

Negative-weights suppression in Monte Carlo samples

# Cell resampling in McMule at NNLO

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## this is very much WIP

- I had to put this project on pause for quite a long time so it's still WIP
- please don't expect any fancy results, this is a **w**orkshop talk

the cleverness is from Jeppe, Andreas, Daniel

- I've implemented this in a MC
- and have a few fun ideas & observations to share



## fixed-order NNLO QED framework

- provided: matrix elements by us or others
- output: **physical cross section** for any physical observable
- McMULE: phase space generation, subtraction, stabilisation, integration, etc.
- all leptonic  $2 \rightarrow 2$  processes in QED at NNLO (+ a few others)
- integrator & generator
- user defines cuts through arbitrary function that is loaded at run time

Get the code here: <https://mule-tools.gitlab.io>

Read the docs here: <https://mcmule.readthedocs.io>



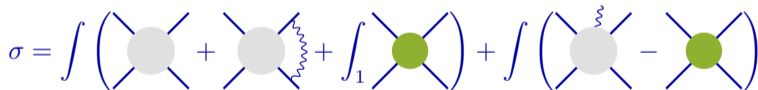
McMULE

process	experiment	physics motivation	order
$e\mu \rightarrow e\mu$	MUonE	HVP to $(g-2)_\mu$	NNLO+
$lp \rightarrow lp$	AMBER, PRad, ULQ2, ...	proton radius and weak charge	NNLO
$eN \rightarrow eN$	PRad, ULQ2	background	NNLO-
$e^-e^- \rightarrow e^-e^-$	Prad 2	normalisation	NNLO
	MOLLER, ...	$\sin^2 \theta_W$ at low $Q^2$	
$e^+e^- \rightarrow e^+e^-$	any $e^+e^-$ collider	luminosity measurement	NNLO
$ee \rightarrow ll$	VEPP, BES, Daphne, ...	$R$ -ratio	NNLO+
	Belle	$\tau$ properties	
$ee \rightarrow \gamma\gamma$	Daphne	dark searches	NNLO-
	any $e^+e^-$ collider	luminosity measurement	
$e\nu \rightarrow e\nu$	DUNE	flux & $\sin^2 \theta_W$	NNLO-
$\mu \rightarrow \nu\bar{\nu}e$	MEG	ALP searches	NNLO+
	DUNE	beam-line profiling	
$\mu \rightarrow \nu\bar{\nu}e\gamma$	MEG, Mu3e, Pioneer	background	NLO
$\mu \rightarrow \nu\bar{\nu}eee$	MEG, Mu3e	background	NLO
$ee \rightarrow \pi\pi$	VEPP, BES, Daphne, ...	$R$ -ratio	NLO
$ee \rightarrow ll\gamma$	VEPP, BES, Daphne, ...	$R$ -ratio	NNLO-

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$e\mu \rightarrow e\mu$	MUonE	HVP to $(g-2)_\mu$	NNLO+
$lp \rightarrow lp$	AMBER, PRad. <b>ULQ2</b> . ...	proton radius and weak charge	NNLO
$eN \rightarrow eN$	PRad, ULQ2		NNLO-
$e^-e^- \rightarrow e^-e^-$	Prad 2	n	NNLO
$e^+e^- \rightarrow e^+e^-$	MOLLER, ..	$\propto W Q^2$	NNLO
$ee \rightarrow ll$	any $e^+e^-$ cc	measurement	NNLO+
$ee \rightarrow \gamma\gamma$	VEPP, BES, Belle		NNLO+
$ee \rightarrow \gamma\gamma$	Daphne	s	NNLO-
any $e^+e^-$ cc		measurement	NNLO-
$e\nu \rightarrow e\nu$	DUNE	$h_W$	NNLO-
$\mu \rightarrow \nu\bar{\nu}e$	MEG		NNLO+
	DUNE	goal: world domination	
$\mu \rightarrow \nu\bar{\nu}e\gamma$	MEG, Mu3e, Pioneer	background	NLO
$\mu \rightarrow \nu\bar{\nu}eee$	MEG, Mu3e	background	NLO
$ee \rightarrow \pi\pi$	VEPP, BES, Daphne, ...	$R$ -ratio	NLO
$ee \rightarrow ll\gamma$	VEPP, BES, Daphne, ...	$R$ -ratio	NNLO-



- written in Fortran 2008, compiled with meson+ninja, toolkit in python3.9
- links to OpenLoops [Buccioni, Lang, Lindert, Maierhöfer, Pozzorini, Zhang, Zoller 19], Collier [Denner, Dittmaier, Hofer 16], handyG [Naterop, Signer, YU 18]
- matrix elements provided as function pointers
- automatic stabilisation for soft emissions at one-loop using the LBK theorem [Engel, Signer, YU 21; Balsach, Bonocore, Kulesza 23]
- automatic IR subtraction using the FKS<sup>ℓ</sup> scheme [Engel, Signer, YU 19]

$$\sigma = \int \left( \text{tree} + \text{loop} + \int_1 \text{FKS} \right) + \int \left( \text{tree} - \text{FKS} \right)$$


- defaults can be overridden if more control is needed
- histogramming can be done in MCMULE or externally (LHEF, HepMC3)

## McMule is designed as an integrator

- calculate arbitrary differential distributions
  - event generation by just dumping momenta to file (“garden hose approach”)
  - if  $r \times N$  of  $N$  weights are negative, we need  $\propto 1/(1 - 2r)^2$  events
- ⇒ reduce  $r$  as much as possible by cancelling negative weights as early as possible
- optimisations from splitting integrand goes away



$$\begin{aligned}
 \sigma_{\text{NNLO}} = & \int_n \left( \text{diagram 1} + \text{diagram 2} + \text{diagram 3} \right) \\
 & + \int_{n+1} \left( \text{diagram 4} + \text{diagram 5} \right) \\
 & + \int_{n+2} \left( \text{diagram 6} \right)
 \end{aligned}$$

The diagrams are:
 

- Diagram 1: A grey circle with four external lines (two incoming, two outgoing).
- Diagram 2: A grey circle with four external lines, one of which is a wavy line.
- Diagram 3: A grey circle with four external lines, one of which is a wavy line.
- Diagram 4: A grey circle with four external lines, one of which is a wavy line.
- Diagram 5: A grey circle with four external lines, one of which is a wavy line.
- Diagram 6: A grey circle with four external lines, one of which is a wavy line.

$$\begin{aligned}
 \sigma_{\text{NNLO}} = & \int_n \left( \text{diagram 1} + \text{diagram 2} + \text{diagram 3} + \int_1 \left[ \text{diagram 4} + \text{diagram 5} \right] \right) \\
 & + \int_{n+1} \left( \text{diagram 6} + \text{diagram 7} - \text{diagram 8} \right) \\
 & + \int_{n+2} \left( \text{diagram 9} \right)
 \end{aligned}$$

The diagrams are:
 

- diagram 1: grey circle with 4 external lines
- diagram 2: grey circle with 3 external lines and 1 wavy line
- diagram 3: grey circle with 2 external lines and 2 wavy lines
- diagram 4: green circle with 4 external lines
- diagram 5: green circle with 3 external lines and 1 wavy line
- diagram 6: grey circle with 3 external lines and 1 wavy line
- diagram 7: grey circle with 2 external lines and 2 wavy lines
- diagram 8: green circle with 4 external lines
- diagram 9: grey circle with 2 external lines and 2 wavy lines

we have negative weights in

- at NLO we have  $n$ -particle event

$$\begin{aligned}
 \sigma_{\text{NNLO}} = & \int_n \left( \text{grey circle} + \text{grey circle with wavy line} + \text{grey circle with wavy line} + \int_1 \left[ \text{green circle} + \text{green circle} \right] + \int_2 \text{orange circle} \right) \\
 & + \int_{n+1} \left( \text{grey circle with wavy line} + \text{grey circle with wavy line} + \int_1 \left[ \text{green circle} - \text{green circle} \right] \right) \\
 & + \int_{n+2} \left( \text{grey circle with wavy line} - \text{green circle with wavy line} + \text{orange circle} \right)
 \end{aligned}$$

we have negative weights in

- at NLO we have  $n$ -particle event
- at NNLO we have  $(n + 1)$ -particle and  $n$ -particle events

$$\begin{aligned}
 \sigma_{\text{NNLO}} = & \int_n \left( \text{tree}_1 + \text{tree}_2 + \text{tree}_3 + \int_1 [\text{loop}_1 + \text{loop}_2] + \int_2 \text{loop}_3 \right) \\
 & + \int_{n+1} \left( \text{tree}_4 + \text{tree}_5 + \int_1 \text{loop}_4 - \text{loop}_5 - \text{loop}_6 \right) \\
 & + \int_{n+2} \left( \text{tree}_6 - \text{loop}_7 + \text{loop}_8 \right)
 \end{aligned}$$

we have negative weights in

- at NLO we have  $n$ -particle event
- at NNLO we have  $(n + 1)$ -particle and  $n$ -particle events involving loops

$$\begin{aligned}
 \sigma_{\text{NNLO}} = & \int_n \left( \text{tree}_n + \text{tree}_{n+1} + \text{tree}_{n+2} + \int_1 [\text{loop}_n + \text{loop}_{n+1}] + \int_2 \text{loop}_2 \right) \\
 & + \int_{n+1} \left( \text{tree}_{n+1} + \text{tree}_{n+2} + \int_1 [\text{loop}_{n+1} - \text{loop}_{n+2}] \right) \\
 & + \int_{n+2} \left( \text{tree}_{n+2} - \text{loop}_{n+2} + \text{loop}_2 \right)
 \end{aligned}$$

we have negative weights in

- at NLO we have  $n$ -particle event
  - at NNLO we have  $(n + 1)$ -particle and  $n$ -particle events involving loops
- ⇒ use cell resampling (cres) [Andersen, Maier 21]

## two observations

- 1 cross section  $\sigma = \int_{\mathcal{C}} d\sigma > 0$ , irregardless of the size of integration region  $\mathcal{C}$
- 2 experiments have a finite resolution  
(we already knew that because we can't see soft photons)

## algorithm to remove negative weights [Andersen, Maier 21]

- pick an event with  $w_i < 0$
- find nearby events until  $\sum_{i \in \mathcal{C}} w_i > 0$
- if  $\mathcal{C}$  gets too big (events become resolvable), abort
- else  $w_i \rightarrow \frac{\sum_{j \in \mathcal{C}} w_j}{\sum_{j \in \mathcal{C}} |w_j|} w_i$

we can remove negative weights without biasing physical observables!

## McMule's provides signal and background models at NNLO

- $ep \rightarrow ep$  scattering experiment at RARIS, Tohoku University (also  $e-^{12}\text{C}$  and  $e-D$ )
- measurement is at ultra-low  $Q^2 \rightarrow$  measure the proton (deuteron) radius
- $E_{\text{beam}} = 50 \text{ MeV}$ ,  $17 \text{ MeV} \leq \sqrt{Q^2} \leq 90 \text{ MeV}$
- measure scattering  $\theta_e$  and  $|\vec{p}_e|$  of outgoing electron in lab frame
- require  $48^\circ < \theta_e < 52^\circ$  and  $|\vec{p}_e| > 46 \text{ MeV}$

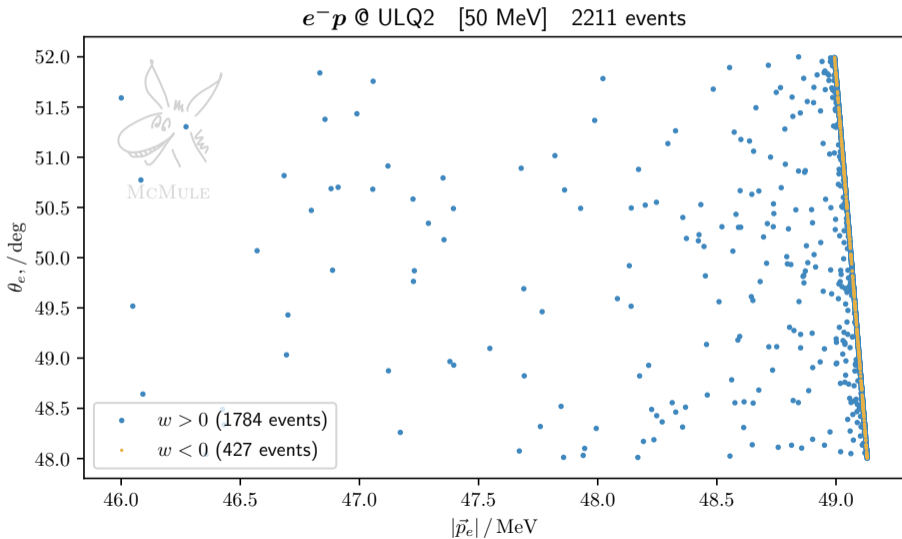


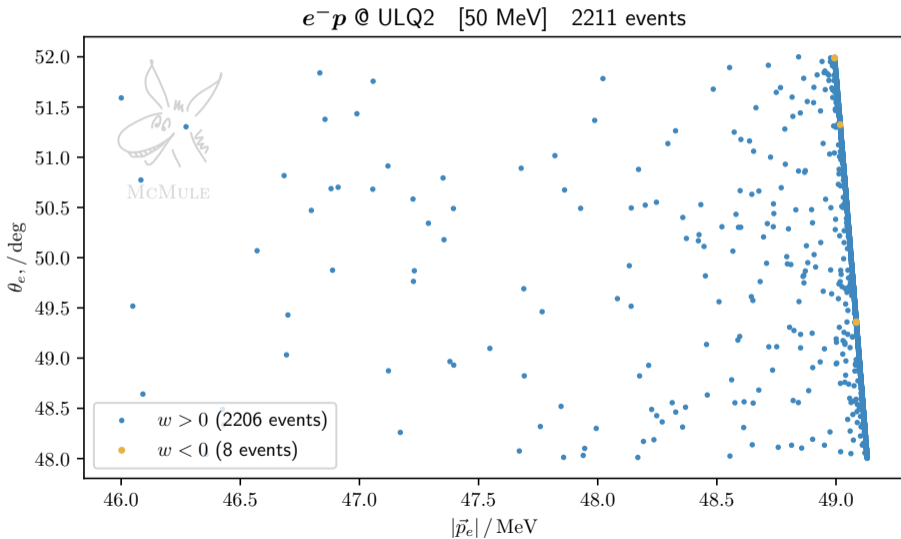
### event generation with McMule

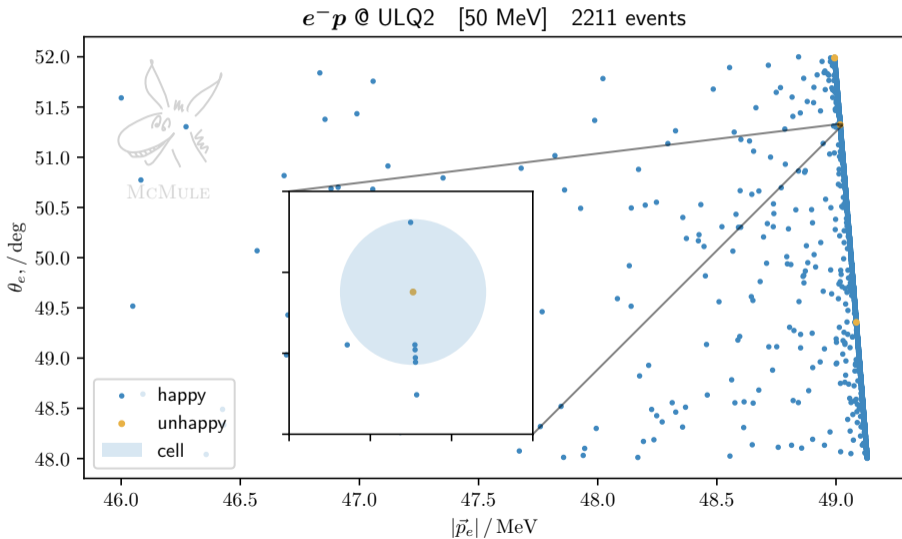
- event distance for resampling: 
$$d(\mathcal{E}^{(1)}, \mathcal{E}^{(2)}) = \sqrt{\left| \frac{\theta_e^{(1)} - \theta_e^{(2)}}{\text{deg}} \right|^2 + \left| \frac{|\vec{p}_e^{(1)}| - |\vec{p}_e^{(2)}|}{\text{MeV}} \right|^2}$$
- resolution parameter  $d < d_{\text{max}} = 0.0045$

Note  $\alpha_{\text{QED}} \ll \alpha_s \Rightarrow$  need many more events

Order	$\xi_c$	$N$	$r$	$[w_{\min}, w_{\max}]/\langle w \rangle$	feature
LO	n/a	99.7M	0.0%	$[0.03, 7.7]$	
NLO	0.1	220M	0.5%	$[-3.6, 3.6] \times 10^7$	
	1.0	216M	3.5%	$[-2.1, 2.1] \times 10^6$	
NNLO	0.1	21.1G	0.7%	$[-8.6, 8.6] \times 10^7$	
	1.0	19.8G	9.2%	$[-2.3, 2.3] \times 10^8$	







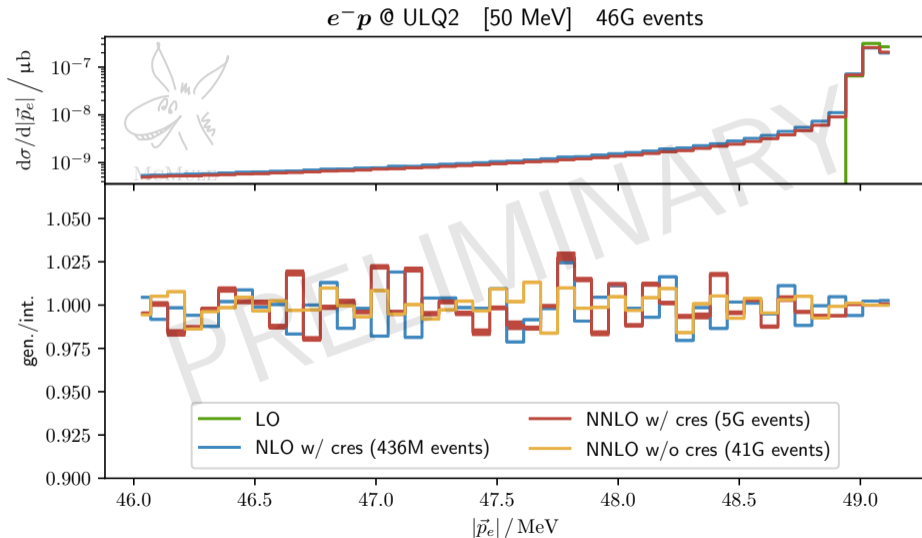
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NLO	0.1	220M	0.5%	$[-3.6, 3.6] \times 10^7$	cres
			0.1%	$[-1.3, 19] \times 10^3$	
NNLO	1.0	216M	3.5%	$[-2.1, 2.1] \times 10^6$	cres
			0.3%	$[-7.0, 26] \times 10^3$	
	0.1	21.1G 3.6G	0.7%	$[-8.6, 8.6] \times 10^7$	cres
			0.1%	$[-6.9, 6.9] \times 10^5$	
1.0	19.8G 1.2G	9.2%	$[-2.3, 2.3] \times 10^8$	cres	
		0.5%	$[-3.3, 2.4] \times 10^4$		

Note  $\alpha_{\text{QED}} \ll \alpha_s \Rightarrow$  need many more events

Order	$\xi_c$	$N$	$1/\langle w \rangle$	feature
LO	n/a	90		
NLO	0.1	20	$10^7$	
	1.0	20	$10^3$	crs
NNLO	0.1	20	$10^6$	
		30	$10^3$	crs
	1.0	10	$10^7$	
		10	$10^5$	crs
	10	$10^8$		
	10	10	$10^4$	crs





we still have some negative events  $\Rightarrow$  subsampling

① perform normal sampling

⑤ perform cell resampling

we still have some negative events  $\Rightarrow$  subsampling

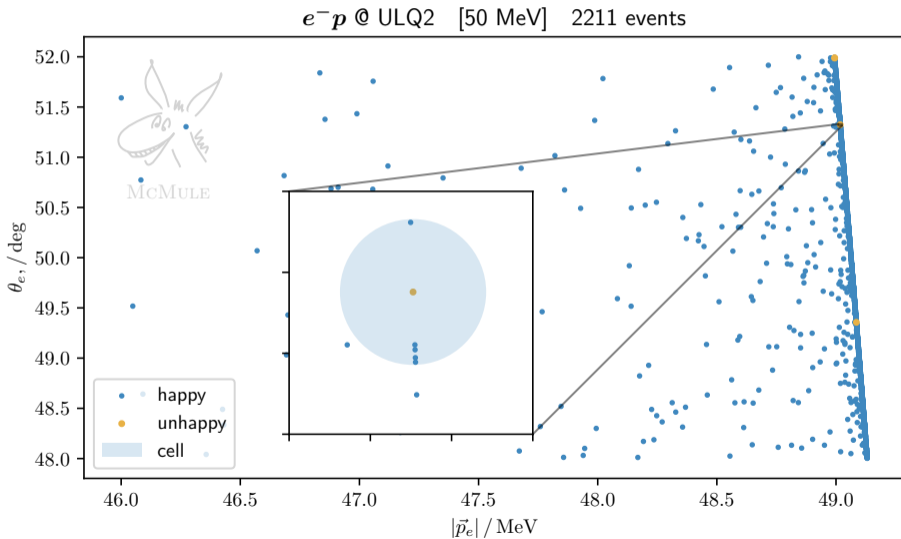
- ① perform normal sampling
- ② dry-run cell resampling: build cells but **do not** change weight
- ③ for each unhappy cell  $\mathcal{C}$  that would've grown too large
  - ① ask MC to sample again
  - ② reject event if  $d(\mathcal{E}, \text{seed of } \mathcal{C}) > d_{\max}$
- ④ merge new and old event sets
- ⑤ perform cell resampling

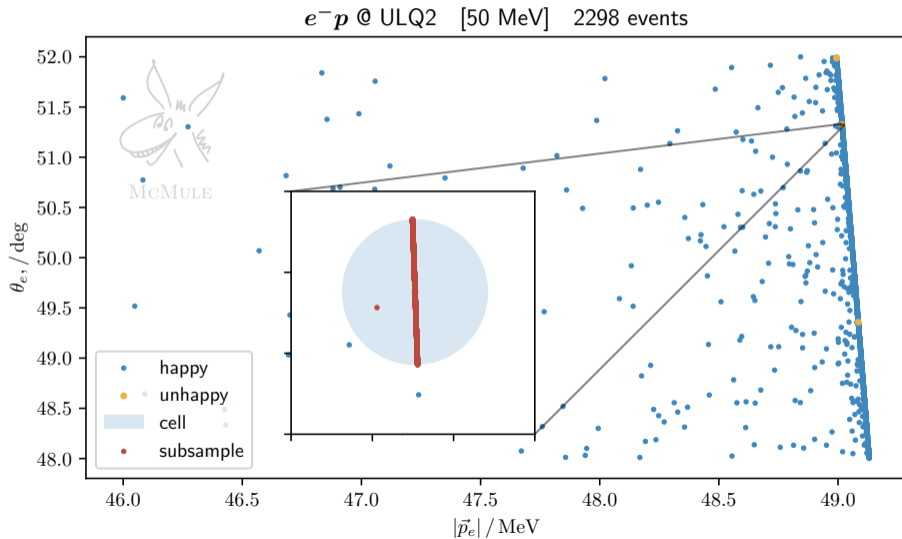
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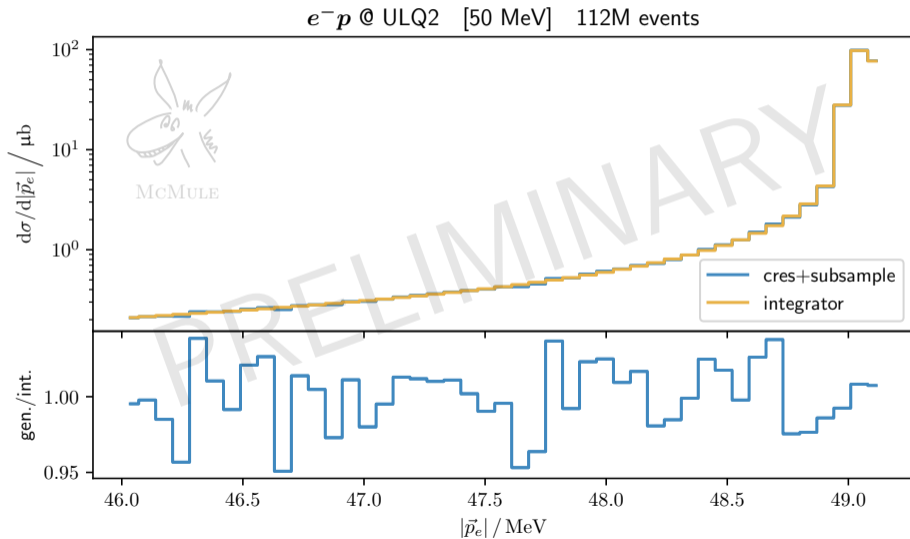
- ① perform normal sampling
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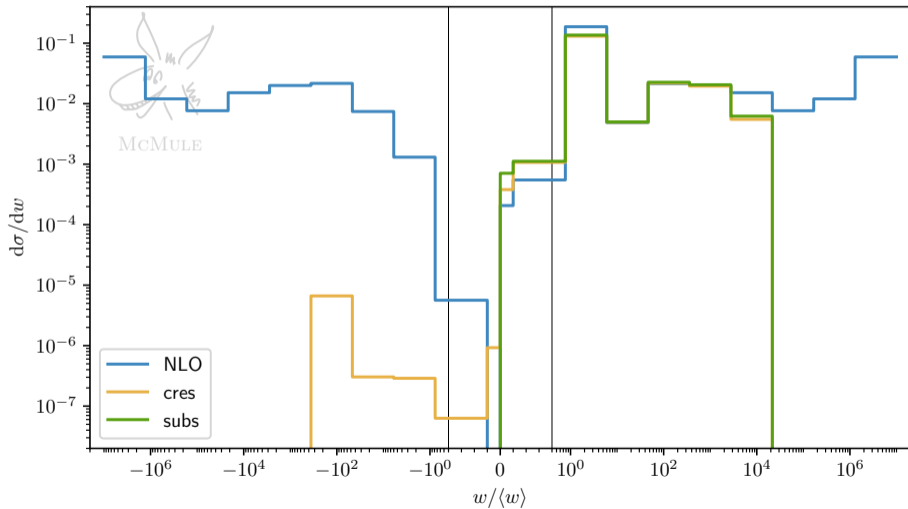
notes

- this will change  $\sigma$ . this is okay because our previous estimate for  $\int_{\mathcal{C}} d\sigma$  was wrong
- interactions between cells makes this more complicated
  - cells can be unhappy even if resampling succeeds
  - subsampling might think it solved all problems but didn't









Note  $\alpha_{\text{QED}} \ll \alpha_s \Rightarrow$  need many more events

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LO	n/a	99.7M	0.0%	$[0.03, 7.7]$	
NLO	0.1	220M	0.5%	$[-3.6, 3.6] \times 10^7$	cres subs
		51M	0.1%	$[-1.3, 19] \times 10^3$	
	1.0	216M	0	$[+0.0, 1.6] \times 10^4$	cres subs
		61M	3.5%	$[-2.1, 2.1] \times 10^6$	
NNLO	0.1	21.1G	0.7%	$[-7.0, 26] \times 10^3$	cres
		3.6G	0.1%	$[-8.6, 8.6] \times 10^7$	
	1.0	19.8G	9.2%	$[-6.9, 6.9] \times 10^5$	cres
		1.2G	0.5%	$[-2.3, 2.3] \times 10^8$	
				$[-3.3, 2.4] \times 10^4$	

Note  $\alpha_{\text{QED}} \ll \alpha_s \Rightarrow$  need many more events

Order	$\xi_c$	$\Lambda$	$]/\langle w \rangle$	feature
LO	n/a	99		
NLO	0.1	2: 5:	$10^7$ $10^3$	pres subs
	1.0	2: 6:	$10^6$ $10^3$	pres subs
NNLO	0.1	2: 3:	$10^7$ $10^5$	pres
	1.0	19.8G 1.2G	9.2% 0.5%	$[-2.3, 2.3] \times 10^8$ $[-3.3, 2.4] \times 10^4$



## summary

- McMule is a (mostly  $2 \rightarrow 2$ ) NNLO code for QED
- event generation at  $2 \rightarrow 2$  NNLO **works** but leads to many negative weights
- cell resampling can reduce this problem
- subsampling might be able to (all but) eliminate it

## outlook

- NNLO cell resampling needs more robust testing
- subsampling at NLO needs more validation
- test subsampling at NNLO
- how does this perform beyond  $2 \rightarrow 2$  NNLO:  $2 \rightarrow 3$  NNLO,  $2 \rightarrow 2$  N<sup>3</sup>LO, resummation





f.l.t.r.: S.Kollatzsch (Zurich & PSI), A.Signer (Zurich & PSI), V.Sharkovska (Zurich & PSI), S.Gündogdu (Zurich & PSI), D. Moreno (PSI), A.Coutinho (IFIC), Y.Ulrich (Liverpool), D. Radic (Zurich & PSI), L.Naterop (Zurich & PSI), M.Rocco (Turin)  
not shown: P.Banerjee (Cosenza), Y.Fang (ETHZ), A.Gurgone (Pavia), R.Krolzig (Zurich), F.Hagelstein (Mainz), M.Ronchi (Mainz), N.Schalch (Oxford), P.Wahlen (Zurich)



McMULE

[mule-tools.gitlab.io](https://mule-tools.gitlab.io)