



# Summary on Deep Dive: ML Models Publication

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## Where is (or will be) ML used in CMS?

Front-end electronics	• Fast ML on ASICs for data compression in Phase 2 HGCAL		
Trigger	<ul> <li>Fast ML on FPGAs for Run 3 &amp; Phase 2 L1 trigger and 40 MHz scouting</li> </ul>		
DQM	<ul> <li>Automated data certification</li> <li>Online anomaly detection (ECAL, HCAL, muon system)</li> </ul>		
Simulation	<ul> <li>Calorimeter simulation with generative models</li> </ul>		
Reconstruction	<ul> <li>Energy and mass regression (e.g., MET, photons, electrons, jets)</li> <li>PU mitigation</li> <li>Clustering (e.g., calorimeter, jets, vertexing)</li> <li>Particle flow</li> </ul>		
Analysis / object ID	<ul> <li>Tau leptons, heavy flavour / boosted / displace jets tagging</li> <li>Event classification</li> <li>Background estimation</li> <li>Uncertainties evaluation</li> </ul>		

# A growing number of ML technical papers

<u>Code</u>	Name
MLG-23-001 » <u>Mc</u> I - show I - CDS I - CSBS	Portable Acceleration of CMS Mini-AOD Production with Coprocessor
MLG-23-002 » <u>Mc</u> - show	ML techniques for identification of anomalous jets
MLG-23-003 » <u>Mc</u> I - show	ABCD background estimation method with ML for a Stealth and RPV t
MLG-23-004 » <u>MC</u> - show	Neural Autoregressive Flows for Data-driven background estimation
MLG-23-005 » <u>Mc</u> I <b>v</b> show	ML aspects of ML-based STXS measurements in Higgs to tau tau

Most are companion to a physics results paper indicating that the **complexity and innovation in the ML technical work** behind cannot be simply summarized anymore with a citation of external work

### Why publish ML models?

#### To preserve, reuse, and reinterpret our results!

**Executive summary.** To achieve their full scientific impact, HEP experiments need to integrate extensive data and analysis preservation efforts into their publication processes, alongside the communication of results in reusable form and preservation of data products, and making event-level data publicly available. Without this, the influence of the hundreds of published analyses from the LHC, HL-LHC, EIC, and other future experiments will be limited mainly to the physics ideas in vogue at the time the collaboration collected their data. The public investment in experimental programs underscores the importance of going beyond the original paper publication and ensuring that analyses continue providing scientific value in perpetuity.

Snowmass '21: Data and Analysis Preservation, Recasting, and Reinterpretation <u>arXiv:2203.10057</u>

### **Reinterpretation: concept and workflow**

**Reinterpretation** consists of recoding a published analysis from scratch for the purpose of interpreting it in terms of other physics models not interpreted in the original publication. Usually done by phenomenologists to test their favorite physics model.

- An analysis code is rewritten outside the original experimental frameworks.
  - Analysis recoding is done less accurately compared to the original experimental code, since detector information does not exist in full detail in public simulation tools.
  - Public tools exist (by phenomenologists, experimentalists, also by ATLAS).
- Monte Carlo simulated events for the signal models are produced.
- Analysis code is run on the events to obtain predicted signal counts / efficiencies.
- Predicted signal counts are used together with observed data and background estimation results from the experimental publication to calculate limits.

IMPORTANT: Must validate the analysis by reproducing the experimental interpretation. e.g. try to obtain cutflows, limits consistent with those given in the paper.

#### From Sezen's talk at Deep Dive

# **Challenges of publishing ML models**

An analysis that uses ML heavily is much less accessible than a traditional cut & count analysis based on human-engineered features

- Providing sufficient model metadata (e.g. input preprocessing, etc.)
- Sharing models on an appropriate platform to enable discoverability (e.g. Huggingface, Zenodo, HEPData, etc.) + cross-referencing CMS analysis/publication
- Ensuring the model is in a persistent format (e.g. that can be read by future versions of software)
- Ensuring reusability of the model in simplified public simulation (e.g. Delphes)
- Adhering to Findable, Accessible, Interoperable, and Reusable (FAIR) Principles

### **Deep Dive on ML models publication**

#### Afternoon (CMS)

Discussion

			http	s://i	ndico.cern.ch/event/1355548/
		13:00	Flash Sim		
			Speaker: Andrea Rizzi (Universita & INFN Pisa (IT))		
Morning	(non CMS)		FlashSim.mp4 🔗 slides		
10:00	Introduction Speakers: Javier Mauricio Duarte (Univ. of California San	13:20	Discussion	Afternoo	n (CMS)
	B GMT20240129-090	12.20	Inputs from BTV	15:30	EXO-22-026: Searching for new physics detecting anomalies in jets Sneaker: 02 Amram (Fermi National Accelerator Lab. (US))
		13.30	Speaker: Ming-Van Lee (Phainingh Wastfachingha Taph, Hach, (DE)		CASE_reinterpretati
10:10	Discussion		BTV ML.pdf BTV.mp4	15:45	Discussion
10:20	Les Houches recommendations summary Speaker: Sezen Sekmen (Kyungpook National University (Ki	13:40	Discussion	15:55	EXO-22-015: Search for Emerging Jets with full Run 2 data Speaker: Yi-Mu Chen (University of Maryland (US))
	LesHouches.mp4 A SekmenLHML2301	13:50	Inputs from JME	16:10	Discussion
10:50	Discussion		Speaker: Anna Benecke (Universite Catholique de Louvain (UCL) (F 20240129_JME_Inp	16:20	SUS-23-001: Search for Stealth/RPV stops using Double DisCo neural network method Speaker: Joshua Hiltbrand (Baylor University (US))
11:00	Surrogate model Speaker: Sebastian Guido Bieringer (Hamburg University	14:00	Discussion	16:35	GM120240129-151 MLG23003_202401
	SurClass.pdf SurrogateModel.mp4	14:10	Inputs from cross-POG	16:45	EXO-22-020: Search for new physics with at least one displaced vertex and missing energy Speaker: Ang Li (Austrian Academy of Sciences (AT))
11:20	Discussion		Speaker: Dr Jean-Roch Vlimant (California Institute of Technolog xPOG_MLDeepDive XPOG.mp4	17:00	Discussion
11:30	ML model release in ATLAS	I		17:10	FAIR AI Models and FAIR4HEP
	Speaker: Lukas Alexander Heinrich (Technische Universit	14:20	Discussion		Speaker: Dr Eliu Huerta
	ATLAS.mp4 🔑 ML_Publish_Models	14:30	Statistical results publication in CMS	17:30	
11:50	Discussion		Speaker: Piergiulio Lenzi (Universita e INFN, Firenze (IT))		
			CAT_DeepDive_MLp		

#### **Recommendations from Les Houches**

#### Les Houches guide to reusable ML models in LHC analyses

Jack Y. Araz<sup>1</sup>, Andy Buckley<sup>2</sup>, Gregor Kasieczka<sup>3</sup>, Jan Kieseler<sup>4</sup>, Sabine Kraml<sup>5</sup>, Anders Kvellestad<sup>6</sup>, Andre Lessa<sup>7</sup>, Tomasz Procter<sup>2</sup>, Are Raklev<sup>6</sup>, Humberto Reyes-Gonzalez<sup>8,9,10</sup>, Krzysztof Rolbiecki<sup>11</sup>, Sezen Sekmen<sup>12</sup>, Gokhan Unel<sup>13</sup>

#### Abstract

With the increasing usage of machine-learning in high-energy physics analyses, the publication of the trained models in a reusable form has become a crucial question for analysis preservation and reuse. The complexity of these models creates practical issues for both reporting them accurately and for ensuring the stability of their behaviours in different environments and over extended timescales. In this note we discuss the current state of affairs, highlighting specific practical issues and focusing on the most promising technical and strategic approaches to ensure trustworthy analysis-preservation. This material originated from discussions in the LHC Reinterpretation Forum and the 2023 PhysTeV workshop at Les Houches.

#### Keywords

BSM; Tools; Machine-learning; Reinterpretation.

1	Introduction
2	Mechanisms and examples
3	Analysis design
4	Material for implementation and validation
5	Surrogate models
6	Summary and conclusions

#### https://arxiv.org/abs/2312.14575

## ML model design: checklist

For BDTs: <u>petrify-bdt</u> is a effort from within HEP to provide a more dependency-free way of preserving and executing BDTs: read framework-specific BDT models (e.g. TMVA XML) and output standard-library C++ and/or Python code

- Use machine-learning software that can be easily converted to a stable interchange format supported by open-source tools.
  - The ONNX and LWTNN JSON formats are the current most stable options for NNs.
- Alternatively, if possible, export the ML model to executable code without dependencies beyond standard libraries.
- Preserved networks should be runnable with as few dependencies as possible from an API to a compiled language (e.g. C++), not just from Python.
- Avoid over-complexity in network design, e.g. not using customised layers or custom activation functions if the application does not require them. Ensure the chosen architecture has sufficient preservation-format support, particularly with ONNX.
- Where possible, and especially if the model is dominated by simple kinematic inputs, avoid input features that are heavily dependent on detector and reconstruction details.
- Where inputs are heavily detector-based, in addition to preserving the ML model itself, provide detailed efficiency maps (including mistag rates) or an equivalent surrogate network using less detector-sensitive input features (see Section 5).

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# Implementation & Validation: checklist

From Sezen's talk at Deep Dive

- Provide exact definitions (including units, ordering and conventions) of network input features, either as code examples or documentation.
- Provide a sample of input features and output values for technical validation.
- Provide *plots of input and output variables* for validation samples, if possible, with some indication of feature importance, as analysis supporting data.
- Provide *cut-flow information*, both before and after any ML-based selections.
- Validated and runnable published analysis code can be the clearest expression of both the general analysis logic and the specific interfacing with the ML functions.
- *Full descriptions of the physics models* used to generate the information above, e.g. SLHA files and generator run cards, are essential inputs to validating any serious reinterpretation
- ML training/evaluation code might not be essential in most cases but it is certainly encouraged (to be seen case by case)
- These guidelines go together with usual analysis preservations ones (e.g. analysis logic and analysis code/snippets, likelihoods cutflows, distributions, etc...)

#### Some examples from ATLAS

#### ATLAS published three Analyses with ONNX

(+ 1 Analyses that store PyTorch specific serialization)

EUROPEAN ORGANISATION FOR NUCLEAR RESEARCH (CERN)Image: Image:	EUROPEAN ORGANISATION FOR NUCLEAR RESEARCH (CERN)         Image: CERN-EP-2021-086         DIT IN THE SECTION FOR REPART OF THE SECTION OF THE	EUROPEAN ORGANISATION FOR NUCLEAR RESEARCH (CERN)Image: Colspan="2">Image: Cern-Ep-2022-213DiferenceDiferenceDiferenceSearch for supersymmetry in final states with missing transverse momentum and three or more b-jets in 139 fb <sup>-1</sup> of proton-proton collisions at $\sqrt{s} = 13$ TeV with the ATLAS detectorThe ATLAS CollaborationA search for supersymmetry in volving the pair production of gluinos decaying via off-shell third-generation squarks into the lightest neutralino ( $f_1^0$ ) is reported. It exploits LHC proton- proton collision data at a center-of-mass energy of a 13 TeV with an integrated luminosity of 139 fb <sup>-1</sup> ollected with the ATLAS detector from 2015 to 2018. The search uses events
139 fb <sup>-1</sup> of proton-proton collision data collected by the ATLAS detector at the LHC in         2015-2018 at a centre-of-mass energy of 13 TeV. Dedicated techniques were developed for         the reconstruction of displaced jets produced by LLPs decaying hadronically in the ATLAS         hadronic calorimeter. Two search regions are defined for different LLP kinematic regimes.         The observed numbers of events are consistent with the expected background, and limits for         cavard banchmark signals are determined. For a SM Higgs bocon with a mass of 125 CeV	A search for R-parity-violating supersymmetry in final states characterized by high jet multiplicity, at least one isolated light lepton and either zero or at least three <i>b</i> -tagged jets is presented. The search uses $139 \text{ fb}^{-1}$ of $\sqrt{s} = 13 \text{ TeV}$ proton–proton collision data collected by the ATLAS experiment during Run 2 of the Large Hadron Collider. The results are interpreted in the context of <b>P</b> parity violating supersymmetry models that fortune plains production	<ul> <li>proton collision data at a centre-of-mass energy \$\sqrt{e}\$ = 13 TeV with an integrated luminosity of 139 fb<sup>-1</sup> collected with the ATLAS detector from 2015 to 2018. The search uses events containing large missing transverse momentum, up to one electron or muon, and several energetic jets, at least three of which must be identified as containing b-hadrons. Both a simple kinematic event selection and an event selection based upon a deep neural-network are used.</li> <li>No classificant average about the analytical baskaround is found. In classificat models involving</li> </ul>

#### https://www.hepdata.net/ record/ins2043503

https://www.hepdata.net/ record/ins1869040

https://www.hepdata.net/ record/ins2182381

#### From Lukas talk at Deep Dive

#### Some examples from ATLAS

ATLAS started with publishing TMVA XML (which in turn can be used with petrify-bdt) or petrify-bdt standalone code directly

hadronic calorimeter. Two search regions are defined for different LLP kinematic regimes. The observed numbers of events are consistent with the expected background and limits for	EUROPEAN ORGANISATION FOR NUCLEAR RESEARCH (CERN) EUROPEAN ORGANISATION FOR NUCLEAR RESEARCH (CERN) DIFED 06 (2022) 005 DOI: 10.1007/JHEP06(2022)005 CERN-EP-2022-00 19th August 202 Search for neutral long-lived particles in <i>p p</i> collisions at $\sqrt{s} = 13$ TeV that decay into displaced hadronic jets in the ATLAS calorimeter The ATLAS Collaboration A search for decays of pair-produced neutral long-lived particles (LLPs) is presented using 139 fb <sup>-1</sup> of proton-proton collision data collected by the ATLAS detector at the LHC in 2015-2018 at a centre-of-mass energy of 13 TeV. Dedicated techniques were developed for the reconstruction of displaced jets produced by LLPs decaying hadronically in the ATLAS hadronic calorimeter. Two search regions are defined for different LLP kinematic regimes. The observed numbers of events are consistent with the expected becknowl and limits for	EUROPEAN ORGANISATION FOR NUCLEAR RESEARCH (CERN)         Image: Colspan="2">Image: Cernet is a constrained of the supersymmetric partners of quarks and gluinos in final states with jets and missing transverse momentum using 139 fb <sup>-1</sup> of $\sqrt{s} = 13$ TeV $p$ collision data with the ATLAS detector         The ATLAS Collaboration         A search for the supersymmetric partners of quarks and gluinos in final states and missing transverse momentum using 139 fb <sup>-1</sup> of $\sqrt{s} = 13$ TeV $p$ collision data with the ATLAS detector         The ATLAS Collaboration
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#### https://www.hepdata.net/record/ins2043503

#### https://www.hepdata.net/record/ins1827025

From Lukas talk at Deep Dive

# Surrogate models

- Main problem: the theorist might use a Delphes-simulated signal which differs from full CMS simulation → wrong response of the ML model
- A surrogate model as solution: neural network trained to replicate the output of the original ML model but using input events with a simpler set of attributes



### Surrogate model: toy setup



### FlashSim

- Universal, fast ML-based end-to-end simulation
- Targets: quickly retrainable, fast as Delphi's, accuracy between FastSim and FullSim



From Andrea's talk at Deep Dive

#### **FlashSim Performance**



### **FlashSim Scenarios**

- Publish FlashSim model(s) to enable reinterpretation on new generated signal
- Several possible scenarios envisioned: (1) fully general NANOAOD, (2) analysis-specific ntuples, (3) final analysis observables



### Where do we start?

- In general, any analysis using simple NN (or BDT) should at least publish in HEPData the ONNX model (petrify-bdt/xml for BDTs) similarly to what ATLAS did
  - Important to document all aspects of the model, e.g. expected use/performance, input preprocessing, etc. along the lines of a Hugging Face model card: <u>https://huggingface.co/docs/hub/en/model-cards</u>
- Other analyses using less reusable models and inputs will require a case by case discussion
  - e.g., publish training code with toy dataset and/or train surrogate model
- We considered a few analyses and a few POGs papers where we can start applying recommendations

#### **PAG Feedback**

- Several analyses shared feedback on challenges and opportunities
- EXO-22-026: Searching for new physics detecting anomalies in jets (CASE)
  - Weakly supervised models require retraining for new signals => Publish training code alongside example trained models
- SUS-23-001: Search for Stealth/RPV stops using Double DisCo neural network method
  - Several analyses use CMS-specific information not available in Delphes, e.g. b-tagger discriminants => Need FlashSim or similar surrogate model solution to enable reinterpretation
- EXO-22-015: Search for Emerging Jets with full Run 2 data
- **EXO-22-020:** Search for new physics with at least one displaced vertex and missing energy

### **POG Feedback**

#### b-hive : An object-tagging and ML framework



MLG+POG publications currently under discussion

→ candidates for ML model release:

- AK8 Particle Transformer
- AK4 Particle Transformer
- DeepMET
- ABCNet for PU mitigation

#### **FAIR AI Models**

• What is the right way to share training code?

• Can leverage "cookie cutter" project structure <u>https://github.com/FAIR4HEP/</u> cookiecutter4fair

		LICENSE Makefile CITATION.cff README.md data Local processed raw	<- License for reusing code <- Makefile with commands like `make data` or `make train` <- Standardized citation metadata <- The top-level README for developers using this project <- The final, canonical data sets for modeling <- The original. FAIR, and immutable data dump
IOP Publishing	Mach. Learn.: Sci. Technol. 4 (2023) 045062 https://doi.org/10.1088/2632-2153/ad12e	Dockerfile	For building a containerized environment
	MACHINE LEARNING Science and Technology	docs	<- A default Sphinx project for documentation; see sphinx-doc.org for details
	DADED	— models	<- Trained and serialized models, model predictions, or model summaries
CrossMark OPEN ACCESS	FAIR AI models in high energy physics	— notebooks	<- Jupyter notebooks. Naming convention is a number (for ordering), the creator's initials, and a short `-` delimited description, e.g. `1.0-jqp-initial-data-exploration`.
RECEIVED 21 December 2022	Philip Harris <sup>®</sup> <sup>(6)</sup> , Raghav Kansal <sup>1</sup> <sup>(6)</sup> , Daniel S Katz <sup>2</sup> <sup>(6)</sup> , Ishaan H Kavoori <sup>1</sup> , Volodymyr V Kindratenko <sup>2</sup> <sup>(6)</sup> , Farouk Mokhtar <sup>1,6</sup> <sup>(6)</sup> , Mark S Neubauer <sup>2</sup> <sup>(6)</sup> , Sang Eon Park <sup>3</sup> <sup>(6)</sup> , Melissa Quinnan <sup>1</sup> <sup>(6)</sup> , Roger Rusack <sup>7</sup> <sup>(6)</sup>	- references	<- Data dictionaries, manuals, and all other explanatory materials
REVISED 27 October 2023 ACCEPTED FOR PUBLICATION 6 December 2023	and Zhizhen Zhao <sup>3</sup> <sup>1</sup> University of California San Diego, La Jolla, CA 92093, United States of America <sup>2</sup> University of Illinois at Urbana-Champaign, Urbana, IL 61801, United States of America <sup>3</sup> Argonne National Laboratory. Lemont. IL 60439. United States of America	└── reports └── figures	<- Generated analysis as HTML, PDF, LaTeX, etc. <- Generated graphics and figures to be used in reporting
PUBLISHED 29 December 2023	<ol> <li><sup>4</sup> The University of Chicago, Chicago, IL 60637, United States of America</li> <li><sup>5</sup> Massachusetts Institute of Technology, Cambridge, MA 02139, United States of America</li> <li><sup>6</sup> Halıcıoğlu Data Science Institute, La Jolla, CA 92093, United States of America</li> </ol>	<pre> requirements.txt</pre>	<- The requirements file for reproducing the analysis environment, e.g. generated with `pip freeze > requirements.txt`
Original Content from this work may be used under the terms of the Creative Commons Attribution 4.0 licence. Any further distribution of this work must	<ul> <li><sup>7</sup> The University of Minnesota, Minneapolis, MN 55405, United States of America</li> <li>* Author to whom any correspondence should be addressed.</li> <li>E-mail: jduarte@ucsd.edu</li> <li>Keywords: FAIR, AI, high energy physics, Higgs boson, ML</li> </ul>	└── setup.py └── src └──initpy	<pre>&lt;- Makes project pip installable (`pip install -e .`) so src can be imported &lt;- Source code for use in this project &lt;- Makes `src` a Python module</pre>
maintain attribution to the author(s) and the title of the work, journal citation and DOI.	Abstract The findable, accessible, interoperable, and reusable (FAIR) data principles provide a framework	└── data └── make_datas	<- Scripts to download or generate data set.py
	for examining, evaluating, and improving how data is shared to facilitate scientific discovery. Generalizing these principles to research software and other digital products is an active area of research. Machine learning models—algorithms that have been trained on data without being	features	<- Scripts to turn raw data into features for modeling tures.py
	explicitly programmed—and more generally, artificial intelligence (AI) models, are an important target for this because of the ever-increasing pace with which AI is transforming scientific domains such as experimental high energy physics (HEP). In this paper, we propose a practical definition of FAIR principles for AI models in HEP and describe a template for the application of these principles. We demonstrate the template's use with an example AI model applied to HEP, in which a graph neural network is used to identify Higgs bosons decaying to two bottom quarks. We report on the robustness of this FAIR AI model is portability across hardware architectures and coffurer.	<pre>models     predict_mc     train_mode     visualization</pre>	<- Scripts to train models and then use trained models to make predictions odel.py el.py
	frameworks, and its interpretability.	tox.ini	.py <- Tox file with settings for running `tox`: see tox.readthedocs.io

### Conclusions

- Questions considered:
  - what are the best practices for sharing ML models in industry? in other sciences? in HEP?
  - how do we make published CMS ML models easy to find / linked to the paper?
  - how do we make published CMS ML models the most useful for reinterpretation?
  - what formats are CMS ML models currently stored in?
  - what types of inputs do CMS ML models use (low-level CMS-specific inputs? high-level particle inputs?)
  - how do we determine when a CMS ML model should be published (or just an efficiency map?)
  - should we release training code as well?
- Goal: draft internal CMS recommendations to publish CMS ML models for physics/ML papers as part of the publication pipeline
  - similar to HEPData requirements
- First attempts will not be the optimal but we need to start from somewhere...

#### **RAMP Seminars**

Preserving the just the pure model is not enough. Important Forum to bring together those who publish and those who re-use to check e.g. limitations, option questions, etc



#### https://indico.cern.ch/event/1083851/

#### https://indico.cern.ch/event/1233294/

# Backup

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AH! TINDABLE

Image: <u>book.fosteropenscience.eu</u>

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F1. (meta)data have **unique** and **persistent** identifier

F2. data are described with rich metadata

F3. metadata specify the data identifier

F4. (meta)data are registered or indexed in a searchable resource



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A1. (meta)data are retrievable using standardized protocol A1.1 protocol is open, free, and universally implementable A1.2 protocol allows for authentication and authorization A2. metadata are accessible, even when the data is not



ACCESSIBLE

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TINDABLE

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I1. (meta)data use a formal, shared, and broadly applicable language for knowledge representation

I2. (meta)data use **vocabularies** that follow FAIR principles

I3. (meta)data include qualified references to other (meta)data





DOI 10.107/8.797

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ACCESSIBLE

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I3. (meta)data include qualified references to other (meta)data

R1. (meta)data have a plurality of accurate and relevant attributes

R1.1. (meta)data have clear and accessible data usage license

- R1.2. (meta)data are associated with their provenance
- R1.3. (meta)data meet domain-relevant community standards



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