Status and progress of SHERPA

Parton Showers and Resummation 2023 in Milan

June 6 2023

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on behalf of the SHERPA collaboration

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MCnet

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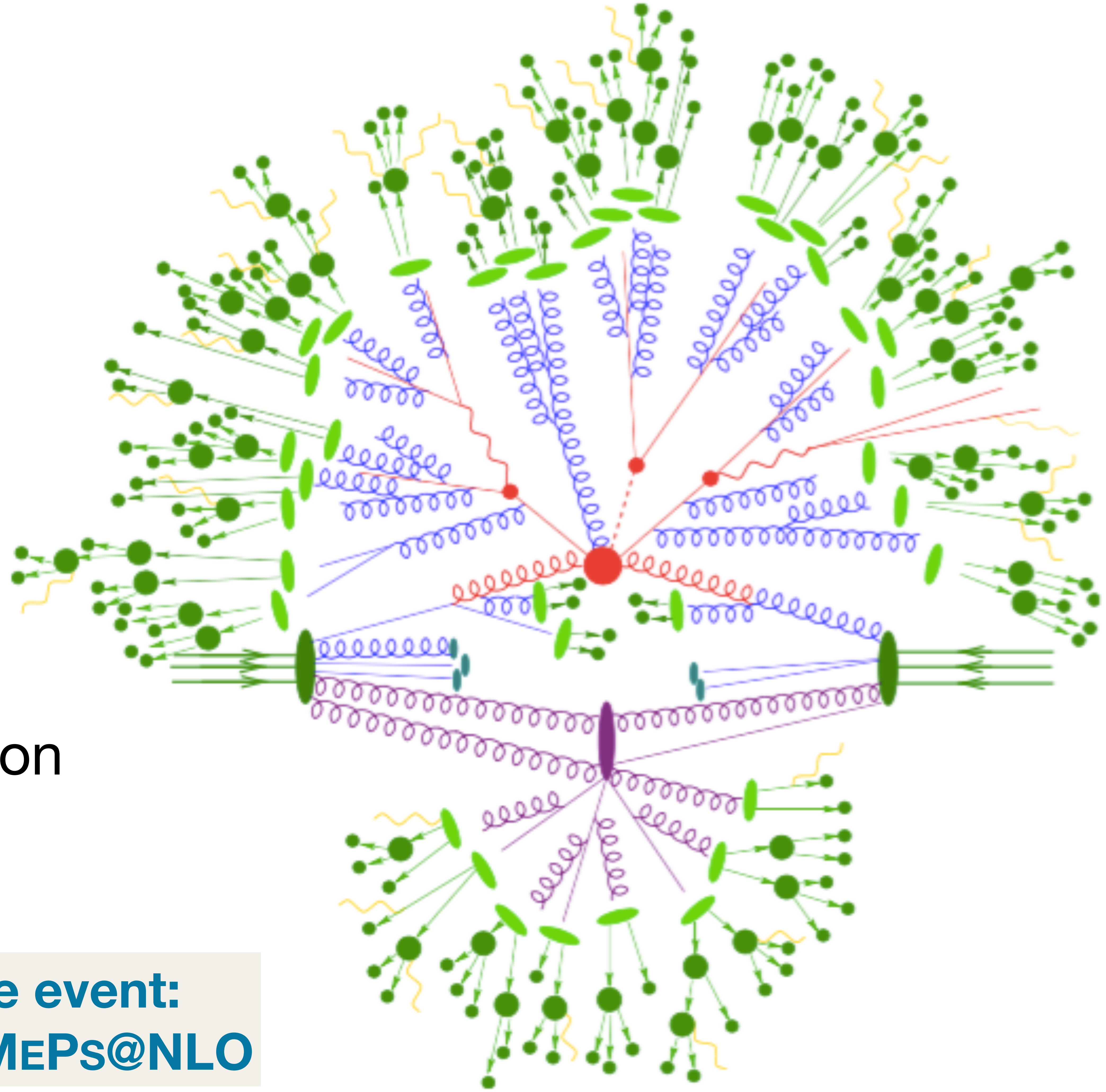
The SHERPA event generator framework

v2.2 release series [SHERPA collab. 1905.09127]

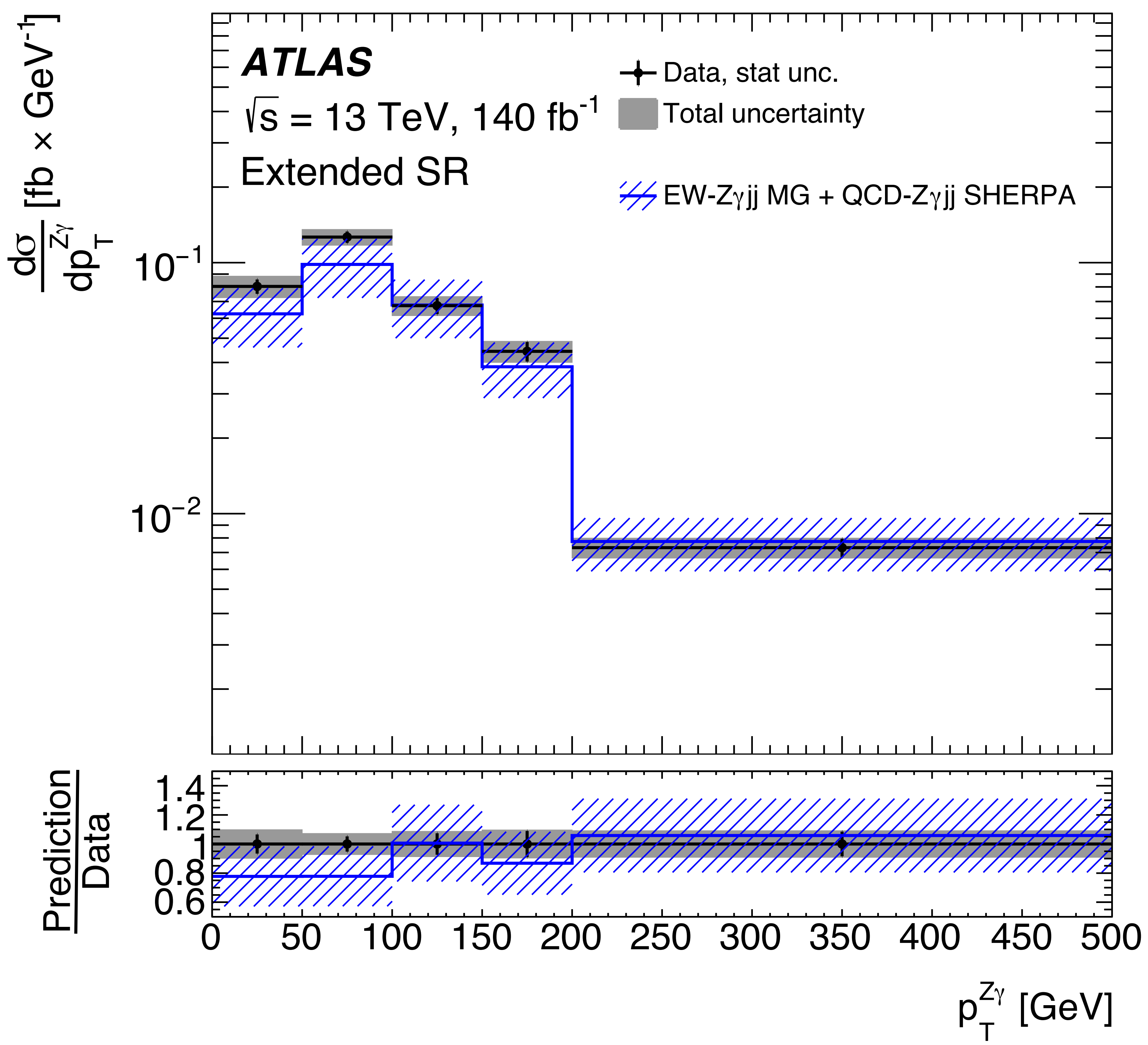
- Two multi-purpose matrix element (ME) generators:
  AMEGIC, COMIX
- Two parton showers (PS) generators:
  CSSHOWER, DIRE
- A multiple interaction simulation à la PYTHIA
- A cluster fragmentation module
- A hadron and τ-lepton decay package
- A higher-order QED generator using YFS resummation
- Many add-ons

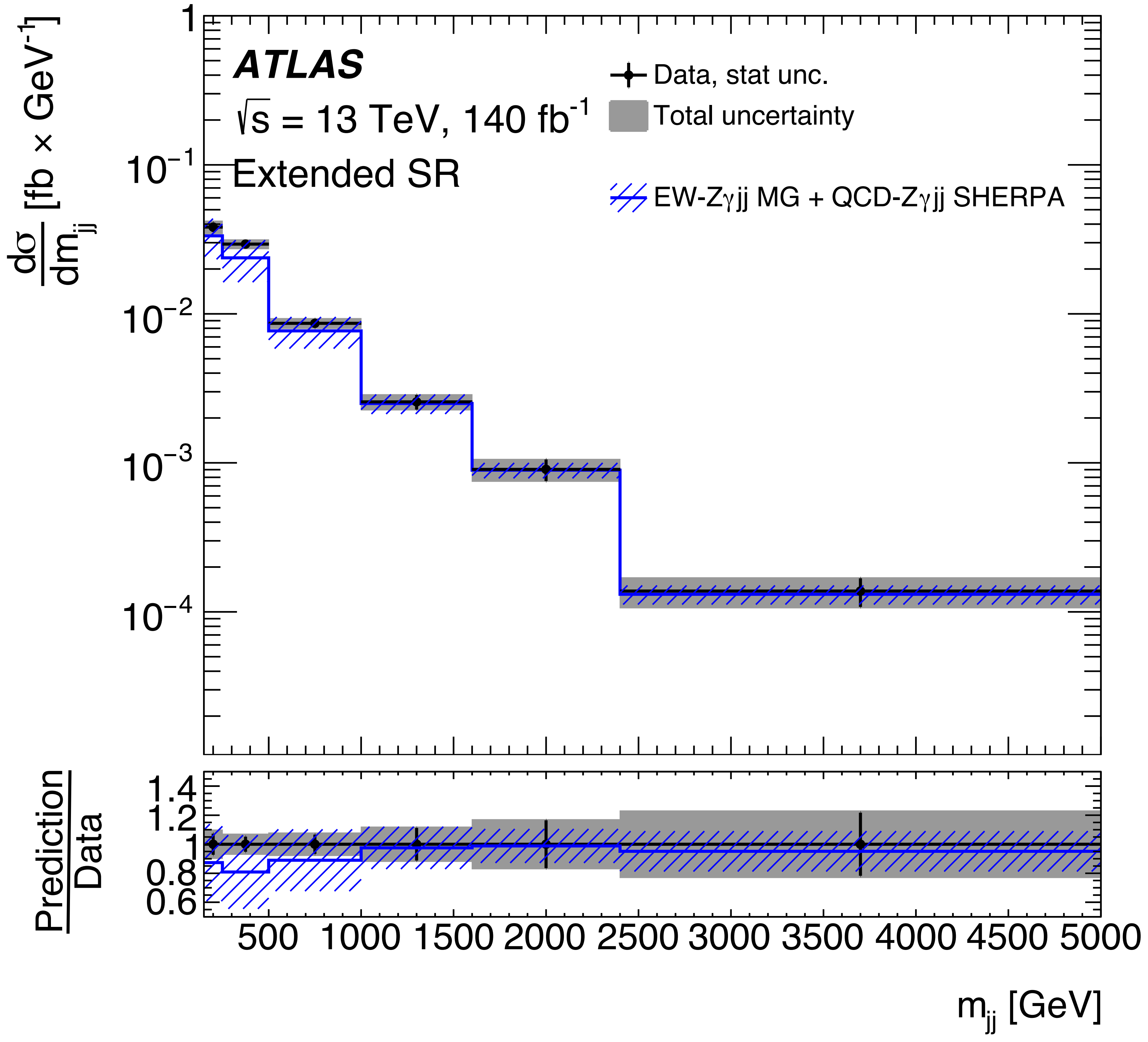


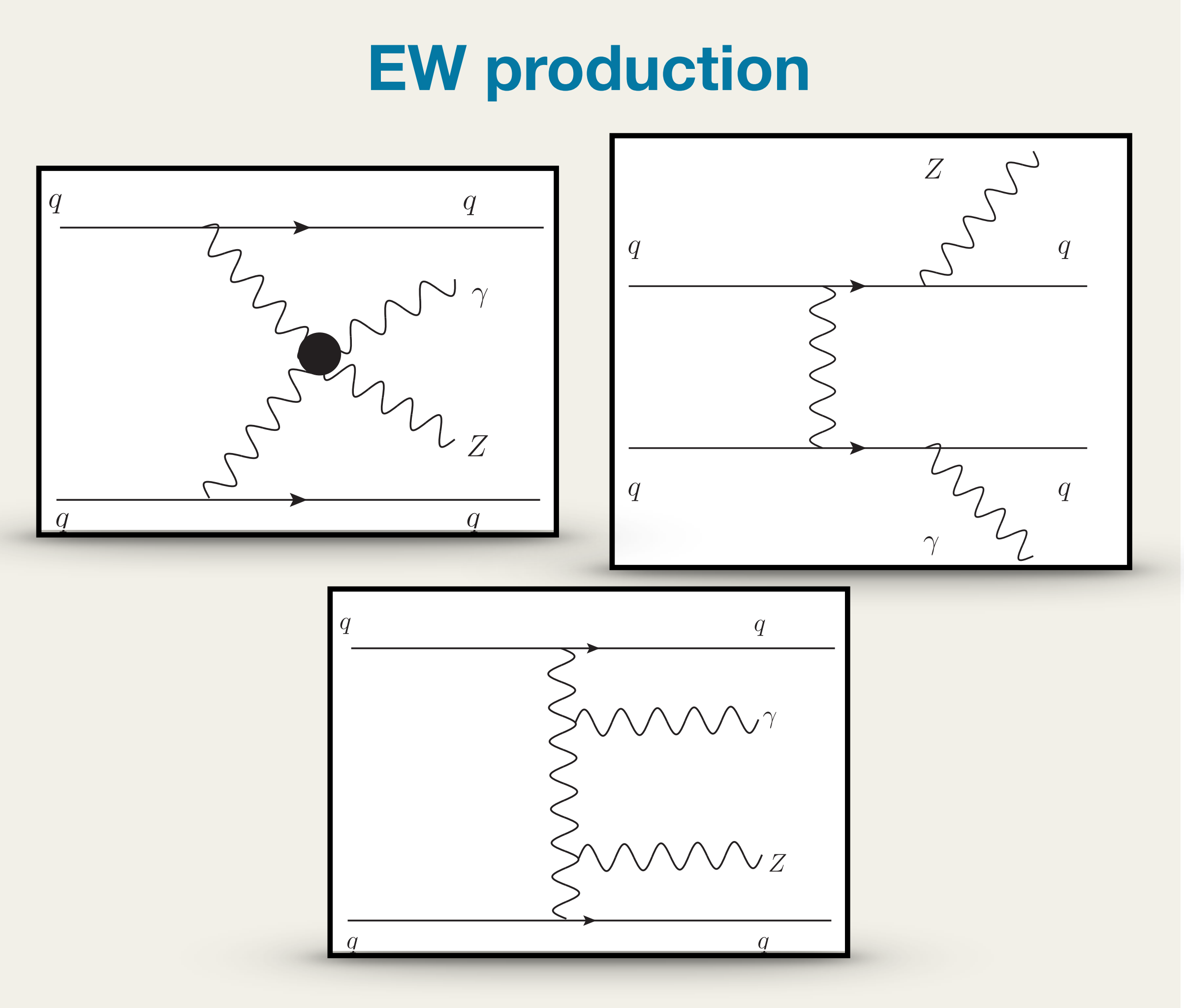
SHERPA's Traditional strength is the perturbative part of the event:
LO, NLO, NNLO, LOPS, NLOPS, NNLOPS, MEPS, MENLOPS, MEPS@NLO

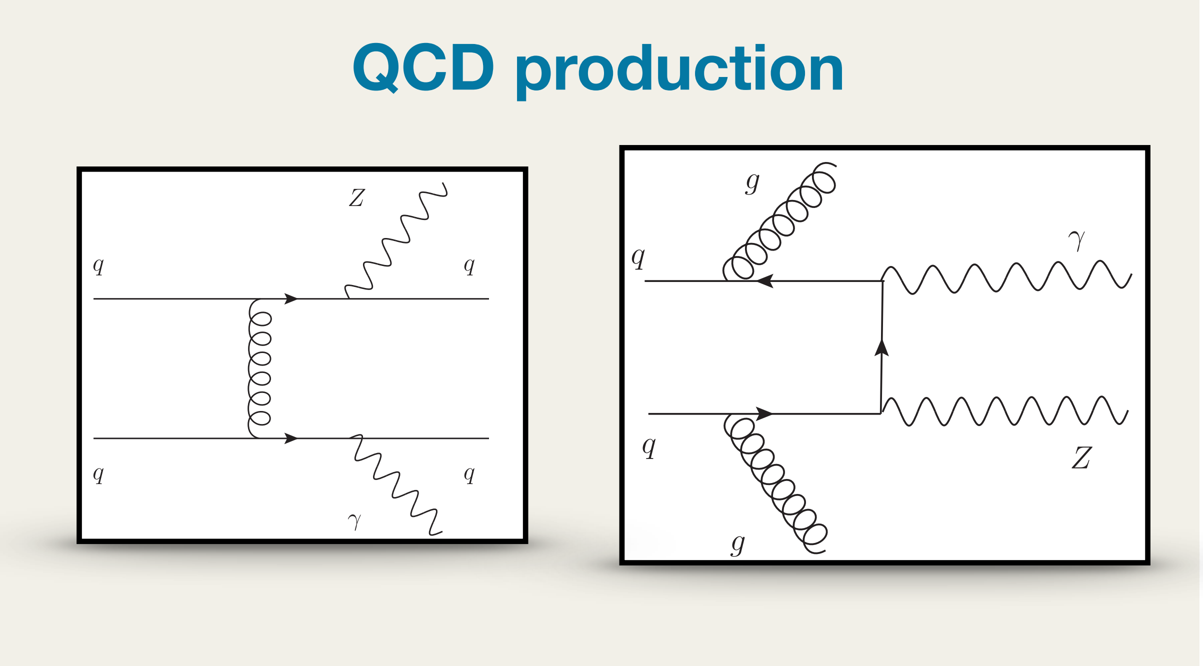
Showcase I

ATLAS Observation of electroweak Zγjj production [ATLAS collab. 2305.19142]







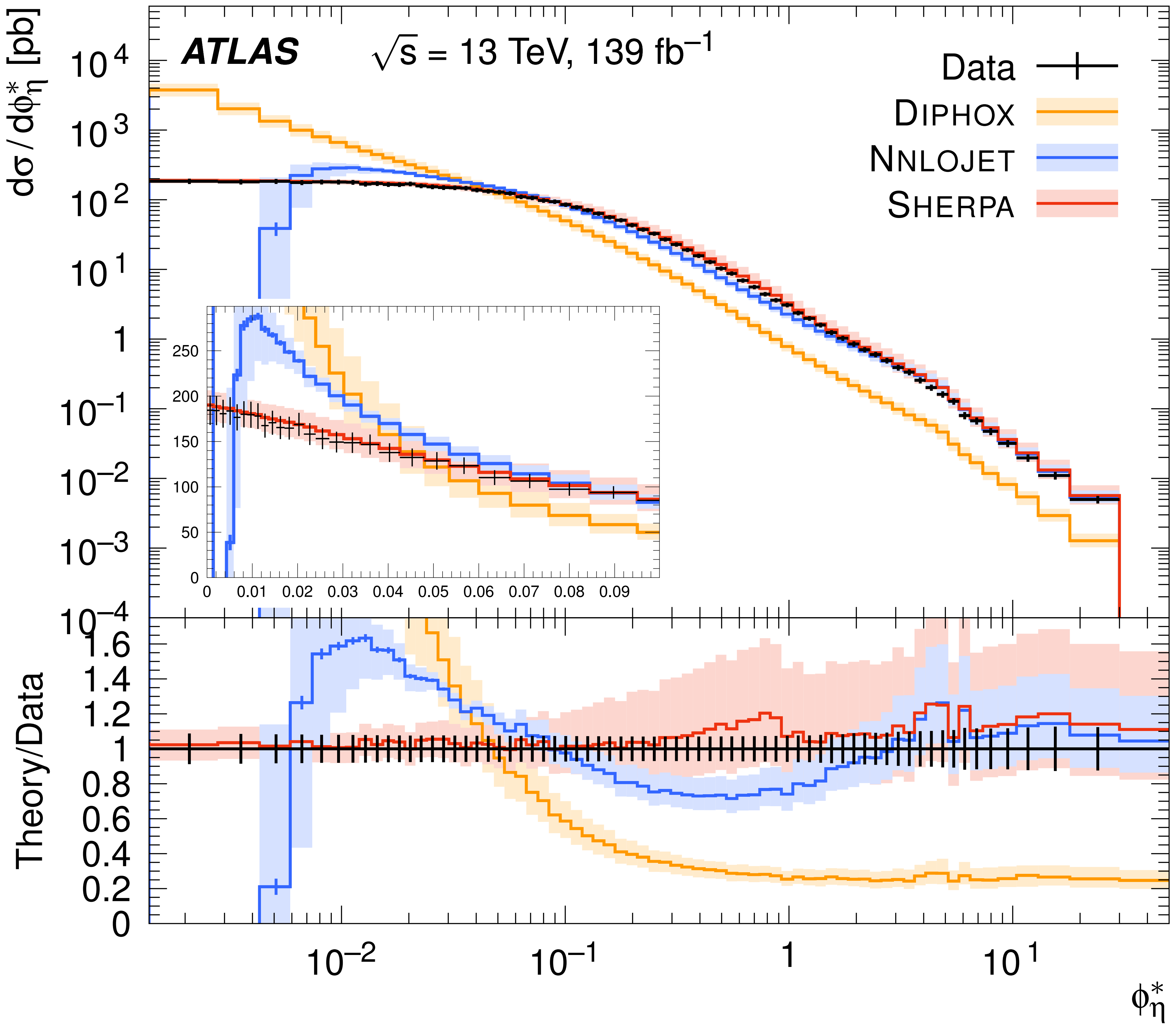


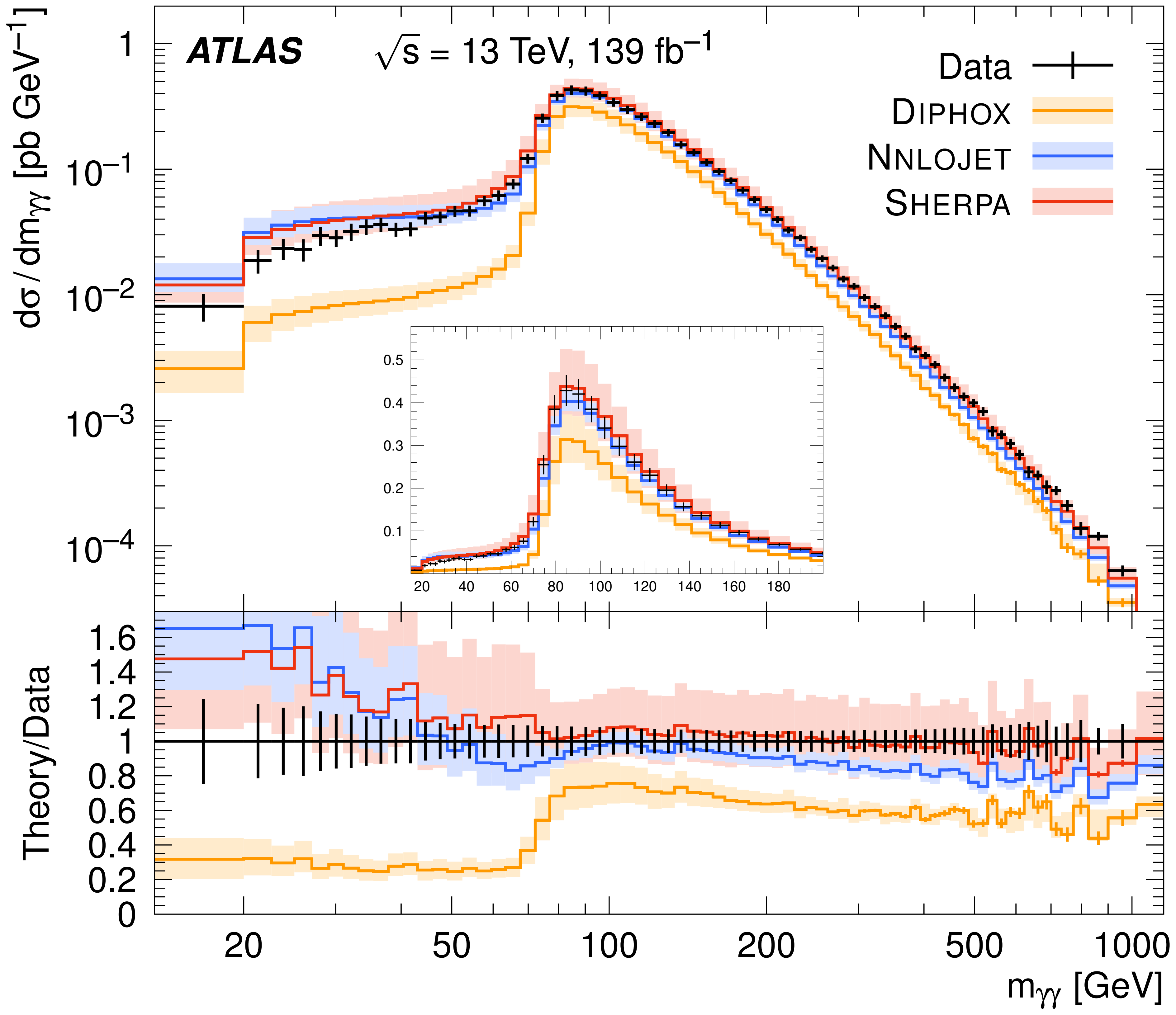
- MG5_aMC@NLO for EW production, Sherpa+OpenLoops for QCD production
- QCD production MEPS@NLO $pp \to Z\gamma jj + 0{,}1j\,@\,\mathrm{NLO} + 2{,}3j\,@\,\mathrm{LO}$
- “Differential cross-section measurements […] found to be consistent with the SM predictions.“

Showcase II

ATLAS prompt diphoton production [ATLAS arXiv:2107.09330]

SHERPA MEPS@NLO diphoton production: $\gamma\gamma + 0{,}1j\,@\,\mathrm{NLO} + 2{,}3j\,@\,\mathrm{LO}$, loop-induced $gg \to \gamma\gamma\,@\,\mathrm{LO}$





SHERPA MEPS@NLO has larger uncertainties than NNLO calculation, but provides excellent description throughout phase space.

Status and progress of SHERPA

Efficiency

Precision

Simone Amoroso's demands

SHERPA status (checkmarks mine)

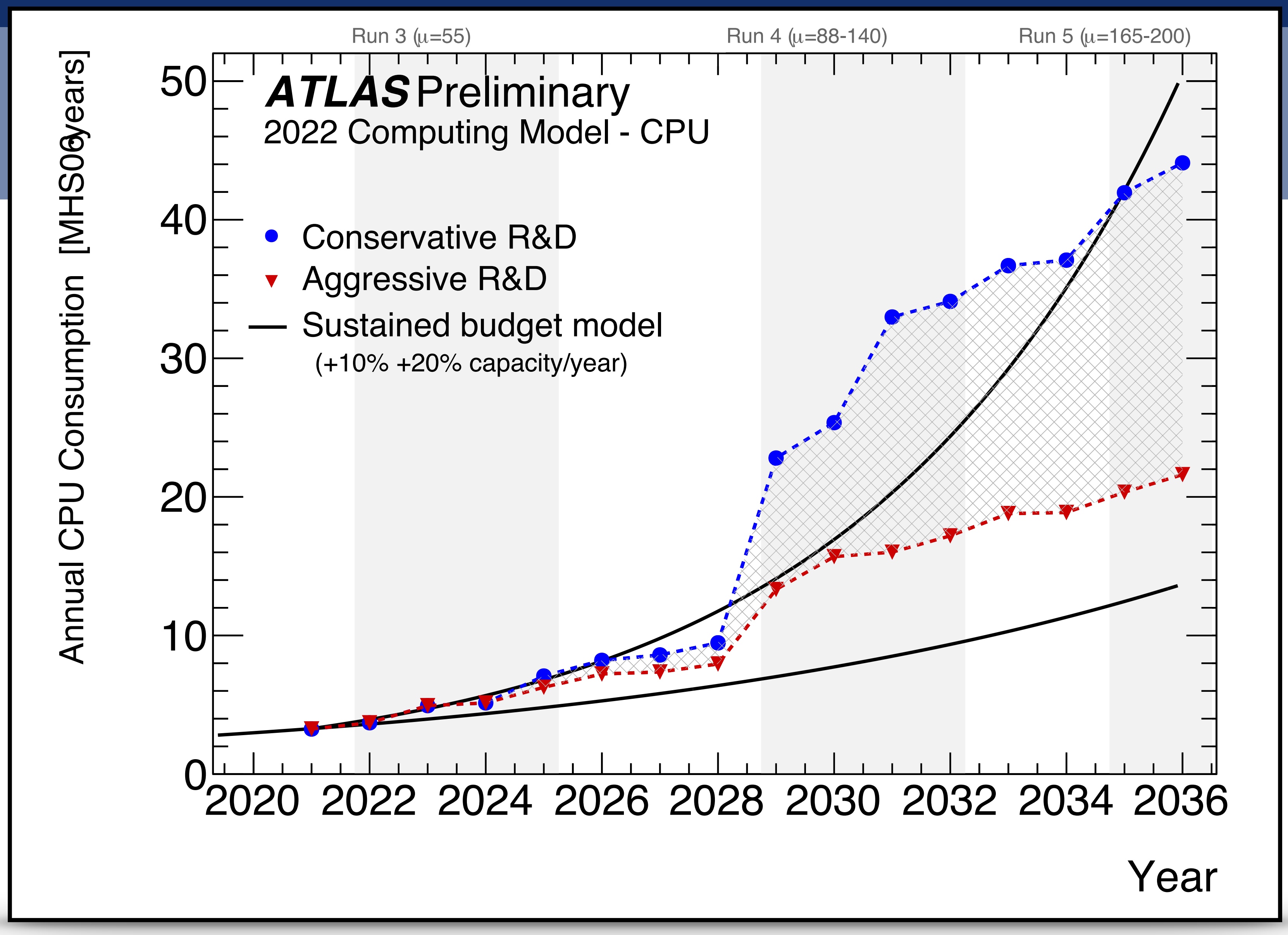
Computing aspects		
We don't just need better generators, we also need to run them at scale	✓	
Public, fast, scalable	✓	[Höche, Prestel, Schulz 1905.05120]
Small fraction of negative weighted events	(✓)	[Danziger, Höche, Siegert 2110.15211] [ATLAS 2112.09588]
Fast and efficient reweighting at least for scale and PDF variations	✓	[EB et al. 2209.00843]
Simple and efficient biasing in phase space (to populate tails)	✓	
Support for heterogeneous computing (?)	WIP	[EB, Giele, Höche, Isaacson, Knobbe 2106.06507]

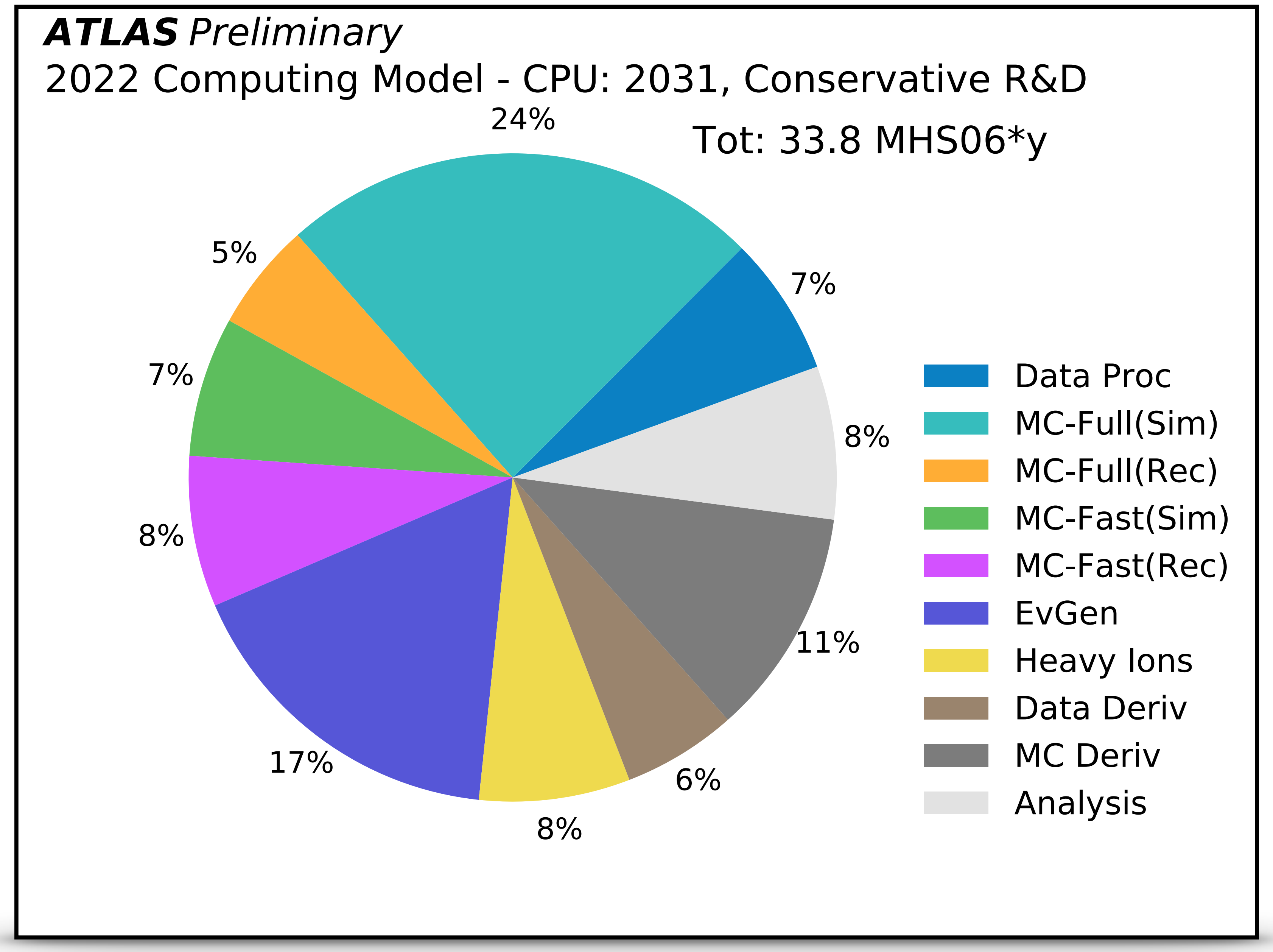
Sherpa+LHAPDF Performance for (HL-)LHC

Overall profiling and tuning [EB et al. 2209.00843]

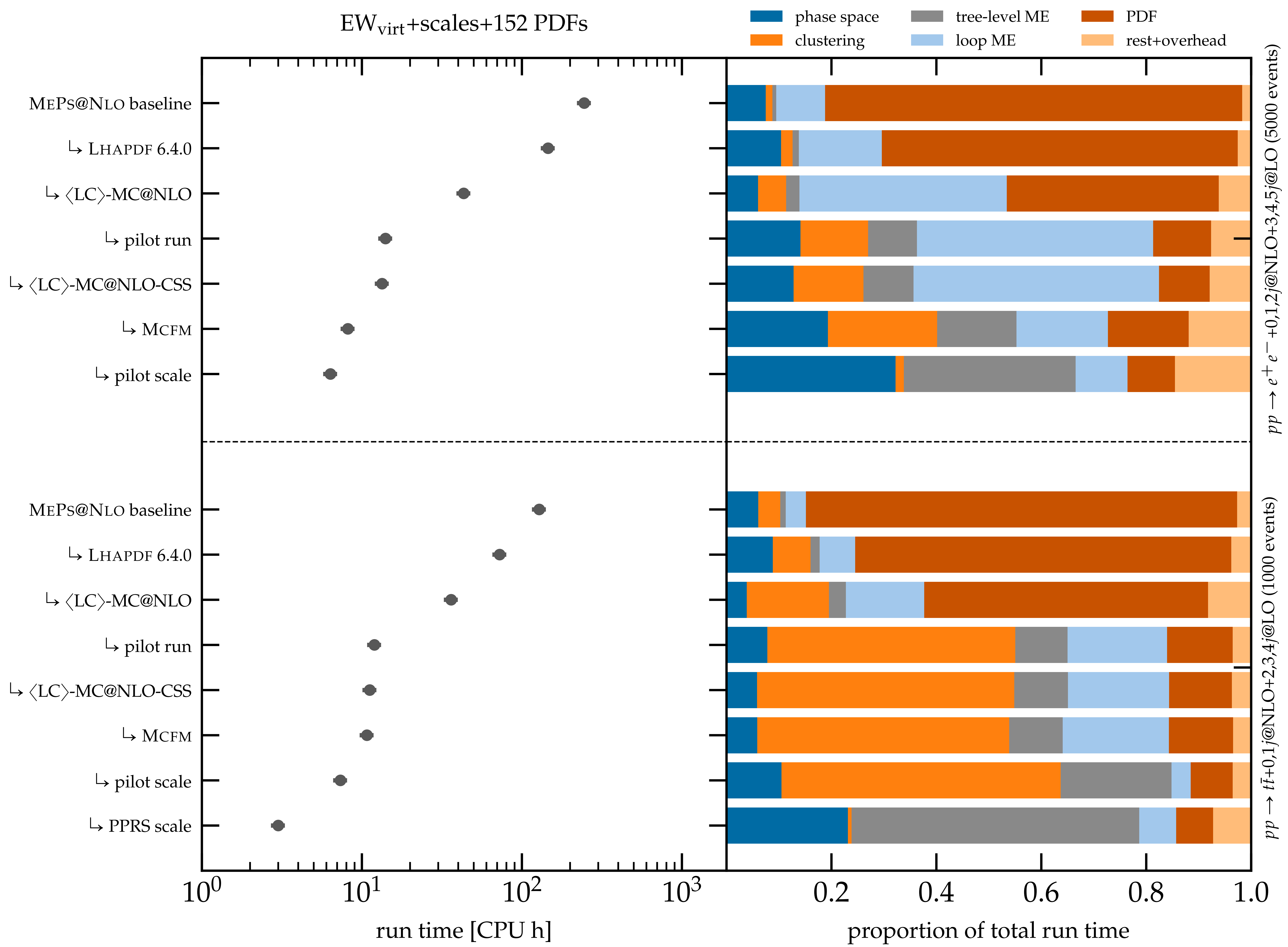
- Latest projection for computing resources: significant part is MC event gen.
- (HL-)LHC measurements in danger of being limited by MC statistics
- Explore reduction of CPU footprint for heaviest use cases, e.g. ATLAS default setup $Z + 0{,}1{,}2j\,@\,\mathrm{NLO} + 3{,}4{,}5j\,@\,\mathrm{LO}$

1. LHAPDF improvement
2. ⟨LC⟩-MC@NLO: reduce matching accuracy to leading colour, neglect spin correlations, i.e. S-MC@NLO → MC@NLO
   also useful to reduce negative event fractions [Danziger, Höche, Siegert 2110.15211]
3. pilot run: minimal setup until PS point accepted, then rerun full setup
4. ⟨LC⟩-MC@NLO-CSS: defer MC@NLO emission until after unweighting
5. use analytical loop library where available
   here: OpenLoops → MCFM via interface [Campbell, Höche, Preuss 2107.04472]
6. pilot scale definition in pilot run that requires no clustering
   small weight spread by correction to correct scale





SHERPA+LHAPDF Performance for (HL-)LHC [EB et al. 2209.00843] – Results



→ 39× speed-up for ATLAS $e^+e^- +$ jets setup

→ 43× speed-up for ATLAS $t\bar{t} +$ jets setup

Why stop here?

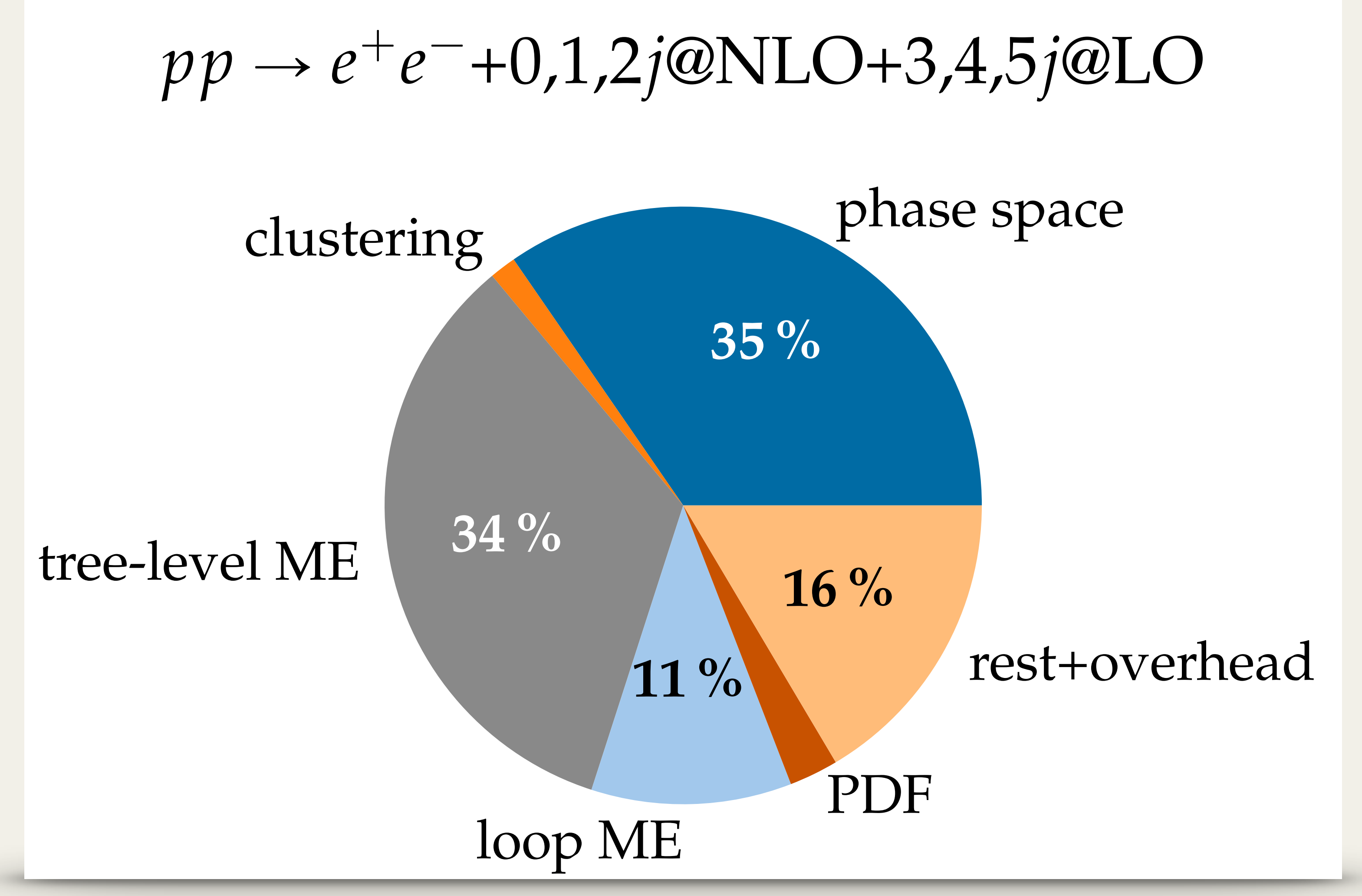
Port bottlenecks to GPU to increase physics range further

- HPC hardware increasingly heterogeneous
- other ongoing MC@GPU efforts: MadGraph5_aMC@NLO, pySecDec, MadFlow [Valassi et al. 2303.18244], [Heinrich et al. 2305.19768], [Carrazza et al. 2106.10279]; also see Olivier Mattelaer's talk (Wed)
- After tuning, tree-level ME and phase-space nearly 70 % of CPU usage
- Ongoing development from scratch of both components on CPU & GPU
  - concentrate on heavy hitters (V+jets, tt+jets)
  - pick & adapt algorithms for GPU architecture
  - new ME generator Pepper (previously BlockGen) [EB, Giele, Höche, Isaacson, Knobbe 2106.06507]
  - new phase-space generator Chili [EB et al. 2302.10449]

➡ GPU accelerated production of (unweighted) parton-level events

- Write out partonic unweighted event files (LHE-like HDF5), read-in to Sherpa (or any generator) for showering, merging and soft physics
- Bonus: reuse of expensive partonic events samples, e.g. for fast shower/hadronisation uncertainty studies etc.
- very useful for Machine Learning studies, since training can happen exclusively on GPU

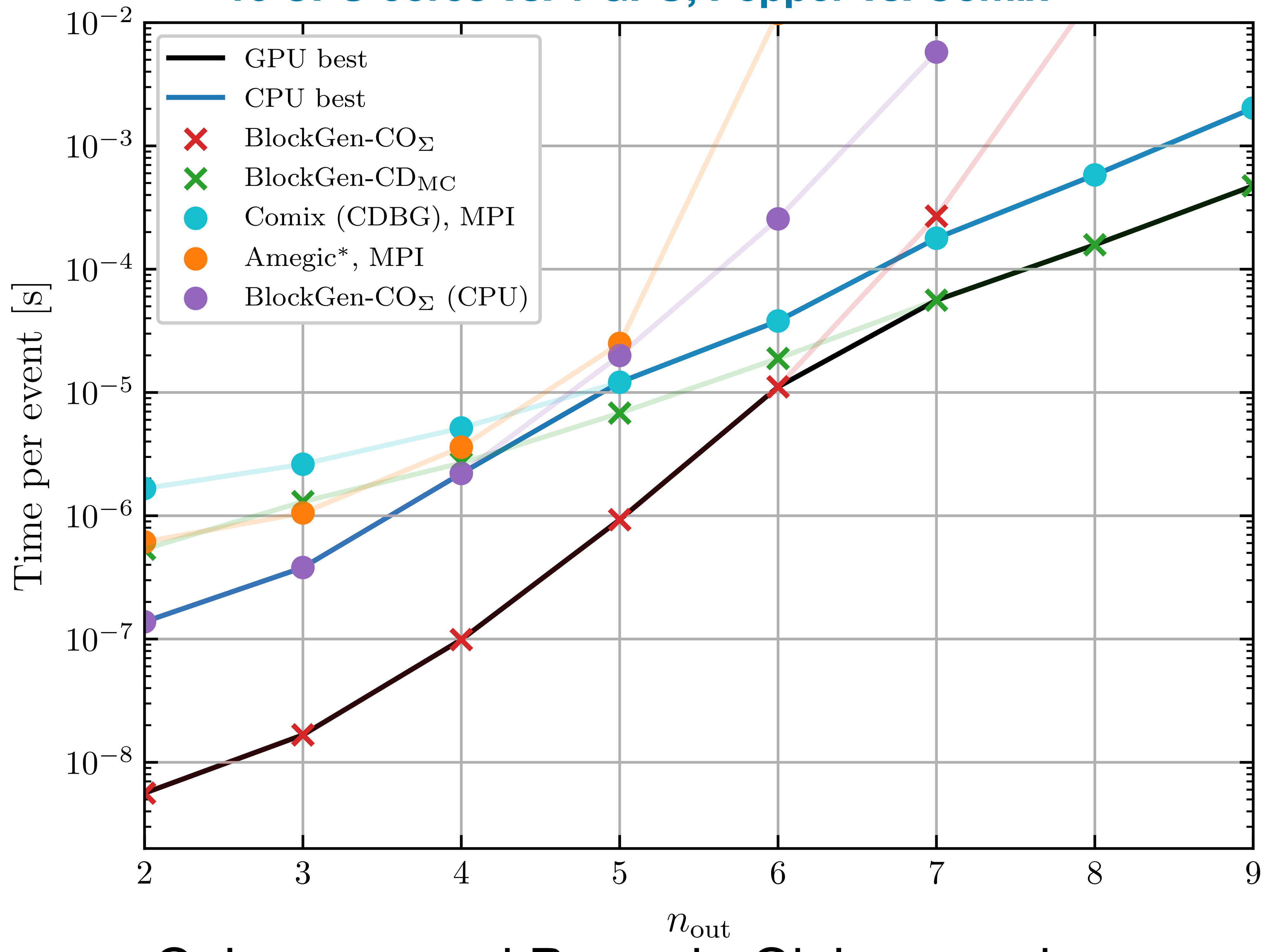
Relative CPU timing after tuning [EB et al. 2209.00843]:



Why stop here?

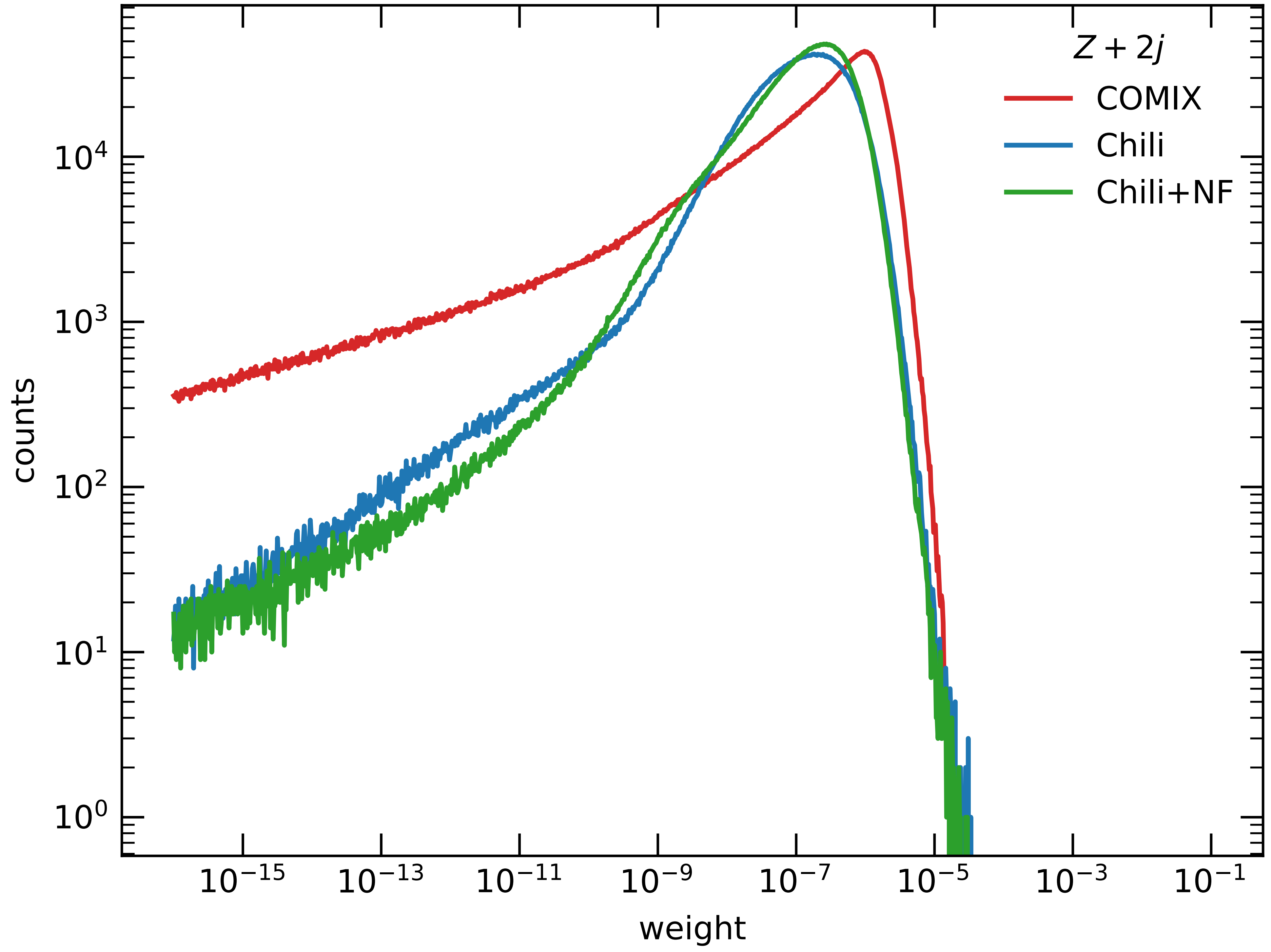
Port bottlenecks to GPU to increase physics range further

16 CPU cores vs. 1 GPU, Pepper vs. Comix



→ Color-summed Berends-Giele recursion on GPU gives best performance in relevant multiplicity range, up to 150× speed-up

Weight distribution for Chili phase-space sampling, Chili vs. Comix



→ traditional phase-space parametrisation contains many channels that are not relevant for standard LHC event samples; CHILI uses much simpler (MCFM inspired) structure while achieving comparable sampling efficiency

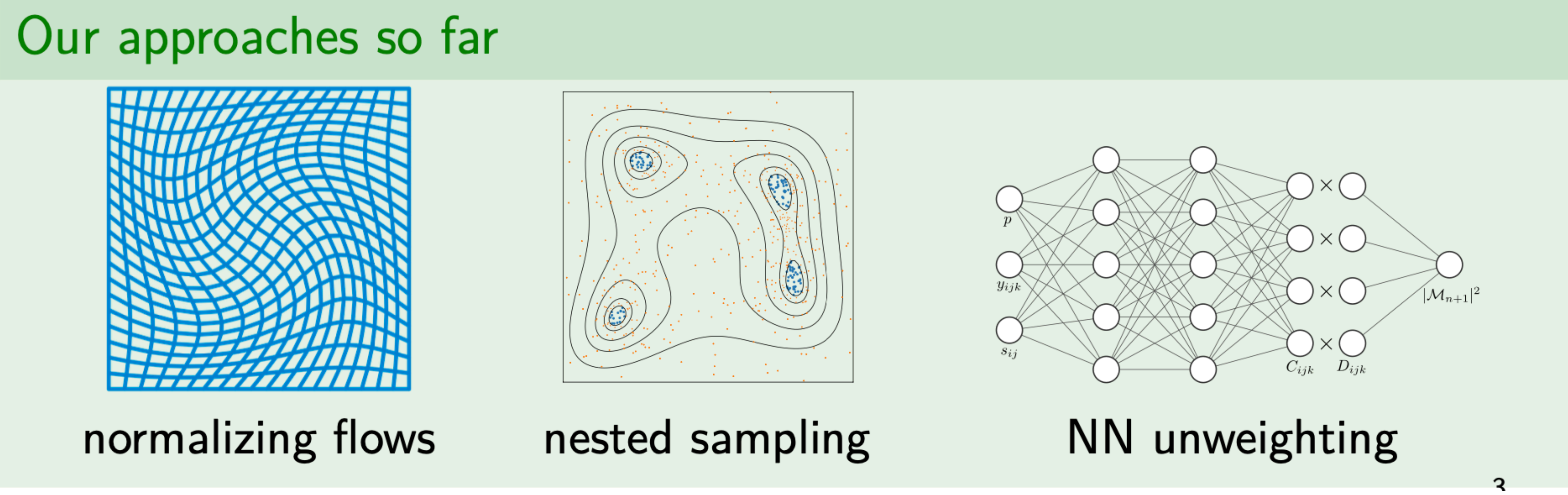
Upcoming publication of GPU-accelerated partonic event generator

Machine Learning assisted event generation

paradigm: improve efficiency, but don't compromise on accuracy

Focus on same bottlenecks: partonic matrix elements, phase-space sampling.

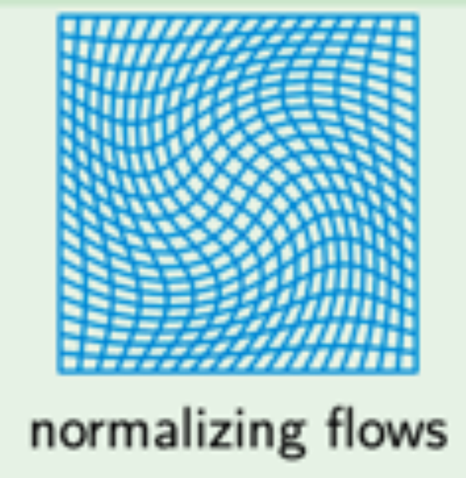
Make use of our Physics understanding.

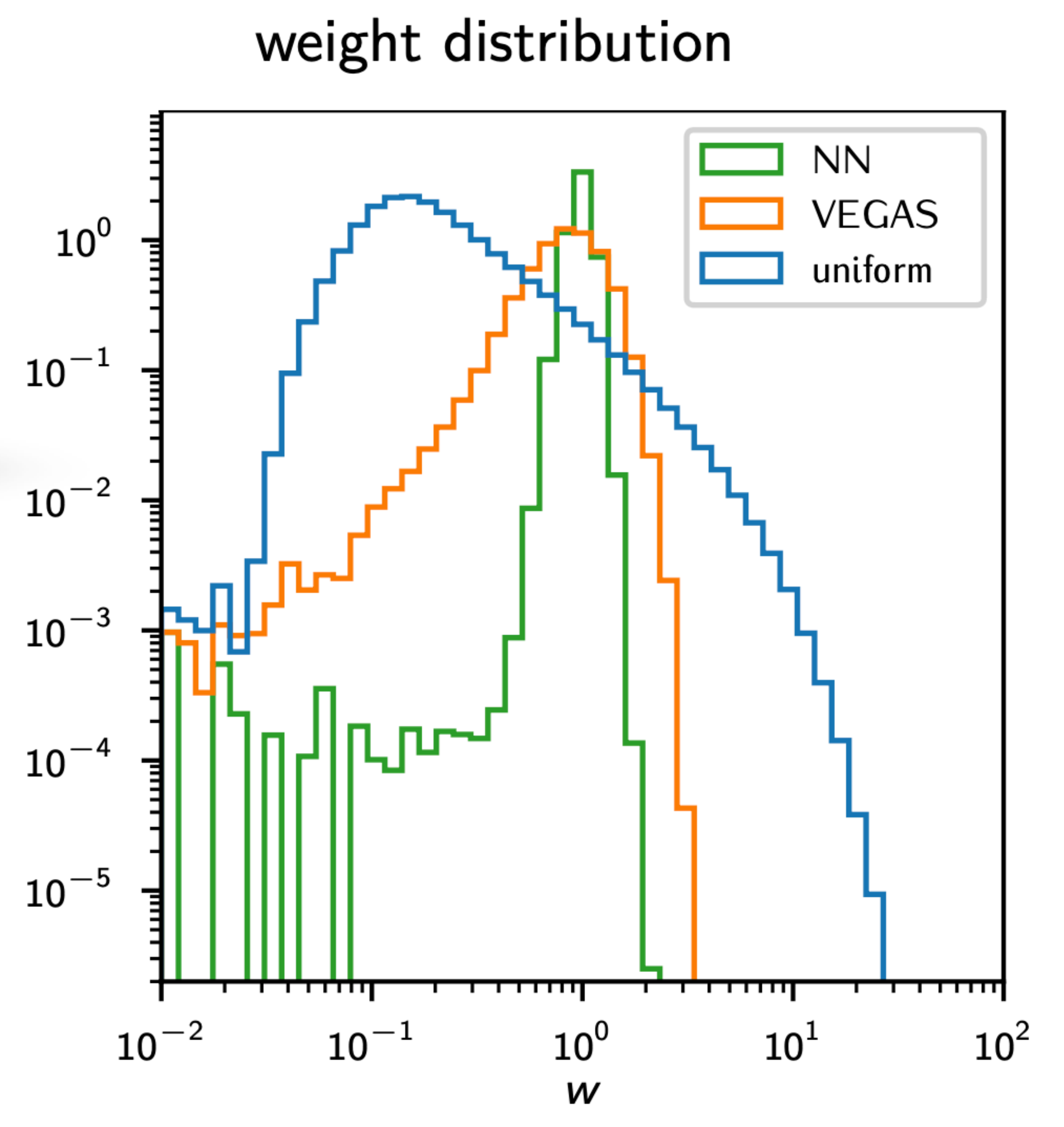


- Diffeomorphism parametrised by NN
- Drop-in replacement for VEGAS to optimise sampling

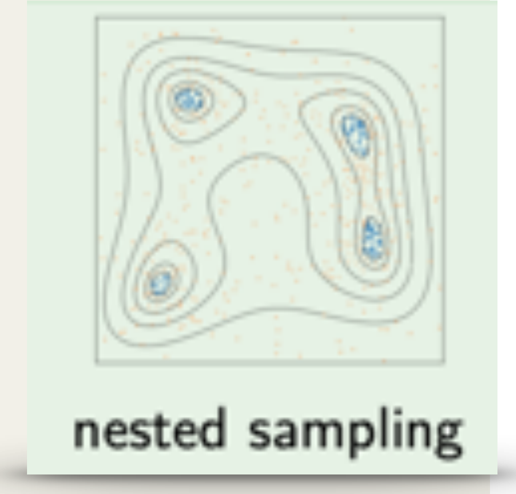
- Bayesian inference to optimise sampling
- Rich tooling available
- Short Markov chains: non-zero but low auto-correlation

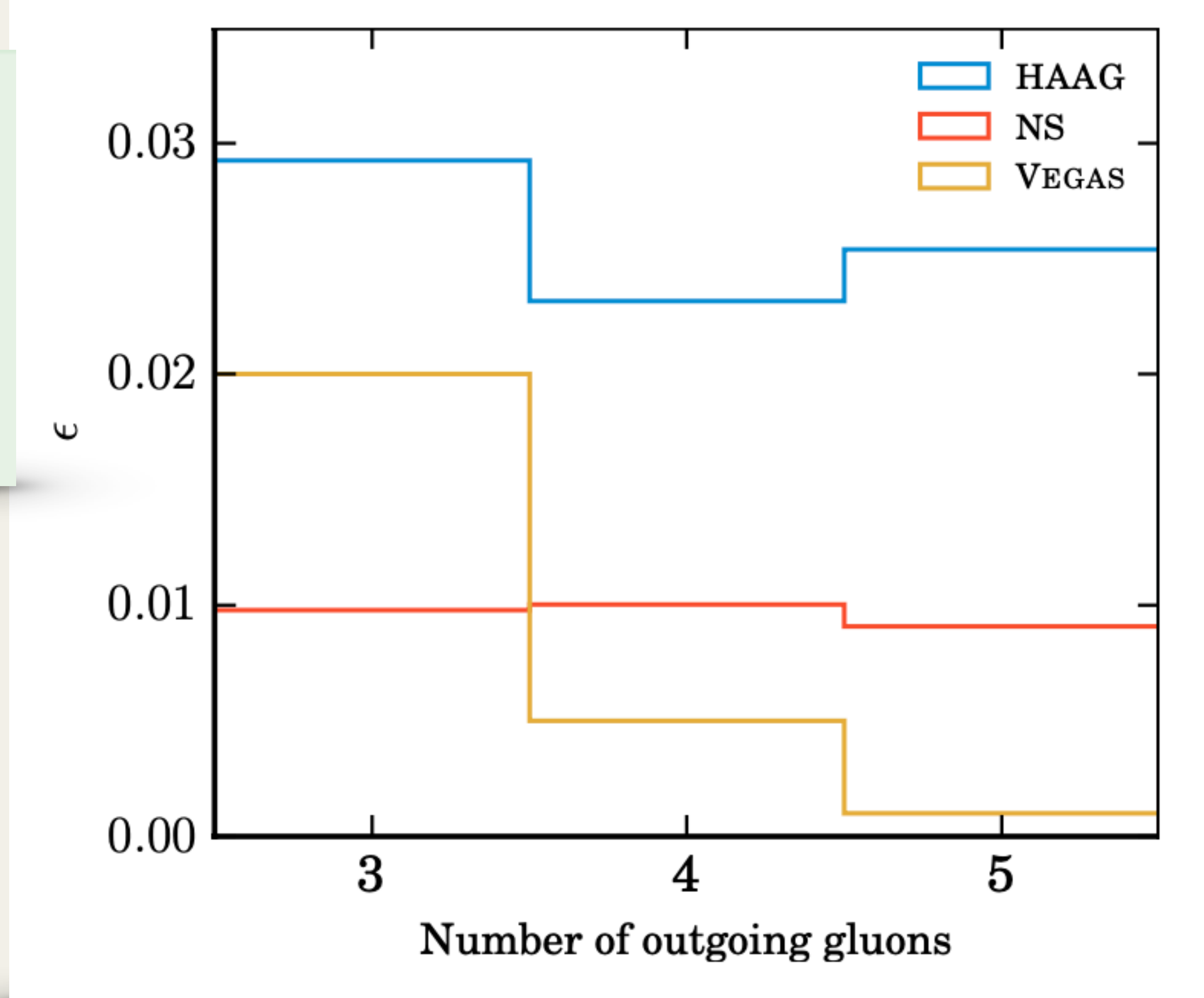
- use fast NN-based surrogate to reduce expensive ME evaluations
- recover true distribution by second unweighting step with exact ME



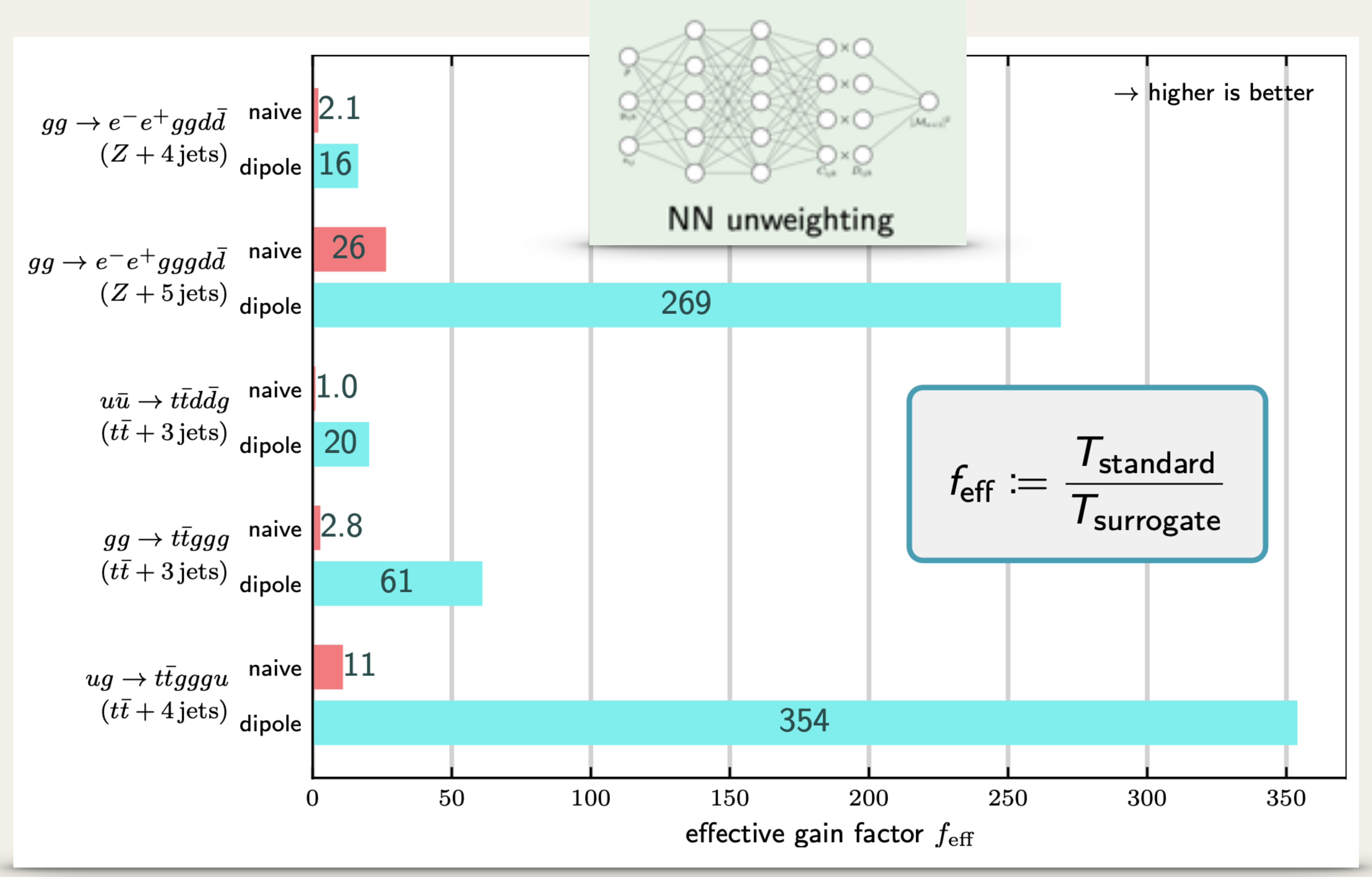


[EB, Janßen, Knobbe, Schmale, Schumann 2001.05478],
[Gao, Höche, Isaacson, Krause, Schulz 2001.10028]





[Handley, Janßen, Schumann, Yallup 2205.02030]



[Danziger, Janßen, Schumann, Siegert 2109.11964]
[Janßen, Maître, Schumann, Siegert, Truong 2301.13562]

- **Significant improvements for simple cases**
- **good scaling for sampling not yet solved/proven …**
- **… but NN unweighting offers working solution**

Status and progress of SHERPA

Efficiency

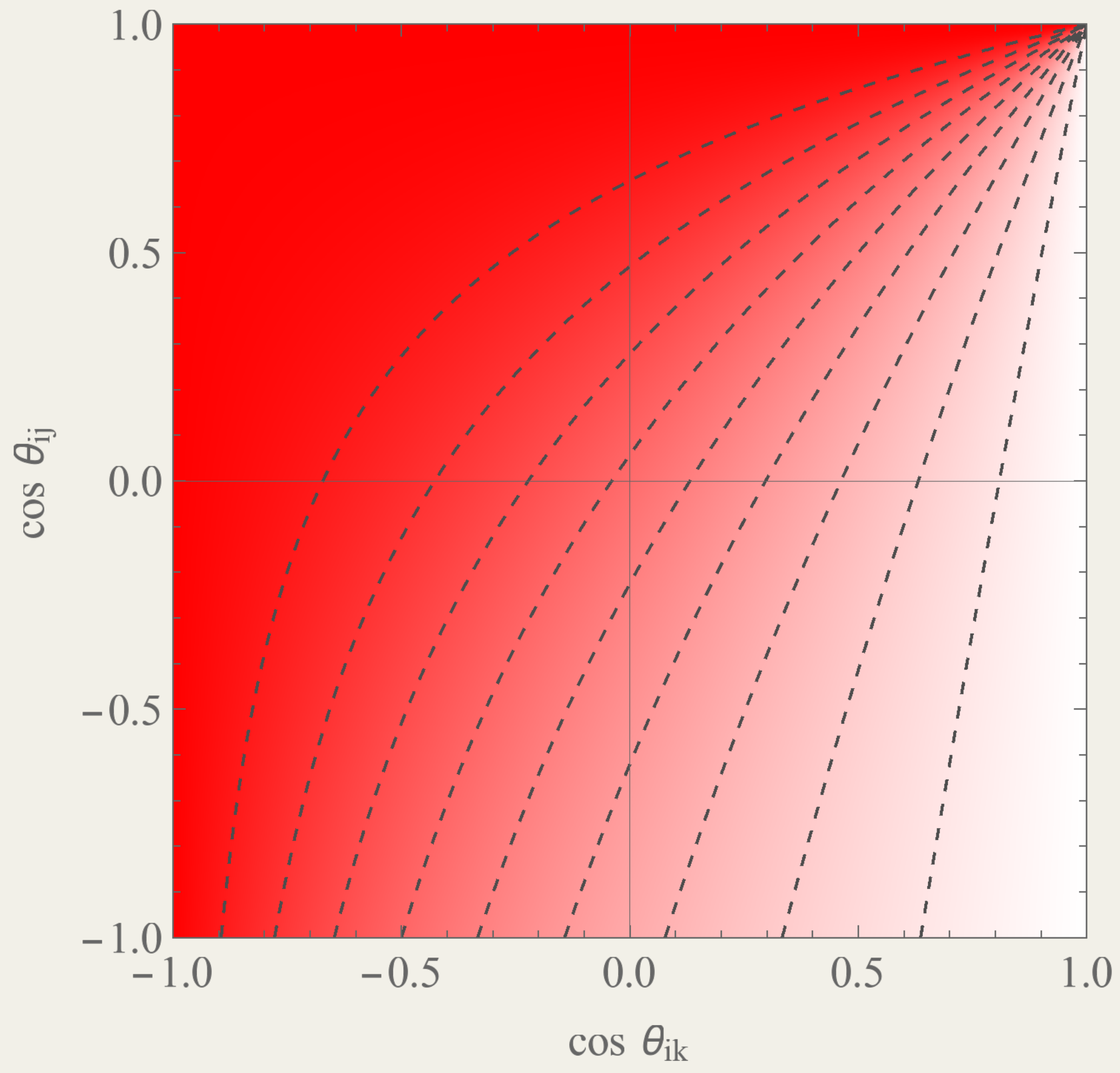
Precision

New NLL-accurate shower algorithm

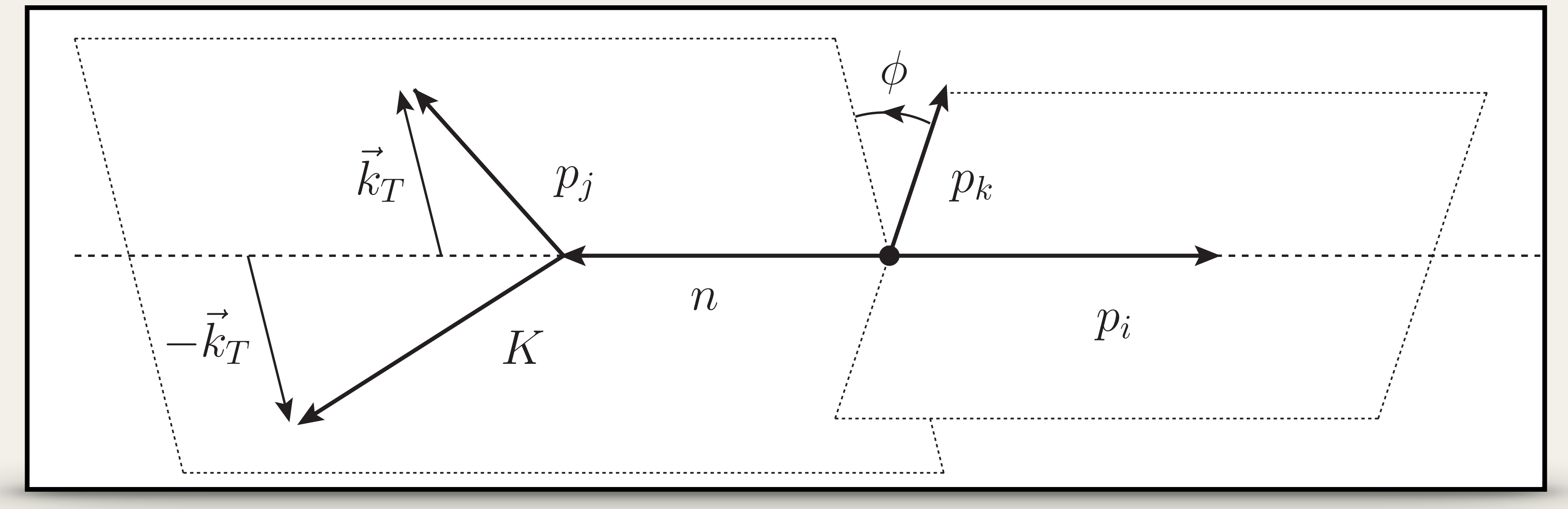
ALARIC → see D. Reichelt's talk (Wed) for details

- Framework to quantify log accuracy of parton showers established in [Dasgupta et al. 1805.09327, 2002.11114], also see Silvia Ferrario Ravasio's talk (Wed) & more refs. therein
- NLL accuracy requires that kinematics mapping of $n \to n+1$ phase space should not distort effects of pre-existing emissions on observables
  - extract NLL relevant effects by taking limit $\alpha_s \to 0$ at fixed $\lambda = \alpha_s \log v$, where v = resummed observable
  - PANSCALES developed & proven to fulfill requirements See Silvia's and Alexander Karlberg's talks (Wed) & refs. therein
  - pre-existing showers in SHERPA do not meet this requirement
- new shower ALARIC [Herren Höche Krauss Reichelt Schönherr 2208.06057]
  - partial fractioning of eikonal → positive definite splitting function with full phase space coverage inspired by Catani & Seymour's treatment of identified hadrons
    - price: dependence of splitting functions on azimuthal angle
  - global kinematics scheme enables analytic proof of NLL accuracy + numerical validation

ALARIC's positive-definite radiator function



ALARIC's emission kinematics with ϕ dependence



New NLL-accurate shower algorithm

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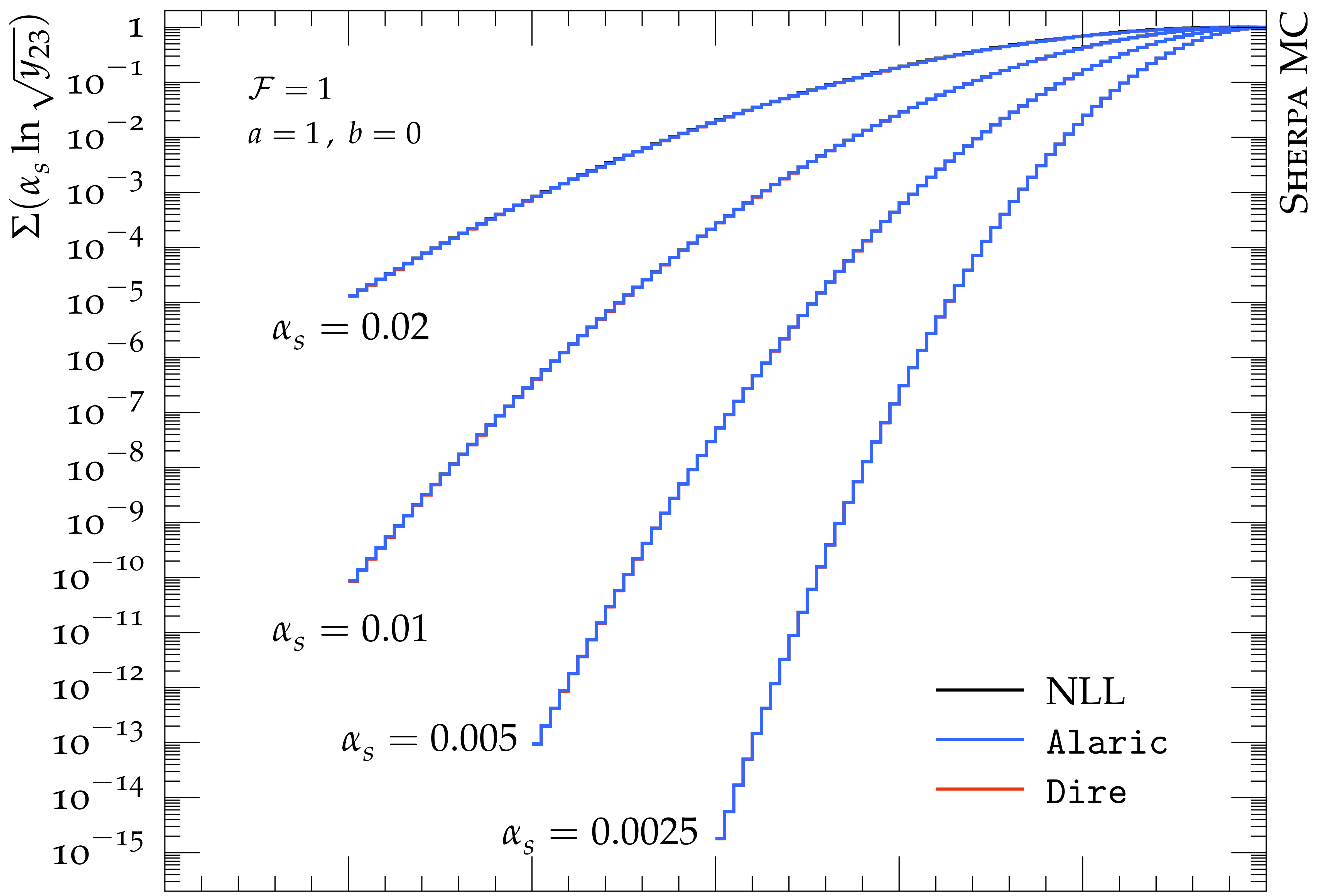
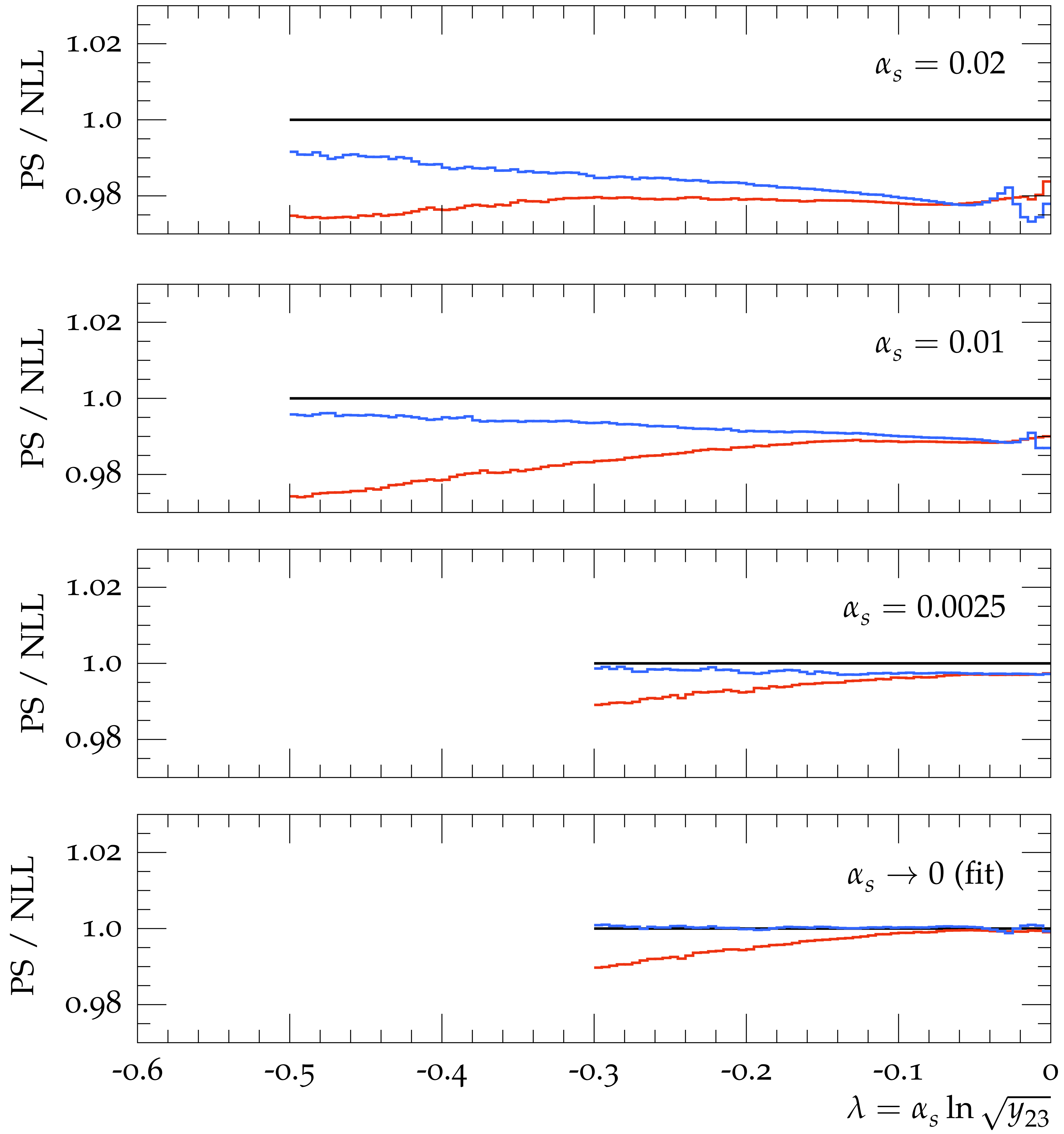
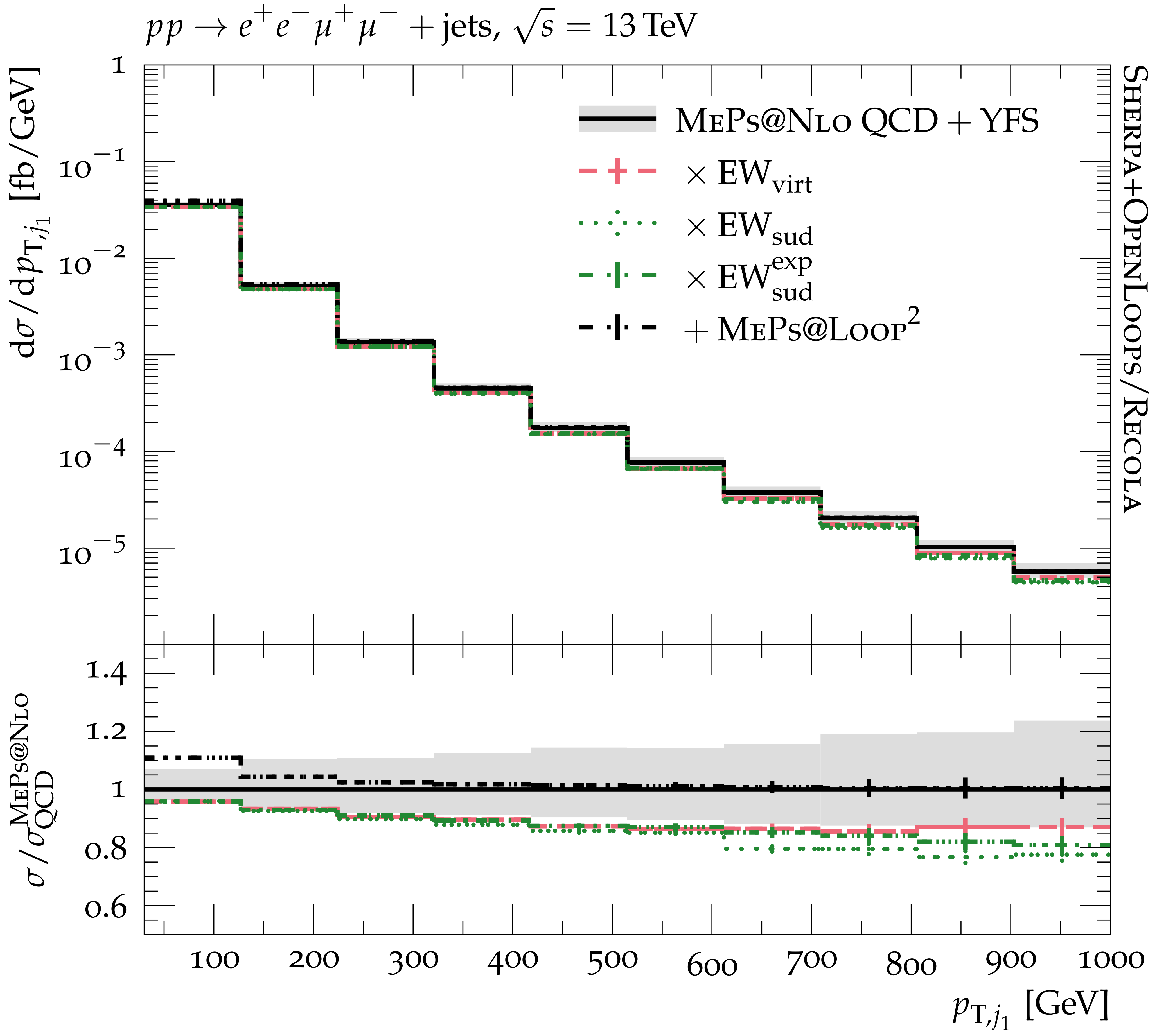




- Numerical Study taking limit $\alpha_s \to 0$ at fixed $\lambda = \alpha_s \log v$
- v = $2 \to 3$ clustering scale (Cambridge algorithm)
- DIRE has large deviations, but ALARIC flat wrt. NLL ✓

EW Sudakov logarithms

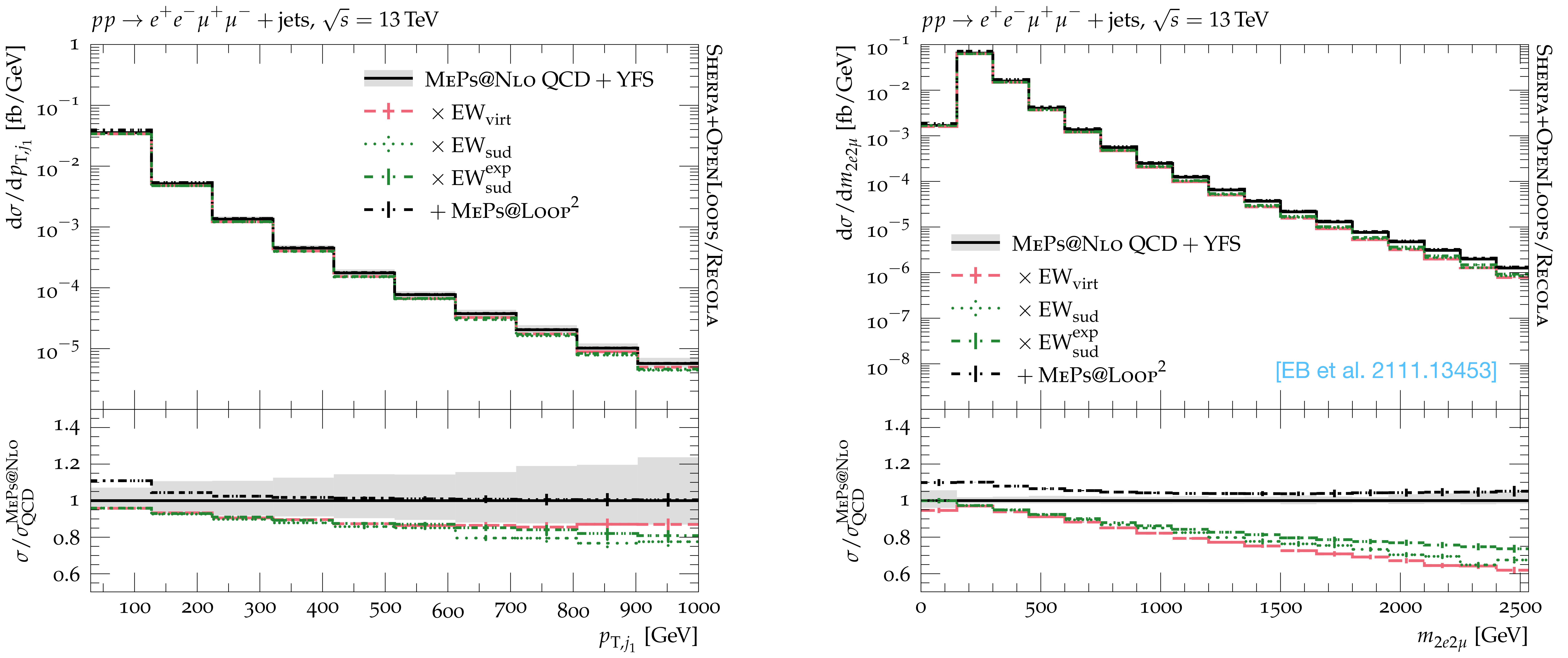
Automated implementation for all processes



- Corrections due to soft/coll. EW gauge bosons coupled to external legs in high-energy limit (e.g. $p_T \gtrsim 1$ TeV → $\mathcal{O}(10\,\%)$ corrections)
- Corrections worked out in full generality [Denner, Pozzorini (2001) hep-ph/0010201]
- partial implementation in AlpGen [Chiesa et al 1305.6837]
- In Sherpa fully automated as universal ME-level corrections [EB, Napoletano 2006.14635]
- Applied to MEPS@NLO diboson production $pp \to 0,1j@\text{NLO} + 2,3j@\text{LO}$ [EB et al. 2111.13453]
  - EW$_{virt}$ for $\mathcal{S}$ events, EW$_{sud}$ for $\mathcal{H}$ and LO events
  - YFS resummation for QED FSR

EW Sudakov logarithms

Automated implementation for all processes

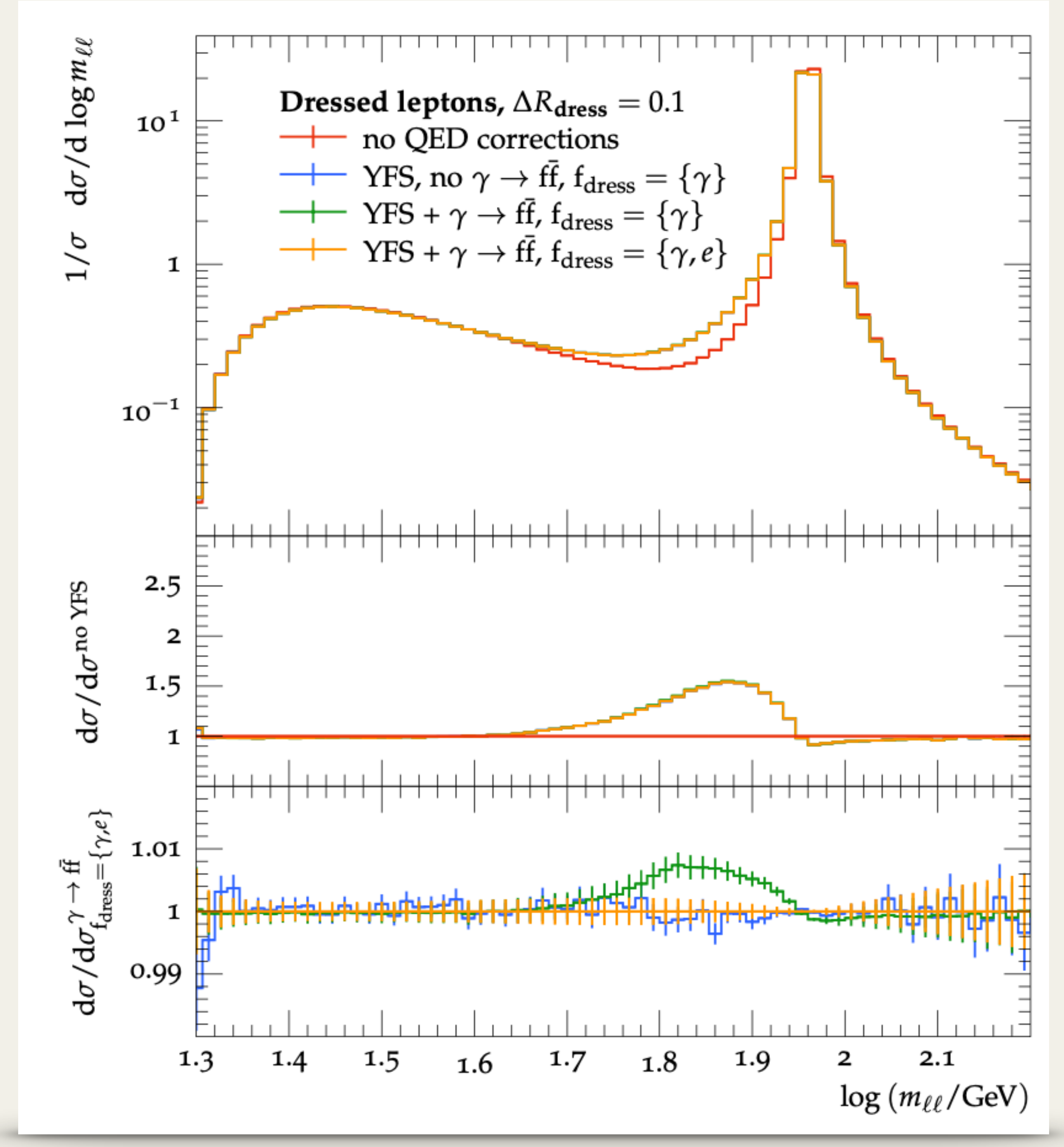


(Approximate) EW corrections outside of MEPS@NLO QCD uncertainty band

Resumming soft photons with YFS

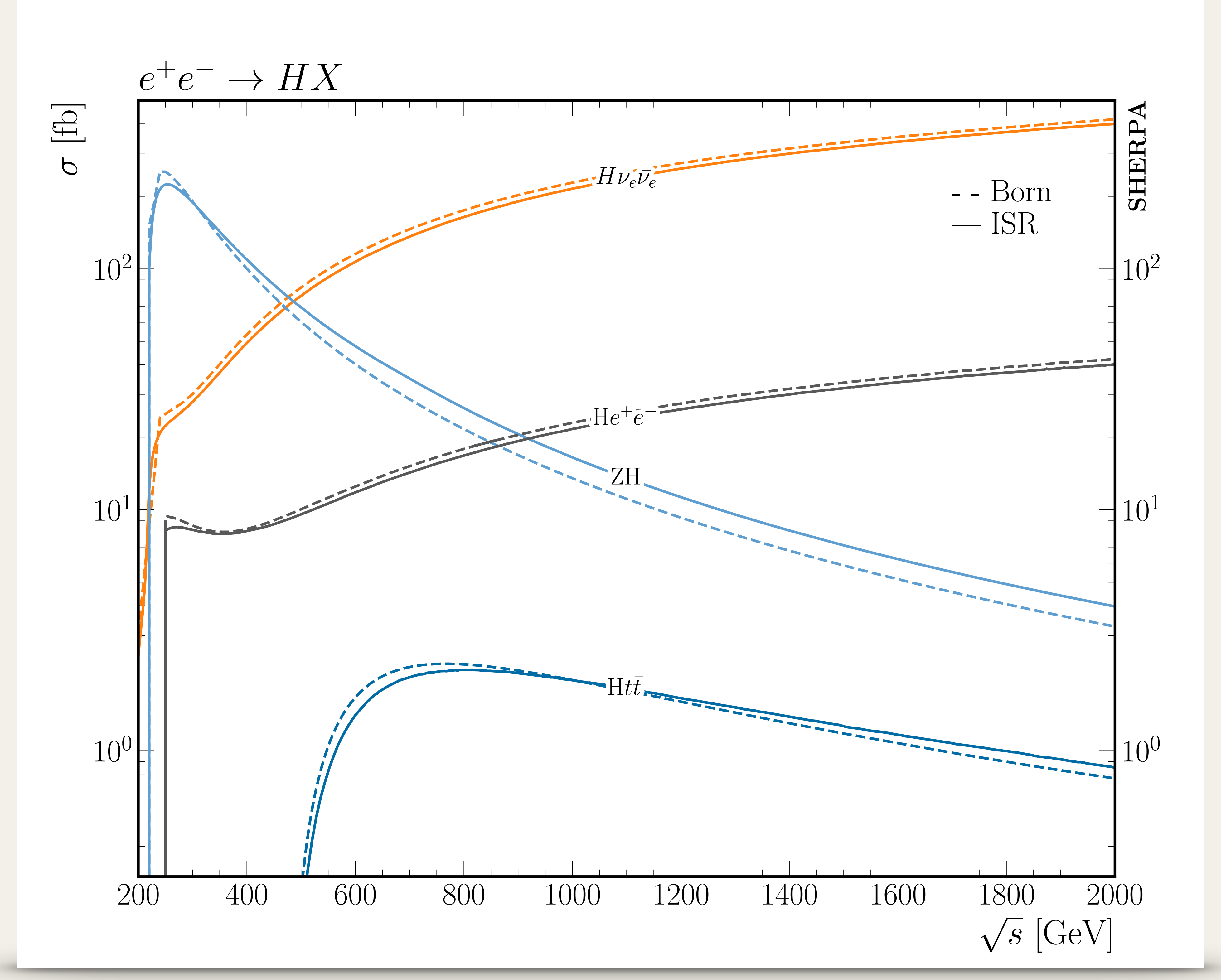
Recent developments in SHERPA

- photon splitting $\gamma \to e^+e^-$ [Flower, Schönherr 2210.07007]
- Example: Dilepton invariant mass for $pp \to e^+e^-$:



Corrections up to 1 %, can be reigned in by refined dressing algorithm

- YFS in ISR for future lepton colliders [Krauss, Price, Schönherr 2203.10948]
- Application to Higgsstrahlung processes at lepton collider:



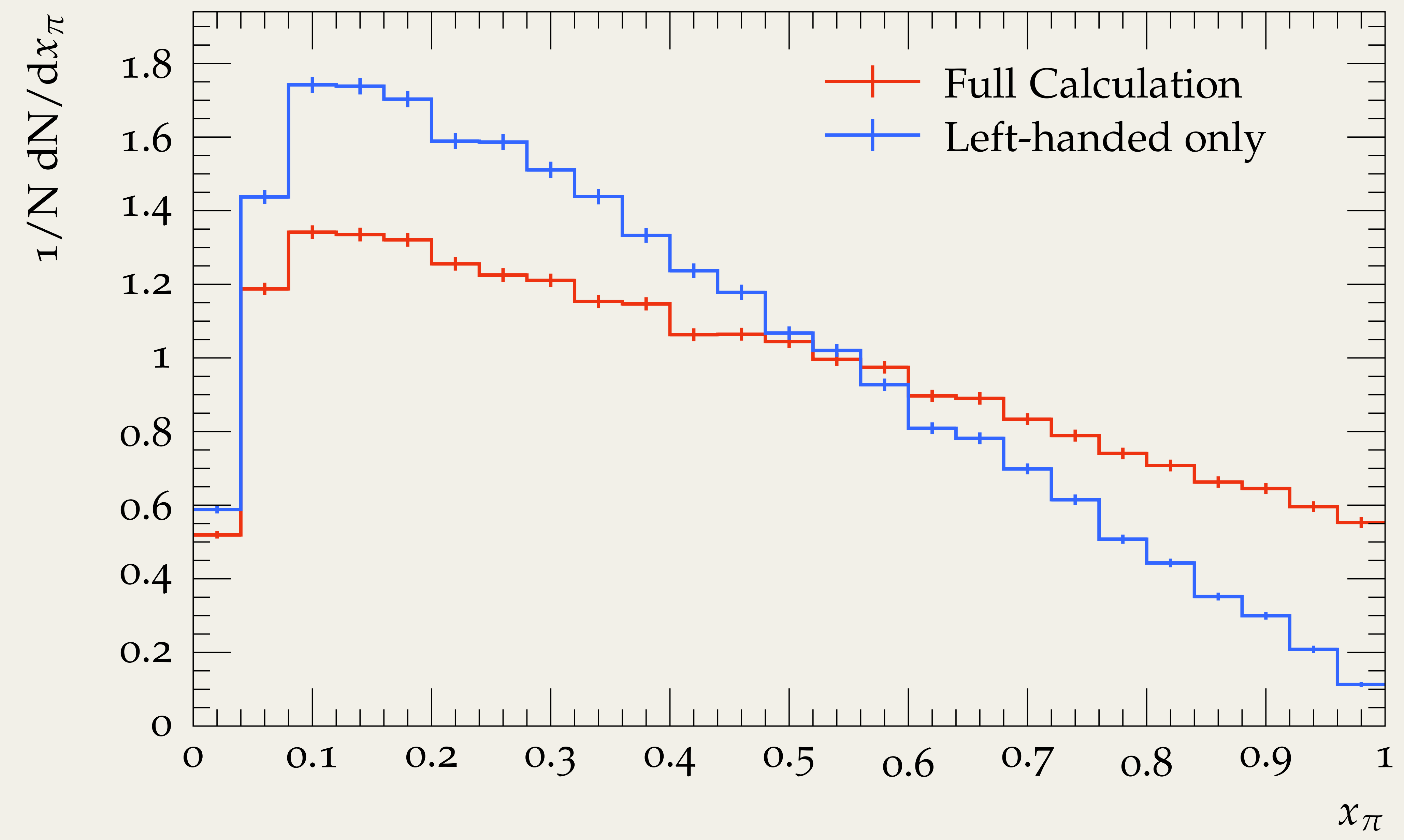
Process-independent implementation of YSF for ISR

Neutrino physics

ACHILLES + SHERPA

- ACHILLES is a newly developed neutrino event generator
  [Höche, Isaacson, Lopez Gutierrez, Rocco 2110.15319]
- paradigm: transfer LHC expertise+tooling in neutrino physics, developed in close collaboration with SHERPA
  - ACHILLES for nuclear physics effects
  - SHERPA's COMIX for calculating leptonic currents, incl. BSM effects via Comix' UFO interface
  - study of ν_τ needs control over angular distribution of τ-lepton decay products
    - use interface to SHERPA for decays, incl. spin correlations across production and decays, QED showers [Isaacson, Höche, Siegert, Wang 2303.08104]
- other use as a module: GENEVA + SHERPA as a shower in HH production [Alioli et al. 2212.10489]
  Also see Alessandro Broggio's talk (Wed)

Momentum fraction for tau decay to single pion folded over DUNE's far-detector flux



→ improved description over conventional fully left-handed assumption of other neutrino generators

BSM physics

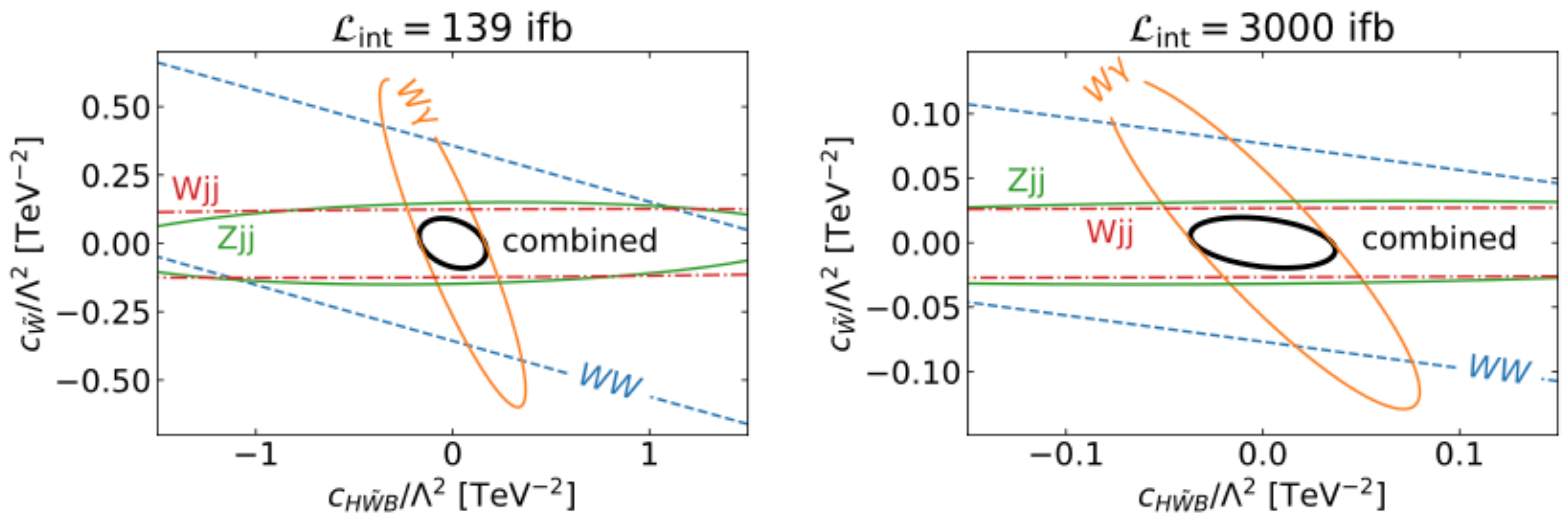
via UFO interface [Höche, Kuttimalai, Schumann, Siegert 1412.6478]

- full support for UFO model [Degrande et al. CPC183(2012)1201]
- UFO2 ongoing [Darmé et al. 2304.09883]
- Lorentz and colour structures built fully automatically
- automatic inclusion in hard decay module
  - identification of all $1\to2$ and $1\to3$ decay channels and calculation of LO widths
  - can select individual channels
  - spin correlations using spin density matrices [Richardson JHEP11(2201)029, Knowles CPC58(1990)271]

BSM physics

Calculating AGC limits using Sherpa+UFO [Bieközter, Gregg, Krauss, Schönherr 2102.01115]

- LO multi-leg with SMEFT model defined via UFO
- use public ATLAS and CMS SM measurements to constrain SMEFT parameters



Conclusions

Status and progress of SHERPA

Conclusions

- **Efficiency improvements** (= increase physics range)
  - tuning exercise → factor-40 speed-up for heavy hitter ATLAS setups
  - porting bottlenecks to GPU → PEPPER+CHILI, interfaced with Sherpa via HDF5
  - ML assisted event generation → NF, Nested Sampling, NN unweighting
- **Precision physics**
  - new NLL-accurate shower ALARIC
  - Fully automated $\mathrm{EW}_{\mathrm{sud}}$ logarithms: application to ZZ production
  - YFS developments: $\gamma \to e^+e^-$ splittings and ISR
  - Neutrino physics via ACHILLES+SHERPA
  - BSM physics via UFO

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  } **FO calculations**

- **Precision physics**
  - new NLL-accurate shower ALARIC
  - Fully automated EW_{sud} logarithms: application to ZZ production
  - YFS developments: $\gamma \to e^+e^-$ splittings and ISR

  } **Log accuracy**

  - Neutrino physics via ACHILLES+SHERPA
  - BSM physics via UFO

Status and progress of SHERPA

Backup

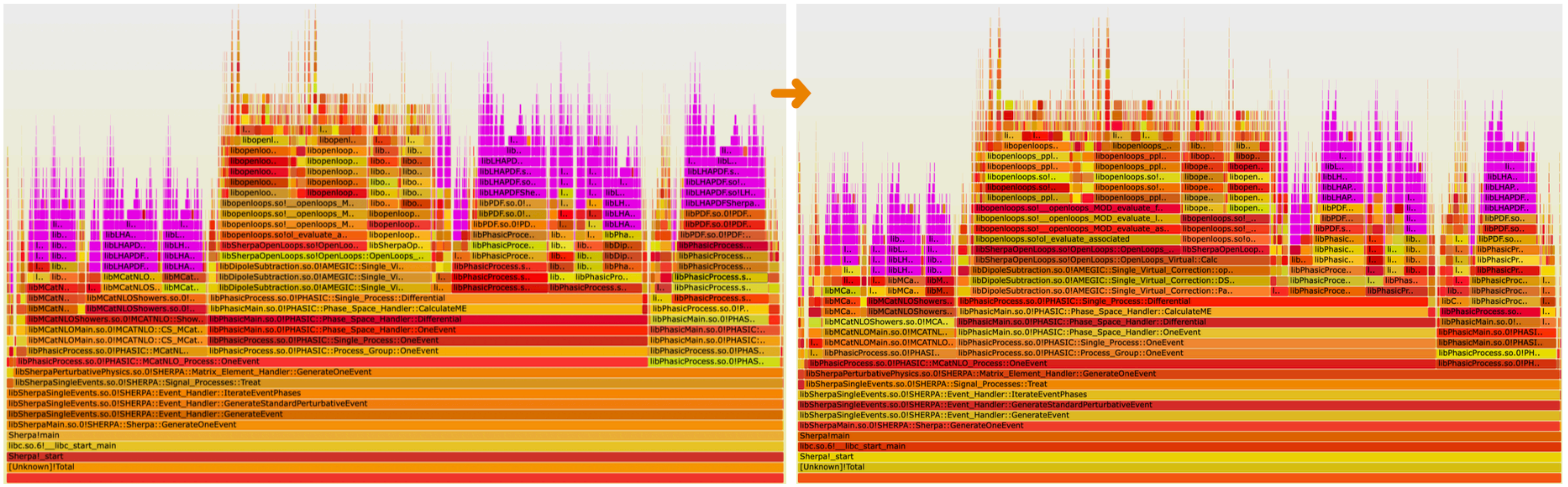
SHERPA+LHADPF Performance for (HL-)LHC

Overall profiling and tuning [EB et al. 2209.00843]

LHAPDF 6.2.3 → 6.4.0

- PDF grid caching for given (x, Q^2) point
  - repeated calls for different flavours / replicas benefit
  - caller side might need to reorder calls to benefit
- Use same interpolation grid structure across flavours
- Cache universal terms of polynomial interpolation
- up to 3x faster for single flavour, ~10x for all flavours

Sherpa flamegraph for ATLAS V+jets setup before/after LHAPDF 6.4.0

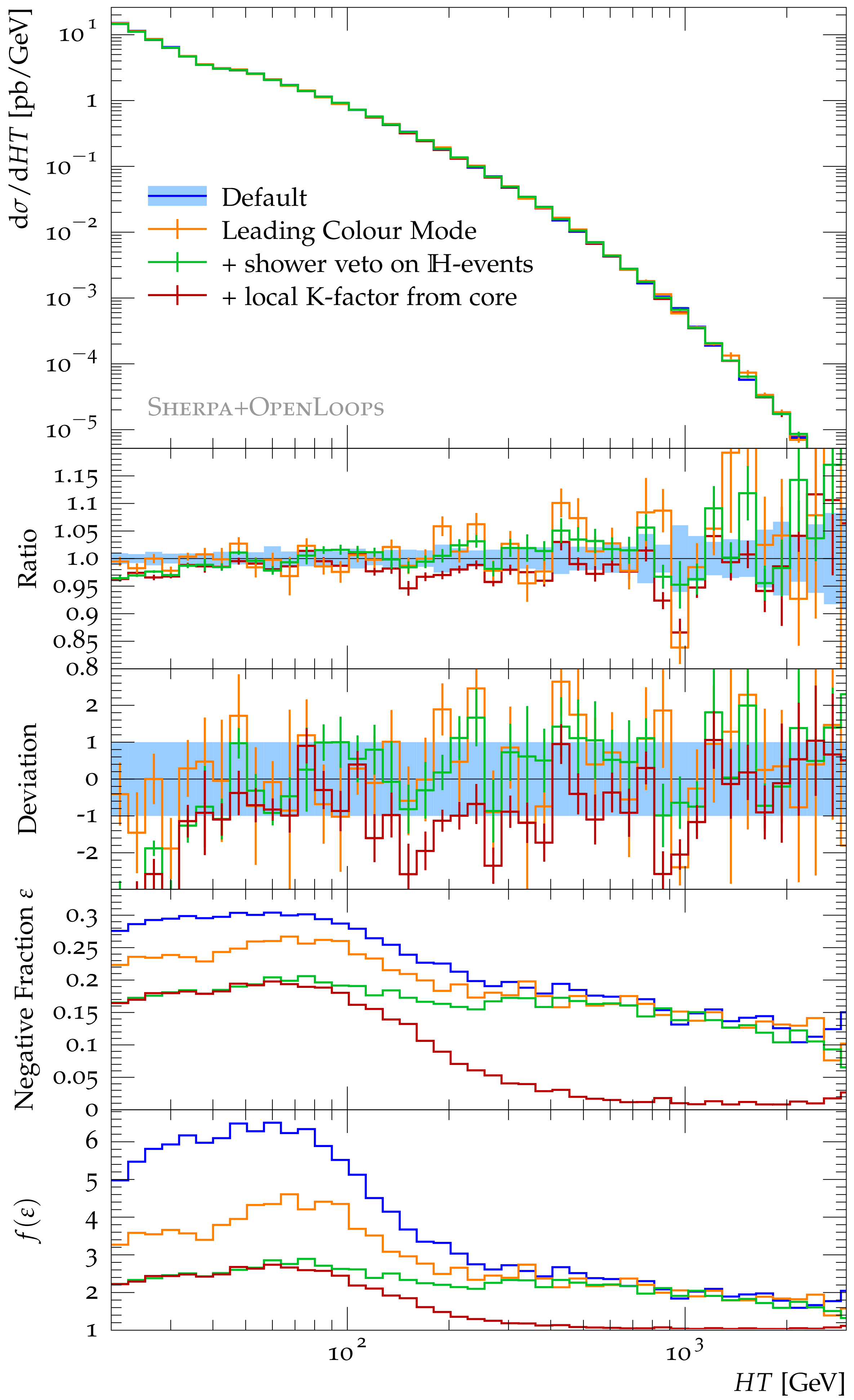


[Andy Buckley, Max Knobbe]

Negative weight fractions

Danziger, Höche, Siegert, arXiv:2110.15211, ATLAS arXiv:2112.09588

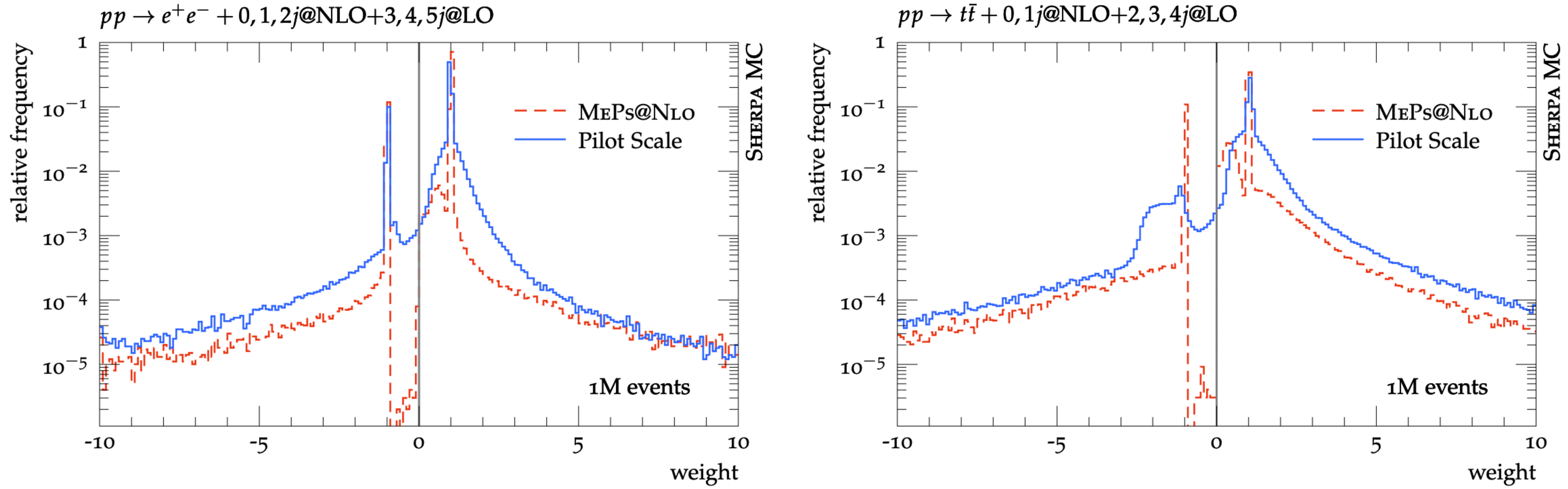
- explored three methods to improve the neg. weight fraction in SHERPA
  1) reduce matching accuracy to leading colour, neglect spin-correlations
  2) include jet veto on $\mathbb{H}$-events, as originally formulated in arXiv:2012.5030
  3) use local K-factor in NLO→LO merging from core configuration instead of highest multiplicity
- public since SHERPA-2.2.8 (Sep '19)



SHERPA+LHADPF Performance for (HL-)LHC

Overall profiling and tuning [EB et al. 2209.00843]

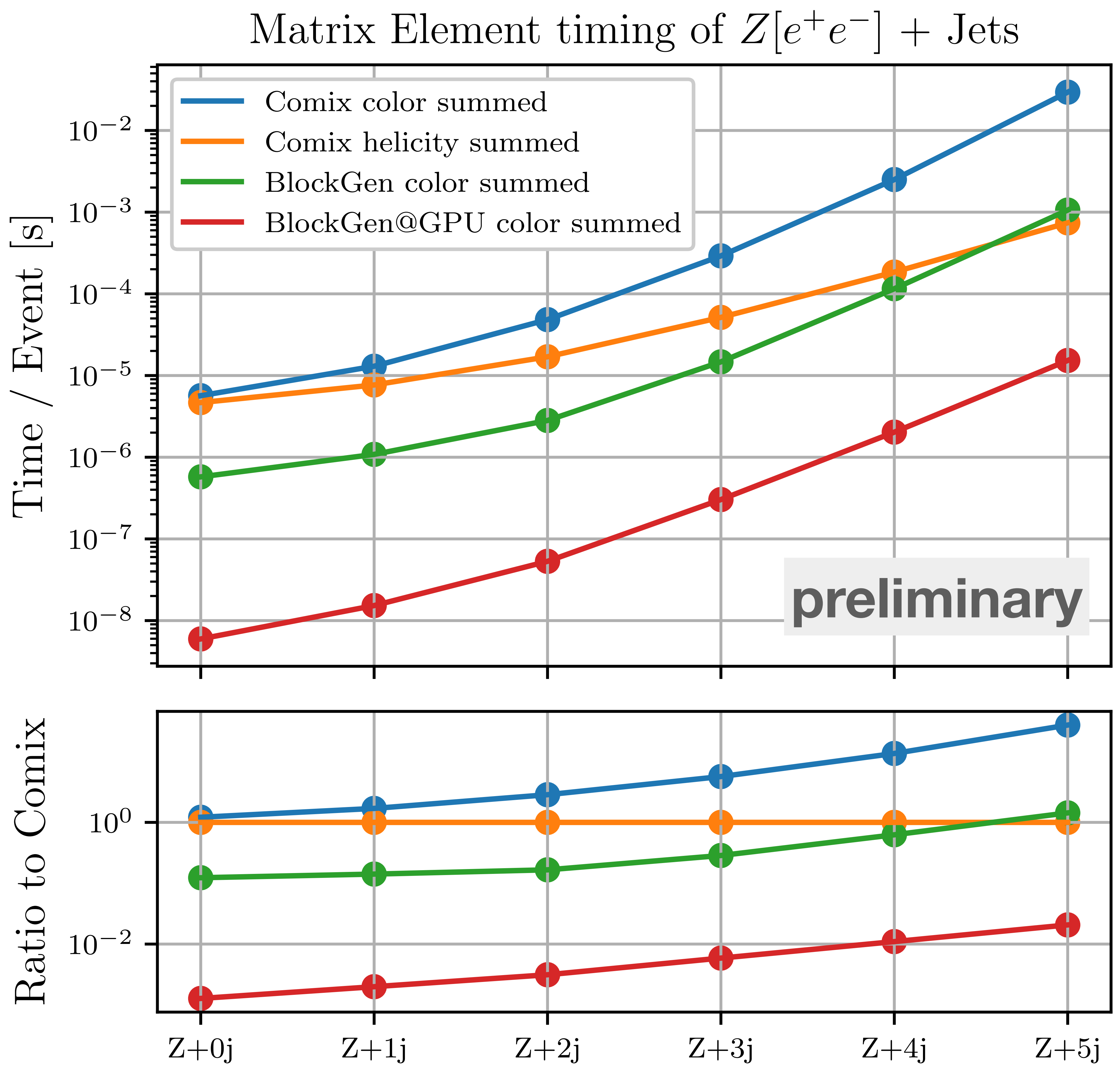
weight distribution broadening due to the use of a Pilot scale



- effective reduction in efficiency from using the pilot scale typically $\lesssim 2$
- computing time reduction reduced by this, but in most cases still beneficial

Port bottlenecks to GPU

PEPPER vs. COMIX runtime per partonic event



Port bottlenecks to GPU

CHILI vs. COMIX runtime for given accuracy target

Process / MC accu	Default PS Time	Default PS # pts	New PS Time	New PS # pts
W+1j / 1‰	4m 52s	10.3M	2m 32s	3.10M
W+2j / 3‰	17m 12s	5.52M	13m 52s	2.53M
W+3j / 1%	46m 24s	7.48M	20m 16s	1.15M
H+1j / 1‰	2m 20s	1.83M	1m 36s	1.50M
H+2j / 3‰	4m 36s	2.32M	4m 4s	0.71M
H+3j / 1%	18m 12s	2.32M	12m 56s	0.63M

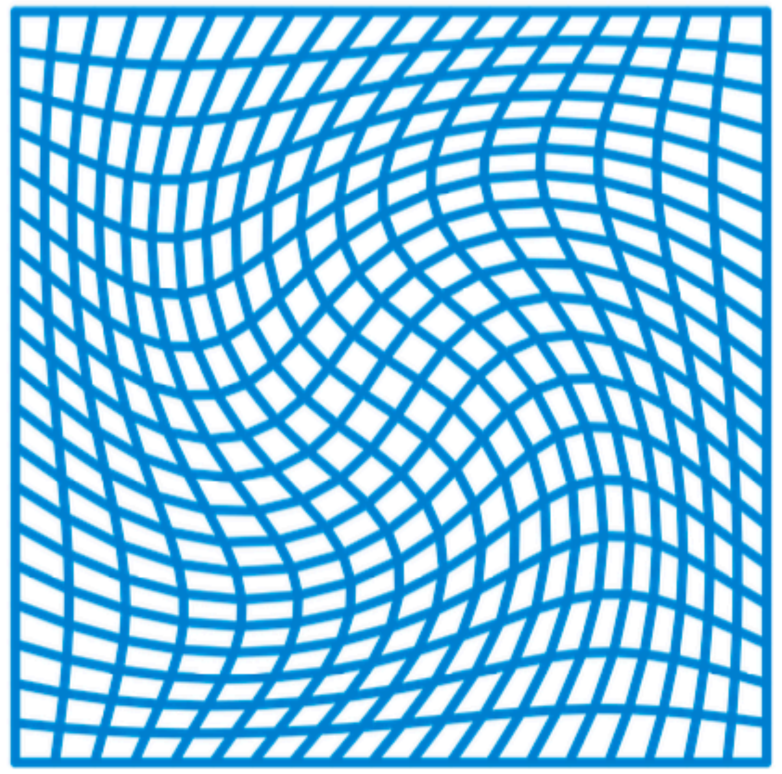
Process / MC accu	Default PS Time	Default PS # pts	New PS Time	New PS # pts
$t\bar{t}$+0j / 1‰	4m 38s	3.15M	4m 0s	3.59M
$t\bar{t}$+1j / 3‰	3m 12s	1.38M	3m 4s	1.47M
$t\bar{t}$+2j / 1%	11m 58s	1.47M	11m 20s	0.89M
2j / 1‰	12m 48s	2.98M	7m 44s	1.80M
3j / 3‰	22m 48s	6.80M	23m 12s	2.39M
4j / 1%	1h 25m	6.95M	50m 24s	0.91M

[EB et al. 2302.10449]

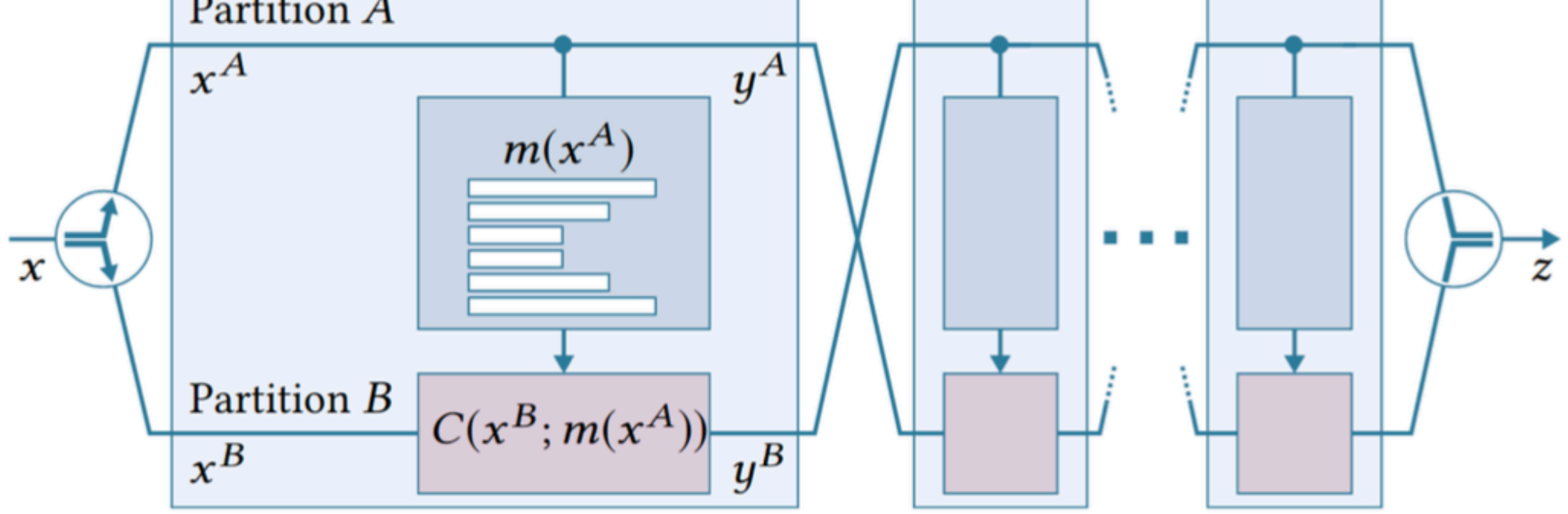
Normalizing Flows

Slide by Timo Janßen

- diffeomorphism parameterized by NNs
- layered mapping: $h = h_L \circ \cdots \circ h_2 \circ h_1$
- each coupling layer transforms part of input
- triangular Jacobian $\rightsquigarrow$ determinant costs $\mathcal{O}(d)$
- replacement for VEGAS



©wikimedia.org File:Diffeomorphism of a square.svg



Müller et al.: SIGGRAPH 2019

Normalizing Flows

Gain factors for V + n jets [Gao et al. 2001.10028]

unweighting efficiency $\langle w \rangle / w_{\max}$		LO QCD $n=0$	LO QCD $n=1$	LO QCD $n=2$	LO QCD $n=3$	LO QCD $n=4$	NLO QCD (RS) $n=0$	NLO QCD (RS) $n=1$
$W^+ + n$ jets	Sherpa	$2.8 \cdot 10^{-1}$	$3.8 \cdot 10^{-2}$	$7.5 \cdot 10^{-3}$	$1.5 \cdot 10^{-3}$	$8.3 \cdot 10^{-4}$	$9.5 \cdot 10^{-2}$	$4.5 \cdot 10^{-3}$
	NN+NF	$6.1 \cdot 10^{-1}$	$1.2 \cdot 10^{-1}$	$1.0 \cdot 10^{-2}$	$1.8 \cdot 10^{-3}$	$8.9 \cdot 10^{-4}$	$1.6 \cdot 10^{-1}$	$4.1 \cdot 10^{-3}$
	Gain	2.2	3.3	1.4	1.2	1.1	1.6	0.91
$W^- + n$ jets	Sherpa	$2.9 \cdot 10^{-1}$	$4.0 \cdot 10^{-2}$	$7.7 \cdot 10^{-3}$	$2.0 \cdot 10^{-3}$	$9.7 \cdot 10^{-4}$	$1.0 \cdot 10^{-1}$	$4.5 \cdot 10^{-3}$
	NN+NF	$7.0 \cdot 10^{-1}$	$1.5 \cdot 10^{-1}$	$1.1 \cdot 10^{-2}$	$2.2 \cdot 10^{-3}$	$7.9 \cdot 10^{-4}$	$1.5 \cdot 10^{-1}$	$4.2 \cdot 10^{-3}$
	Gain	2.4	3.3	1.4	1.1	0.82	1.5	0.91
$Z + n$ jets	Sherpa	$3.1 \cdot 10^{-1}$	$3.6 \cdot 10^{-2}$	$1.5 \cdot 10^{-2}$	$4.7 \cdot 10^{-3}$		$1.2 \cdot 10^{-1}$	$5.3 \cdot 10^{-3}$
	NN+NF	$3.8 \cdot 10^{-1}$	$1.0 \cdot 10^{-1}$	$1.4 \cdot 10^{-2}$	$2.4 \cdot 10^{-3}$		$1.8 \cdot 10^{-3}$	$5.7 \cdot 10^{-3}$
	Gain	1.2	2.9	0.91	0.51		1.5	1.1

Nested Sampling

Slide by Timo Janßen

Nested Sampling

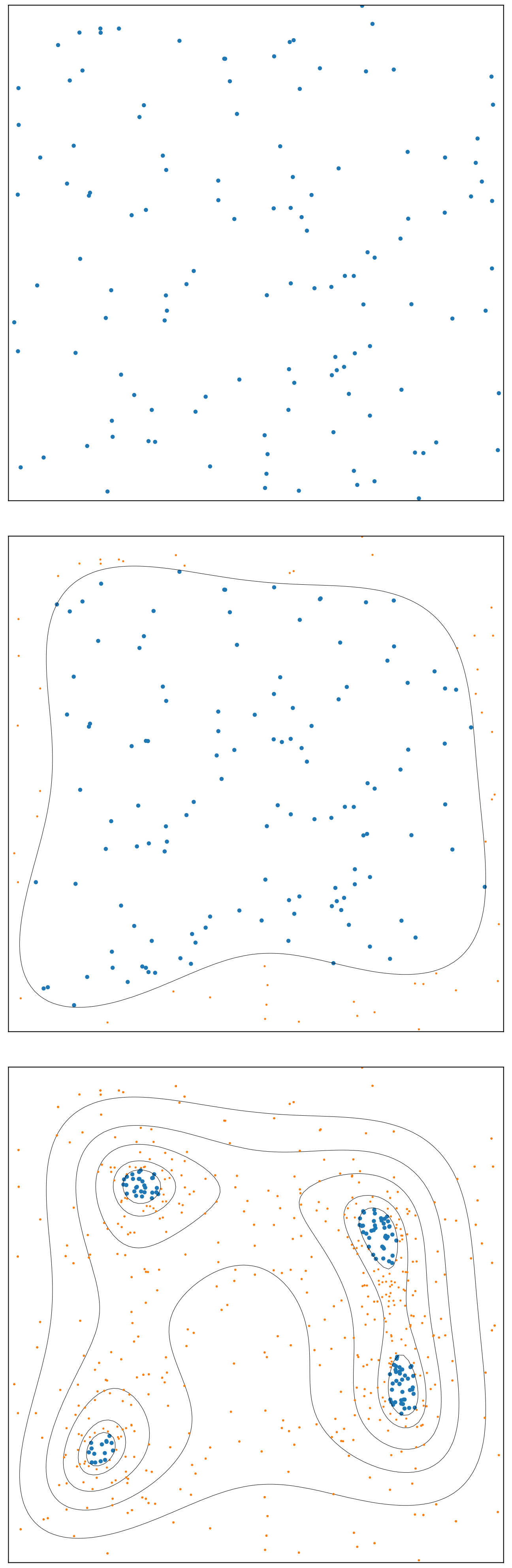
Meta algorithm

- draw ensemble of live points (uniformly)
- sort in order of likelihood, $\mathcal{L}$
- replace $\mathcal{L}_{\text{min}}$ by sampling uniformly, requiring $\mathcal{L} > \mathcal{L}_{\text{min}}$
- repeat until termination criterion reached
- dead points form representative sample of target distribution

Implementation

- PolyChord (Handley et al., 2015)
- use slice sampling (R. Neal, 2003) to evolve live points

$\rightarrow$ many short Markov chains $\rightsquigarrow$ low autocorrelation



J. Skilling: AIP Conference Proceedings **735**, 395 (2004)

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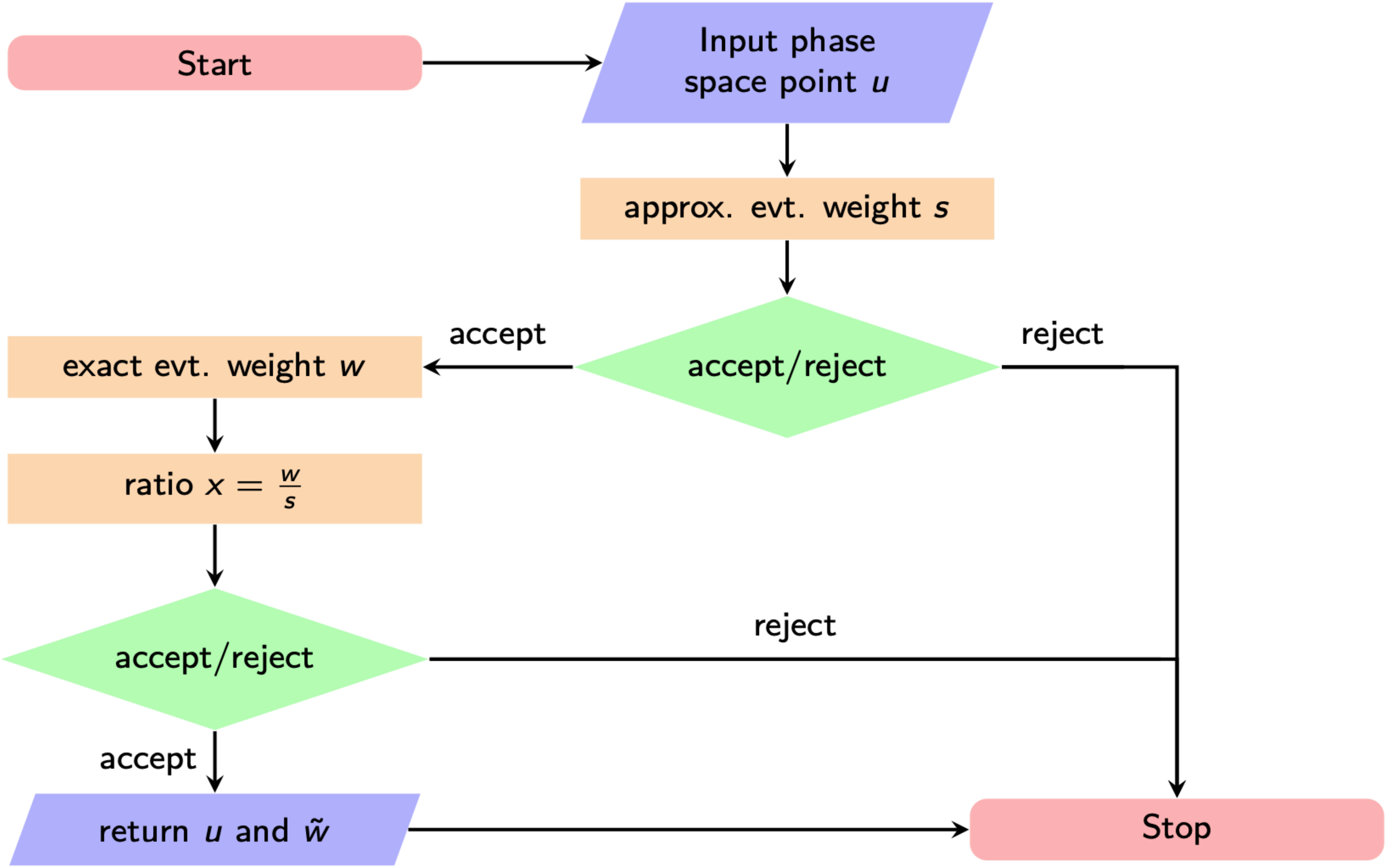
Surrogate unweighting

Algorithm [K. Danziger, TJ, S. Schumann, F. Siegert: SciPost Phys. 12, 164 (2022)]



Surrogate unweighting

Slide by Timo Janßen

Factorisation-aware matrix element emulation

soft/collinear factorisation properties

$$|\mathcal{M}_{n+1}|^2 \to |\mathcal{M}_n|^2 \otimes \mathbf{V}_{ijk}$$

[Catani, Seymour Nucl.Phys. B485 (1997) 291-419]

Ansatz

$$\langle|\mathcal{M}|^2\rangle = \sum_{\{ijk\}} C_{ijk} D_{ijk}$$

- $D_{ijk} = \langle V_{ijk}\rangle / s_{ij}$: spin-averaged Catani-Seymour dipoles divided by kinematic invariant
- C_{ijk}: coefficients fit by neural network

D. Maître, H. Truong: JHEP 11 (2021) 066

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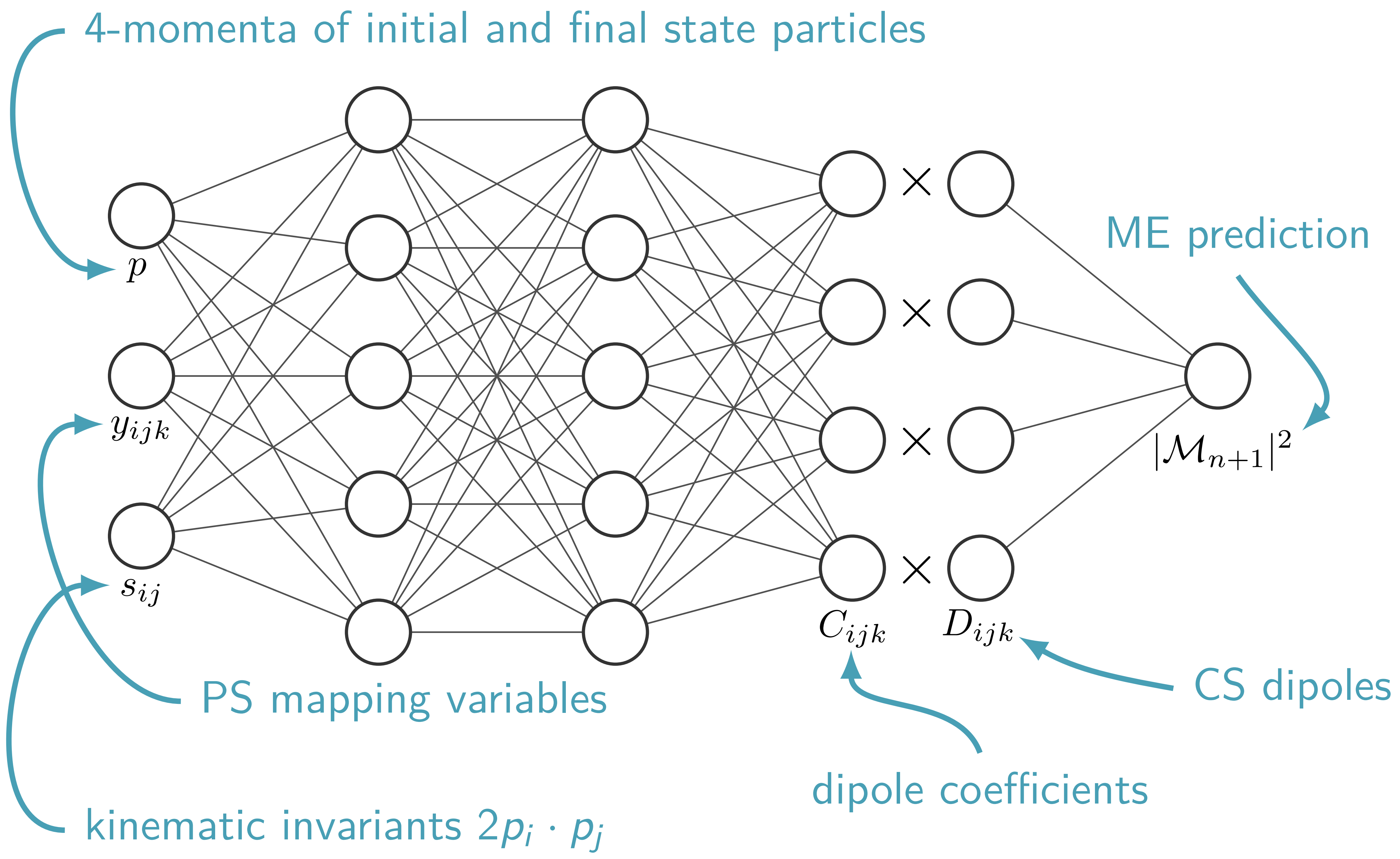
Surrogate unweighting

Slide by Timo Janßen

Factorisation-aware matrix element emulation



D. Maître, H. Truong: JHEP 11 (2021) 066

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EWvirt & EWsud

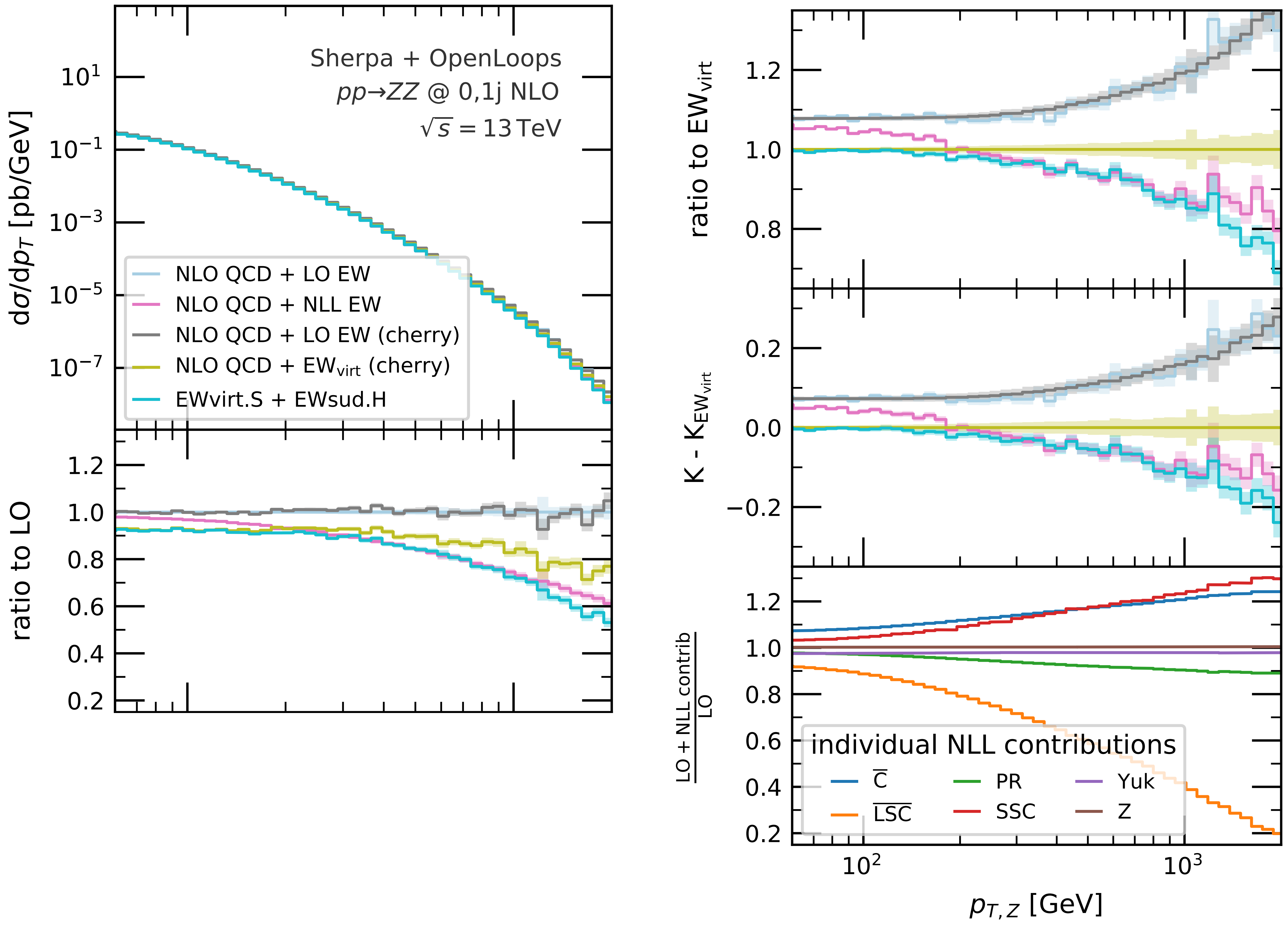
Comparative study in ZZ production

[EB et al. 2111.13453]

- Both schemes capture dominant logs in Sudakov region
- EWvirt:
  - subleading Born (can be sizable, e.g. in 3-jet production) [Reyer Schönherr Schumann 1902.01763]
  - approx. integrated real emission
  - finite terms in virtual loop
  - not applied to real-emission events
  - no subleading logs from RG
  - requires virtual loop ME
- don't expect perfect agreement, but so far we see K factors consistent within couple percent
- **proposal**: apply EWvirt to lower multis and EWsud to real-emission terms and higher multis, in a single merged sample („Hybrid“)

preliminary, MEPS@NLO ZZ production, 0,1j@NLO, 3,4j@LO

Hybrid: EWvirt.S + EWsud.H + EWsud.j4



Collider reach

- Plot taken from a talk by Marek Schönherr
- How far the integrated luminosity takes us into the Sudakov region