UNIVERSITY OF LIVERPOOL

Computing & Software developments for HEP

Eduardo Rodrigues, for several colleagues (see names in pages)

Particle Physics Annual Meeting, Liverpool, 18th – 19th May 2023

MC work – GENIE Monte Carlo generator

Costas Andreopoulos, Marco Roda, Julia Tena-Vidal (now a post-doc at TAU)

- **Liverpool-led event generator**, simulating neutrino interactions from MeV to PeV energy scales.
- A **bridge between theory and experiment**
- **Used by all modern neutrino experiments** - Primary GENIE reference has ~1,100 citations!
- The GENIE group leads **influential phenomenological work**

http://www.genie-mc.org

Recent development focus:

- Construction and characterisation of several alternative comprehensive neutrino models; Evaluation of modelling uncertainties
- Hadronization re-tuning and alternative hadronic re-interaction models
- Very-high energy interactions (NLO DIS model) to support neutrino telescopes and CERN FPF experiments
- Rare processes (e.g. NC single-photon production)
- Electron scattering (extracting neutrino modelling constraints from complementary electron-nucleus scattering data)
- BSM models (Dark Neutrinos, Boosted Dark Matter, Heavy Neutral Lepton simulations)
- Leading global analysis of neutrino scattering data
- Effort towards GENIE Argon tune (SBN, DUNE)

Genie
UNIVERSAL NEUTRINO GENERATOR & GLOBAL FIT

Recent GENIE papers led by the Liverpool team:

- Neutrino-nucleus CC0π tuning in GENIE v3, PRD 106 (2022) 11, 112001
- Hadronization model tuning in GENIE v3, PRD 105 (2022) 1, 012009
- Bare nucleon cross-section tuning in GENIE v3, PRD 104 (2021) 7, 072009
- Recent highlights in GENIE v3, Eur.Phys.J.ST 230 (2021) 24, 4449-4467

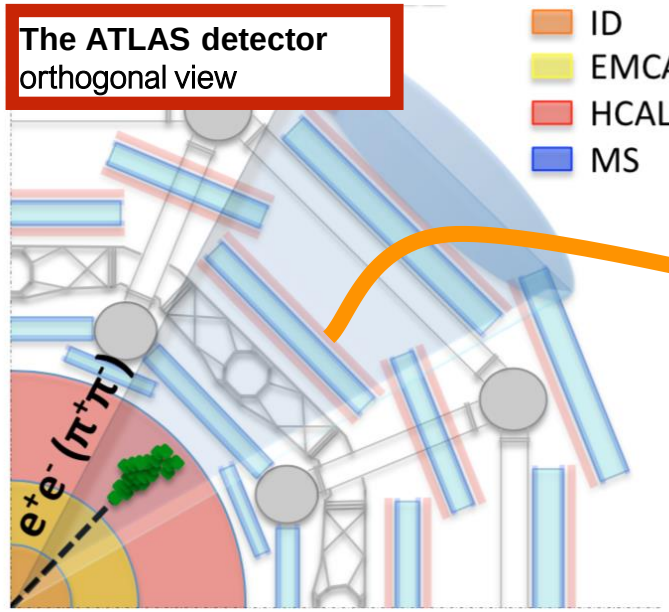
AI/ML work – (x)AI models for HEP

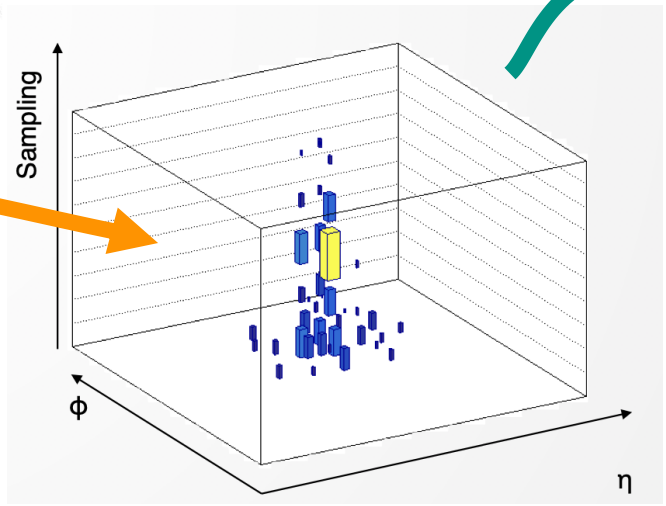
ATLAS members **M. D'Onofrio (PI), J. Carmignani and C. Sebastiani** are involved in the international consortium **MUCCA** consortium - *Multi-disciplinary Use Cases for Convergent new Approaches to AI Explainability* - funded by CHIST-ERA (EPSRC) to develop, understand and interpret AI methods

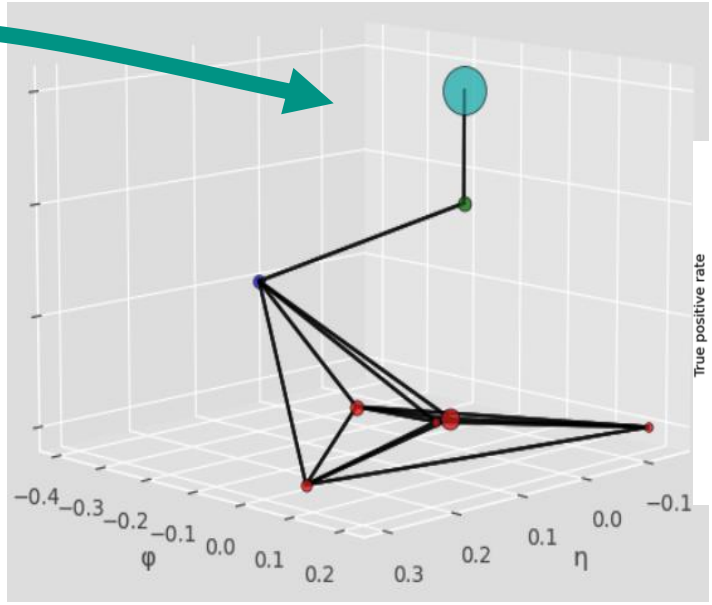
Overarching **strategy**: study this in *heterogeneous* use-cases: High Energy Physics (ATLAS analysis and online trigger), medical imaging, diagnosis of pulmonary, tracheal and nasal disease, Neuroscience.

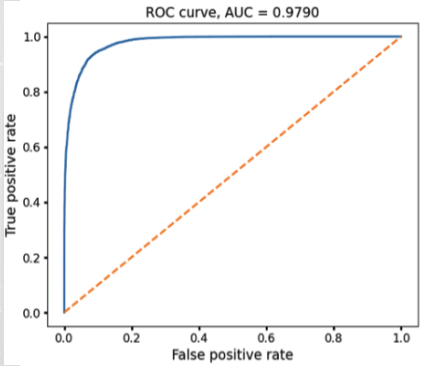
Example for one of the Liverpool deliverables: improve capability to search for dark sector – long-lived dark photons

The ATLAS detector
orthogonal view









Excellent performance

Exploit the calorimeter granularity to parametrise the energy deposits: x, y, z, energy

PUBLISHED – use 3D jet images:
- Train a CNN
- Very sparse images -> sub-optimal

https://arxiv.org/abs/2206.12181

DEVELOPED – Use Graphs NN:
- Train a fully optimised GNN
- Small cloud space objects
- Efficient and easy to manipulate

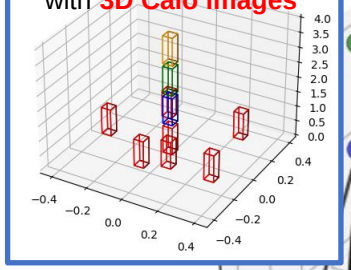
AI/ML work – xAI learning process

- Compare different training models: freeze best one
- Choice of initial conditions (physics driven): Train and test GNN w/o selections on number of nodes/number of subgraphs to identify the best setup for distances (DR) within a single calo-layer and different calo layers
- Graphs pre-processing: remove isolated nodes (1 or 2) and subgraphs not connected to the core graph
- Compare different explainer methods to find the best one for HEP use cases —> so far, considering two orthogonal approaches: Saliency Maps and inductive bias (Trac-In) models.

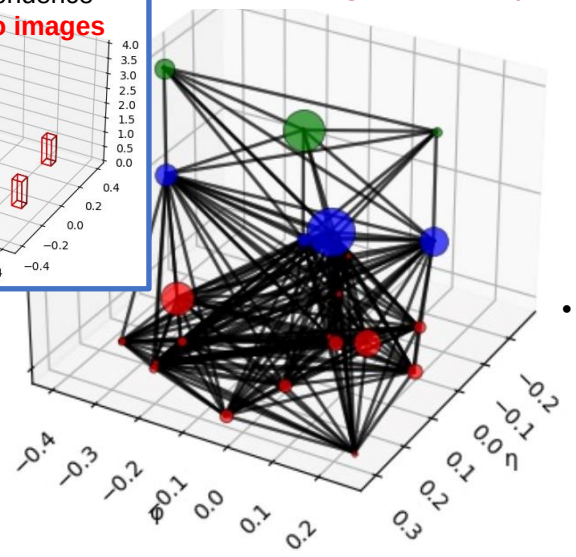
How does a signal look like?

True label: 0, predicted label: 0, predicted prob: 0.00

Full correspondence with **3D Calo images**

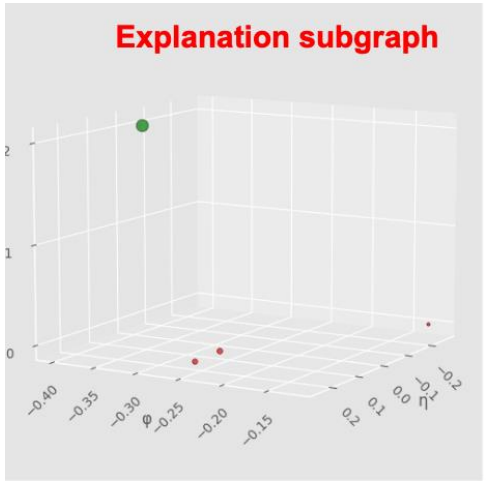


True negative example



Saliency maps

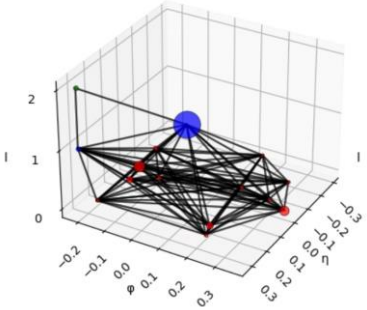
- Top 4 influential nodes



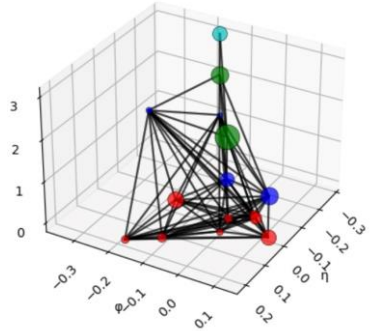
- Top influential data from training dataset

Trac-in model

Proponent (background event)



Opponent (signal event)



Currently finalising the studies targeting a paper by end of summer, and applying similar techniques to other BSM searches (Supersymmetry) and for identification and classification of tau-lepton decaying hadronically at ATLAS

Quantum Computing work – Neutrino physics

Costas Andreopoulos

- Strategic collaborative project with the Fermilab Quantum Institute
- Liverpool awarded 2 PhD positions, nominally to start in October this year
  - Further info at https://inspirehep.net/jobs/2620740 (advert now closed)

- Idea: simulate QCD on quantum computers, leverage qudits (N-level generalization of the qubit)
- Key goal for neutrino physics: attack the problem of fermion scattering from a "top-down" phenomenological perspective through deep inelastic scattering and hadronization studies designed to contextualize the quantum simulation work and connect it to intermediate-term physics goals at experiments like DUNE

Quantum Computing work – @ LHCb

Eduardo

- Work done within LHCb DPA's R&D work package on "Innovative Analysis Techniques"

- At the moment we have efforts from 2 institutes, with several people involved
  - I'm involved as PL, e,g. for discussions with CERN QTI / Openlab. No hands-on work so far from me

- The first DPA project paper … is a paper on Quantum Computing !
  - First application of QML to the task of jet charge identification:
    "Quantum Machine Learning for b-jet charge identification", JHEP 08 (2022) 014
  - Actually got some great attention and coverage,
    e.g. https://news.liverpool.ac.uk/2022/08/04/first-studies-with-quantum-machine-learning-at-lhcb/

- LHCb colleagues presented 1 talk + 1 poster on "Quantum Computing Applications at LHCb"
  at QT4HEP workskop ("International Conference on Quantum Technology for High-Energy Physics"), Nov. 2022, CERN

- Future engagement from Liverpool to be clarified …

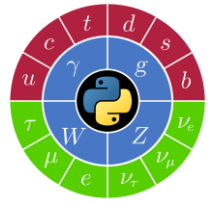
Community work – HSF, PyHEP

HSF – HEP Software Foundation

https://hepsoftwarefoundation.org/

- Continue to be part of the coordination team
- Great way to get to know about (community, but not only) activities across experiments and working groups
- E.g.: we know we will be asked again this year by the LHCC on input on
  "Common Software Projects: Data Science Tools for Analysis" as part of their HL-LHC review
  (our 2021 report: https://arxiv.org/abs/2202.02194)

HSF PyHEP "Python in HEP" WG



- Co-convener of the WG. A key activity are the workshops
- PyHEP series of workshops turning 5 this year!
- First year with 2 workshops:
  - Standard, online PyHEP 2023 – intended since the onset for both developers and physicists

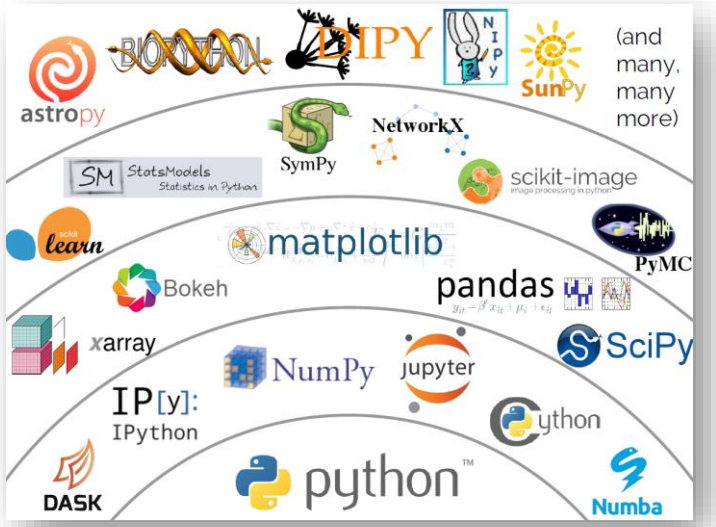
> The **PyHEP workshops** are a series of workshops initiated and supported by the HEP Software Foundation (HSF) with the aim to provide an environment to discuss and promote the usage of Python in the HEP community at large. Further information is given on the PyHEP WG website.

  - First PyHEP.dev – "in-person, informal workshop for developers of Python software in HEP to plan a coherent roadmap and make priorities for the upcoming year"

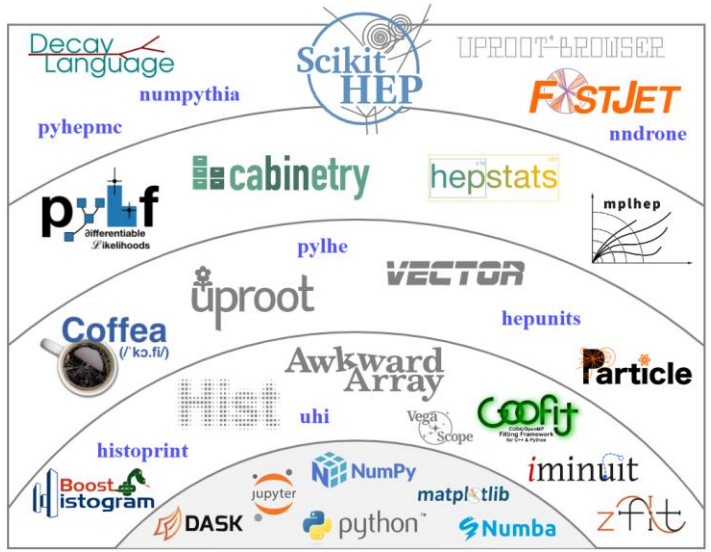
Community work – Scikit-HEP project

- Grand idea = elaborate a domain-specific scientific ecosystem à la SciPy for Particle Physics

https://scikit-hep.org/



Jake VanderPlas,
The Unexpected Effectiveness of Python in Science,
PyCon 2017



Scikit-HEP project packages + other projects (e.g. Coffea)

- A set of tools, not a single (monolithic) toolkit, with interoperability between tools where relevant
- Build(ing) a community of developers and users, hence community-driven and community-oriented project
- Used by several projects and experiments, many analysts (maybe you ;-)?)
- These days: I devote the time I can, still maintain a few packages. Interested? Get in touch!

Community work – “outputs”

- This type of work, while “in my free time” and in parallel, does produce “outputs”:

- Talks:
  - At PyHEP 2022 workshop (e.g. update on my Scikit-HEP project packages)
  - Invited talk "Scikit-HEP project - on making our work citable“ at "Software Citation and Recognition in HEP" workshop, November 2022

- CHEP 2023 (May 2023): co-convener of Track 5 on "Sustainable and Collaborative Software Engineering“

- Publications:
  - "Awkward Packaging: building Scikit-HEP“, Proceedings of SciPy 2022, doi:10.25080/majora-212e5952-012
  - Report of HSF IRIS-HEP Second Analysis Ecosystem Workshop, May 2022, doi:10.5281/zenodo.7003962

C&SW UK wide – SWIFT-HEP project

Eduardo, others in the future

https://swift.hep.ac.uk/

- SWIFT-HEP = SoftWare and InFrastructure Technology for High Energy Physics
- UK-wide project similar to US's IRIS-HEP, but much smaller in size in this "phase 1" 3-year period April 2021 - March 2024
  - 5 work packages

- Liverpool so far lightly involved via me as WP5 "Data Analysis" co-convener
- Other co-convener from Bristol. They have a half-paid post-doc working on WP5 (the only hire here)
- Interest in "analysis facilities" (term is broad ;-))
- Work so far done on bridging DIRAC with tools such as Dask for parallel computing
- Phase 1 deliverable will be a little proof-of-concept having Dask and DIRAC talk to each other

- First thoughts towards a bigger phase 2 ongoing … Opportunity to engage, propose, and eventually get a share of the pot
- SWIFT-HEP (can) differentiate(s) from IRIS-HEP in that it targets beyond HL-LHC experiments, e.g. LZ

- There will be a dedicated discussion on the future strategy for computing in the upcoming PPAP meeting (6-7 July).
  PPAP will invite people from GridPP, IRIS, SWIFT-HEP and DIRAC to discuss
  ⇒ maybe pass on any thoughts to me and I will convey them to SWIFT-HEP's PI?
  ⇒ e.g. maybe convey push towards (more) GPUs in GridPP?