An efficient and sustainable approach to precision simulations at the (HL-)LHC

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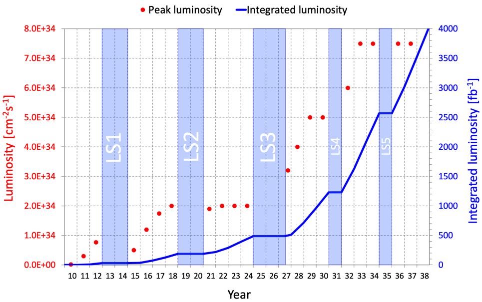
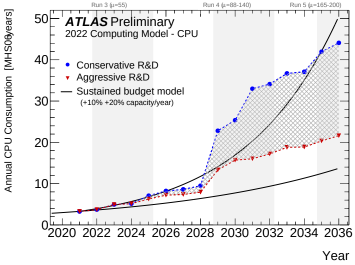
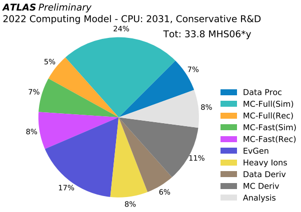
Expected computing requirements

- projected evolution of computing resources sees cost of event generation on par with detector simulation
- LHC measurements in danger of being limited by Monte Carlo statistics







[CERN-LHCC-2022-005]

Targeted optimisation of CPU-based event generation

- Most event generation CPU spent on multi-leg NLO calculations [JHEP 08 (2022) 089]
  - used for main Standard Model processes: extremely large event sample sizes
  - relevant to measurements and searches alike

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- Study CPU performance of Sherpa MEPS@NLO calculations for $e^+e^- + 0, 1, 2j$@NLO$+3, 4, 5j$@LO and $t\bar{t} + 0, 1j$@NLO$+2, 3, 4j$@LO
  - introduction of pilot run in Sherpa brings a factor 5 improvement
  - using analytic QCD loop amplitudes in the unweighting brings another factor 1.5
  - detailed write-up presented in [EPJC 82 (2022) 12]

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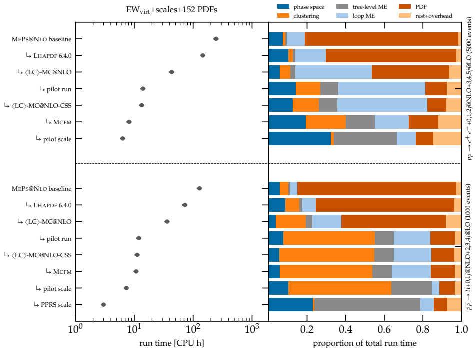
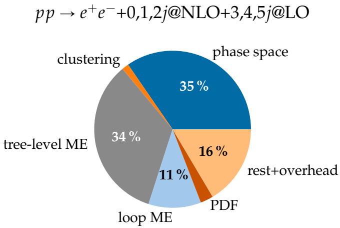
cumulative speed-ups for:	$pp \to e^+e^-$ + jets			$pp \to t\bar{t}$ + jets		
	runtime [CPU h/5k events]			runtime [CPU h/5k events]		
setup variant	old	new	speed-up	old	new	speed-up
no variations	20 h	5 h	4×	15 h	8 h	2×
EW_{virt}	35 h	5 h	6×	20 h	8 h	2×
EW_{virt} +scales	45 h	5 h	7×	25 h	8 h	4×
EW_{virt} +scales+100 PDFs	90 h	5 h	15×	55 h	8 h	7×
EW_{virt} +scales+1000 PDFs	725 h	8 h	78×	440 h	9 h	51×

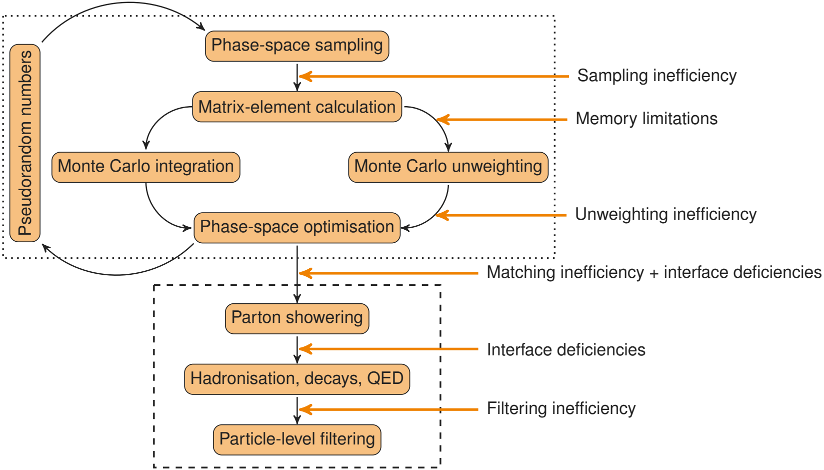
Case study: ATLAS baseline configuration





➜ CPU consumption **overall improved by factors of $\times$39 and $\times$43** for V+jets and $t\bar{t}$+jets

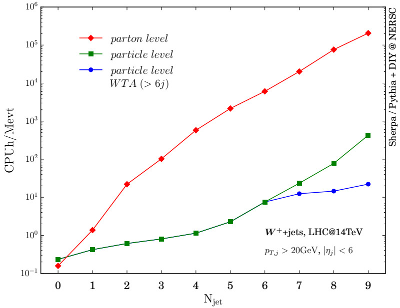
Typical MC production chain

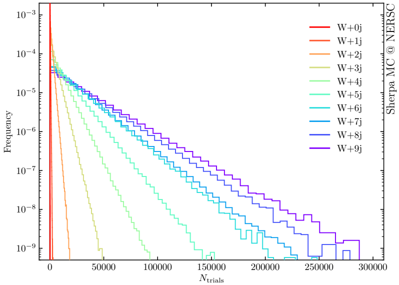


→ Lack of active development on infrastructure tools (LHE, HepMC, ...) set to become major bottleneck going forward

Parton vs particle level

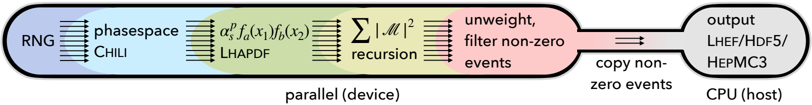
- Scaling of parton- and particle level analysed in [**PRD 100 (2019) 1**]
- cost of showering matrix elements with extra emissions **dominated by parton level**
  - number of diagrams grows factorially with every additional emission (at best exponentially when exploiting recursions a la `COMIX`)
- low-multiplicity matrix elements cheaper to regenerate entirely than to store on disk





Introducing Pepper: a portable ME generator for the HL-LHC

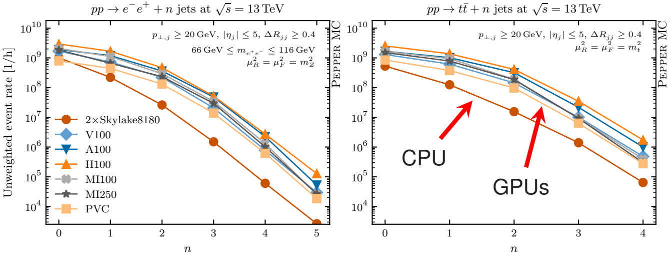
- Focus on highest multi (e.g. $e^+e^- + 5$, $t\bar{t} + 4$)
  this is beyond small scale computing → WLCG / HPC
- 10–20 years ago: Homogeneous CPU+RAM architectures
- This is undergoing a big change (partly due to AI trends)
  - HPC moves to exascale era → scalability
  - GPU acceleration → portability
- 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

Comparing runtimes on relevant architectures

- 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

Portability: Aurora example

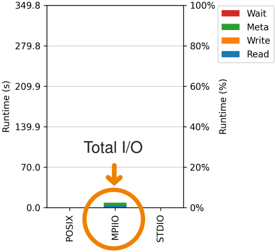
- Estimate "roughly 330 billion [leptonically decaying V+jets] events" required for HL-LHC [arXiv:2112.09588]
  - "SHERPA 2.2.11 setup would exceed budget by 16%"
- Assuming all 330 billion events are $Z + 4j$, production cost at parton-level would be:
  - 240M CPUh COMIX @ Intel E5-2650 v2 CPU
  - 380k GPUh PEPPER @ Nvidia A100 → **This would be 8h on Aurora (with PVC)**

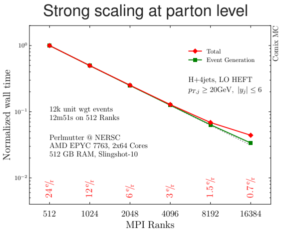
Introducing LHEH5

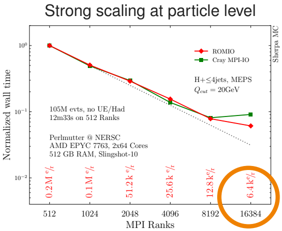
- established LHEF format is based on XML
  - flexible enough to add any desired feature
  - poses a challenge for I/O operations at scale
- new efficient LHE-like data format based on HDF5+HighFive proposed in [PRD 109 (2024) 1]

Name	Data type	Contents
VERSION	3 × int	Version ID
INIT	10 × double	beamA, beamB, energyA, energyB, PDFgroupA, PDFgroupB, PDFsetA, PDFsetB, weightingStrategy, numProcesses
PROCINFO	6 × double	procId, npLO, npNLO, xSection, error, unitWeight
EVENTS	9 × double	pid, nparticles, start, trials, scale, fscale, rscale, aqed, aqcd
PARTICLES	13 × double	id, status, mother1, mother2, color1, color2, px, py, pz, e, m, lifetime, spin
CTEVENTS	9 × double	ijt, kt, i, j, k, z1, z2, bbpsw, tlpsw
CTPARTICLES	4 × double	px, py, pz, e

I/O performance





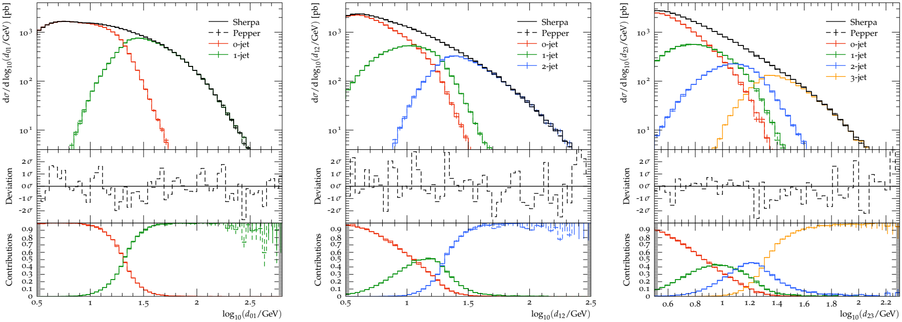


105M events / min

- ➜ overall I/O time reduced to below 1s per rank
  - ➜ time spent in I/O operations less than 5% when reading 128.85 GiB
- ➜ ideal for accessing back-fill queues at large computing centres

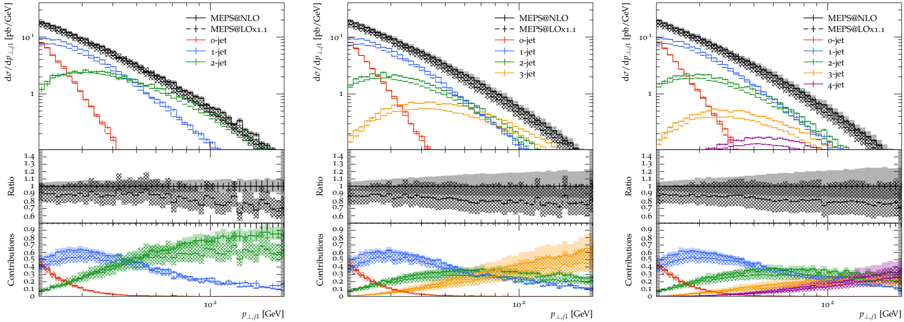
Comparison of parton-level event generators

- validated for standard candle processes (Z+jets shown) at various multiplicities
- can mix and match generators to reduce computing time to the absolute minimum required for event simulation



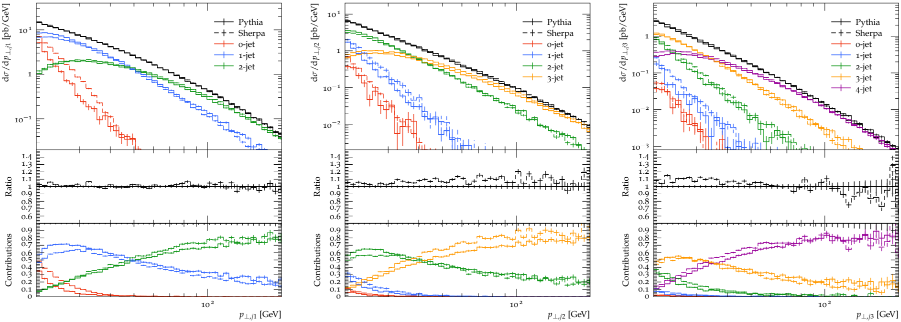
Improved modelling through high-multiplicity final states

- simulation of additional radiation at tree level clearly necessary for proper physics modelling of high-multiplicity final states
- hatched bands indicate the scale uncertainties from 7-point scale variations at LO, solid bands represent the corresponding band at NLO
- uncertainties inevitably increase with additional jet multiplicities as more of the phase space is systematically varied



More robust uncertainty estimates

- LHEH5 enables efficient substitution of various parts in the event generation chain
  - already supported by Pepper, Sherpa and Pythia!
- 10 % uncertainty seen in Z+jets due to different algorithmic choices in the parton showers



Future event generation workflows

- Approach 1: produce parton-level samples centrally with input from the MC developers, provide them in a shared space for all experiments
  - experiments run their preferred shower setup (✔)
  - allows for affordable plug & play between different models (✔)
  - lowers cost threshold for reproducing larger setups after some time if need be (✔)
  - requires more storage for parton-level events (✘)
  - new infrastructure needs to be set up and maintained (✘)

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  - new infrastructure needs to be set up and maintained (✘)
- Approach 2: run everything in one go, harnessing heterogeneous resources, possibly with in-memory transfer of GPU-accelerated calculation components
  - no intermediate storage for parton level events needed (✔)
  - minimal infrastructure changes required (✔)
  - parton-level events continue to cost twice as strictly necessary (✘)
  - regenerating larger setups from scratch will become painful (✘)

Summary

- computing cost of traditional CPU-based multi-leg event generation significantly reduced by factor 40–80 following dedicated profiling
- first production-ready portable LO event generator allows to incorporate GPU resources into high-precision simulations
- new `LHEH5` format allows for efficient parton-level event generation
  - excellent I/O performance for massive MPI applications
  - additional factor 3–6 speed-up for traditional grid resources
- new tools chain facilitates more robust uncertainty estimates of parton-shower effects
- allows better exploitation/recycling of existing resources in subsequent large-scale production campaigns
- seeing latest performance improvements reflected in up-to-date projections from the experiments paramount for defining appropriate objectives going forward

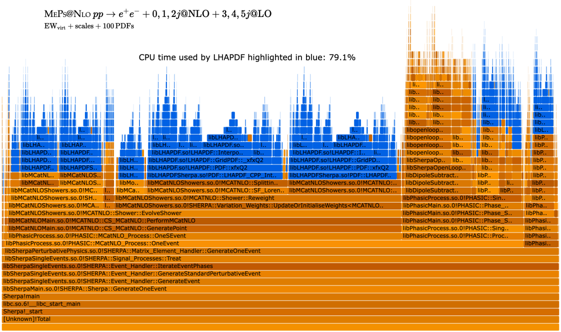
Backup

Initial profiling exercises

- first generator CPU profiling done by Tim Martin suggested per-event CPU dominated by LHAPDF

- graph shows PDF calls highlighted in blue (using LHAPDF 6.2.3)

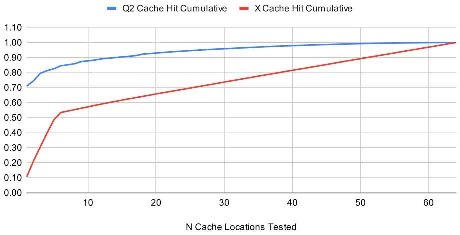
- maybe not completely surprising: multiweights originally not designed with hundreds of variations in mind [EPJC 76 (2016) 11]



- explore two approaches in parallel: make LHAPDF faster and rework LHAPDF call strategy

Improving LHAPDF

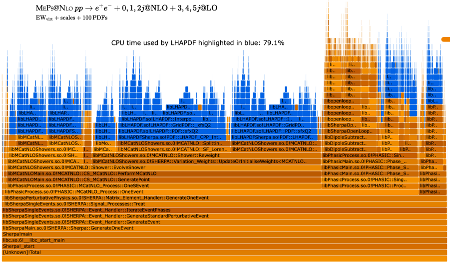
- first PDF-grid cache introduced in v6.3.0
  - rendered ineffective by PDF-call strategy used in Sherpa
  - nevertheless useful as case study

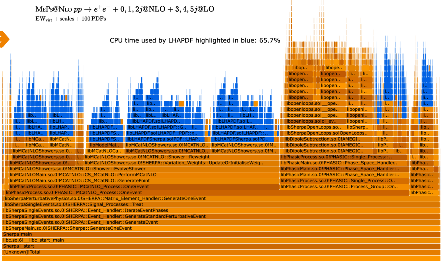


- follow-up release v6.4.0 with improved interpolation logic
  - revised cache implementation with improved memory layout (but well-matched call strategy in the generator still crucial)
  - pre-computation of shared coefficients of the interpolation polynomial along (x, Q^2) grid lines
  - results in factor 3 speed-up for single flavour computations
  - can achieve factor 10 speed-up when combining with multi-flavour caching

Impact of new LHAPDF

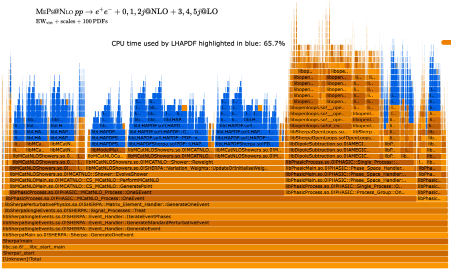
- ATLAS V+jets setup **overall 30% faster** using new LHAPDF release
  - switching from old ATLAS production default v6.2.3 to new v6.4.0 release

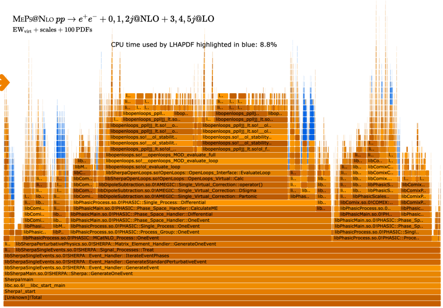




Internal restructuring and pilot run

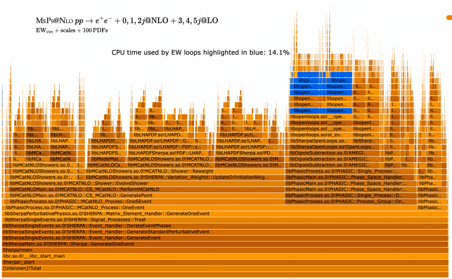
- perform the unweighting using a minimal setup and once an event is accepted, rewind RNG state and re-calculate accepted event using all the bells and whistles
- **achieves factor 5 speed improvement** for ATLAS setup (using LHAPDF 6.4.0 yields additional 6% speed-up)
- pilot run reduces CPU spent on evaluating PDFs to below 10%

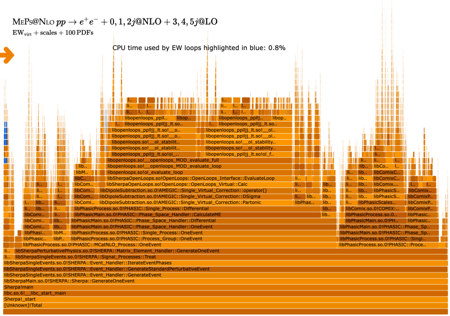




Internal restructuring in Sherpa 2.2.12: the pilot run

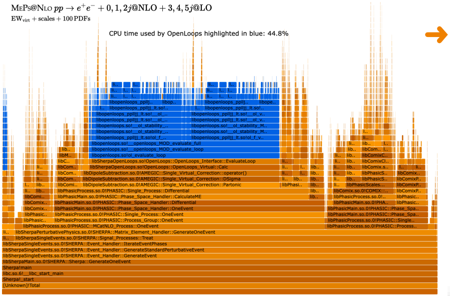
- CPU spent on calculating EW one-loop amplitudes going from 19% down to 0.8% when using the pilot run with the ATLAS V+jets setup
- nevertheless, $\sim$40% of the CPU still spent on calculating QCD loops



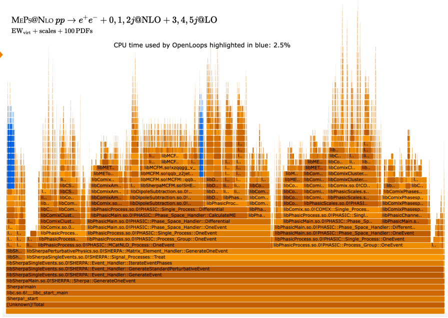


Analytic vs numerical QCD loop amplitudes

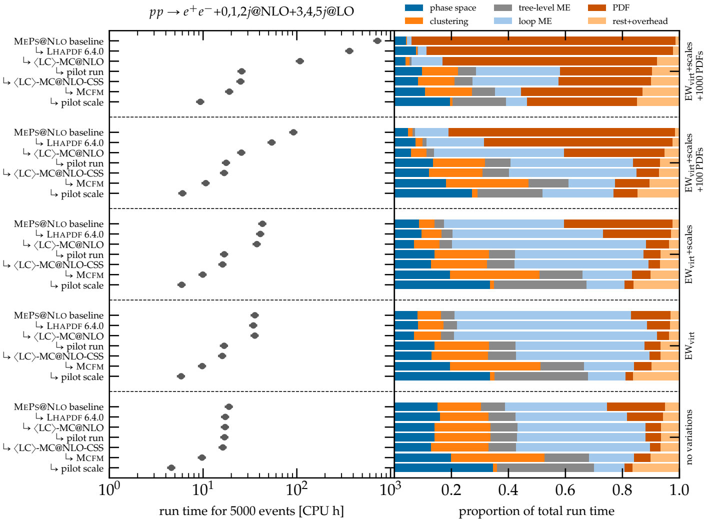
- ➜ employ analytic one-loop amplitudes (if available) in the pilot run using Sherpa-MCFM interface [EPJC 81 (2021) 12]
- ➜ yields **additional ∼35% speed improvement** for the V+jets setup



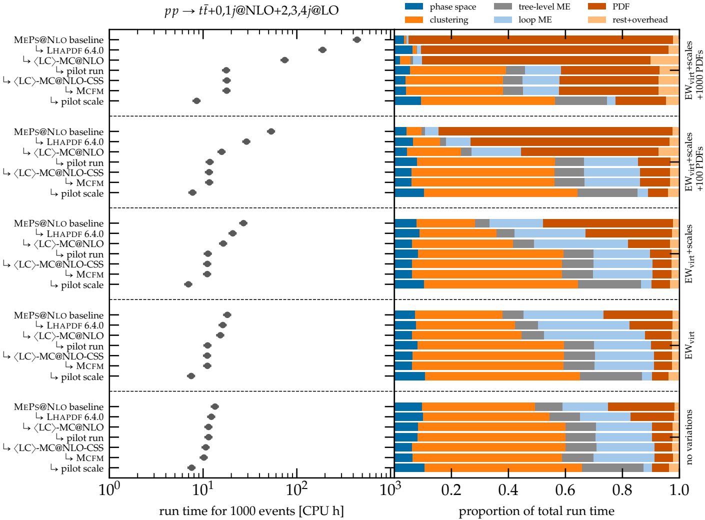
➜



Breakdown of CPU budget in $V+$jets

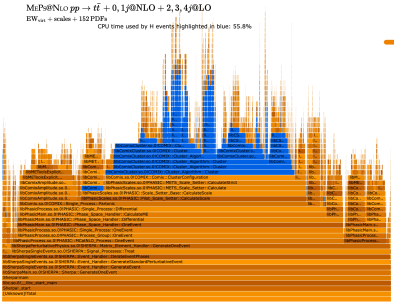


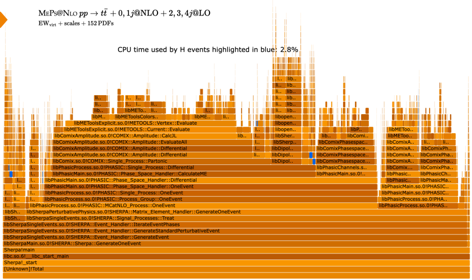
Breakdown of CPU budget in $t\bar{t}$+jets



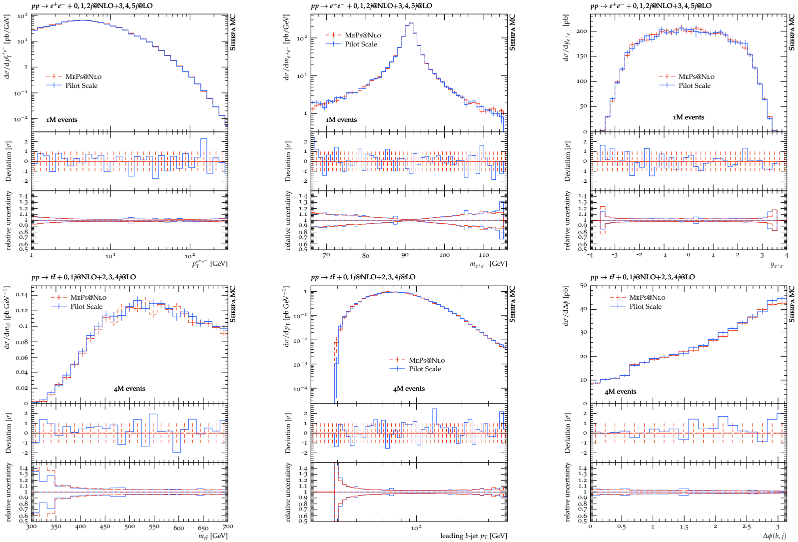
Cluster-independent scale definition

- ➜ employ clustering-independent scale definition ($H_T'/2$) for $\mathcal{H}$-events in $t\bar{t}$+jets (already used in V+jets baseline setup)
- ➜ yields **additional factor 2 speed-up** of the overall run time



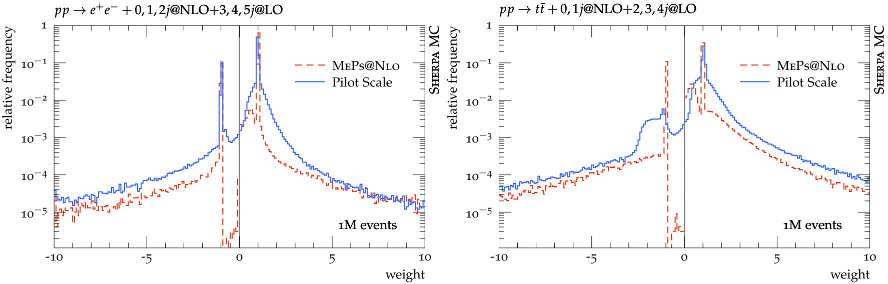


Comparison of MEPS@NLO vs Pilot Scale strategy



Weight distribution for pilot scale

- weight distributions for partially unweighted events after matching and merging:



- second unweighting would reduce the efficiency by less than factor 2 for large N_{events}

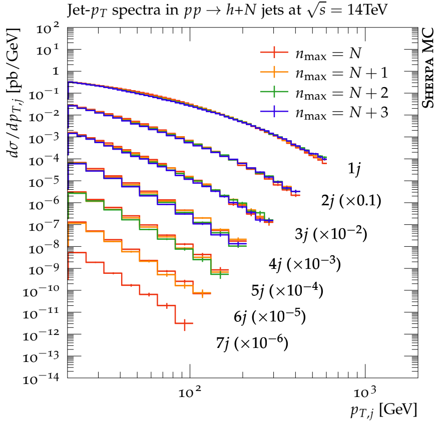
Benchmarking with state-of-the-art event generators

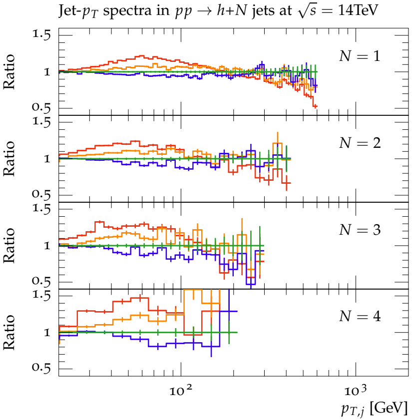
- comparison of Sherpa's COMIX with PEPPER+CHILI, on a single core Intel(R) Core(TM) i3-8300 CPU at 3.70GHz with 8MB L3 cache.
- samples generated with a given target for the total cross section uncertainty ("Tot. unc.")
- "Speed-up" gives the walltime gain factor of PEPPER+CHILI vs. COMIX
- PEPPER+CHILI: $Z + 0, 1j$ generated using helicity summing, while the higher ones use helicity sampling, thereby achieving the best possible performance in each case
- factorial scaling in PEPPER causes COMIX to win at very high multiplicities

Process	Tot. unc. [%]	Sherpa (Comix)			Pepper+Chili			Speed-up
		Walltime [s]	Mem. (USS) [MB]	Eff. [%]	Walltime [s]	Mem. (USS) [MB]	Eff. [%]	
Z+0j	0.089	68	62	22	10	40	43	6.8
Z+1j	0.19	76	66	5.3	31	33	10	2.5
Z+2j	0.99	92	64	0.28	10	35	1.4	9.2
Z+3j	3.8	95	65	0.037	36	43	0.097	2.6
Z+4j	14	122	115	0.0050	71	133	0.016	1.7

Case study: Higgs plus many jets at LO

- $H + 0, 1, 2, 3, 4, 5, 6, 7j$@LO, ratios normalised to $n_{\text{max}} = 2$
- maximum jet multiplicity (n_{max}) set to the number of measured jets, N (red), $N + 1$ (green), $N + 2$ (blue) and $N + 3$ (purple)





Case study: Higgs plus many jets at NLO

- $H + 0, 1, 2j$@NLO$+3, 4, 5, 6, 7j$@LO, ratios normalised to $n_{\max} = 2$
- maximum jet multiplicity ($n_{\max}$) set to the number of measured jets, N (red), $N + 1$ (green), $N + 2$ (blue) and $N + 3$ (purple)