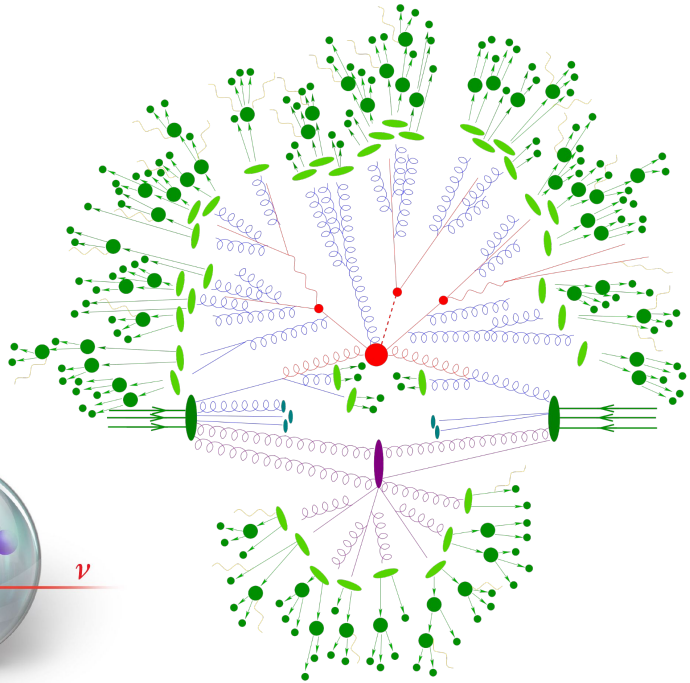
Tools, MC, ML and all that*

Stefan Höche, Josh McFayden, Simon Plätzer, Vinnie Mikuni

*Wiki to be updated
Also consider “Les Houches” 2021:
https://indico.in2p3.fr/event/24331/timetable/#20210614.detailed

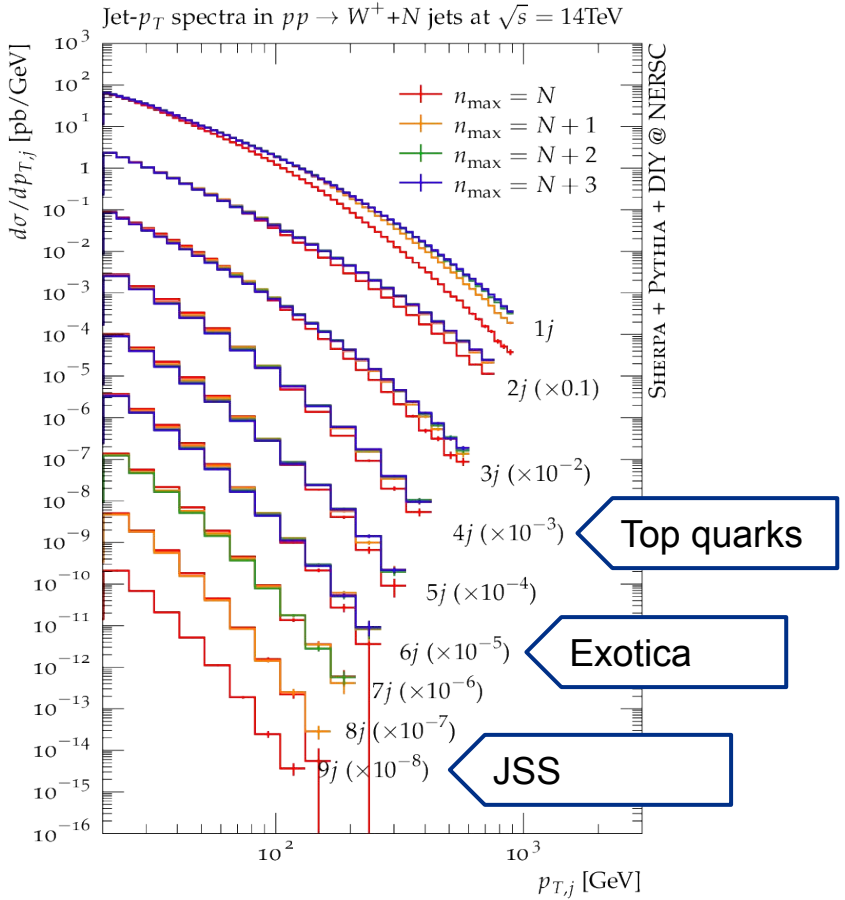
Event generators

- Recent survey of the field (Snowmass 2021)
  [Campbell et al.] arXiv:2203.11110
  - Fixed-order calculations
  - Resummation
  - Parton showers
  - Non-perturbative physics
- Many inspiring ideas
  - New experimental challenges
  - Unconventional signatures
  - Precision calculations
  - Cross-experimental aspects
  - Computing challenges



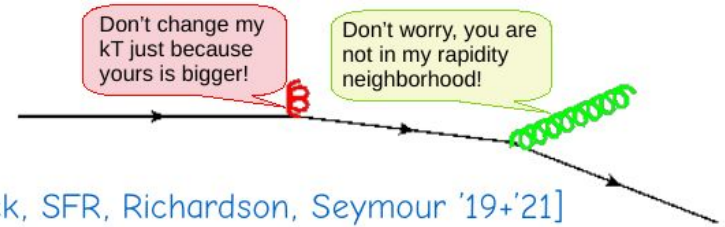
QCD Matching & Merging

- Strong focus at previous workshops, multiple comparative studies
  - Some open questions: negative weights, uncertainties from jet definitions, …
- NNLO matching existing, but further dev needs
  - Deeper understanding of showers and underlying resummation properties
  - Fully differential matching
- Combination of different resummations
  - HEJ (high-energy resummation + PS)
  - Geneva (SCET-I or -II resummation + PS)
- Pheno studies of most uncertain simulations
  - Pure jets
  - Heavy Flavor
  - Hard photons
  - ttV

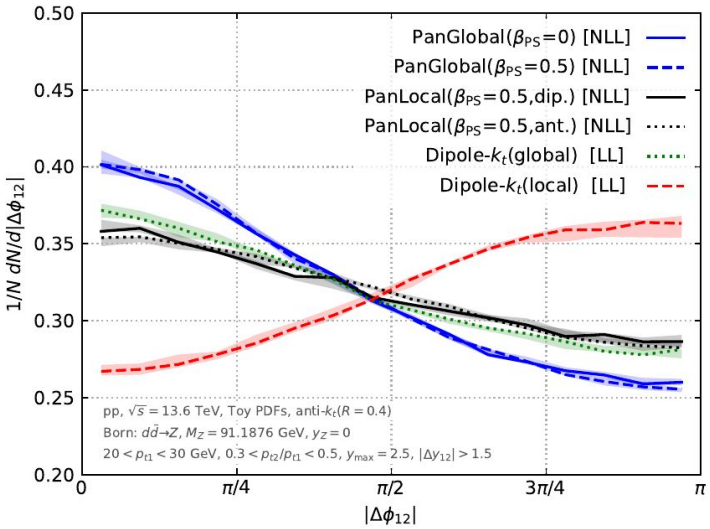


Shower development & accuracy

- Benchmark comparisons between improved shower algorithms
  - Phenomenological impact
  - Full simulations vs resummation (plus had)?
  - Decisive observables – Lund planes, correlators?
- Theoretical development
  - Splitting functions and partitionings
  - Formulation/derivation of algorithms, amplitude evolution
  - Next-to-leading power corrections?
- Study of subleading colour effects
  - Tools and accuracy of available calculations
  - Effective approximations?
- Interplay with hadronization
  - To what extent is perturbative accuracy sufficient?

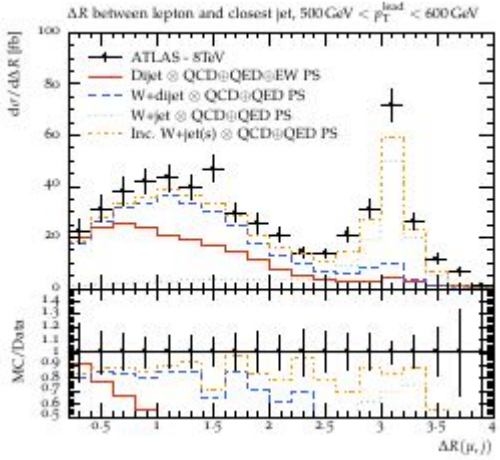


[Bewick, SFR, Richardson, Seymour '19+'21]

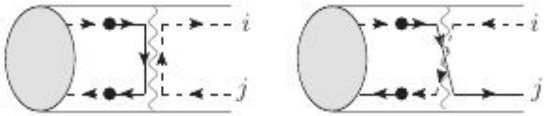


Electroweak physics in event generators

- What can we do about QCD + QED in showers?
  - NLL accurate?
  - Initial state evolution?
- Taking stock of electroweak contributions
  - Compare different approaches: quasi-collinear, Sudakov logs, soft structure?
  - What are the needs to have a fully reliable electroweak evolution available?
  - What fixed-order studies would we need to consider?
  - How do we define observables at all?
- Elephant on this slide: simulations at 100(s) TeV?
- Sudakov logs (?) and ttW?



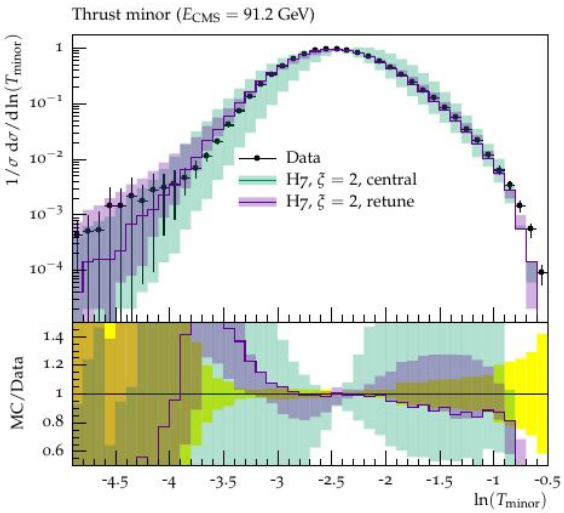
[Massoumina, Richardson ‘20]



[Plätzer, Sjödahl ‘21]

Comprehensive uncertainties

- Continue studies initiated at LH ‘17 and ‘19
  - Detailed study of perturbative/non-perturbative interplay
  - Shower variations and retuning
  - Impact of matching and merging
- The role of the shower cutoff
  - Theoretical meaning and interpretation
  - Practicalities in tuning and uncertainties
  - Relation to analytic hadronisation corrections
- Technical considerations
  - Interoperability of models
  - On-the-fly and branched events? Extensions of HepMC towards this?
  - Reliability of reweighting algorithms and their improvements



[Les Houches ‘17]

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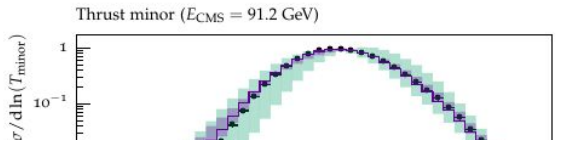
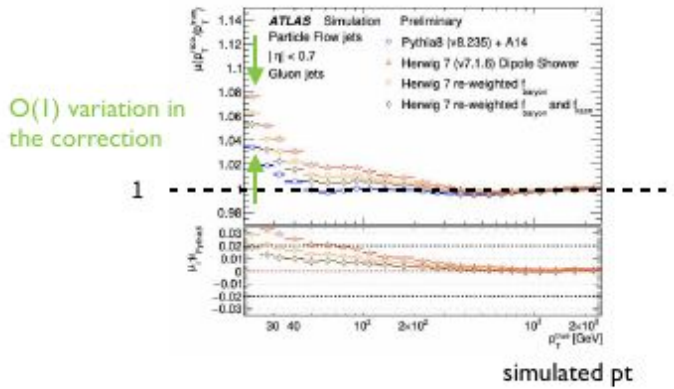


deviation of reconstructed pt

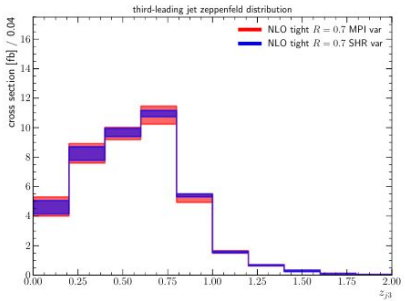


simulated pt

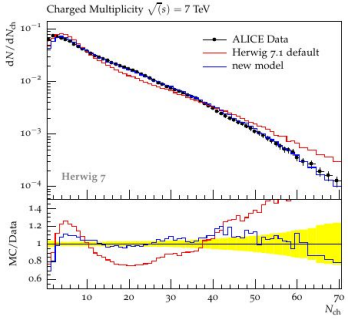
[ATLAS-PUB-2022-021]

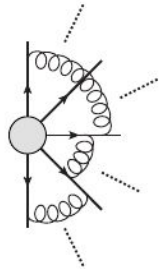
Hadronization & multi-parton interactions

- How well do models extrapolate
  - Different energy ranges
  - Different observables
  - Different processes
- How much lack of perturbative ignorance are models sweeping under the carpet?
  - Do we see roads to determine this from first principles?
  - E.g. interplay colour reconnection and subleading-N improvement



[Bittrich et al. ‘21]

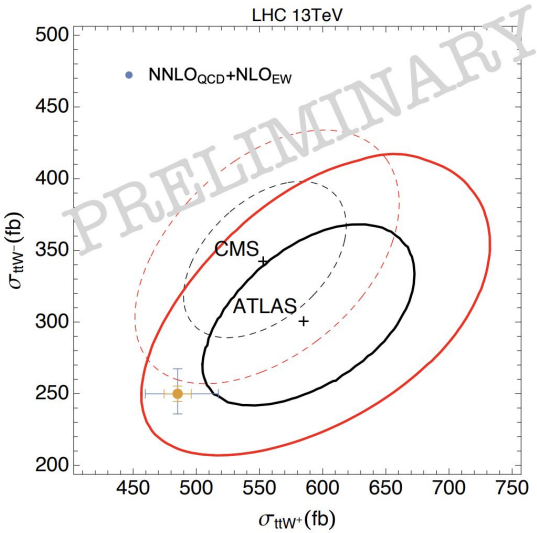


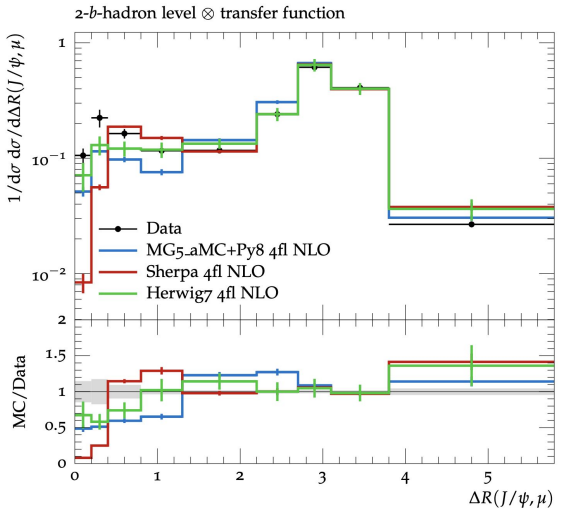


[Gieseke, Kirchgaesser, Plätzer, Siodmok ‘18]

Specific studies

- VBS and VBF
  - Radiation patterns, jet vetoes, impact of MPI
- ttW puzzle
  - Latest NNLO prediction does not resolve tension seen in Run 2 data
    - But only looking at one (fixed) scale
  - Any more theory considerations?
    - Uncertainty recipe for experiments
- Analysis of latest heavy flavour analyses?
  - Extension of 2017 study?
  - New HF measurements available





Tool platforms & interfaces

- Availability of generator setups, versions and event samples
  - DOI
  - Zenodo? HepData? Rucio/eos?
  - Containerisation of generators and rivet - even of Les Houches analyses?
- Benchmarking/accounting
  - Better ways to assess CPU(/memory/GPU) performance of generators
  - Both standalone and the use inside experiments
- Event sample bazar – shared between experiments and pheno groups
  - Possibly at intermediate steps
  - Common HDF5 structure: would this be a LHEF 4.0?
- Existing LHEF
  - What updates are needed? Additional scales?

Tool platforms & interfaces, continued

- Novel Monte Carlo methods and algorithms
  - Use of ML
  - Resampling, event sample paradigm
  - Negative-weight removal (also “resampling”)
- Interfaces to matrix element providers
  - Status and use cases of BLHA – are updates needed?
  - Pick up on full amplitude interfaces again? Confront with new shower paradigms.
- Modular framework for event generation?
  - Possibility to switch in/out different physics models
  - Easier platform for code optimisation?

Portability of event generators

- Multiple efforts to create vectorized code & GPU-based solutions
  - MadGraph / MadEvent
  - Pepper / Chili (formerly BlockGen)
- Community support needed
  - Currently: Proof-of-concept development within HSF & HEP-CCE
  - Long-term future depends on usage for actual science runs
  - Will LHC experiments commit to
    - Use portable generator technology in their workflows
    - Use heterogeneous computing resources at scale (e.g. national HPC centers)

Workforce and community development

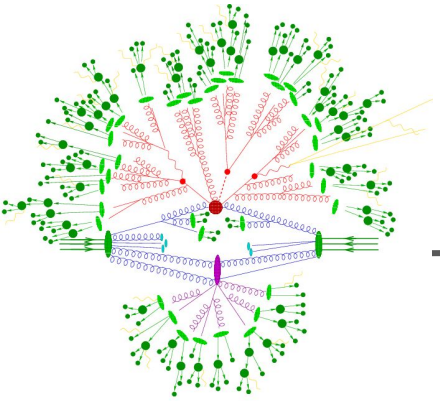
- Situation of MCnet
  - Funding ran out, but still existing as a network
  - Schools and meetings continued
  - Discussion of forming LHCC Generators WG

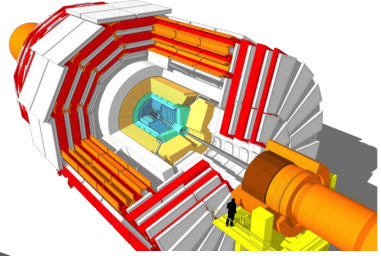
- Situation of event generators
  - Project-based work typically highly sought after (excellent rewards structure)
  - Support work typically badly neglected (non-existent rewards structure)
    - Technical work could be supported externally via
      e.g. experiments and/or software experts
    - Can be hard to make work in practise, but recent positive examples
      - MG4GPU, SWIFTHEP

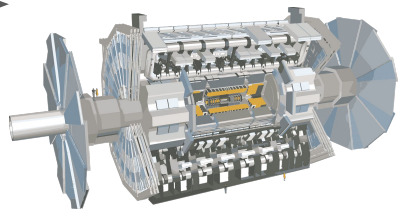
Cross-cutting discussions and development efforts

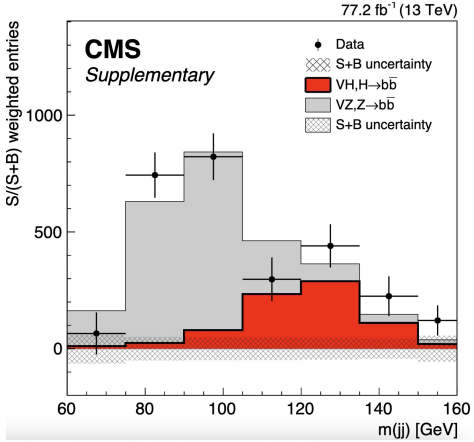
- Several possible areas of engagement beyond LHC
  - Nuclear, Neutrino, Astro physics
  - Some of the next big HEP facilities:
    - EIC, DUNE, FPF

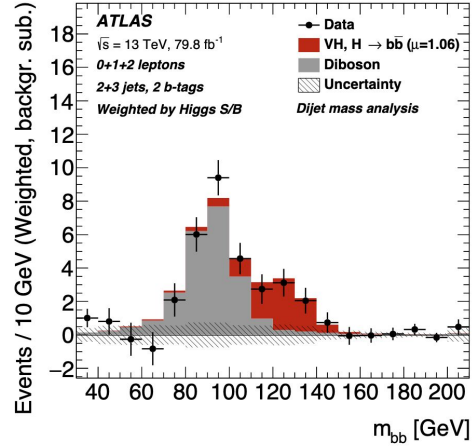
- Significant overlap in physics and technical expertise
  - MC tuning, HepMC, Rivet
  - DIS, nuclear structure functions, neutrino cross sections, forward charm
    - E.g. impact of FPF PDF constraints on precision (e.g. mW)?
    - E.g. forward charm and cosmic ray muon anomaly?



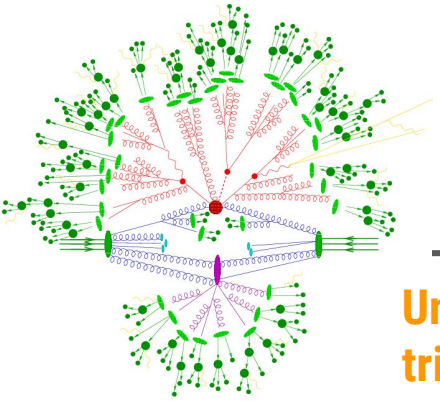




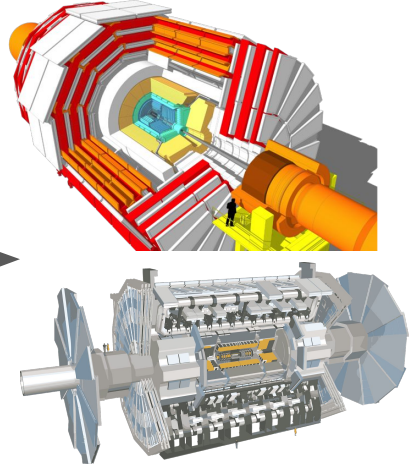




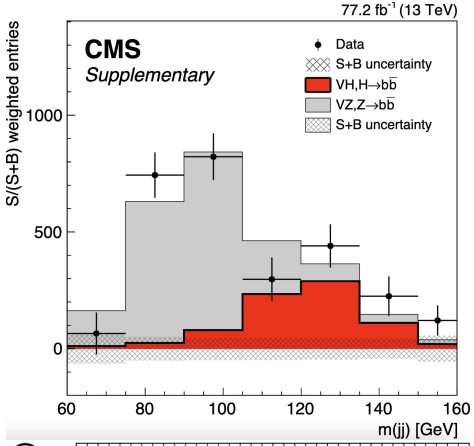
DELPHES
fast simulation



Unfolding, triggering



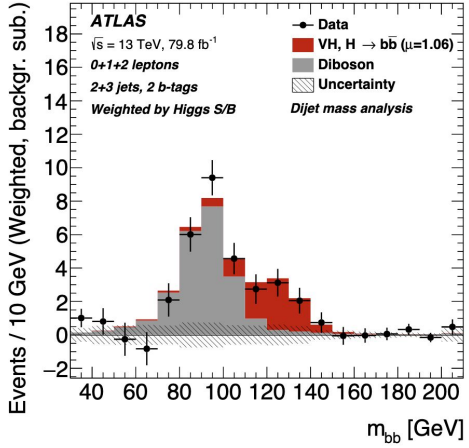
Calibration, Data Curation, PID



ME calculation, hadronization, MC sampling, PDF fits

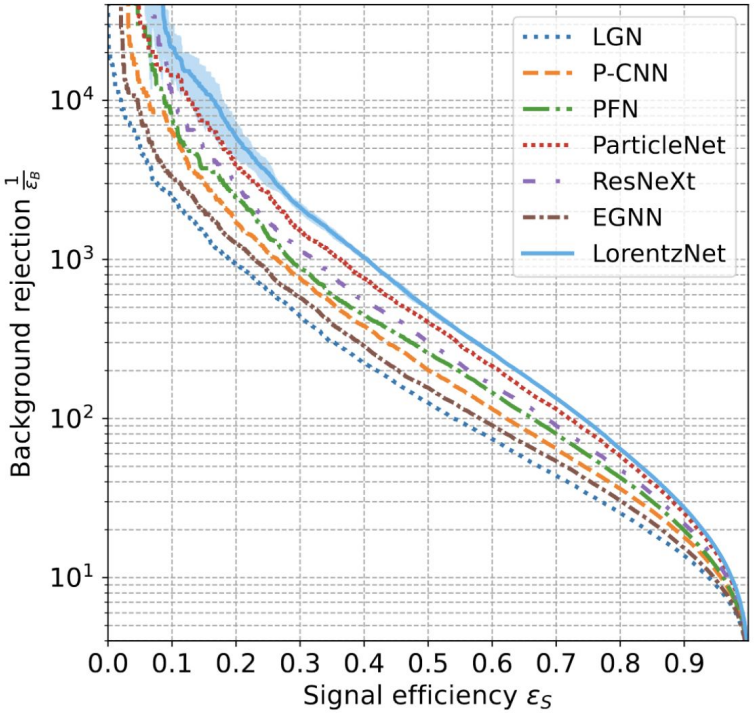
Fast Simulation, Experimental design

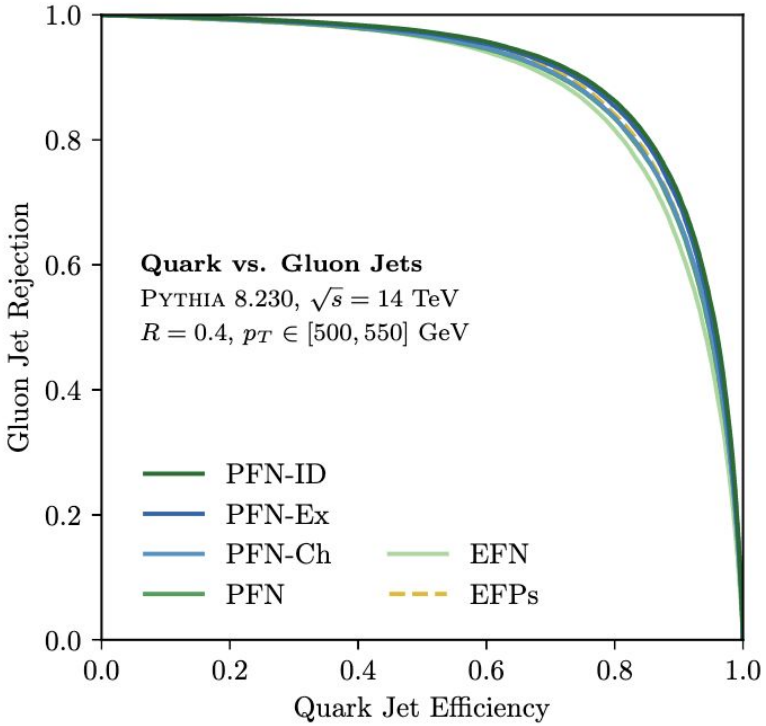
Pattern Recognition, Classification



DELPHES
fast simulation

ML for SM: Jet Physics

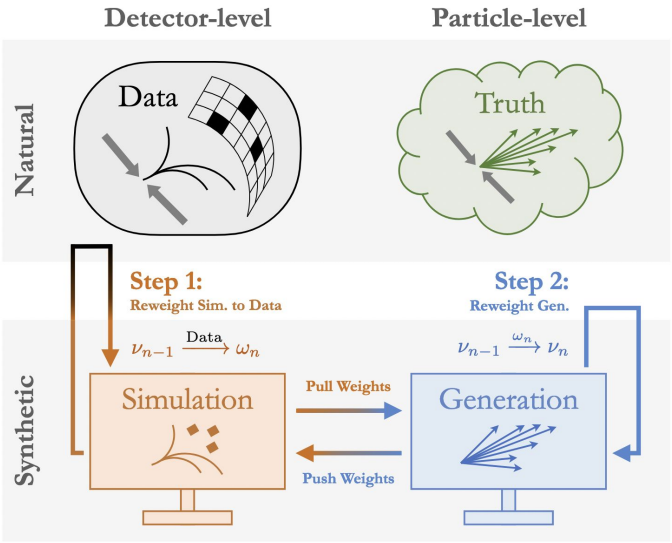


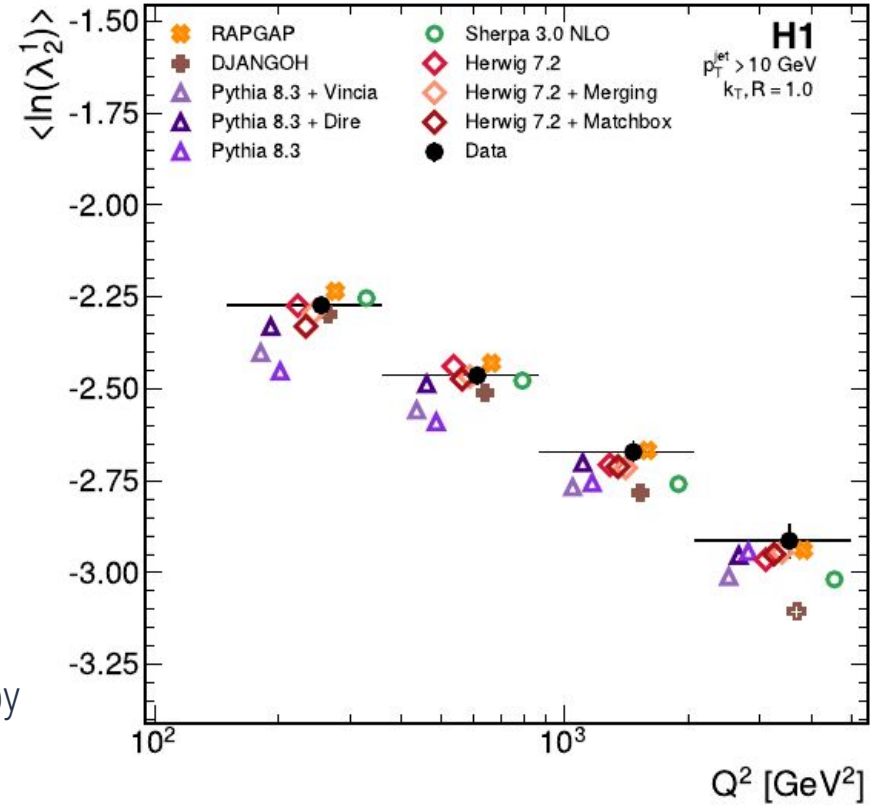


Modern **jet taggers** are very performant and crucial to many experimental measurements

- Recent interest in explicitly enforcing **symmetries**, like **Lorentz group equivariance**, or designing algorithms with specific properties, such as **Infrared and Collinear safety**
- **What properties do we want these algorithms to have?**

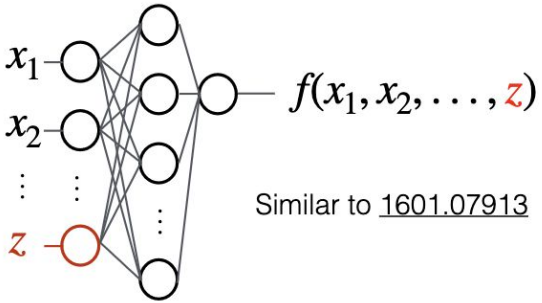
ML for SM: Unfolding





- **Unbinned and high dimensional** unfolding enabled by ML methods using collider data already published
- Easy to unfold **functions of the data: unbiased** unfolding of the moments of distributions
- New opportunities for unfolding: **Energy correlators, track functions**
- **What should we unfold?**

ML for SM: Uncertainties

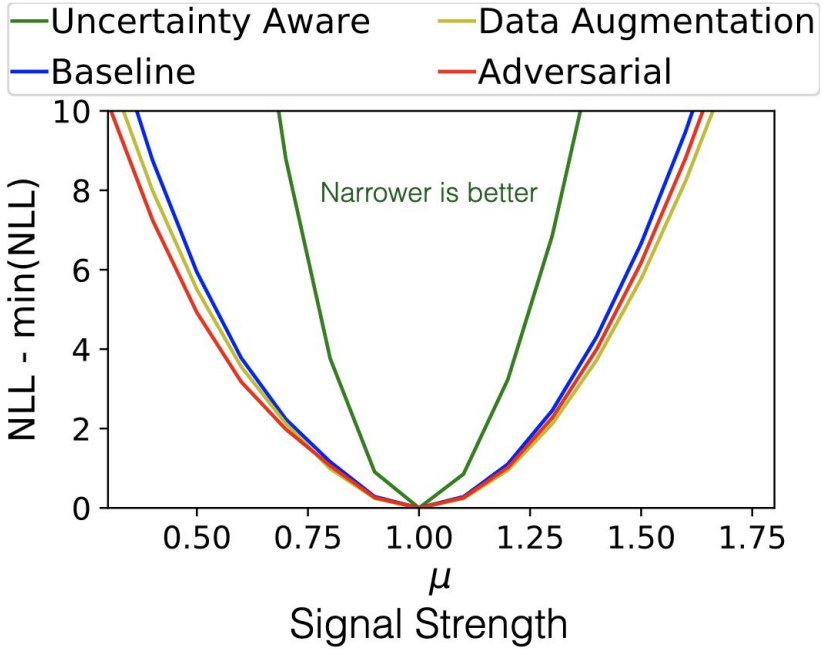


Similar to 1601.07913

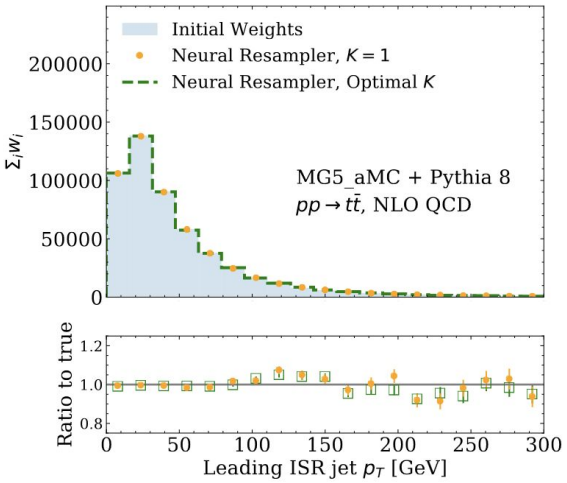
Repeat for each hypothesis z

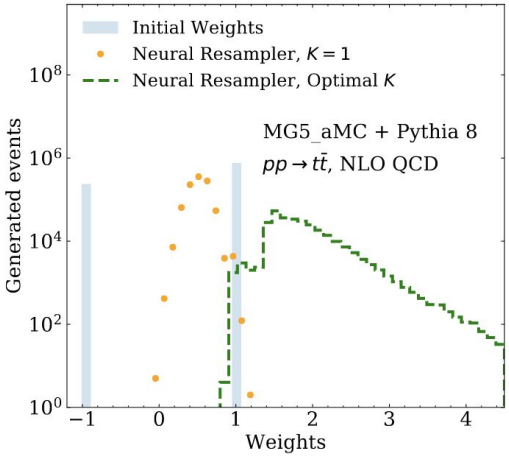
Data with Z = ?

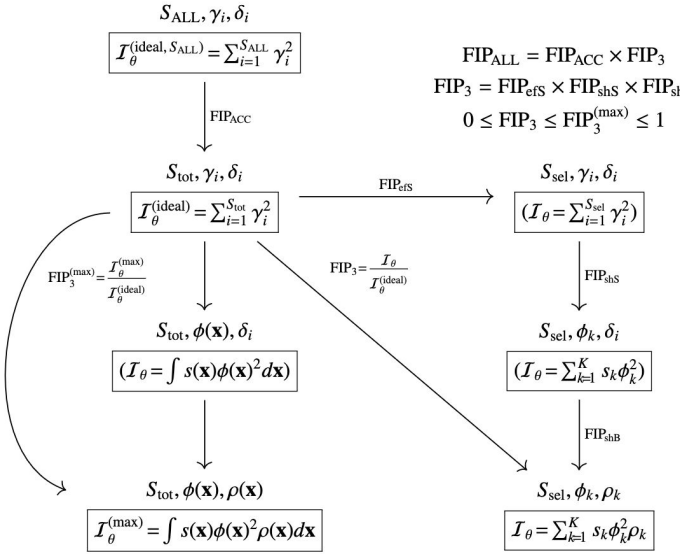
- Train your favorite classifier to be **parametrized** by the main uncertainties of your measurement
- Get the **best classifier** for a given value of the nuisance
- More **precise** final measurements with algorithms that account for uncertainties in the training phase
- **Which measurements would benefit the most?**



ML for SM: Reweighting







- Removing **negative weights** from MC generators
- Interpolating between **different simulation parameters**
  - Can also be used for **Experimental design** and to find the theoretical limit for the **best precision** on the parameter that you could extract from a sample with an ideal detector

ML for SM: Fast MC Simulation

Event Generation with Normalizing Flows

Christina Gao,[1] Stefan Höche,[1] Joshua Isaacson,[1] Claudius Krause,[1] and Holger Schulz[2]
[1]*Fermi National Accelerator Laboratory, Batavia, IL, 60510, USA*
[2]*Department of Physics, University of Cincinnati, Cincinnati, OH 45219, USA*

Unweighting multijet event generation using factorisation-aware neural networks

T. Janßen[1], D. Maître[2], S. Schumann[1], F. Siegert[3], H. Truong[2]

Towards a Deep Learning Model for Hadronization

Aishik Ghosh,[a,b] Xiangyang Ju,[b] Benjamin Nachman,[b,c] and Andrzej Siodmok[d]

`PDFFlow`: parton distribution functions on GPU

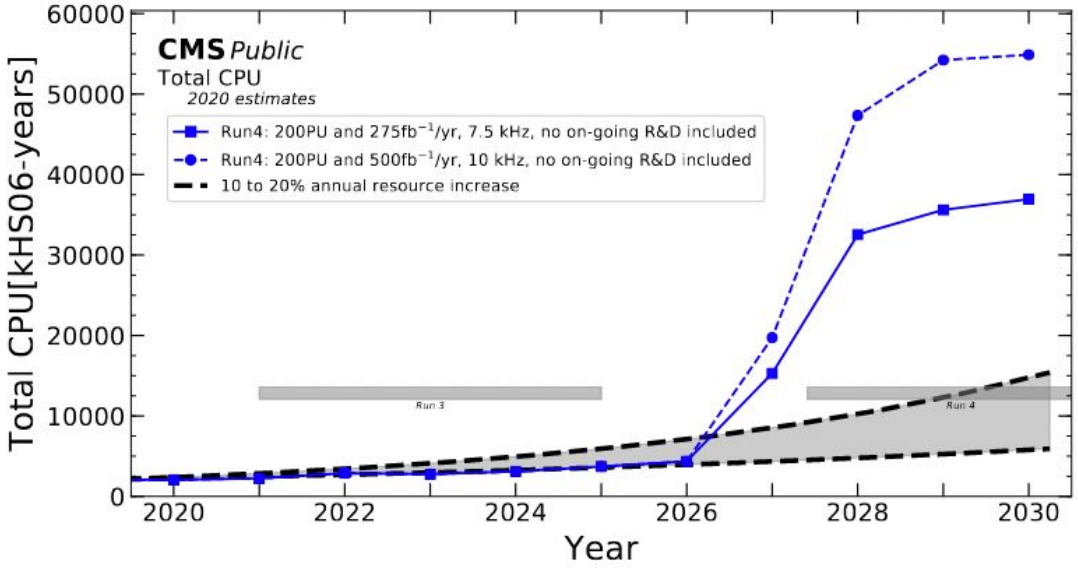
Stefano Carrazza[a,*], Juan M. Cruz-Martinez[a], Marco Rossi[a,b]

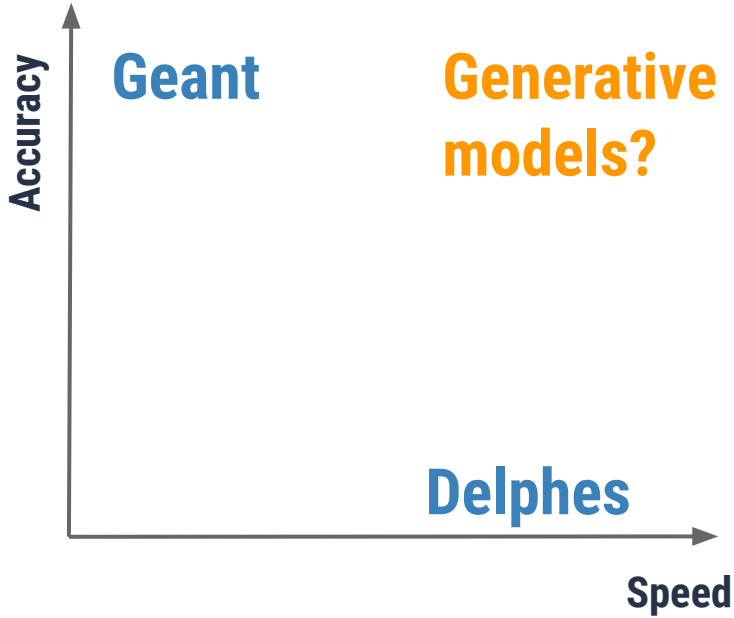
`MCNNTUNES`: tuning Shower Monte Carlo generators with machine learning

Marco Lazzarin[a], Simone Alioli[b], Stefano Carrazza[a]

- **Accelerate** theory predictions by speeding up slower calculations with **hardware** (GPU support) or **software** innovations:
  - Hadronization
  - Phase-space integration
  - Matrix-element estimation
  - Tuning

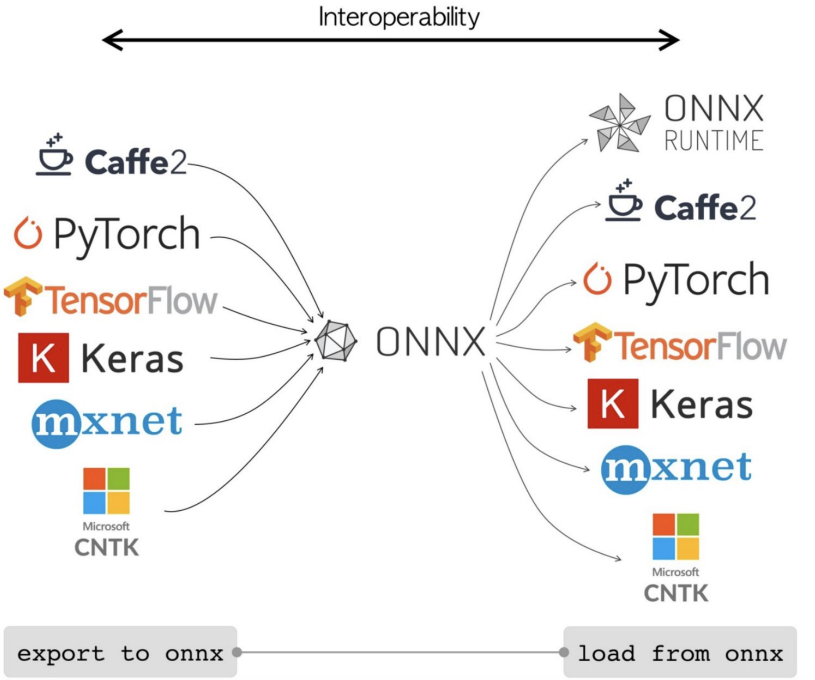
ML for SM: Fast Detector Simulation





- **Detector simulation** becomes computationally prohibitive with current strategy
  - We need **billions** of simulated events to cover different physics processes
  - **Multiple independent theory predictions** to cross check different measurements
- Machine learning provides an exciting alternative for **fast simulation**
- **What are the challenges to incorporate models inside current software?**

ML for SM: Interoperability



- **Inference as a service** leverage remote resources and take advantage of different computing centers/cloud computing
- **SONIC/TRITON**

- **Deployment** of new algorithms within the current software framework is often not straightforward
- Needs to leverage **modern hardware** (when available)
- Software **maintenance** and **reproducibility** are necessary
- **How about other GPU capable workflows? What is the performance gain?**

ML for SM

- Modern **data analysis** methods and **machine learning** are a **fundamental part of collider physics**
- **New** and **exciting opportunities** to leverage the sudden **increase in computational power** and **flexibility** to extend our **scientific reach**
- **Facilitate the communication** between different research communities and promote **interdisciplinarity**