PEPPER

A Portable Parton-Level Event Generator for the HL-LHC

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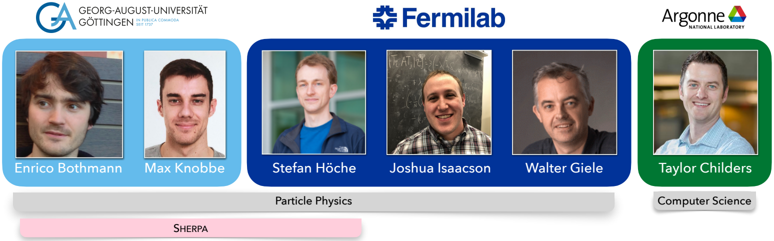
About

About this Talk

- PEPPER: **P**ortable **E**ngine for the **P**roduction of **P**arton-level **E**vent **R**ecords
- General overview, discuss performance/portability aspects

About the Team



Introduction

Why improve computing performance?

- High statistics at HL-LHC & excellent detector performance

  $\rightarrow$ Need for precise MCEG simulations

  $\rightarrow$ Poor MCEG performance can limit experimental success

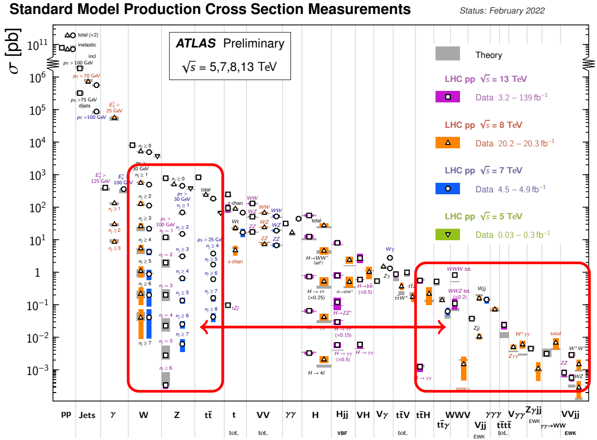
  [HSF Physics Event Generator WG] arXiv:2004.13687, arXiv:2109.14938

What dominates the computing budget?

- Which physics processes?
- Parton or particle level?
- Which final-state jet multiplicities?

In contrast to computers, human resources are scarce.
We can't afford to make incremental improvements.

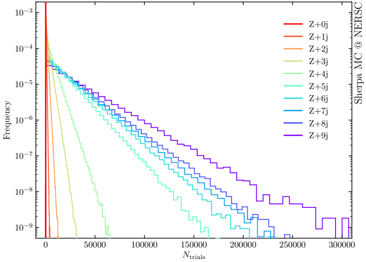
Which physics processes?



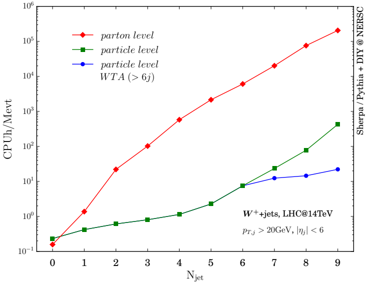
[ATLAS] https://twiki.cern.ch/twiki/bin/view/AtlasPublic/StandardModelPublicResults

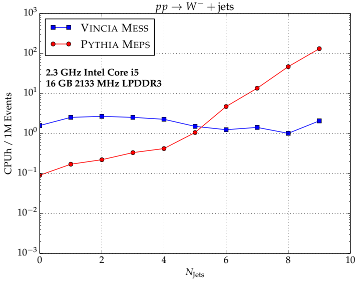
- Signals: High multiplicity but comparably low complexity
- Main backgrounds: High multiplicity and high complexity

- ATLAS' state-of-the-art SHERPA samples
  - $pp \to e^+e^- + 0, 1, 2$j@NLO $+ 3, 4, 5$j@LO
  - $pp \to t\bar{t} + 0, 1$j@NLO $+ 2, 3, 4$j@LO
- Majority of time (60–80 %) spent in tree-level matrix elements (ME) and phase space (after extensive optimization & usage of analytic loop MEs [EB et al.] arXiv:2209.00843)
- Reason: low unweighting efficiencies and expensive ME for high jet multiplicities [Höche,Prestel,Schulz] arXiv:1905.05120



Timing distribution: scaling with multiplicity





- Hard scattering simulation much more demanding than particle-level remainder [Höche,Prestel,Schulz] arXiv:1905.05120
- Complexity of merging ME&PS can be reduced to achieve linear scaling using sector showers [Brooks,Preuss] arXiv:2008.09468 so not a problem in principle

Algorithms: matrix element

Figure of merit

unweighted event generation throughput for highest jet multiplicity

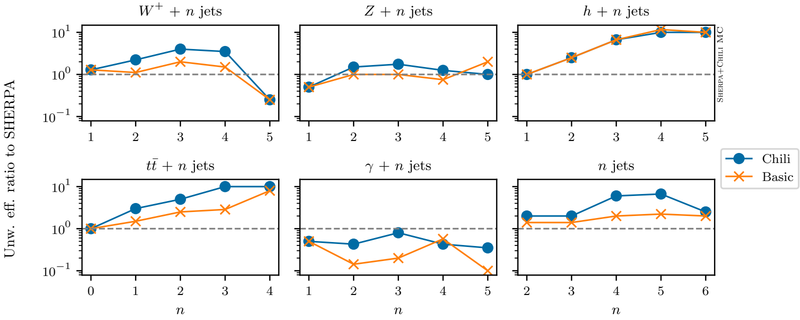
e.g. $pp \to e^+e^- + 5j$, $pp \to t\bar{t} + 4j$ or more

- Berends–Giele recursion for best multi-jet scaling behaviour
- Colour summing for lockstep GPU evaluation
  - Use minimal colour basis developed by amplitude community $\mathcal{O}((n-1)!^2) \to \mathcal{O}((n-2)!^2)$

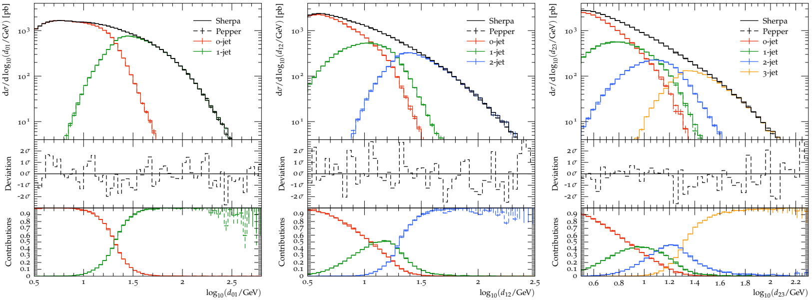
    [Melia] arXiv:1304.7809 arXiv:1312.0599 arXiv:1509.03297

    [Johansson,Ochirov] arXiv:1507.00332
  - Our implementation generalises it to $\ell\ell$+jets amplitudes
- Helicity sampling to avoid additional 2^n scaling

- CHILI phase-space generator uses simple (MCFM-inspired) structure: one t-channel + adjustable number of s channels
  [EB et al.] arXiv:2302.10449
  - Portable (ported builtin CHILI in PEPPER)
  - RAMBO-like speed
  - Efficiency on par with recursive COMIX phase-space
    - $\rightarrow$ Ideal to provide on-device ML training data for many jets

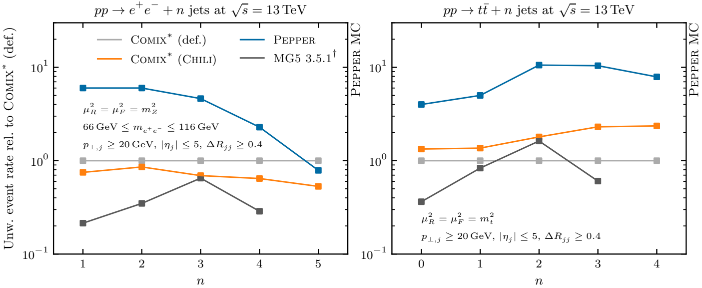


- PDF via LHAPDF, ported to CUDA and Kokkos
- Particle-level simulation via Sherpa or Pythia
  → LHEH5-based framework [EB et al.] arXiv:2309.13154 → Chris' talk



- Test of complete LHEH5-based simulation pipeline with Pepper+Sherpa [EB et al.] arXiv:2309.13154
- Additional 3× speed-up for ATLAS MEPS@NLO $pp \to e^+e^- +$ jets set-up → Sherpa v2.3.0 (Sep '23)

Baseline unweighted event generation performance



- Unweighted event throughput compared to COMIX*
- Constitutes baseline single-threaded performance of currently available competitive algorithms
- Novel standalone PEPPER performs better than COMIX, but PEPPER's real goal is portability [EB et al.] arXiv:2311.06198

Numbers generated on Intel Xeon E5-2650 v2

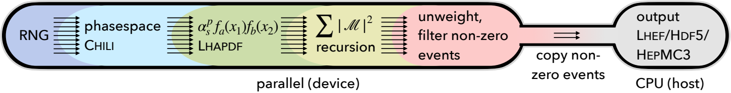
* Partonic processes split into to g/q groups (not SHERPA standard)

† Modified to match efficiency convention of [Gao et. al] arXiv:2001.10028

- Many computing vendors, heterogeneous architectures
- (Pre-)Exascale computing systems intentionally diverse

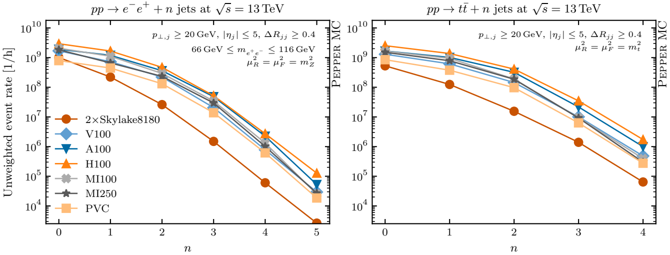
Portability is baked into PEPPER

- Focus on highest multi (e.g. $e^+e^- + 5$, $t\bar{t} + 4$)
  this is beyond small scale computing → WLCG / HPC
- 10–20 years ago: Homogeneous CPU+RAM architectures
- This is undergoing a big change (partly due to AI trends)
  - HPC moves to exascale era → scalability
  - GPU acceleration → portability
- PEPPER addresses both aspects with MPI, HDF5 and Kokkos
- PEPPER parallelises the entire parton-level event generation:



- Tested Xeon CPU, Intel/AMD/Nvidia GPU, HPC systems
  - ✓ Covers all (pre-)exascale architectures on previous slide
  - ✓ Scalable from a laptop to a Leadership Computing Facility

- Excellent performance across a wide range of architectures
- Portability provided by Kokkos: one code-base compiled for different architectures



MEvents / hour	2×Skylake8180	V100	A100	H100	MI100	MI250	PVC
$pp \to t\bar{t} + 4j$	0.06	0.5	1.0	1.7	0.4	0.3	0.3
$pp \to e^-e^+ + 5j$	0.003	0.03	0.05	0.1	0.03	0.03	0.02

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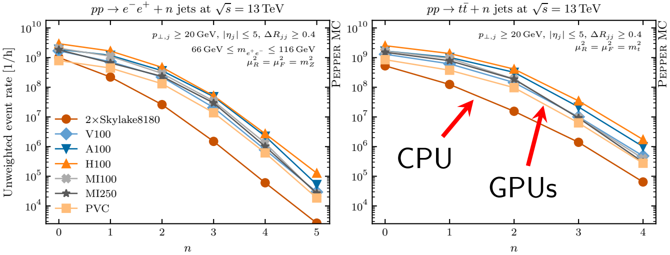

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Portability: Aurora example

- Estimate "roughly 330 billion [leptonically decaying V+jets] events" required for HL-LHC [ATLAS] arXiv:2112.09588
  - "**Sherpa 2.2.11 setup would exceed budget by 16%**"
  - Assume all 330 billion events are Z+4j
    Production cost at parton-level would be:
    - 240M CPUh Comix @ Intel E5-2650 v2 CPU
    - 380k GPUh Pepper @ Nvidia A100 →

This would be 8h on Aurora (with PVC)

Conclusions and outlook

Status

- ✓ Portable parton-level multi-jet event generator PEPPER
  Achieves scalability from a laptop to a Leadership Computing Facility

Outlook

- Use synergies PEPPER/CHILI $\leftrightarrow$ on-device training $\leftrightarrow$ ML
- Add more processes to PEPPER, work towards NLO

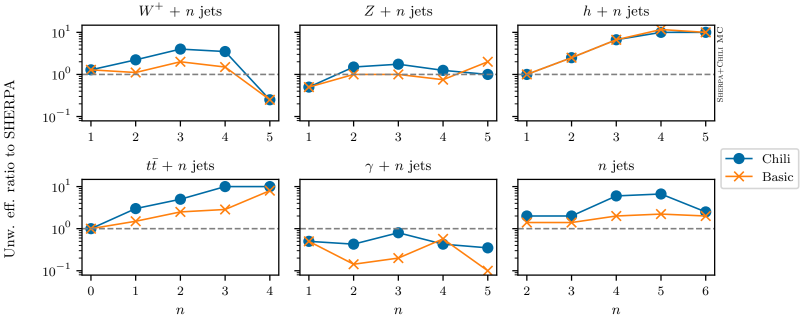
Discussion points

- Regularly updated per-process event generation cost data from ATLAS & CMS? (time/energy/money/. . .)
- Can we get together and establish HPC/GPU workflows with hep-ex & LCFs? (Usability $\leftrightsquigarrow$ Flexibility, Portability . . .)
- Expected adoption of HPC resources by LHC computing?

5 Backup

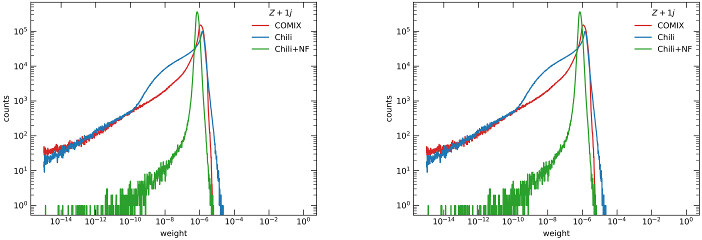
Simple & portable phase space

- CHILI phase-space generator uses simple (MCFM-inspired) structure: one t-channel + adjustable number of s channels
  [EB et al.] arXiv:2302.10449
  - Portable (e.g. basic or "mild" CHILI in PEPPER)
  - RAMBO-like speed
- Performance of basic CHILI (single channel) on par with recursive phase-space in COMIX see also figure on slide 9



Simple & portable phase space: applications & NIS

- What to do with CHILI? (stand-alone library ↗)
  - Simplicity & portability → used in PEPPER v1 as default
  - Speed → public parton-level SHERPA version for HPC ↗
- One/few channels + speed + portability → good fit for ML
- Example: Neural Importance Sampling
  Proof-of-principle [EB et al.] arXiv:2001.05478
  i-Flow+SHERPA [Isaacson et al.] arXiv:2001.10028 arXiv:2001.05486
  MADNIS [Heimel et al.] arXiv:2212.06172 arXiv:2311.01548 → Theo's talk
- CHILI+MADNIS quick'n'dirty [EB et al.] arXiv:2302.10449



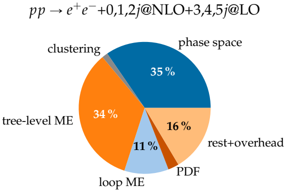
- Future: SHERPA v3.x, on-device NN training with PEPPER

(Some) Components of a MC Computation

$$\sigma_{pp\to X_n} = \sum_{ab} \int dx_a dx_b d\phi_n f_a(x_a, \mu_F^2) f_b(x_b, \mu_F^2) \times |\mathcal{M}_{ab\to X_n}|^2 \Theta(p_1, ..., p_n)$$

Components we need to consider:

- Tree-level Matrix elements
- Phase space generation
- PDF's



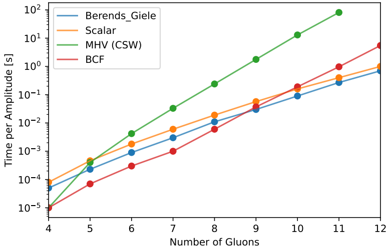
→ Large portion of MC time spend in ME + PS

[EB et al.] arXiv:2209.00843 → Chris' talk

The Amplitudes

- Strategies to compute tree-level amplitudes
  1. Berends-Giele like recursion
  2. Scalar
  3. MHV (CSW)
  4. BCF
- Rely on performance studies from early 2000's
  hep-ph/0602204,hep-ph/0607057
- We are interested in best scaling behaviour / performance for multi-jet processes

⇒ **Choice: Berends-Giele recursion**



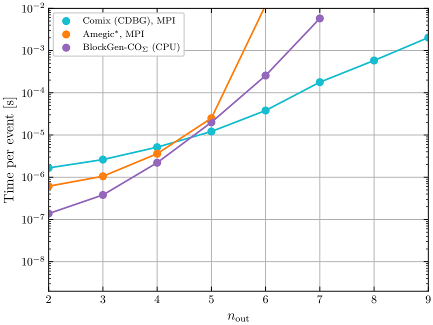
Based on numbers from hep-ph/0602204

Benchmark performance for gluon-only Color-treatment:

- Compare different color treatments: color-dressing/summing/sampling
- Color-sampled algorithms scale similar to color-summed approaches
- Color-summing scales worse than color-dressing, but faster up to roughly 5-6 outgoing jets
- Caveat: Color-sampling comes with penalty factor from slower convergence

⇒ **Algorithmic choice: Sum colors** Helicity-treatment:

- Picture less clear, still allow multiple options



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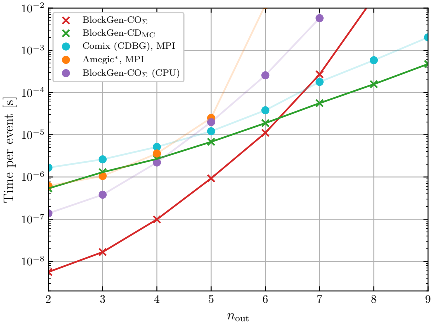

The Color & Helicity Sum [EB, Giele, Höche, Isaacson, Max Knobbe, 2106.06507]

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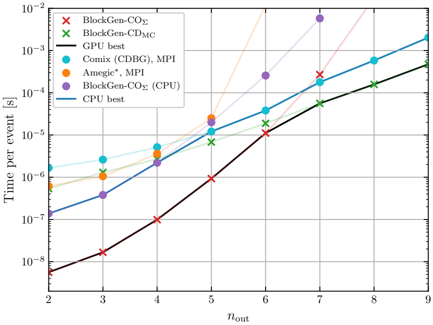
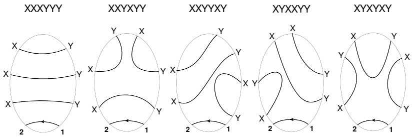


From Gluon-only to V+Jets

- Introduce spinors (Weyl for massless, Dirac for massive particles)
- Add more general QCD three point vertices
- Straight-forward for helicity-sum and Berends-Giele recursion
- First time in a code aimed for production: use minimal QCD color-basis $\{A(1, 2, \sigma), \sigma \in \mathrm{Dyck}\}$

  [T. Melia 1304.7809 & 1312.0599 & 1509.03297; H. Johansson, A. Ochirov, 1507.00332]

  → Allows to fix one fermion line, remaining permutations are given by Dyck-Words
  → Four particle Dyck Words: ()(), (())
  → Significantly fewer amplitudes to compute
- Include EW particles after QCD basis has been set up



[1304.7809]

Phase space generator: CHILI [SciPost Phys. 15 (2023) 169]

- Differential phase space element for an n-particle final state

$$\mathrm{d}\Phi_n(a,b;1,\ldots,n) = \left[\prod_{i=1}^{n} \frac{\mathrm{d}^3\vec{p}_i}{(2\pi)^3\,2E_i}\right] (2\pi)^4\delta^{(4)}\left(p_a+p_b-\sum_{i=1}^{n} p_i\right) .$$

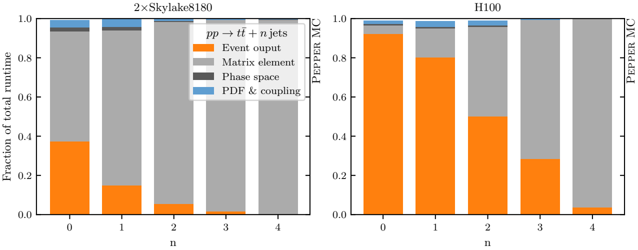
- Standard factorization formula

$$\mathrm{d}\Phi_n(a,b;1,\ldots,n) =$$

$$\mathrm{d}\Phi_{n-m+1}(a,b;\{1,..,m\},m{+}1,\ldots,n)\,\frac{\mathrm{d}s_{\{1,..,m\}}}{2\pi}\,\mathrm{d}\Phi_m(\{1,..,m\};1,\ldots,m) .$$

- Use t-channel + adjustable number of s-channels
- Basic strategy: use single t-channel and only add s-channel resonances when required
  $\rightarrow$ easy to combine with Vegas
  $\rightarrow$ lean implementation allows for portability

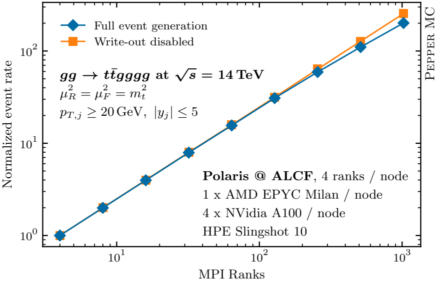
Timing details

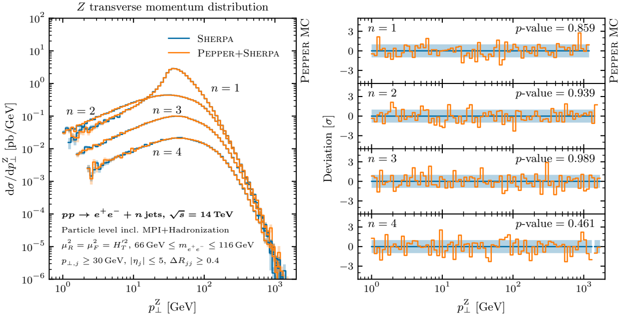


- Lower multiplicities are limited by write-out speed
  $\rightarrow$ No more need for computing improvements, but faster I/O
- Computing becomes relevant component only for large multiplicities

Scalability

- Test scalability for up to 1024×A100's
- Scaling violation due to I/O problems
  → currently investigated at ALCF
- Equivalent technology to [2309.13154]
  → established scaling to up to 16k threads at NERSC
- These problems don't show up for a couple of nodes or low data volume
  → important benchmark





- Validated against SHERPA
  → for $V + j$, $t\bar{t}$+j, single multiplicity and multi-jet merged
- Writeout of HDF5 files, processable via SHERPA & PYTHIA