

Finanziato dall'Unione europea NextGenerationEU

Ministero dell'Università e della Ricerca





Advanced Machine Learning. Flash Simulation and bleeding edge applications

FlashSim: February status report

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Who we are

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Staff members:

- Alessandro Bombini ^j, INFN
- Giuseppe Piparo[/], INFN
- Maurizio Martinelli^a, Università Milano Bicocca
- Simone Capelli ^a, Università Milano Bicocca
- Federica Maria Simone ^{*i*}, Politecnico di Bari
- Nicola De Filippis ^{*i*}, Politecnico di Bari
- Vieri Candelise ^{*h*}, Università di Trieste
- Giuseppe Della Ricca^{*h*}, Università di Trieste
- Valentina Zaccolo ^k, Università di Trieste
- Mattia Faggin ^k, Università di Trieste
- Lorenzo Rinaldi ^e, Università di Bologna
- Piergiulio Lenzi ^g, Università di Firenze
- Vitaliano Ciulli ^g, Università di Firenze
- Sharam Rahatlou^h, Università Roma 1
- Daniele del Re ^{*h*}, Università Roma 1
- Lorenzo Capriotti ^{*f*}, Università di Ferrara
- Francesco Conventi^e, Università di Napoli
- Francesco Cirotto ^e, Università di Napoli

PhD students:

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- Francesco Vaselli ^c, Scuola Normale Superiore di Pisa
- Matteo Barbetti ^{*b*}, Università di Firenze
- Muhammad Numan Anwar ^j, Politecnico di Bari
- Benedetta Camaiani ^g, Università di Firenze
- Alkis Papanastassiou ^g, Università di Firenze
- Antonio D'Avanzo ^e, Università di Napoli

External collaborators:

• Andrea Rizzi ^c, Università di Pisa

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Ongoing activities				
O ALICE - Timing-based vertex-reconstruction validation for the triggerless	DAQ			
 ATLAS - Fast simulation ATLAS - 4D reconstruction algorithms ATLAS - Anomaly detection for full-hadronic final states 	 LHCb - Lamarr (Flashsim) - PID and Calorimetry LHCb - Lamarr (Flashsim) - Tracking 			
CMS - Flashsim	LHCb - F	Parametrization of Chere	enkov detector path inR tive solid-state detector	CH detectors
CMS - Theory-independent classifiers for CMS using domain adaptation	LHCf - R	econstruction of multip	le calorimetric clusters]
		Simulatio Reconstr Monitori Data ana	on ruction ng lysis	

Hear-beat survey: responses

- LHCf Reconstruction of multiple calorimetric clusters: *up and running*
- LHCb Flash simulation of resistive solid-state detectors: *up and running*
- LHCb Tracking parametrizations for Flash Sim: *up and running*
 - Repo: https://qithub.com/s-capelli/lb-trksim-train/tree/notebooks-bicocca
 - Abstract at ACAT 2024 accepted as poster
- LHCb Tracking parametrizations for Particle ID and Calorimetry: *up and running*
- CMS Data anomaly detection for data validation and certification: *up and running*

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- Abstract to AISSAI2024 accepted!
- Repo: <u>https://qithub.com/fsimone91/MuonAE</u>
- ALICE Reconstruction of Omega decays with ML techniques: *restarting*

The current setup made available by AI_INFN is a too scattered into many R&D clusters were different R&D are being performed. We need to converge quickly to a more stable setup. Can we have a formal request for resources to INFN CSN5?

We receive many complaints on the stability and performance of MinIO (DataCloud will phase it out). Can we kindly push for a quick convergence on the identification of a cloud storage solution.

Advanced ML: flash simulation and other applications

Development of algorithms for flash simulation

Effort focused on the development of algorithms for the flash simulation.

Presentation at WP2 meeting, Sept. 26 ^t	^h 2023
A brief introduction to Physics Informed Neural Networks	N are
Basic recipe - graphically represented $\mathcal{F}[\mathbf{u}(\mathbf{z}),\mathbf{z},\gamma] = \mathbf{J}(\mathbf{z}), \mathbf{z}\in\Omega$	
1. Geometry sampler via tessellation $\{z_i\}_{i=1,\dots,N} \in \Omega$ $\mathcal{B}[\mathbf{u}(\mathbf{z}), \mathbf{z}] = \mathbf{g}(\mathbf{z}), \mathbf{z} \in \partial \Omega$	
2. A deep Neural Network (e.g., using Fylorch) $\mathcal{U}_{\theta}(z) \leftarrow DINN[\theta; z]$ 3. A PDE-defining operator (e.g., using Pylorch Autograd) $\mathcal{F}[\hat{u}_{\theta}(z), z, \gamma], \mathcal{B}[\hat{u}_{\theta}(z), z, \gamma]$	Hands-
$ \begin{array}{c} (4. \text{ An optimisation algorithm (e.g., SSD, ADAM L.BFGS)} \\ \hline \\ Governing Equation \\ \hline \\ G_{2n-1} \subset [J] \left[J \left[\int_{0}^{\infty} \frac{dn}{2} \frac{dn}{2} \frac{d^{2}}{2} \left[\int_{0}^{\infty} \frac{dn}{2} \frac{dn}{2} \frac{d^{2}}{2} \left[\int_{0}^{\infty} \frac{dn}{2} \frac{dn}{2} \frac{d^{2}}{2} \left[\int_{0}^{\infty} \frac{dn}{2} \frac{dn}{2} \frac{dn}{2} \left[\int_{0}^{\infty} \frac{dn}{2} \frac{dn}{2} \frac{dn}{2} \left[\int_{0}^{\infty} \frac{dn}{2} \frac{dn}{2} \left[\int_{0}^{\infty} \frac{dn}{2} \frac{dn}{2} \frac{dn}{2} \left[\int_{0}^{\infty} \frac{dn}{2} \frac{dn}{2} \frac{dn}{2} \left[\int_{0}^{\infty} \frac{dn}{2} \frac{dn}{2} \frac{dn}{2} \left[\int_{0}^{\infty} \frac{dn}{2} \frac{dn}{2} \frac{dn}{2} \right] \right] \right] \right] \right] $	CO Open in C
	Authors: M.
$\left(\begin{array}{c} \mathbf{r} \\ \mathbf{r} \\$	Date created
$\mathcal{L}_{\pi} = \frac{1}{ \psi } \sum_{a,b,v} u-d x,t _{2}^{2}$	Last modifie
Input Hidden Layers Output AD Losses Optimise	Description:

Generative A	dversa	rial Ne	Networks PIDGAN [LHCb]				
Algorithms*	Avail	Test	Lipschitzianity**	Design inspired by	Tutorial		
GAN			×	<u>1, 8, 9</u>	Open in Colab		
			×	<u>2, 8, 9</u>	CO Open in Colab		
LSGAN			×	<u>3, 8, 9</u>	Open in Colab		
WGAN				<u>4, 9</u>	CO Open in Colab		
WGAN_GP				<u>5, 9</u>	CO Open in Colab		
				<u>6, 9</u>	CO Open in Colab		
WGAN_ALP			2	<u>7, 9</u>	CO Open in Colab		
BceGAN GP				<u>2, 5, 9</u>	CO Open in Colab		
BCeGAN_ALP			2	<u>2, 7, 9</u>	CO Open in Colab		

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Hands-on Deep Generative Models

Tutorial [CMS]

👩 Open in Colab 🖹 Open in Kaggle 💽 Open in GitHub

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Authors: M. Barbetti (INFN-CNAF), S. Capelli (INFN-MiB), F. Vaselli (INFN-Pisa) Date created: 30/10/2023

Last modified: 12/11/2023

Description: This hands-on demonstrates how deep generative models succeed in reproducing the high-level response of a generic HEP experiment, offering a viable solution to reduce the pressure on the computing budget for simulation production. In particular, in this notebook we will test the performance of Generative Adversarial Networks and Normalizing Flows to parameterize the errors introduced during the detection and reconstruction of high-energy particle jets using the CMS detector.

Documentation

- Ph.D. Thesis Matteo Barbetti
- Advanced Hackathon of ML-INFN [link]
- Notebooks on Lamarr Tracking [<u>link</u>]

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- Doxygen on SQLamarr [<u>link</u>]
- PIDGan tutorials [link]



UNIVERSITÀ Degli studi

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> The *flash-simulation* paradigm and its implementation based on Deep Generative Models for the LHCb experiment at CERN

> > Matteo Barbetti

Dissertation presented in partial fulfillment of the requirements for the degree of Doctor of Philosophy in Smart Computing



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Infrastructure for training

Uploaded to GitHub the Helm chart of the Kubernetes platform to access GPU resources in cloud: <u>https://github.com/landerlini/ai-infn-platform</u>
 Features:

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- \circ $\$ JupyterHub with IAM token authentication
- POSIX interface INFN Cloud MinIO
- Multi-node distributed filesystem based on NFS
- Rudimental batch system, tested for Geant4-based simulations
- Missing feature for the needs of the Flagship: **cvmfs**.
 - Checked with WP5 the feature does not break the offloading model based on InterLink
 - I would like and endorsement of CSN5 before requesting support for ICSC usecases on these resources
- DNS entry registered, deployment still not ready to production: <u>hub.ai.cloud.infn.it</u>
- 4 flagship use-cases tested on development clusters (see below).

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Infrastructure for validation

The validation workflow for Lamarr (LHCb flashsim) has been ported to Snakemake, but it has not been containerized yet.

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It has been tested locally for the decay $B \rightarrow \chi_c K$ showing promising results for charged particles and photons, but more tests are needed to validate the full pipeline.



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KICSC





KPI ID	Description	Acceptance threshold	2024-02-13
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	1 M events (completed: 0.1%)
KPI2.2.1.2	N _{EXP} experiments have tested a machine-learning based simulation	N _{EXP} >= 2	0 experiment (completed: 0%)
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	3 use-cases (since Sept. '23) (completed: 100%)
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	4 use-cases (completed: 80%)

KPIs

List of conferences for KPI2.2.1.3

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- L.A., Generative models at the LHC, ALPACA workshop 2023, Trento
- B. Camaiani, Example of adaptation domain in High Energy Physics, XAI 2023, Milano

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• A. Papanastassiou, "Anomaly detection with autoencoders for data quality monitoring in HEP", XAI 2023, Milano

Abstract accepted (not counted in KPIs, yet. Right?)

- Lamarr: implementing the flash-simulation paradigm at LHCb, ACAT 2024
- F. Simone, Anomaly detection for data quality monitoring of the CMS detector, AISSAI 2024



List of use-cases tested on the platform (%)

- Lamarr, the ultra-fast simulation option for the LHCb experiment (tracking parametrizations)
- Lamarr, the ultra-fast simulation option for the LHCb experiment (particle identification and neutral reconstruction parametrizations)
- Theory-independent classifiers for the data analysis with the CMS experiment
- Machine-learning-based simulation of the response of resistive solid-state detector to the charge generated by a traversing minimum-ionizing particles

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Date

Date



Date Bi-weekly meeting of Spoke 2 - WP 2

On resources

The HPC bubbles requested by this flagship should be commissioned by summer 2024.

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In the meanwhile:

- Compute:
 - ML_INFN is providing GPUs for <u>interactive development</u> (no batch)
 - some of us is starting playing with *Leonardo Booster* for practicing <u>ML with batch jobs</u> (spoke, please clarify rules and procedures)
 - ML_INFN plans for experimental support for batch jobs since early 2024, (but very tight schedule)

• Storage:

- cache and ephemeral storage is available through INFN Cloud (few TB)
- "permanent" storage for data relevant for audit under discussion,
 for the time being, we are encouraged using <u>minio.cloud.infn.it</u>

Get in touch! The machinering is slowly starting to spin, since getting accustomed to the environment may require time, if you plan to use ICSC resources at some point, we suggest you start practicing with the temporary, resource-limited environment we have now.

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