

COLLATED SLIDES AND CONTRIBUTIONS





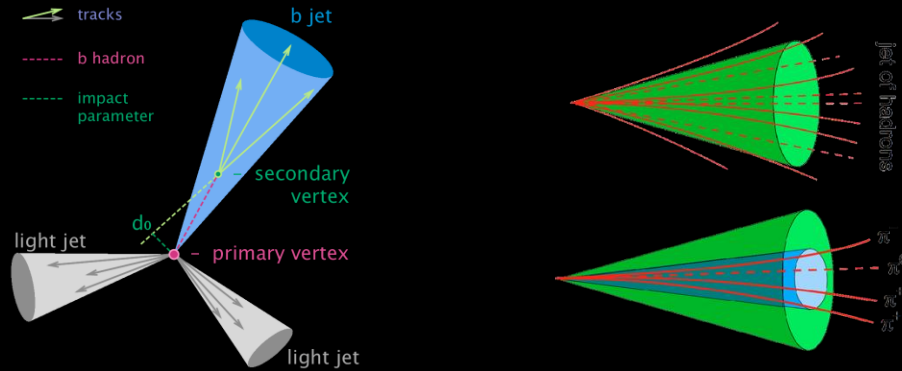
Thanks for all contributors

- Particle physics:
 - Trigger/Data analysis at collider experiments: ATLAS, LHCb
 - Nuclear physics:
 - Data analysis at hadron colliders
 - CMP:
 - Application to cancer research, spectroscopy, chemical physics
 - AS:
 - CI activities overview, Beam studies
 - Physics education:
 - AI in education
- Not included but on-going:
- AI for visual inspections of detectors (ATLAS upgrade)
 - AI for gamma-ray detector developments (NP, Tom Wonderley – PhD with Andy Boston)

CHALLENGING
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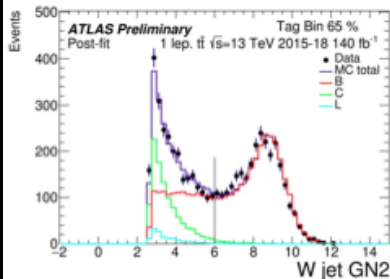
Particle physics: ATLAS

Physics objects reconstruction: b-jets and taus



ATLAS Flavour Tagging (A Mehta, N Rompotis)

- Calibration of a Graph Neural Network classifier to identify jets that are initiated by heavy-flavour quarks
- Liverpool has been working in this for years and has published several results



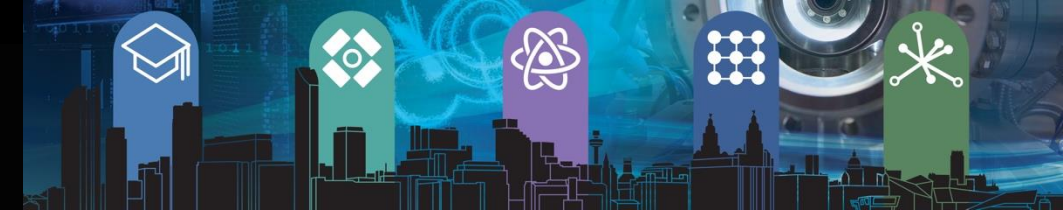
example of the graph neural network output on jets from W boson decays

Latest public result:

<https://atlas.web.cern.ch/Atlas/GROUPS/PHYSICS/PLOTS/FTAG-2023-05/>

Latest paper:

<https://atlas.web.cern.ch/Atlas/GROUPS/PHYSICS/PAPERS/FTAG-2020-08/>



MD'O, Jordy Degens, Nikos Rompotis, Rob McNulty, Mehul Depala

2) τ -Leptons & QCD Jets

τ -leptons

- Heaviest known lepton (1.77 GeV) [3]
- 5 hadronic decay modes (Table 2.1)
- Hadronic Decay BR: 65% [3] to collimated jets with low number of tracks and small decay probability

Table 2.1: Hadronic decay modes of the τ -lepton, and their corresponding labels used in this analysis

Hadronic Decay Modes	Label
$\tau^\pm \rightarrow \pi^\pm \nu_\tau$	1p0n
$\tau^\pm \rightarrow \pi^\pm \nu_\tau \pi^0$	1p1n
$\tau^\pm \rightarrow \pi^\pm \nu_\tau \geq 2\pi^0$	1pXn
$\tau^\pm \rightarrow \pi^\pm \pi^\mp \pi^\pm \nu_\tau$	3p0n
$\tau^\pm \rightarrow \pi^\pm \pi^\mp \pi^\pm \nu_\tau \geq \pi^0$	3pXn

QCD Jets (Main Background Source)

- Contains many tracks and occur more often than the τ -decays
- Same particles in jet as in τ -decays (e.g. π^\pm , π^0)

Unified Model Graph Neural Network (GNN)

Proposed

- ARMA convolutional layers [5]
- Combination of input variables from both ID and DMC
- Inputs can be unordered sets with varying lengths

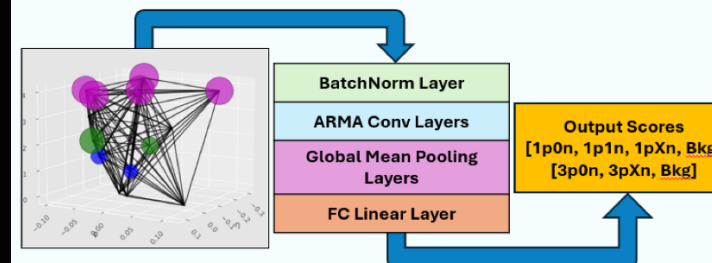


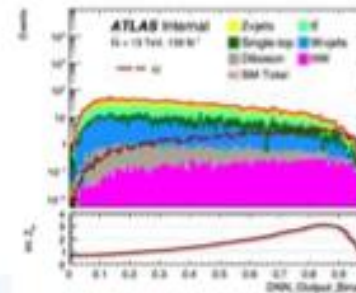
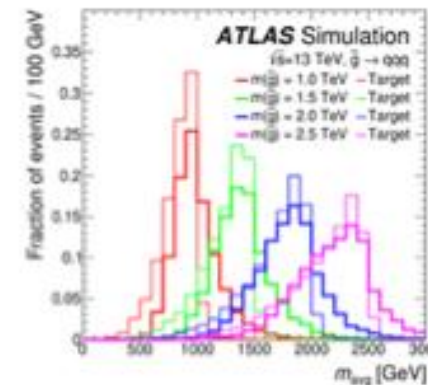
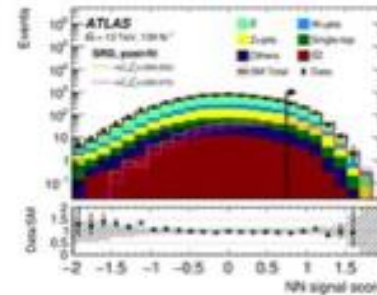
Figure 5.1: Proposed GNN Architecture. From left to right; graph input, passed through the layers of the GNN, which is then given a multiclassification score



Particle physics: ATLAS – data analysis

Overview (Recent & On-going)

- Search for top+charm+MET ([arxiv:2402.12137](https://arxiv.org/abs/2402.12137))
 - Neural Network (NN) to isolate signal from background using general kinematic features of an event
 - Dedicated c-tagging ML algorithm to ID c-jets (objects within the event)
- Search for RPV gluinos in multi-jet final state ([arxiv:2401.16333](https://arxiv.org/abs/2401.16333))
 - Deep NN, using attention mechanisms taking inspiration from transformer models → A first in ATLAS data-analysis
 - Identify on a individual event basis which jets belong to specific gluino decays
- Measurement of ttZ with Z→nunu (Internal for now)
 - Deep NN's trained to isolate signal (ttZ) from background based on event-level variables for potential SM (first) observation
- (And more experience over the last ~5 years, xGB etc)



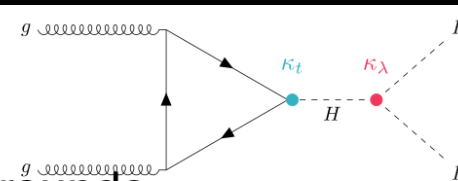
John Anders



Particle physics: ATLAS and future colliders

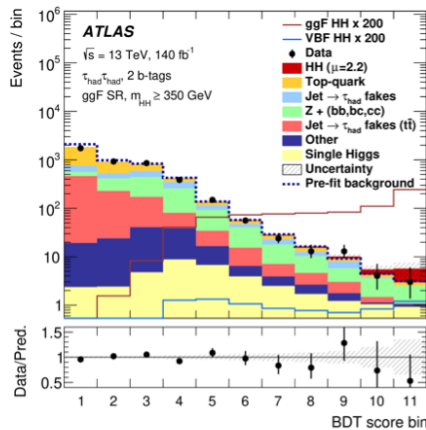
Di-Higgs studies

Measuring DI-Higgs allows to determine shape of Higgs potential
Extremely challenging due to tiny cross-sections and huge backgrounds



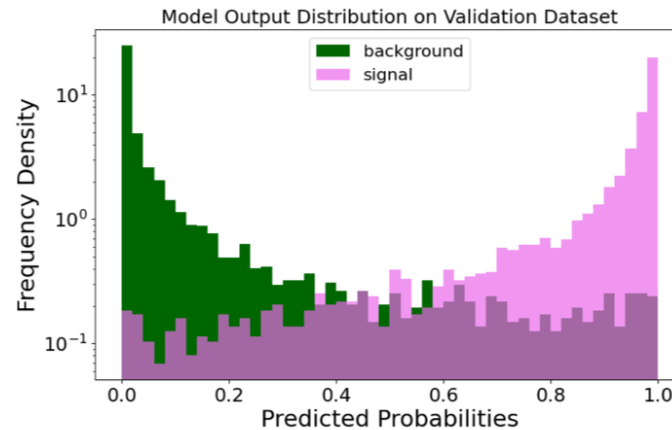
LHC ATLAS $bb\tau\tau$

- Use BDT to separate signal from background
- Studies on using Attention transformer network
- Allows for order of magnitudes separation of signal and background
- Carl/Jordy/Bhupesh
- Use MVA for reconstructing the di-tau system with undergrad student



FCC $bb\tau\tau$

- FCC-hh could produce abundant Higgs pairs
- Use GNN to estimate sensitivity to measure HH
- Carl/Monica/Jordy + 2 undergrad students

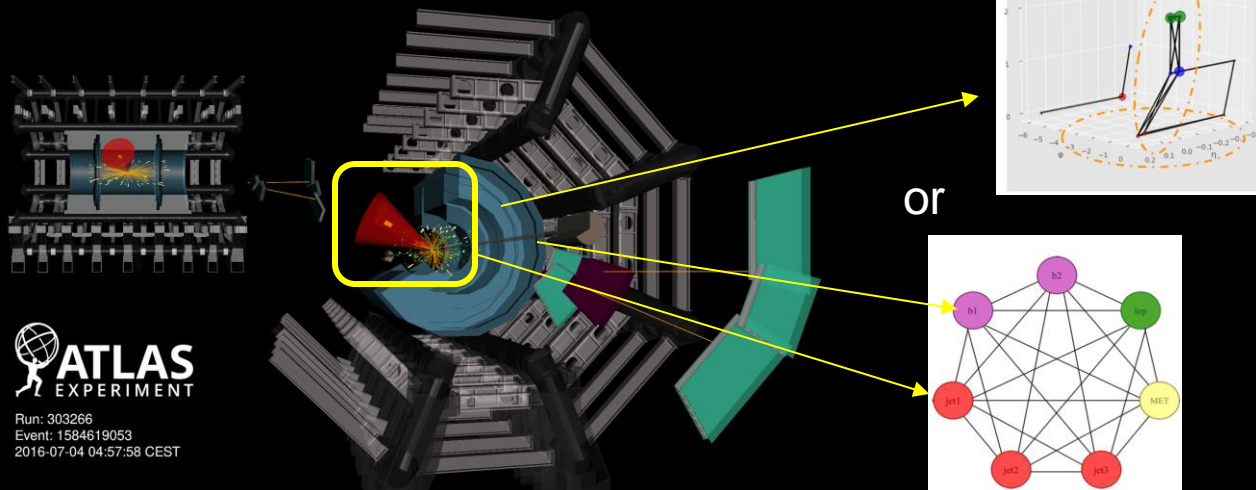


Jordy Degens
Carl Gwilliam
Bhupesh Dixit
(FCC)Monica D'Onofrio



Particle physics: ATLAS and diverse applications

Searches for SUSY and dark photons: problem to be addressed → **event classification and process discrimination** in large and diverse datasets for discovery



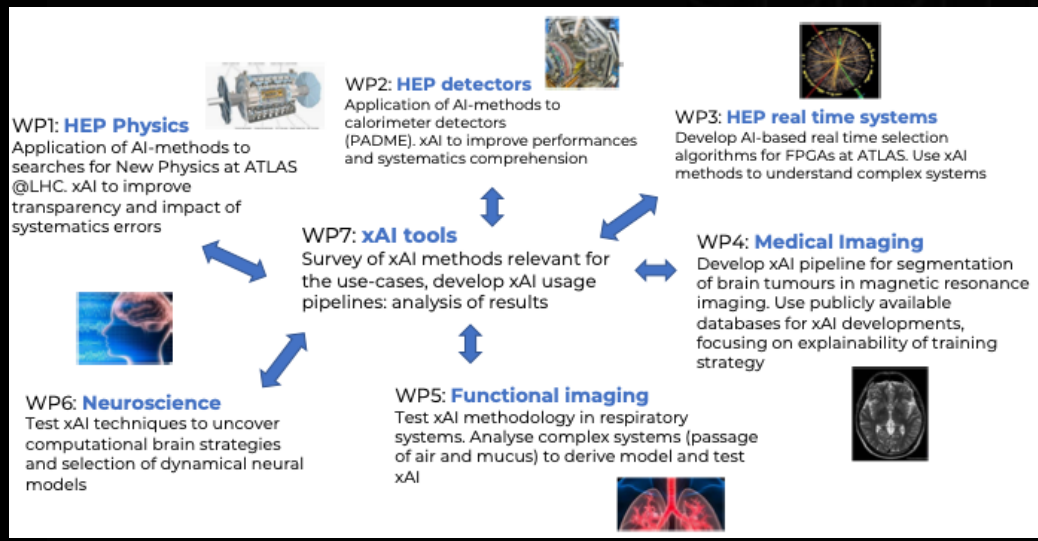
ATLAS
EXPERIMENT
Run: 303266
Event: 1584619053
2016-07-04 04:57:58 CEST

How-to: GNN and beyond:

- Datasets building with diverse inputs
- Graph pre-processing, graph-based models built and trained
- Model optimization, xAI (Saliency Maps, TracIn)
- Simple GNN, GNN attention transformers, autoencoders developed, tested and compared

Pipelines for AI and xAI applicable to diverse fields: MUCCA consortium (MD' O P + postdocs and students working on this in the past few years)

Goal to study xAI in heterogeneous cases *quantifying strengths* and *solving weaknesses* of new and state of the art methods on Deep Learning applications





From PP to broader application (2)

- PP skills applicable to other disciplines:
 - Healthcare:

Title: The use of AI models for predictions in Age-related Macular Degeneration and Diabetic Retinopathy

Student: Robert McNulty (Liv.inno student, co-funded by ARO)

Where: Institute of Life Course and Medical Science (ILCaMS) at UoL

Supervisors [Physics] Dr. Nikos Rompotis (P), Prof. Monica D'Onofrio (S),
[Externals] Prof. Yalin Zheng, Dr. Philip Burgess + Richard Spragg (ARO)

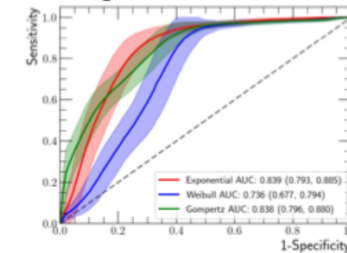


• Age-related Macular Degeneration (AMD)

<https://www.nhs.uk/conditions/age-related-macular-degeneration-amd/getting-diagnosed/>

Project ongoing:
Classification and time-to-progression of AMD with/without treatment using Machine Learning, working with Prof. Yalin Zheng

Figure 1: ROC curves for three time-to-progression (survival) models, shown with a 95% confidence interval for exponential (red), Weibull (blue), and Gompertz (green) survival functions for AMD, with the time prediction at 2 years.



• Diabetic retinopathy (DR)

<https://www.nhs.uk/conditions/diabetic-retinopathy/>

To start soon:
Investigating the performance of an AI algorithm in detecting variable thresholds of referable DR and prediction of the time-to-progression of DR, working with Dr Philip Burgess

- Space: apply AI from PP to detection of gravity anomalies in asteroids through the inverse gravity problem (joint PhD project with Space Engineering and ESA, MD'O)
- But also initiatives for training: EPSRC sponsored school (within MUCCA project), School organized in Sept 2023: [From Graph Neural Networks to Explainable AI: comprehending and trusting Machine Learning algorithms](#)



Particle physics: LHCb

- *LHCb data reconstruction*: problem to be addressed → fast and efficient reconstruction of tracks in busy environment. **How-to**: ML-tracking on FPGAs algorithms, performing all the data organisation steps prior to a track fit being performed.
- Several contributions to the experiments in this respect ...

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Particle physics: LHCb

Eduardo Rodrigues (LHCb experiment)

Active in several Computing & Software endeavours, some very much connected with Data Science:

- In LHCb – was until recently the Data Processing & Analysis project leader (offline)
- [HSE](#) (HEP Software Foundation) Steering Group member
- HSF PyHEP («Python in HEP») co-convener
- Member of the UK [SWIFT-HEP](#) project (SoftWare and InFrastructure Technology for High Energy Physics) and previously co-convener for the Data Analysis WG
- Founder of the [Scikit-HEP](#) project (community-driven and community-oriented project with the aim of providing Particle Physics at large with a Big Data ecosystem for data analysis in Python)

Recent relevant publications:

- PyHEP.dev 2024 Workshop Summary Report**
A. Alshetri et al., Report of PyHEP.dev 2024 developer's workshop, Aachen (Germany), 26-30 August 2024
e-print [arXiv:2410.02112 \[hep-ex\]](#)
- Analysis Facilities White Paper**
[arXiv:2404.02100 \[hep-ex\]](#), HSF-TN-2024-01
- FunTuple: A New N-tuple Component for Offline Data Processing at the LHCb Experiment**
A. Mathad et al., Comput Softw Big Sci (2024) 8, 6, [doi:10.1007/s41701-024-00116-1](#)
(e-print [arXiv:2310.02433 \[physics.data-an\]](#))

Particular interests:

- Analysis software in general and especially Data Science related and oriented packages/libraries
- Future Analysis Facilities for HEP analysis at scale on heterogeneous resources



Particle physics: LHCb

Eduardo Rodrigues – Scikit-HEP project

- ❑ Used by many, including ATLAS, CMS, LHCb, Belle II, KM3NeT
- ❑ Key design is a direct connection with the scientific Python ecosystem (array programming in particular)
- ❑ “Shell ecosystem” from Data Science pillars to HEP domain specific libraries,



Basics
Awkward(array)
Vector
Hepunits

Data manipulation & interoperability
uproot
uproot-browser
hepconvert

Fitting and Statistics
iminuit
pyhf
cabinetry
resample
hepstats

HEP specific libraries and interfaces to HEP libraries
Particle
DecayLanguage
fastjet
pylhe
pyhepmc

Histogramming
boost-histogram
Hist
histoprint
UHI

Visualisation
mplhep

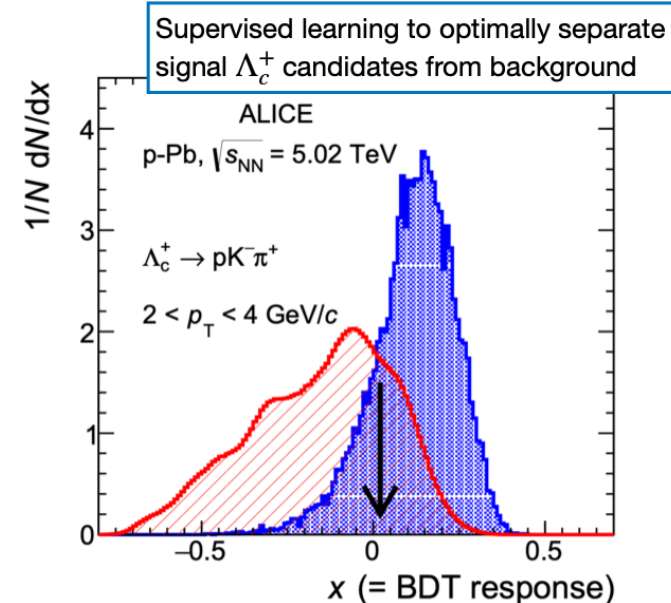


Nuclear Physics: ALICE

ALICE group activities 1) ML within ALICE

- Liverpool ALICE group have made significant contributions to AI/Machine Learning (ML) applications within ALICE
- **ML to improve charmed hadron production measurements:**
 - Lead authors/analysers on first ALICE paper that uses ML (Boosted Decision Trees) for classification task - improve signal extraction of charmed baryon Λ_c^+ to measure its production cross section
 - Lead involvement in further development of ML tools for charm and beauty hadron production measurements within ALICE, lead involvement in papers which further utilised these techniques
 - Use of ROOT (TMVA) or python (XGBoost,scikit-learn) tools
 - Improvements in statistical uncertainties, allowed measurements that would not be possible otherwise (e.g. Λ_c^+ production in Pb-Pb collisions)
- **ML to make jet energy corrections:**
 - Collaborating with ALICE colleagues in Derby on use of ML to correct for detector effects when measuring jets (detector resolution + tracking efficiency)
 - Exploring 'OmniFold' - new unfolding technique which uses neural networks for this task - multi-dimensional correction made possible
 - Relevant for other HEP experiments which make similar measurements

ALICE Collaboration: *JHEP* 04 (2018) 108
Phys.Rev.Lett. 127 (2021) 20, 202301
Phys. Rev. C 104 (2021) 054905
Phys. Lett. B 839 (2023) 137796



Jaime Normann

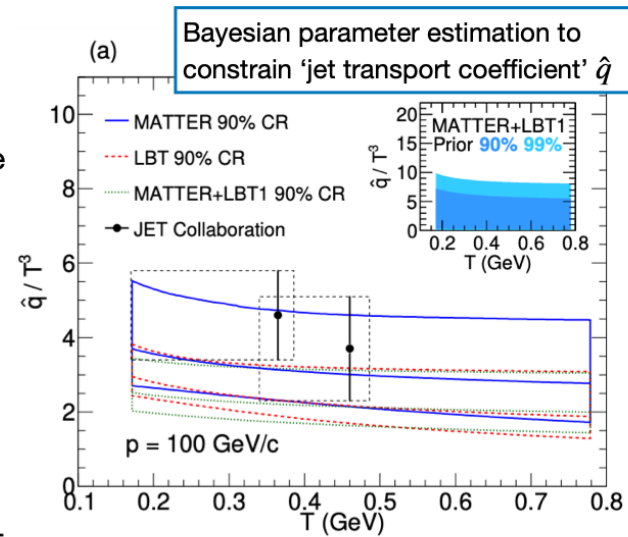


Nuclear Physics: ALICE

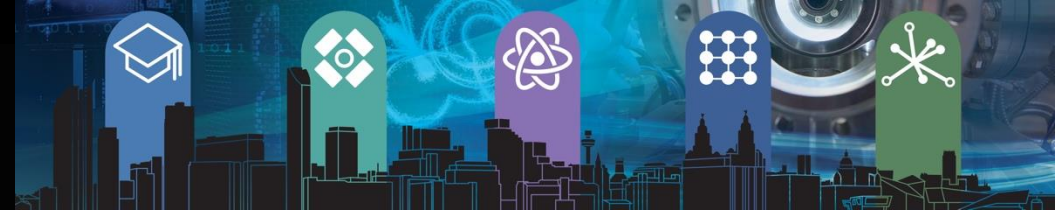
ALICE group activities 2) JETSCAPE

- ALICE group joined JETSCAPE collaboration (<https://jetscape.org/>) recently
- US-based interdisciplinary collaboration developing software framework which provides a systematic, rigorous approach to simulating relativistic heavy-ion collisions
- Use in theory-data comparisons - **Bayesian inference to constrain properties of the Quark-Gluon Plasma**
 - Significant computing resources needed to sample model parameter phase space - cutting edge ML approaches in development within collaboration
 - Relevant for other fields which encounter similar challenges
- We have been awarded 500k HPC CPU hours on CDS3 (started October)
 - Application through IRIS - digital research infrastructure to support STFC science, which allocates computing resources
 - CDS3 - one of EPSRC Tier2 national HPC facilities at University of Cambridge
 - Plan to be used for/contribute to next-generation Bayesian analyses with JETSCAPE
 - LIV.INNO-funded student will spend 50% of their time on this project
 - Close collaboration with colleagues at LBNL Berkeley

JETSCAPE collaboration: *Phys.Rev.C* 104 (2021) 2, 024905
arxiv:2408.08247



Jaime Normann



CMP

Tim Veal group used density functional theory in combination with a machine-learning approach to screen nearly one million potential structures, thereby developing a robust atomistic model of the highly complex γ -phase of gallium oxide. Theoretical results were compared with surface and bulk sensitive soft and hard X-ray photoelectron spectroscopy, X-ray absorption spectroscopy, spectroscopic ellipsometry, and photoluminescence excitation spectroscopy measurements of the occupied and unoccupied states of γ -Ga₂O₃

Tackling Disorder in γ -Ga₂O₃

LE Ratcliff et al., *Advanced Materials*, 2204217, 34 (2022)

Liverpool Diagnostic Infrared Wand

Methodology

Analysis of infrared spectral images with with patented algorithm¹. (LUMOS IR imaging instrument)

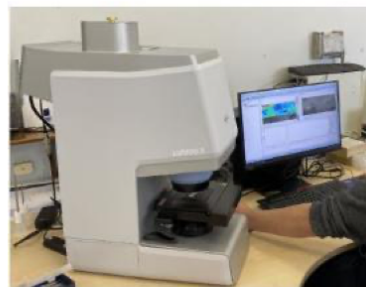
Physics Team

Steve Barrett, James Ingham, Caroline Smith, Paul Unsworth, Peter Weightman

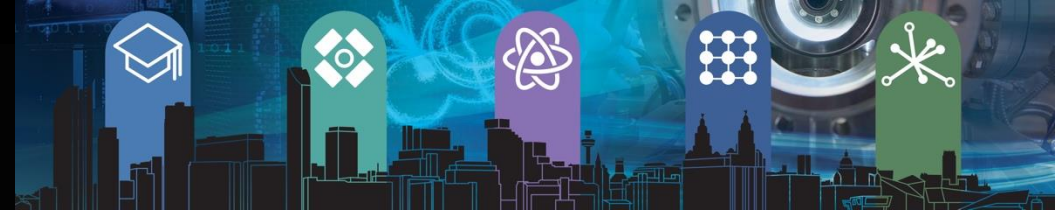
Apparatus available for collaboration

LUMOS

IR Spectral Imaging
Diffraction Limited



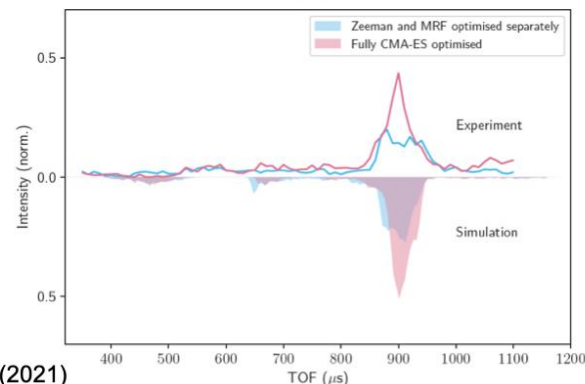
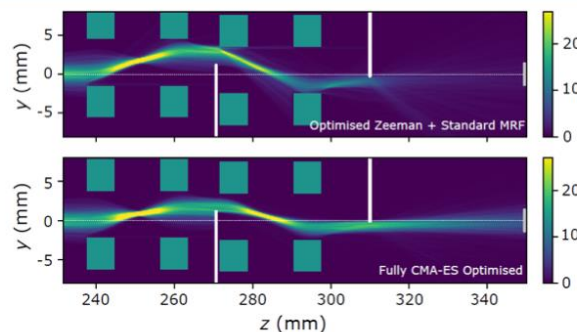
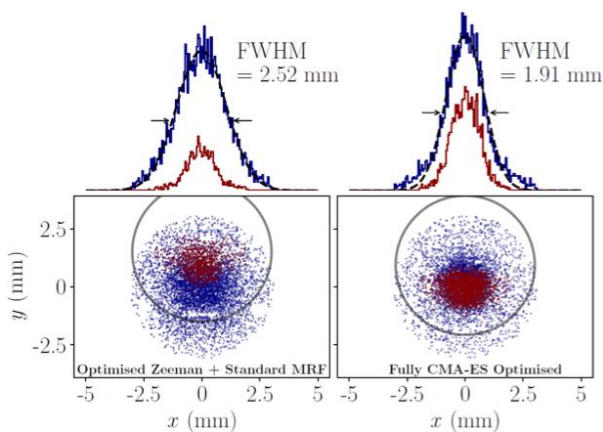
¹ Ingham, Barrett and Weightman, "A method of selecting discriminating wavelengths of radiation for use in absorption spectroscopy". WIPO International Publication Number: WO 2019/197806 A1 Filed 5/4/19. Granted (EU, US, Japan).



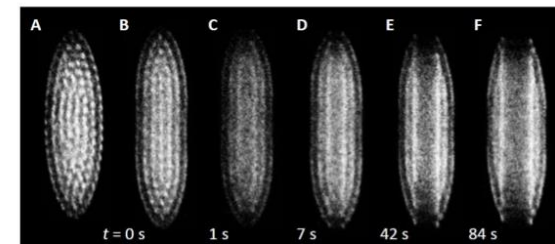
CMP

AI and ML in Chemical Physics Research

- We use evolutionary strategies (CMA-ES) to optimise our experimental parameters
- Achieve up to 50% increase in target particle transmission and improved beam purity



- Alongside collaborators at Birmingham, we are training a neural network to analyse experimental Coulomb crystal images on-the-fly. At present, crystal image analysis is reliant on molecular dynamics simulations that can take days (or even weeks) to run on Barkla.



O. Mohamed*, L. Y. Wu* et al., *Rev. Sci. Instrum.* **92**, 093201 (2021)

- Brianna et al.
- Issue raised about infrastructure needs (to be discussed)



UNIVERSITY OF
LIVERPOOL

Data Science and AI in the Accelerator Science Cluster

Prof Dr Carsten P Welsch



ACCELERATOR SCIENCE – R&D STRATEGY

- In the next decade we will focus on the **LHC** at CERN, where we lead the development of gas jet monitors for the high luminosity upgrade, and other collider options; on the exploitation of the **CLARA** facility on Daresbury campus to explore next-generation FEL technologies; on the development and exploitation of the new facilities **PERLE and RUEDI**; and on the optimization of low energy beam transport and efficient injection into traps at the Antiproton Decelerator, in particular contributions to **AEgIS**.
- As part of **AWAKE**, we will continue our efforts on novel (high gradient) acceleration techniques. Following the successful demonstration of proton-driven wakefield acceleration in 2018, we are leading the development of novel diagnostics that will give more detailed insight into the physics of the acceleration process and also benefit other large scale plasma accelerator projects such as **EuPRAXIA**. We will also expand simulation and experimental studies into micro-accelerators using carbon nanotubes and dielectric structures.
- We will carry out R&D into a **movable accelerator for heritage studies**; least invasive **beam and dose monitors** to help improve patient treatment and medical accelerator operation; continue to develop and optimize **novel low dose 3D X-ray imaging systems** with Adaptix; carry out R&D into **Smart Health Tracking** with ViBo Health; drive **quantum technologies** for accelerator applications; grow our **spinout company D-Beam**, targeting a product portfolio that benefits accelerator facilities around the world.

Frontier
Accelerators

Novel
Accelerators

Accelerator
Applications

A backbone of all three areas above will be our continued leadership in **Data Intensive Science** through large-scale structured training programs.

R&D PROJECTS INCLUDE/D

*Academic and
research staff, many
PhD students*

LIV.INNO

- Beam gas curtain monitor for the High Luminosity LHC
- 'Green' Photocathodes for the Generation of High-Brightness Electron Beams
- Optimization of low-dose, low cost mobile 3D x-ray imaging
- Reconstruction of Transverse Beam Distribution using Machine Learning
- Optical transition radiation diagnostics for low energy ion beams
- Longitudinal Density Monitor for the Large Hadron Collider

LIV.DAT

- Advanced optics concepts for HLLHC
- Betatron Radiation from Underdense Plasma
- Dielectric laser acceleration of relativistic beams
- Particle Acceleration in Carbon Nano Tubes
- Beam Induced Fluorescence monitor for high-intensity beams

CURRENT R&D ACTIVITIES

- **Beam diagnostics:** AI for real-time data analysis, noise reduction, and anomaly detection
- **Beam dynamics and control:** Machine learning algorithms for real-time feedback, control and optimization of beam parameters
- **Fault prediction and prevention:** Predictive maintenance models detect anomalies in accelerator components, helping reduce downtime and improve the longevity of critical parts.
- **Simulation and modelling:** Large datasets to improve HPC and Monte Carlo simulations, making them faster and more accurate, particularly when it comes to interactions within particle beams.
- **Optimization of accelerators and beamlines:** Machine learning techniques to optimize beamline parameters and configurations based on real-time data, enhancing efficiency and throughput of experimental setups.
- **Control system automation:** AI algorithms to dynamically adjust settings in response to changing conditions, improving efficiency and reliability.

FUTURE ACTIVITIES AND OPPORTUNITIES

- **ARTIFACT** – (unsuccessful) 10M€ Horizon Europe proposal, however, now basis for pan-European partnership with Liverpool as founding member;
- **New lecturer** – Dr Andrea Santamaria Garcia, starting 1 February 2025
- **LIV.AI** – future centre for doctoral training based on LIV.DAT and LIV.INNO training concepts, structure and partnerships
- **Energy efficiency and resource optimization:** Using AI to minimize operational costs and environmental impact.
- **Accelerator Design Optimization:** AI-driven optimization techniques to meet ever more demanding performance criteria.
- **(Detector design and calibration:** Using AI to refine sensitivity and ensure accurate data collection)

AS and CI



CHALLENGING

On going work

- Machine learning framework for prediction of beam parameters in a space charge dominated beams
- Machine Learning framework for prediction of output parameters for 3D chest imaging-OPTIX

Future work

- ML for betatron radiation for beam diagnostic (PIC code, with PywarpX)- Debdeep
- Image based convolution neural network (OptiX, Alex)
- STFC/ASTEC CLARA sensor data—Virtual Sensors (Dave, Amelia, Joe)

Difficulties

- Network issues as I am working from Cockcroft Institute
- Delayed IT service help (1 week gone to just connect the WarpX to python utility. Still no success)
- Lack of Teamwork to Identify AI/ML problems

Mahesh Thorat

- Other activities include LIV.INNO projects on AS topics
- New lecturer starting in Feb 2025 focused on AI applications to AS

Applications of Data Science and AI in PER

Andrew Low

1. Predictive Analytics for Student Outcomes

- Machine learning models to forecast student performance, degree classifications, and retention rates.
- Identification of at-risk students and data-driven interventions to support students.

2. Personalised and Adaptive Learning Systems

- Development of AI platforms that personalise learning and offer real-time feedback
- Intelligent tutoring systems that simulate one-to-one instruction

3. NLP for automated feedback and text analysis

- Automated marking and feedback of written work using pre-defined rubric
- Thematic analysis of student survey and interview responses to support qualitative analysis



PER at Liverpool

Predictors and Socio-Demographic Disparities in STEM Degree Outcomes: A UK Longitudinal Study using Hierarchical Logistic Regression

Andrew Low and Yasemin Kalender
Department of Physics, University of Liverpool
(Dated: November 5, 2024)

Socio-demographic disparities in STEM degree outcomes impact the diversity of the UK's future workforce, particularly in fields essential for innovation and growth. Despite the importance of institution-level, longitudinal analyses in understanding degree awarding gaps, detailed multivariate and hierarchical analyses remain limited within the UK context. This study addresses this gap by using a multivariate binary logistic model with random intercepts for STEM subjects to analyse predictors of first-class degree outcomes using a nine-year dataset (2013/14 to 2021/22) from a research-intensive Russell Group university. We find that prior academic attainment, ethnicity, gender, socioeconomic status, disability, age, and course duration are significant predictors of achieving a first-class degree, with Average Marginal Effects calculated to provide insight into probability differences across these groups. Key findings reveal that Black students face a significantly lower likelihood of achieving first-class degrees compared to White students, with an average 16% lower probability, while students graduating from 4-year degree programmes have an average 24% higher probability of achieving a first-class degree relative to those on 3-year programmes. Although male students received a higher proportion of first-class degrees overall, our multivariate hierarchical model shows higher odds for female students, underscoring the importance of model choice when quantifying awarding gaps. Baseline odds for first-class outcomes rose considerably from 2015/16, peaking in 2020/21, indicating possible grade inflation during the COVID-19 pandemic. Interaction effects between socio-demographic variables and graduation year indicate stability in ethnicity, disability, and socioeconomic awarding gaps but reveal a declining advantage for female students over time. These findings contribute to the literature and provide a transferable, evidence-based framework for departments and institutions to monitor awarding gaps, helping to guide the development of targeted, equity-driven policies that support a diverse and inclusive STEM workforce in the UK.

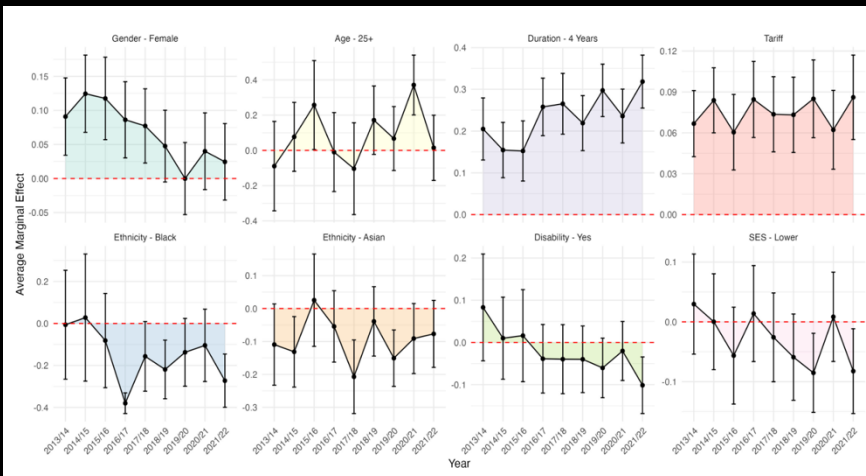
1. Data science:

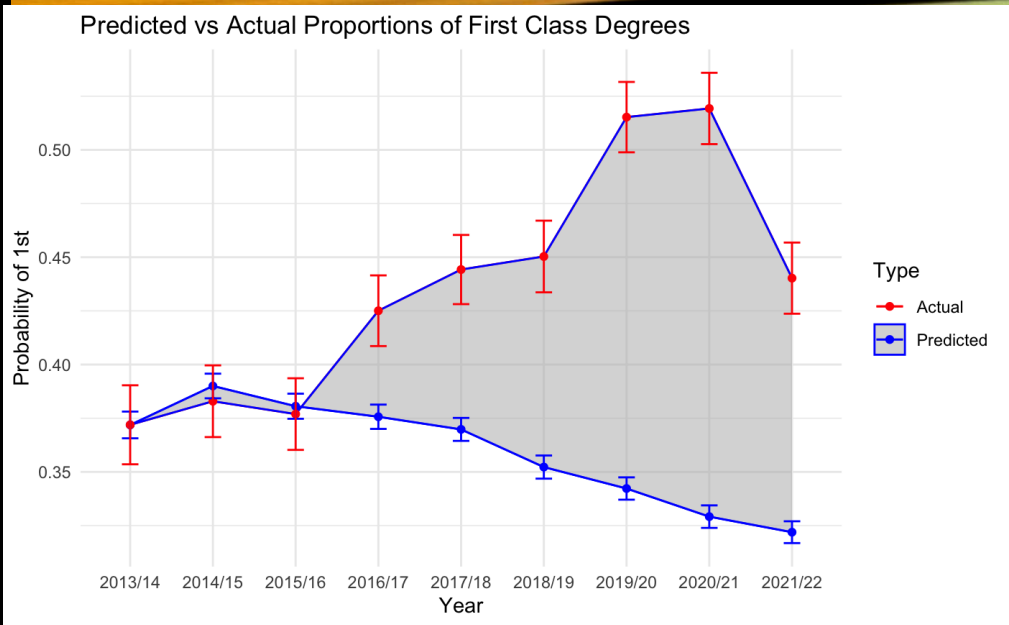
- Using multivariate hierarchical logistic regression to quantify and track physics degree awarding gaps.

- Development of framework for departments/institutions to test impact of strategic interventions

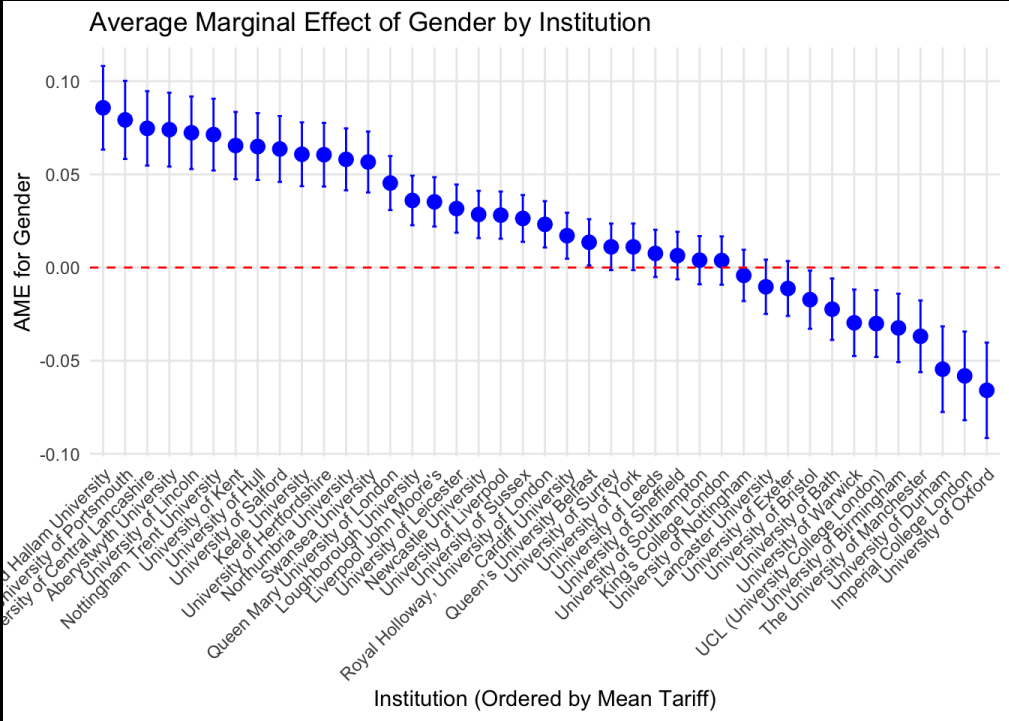
-Applications of Bayesian Inference for complex educational models and sparse data

-Student recruitment/retention analysis





How do you quantify “unexplained” grade inflation in UK Physics Degree Programmes?



Using HLM to explore Institutional Selectivity and Gendered Disadvantage in Physics



Data Dialogue with ChatGPT: Using Code Interpreter to Simulate and Analyse Experimental Data

Andrew Low¹ and Z. Yasemin Kalender¹

¹*Department of Physics, University of Liverpool, Liverpool, UK, L69 7ZE**

Artificial Intelligence (AI) has the potential to fundamentally change the educational landscape. Chatbot's such as ChatGPT allow users to engage in conversations that mimic human interactions. So far, much of the physics education research relating to AI has focused on lecture-based assessment and the ability of ChatGPT to answer conceptual surveys and traditional exam-style questions. In this study, we shift the focus by investigating ChatGPT's ability to complete an introductory mechanics laboratory activity by using Code Interpreter, a recent plugin that allows users to generate and analyse data by writing and running Python code 'behind the scenes'. By uploading a common 'spring constant' lab activity using Code Interpreter, we investigate the ability of ChatGPT to interpret the activity, generate realistic model data, produce a line-fit, and calculate the reduced chi square statistic. By analysing our interactions with ChatGPT, along with the Python code generated by Code Interpreter, we assess how the quality and accuracy of ChatGPT's responses depends on different levels of prompt detail. We find that although ChatGPT is capable of completing the lab activity and generating plausible-looking data, the quality of the output is highly dependent on the detail and specificity of the text prompts provided. We find that the data generation process adopted by ChatGPT in this study leads to heteroscedasticity in the simulated data, which may be difficult for novice learners to spot. We also find that when *real* experimental data is uploaded via Code Interpreter, ChatGPT is capable of correctly plotting and fitting the data, calculating the spring constant and associated uncertainty, and calculating the reduced chi square statistic. This work offers new insights into the capabilities of Code Interpreter within a laboratory setting and highlights a variety of text-prompt strategies for the effective use of Code Interpreter in a lab context.

2. Use of AI tools:

- Data simulation in undergraduate labs
- Approaches to physics problem solving using ChatGPT
- Exploring the AI divide – who uses it, and how
- NLP to understand student experience

Ellen Oldershaw: Bell Burnell Graduate Scholarship Fund Awardee 2024

Ellen's work has the potential to change the way physics is taught in higher education in the UK, making it more accessible to students from minority backgrounds.

*'Machine Learning and AI in
Physics Education Research'*

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AIMS, OPPORTUNITIES, CHALLENGES

- PER is new and emerging field in UK
- Opportunity for Liverpool to be a leader in the field
- Many UK institutions are unfamiliar with PER applications of data science/AI, but keen to learn
- Share knowledge e.g. delivering seminars in Glasgow and Edinburgh this month
- Organising series of methodology workshops for PER community in collaboration with University of Edinburgh
- Establish annual PER UK conference – host at Liverpool
- Significant institutional barriers
- Significant funding issues: no money = no PhD students