MC toolchain lessons from the LHC

From supporting tools to MC production

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LHC experience and the MC toolchain

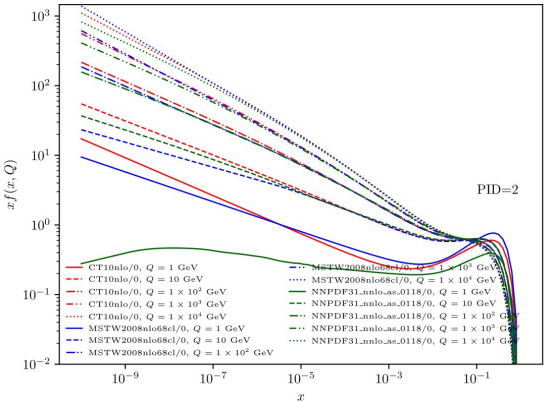
- **The LHC has (among a few other things) seen huge developments in the sophistication of the MC ecosystem**
  - As will be discussed, the physics content of the generators is a world away from pre-LHC:
    - NLO, multileg matching & merging, weighted variations, …
  - But also the "supporting tools":
    - Event formats: HepMC, LHE, HDF5LHE, …
    - Parton densities: LHAPDF universal format and interpolators
    - Validation: HZTOOL → Rivet
    - Tuning: Professor and Apprentice toolkits plus e.g. Autotune
    - BSM interpretation, detector fast-sim, generative ML… *not for today!*

- **I'll give a whistle-stop tour of what's available**

- **And also some practical, logistical and social lessons learned**

Before the MC: LHAPDF parton density library

- **PDFs are a crucial input to MC**
  - Also a key *output* of ep/eA colliders, of course…
  - Need a functional library of (~1500…) established fits
  - Now standard to expect a *error set* for each fit
- **LHAPDF**
  - Library evolved out of Les Houches workshops ~ 2001
  - Backward compatibility with original CERN PDFLIB
  - Gradually extended for error sets, but crumbling F77 and patchwork of incompatible submitted evolution codes…
  - Rewritten in C++ for v6: single data format, decoupled from lib; use internal set of interpolator routines
  - Far more maintainable; has seen speed improvements, GPU interface, extended uncertainty specs, …
  - **Connection between global fits and GPDs? Machinery?**



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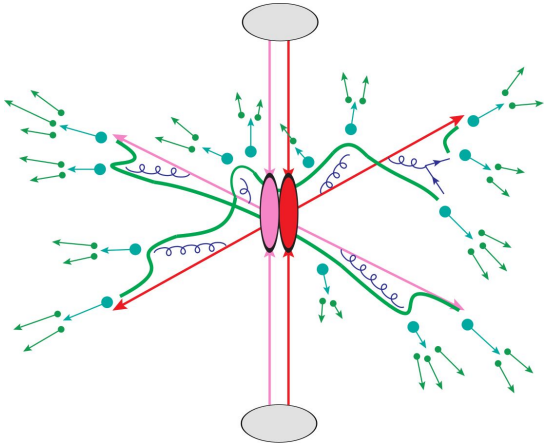
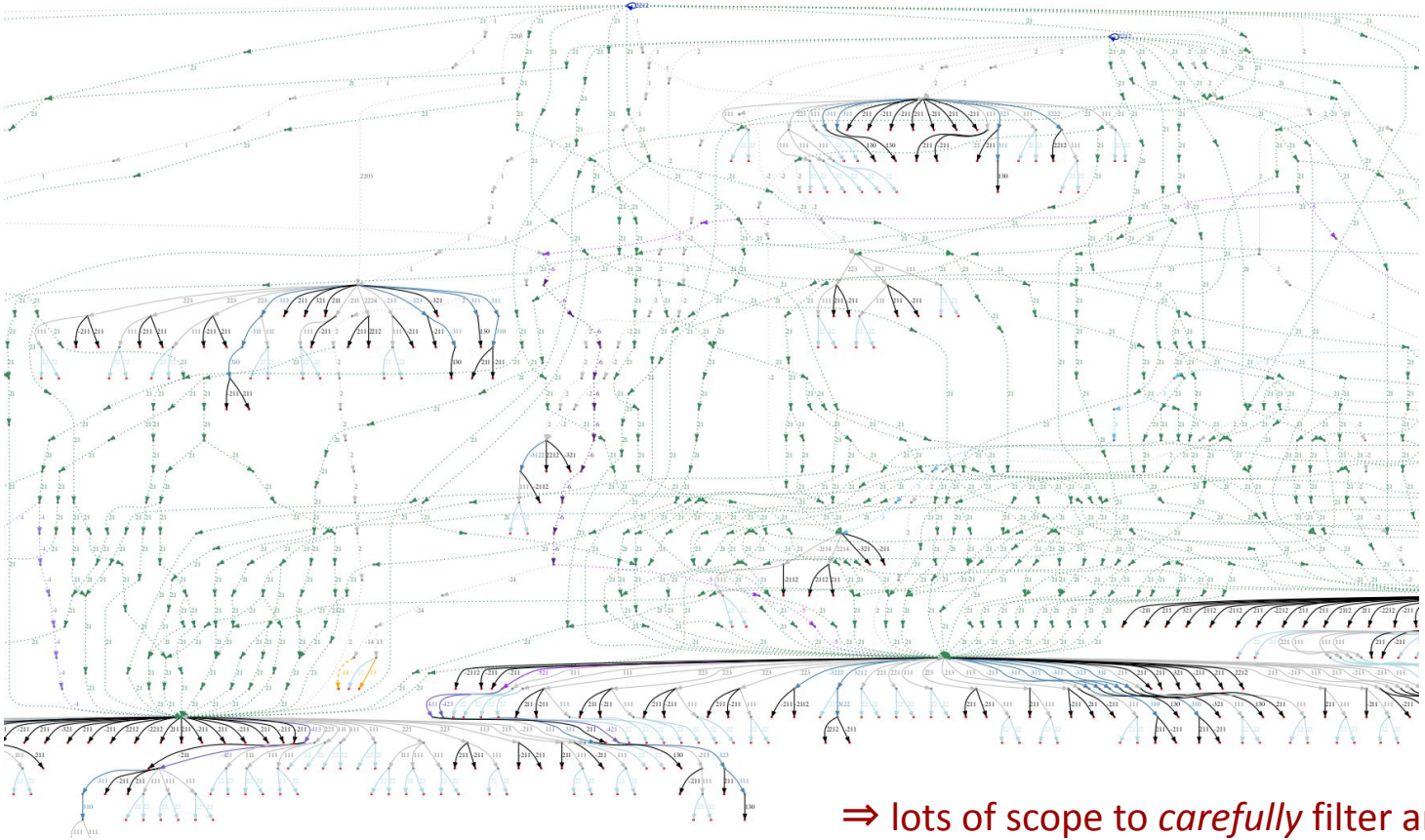
Event formats: from LHE to HepMC

- **Generators**
  - MC codes split between ME and shower+hadronisation generators, e.g. MG5_aMC, PoWHEG, WHiZard (+ loops) vs Pythia, Herwig and Sherpa (which actually does both)
  - Loosen technical coupling via intermediate file formats: LHE (and successor) at ME level, HepMC at hadron level.
- **LHE / HDF5LHE**
  - Minimal format written for mapping LHA common blocks.
  - Designed for small, usually partonic, process exchange.
  - Quasi-XML →parallel-I/O HDF5 for HPC work.
- **HepMC**
  - As much an in-memory interface & data structure as a file format: designed for *general* representation of events
  - NB: "truth" is not "true"! Primarily a record of the algs



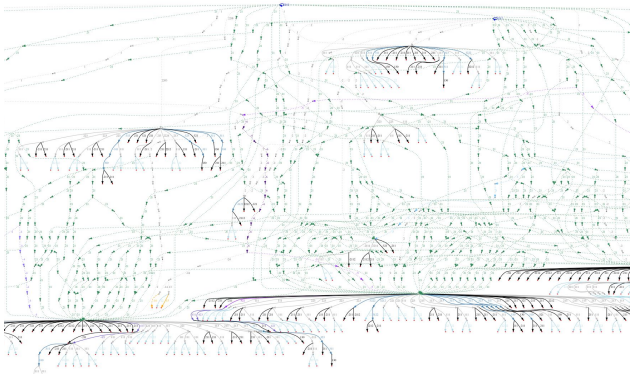
HepMC example (⅓ of a Py8 *pp*→ttbar event)



⇒ lots of scope to *carefully* filter and reduce

HepMC history and content

- **History**
  - General graph model, of GenParticles and GenVertices
  - v1 in 2001: raw pointers, lack of standardisation
  - v2 in 2008: resolve expt forks and CLHEP dep, adds units
  - v3 in ~2019: smart ptrs, resolve constness inconsistencies, clarify ownerships, no barcodes, attributes, make memory contiguous → ROOT-friendly



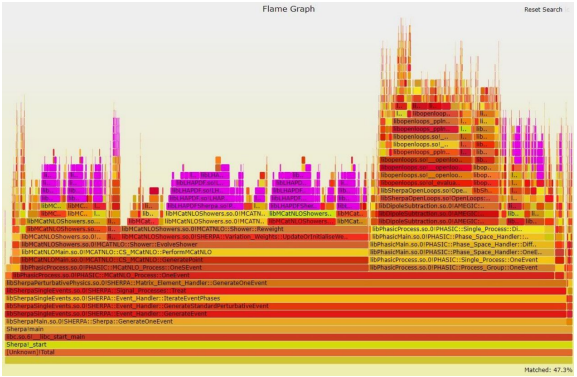
- **Standardisation**
  - v2 introduced standardisation of particle status codes (and later vertex statuses, but these are far less used)
  - More recent MCnet consensus on standard multiweights

- **Gaps**
  - Lack of event-file manipulation tools: shouldn't have to code!
  - Spins and polarizations still second-class. Need push to pass full e.g. spinor info, avoid guesswork

Computational performance

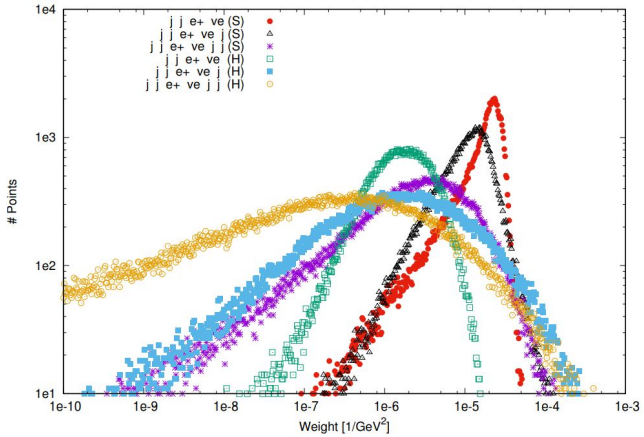
Bulk of LHC evgen CPU in multileg NLO *V*+jets, *tt*

- Don't forget associated packages, e.g. LHAPDF, HepMC
- 40% of Sherpa CPU was in PDFs! Joint projects to address:
  - reduce PDF calls ✓ (pilot runs, restructure code) ⇒
  - speed PDF computation ✓ (~~cache~~, vector, GPU, ipol)
  - optimise transcendental functions, specialise, … ~



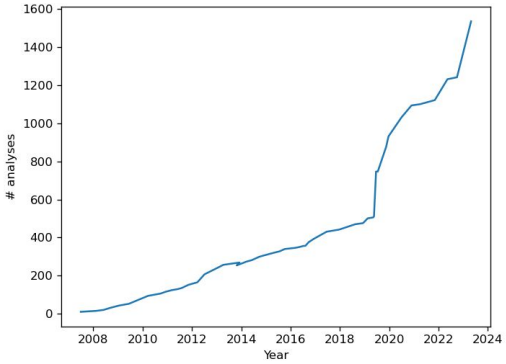
New architectures (?)

- GPUs, other accelerators, vectorisation: nascent efforts, not mainstream, focus on ME since shower etc. trivially parallelisable
- Focus on new gen strategies using HPC
  - Why are multiple experiments duplicating CPU on generating the same expensive algebraic ME results?
  - Logistics of GPU on Grid look bad: use systems to best match requirements ⇒ improved event formats and manipulation tools for HPC ⟶ HTC interchange



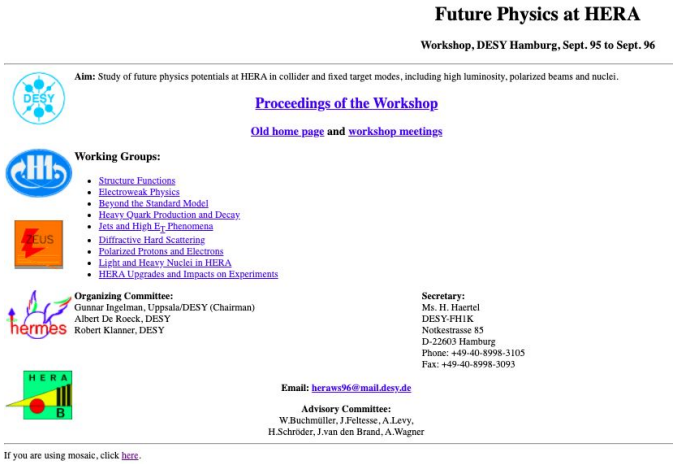
MC analysis and validation: Rivet

- **Rivet is the "LHC standard" MC analysis toolkit**
  - More broadly aiming to preserve the logic of data analyses and encourage expt-pheno collaboration
  - Availability of runnable analysis code is a game-changer!
  - Central to a *community* of analysis reinterpretation tools
- **Code-wise, a C++ core and Python tools. Some good ideas:**
  - Fiducial / generator-independence emphasis
  - Integration with HepData (v4 release and new stats backend)
  - 1500-2000 analyses
- **Used in both MC and measurement-analysis communities: always room to grow more. Strong *network effects***
  - Requires active support in experiments, conveners who "get it". Lightweight reinterpretation is accessible: powerful complement to "full" analysis preservation. Also needs stats/data: HepData, HS3, ML models, … plan in advance!



From HZTool to Rivet

- **The idea of preserving experimental analyses for MC validation was born out of HZTOOL**
  - HERA (H1 and ZEUS) DIS and photoproduction
  - Probing low-*x*, semi-perturbative physics:
    DIS with Q^2 ~ 4 GeV^2; jet p_T ~ 5 GeV; diffraction
  - Many "state of the art" models only in MCs
  - Much confusion about comparing like-with-like between generators, experiments, and analyses
  - HZTool (Fortran) for cross-experiment comparisons of similar measurements modulo cut differences
- **Direct line to Rivet, 10 years later: "HZ mark two"**
  - UK e-science funding; adopted by EU MCnet network



Future Physics at HERA

Workshop, DESY Hamburg, Sept. 95 to Sept. 96

Aim: Study of future physics potentials at HERA in collider and fixed target modes, including high luminosity, polarized beams and nuclei.

Proceedings of the Workshop

Old home page and workshop meetings

Working Groups:

- Structure Functions
- Electroweak Physics
- Beyond the Standard Model
- Heavy Quark Production and Decay
- Jets and High E_T Phenomena
- Diffractive Hard Scattering
- Polarized Protons and Electrons
- Light and Heavy Nuclei in HERA
- HERA Upgrades and Impacts on Experiments

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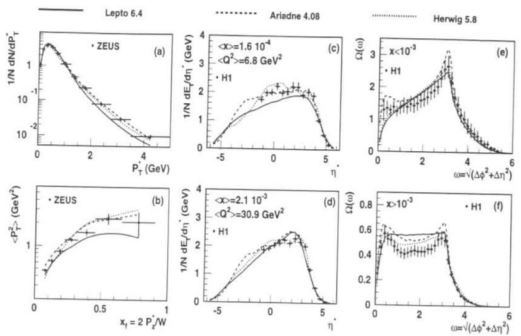
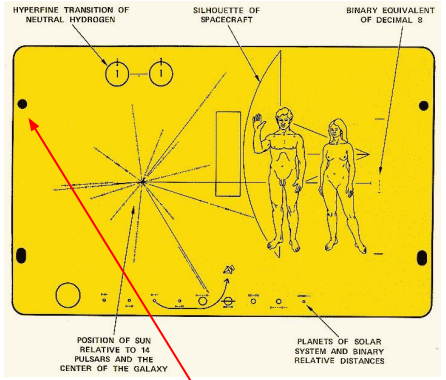


Figure 1: *The transverse momenta dN/dp_T (a) and the 'seagull' plot $\langle P_T^2 \rangle \times x_F$ (b) of single particles in the positive hemisphere of the hadronic center of mass. The transverse energy flow $dE_T/d\eta$ in a low (c) and high (d) x and Q^2 bin. The transverse energy-energy correlations for $x > 10^{-3}$ (e) and $x < 10^{-3}$ (f).*

Lessons learned

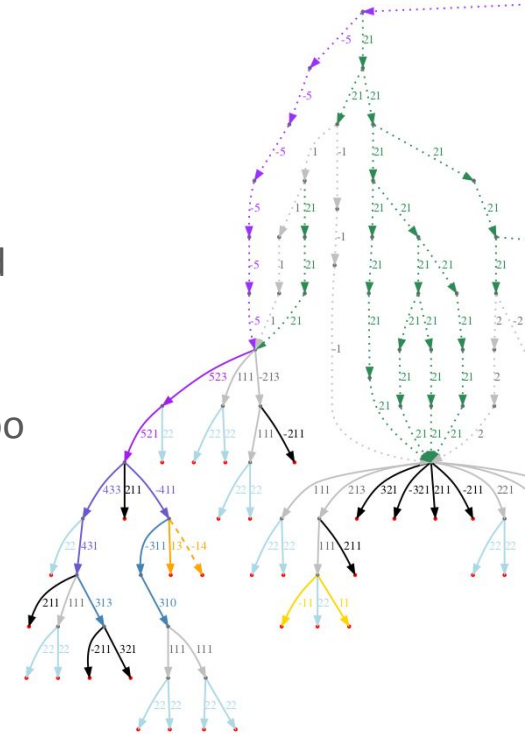


- **A simple/obvious idea, with surprising impact:**
  - **Reproducing a key plot (or not) is *powerful***
    - ⇒ *understand physics, communicate issues, improve MCs*
  - **A *common language* for phenomenology and experiment**
- **But…**
  - "Obvious" to use partons, bosons, etc. direct from the event graph
  - Frequently unphysical, depend on approximations. May not even exist!
  - Scalability of many analyses to new MCs means avoiding gen-dependence
    - **⇒ predict "real" observables, from well-defined final states**
- **Standardisation: boring but important**
  - (physical) event format conventions, statuses, PDG particle numbering, weights…
- **Scalability**
  - Lots of expensive operations are repeated: sharing calculations is essential

Physically safe analysis methods

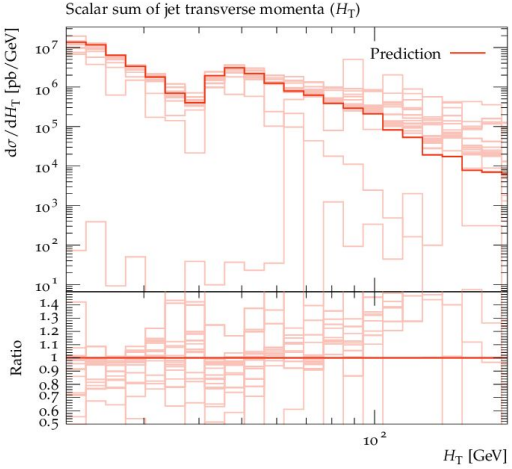
Avoiding unstandardised event-graph features was pragmatic, but led to some genuine physical insights:

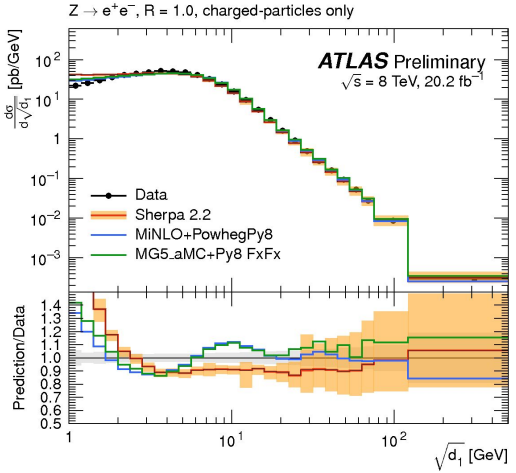
- **Refining the "fiducial analysis", define *unfolding targets***
- **Hadronisation as a "decoherence barrier"**
  use the natural dividing line between the quantum-interfering hard process & semi-classical decays: ~ no tempting partons!
- **Bringing truth tagging closer to reco**
  first releases used *b*-ancestry of jet constituents to set HF labels: too inclusive! ⇒ *associate* the hard-fragmenting, weakly-decaying *B*
- **Promptness/directness tests**
  don't identify a particle "from the hard process"; do it backward. Label as *indirect* via recursive checks for hadron parentage
- **Dressed leptons**
  we now primarily *dress* truth leptons with their photon halo



Multiweights and re-entry

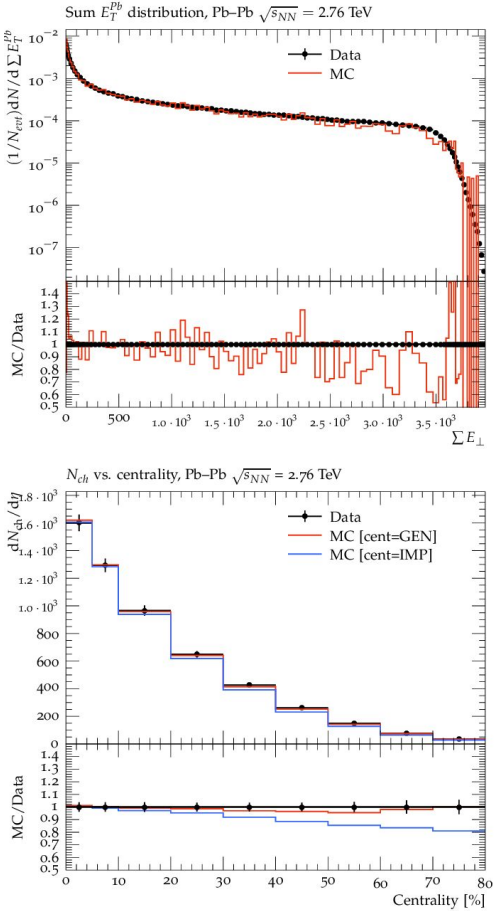
- **MC weight vectors allow expression of increasingly complex theory uncertainties.** But a burden for analysis chains: have to propagate and correctly combine O(200) weight streams!
- **Rivet 3: complex automatic handling of weights**
  ~invisible to users: data objects *look* like histograms etc. but are secretly multiplexed
- **Can now re-call finalisation to combine runs:**
  RAW histogram stage preserves pre-finalize objects
  ⇒ "re-entrant" perfect rivet-merge-ing
  Key for e.g. *pA/pp or W/Z* ratios, + BSM recasting
- **Data types are important:** glimpses of a fully coherent separation of semantics from presentation





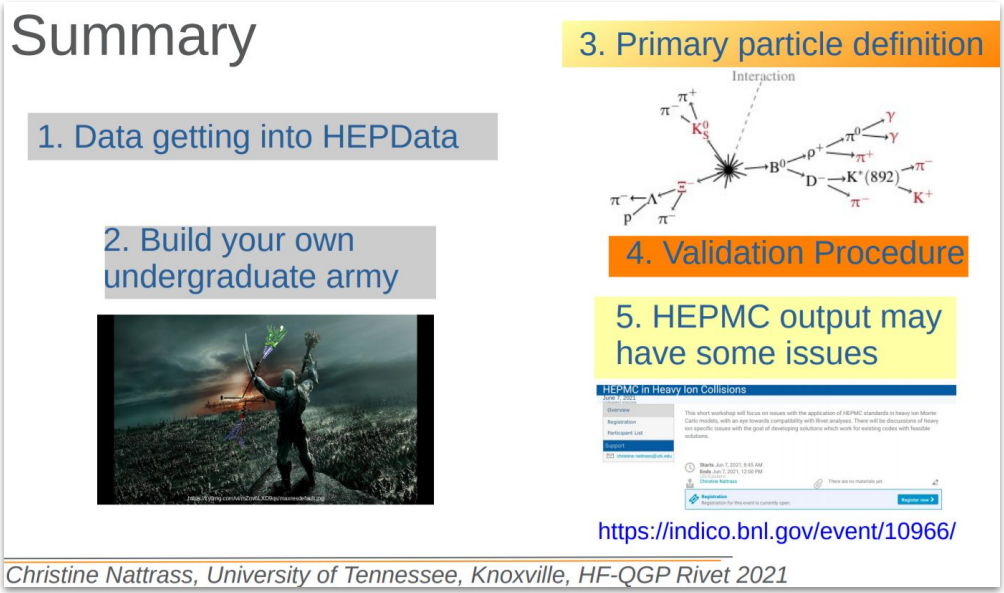
Heavy-ion physics preservation

- "Adding heavy-ion support" sounds trivial!
- Actually nuanced ⇒ lots of structural impacts
  - HI observables often require centrality-fraction calibration curves: we need a 2-pass run.
  - Flow observables, event/event correlations… all centrality-binned!
  - Swappable definitions: few HI generators are general-purpose enough to do "everything"
- All supported "out of the box" since v3
  - Paper: https://arxiv.org/abs/2001.10737
  - Core development tool for Pythia/Angantyr: authors and ALICE (etc.) collaborators providing analyses
- **Should be well-placed for EIC HI requirements**



HI *community engagement*

- **Great "spontaneous" engagement from within BNL HI. Several productive workshops**



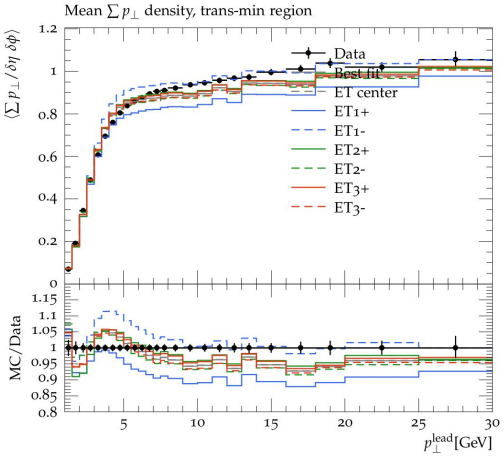
- HepData, Rivet
- Better ex/ph communication
- Faster model/data comparisons
- Addressing issues with formats and incomplete models
- Undergrad army!

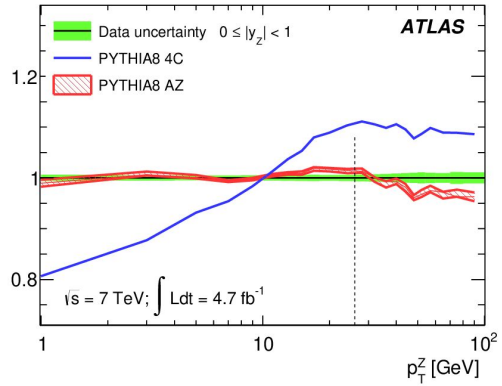
Work reactivated recently, very relevant overlap with EIC community

Applications: from tuning to…

***First* "killer app": huge pre-LHC soft-QCD uncertainties:**

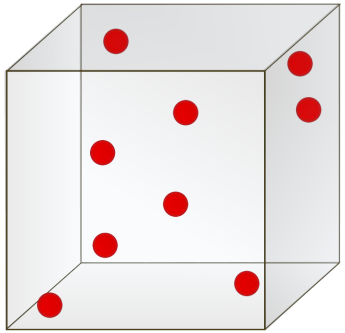
- **Tuning required Rivet analyses from expt**
- **Feed in to underlying event, pile-up, etc. modelling**
  - Better tunes ⇒ better analysis, better results
  - Impact: LEP and Tevatron analyses published for ~10 years suddenly got *used*! And cited…
    - ⇒ ATLAS tunes, CMS tunes, eigentunes…
    - ⇒ Rapid responses to preliminary data
  - Model development: matching & merging, addition of MPI energy-evolution & colour-reconnection to Herwig, …
- More recently, use of Rivet's analysis collection for *BSM, Higgs EFT, PDF fits (see Anjelo's talk after), …*
  - **Good analysis preservation enables new ideas**



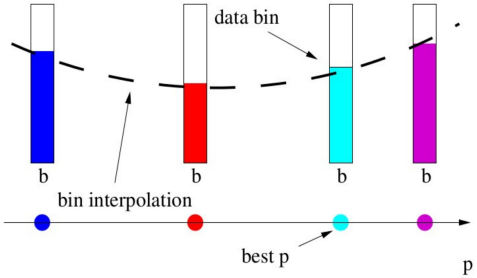


Speaking of tuning… Professor/Apprentice

- **MC models contain O(10-30) influential free parameters, typically in non-perturbative parts**
  - Fragmentation kinematics, cluster and string splittings, flavour and meson/baryon mixtures, MPI, shower scales
  - No *a priori* predictions ⇒ "tune" to match data
  - As much data as possible — within model capabilities



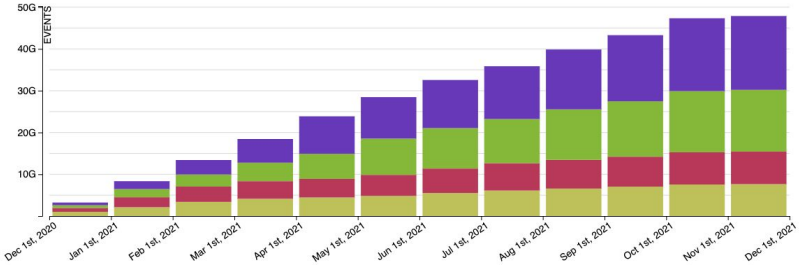
- **Professor (2009) and Apprentice (2021) semi-automate the fit, with a surrogate-model approach**
  - **pre-sample** from the MC parameter (sub-)space
  - **parallel-execute** a comprehensive set of MC runs with (Rivet) analysis → histogram predictions vs data
  - **parametrise** the response of *each bin* to the parameters
  - **⇒ usual iterative fit to reference data**



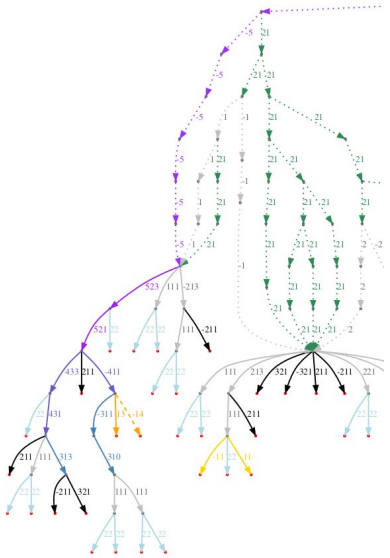
- **Supported & developed… but currently at "best effort" level**

LHC experience of MC production logistics

- **Both ATLAS and CMS batch MC event generation in *campaigns* of O(50 Gevt)**
  - ➢ not every year: often reuse+extend evgen



- **Running generators at scale introduces exciting new failure modes!**
  - ➢ rare numerical issues
  - ➢ configuration mistakes *very* costly
  - ➢ requires serious software and configuration management



- **MC generation has particularly strong *upward* CPU scaling**
  - ➢ analysers have accustomed to MC being a good proxy for data.
  - ➢ *Always* demand for next order in precision
    - ⇒ typically costs an *order of magnitude* more CPU!
  - ➢ sometimes the right answer is “no”... match precision to requirements! [While being impressed it’s *possible*]

Code management and integration

- **Code and build management**
  - LHC experiment software mostly built on LCG software bundles
  - Generators included via GenSer project: integrate release tarballs, perform basic tests
  - Used directly by ATLAS and LHCb, tarballs by CMS, not by ALICE
  - Experiment frameworks need “glue” packages to pick up compiled generators. Library version compatibility, e.g. FastJet & HepMC, not always coherent…
  - Not 100% clear the intermediate has been worth it: generators are out-of-the-box packaged following far more usable software methods than in the Fortran era

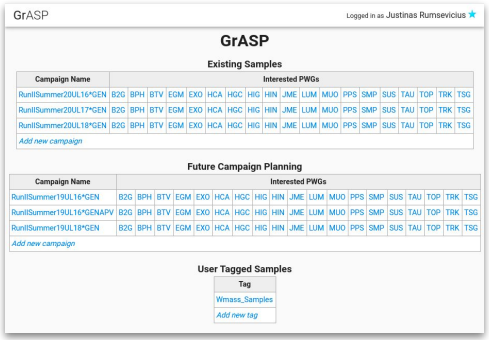
- **Experiment-framework interfacing**
  - Dedicated packages for each generator — configurations *still* not all programmatically friendly (Powheg, MG5). Do as a little physics as possible in interfaces!
  - Documentation: prefer repo READMEs to wikis!!
  - Post-proc event-graph testing and fixing: flag common problems like unknown PIDs, broken graphs, unexpected displaced vertices, E & p imbalances…

Sample-configuration management

- **Python job options (JOs) in both ATLAS and CMS**
  - O(10,000-1,000,000) sample configurations: jet slices, heavy-flavour filtering, BSM param-scans, other enhancement-biasing…
  - New ones *will* be made by non-experts, via copy & paste ⇒ validation essential!
  - Vigilance needed to identify common elements and manage common JO snippets. Chain snippets for e.g. standard params, tunes, modes, …

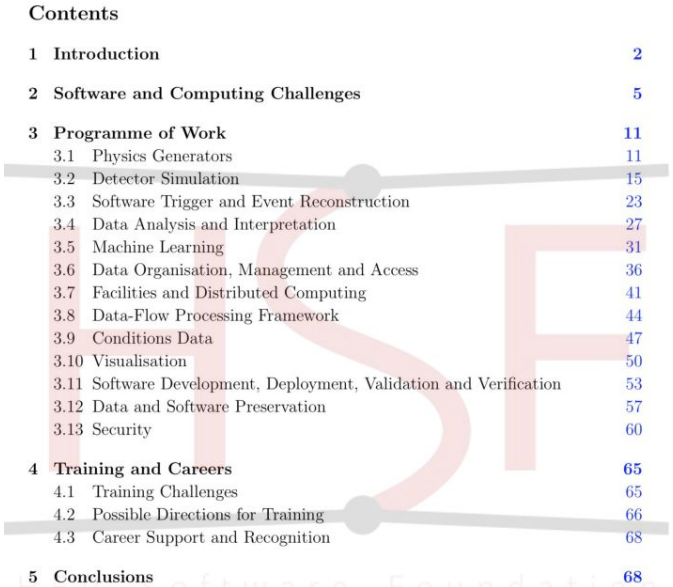
- **Managing sample requests & production status**
  - "Keep it simple. I'm sure a GitLab issue would work just fine". GitLab is great…
  - CMS more sophisticated than ATLAS: dedicated Web apps, e.g. GrASP, vs Twiki+GSheets+JIRA+…
  - Not "interesting", not physics, but needs effort and dev time

- **Distribution**
  - JO updates far too frequent to include in sw releases. Sync via CVMFS or tarballs. Need *versioning*: configs need to be exactly repeatable, for sample extensions



Physics content & communication

- **Experiment generator experts rely on MC authors**
  - Get direct bug/task reporting with authors
  - Need regular interaction, understanding of different motivations and incentives (theory vs exp worlds)
  - Need ability to supply standalone configs to authors: they can't do anything with JOs ⇒ design interfaces with ability to dump standalone steering files
  - don't try to be too clever!
- **Standardising**
  - Work with authors to standardise: formats, systematics weight structure, PDG codes
  - evolving and enforcing standards makes everything better/clearer in the long run


Contents

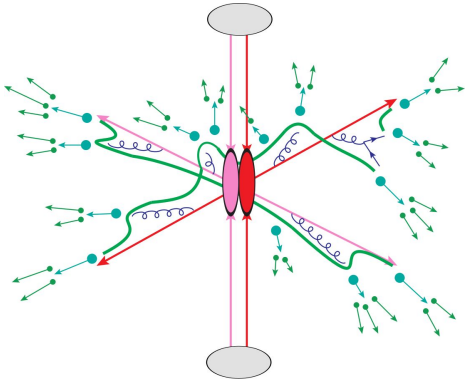
Summary / thoughts

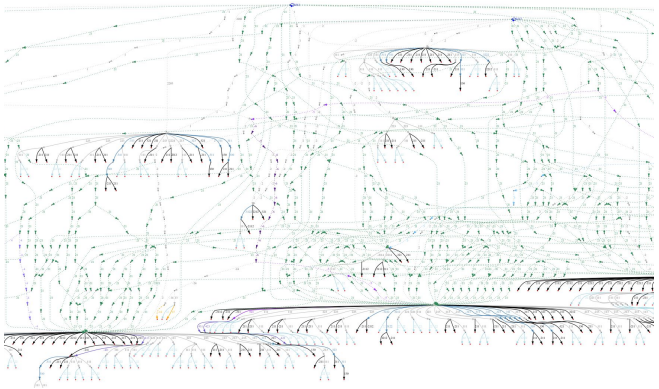
- **We have a well-developed toolchain of supporting codes around the MC generators themselves.**
  - From MCnet historically, schemes like UK SWIFT-HEP helping: more please! Note MC tools workshop here at the end of June
  - Most tools like LHE, HepMC, LHAPDF, Rivet, Prof… not funded!
- **As well as production tools, analysis preservation matters**
  - Completes the virtuous cycle from theory to exp and back
  - Rivet+HepData are ready for EIC: key is incorporation of preservation in experiment procedures and incentives
  - Reusability enhances analysis/publication impact, and provides fruitful exp/th collaboration, esp for junior scientists
- **Lots of LHC-era experience in production scaling and issues**
  - Mistakes are costly! Let's avoid having to re-learn the hard way. LHC-EIC communication routes? Tool re-use? Investment in process

Backup slides

MC generation

- **MC generation is where theory meets experiment**
  - The fundamental *pp, pA, AA* collision, *sans* detector
- **Components of an "exclusive" event-generator chain:**
  - QFT matrix element sampling at fixed-order in QCD
  - *Dressed* with approximate collinear splitting functions, iterated in factorised Markov-chain "parton showers"
  - FS parton evolution terminated at Q ~ 1 GeV: phenomenological hadronisation modelling
  - Mixed with multiple partonic interaction modelling
  - Finally particle decays, and other niceties
- **Modern HEP is hostage to shower MCs!**
  - The main mechanism for translating theory to experimental signatures, from QCD to BSM
  - Generally very complex modelling and output

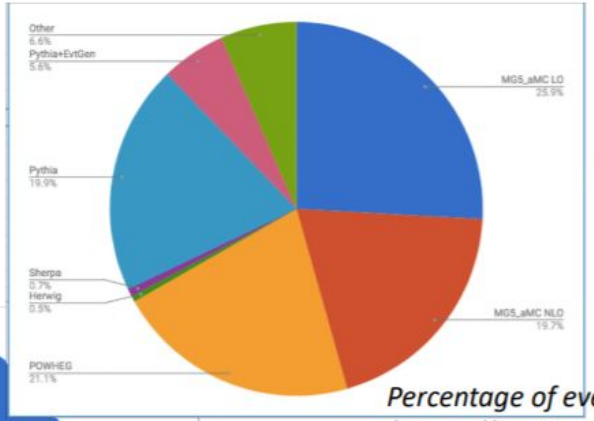




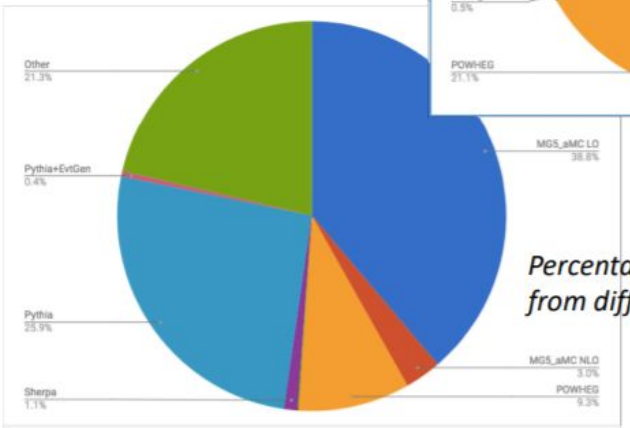
Generator balance

- **CMS has a particularly strong reliance on MG5_aMC and Pythia**
  - 97% Pythia showering!
  - few percent Herwig and Sherpa variations
- **ATLAS a much broader set of generators:**
  - Sherpa NLO for *V*+jets, and *VV* processes
  - Powheg+Pythia for *tt*
  - MG5 LO for most BSM

→ *Approximate and based on 2016 MC campaign*



Percentage of events from different generator



Percentage of samples from different generators

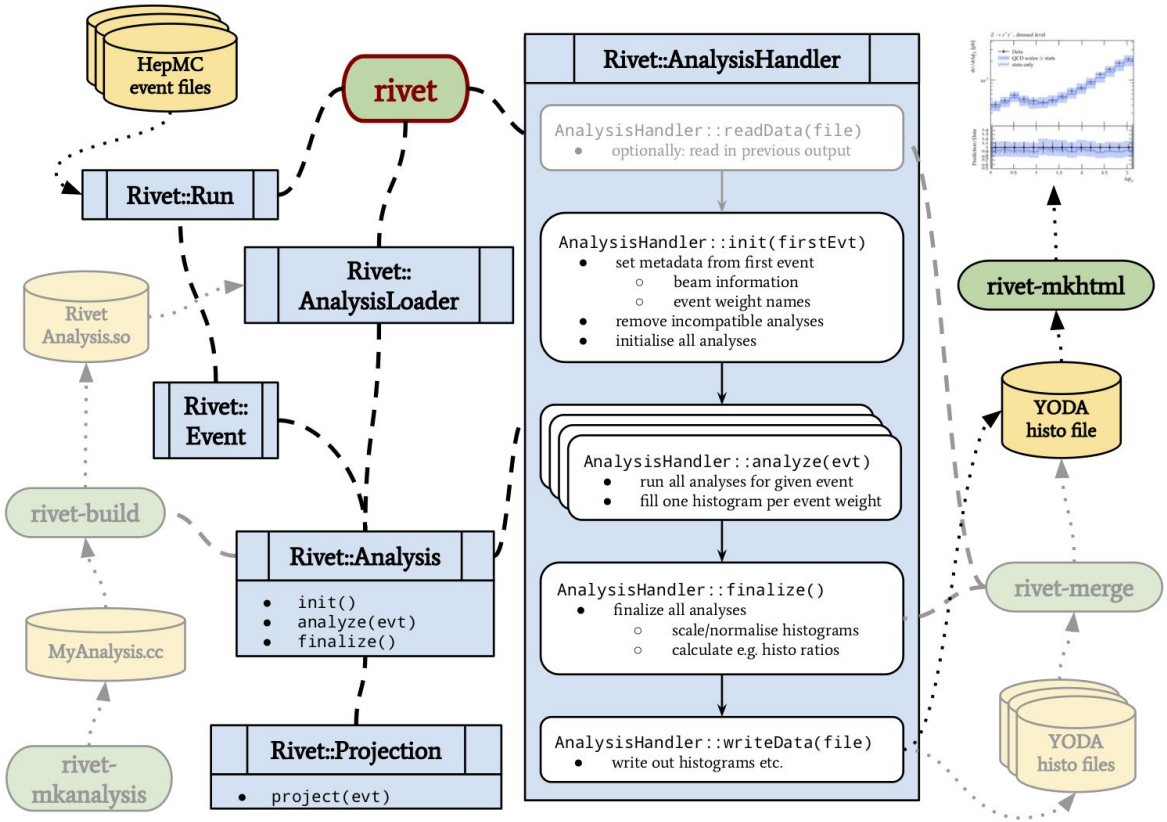
from Efe Yazgan, CMS

Generation practicalities

- **Logistics of bulk NLO production**
  - With “generator generators”, job splitting to O(1kevt) → don’t waste time rebuilding the model and remapping the phase-space (integration) in each job
  - Prebuild “gridpacks” storing results of integration: produced privately on HPC. Gridpack distribution with JOs / via CVMFS
  - LHE generation and tracking correspondence to showered HepMC event (esp. with post-shower event-filtering). Embed in HepMC3?
- **Weighting, filtering and enhancement**
  - Systematics weights: currently O(100) for ME scales, PDFs, sometimes shower vars
  - Post-hoc filtering: focus samples on flavour combinations & phase-space of interest
  - Increasingly “enhancing” phase-space coverage with biased sampling and counter-weights: adaptive samplers in multileg codes “learn” biases, so efficient
- **Data formats**
  - Automatic persistency is overrated — if any risk of change, use dedicated TP converters to persist key event info and handle compatibility. Annoying, but…
  - Downstream analysis formats: reduce event graph to collections of standard e.g. (many different) truth jets with truth flavour-tags dressed leptons, truth MET, etc.

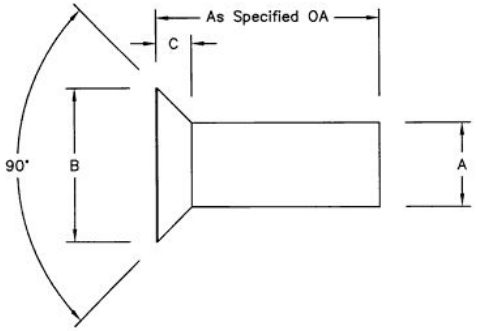
The result

- **Rivet v3 structure**
  arXiv:1912.05451
- Streamlined set of tools from analysis coding to event processing to plotting (and other applications)
- And a key gateway to connect data analysis to theory (and back again)



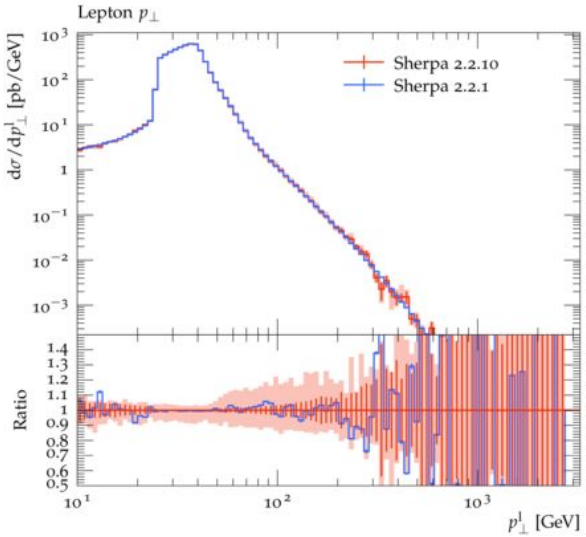
Designing Rivet

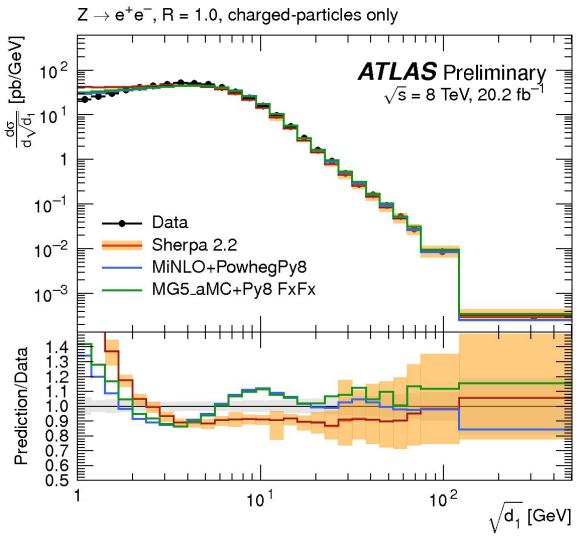
- **Ease of use**
  - **Big emphasis on “more physics, less noise”!**
  - Minimal boilerplate analysis code, HepData sync
  - Event loop and histogramming basically familiar
  - Tools to avoid having to touch the raw event graph
- **Embeddable**
  - OO C++ library, Python wrapper, sane user scripts
  - Generator independence: communication via HepMC
    - Note HepMC3 HI-support efforts
  - Analysis routines factorised: loaded as “plugins”
- **Efficient**
  - Avoid recomputations via “projection” caching system
- **Physical**
  - **Measurements primarily from final-state particles only**

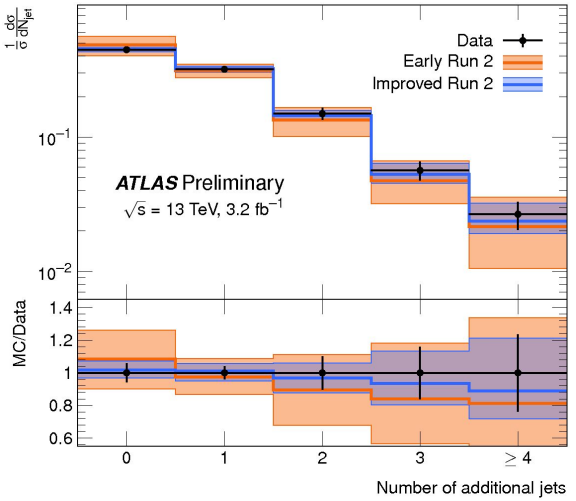


MC systematics bands via multiweights

ATLAS MC studies have been a significant driver of this feature *(thanks to Chris Gutschow)*







- Weight-naming standardisation: see arXiv:2203.08230

Getting & using Rivet

Lightweight analysis preservation is valuable… and easy to start

As either a “user” or analysis author, the barrier is lower than ever: we recommend using our Docker images to get started

Ideal for student projects!

Tutorials available from the Rivet website, a walkthrough in the R3 paper

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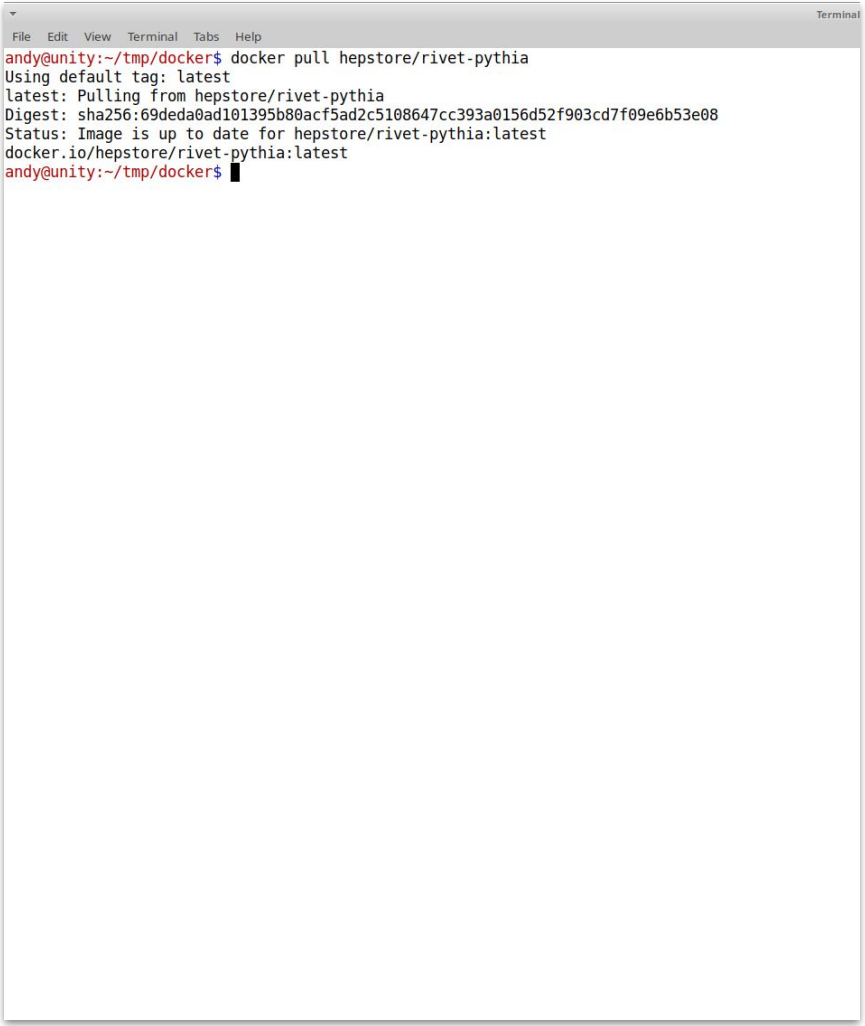

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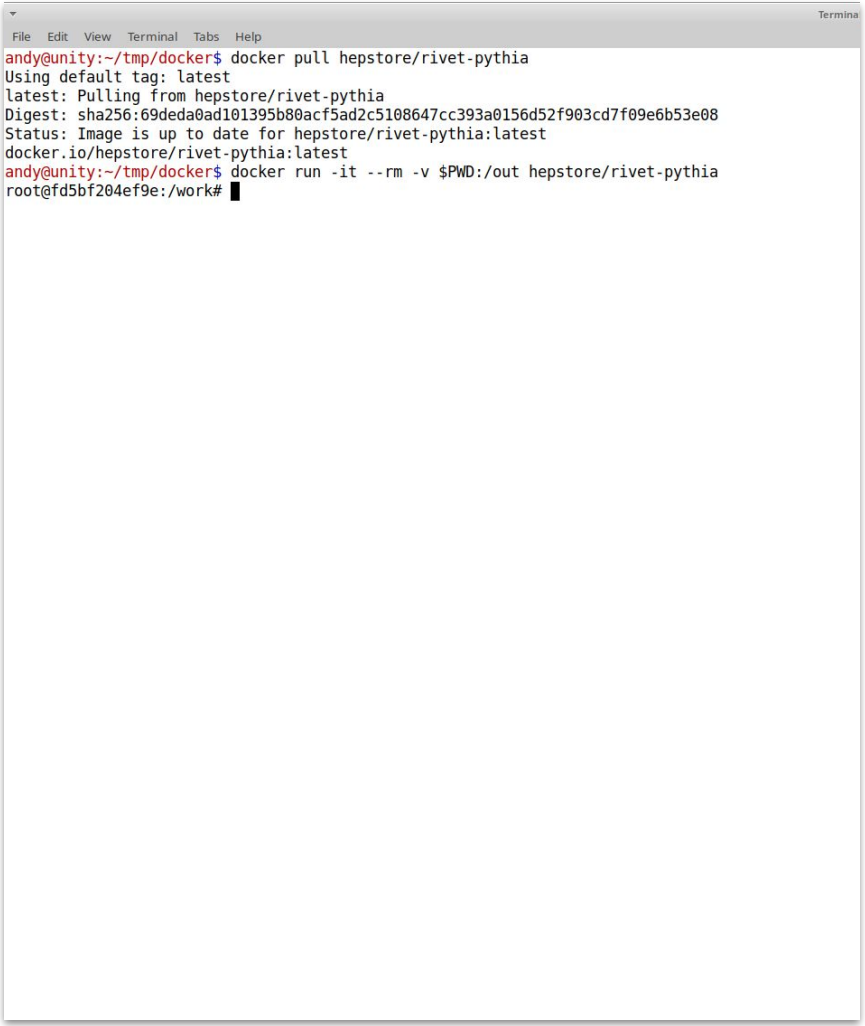

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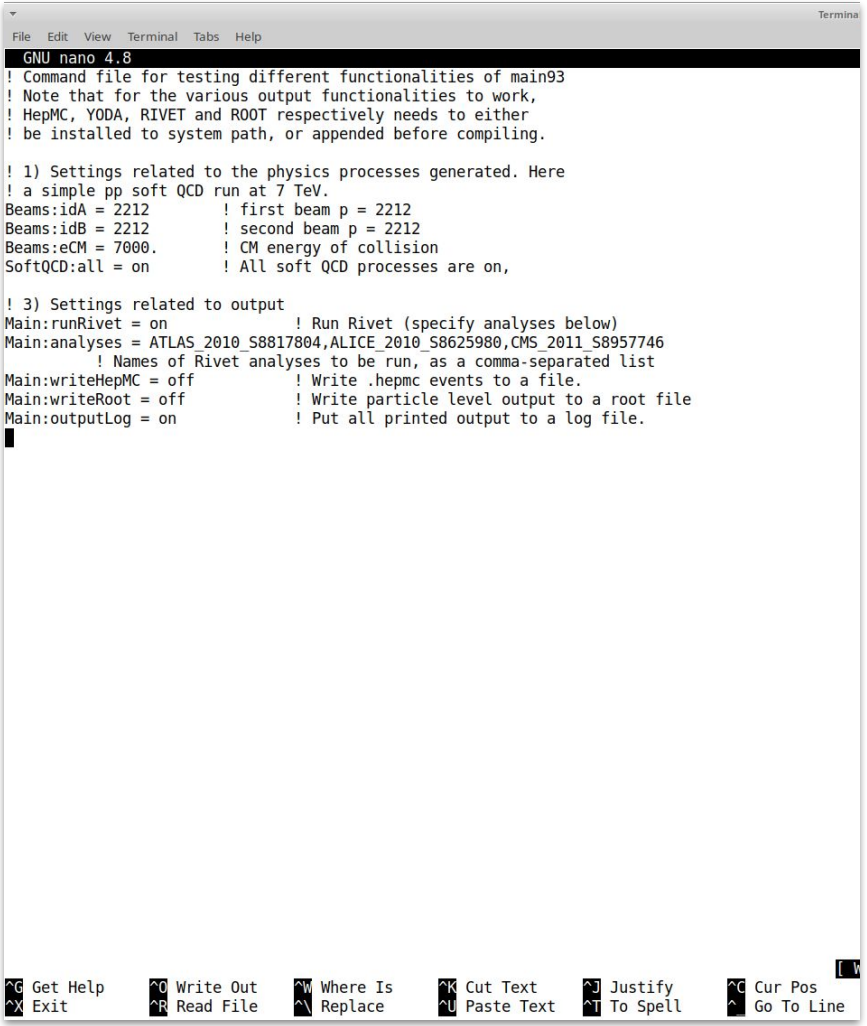

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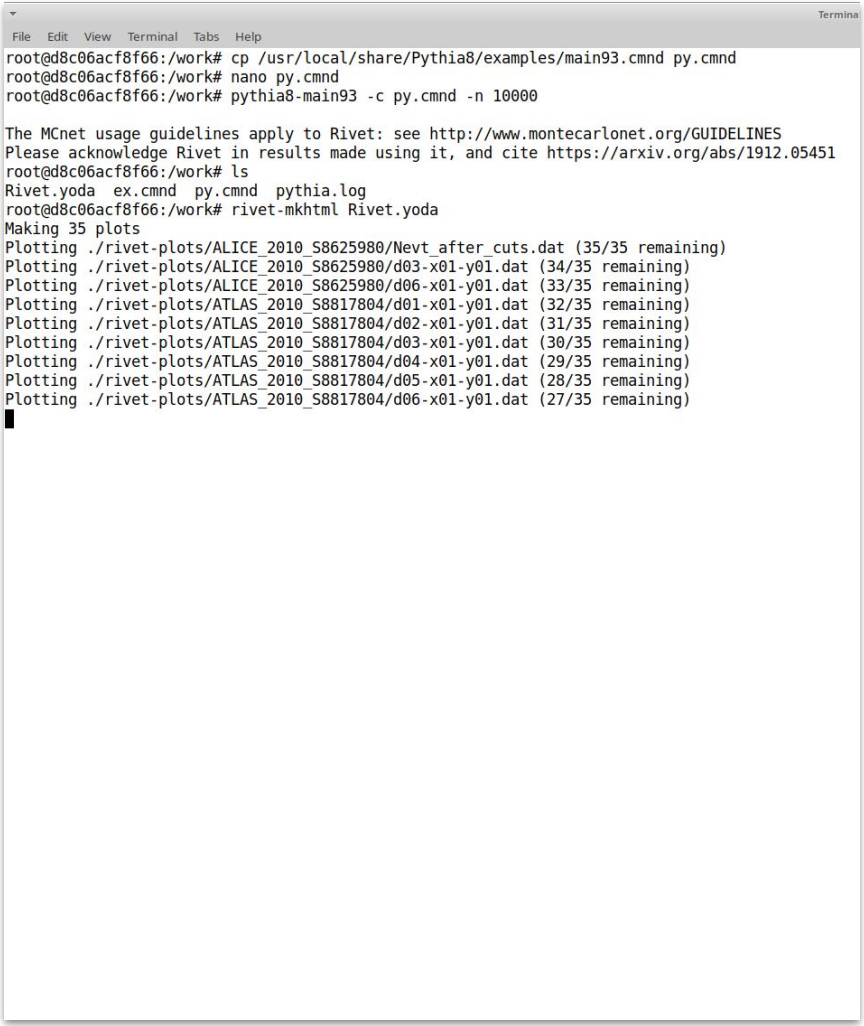

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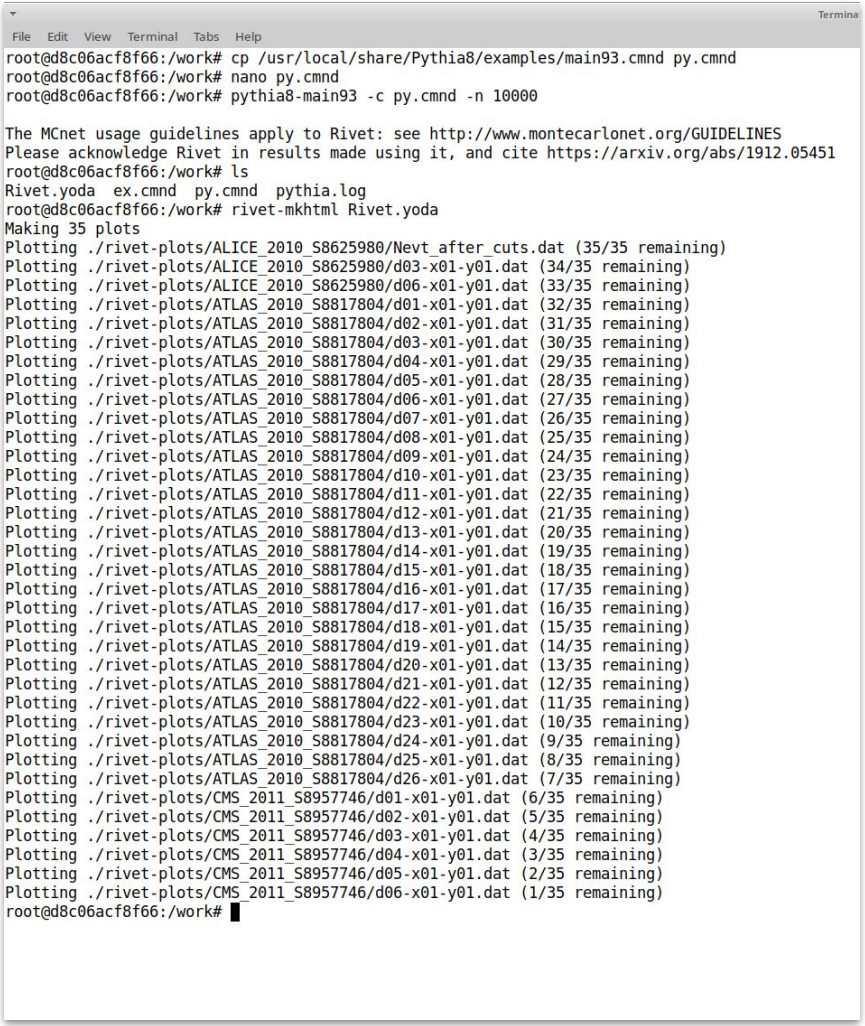

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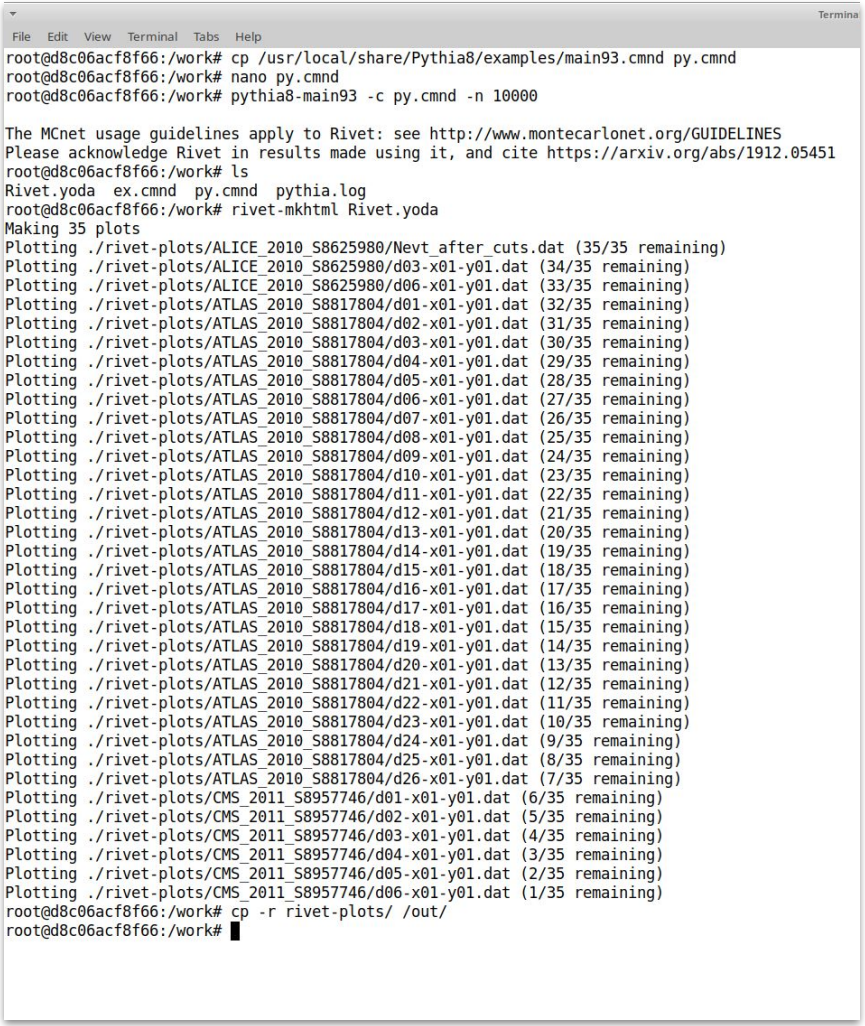

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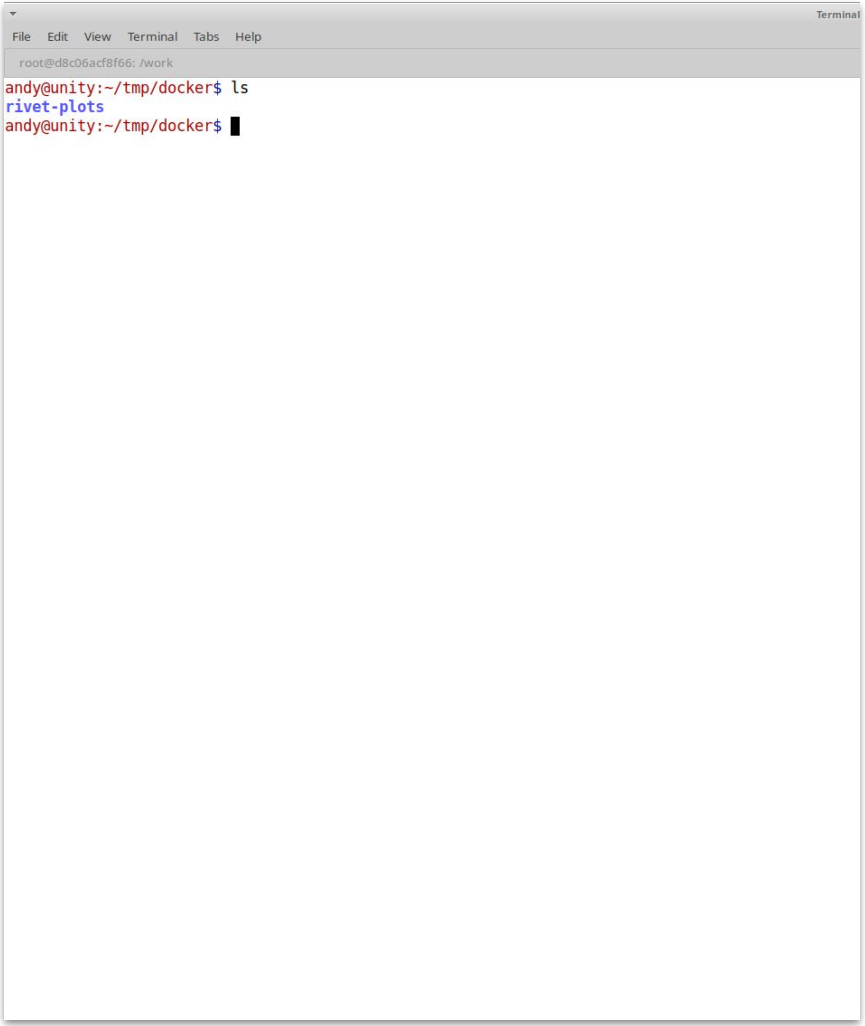

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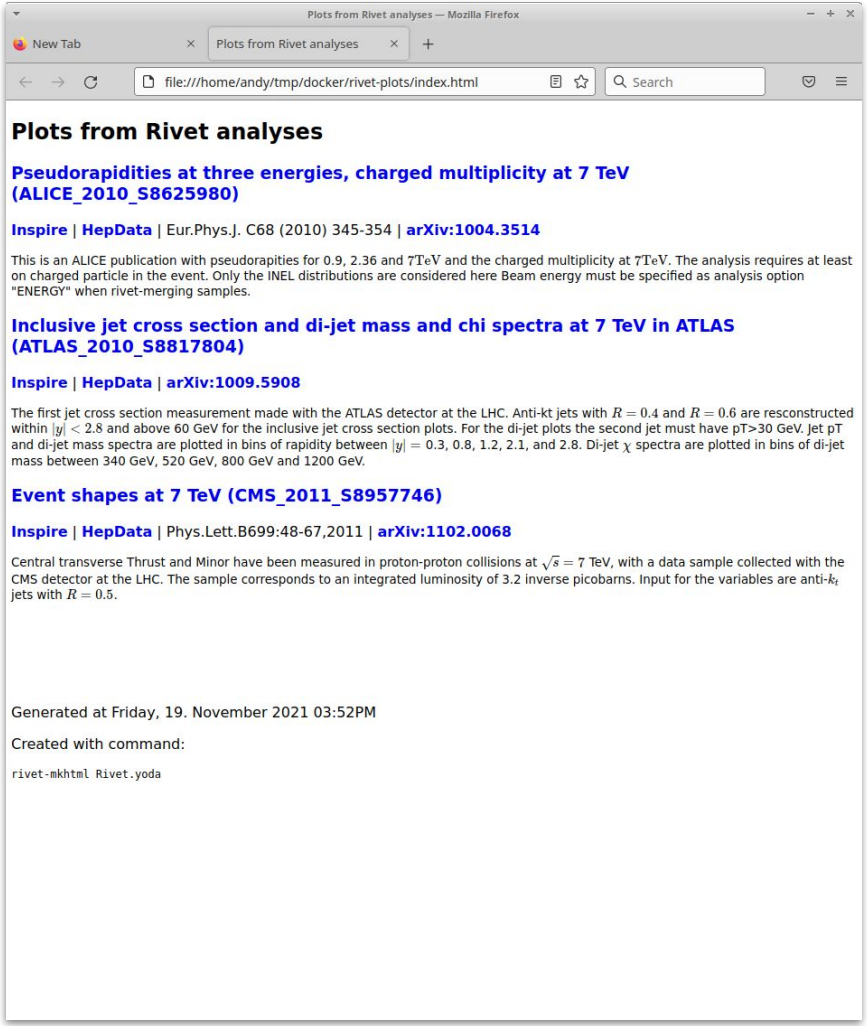

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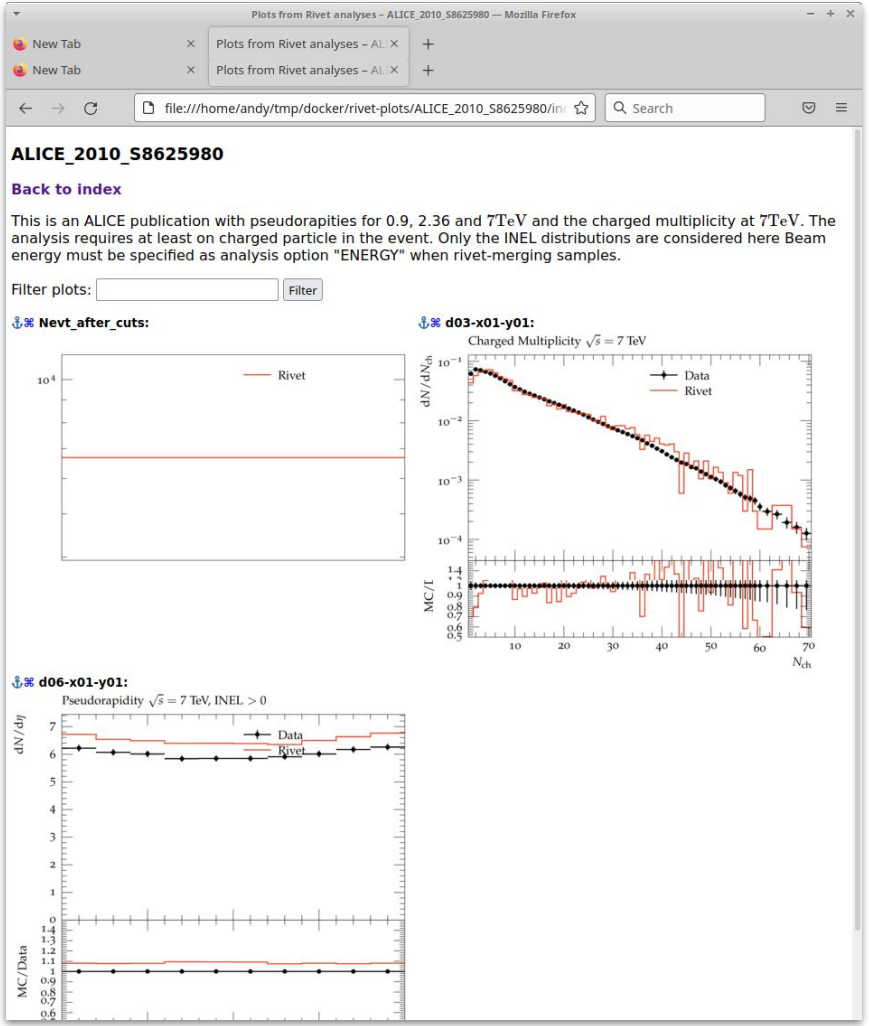
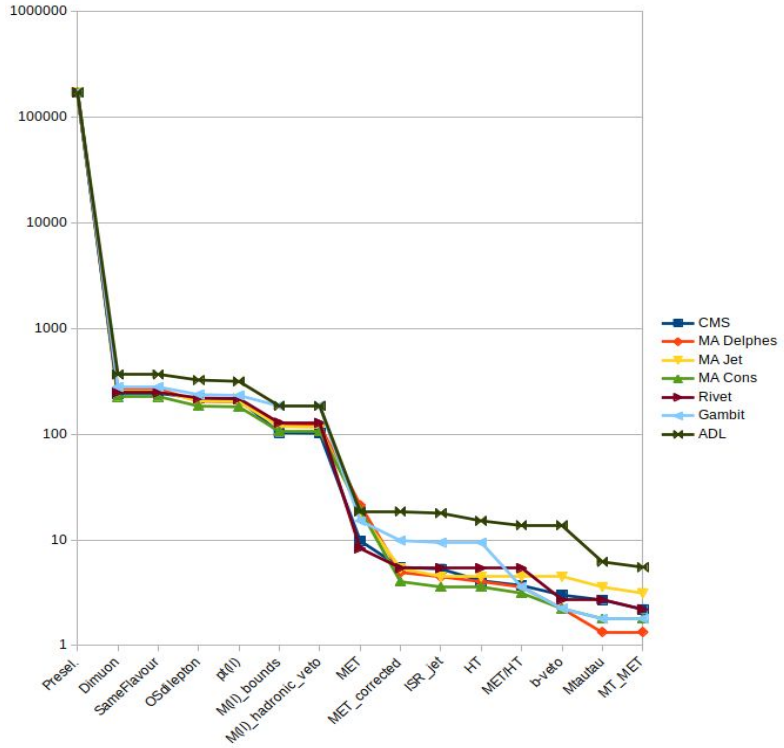


Rivet and BSM-search recasting

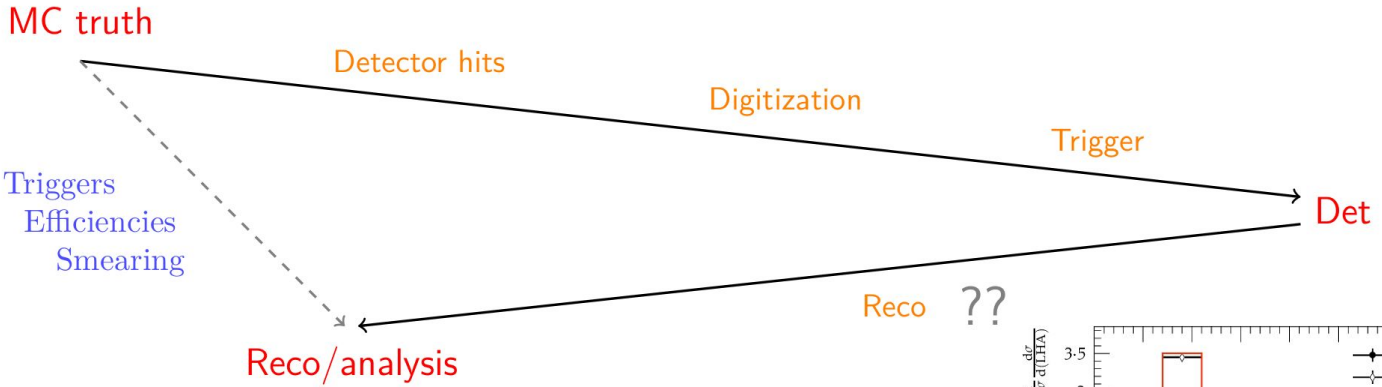
- **Rivet's main emphasis *isn't* BSM direct searches, but there's no reason not to**
  - lots of experiment experience and support
  - efficient scaling-up to hundreds of analyses, with distinct phase-space specific detector/efficiency functions
- **Extra capabilities can lead to novel studies**
  - new areas, collaborations, interested users…



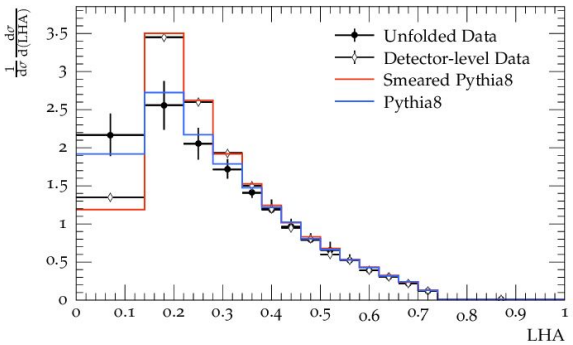
Les Houches 2019 CMS soft-lepton recasting-tools comparison

Detector emulation (but unfold by preference!)

- **Detector smearing built on Rivet's projection system — for reco-level analyses**
  - developed based on GAMBIT ColliderBit experience: no need for "full fast-sim"



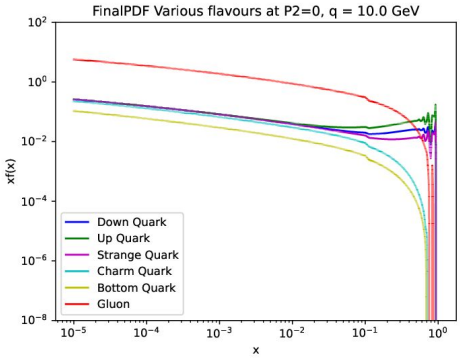
  - like Delphes, but more flexible & can be *analysis-specific* ⇒ MA5 "SFS" mode
  - flexibility allows e.g. "tuned" jet-substructure smearing, systematics studies, …



The future of Rivet

- **Vision: Rivet as a standard for "truth-level" observables**
- Eyes on future colliders, including EIC, cosmic-ray air showers … and nuclear physics, COMPASS? Happy to try!
- Not just standalone, but as a library in pheno & experiment frameworks, too: leverage analysis collection, standardise MC-observable definitions, seamless systematics handling, etc.
- Version 2 features include high-dimensional (and consistent) histogramming, HDF5 aux data, and ONNX machine-learning.
- At its core: a physics-oriented system for physicists to **compare MC predictions to one another and to data, on many simultaneous observables, in myriad ways**

We don't *know* all the use-cases yet.



BSM from “Standard Model”

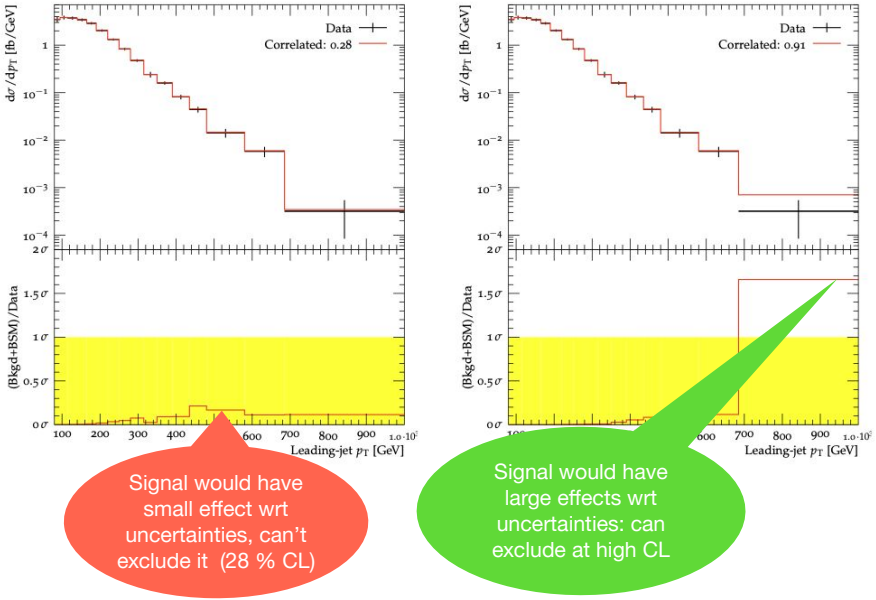
- **Not being focused on *direct* searches doesn’t mean no interest in BSM!**
- **Particle-level measurements *can* achieve high model-independence**
  - Careful definition of fiducial cross-section
  - Control distributions of “hidden variables” which are cut on
  - Reduce model sensitivity in unfolding
- **Rivet used directly in e.g.**
  - TopFitter top quark EFT fits;
  - at core of ATLAS *VH* EFT fits;
  - being integrated into Gambit global fits; and…
- **Contur is getting particular uptake**
  - Inject signal to “SM” measurements: if it’d be statistically distinct, the model is eliminated
  - Rivet gives huge coverage from “many angles”: views on not all, but most BSM signatures

    a new result with Rivet code can be in Contur (or other) BSM fits within *hours*

Contur

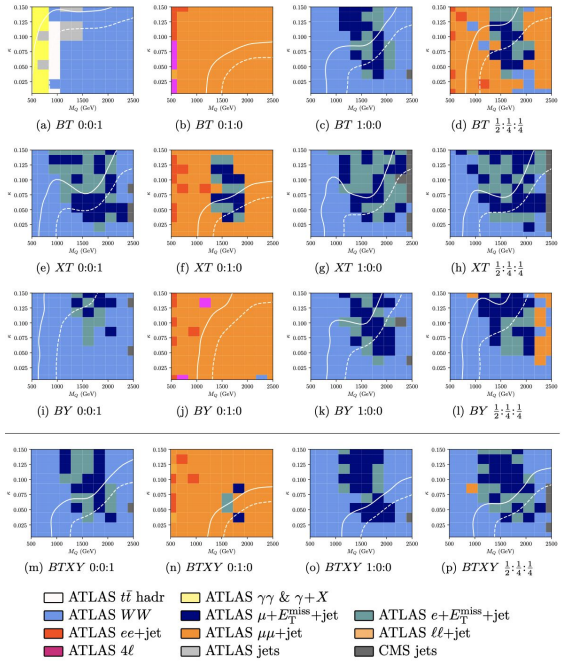
HT Louie Corpe

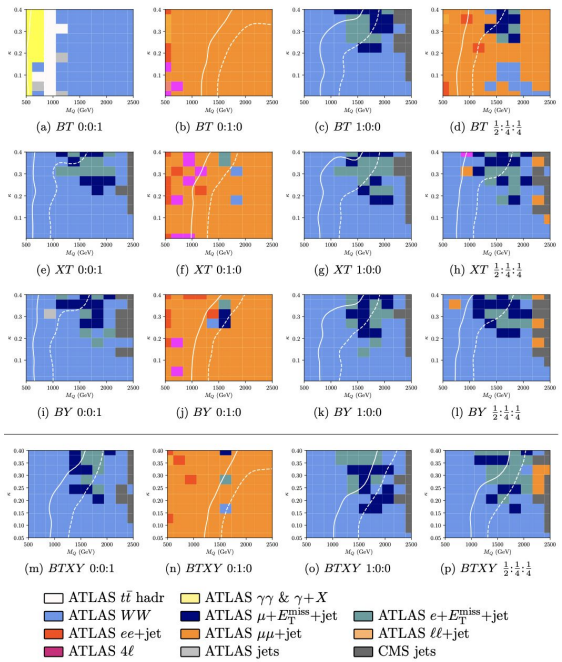
- **Contur is "just" a wrapper on Rivet**
  - Ok, not just! You need to know which analyses are "safe". Another reason for emphasis on final-states and *no cheating*
  - In absence of unambiguous BSM, make zeroth-order assumption that data = SM
  - Can be improved with high-precision SM theory predictions & uncertainties
  - Signal-injection ⇒ care with e.g. ratios & profiles… cf. Rivet "perfect merging"
  - Group analyses in stats-orthogonal "pools". Use (expected) most-constraining element in the pool for setting limits — use correlations when possible to make "bigger" elements
  -

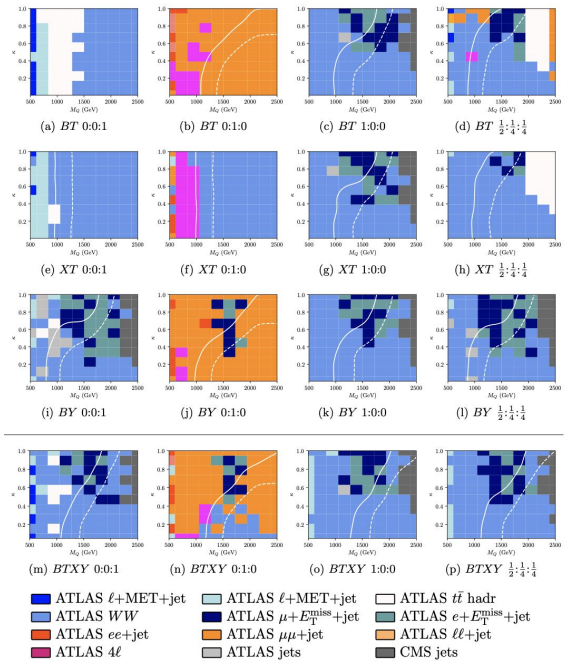


Try doing this with full-sim recast in finite time…

- Contur VLQ review requested a scan of realistic multiplets:
  - 7 multiplets, each with 3 generational couplings, each with 4 W/H/Z-couplings,
  - 300 points per scan, x 30,000 events ⇒ 750M events!







Open questions / discussions on preservation

- **Technical**
  - What obstacles to routine preparation in data / code ecosystem?
  - ML preservations ⇒ validation and regression checks even more crucial (cf. ATLAS-SUS-2019-04 experience)
  - Stability and longevity: how can we ensure the code still does the right thing in 2040? 2050? Beyond? Curation or containers?
- **Validation**
  - Huge pain / obstacle to preservation: figuring out the reference models, add cutflow checkpoints in the code (→re-ordering…)
  - Building cutflows / control distributions into analyses? Link to HepData? Ref HepMC samples on Zenodo?
- **Social**
  - Valuing work that makes science reusable beyond The Paper
  - Current (experimental) perceptions?
  - Phenomenology input? Cross-community collaboration opportunities?
- **AOB?**