FAIR principles for Digital Objects in High Energy Physics A Case Study with Universal FeynRules Output (UFO) Models

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Abstract

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Research in the data-intensive discipline of high energy physics (HEP) often relies on domain-specific digital contents. Reproducibility of research relies on proper preservation of these digital objects. This paper reflects on the interpretation of principles of Findability, Accessibility, Interoperability, and Reusability (FAIR) in such context and demonstrates its implementation by describing the development of an end-to-end support infrastructure for preserving and accessing Universal FeynRules Output (UFO) models guided by the FAIR principles. UFO models are custom-made python libraries used by the HEP community for Monte Carlo simulation of collider physics events. Our framework provides simple but robust tools to preserve and access the UFO models and corresponding metadata in accordance with the FAIR principles.

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Details in our paper <u>arxiv: 2209.09752</u> recently accepted at *SciPost Physics Codebases* Git repositories: <u>https://github.com/Neubauer-Group/UFOManager</u> <u>https://github.com/Neubauer-Group/UFOMetadata/</u>



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The FAIR Principles

- To inspire scientific data management for reproducibility and maximal reusability¹
- Originally proposed for scientific data
- Can be interpreted as guidelines to manage and preserve other Digital Objects (DOs) e.g. research software² , tutorials and notebooks³ , AI and ML models⁴
- Different working groups working on FAIR guidelines for different DOs (e.g <u>FAIR4RS</u>, <u>FAIR</u> <u>workflows</u>, <u>FAIR VREs</u>)

	FAIR DATA PRINCIPLES			
idable:locating DOs in a failsafe fashioncessible:obtaining DOs along with their	AH!	I O I I O I OII O I I O I I O I O	HOW DO YOU OPEN A .XEQ FILE?	
eroperable: context, content, and format being usable across multiple	(C)	f		▶ ₽
usable: computing platforms specifying the context and extent of reusing DOs	Tinbable	Accessible	INTEROPERABLE	REUSABLE

Extending FAIR to Other Digital Objects

- Interpretation of FAIR depends on the nature of the digital content being FAIRified
- Dedicated work being done for interpreting and benchmarking the FAIR principles for a variety of digital objects
- Question: What kind of tools and processes are needed to make HEP DOs FAIR?
- Constraints:
 - FAIRification without interfering with the established 0 practices of developing the DOs
 - Compatible with existing DOs as well as newer content 0
 - Preferably, an end-to-end software system with certain 0 automations incorporated

arxiv: 2212.05081

FAIR AI Models in High Energy Physics

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Abstract. The findable, accessible, interomerable, and reusable (FAIR) data principles have provided a framework for examining, evaluating, and improving how we share data with the aim of facilitating scientific discovery. Efforts have been made to generalize these principles to research software and other digital products. Artificial intelligence (AI) models-algorithms that have been trained on data rather than explicitly programmed-are an important target for this because of the everincreasing pace with which AI is transforming scientific and engineering domains. In this paper, we propose a practical definition of FAIR principles for AI models and create a FAIR AI project template that promotes adherence to these principles. We demonstrate how to implement these principles using a concrete example from recommentation in the intervention of the principles in the principles in the principle in their portability across hardware architectures and software frameworks, and report new insulation of the interpretability of AI predictions by studying the interpretability between FAIR datasets and AI models. Enabled by publishing FAIR AI models, these studie pave the way toward reliable and automated AI-driven scientific discovery

arxiv: 2210.08973

FAIR for AI: An interdisciplinary, international, inclusive, and diverse community building perspective

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Introducing the FAIR Principles for research software

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Universal FeynRules Output (UFO) Models

- UFO models are used for simulating Beyond Standard Model Physics with Monte Carlo generators
- Custom Python libraries that pack necessary physics content as modules
- Designed to be **Interoperable** across multiple generator
- Heavily used in ATLAS and CMS analyses
- No uniform convention for management and citation practices for these models
- Most models are preserved at the <u>FeynRules Model</u>
 <u>Database</u> w/o dedicated metadata preservation or version controlling

Model-independent files	Model-dependent files
	particles.py
initpy	coupling_orders.py
object_library.py	parameters.py
function_library.py	vertices.py
write_param_card.py	couplings.py
	lorentz.py

Why FAIRify UFOs? The Case for UFO Citations

- In many cases, only the theory paper describing the physics model is cited
- The actual digital object i.e. the implementation of the model itself is not always cited
- When cited, no uniform convention is followed
- Often digital repositories are cited, that may be lost/changed when the hosting service or the hosting account becomes inactive

- [220] DM forum repository, *Higgs_scalar UFO model webpage*, https://svnweb.cern.ch/cern/wsvn/LHCDMF/trunk/models/Higgs_scalar_UFO/.
- [221] DM forum repository, Zp2HDM_UFO UFO model webpage, https://svnweb.cern.ch/cern/wsvn/LHCDMF/trunk/models/EW_Higgs_2HDM/.
- [222] DM forum repository, DMS_tloop UFO model webpage, https://svnweb.cern.ch/cern/wsvn/LHCDMF/trunk/models/Monojet_DMS_tloop/.
- [223] DM forum repository, DMScalarMed_loop UFO model webpage, https://svnweb.cern.ch/cern/wsvn/LHCDMF/trunk/models/HF_S+PS/.
- [224] DM forum repository, dmS_T UFO model webpage, https://svnweb.cern.ch/cern/wsvn/ LHCDMF/trunk/models/Monojet_tChannel/contributed_by_Amelia_Brennan/.

From the references in JHEP 05 (2019) 142



Making UFOs FAIR

- Making UFOs FAIR requires consistent standards for
 - preserving the models with persistent identifiers like DOIs (F, A)
 - storing domain-specific enriched metadata (I, R)
 - allowing search and download models (F, R)
- FAIRification should be independent of developing the UFO, compatible with existing models (hence, compatible with both Python 2 and 3)

UFOManager

Dedicated software developed to

- Validate models
- Create enriched metadata
- Store said metadata in dedicated repo
- Publish model in Zenodo with DOI
- Facilitate search and download of models
- Allows version controlling

<u>UFOMetadata</u>

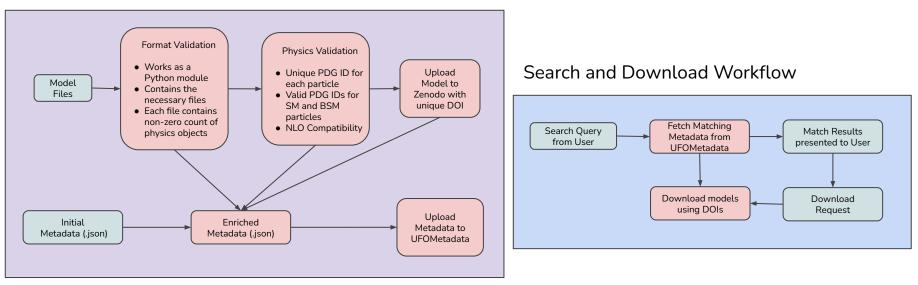
Dedicated repository developed to

- Store metadata of published UFO models
- Validate metadata format with continuous integration

6

UFOManager

Upload Workflow



The Enriched Metadata

{		
	"Author": [
		{"name" : "Luca Panizzi",
		"affiliation": "Uppsala University",
		"contact": "luca.panizzi@physics.uu.se"},
		{"name" : "Benjamin Fuks",
		"affiliation": "Sorbonne University",
		"contact": "fuks@lpthe.jussieu.fr"}
],	
	"Paper_id":	{"doi": "10.1140/epjc/s10052-017-4686-z",
		"arXiv" : "1610.04622"},
	"Description":	"Vector-like Quark UFO Model at NLO QCD
		with four flavour scheme",
	"Model Homepage" :	"https://feynrules.irmp.ucl.ac.be/wiki/NLOModels"
}		

Initial Metadata





"Model name": "Model Doi":	"UFO model for Vector-like Quarks at NLO QCD with four flavor scheme", ""10.5281/zenodo.6977663"",
"Author":	10.5261/201000.09//003 ,
	{"name" : "Luca Panizzi",
	"affiliation": "Uppsala University",
	"contact": "luca.panizzi@physics.uu.se"},
	{"name" : "Benjamin Fuks",
	"affiliation": "Sorbonne University",
	"contact": "fuks@lpthe.jussieu.fr"}
],	
"Paper_id":	{"doi": "10.1140/epjc/s10052-017-4686-z",
	"arXiv" : "1610.04622"},
"Description":	"Vector-like Quark UFO Model at NLO QCD
	with four flavour scheme",
"Model Homepage" :	"https://feynrules.irmp.ucl.ac.be/wiki/NLOModels",
"Number of decays":	10,
"Number of coupling orders":	3, 97,
"Number of coupling tensors": "Number of lorentz tensors":	39.
"Number of parameters":	98,
"Number of vertices":	125.
"Number of propagators":	4,
"Model Python Version":	2,
"Model Version":	1.0,
"Allows NLO calculations":	true,
"All Particles":	{"ve": 12, "ghG~": -82, "y~": -6000008,
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	"c~": -4, "t~": -6, "G0": 250, "u": 2,
	"ve~": -12, "tp": 6000006,
	"x~": -6000005, "G-": -251,
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	"y": 6000008, "e+": -11, "H": 25, "t": 6,
	"vm": 14, "d~": -1, "s~": -3,
	"mu-": 13, "ghG": 82, "bp": 6000007, "a": 22,
	"x": 6000005, "ta-": 15,
	"b∼": -5, "Z": 23,
	"d": 1, "g": 21,
	"W-": -24, "W+": 24,
	"tp~": -6000006, "mu+": -13,
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on faiticies :	"c~": -4, "t~": -6, "u": 2,"ve~": -12,
	"ta+": -15, "vt~": -16, "e-": 11,
	"e+": -11, "H": 25, "t": 6,
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	"b~": −5, "Z": 23,
	"d": 1, "g": 21,
	"W-": -24, "W+": 24,
	"tp~": -6000006, "mu+": -13,
	"bp~": -6000007, "c": 4, "b": 5, },
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New elementary particles .	"bp": 6000007, "x~": -6000005, "x": 6000005,
	"y": 6000008, "tp~": -6000006, "G-": -251,
	"G+": 251, "bp~": -6000007 }
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"Particles with PDG-like IDs":	{"GO": {"charge": 0.0, "spin": 1, "id": 250},
	"bp": {"charge": -1/3, "spin": 2, "id": 6000007},
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	"y ": {"charge": 4/3, "spin": 2, "id": -6000008 },
	"y": {"charge": -4/3, "spin": 2, "id": 6000008 },
	"x": {"charge": 5/3, "spin": 2, "id": 6000005 },
	"bp ": {"charge": 1/3, "spin": 2, "id": -6000007}}

UFOMetadata

- Stores Metadata for FAIRified UFO models
- Interfaces with the Upload script of UFOManager to enable the storage of enriched metadata, and with the Download script to enable search for the right UFO models
- Has a built-in Continuous Integration Workflow to automate the integration of new UFO models

promain + UFOMetadata / Metadata /		Go to file Add file *
^{г-к} yorkiva updated metadata		× 30360ee on Jan 25 🕤 History
DMSimpt_NLO_v1_2_UFO.json	updated metadata	4 months ago
DMspin2.json	updated metadata	4 months ago
SM_with_pNG_UFO.json	updated metadata	4 months ago
SM_with_pNG_UFO_py3.V2.0.json	updated metadata	4 months ago
SUSYQCD_UFO.json	updated metadata	4 months ago
VLQ_v4_5FNS_UFO.json	updated metadata	4 months ago
VLQ_v5_4FNS_NLO_UFO.V2.0.json	updated metadata	4 months ago
VLQ_v5_4FNS_NLO_UFO.V3.0.json	updated metadata	4 months ago
VLQ_v5_4FNS_only3rd_NLO_UFO.json	updated metadata	4 months ago
VLQ_v5_5FNS_NLO_UFO.V2.0.json	updated metadata	4 months ago
VLQ_v5_5FNS_only3rd_NLO_UFO.json	updated metadata	4 months ago
C sgluons_NLO.json	updated metadata	4 months ago
stop_ttmet_NLO.json	updated metadata	4 months ago
l vlq_v4_4fns.json	updated metadata	4 months ago

Summary and Outlook

- The work presented here is a demonstrative example of the kind of tools and approaches needed to FAIRify custom-HEP DOs
- Room for improvement:
 - Seamless integration with existing model repositories and databases
 - \circ ~ Work to be done to include compatibilities with UFO v2.0 ~
 - Making it a part of a more sustainably preserved cyberinfrastructure for development, preservation, dispersion, and citation of UFO models
- Ultimately, we hope to initiate and engage in a larger community-wide discussion on adaptation of FAIR principles for DOs (UFOs and beyond) in HEP



Mark Neubauer



Zijun Wang

References

- 1. Wilkinson, M., Dumontier, M., Aalbersberg, I. et al. The FAIR Guiding Principles for scientific data management and stewardship. Sci Data 3, 160018 (2016). <u>https://doi.org/10.1038/sdata.2016.18</u>
- 2. Chue Hong, Neil P., Katz, Daniel S., Barker, Michelle et al. RDA FAIR4RS WG. (2022). FAIR Principles for Research Software (FAIR4RS Principles) (1.0). <u>https://doi.org/10.15497/RDA00068</u>
- 3. Richardson, R. A., et al. "User-friendly Composition of FAIR Workflows in a Notebook Environment." Proceedings of the 11th on Knowledge Capture Conference. 2021. <u>https://doi.org/10.1145/3460210.3493546</u>
- 4. Katz, D. S., Psomopoulos, F. E., and Castro, L. J. "Working towards understanding the role of FAIR for machine learning." DaMaLOS@ ISWC (2021): 1-7. <u>https://doi.org/10.4126/FRL01-006429415</u>