





Advanced Machine Learning. Flash Simulation and bleeding edge applications

FlashSim: February status report

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Who we are

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- Francesco Vaselli ^c, Scuola Normale Superiore di Pisa
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- Muhammad Numan Anwar ^j, Politecnico di Bari
- Benedetta Camaiani ^g, Università di Firenze
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External collaborators:

• Andrea Rizzi ^c, Università di Pisa





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	100 M events (completed: 10%)
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%)

KPIs





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 being commissioned: Access to CINECA Leonardo: granted Access to CNAF-Tier-1: granted Access to ReCaS-Bari (condor): configuring, see INFN-CLOUD#1704 Access to HPC Bubble Padova (for ENI-PIML IG): upcoming 	
R2	The provisioning model is not ready for production	 Status: CINECA Leonardo: upcoming (G. Bianchini, Spoke O) CNAF-Tier-1: in production ReCaS-Bari: waiting for access HPC Bubble Padova (ENI-PIML IG): waiting for access 	
R3	The recruitment process has limited or delayed success due to the large number of ML positions opening	 Two new post-docs are starting (ENI-PIML IG funds): Alessandro Rosa, INFN Firenze Foundational aspects of Physics Informed Neural Networks Rosa Petrini, INFN Firenze Computing infrastructure for training Physics Informed NN 	

WELCOME





Update on LHCb Flash Sim

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 Opdated InterLink infrastructure

While adding new sites we realized that managing differences between the remote sites at application-level was becoming very challenging.



The plugin structure of InterLink has been redesigned with the goal of a uniform description of the jobs across multiple sites.

For test purpose, the current plugin works without ingress enabled in the resource provider.

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Flash Simulation Workflow – offloaded



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Scalability tests

- Most payloads are single-threaded WLCG-compatible applications
 - Ideal for scalability tests of job-management infrastructure (many small jobs)
- Every job mounts the distributed file system via fuse
- Container images are retrieved via the distributed file system (*should be improved*)

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• Data from one step to the other is exchanged via S3 (small development instance)

Preliminary results.

Can sustain up to 100 concurrent jobs, independently of the provider. Beyond, the metadata engine of the file system (tested both Postgres and Redis) cannot cope with the high number of concurrent connections.

The S3 instance as well suffers for the many concurrent operations.

Comments and next steps

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- 1. 100 job is a ridiculously tiny number if compared to the WLCG frameworks, but
 - a. this infrastructure is intended for AI. Controlling 100 GPU-powered nodes is less ridiculous;
 - b. the bottleneck are *the storage* and *database* infrastructure, where we put no effort and have extremely limited experience \rightarrow it is very likely this threshold could be improved with a better setup (*e.g.* using a Redis cluster, MinIO on bare metal with more-abundant RAM)

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- c. improvements at application level are possible, in particular software distribution
 (for example, simply shipping snakemake in the docker image made a factor 3 on the number of jobs)

 [•] by Gioacchino Vino, DataCloud
- 2. The distributed file system is fragile (with no surprise)

 \rightarrow it hides other offloading-specific instabilities.

To clear-up the offloading-specific aspects, we rewrote the workflow to be as gentle as possible on storage and network, removing dependencies on a distribute fs.

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Flash Simulation Workflow – offloaded – prod

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Comments on the "prod" workflow

Pro

Scale better, enabling tests of the offloading infrastructure itself

Run everywhere, the resulting payload is a single-core, 2-GB memory job, **consistent with WLCG standards**.

Drastically reduce data exchange, ideal for network-bound steps.

Cons

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All steps run in the same node, extremely inefficient for some task (overall CPU efficiency @CNAF: 4%)

Tedious for development, any modification requires **rebuilding** the OCI-image and **invalidating** the cache on the nodes.

> Significantly **more difficult** to setup and submit.

A required step to validate and demonstrate the infrastructure, but not the goal of this flagship.



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Feb. 2025

Events produced in the exercise

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As of today, we have produced 20M with Snakemake and 80M events with the "prod" workflow. Most of these events are Lambda_b decays generated with a Particle Gun.

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Next steps

1. Continue with the production to **keep the system under pressure** and solve problems while they arise (also good for the KPI)

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- 2. Integrate **Leonardo** in the new offloading setup
- 3. Integrate the **HPC Bubble** from Padova
- 4. Validate the infrastructure with *"prod"* workflow
- 5. Reintroduce snakemake and juicefs (and *hetherogeneity*, *GPUs*, ...)

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A recap on Physics Informed Machine Learning

- In Physics Informed Neural Network, the network is the "Ansatz" of a problem defined by a Partial-Difference Equation (PDE).
- The solution is reached by combining information on the PDE, experimental or simulated data, and boundary conditions.
- The solution can be parametric and meshless.
- We are studying two problems relative to the response of solid-state sensors with resistive electrodes, and two-fluid hydrodinamycs.



Figure 1.1 Geometry and working principle of 3D diamond detectors fabricated by electrode graphitization. The dashed line represent a traversing particle depositing energy by ionization.



Lead: Alessandro Bombini

Physics Informed Neural Netorks as interpolator



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Meshless time-dependent simulation with a Neural

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Static simulation

(cheap)

Next steps

- 1. More accurate evaluation of the contribution from the physics is needed.
- 2. Evaluation of the impact of the interpolation on the "physics observables" is in progress (with Garfield++, *Clarissa Buti*)

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3. Prepare an abstract for ACAT?

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After a partial redesign of the offloading infrastructure, we managed to **hit the limit of the distributed file system**. Improvements are possible, but require a more consolidated infrastructure which is still evolving too quickly.

We developed a **"prod" version of the Lamarr validation workflow** designed to run with minimal dependencies on the outside world, designed explicitly for stressing the offloading infrastructure (while doing something still useful...).

With Spoke 0, we are setting up what is needed to offload towards SLURM, enabling adding **Leonardo** and Padova **HPC Bubble** to the resource pools.

The activity on physics-informed machine learning is progressing and is receiving RAC-allocated resources. We should consider applying for a conference in **fall 2025**.





Backup

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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)

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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



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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 PIEIIII	
Storage	25 TB	10 TB	

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• 0.5 M hours from opportunistic borrowing from AI_INFN Platform

Status of the integration of INFN-T1 resources

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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**.



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(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). 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 - 15 / volumeMounts: - name: my-volume mountPath: /cvmfs readOnly: True volumes: - name: my-volume

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persistentVolumeClaim:

claimName: intentionally-not-existing

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

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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:

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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





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[ShubProxy]

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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.



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

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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
 - \circ Slurm submission from edge node icsc01
 - Official interlink slurm plugin

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1	Name Last Modified	<pre>wildcards: runnumber=1142, event_type=12133264, number_of_events=1000 resources: mem mb=2000, mem mib=1908, disk mb=1000, disk mib=954, tmpdir=<tb< pre=""></tb<></pre>	
	envs 29 days ago	D>, millicpu=1000, tolerations=offloading, runtime=7200	
:=	profile	Submitted job 5448 with external jobid 'anderlinil-bender-oct25-09h48m48-440'.	
	rules 27 days ago	[Fri Oct 25 10:13:53 2024]	
-	scripts 2 days ago	Finished job 5378. 95 of 119 steps (80%) done	
	🗅 Snakefile last month	[Fri Oct 25 10:17:31 2024]	
	Y: sql_edm.yaml last month	Finished job 5738. 96 of 119 steps (81%) done	
s	imple 💶 2 🛐 19 🤀 Mem: 2.40 / 8.00 GB	Terminal 3 1 🗘	

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(miniconda3)[lucio@pcl	hcb06 v3]:	\$ k get nodes
NAME	STATUS	ROLES
hub-a100-2	Ready	<none></none>
hub-a100-3	Ready	<none></none>
hub-a102-b	Ready	<none></none>
hub-cpu-2	Ready	<none></none>
hub-master	Ready	control-plane,etcd,master
hub-rtx-2	Ready	<none></none>
hub-rtx-3	Ready	<none></none>
hub-storage	Ready	<none></none>
>infn-tl	Ready	agent
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.



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

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



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Bi-weekly meeting of Spoke 2 – WP 2

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AI_INFN Machine Learning Hackathon with ICSC support

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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: <u>agenda.infn.it/event/43129/</u>



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Welcome to the First edition of the Advanced Artificial Intelligence @ INFN (AI_INFN) hackathon, dedicated to INFN affiliates. This edition is hosted at INFN Sezione di Padova.

Notably, it is the third Hackathon to happen in Person, so please apply only if you are planning to come to Padua. The logistics allow for ~ 20 participants.

AL_INFN hackathons are developed in continuity with ML_INFN hackathons. You may want to check the indico pages of the first (entry level), second (entry level), third (advanced level), fourth (entry level) and fifth (advanced level) editions of ML_INFN hackathons, with most of the talks attached as video files.

The mandatory registration process will be open soon.

In case of a number of registrations exceeding the available positions, the applications will be ranked and selected on the basis of the scientific CV of the applicants and of the order of registration.

The successful applicant will be informed by November 10th. Please do not book hotel/flight before a positive confirmation.

The course is to be considered as "advanced level' for Machine Learning topics. The hackathon will be organized over 3 days, distributed as

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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: <u>agenda.infn.it/event/40829</u>

SOSC 2024 Sixth International School on Open Science Cloud Control Contro Con

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The 6th edition of the International School on Open Science Cloud (SOSC 2024) will be held in Bologna, from 02 to 06 December 2024. The school is organized by INFN, Department of Physics and Astronomy "Augusto Righi" of the University of Bologna, the Departments of Physics and Geology of the University of Perugia and the ICSC Foundation.

The School is multi-disciplinary and targeted at postgraduate researchers including bachelor degree or equivalent in fields such as physics, statistics, computer science, computer vision, biology, medicine, bioinformatics, engineering, working at any research institute, with some experience and interest in data analysis, in computing or in related fields. Applications by university students (undergraduate) will be considered depending on availability and must be accompanied by a letter of reference from a university professor. We embrace diversity and strongly encourage qualified and curtous individuals from all nationalities and backgrounds to apply.

Important dates

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- · Monday 3rd of June applications open
- · Thursday 5th of September acceptance notification sent to the participants
- Saturday 5th of October application closes.
- Application confirmation will be sent to participants by October 20
- Friday 1st of November registration fee payment deadline
 Monday 2nd December student arrivals at Bologna
- Friday 6th of December departure

The SOSC 2024 is also supported by the INFN Commissione Scientifica Nazionale 5 (CSN5) through the initiative "AL_INFN"



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