Towards efficient and sustainable event generation for the HL-LHC

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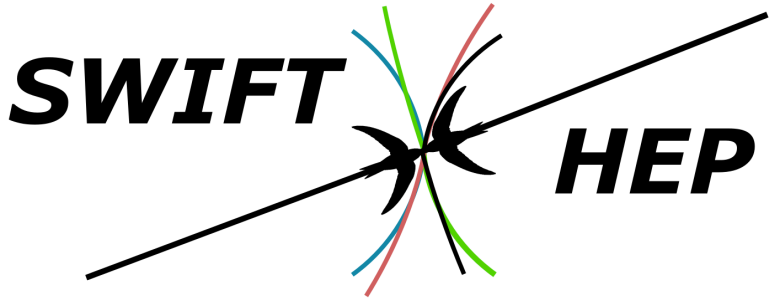
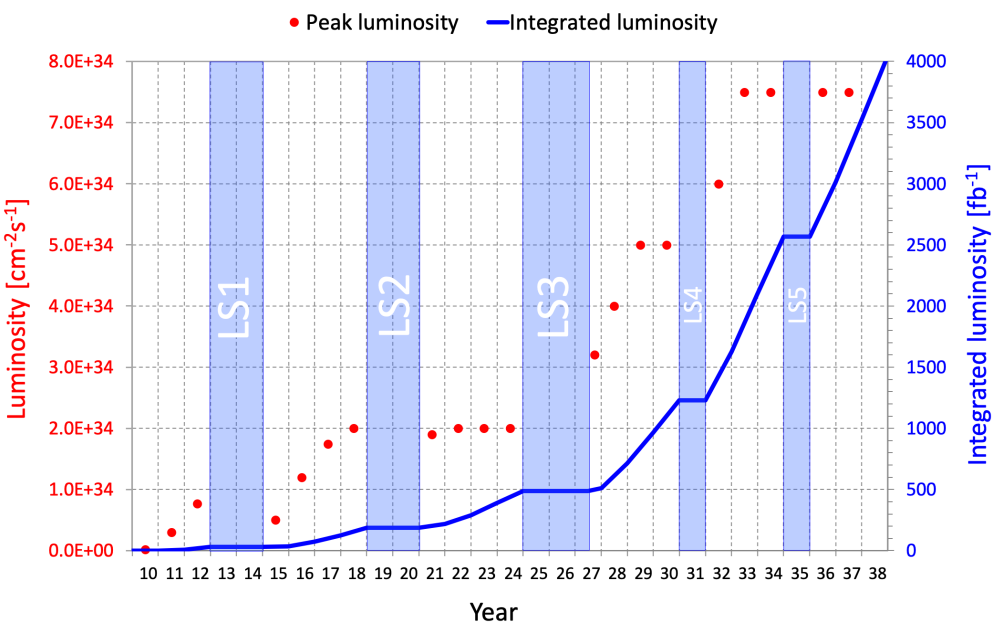
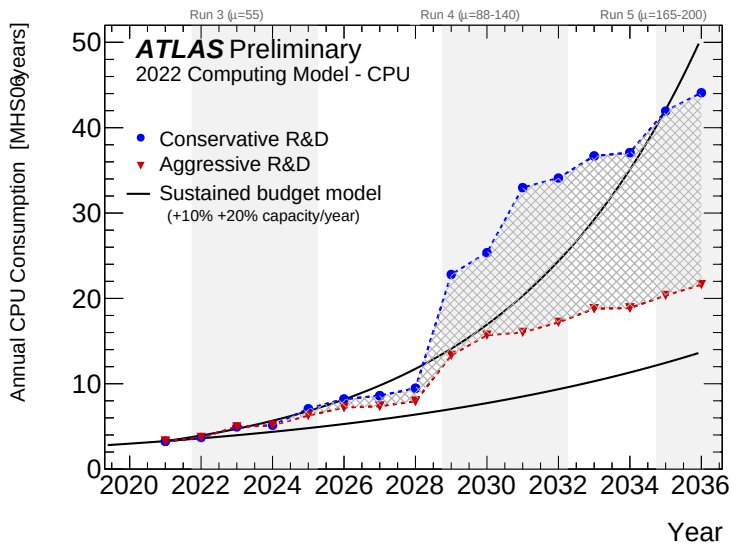
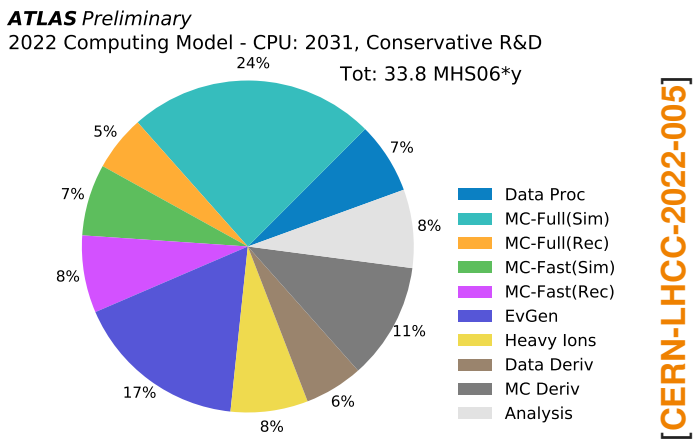


Expected computing requirements

- 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

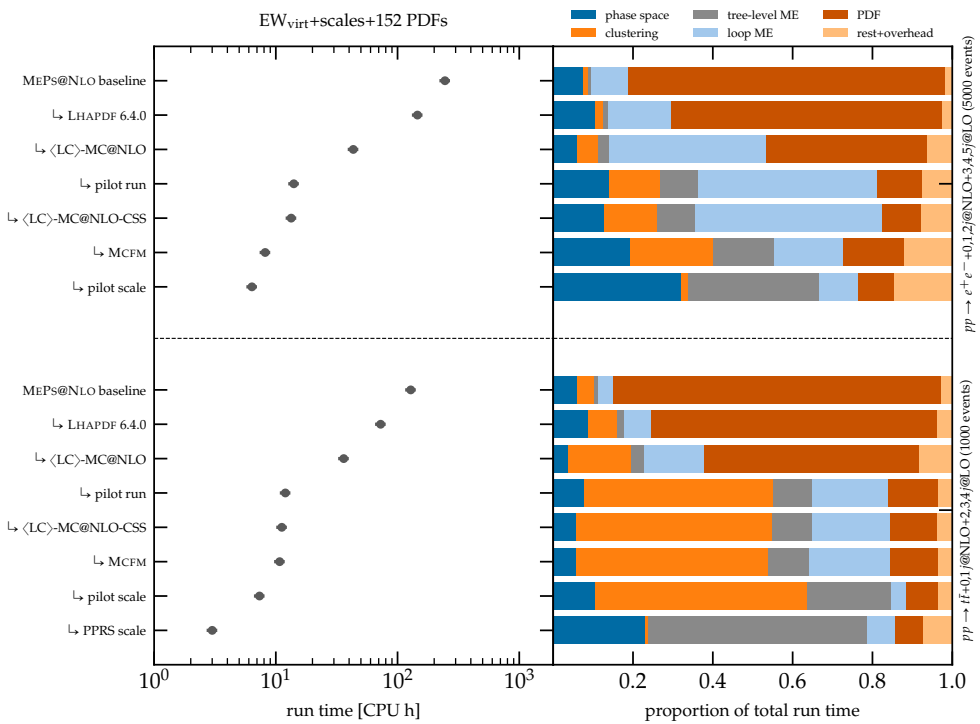






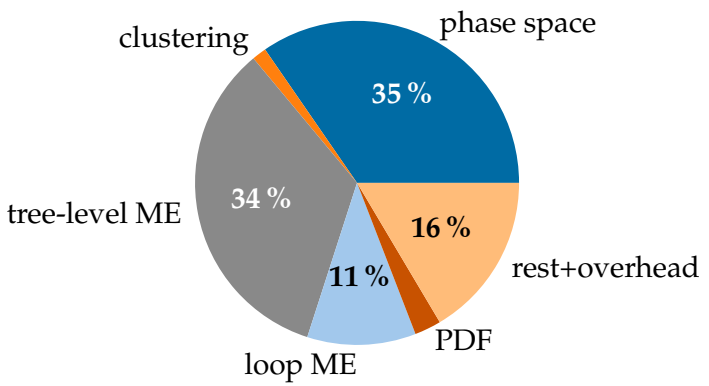
Targeted optimisation of CPU-based event generation

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



[EPJ C82 (2022) 12]

$pp \to e^+e^-$+0,1,2j@NLO+3,4,5j@LO



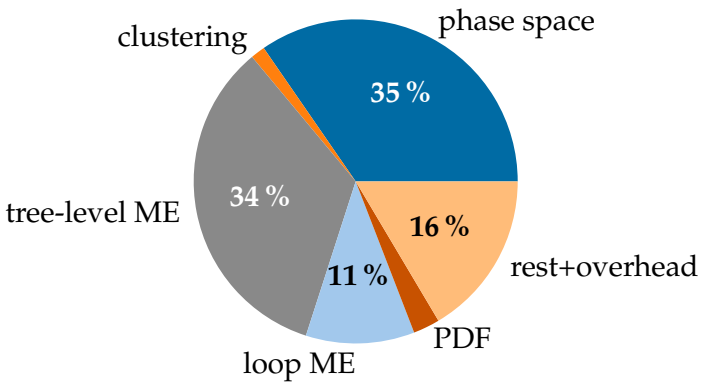
- CPU consumption **overall improved by factors of $\times 39$ and $\times 43$** for V+jets and $t\bar{t}$+jets

Parton-level event generation

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

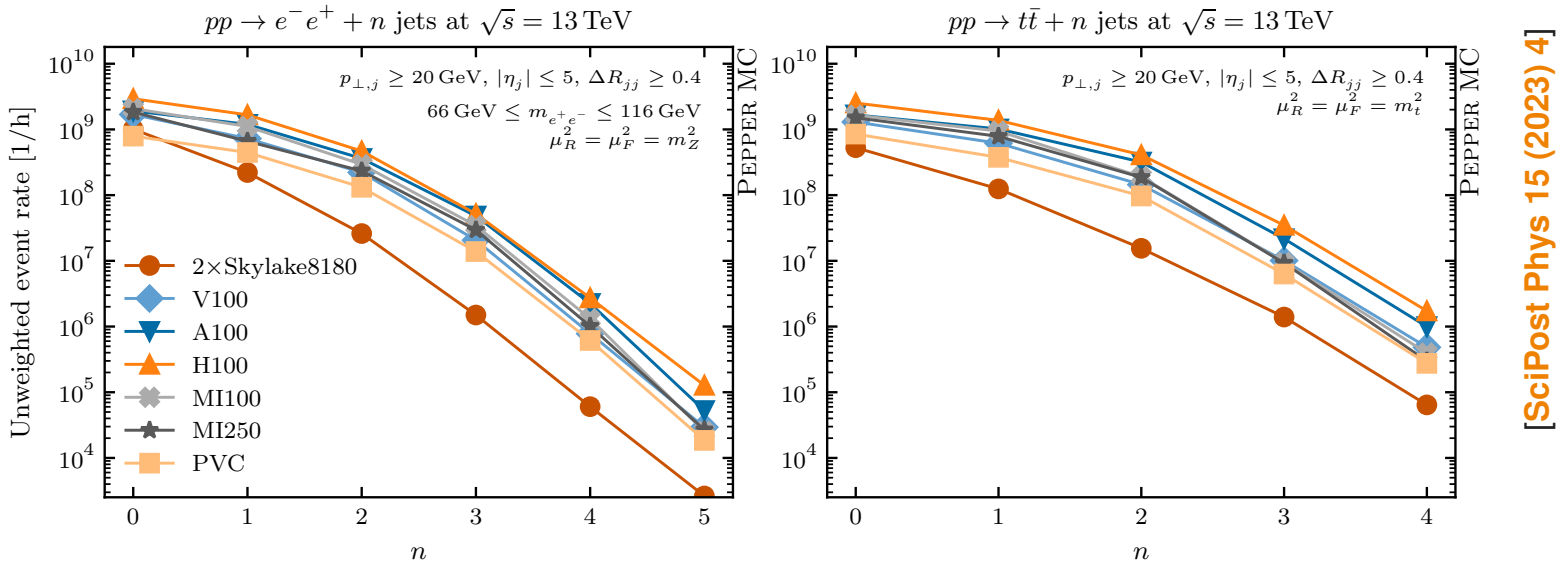
- Large portion of MC time spend in ME+PS
- Components we need to consider:
  - Phase space generation → CHILI
  - PDFs → LHAPDF
  - Tree-level matrix elements → PEPPER

$pp \to e^+e^-$+0,1,2j@NLO+3,4,5j@LO



PEPPER + CHILI: baseline GPU performance

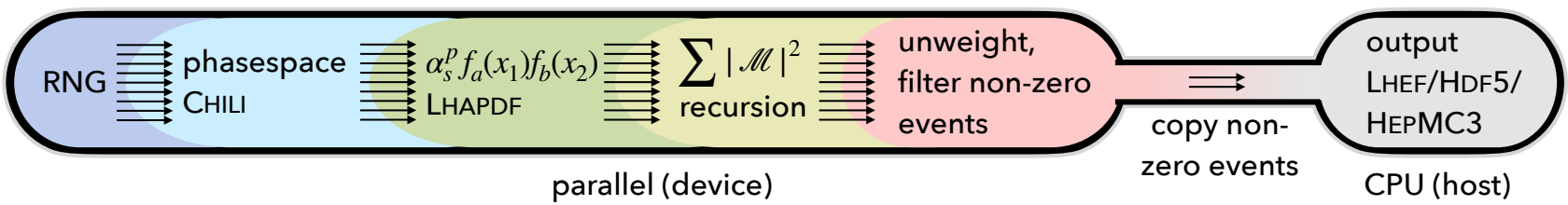
- Excellent performance across a wide range of architectures
- Portability provided by Kokkos: one code-base compiled for different architectures



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
	CPU	**GPUs**					

Portability is key

- Focus on high multiplicities ($e^+e^- + 4$, $t\bar{t} + 3$ or more jets)
  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:



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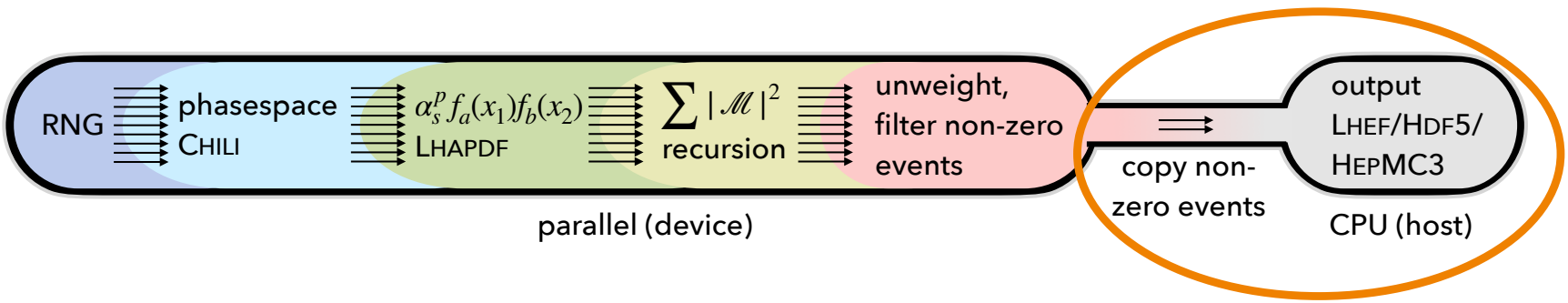
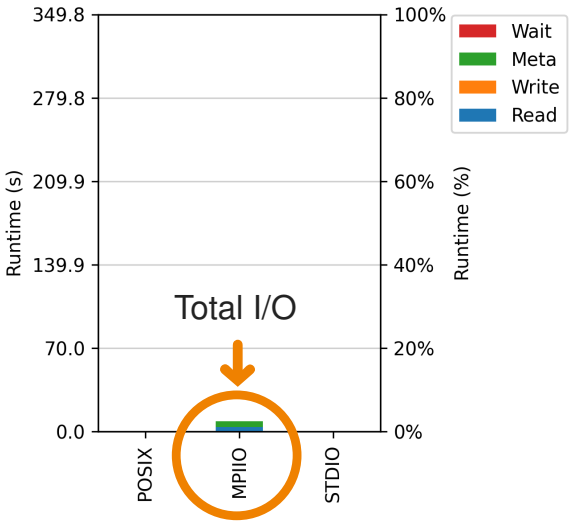


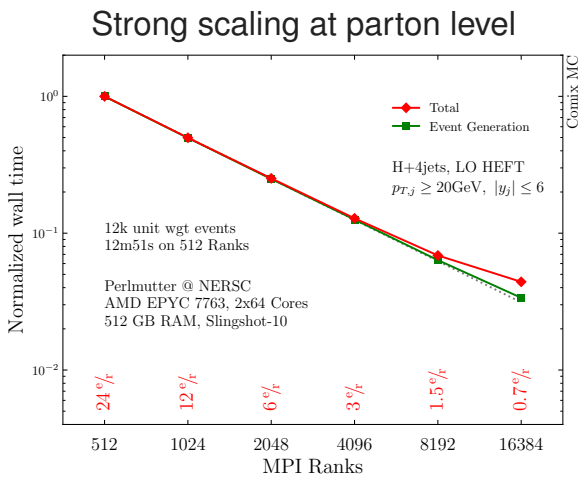
Introducing LHEH5

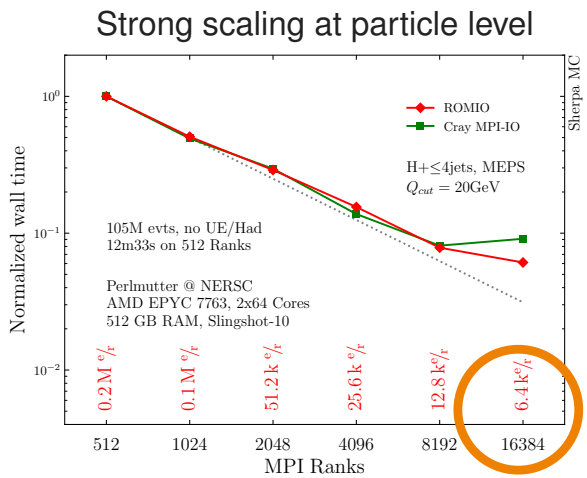
- established LHEF format is based on XML
  - flexible enough to add any desired feature
  - poses a challenge for I/O operations at scale
- new efficient LHE-like data format based on HDF5+HighFive proposed in [PRD 109 (2024) 1]

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





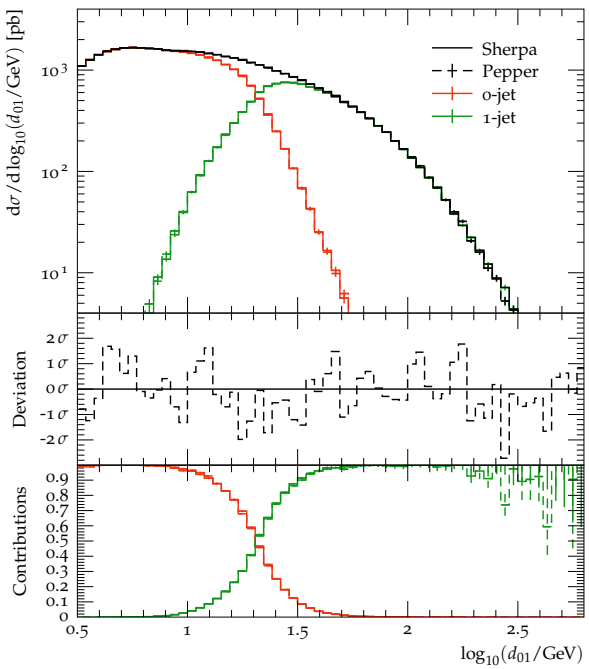


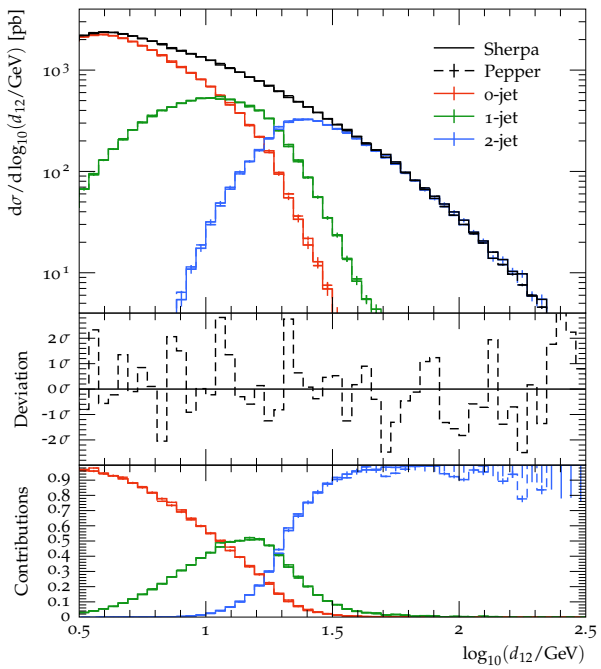
105M events / min

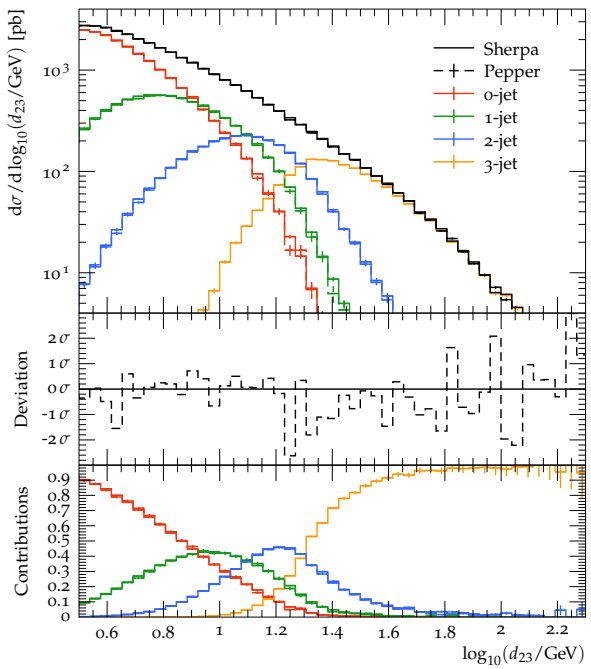
- overall I/O time reduced to below 1s per rank
  - time spent in I/O operations less than 5% when reading 128.85 GiB
- ideal for accessing back-fill queues at large computing centres

Tool-chain integration

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



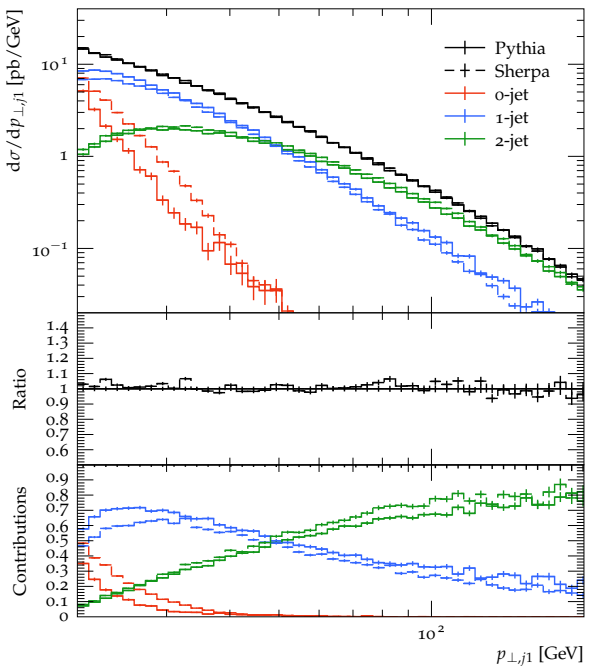


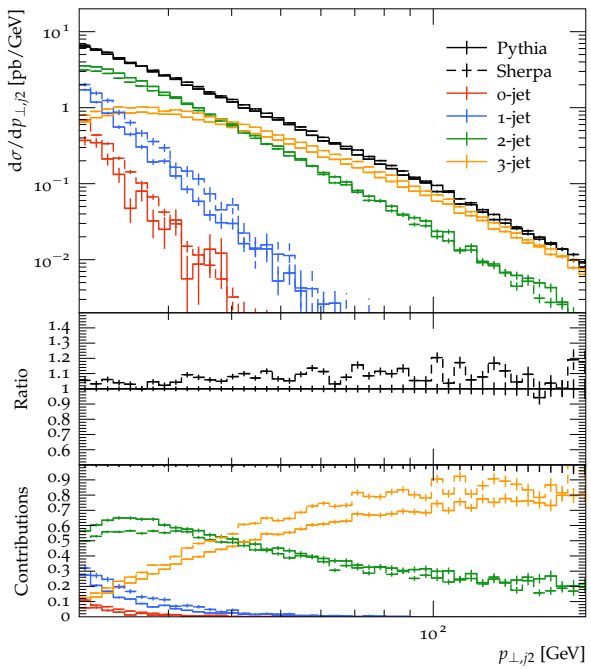


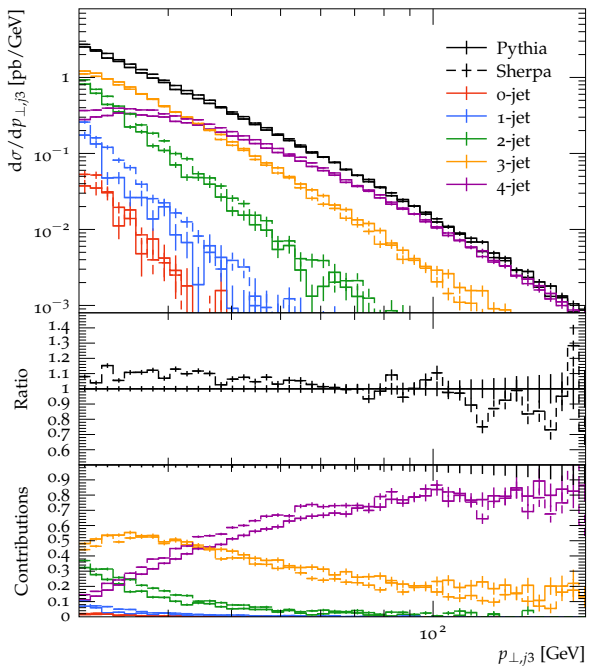
[PRD 109 (2024) 1]

More robust uncertainty estimates

- LHEH5 enables efficient substitution of various parts in the event generation chain
  - already supported by both 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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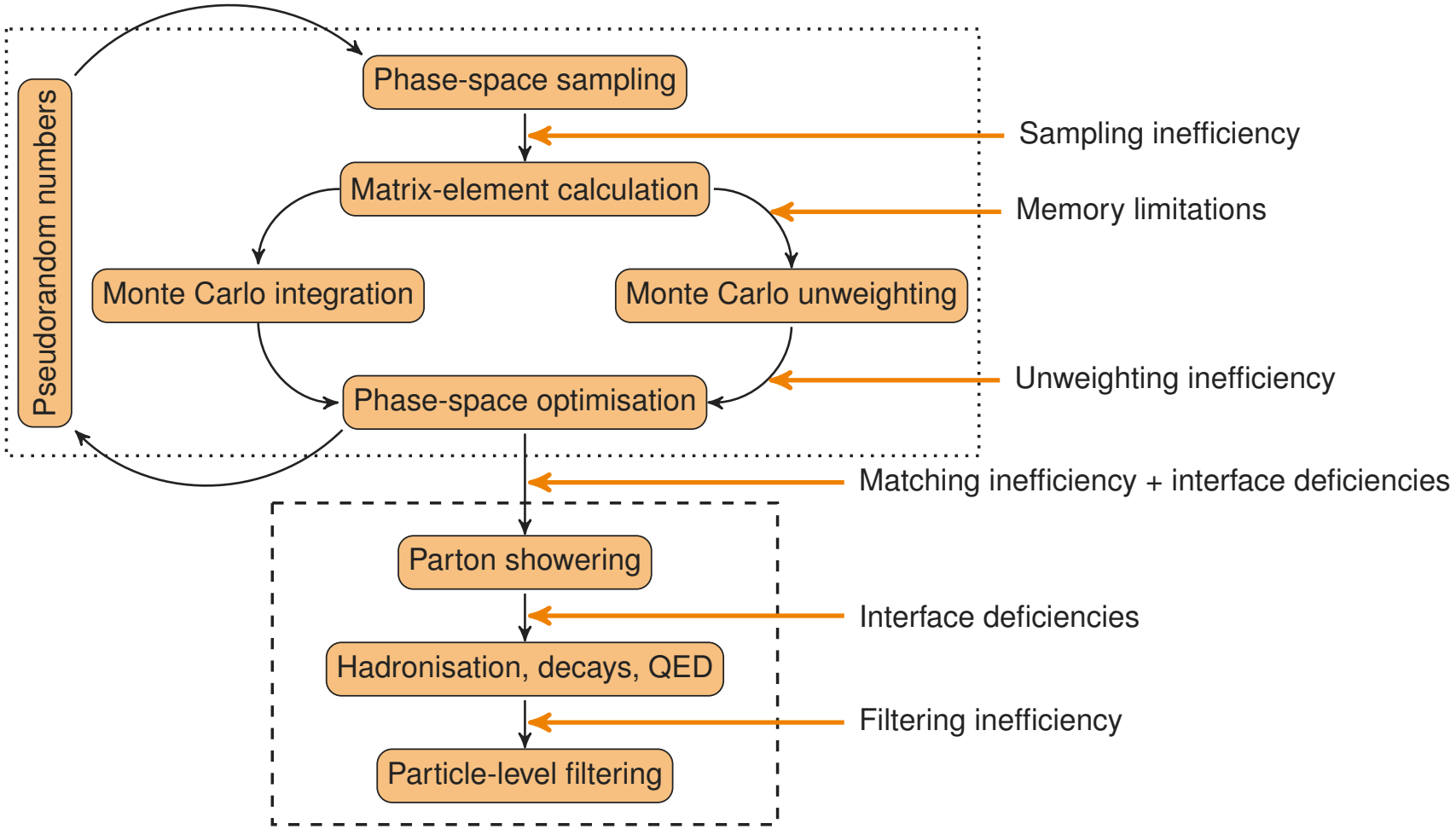
  - requires more storage for parton-level events (✘)
  - new infrastructure needs to be set up and maintained (✘)
- Approach 2: run everything in one go, harnessing heterogeneous resources, possibly with in-memory transfer of GPU-accelerated calculation components
  - no intermediate storage for parton 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 (✘)

Other bottlenecks



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

Outlook

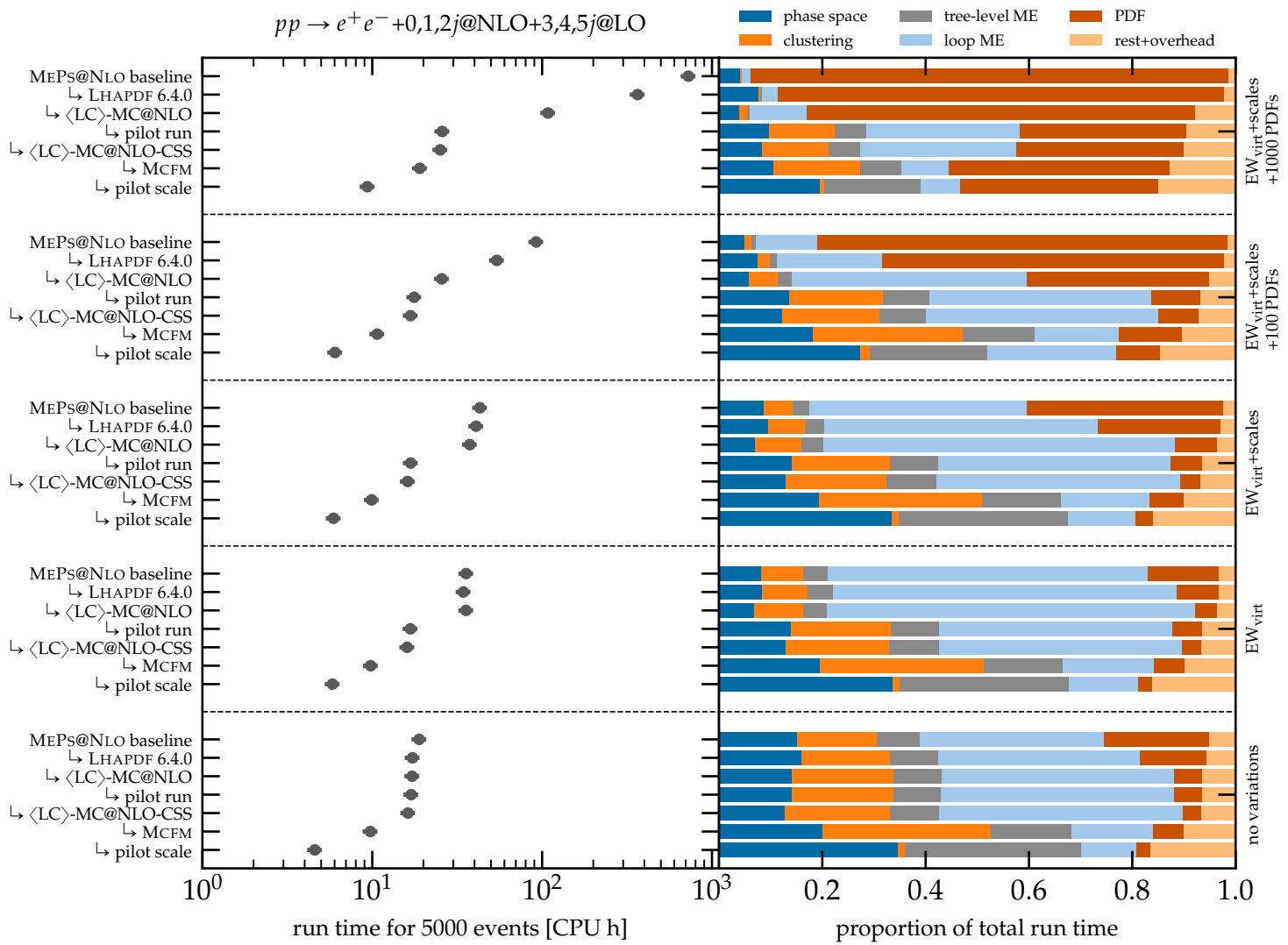
- upcoming [IPPP workshop] on Monte Carlo support tools
- Lots of scope to extend Swift-HEP1 efforts:
  - LHEH5: extend to particle level and put into HEPMC
  - LHAPDF: support for 2D spline fits (also photon PDFs, nucleon PDFs for EIC?)
  - SHERPA: adapt the codebase to better support modern computing architectures and workflows with RSE support
- ... and more:
  - HEPMC: needs systematic profiling in light of HPC usage; extend to efficiently support factorised parton-shower systematics
  - Showers: extend recent reweighting efforts to reduce cost of asssessing non-perturbative uncertainties (hadronisation, MPI, decays) [arXiv:2308.13459]
  - Hadron-decay modelling: community hadronisation and decay packages for efficient generation of complex multi-rare-decay topologies (if there's interest)
- General theme: make event generation maximally HPC friendly and develop the MC infrastructure to deliver the best possible calculations and robust uncertainties

Summary

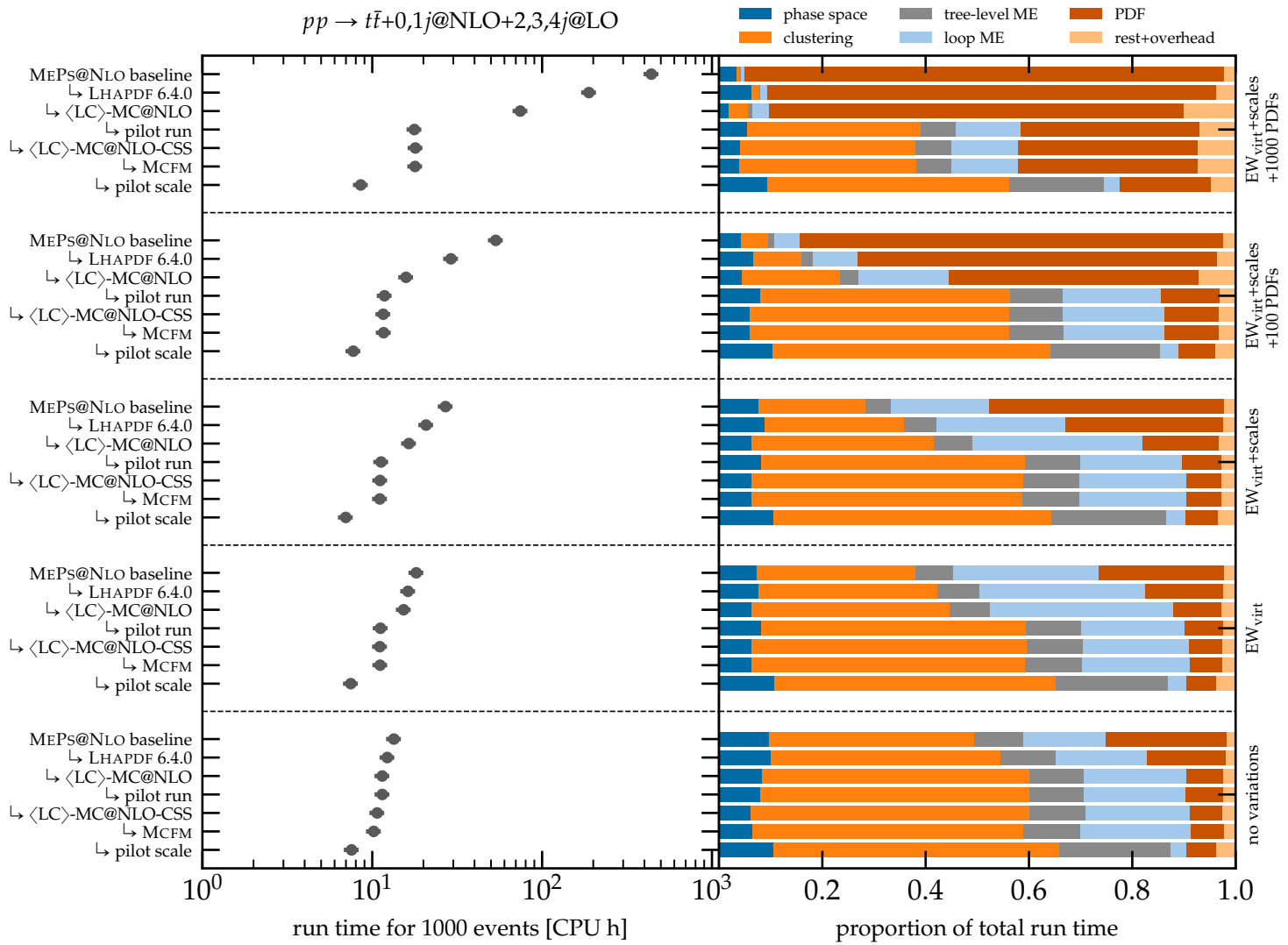
- computing cost of traditional CPU-based multi-leg event generation significantly reduced by factor 40–80 following dedicated profiling [EPJ C82 (2022) 12]
- first production-ready portable LO event generator allows to incorporate GPU resources into high-precision simulations [SciPost Phys 15 (2023) 4]
- this constitutes the first realistic and sustainable approach towards large scale event generation in the HL-LHC era
- well positioned to exploit Leadership Computing Facilities across the world
  - ideally suited for high-precision calculations if quotas can be obtained
- focus now shifting towards better calculations and more robust uncertainty estimates

Backup

Breakdown of CPU budget in V+jets

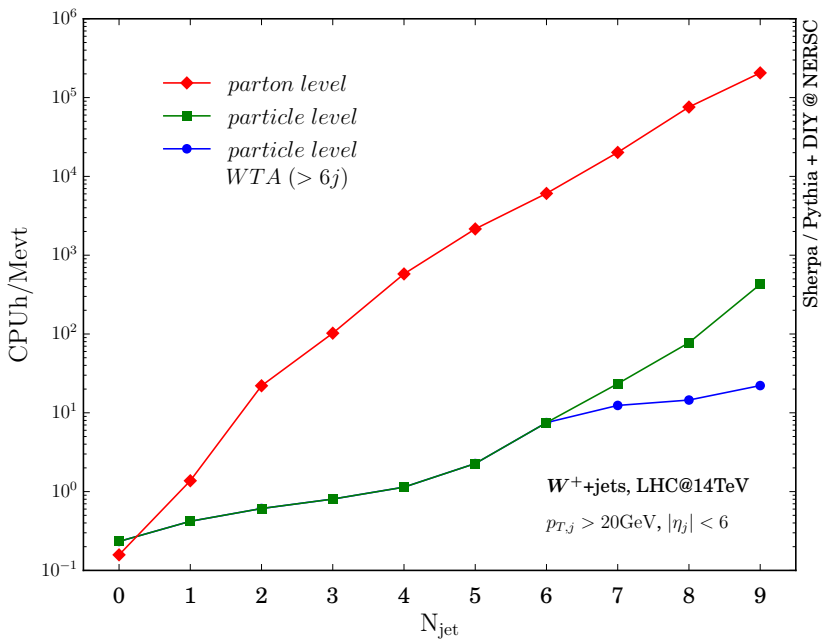


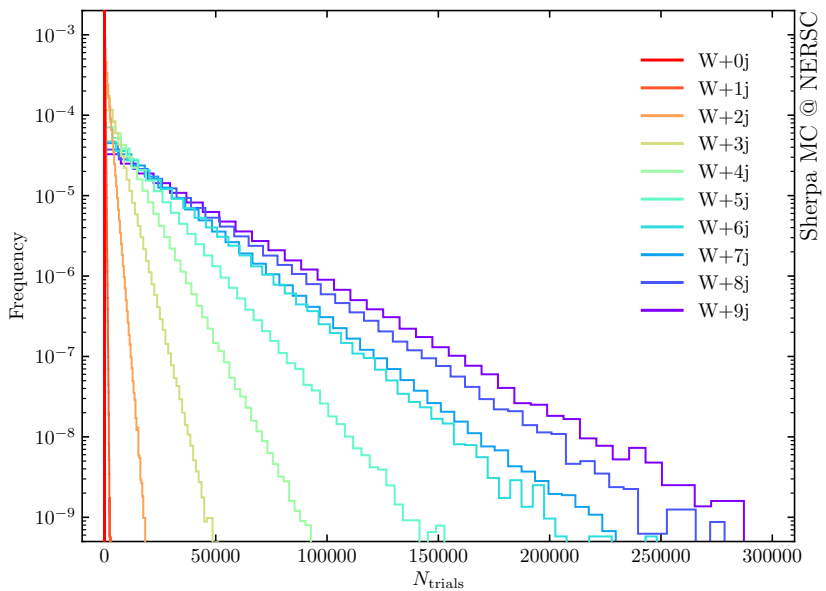
Breakdown of CPU budget in $t\bar{t}$+jets



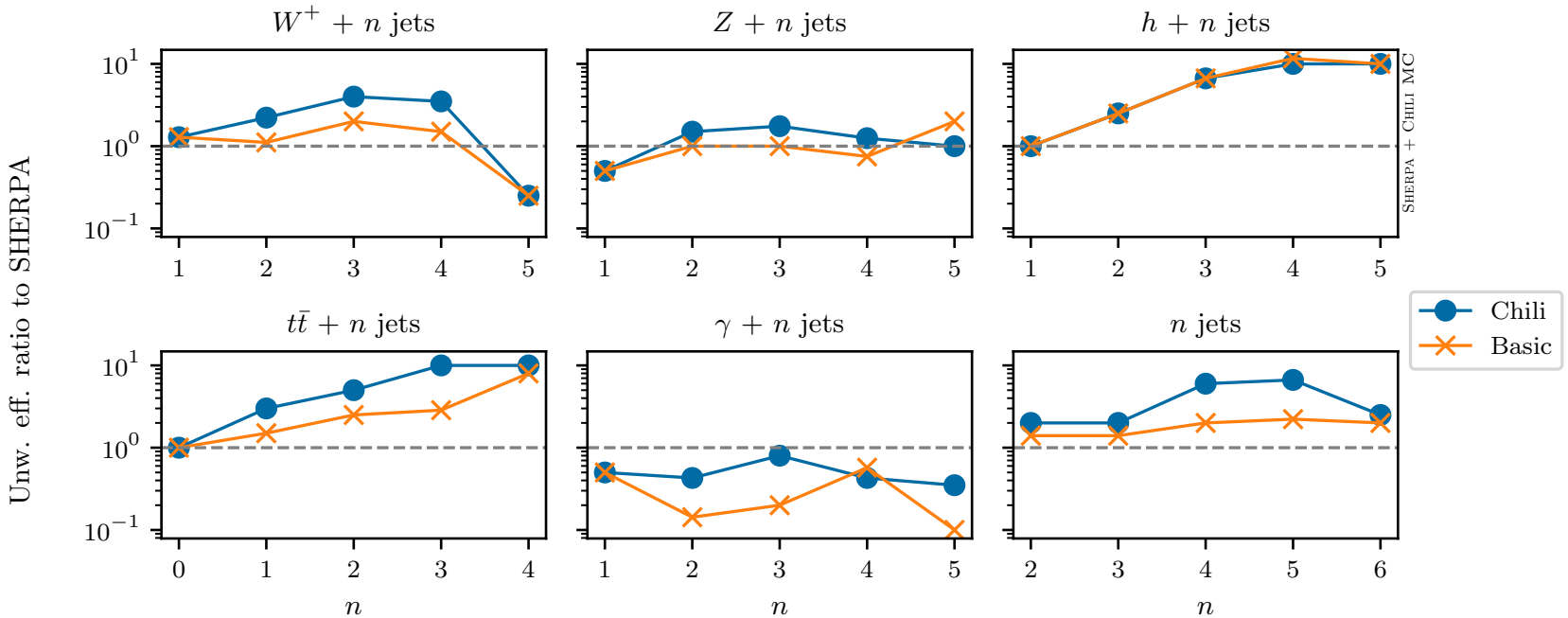
Parton vs particle level

- 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





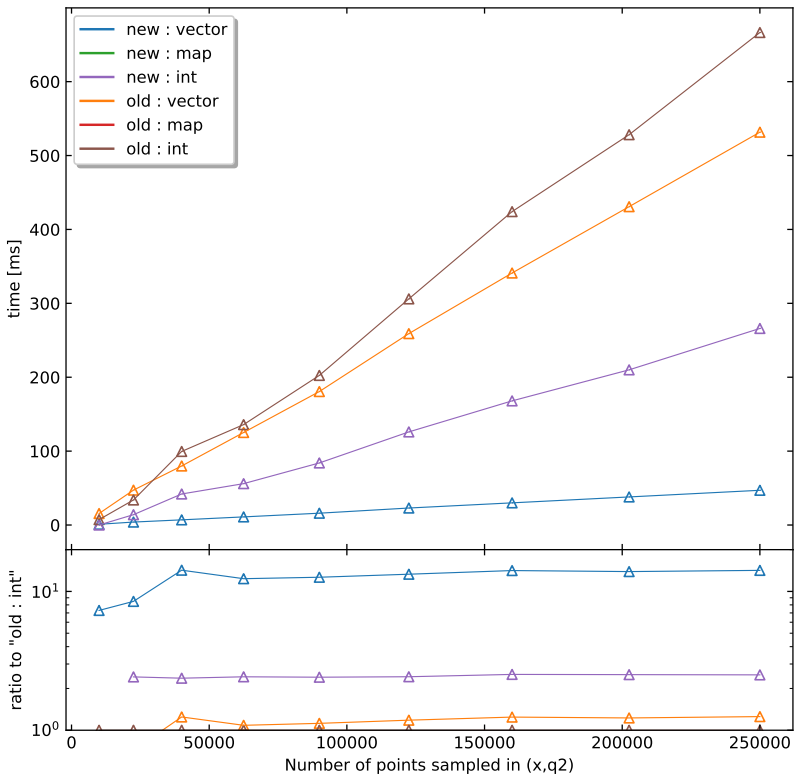
Chili performance compared to SHERPA default



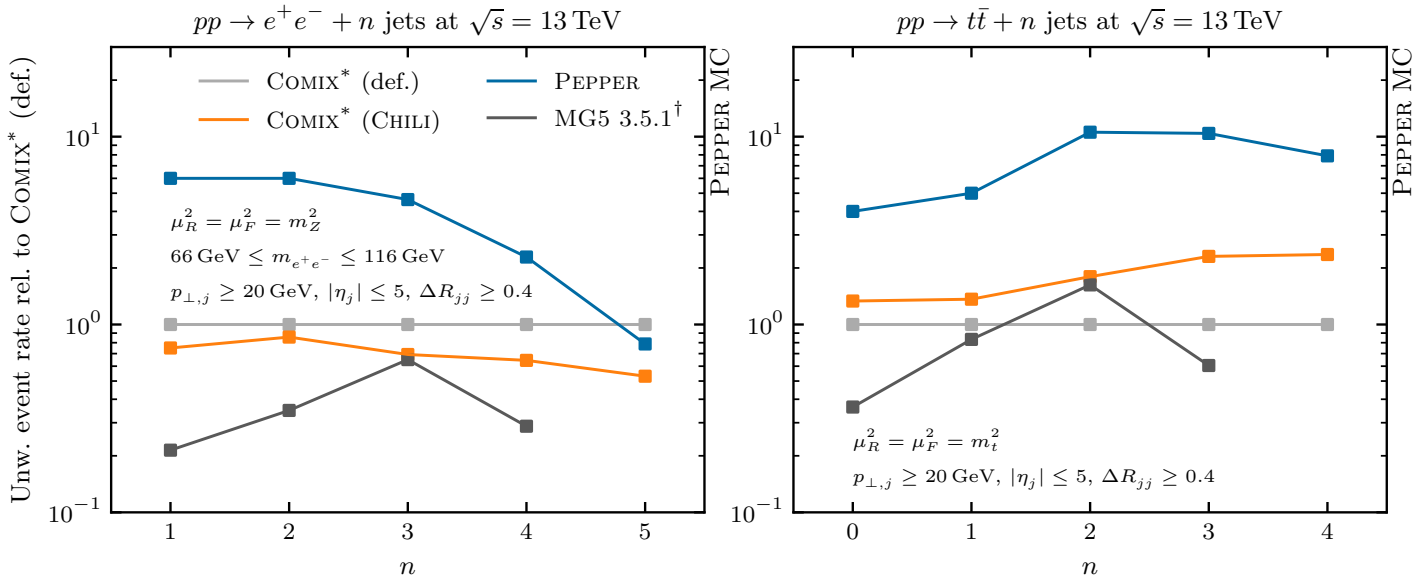
- CHILI phase-space generator uses simple (MCFM-inspired) structure: one t-channel + adjustable number of s channels [SciPost Phys 15 (2023) 4]
  - Portable (ported built-in CHILI in PEPPER)
  - Efficiency on par with recursive COMIX phase-space

Making LHAPDF GPU-ready

- Byproduct of porting exercise
  - PDF evaluations not critical
  - copying of data is
- Huge performance gains
  - 3-10x speedup per PDF evaluation
  - more possible by changing MC workflows
- OpenMPI used for efficient initialisation
  - constant init time vs. infinite init time [PRD 100 (2019) 1]
- Added CUDA + Kokkos interface/version
  - excellent computing performance / accuracy
  - portable version used for the remaining talk



PEPPER + CHILI: baseline CPU performance



- First complete CHILI + PEPPER benchmark
  - Unweighted event throughput compared to COMIX*
  - Constitutes baseline single-threaded performance of currently available competitive algorithms
  - Standalone PEPPER performs better than COMIX, but PEPPER's real goal is portability

Numbers generated on Intel Xeon E5-2650 v2
* Partonic processes split into to *g*/*q* groups (not SHERPA default)
† Modified to match efficiency convention of [PRD 101 (2020) 7]

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

Super-computing for the HL-LHC

- PEPPER runs on all leading systems in EU and U.S.
- ATLAS estimated roughly 330 billion leptonically decaying V+jets events would be required for HL-LHC [JHEP 08 (2022) 089]
- Time for V+j sample:
  - 4h Frontier
  - 6h Aurora
  - 8h Leonardo
  - 15h Lumi