

McMULE for MUonE

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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

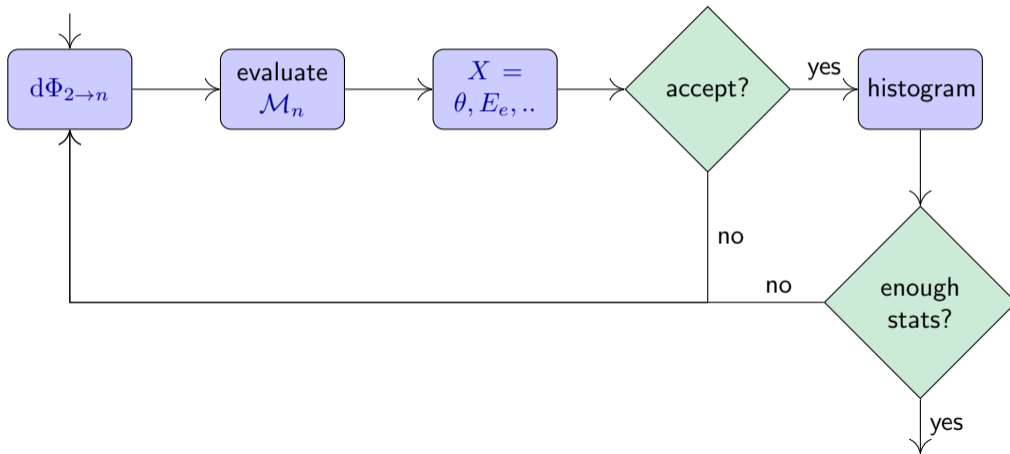
| process | experiment | physics motivation | order |
|---------------------------------------|------------------------|--------------------------------|-------|
| $e\mu \rightarrow e\mu$ | MUonE | HVP to $(g-2)_\mu$ | NNLO+ |
| $lp \rightarrow lp$ | AMBER, PRad, ULQ2, ... | proton radius and weak charge | 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 | τ 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- |

| 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 | | 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- |
| $e\nu \rightarrow e\nu$ | any e^+e^- cc | measurement | NNLO- |
| $\mu \rightarrow \nu\bar{\nu}e$ | DUNE | h_W | NNLO- |
| $\mu \rightarrow \nu\bar{\nu}e\gamma$ | MEG | goal: world domination | NNLO+ |
| $\mu \rightarrow \nu\bar{\nu}eee$ | DUNE | ling | NNLO+ |
| $\mu \rightarrow \nu\bar{\nu}e\gamma$ | 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- |

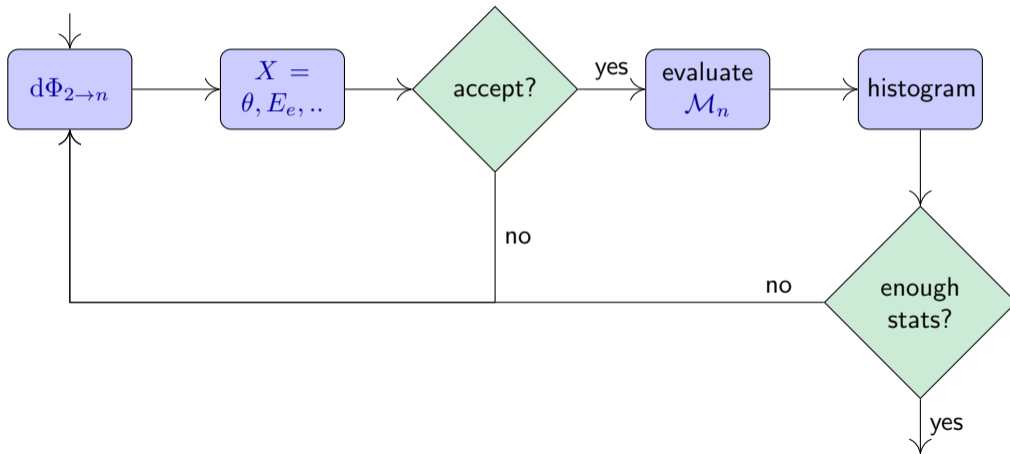


$$\begin{aligned}
 \sigma = & \int d\Phi_2 \left| \begin{array}{c} \text{tree} \\ \text{tree} \end{array} + \begin{array}{c} \text{1-loop} \\ \text{tree} \end{array} + \begin{array}{c} \text{1-loop} \\ \text{1-loop} \end{array} + \begin{array}{c} \text{2-loop} \\ \text{tree} \end{array} + \dots \right|^2 \\
 & + \int d\Phi_3 \left| \begin{array}{c} \text{1-loop} \\ \text{tree} \end{array} + \begin{array}{c} \text{2-loop} \\ \text{tree} \end{array} + \begin{array}{c} \text{2-loop} \\ \text{1-loop} \end{array} + \dots \right|^2 \\
 & + \int d\Phi_4 \left| \begin{array}{c} \text{2-loop} \\ \text{tree} \end{array} + \begin{array}{c} \text{3-loop} \\ \text{tree} \end{array} + \dots \right|^2 \\
 & + \int d\Phi_5 \left| \begin{array}{c} \text{3-loop} \\ \text{tree} \end{array} + \dots \right|^2 \\
 & + \dots
 \end{aligned}$$

a simple analysis assuming X is difficult: a generator



a simple analysis assuming \mathcal{M}_n is difficult: an integrator



why is the theory pipeline different?

- **assumption**: for a pure theory calculation, X is trivial to calculate

```

q3lab = boost_rf(q1,q3)
q4lab = boost_rf(q1,q4)
theta_e = acos(cos_th(ez,q3lab))
theta_m = acos(cos_th(ez,q4lab))

gmu = (q2lab(4)*me+mm**2)/(q2lab(4)*me+me**2)
gam = (q2lab(4)+me)/sqrt(scms)
theta_m_el = atan(2*tan(theta_e)/((1+gam**2*tan(theta_e)**2)*(1+gmu)-2))
bdev = theta_m/theta_m_el

if(Ee<1000.) pass_cut = .false.
if(theta_m<0.3E-3) pass_cut = .false.
!band cut
if(bdev<0.9) pass_cut = .false.
if(bdev>1.1) pass_cut = .false.
    
```

- but \mathcal{M}_n is **really** slow

why is the theory pipeline different?

- **assumption**: for a pure theory calculation, X is trivial to calculate
- but **some parts** of \mathcal{M}_n are very slow
- $\int d\Phi_{n+1}$ is divergent!

what does this mean?

- decide early whether \mathcal{M}_n needs to be calculated
- $\mathcal{M}_n = \underbrace{\mathcal{M}_n^{(0)}}_{\text{fast and large}} + \underbrace{\mathcal{M}_n^{(1)}}_{\text{okay-ish and large-ish}} + \underbrace{\mathcal{M}_n^{(2)}}_{\text{unbelievably slow but small}} + \dots$
- this allowed us to do the first full* **NNLO** calculation of $e\mu \rightarrow e\mu$ [Broggio, Engel, Ferroglia, Mandal, Mastrolia, Rocco, Ronca, Signer, Torres Bobadilla, Zoller, YU 22]
- require a subtraction

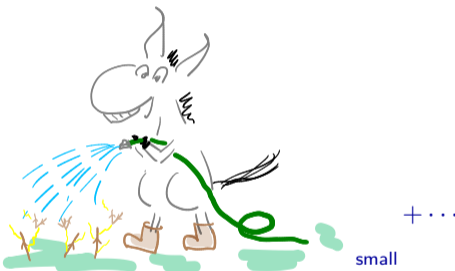
⇒ weights have no probabilistic interpretation

why is the theory pipeline different?

- **assumption**: for a pure theory calculation, X is trivial to calculate
- but **some parts** of \mathcal{M}_n are very slow
- $\int d\Phi_{n+1}$ is divergent!

what does this mean?

- decide early whether Λ
- $\mathcal{M}_n = \underbrace{\mathcal{M}_n^{(0)}}_{\text{fast and large}} + \text{oka} + \dots$



- this allowed us to do the **garden-hose approach** if $e\mu \rightarrow e\mu$ [Broggio, Engel, Ferrogliola, Mandal, Mastrolia, Rosso, Ronca, Singer, Torres Bobadilla, Zoller, YU 22]
- require a subtraction

⇒ weights have no probabilistic interpretation

... at NLO for simplicity

$$\sigma_{\text{NLO}} = \int \text{[tree]} + \frac{\alpha}{4\pi} \int \text{[1-loop]} + \frac{\alpha}{4\pi} \int \text{[2-loop]}$$

- slicing: fairly few negative weights **but** numerically construct $\log \omega_c$

$$= \int \underbrace{\left(\text{[tree]} + \frac{\alpha}{4\pi} \text{[1-loop]} + \frac{\alpha}{4\pi} \int_1 \text{[2-loop]} \right)}_{\text{mostly } > 0} + \frac{\alpha}{4\pi} \int_{\omega > \omega_c} \underbrace{\text{[2-loop]}}_{> 0}$$

- subtraction: easier integration **but** lots and lots of negative weights ($\mathcal{O}(5\%)$ at NLO, more at NNLO)

$$= \int \underbrace{\left(\text{[tree]} + \frac{\alpha}{4\pi} \text{[1-loop]} + \frac{\alpha}{4\pi} \int_1 \text{[2-loop]} \right)}_{\text{mostly } > 0} + \frac{\alpha}{4\pi} \int \underbrace{\left(\text{[2-loop]} - \text{[2-loop]} \right)}_{\text{whatever}}$$

best theory

- early access to improvements
- currently: full NNLO
- future: N³LO, NLP soft resummation
- better handling of hadronic effects
- better numerical stability & efficiency

good experiment

- less complicated detector simulation
 $\mathcal{O}(\text{ms/ev})$
- potentially involving interpolations
and other sources of uncertainties
- can be done with GEANT4

best experiment

- full-blown detector simulation
- full event generation from McMULE
(WIP)
- no modelling uncertainties

good theory

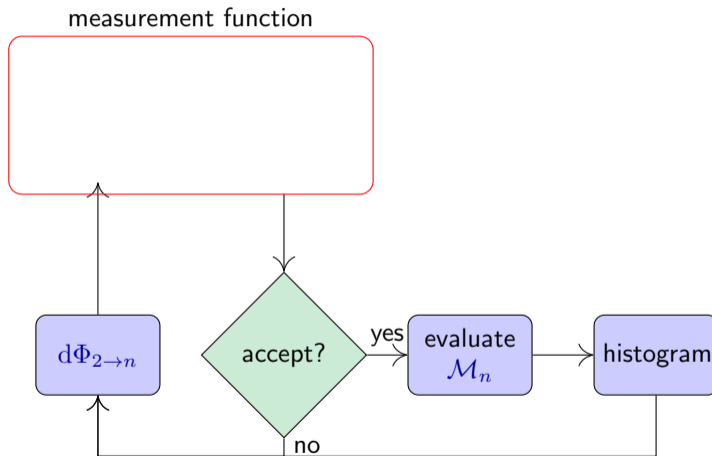
- “only” NNLO
- no early access to features
- significantly increased runtime &
storage requirement



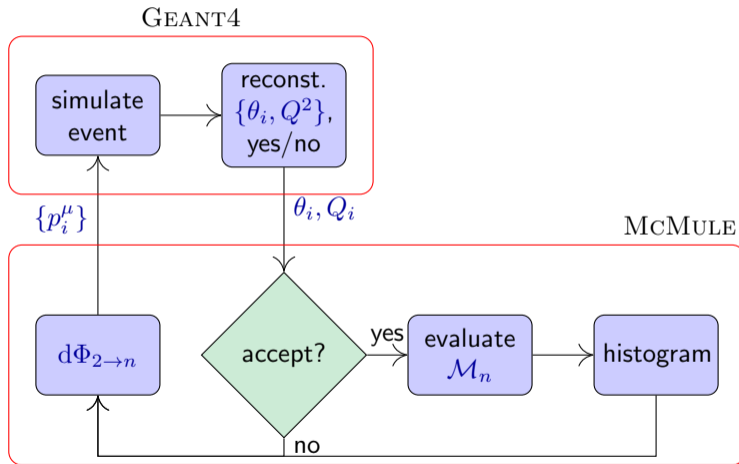
two examples in $ep \rightarrow ep$

ULQ2 (Tohoku University), PRad II (JLab)

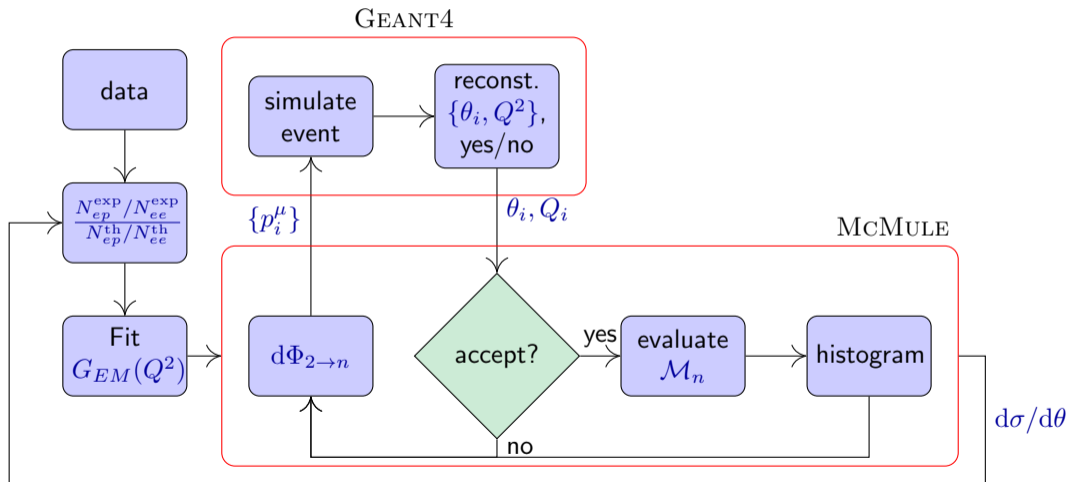
- PRad II is adopting McMULE into their analysis flow



- PRad II is adopting McMULE into their analysis flow



- PRad II is adopting McMULE into their analysis flow



- building & validating generator
- generator efficiency $\sim (w_{\max} - w_{\min})/\langle w \rangle$

| Order | ξ_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% | $[-2.3, 2.3] \times 10^8$ | |

- building & validating generator
- generator efficiency $\sim (r)$

| Order | ξ_c | Λ |
|-------|---------|-----------|
| LO | n/a | 9% |
| NLO | 0.1 | 2% |
| | 1.0 | 2% |
| NNLO | 0.1 | 2% |
| | 1.0 | 1% |



| $]/\langle w \rangle$ | feature |
|-----------------------|---------|
| 10^7 | |
| 10^6 | |
| 10^7 | |
| 10^8 | |

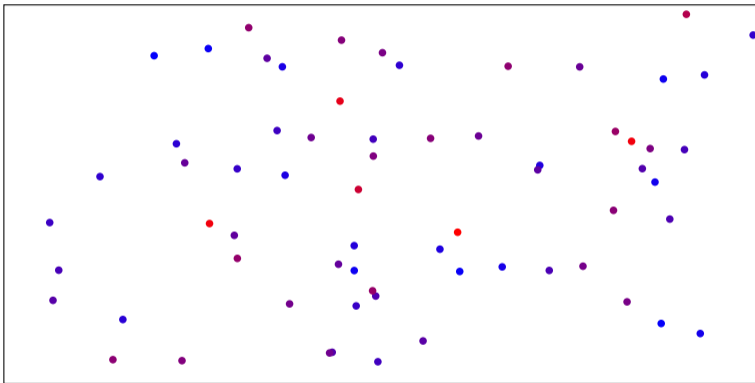
two observations

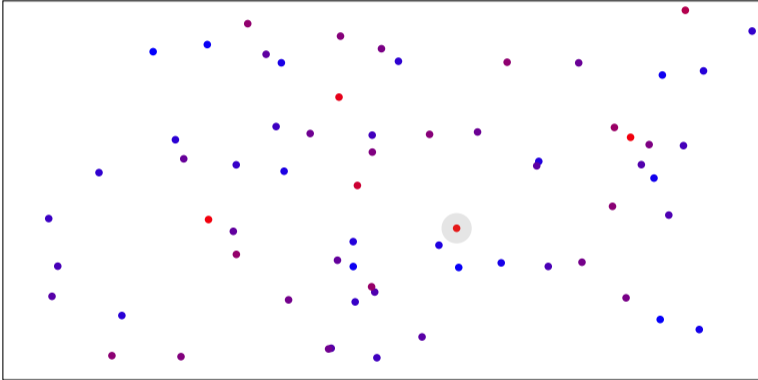
- 1 cross section $\sigma = \int_{\mathcal{C}} d\sigma > 0$, irregardless of the size of integration region \mathcal{C}
- 2 experiments have a finite resolution
(we already knew that because we can't see soft photons)

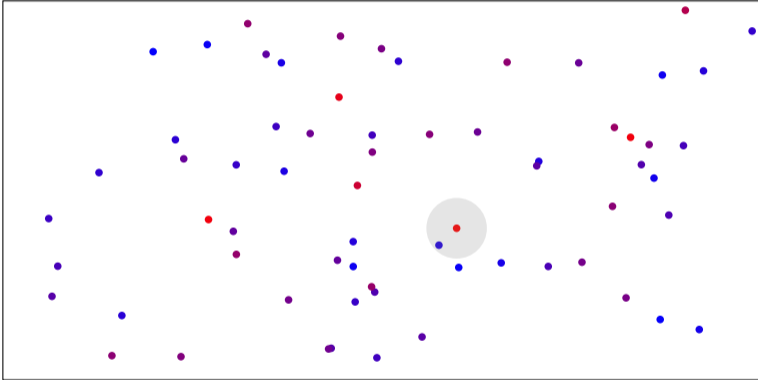
algorithm to remove negative weights [Andersen, Maier 21]

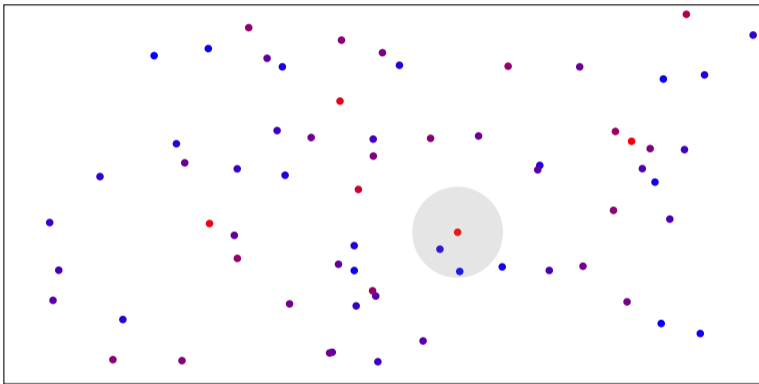
- pick an event with $w_i < 0$
- find nearby events until $\sum_{i \in \mathcal{C}} w_i > 0$
- if \mathcal{C} gets too big (events become resolvable), abort (or add more events)
- else $w_i \rightarrow \frac{\sum_{j \in \mathcal{C}} w_j}{\sum_{j \in \mathcal{C}} |w_j|} w_i$

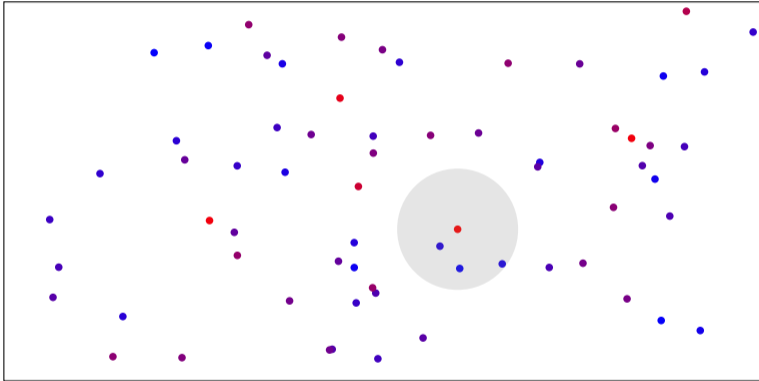
we can remove negative weights without biasing physical observables!

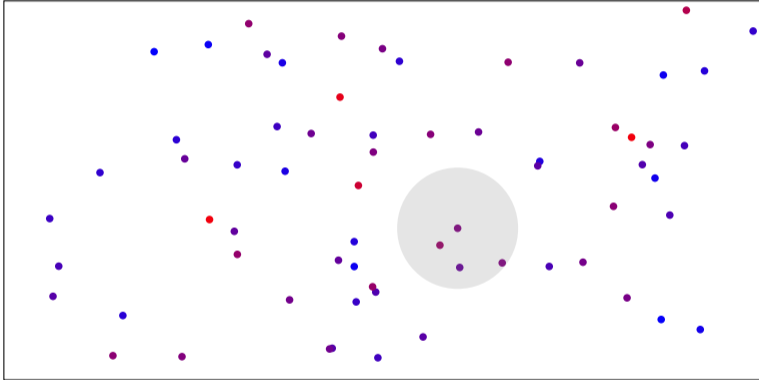


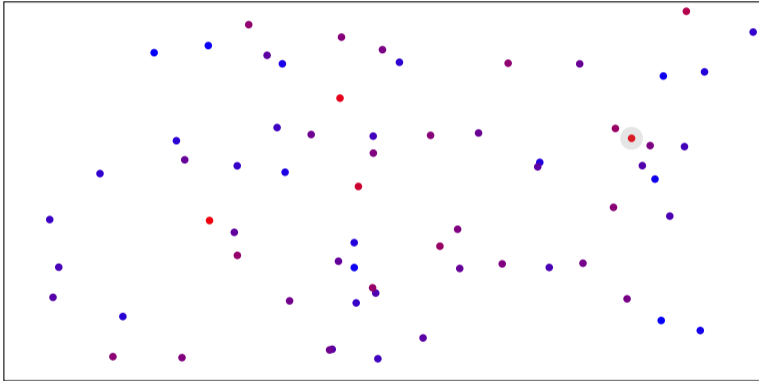


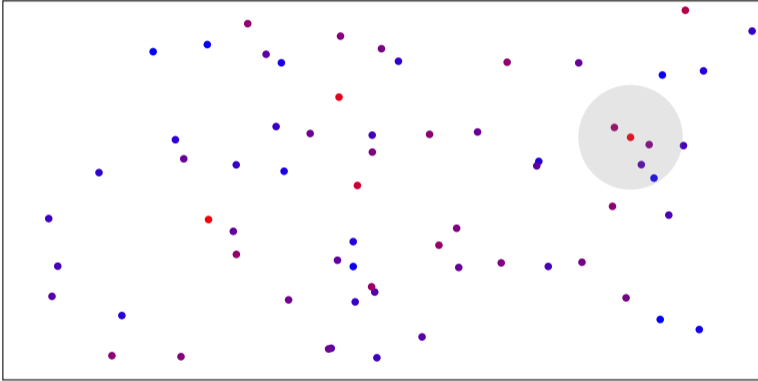


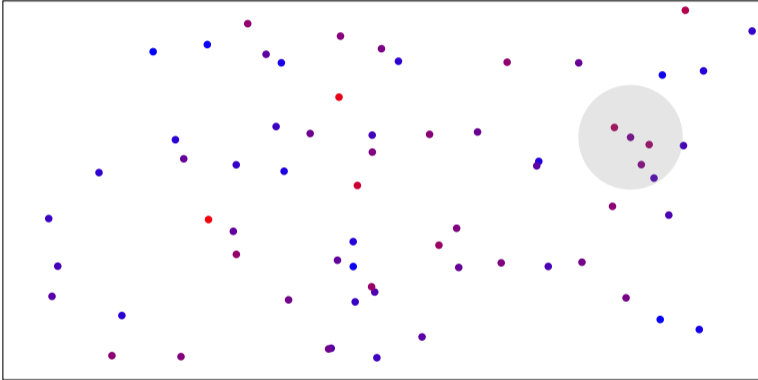


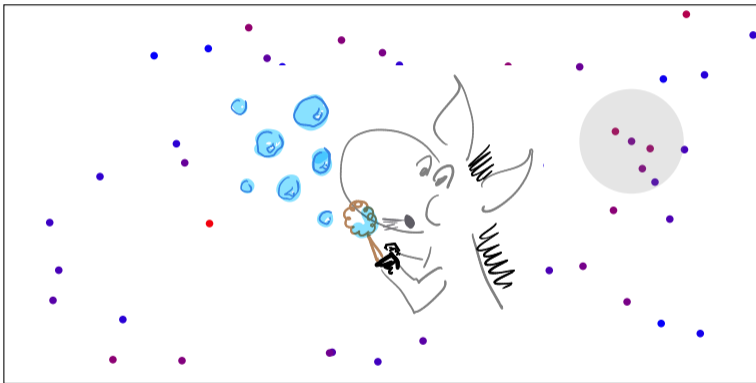






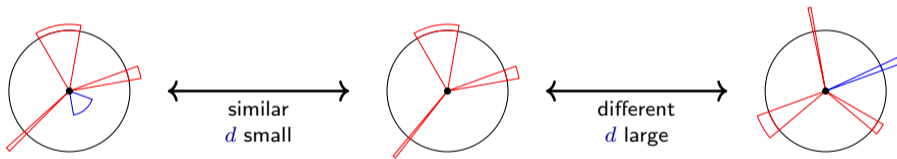






we need to define a metric in event space $d(e_1, e_2) \geq 0$

- doesn't really matter how we do this as long as IR safe
(events with soft photons are near each other)
- ideally: events that look similar are closer to each other than those that don't



- e.g.
$$d(\mathcal{E}^{(1)}, \mathcal{E}^{(2)}) = \sqrt{\left| \frac{\theta_e^{(1)} - \theta_e^{(2)}}{10 \text{ mrad}} \right|^2 + \left| \frac{\theta_\mu^{(1)} - \theta_\mu^{(2)}}{1 \text{ mrad}} \right|^2}$$

- building & validating generator
- generator efficiency $\sim (w_{\max} - w_{\min})/\langle w \rangle$

| Order | ξ_c | N | r | $[w_{\min}, w_{\max}]/\langle w \rangle$ | feature |
|-------|---------------|---------------|---------------------------|------------------------------------------|---------|
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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% | $[-3.3, 2.4] \times 10^4$ | | |

- building & validating generator
- generator efficiency $\sim (w_{\max} - w_{\min})/\langle w \rangle$

| Order | ξ_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% | $[-3.6, 3.6] \times 10^7$ | 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 | 0.3% | $[-7.0, 26] \times 10^3$ | cres |
| | | 3.6G | 0.1% | $[-6.9, 6.9] \times 10^5$ | |
| | 1.0 | 19.8G | 9.2% | $[-2.3, 2.3] \times 10^8$ | cres |
| | | 1.2G | 0.5% | $[-3.3, 2.4] \times 10^4$ | |

- building & validating generator
- generator efficiency $\sim (w - w_{\text{min}}) / (w)$

| Order | ξ_c | Λ | $\sigma / \langle w \rangle$ | feature |
|-------|---------|---------------|----------------------------------------------------------------------------|--------------|
| LO | n/a | 9 | | |
| NLO | 0.1 | 2: 5: | 10^7 10^3 | pres subs |
| | 1.0 | 2: 6: | 10^6 10^3 10^4 | pres subs |
| NNLO | 0.1 | 2: 3.6G | 0.1% $[-6.9, 6.9] \times 10^5$ | pres |
| | 1.0 | 19.8G 1.2G | 9.2% $[-2.3, 2.3] \times 10^8$ 0.5% $[-3.3, 2.4] \times 10^4$ | pres |



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 & subsampling might be able to (all but) eliminate this problem
 - **but** event generator will always lag behind integrator
- ⇒ experiments should develop fast simulations

outlook

- finish & test generator
- go beyond $2 \rightarrow 2$ NNLO: $2 \rightarrow 3$ NNLO, $2 \rightarrow 2$ N³LO, 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: not shown: F.Hagelstein (Mainz), N.Schalch (Oxford), P.Banerjee (Cosenza), M.Ronchi (Mainz), Y.Fang (PSI), G.Billis (PSI), J.Wilson (Liverpool)



McMULE

mule-tools.gitlab.io