

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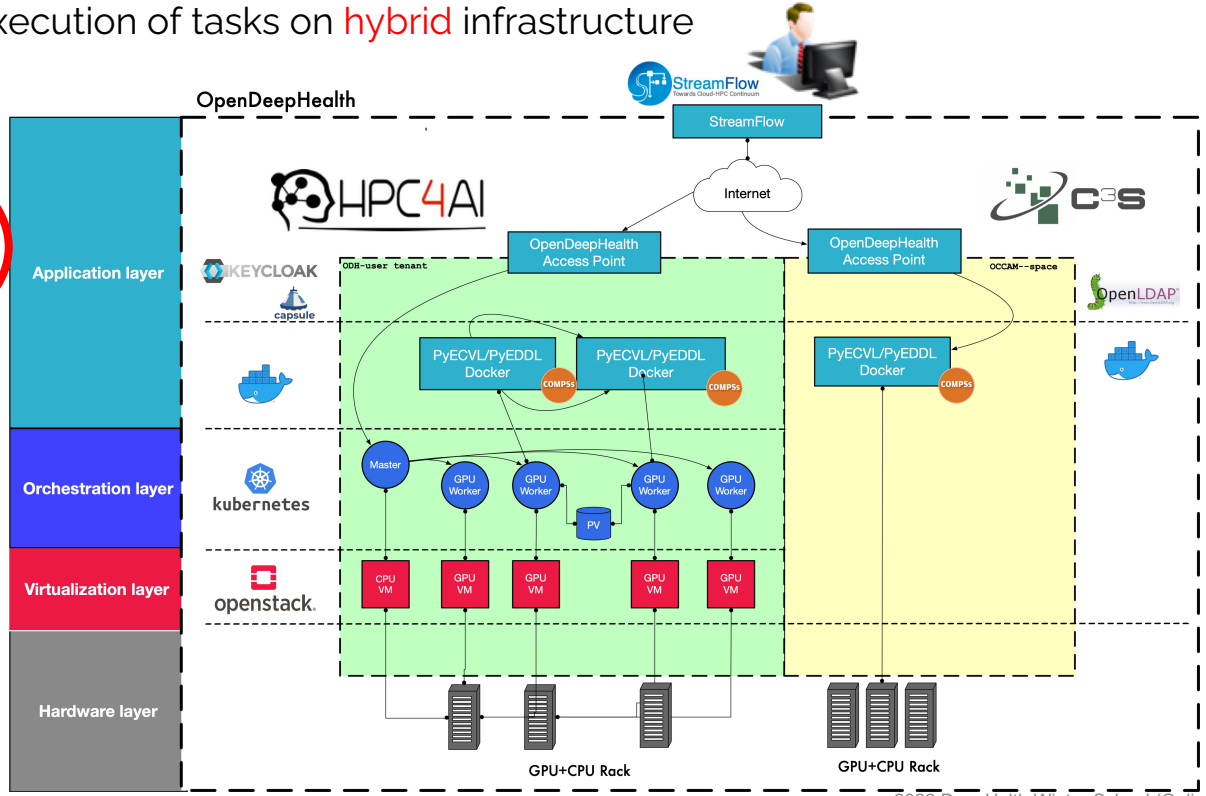
OpenDeepHealth Platform

The **StreamFlow** Workflow Management System (WMS) orchestrates the execution of tasks on hybrid infrastructure

Multi-tenant private Kubernetes for AI training

Literate workflows to write complex distributed pipelines as Jupyter Notebooks



Super Computer cluster providing an elastic virtual farm of containers on bare metal

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Capsule: the Kubernetes multi-tenancy operator

- Capsule leverages the **Kubernetes resources** to handle multi-tenancy at the cluster level;

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- A Tenant can be used to configure various aspects:
  - **Security** (NetworkPolicies, PodSecurityPolicies, allowed Service Kinds, …)

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  - **Resources** (ResourceQuotas, LimitRanges, NodeSelectors, StorageClasses, …)
  - **Services** (available hostnames, CustomResource quotas, integration with running applications through ServiceAccounts, …)

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```yaml
apiVersion: capsule.clastix.io/v1beta1
kind: Tenant
metadata:
  annotations:
    capsule.clastix.io/enable-node-listing: 'true'
spec:
  additionalRoleBindings:
    - clusterRoleName: odh-policy
      subjects:
        - apiGroup: rbac.authorization.k8s.io
          kind: Group
          name: system:authenticated
  ingressOptions:
    allowedHostnames:
      allowedRegex: .opendeephealth.di.unito.it$
    hostnameCollisionScope: Disabled
  namespaceOptions:
    quota: 3
  networkPolicies:
    items:
      - egress:
          - to:
              - ipBlock:
                  cidr: 0.0.0.0/0
                  except:
                    - 252.0.0.0/8
                    - 172.17.7.0/24
                    - 172.20.7.0/24
        ingress:
          - from:
              - namespaceSelector:
                  matchLabels:
                    capsule.clastix.io/tenant: unito
              - namespaceSelector:
                  matchLabels:
                    name: projectcontour
                podSelector:
                  matchLabels:
                    app: envoy
              - podSelector: {}
        policyTypes:
          - Ingress
          - Egress
  nodeSelector:
    pool: unito
  owners:
    - kind: Group
      name: unito-tenant-owners
  serviceOptions:
    allowedServices:
      externalName: true
      loadBalancer: false
      nodePort: false
    externalIPs:
      allowed: []
```

Practically, a Tenant is **a single YAML file to manage all the aspects of multi-tenancy**

Multi-tenant architecture

- Capsule (https://capsule.clastix.io/) for **cluster-level segregation**

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- JupyterHub (https://jupyter.org/hub) for **single-user notebooks**

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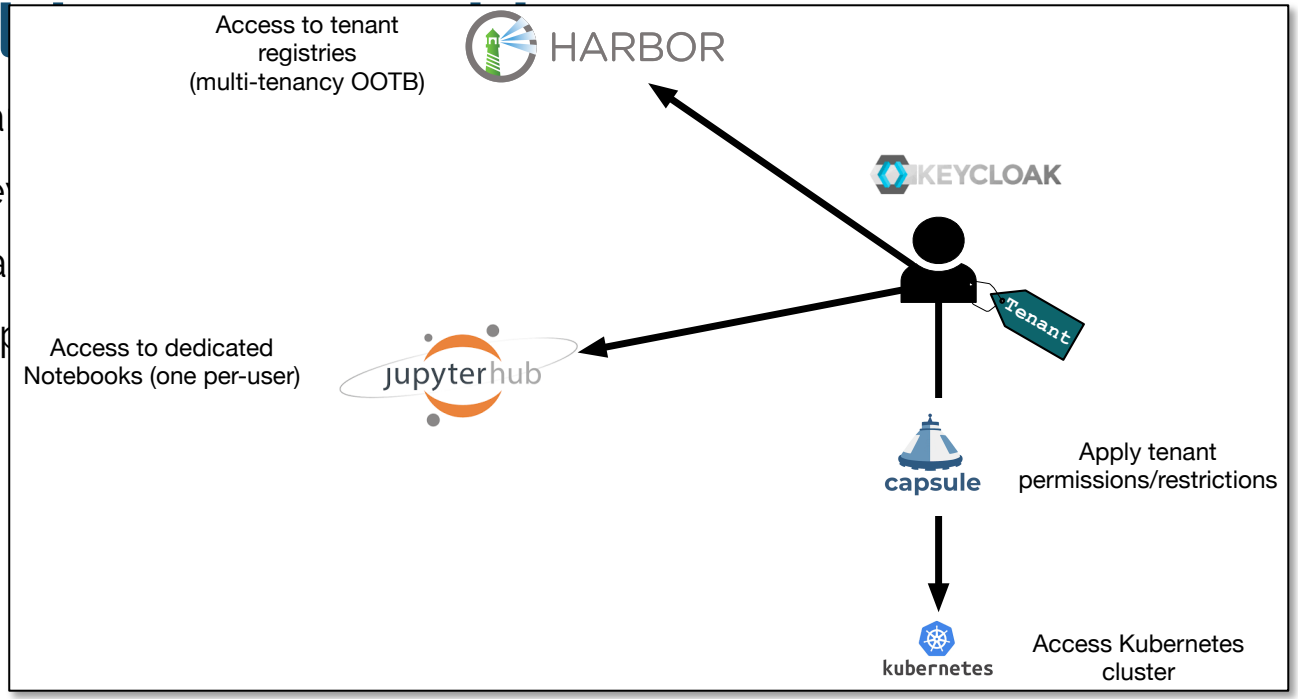

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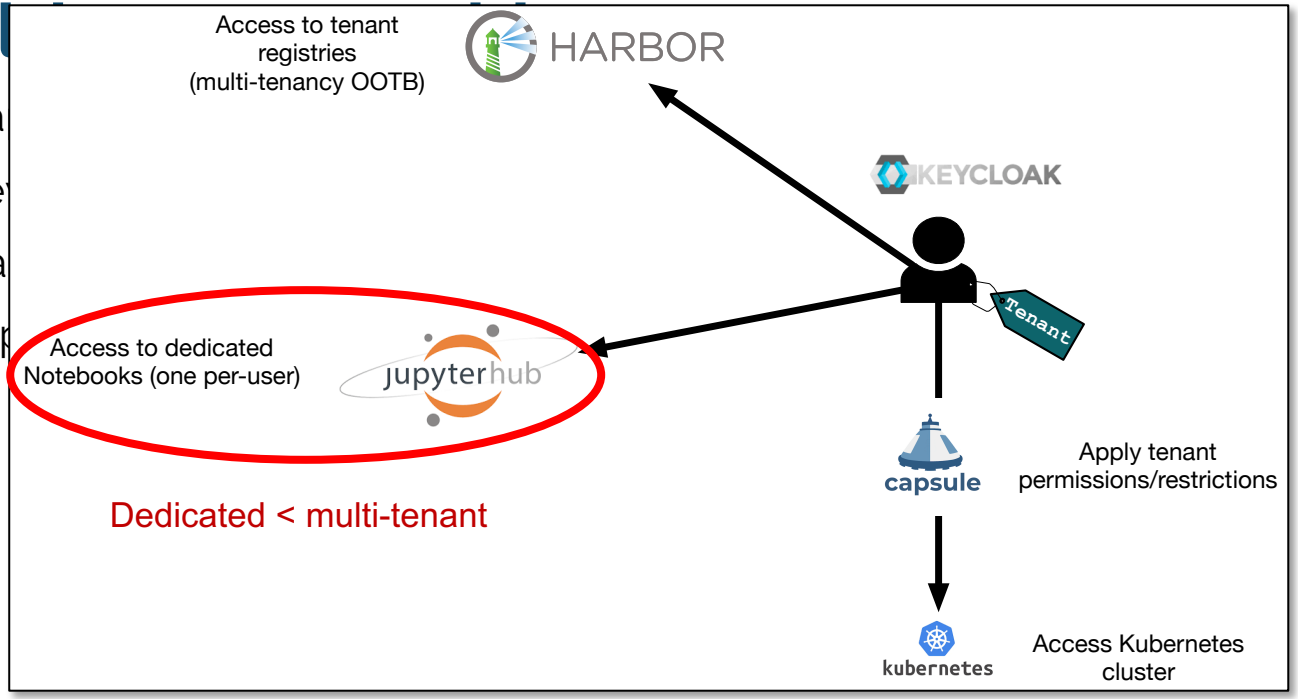

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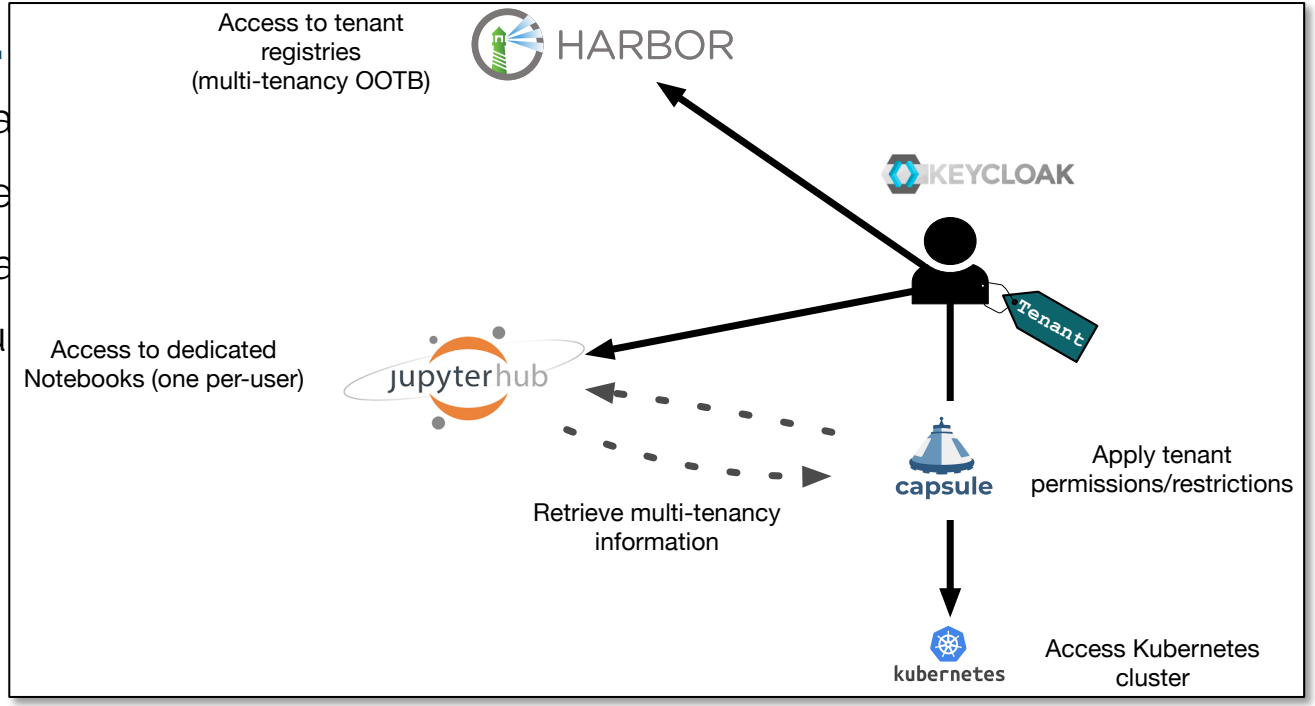

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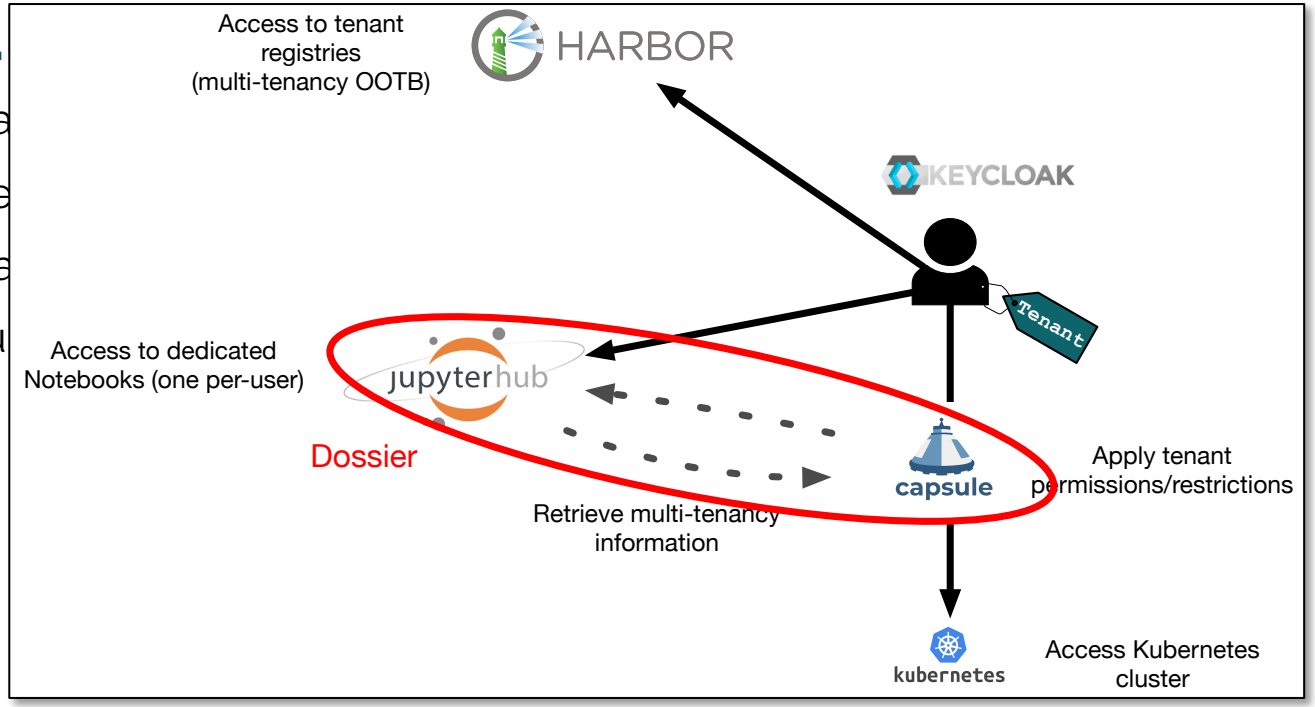

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- Dossier (https://github.com/alpha-unito/dossier) for **multi-tenant distributed Jupyter Notebooks**

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Dossier: Multi-tenant Distributed Jupyter as a Service

- Jupyter-workflow is provided as-a-Service in OpenDeepHealth through a **multi-tenant infrastructure**, called Dossier;

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- Dossier users can offload computation to other infrastructures, either provided by OpenDeepHealth itself (the **Super Computer cluster**) or independently managed by users;
- System administrators can easily manage accounting and security at a **coarse-grain** (namespace groups) and in a **centralised way**.

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DI TORINO

DEEPHEALTH

Thank you!

Iacopo Colonnelli

iacopo.colonnelli@unito.it

https://streamflow.di.unito.it

https://jupyter-workflow.di.unito.it/

https://github.com/alpha-unito/dossier

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