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Advanced Machine Learning. Flash Simulation and bleeding edge applications

FlashSim: *November status report*

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External Partner

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KPIs

KPI ID	Description	Acceptance threshold	2024-09-24
KPI2.2.1.1	N_{MC} billion events obtained from ML-based simulation, as demonstrated by official links in experiments' simulation databases	N_{MC} >= 1	2.3 M events (completed: 0.2%)
KPI2.2.1.2	N_{EXP} experiments have tested a machine-learning based simulation	N_{EXP} >= 2	3 experiment (completed: **150%**)
KPI2.2.1.3	Machine-learning use-cases tested in the context of the CN were presented at N_{CONF} international and national events	N_{CONF} >= 3	17 use-cases (since Sept. '23) (completed: **567%**)
KPI2.2.1.4	N_{UC} different machine-learning use-cases were tested in the context of the CN and made available in git repositories	N_{UC} >= 5	5 use-cases (completed: **100%**)

Risk Analysis

Identifier	Description	Update
R1	The CN is unable to provide the needed resources	We have access to Leonardo resources, and the provisioning model enabling offloading via InterLink has been validated in Integration PoC. Offloading from the AI_INFN Platform is still being commissioned. We have recently gained access to Tier1 resources. HPC Bubbles should be installed in 2024 Q4 and the provisioning model is under discussion.
R2 TODAY	The provisioning model is not ready for production	The provisioning model has been validated on CPU and using simplified backends such as Docker or Kubernetes itself, and recently extended to HTCondor backend. Polishing and refinements are needed to enable offloading to CINECA Leonardo.
R3	The recruitment process has limited or delayed success due to the large number of ML positions opening	All postdoc selected to work on the subject of this flagship planned to start on October 2024 withdrew. A new selection is ongoing, with planned start January 2025.

Flash Simulation

From M. Barbetti's talk @ ICHEP 2024 [LINK]

Fast simulation vs. Flash simulation

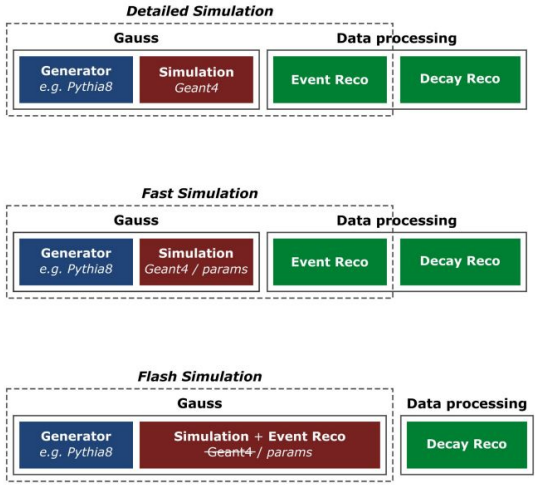
Methods to **speed up** the Geant4-based simulation productions:

- upgrade of the simulation framework (including multi-threading)
- leveraging GPU-acceleration (*e.g.*, use AdEPT, Celeritas)
- reuse of the not-signal part of the event, **ReDecay** [2]

Fast Simulation techniques to parameterize the detector low-level response without relying on Geant4:

- **Point library** for Calorimeters energy deposits [3]
- **Generative Models** (*e.g.*, GAN, VAE) for Calorimeters energy deposits [4]

Flash Simulation (also called *Ultra-Fast* or *parametric*) defines a more radical approach by replacing Geant4 and reconstruction with parameterizations able to **directly transform** generator-level particles into analysis-level reconstructed objects



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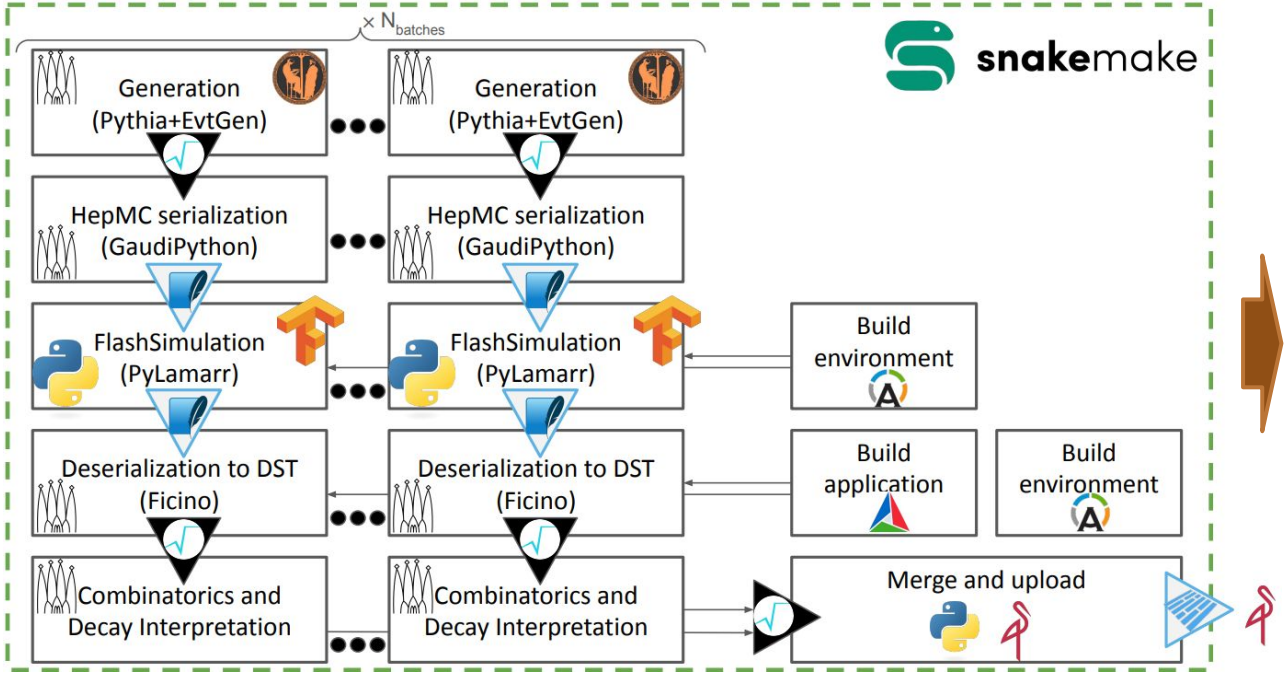
Flash Simulation Workflow

Validation (mixed: HTC, HPC and Cloud)

Training (pure HPC)



Logging (pure Cloud)

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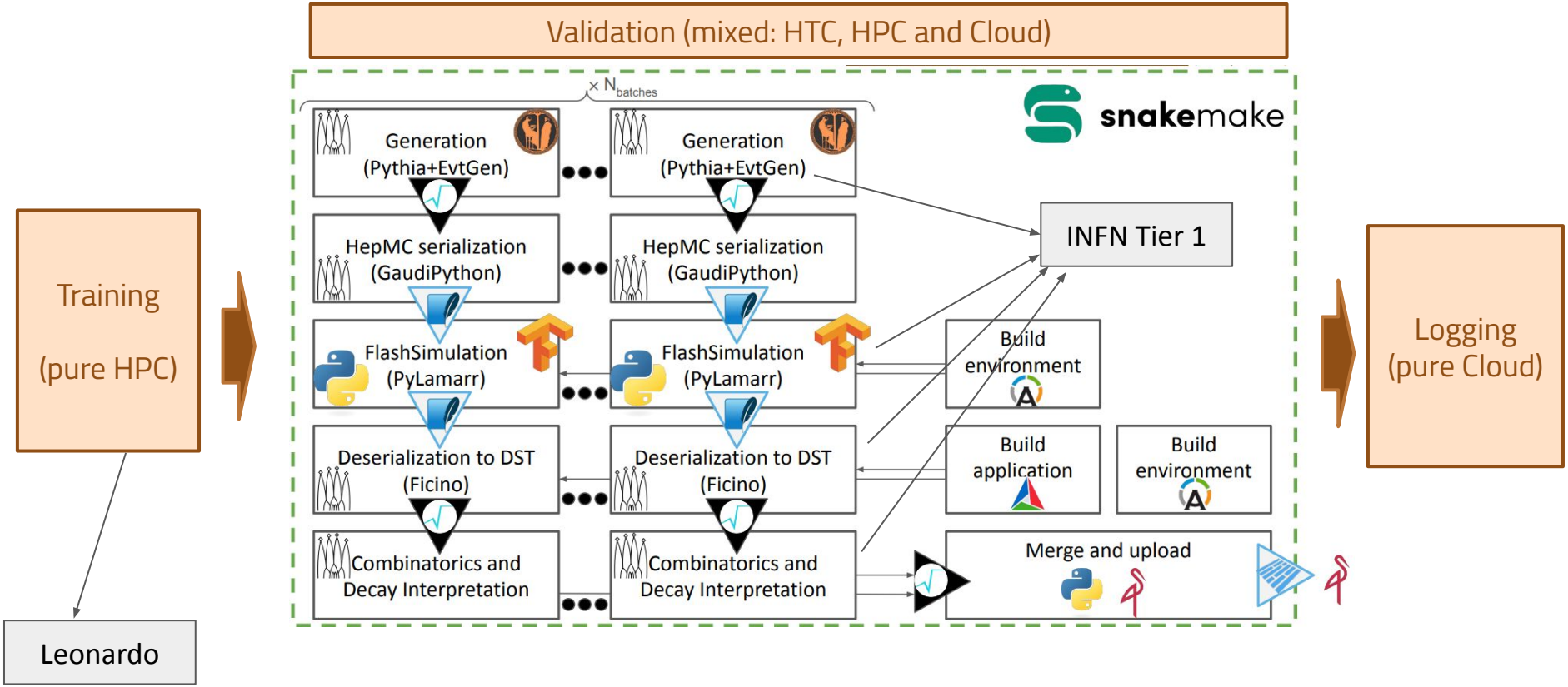
Flash Simulation Workflow – offloaded



Status of the integration of INFN-T1 resources

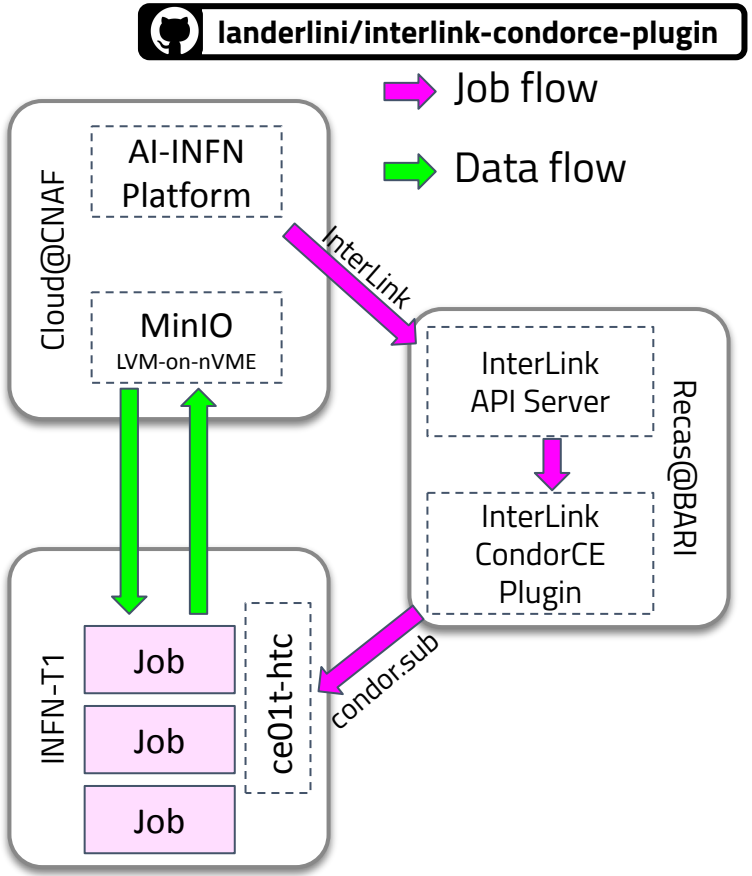
Developing the **HERD Computing Model**,
CNAF defined a CondorCE submitting jobs from remote locations through authentication.

Unfortunately, the CondorCE is not reachable from Cloud@CNAF for network policies, but it is, for example, from ReCaS@BARI.

We developed an **InterLink plugin** sitting in a VM in Bari, accepting InterLink submissions from Cloud@CNAF and forwarding them to CNAF Tier-1 test CE.

The plugin converts the **Kubernetes Pod** specifications into a (possibly rather long) shell script running **Apptainer** containers in multiple subprocesses.

Input and output data is managed through a self-managed **MinIO instance on LVM-on-nVME** hosted in **Cloud@CNAF**.



(re)Defining cvmfs and fuse volumes

Converting Pod's requests to access cvmfs or fuse data should be responsibility of the plugin, as different compute backend may be subject to different rules.

In CondorCE plugin I use generic annotations to define volumes.

For Leonardo, this require hacking the singularity submission command (very verbose).

```yaml
apiVersion: v1
kind: Pod
metadata:
  name: cern-vm-fs
  annotations:
    cvmfs.vk.io/my-volume: sft.cern.ch
spec:
  containers:
    - name: main
      image: ubuntu:latest
      command:
        - /bin/bash
        - -c
        - ls /
      volumeMounts:
        - name: my-volume
          mountPath: /cvmfs
          readOnly: True

  volumes:
    - name: my-volume
      persistentVolumeClaim:
        claimName: intentionally-not-existing
```

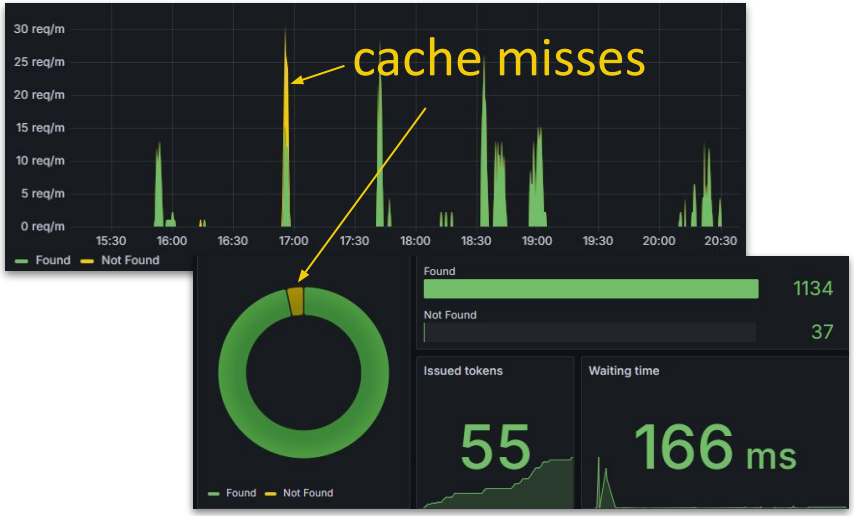
```yaml
apiVersion: v1
kind: Pod
metadata:
  name: fuse-vol
  annotations:
    fuse.vk.io/my-fuse-vol: |
      cat << EOS > /tmp/rclone.conf
      [example]
      type = local
      EOS

      # Mimic a remote
      mkdir -p /tmp
      echo "hello world" > /tmp/file.txt

      # Mount the remote
      rclone mount2 \
        --config /tmp/rclone.conf \
        --allow-non-empty example:/tmp \
        $MOUNT_POINT

spec:
  containers:
    - name: main
      image: rclone/rclone:latest
      command:
        - cat
      args:
        - /mnt/fuse-vol/file.txt
      volumeMounts:
        - name: my-fuse-vol
          mountPath: /mnt/fuse-vol
  volumes:
    - name: my-fuse-vol
      persistentVolumeClaim:  # deliberately fake pvc
        claimName: csi.example.com
```

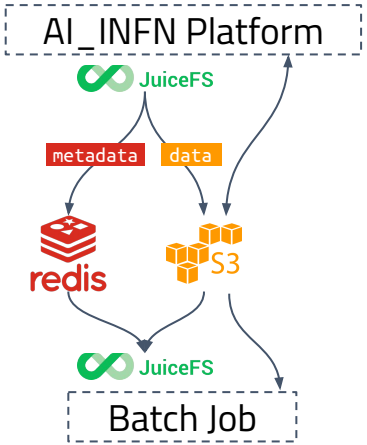
Solving the distributed cache problem

Focus on data flow

A **shared virtual file system** is mounted by the condor nodes with fuse using JuiceFS.

JuiceFS falls back on **MinIO** for the data and **Redis** (part of the AI-INFN platform) for the metadata





[ShubProxy]

Downloading and building docker images into SIF for each jobs

- would cause a periodic bans of CNAF by DockerHub;
- cause large inefficiency in short jobs.

We deployed a simple web application defining a shared cache.

If the image is not available in S3, the web app schedule its build, otherwise it return the built artifact from cache.

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Status of the integration with Leonardo

The slurm plugin in production in Leonardo, does not accept Pod requests from the Flash Simulation workflow.

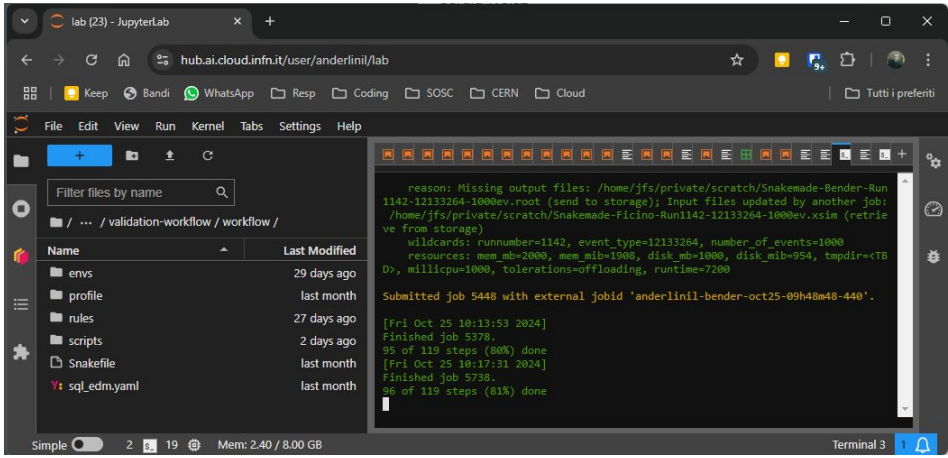
All the building blocks were tested separately and we expect no fundamental reason for the plugin not to work.

Still, some polishing would be needed, probably in a joint debugging session.

Alternatively, we may try to use the CondorCE plugin submitting to slurm.

Combining CNAF Tier-1 and CINECA Leonardo resources

- Kubernetes cluster
  - AI_INFN Platform (RKE2 with Kubernetes 1.27)
  - Virtual Nodes installed manually (no helm chart)
  - Snakemake as workload manager
- Tier1 setup
  - CondorCE (originally developed for HERD) mapped to ce01t
  - InterLink server and dedicated plugin running in a VM in ReCaS
- Leonardo setup
  - Slurm submission from edge node icsc01
  - Official interlink slurm plugin




```
(miniconda3)[lucio@pclhcb06 v3]$ k get nodes
NAME                  STATUS   ROLES
hub-a100-2            Ready    <none>
hub-a100-3            Ready    <none>
hub-a102-b            Ready    <none>
hub-cpu-2             Ready    <none>
hub-master            Ready    control-plane,etcd,master
hub-rtx-2             Ready    <none>
hub-rtx-3             Ready    <none>
hub-storage           Ready    <none>
vk infn-t1            Ready    agent
vk leonardo-virtual-node  Ready    agent
```

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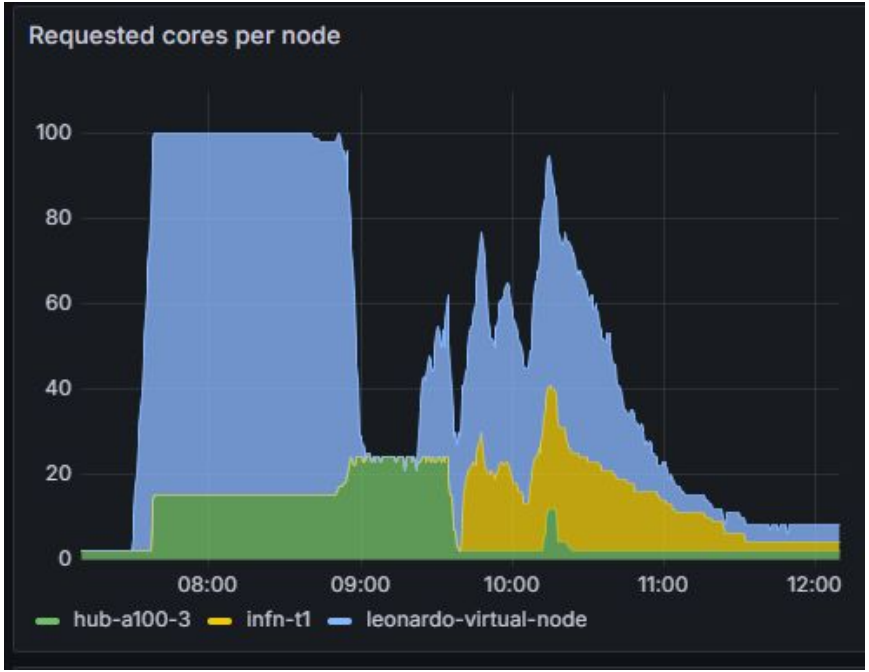
First workflow combining Leonardo DCGP and Tier-1

On October 25th, we run a first workflow combining CPU resources from Tier-1, Leonardo and a local node.

Will perform scalability tests soon.

Known scalability boundary is the size of the allocated buffer (1 TB), nCPU < 1k.

Offloading to Leonardo booster (with GPU payloads) coming soon.



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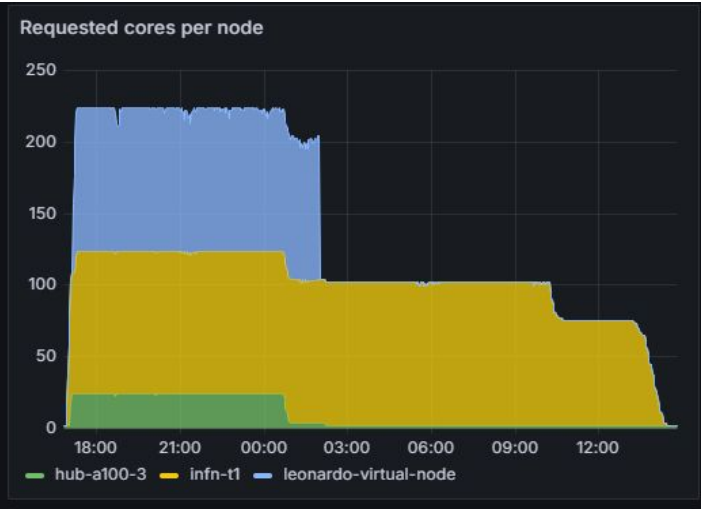
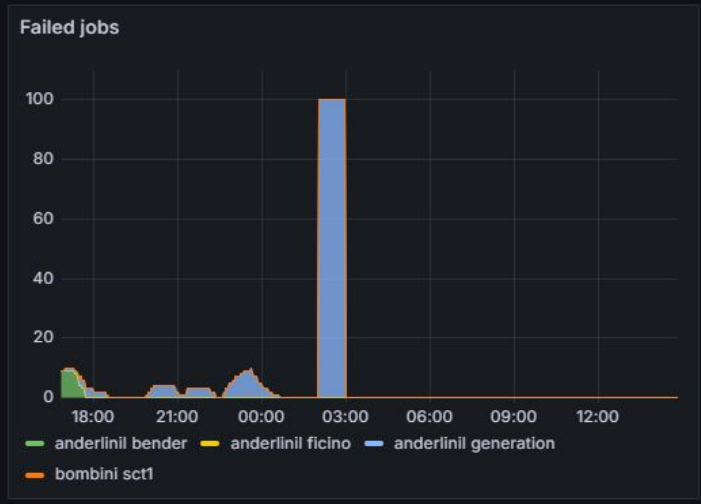
Longer run

Observed a bottleneck in the submission system, we tried submitting a bulk of “long” jobs.



Without entering details, very interesting dynamics, due to the interplay of:

- Node limits
- Kueue Resource Flavor limits
- Backend priority policies



AI_INFN Machine Learning Hackathon with ICSC support

AI_INFN is organizing the AI_INFN hackathon next week covering code-examples for the topics:

- Flash simulation and unfolding with GANs
- Reconstructing experimental data (LHCf)
- Processing of time-dependent NMR images
- Quantum Machine Learning

When: 26 – 28 November 2024

Where: Padova

Link to the agenda: agenda.infn.it/event/43129/

School of Open Science Cloud

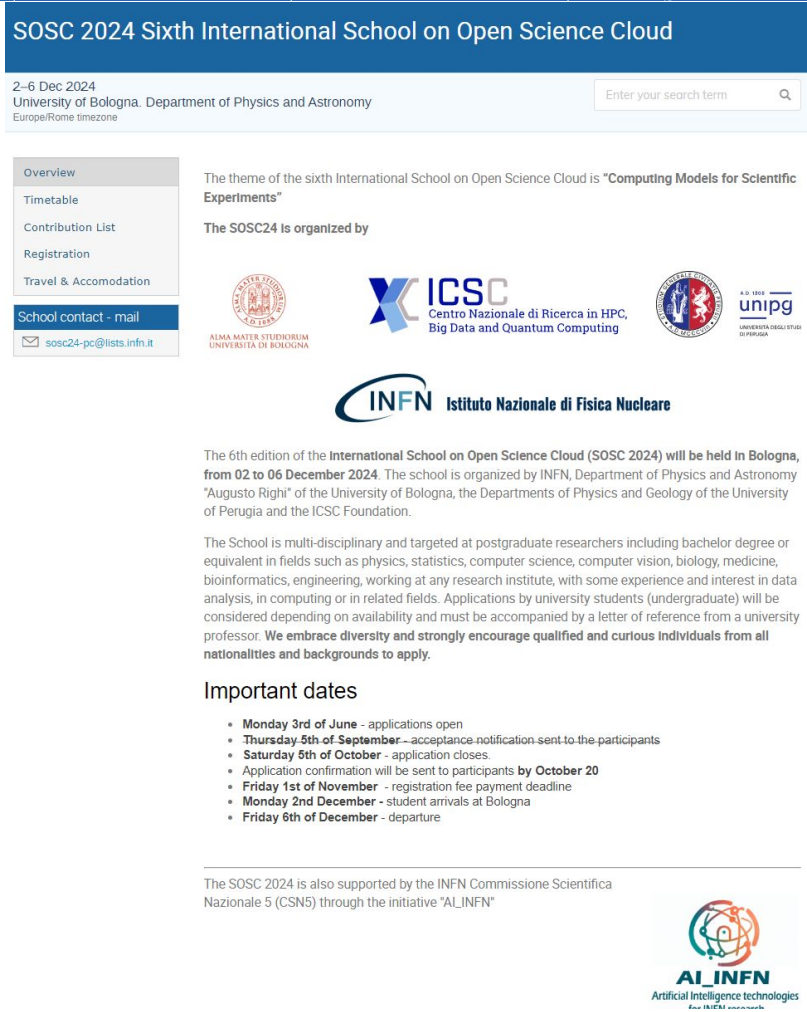
Deep involvement of WP2 people also in the organization of SOSC, including advanced machine learning use-cases of a cloud-based infrastructure.

- Containerization
- Data management
- Computer Vision and Machine Learning
- Distributing workflows

When: 2 – 6 December 2024

Where: Bologna

Link to the agenda: agenda.infn.it/event/40829



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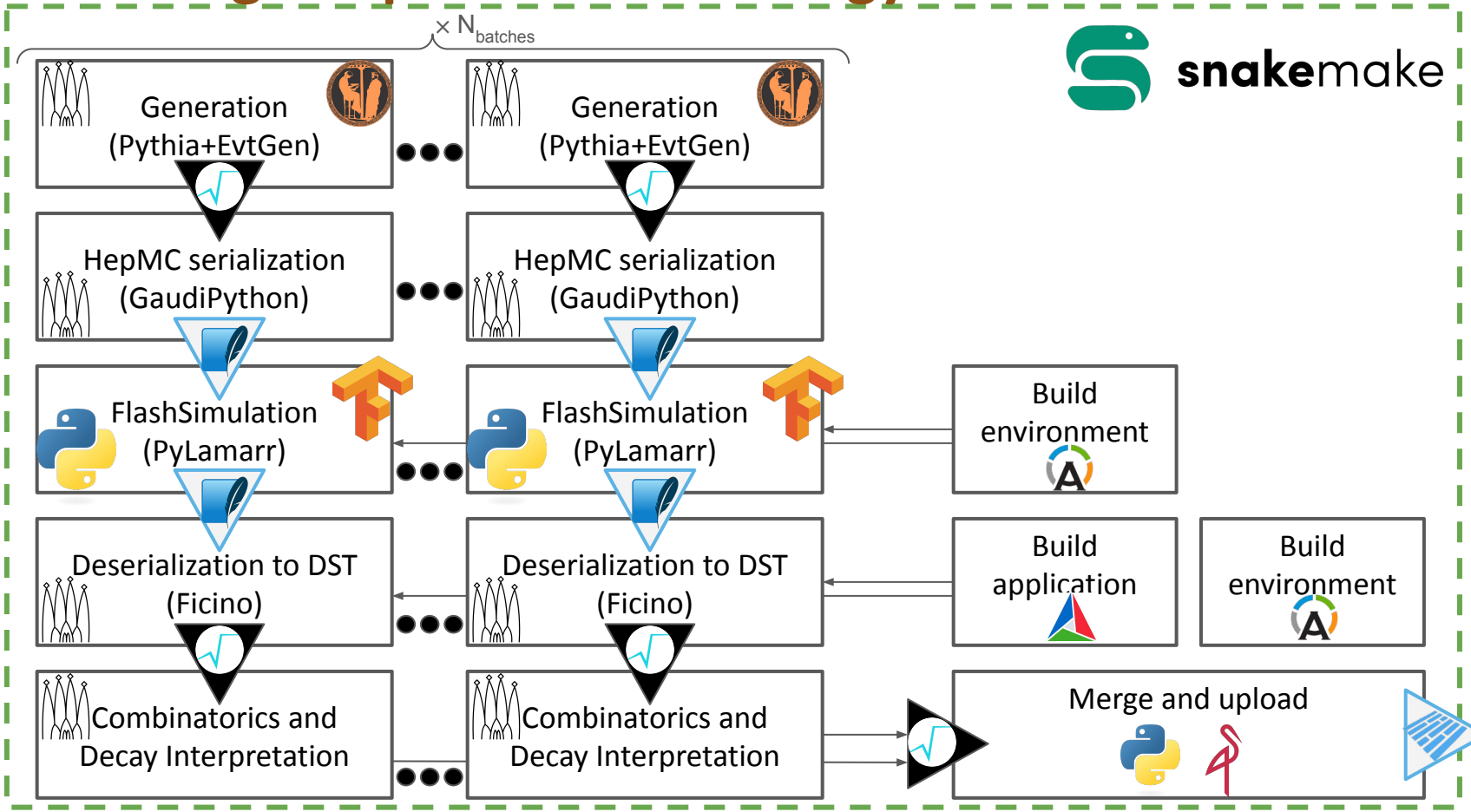
Backup

Recalling the production strategy



Resources

Pythia8 (full event)

Generates the whole proton-proton collision event, with pileup and spill-over.
Then processes all particles with Lamarr and Bender to produce nTuples.

1M events (on 50 parallel jobs) require:

- O(48h) × 50 CPUs
- 0.8 TB of buffer in S3.

Particle Gun (signal-only)

Generates only the heavy hadron decay.
Then processes particles with Lamarr and Bender to produce nTuples.
Less tested than Pythia8 productions

1M events (on **up to** 50 parallel jobs) require:

- O(1h), *limited by submission latency*
- 4 GB of buffer in S3

Requests for the validation part

Resource	Full Request	Strictly required for KPI 1 (Full-Pythia option)
CPU on INFN Cloud	2 M CPU hours	2.4 M CPU hours*
GPU on INFN Cloud	4 H200 for 18 months	0
GPU on Leonardo Booster via InterLink	10000 hours	0
Storage	25 TB	10 TB

Preliminary

- 0.5 M hours from opportunistic borrowing from AI_INFN Platform