Machine Learning for Phase Space Sampling

An exploration for LHC simulated event generation with SHERPA

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Several slides adapted from Steffen Schumann

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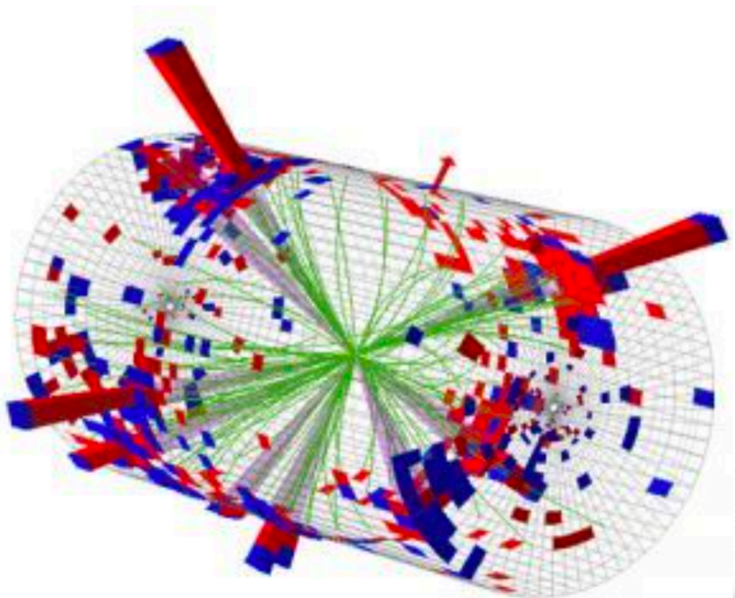
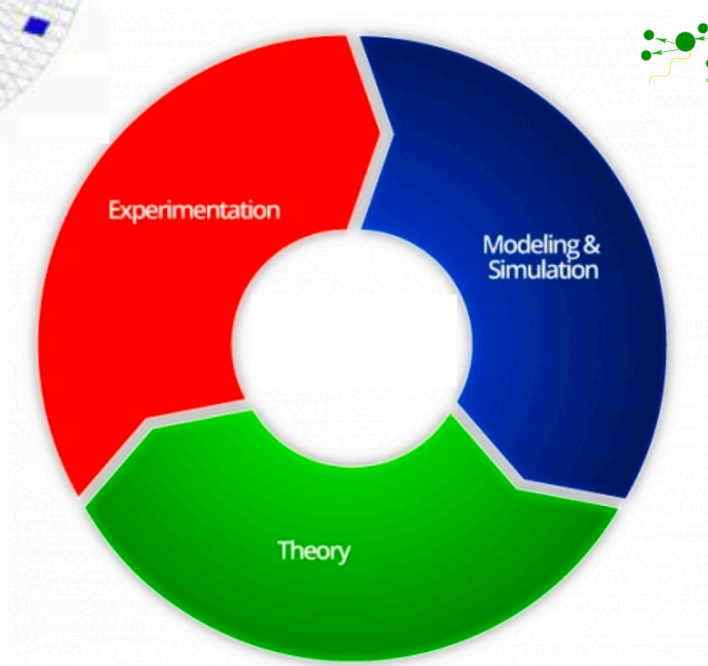
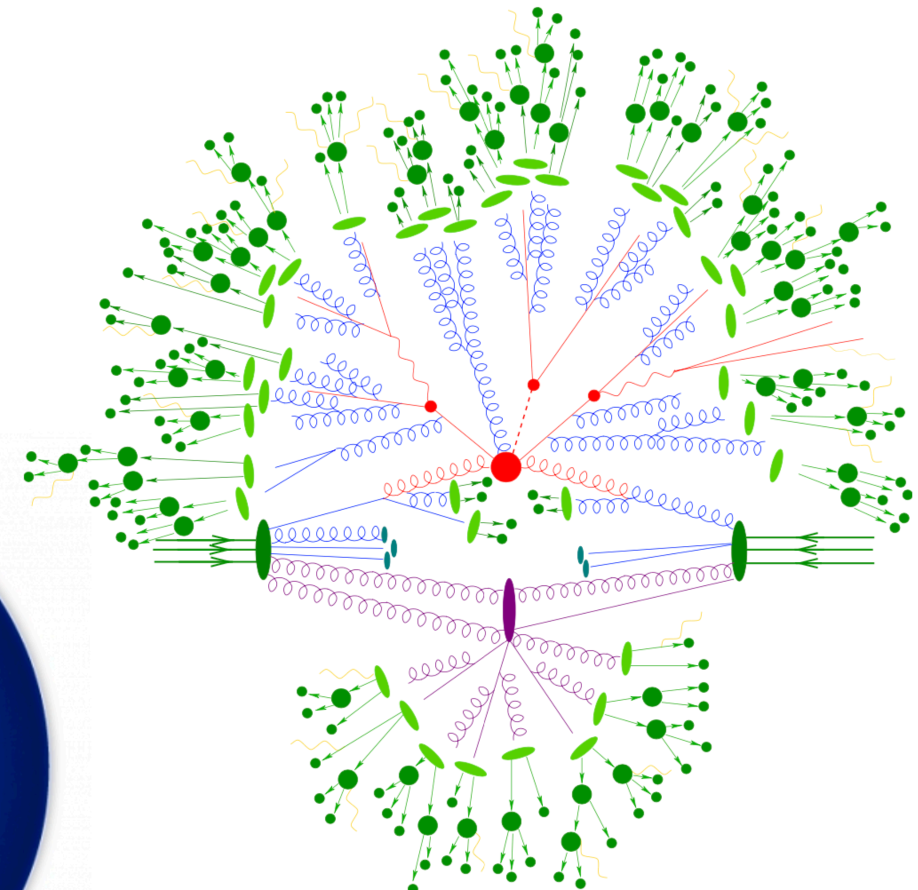
The High Energy Physics Triad







$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + i\bar{\Psi}\not{D}\Psi + h.c.$$

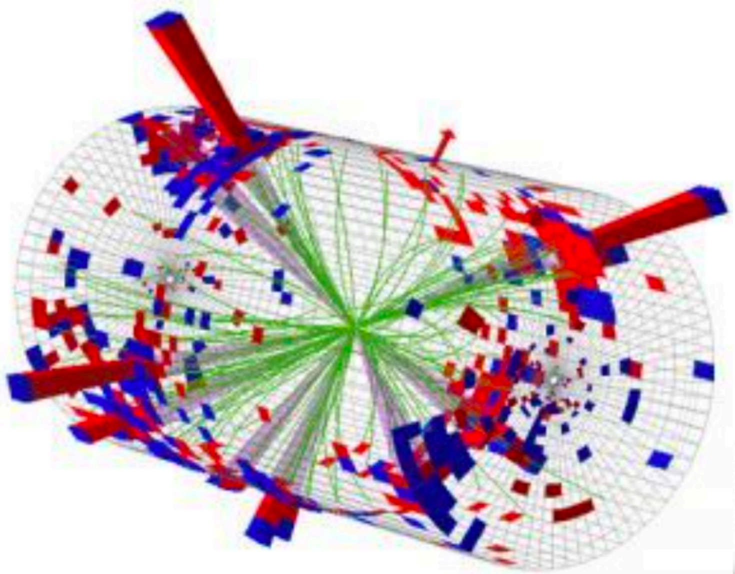
Slide adapted from Stefan Höche

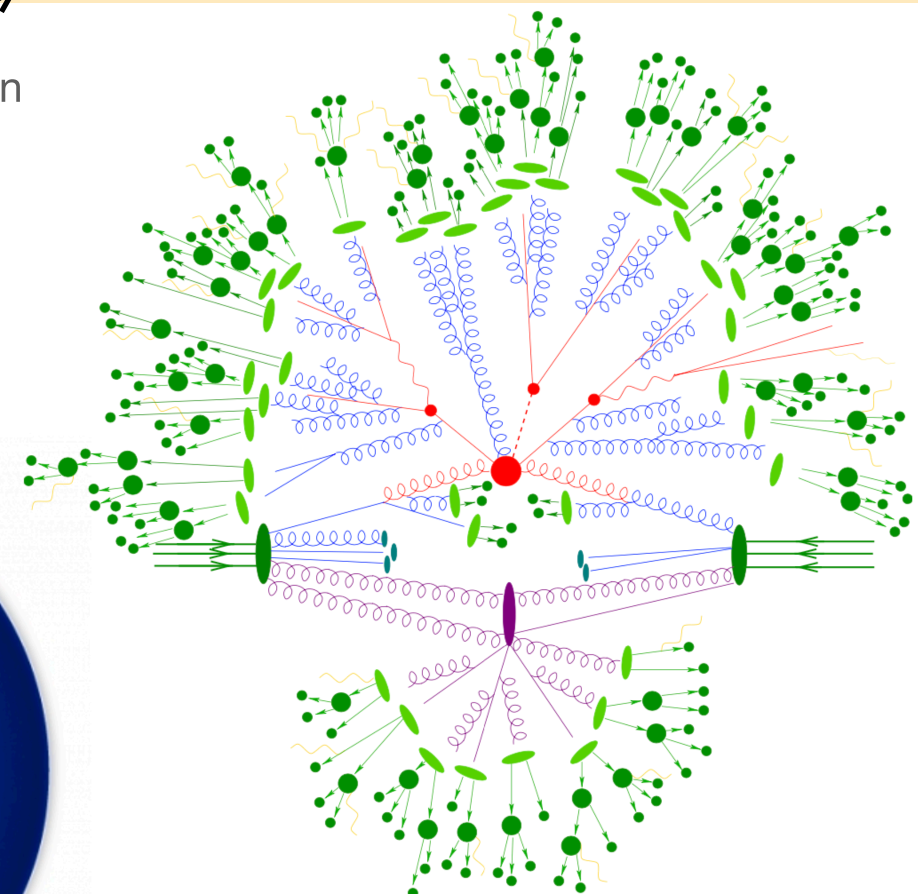
The High Energy Physics Triad

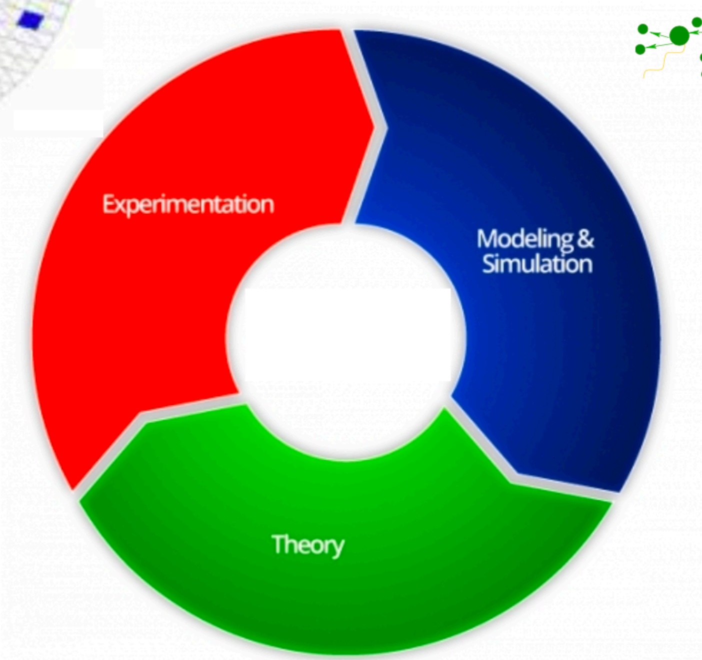
Random collision ▶ Detector response ▶ Trigger ▶ Event Reconstruction ▶ Event Sample

Random numbers ▶ Monte Carlo event generator ▶ Detector simulation ▶ Event Reconstruction ▶ Simulated Event Sample

statistical comparison







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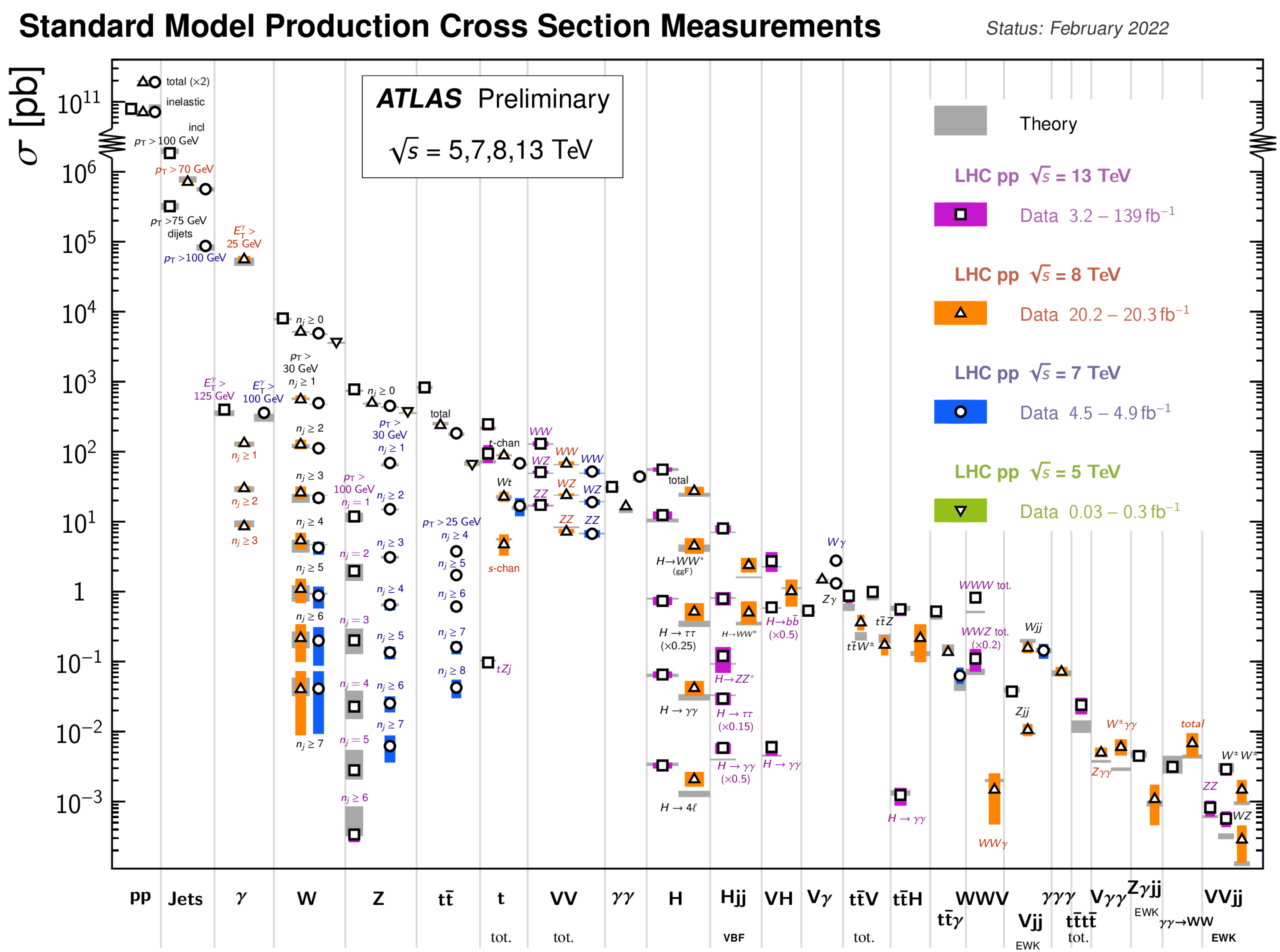
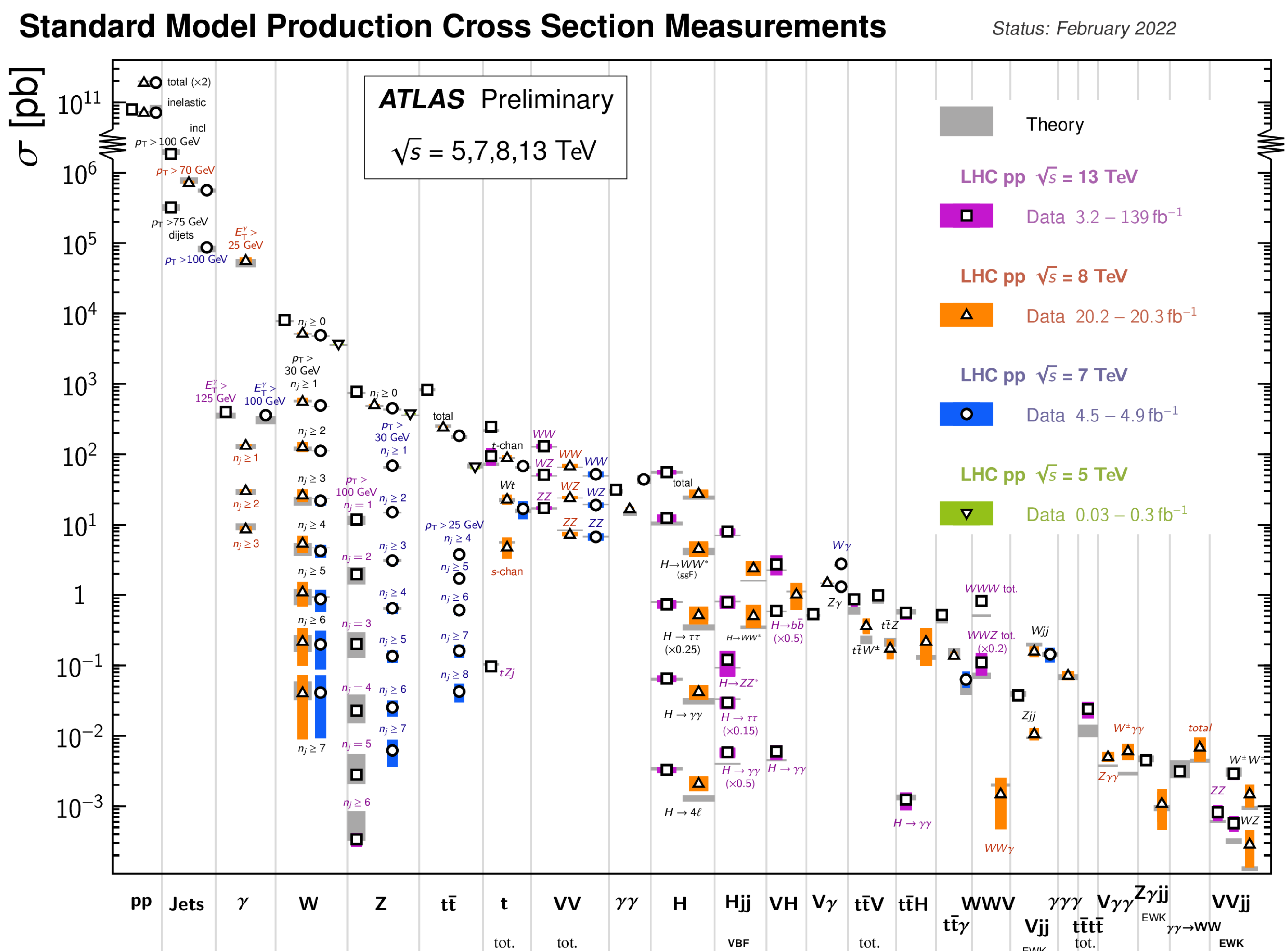
LHC Process Zoo



LHC Process Zoo

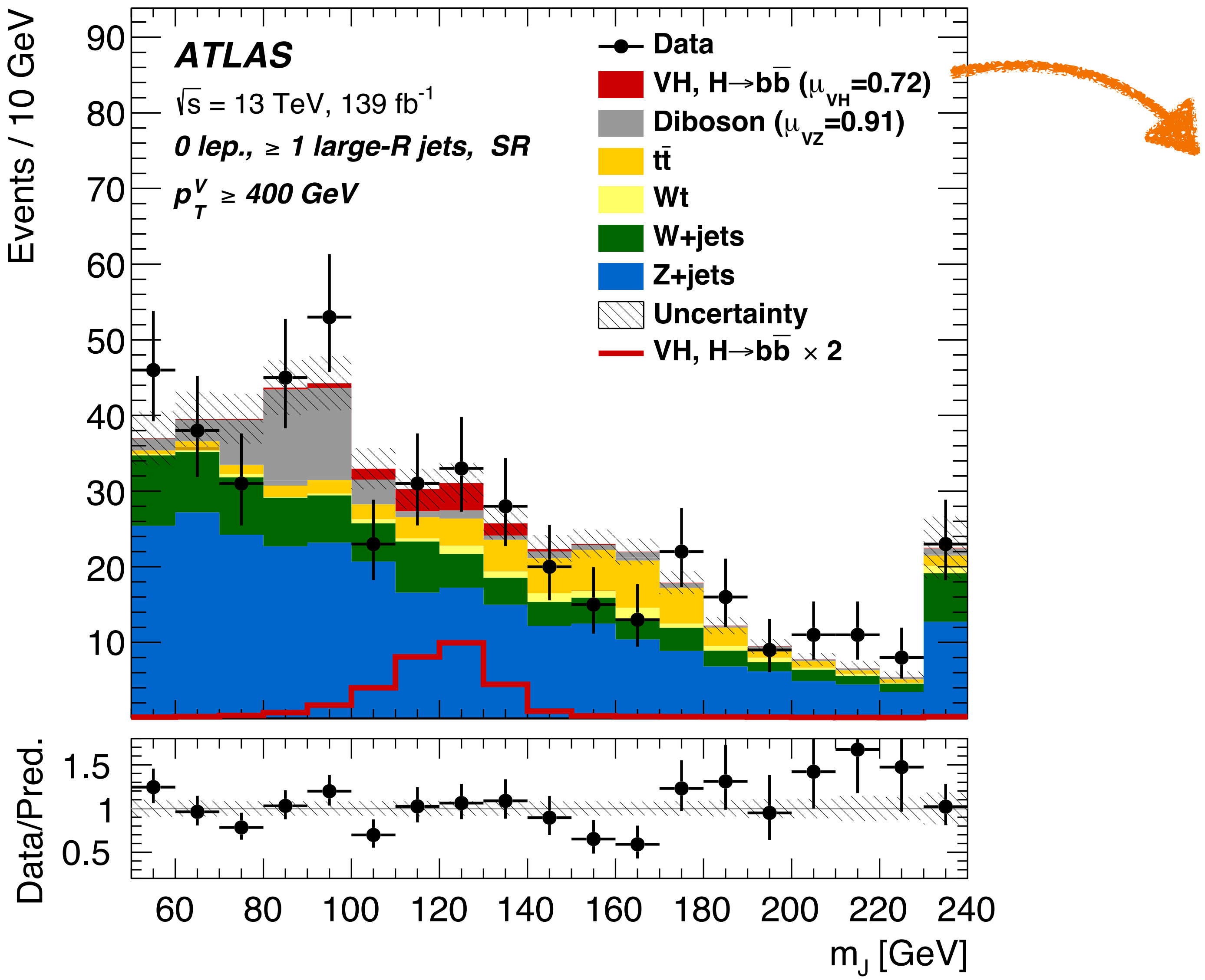


signal processes for SM measurements & BSM searches
often associated with several jets

V+jets: background to most other processes & large rates even with several extra jets

Typical Use Case & Need for Precision

[G. Aad et al. [ATLAS], Phys. Lett. B **816** (2021), 136204]



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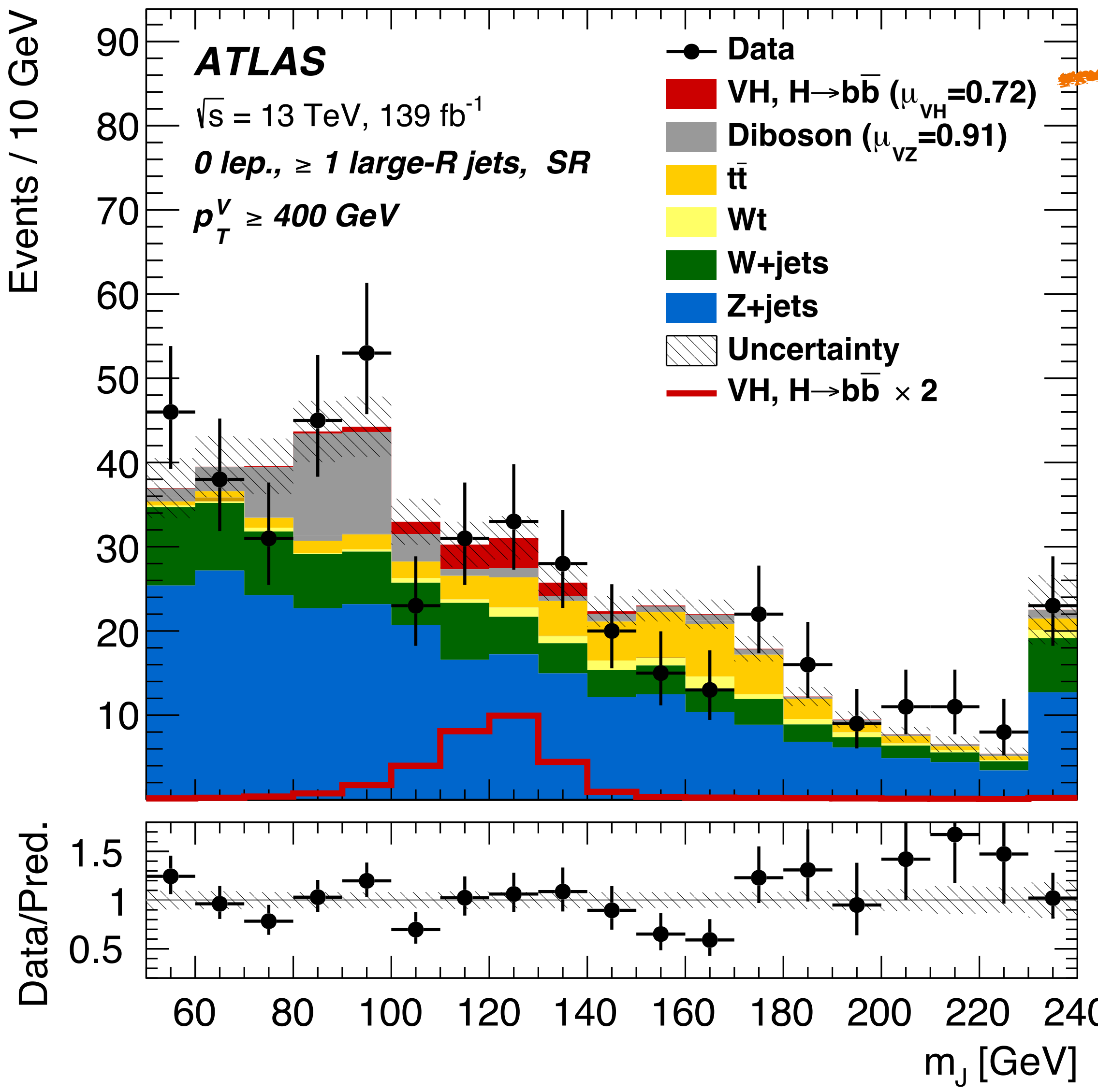

“measured signal yield to that predicted by the Standard Model, is $0.72^{+0.39}_{-0.36}$ ”

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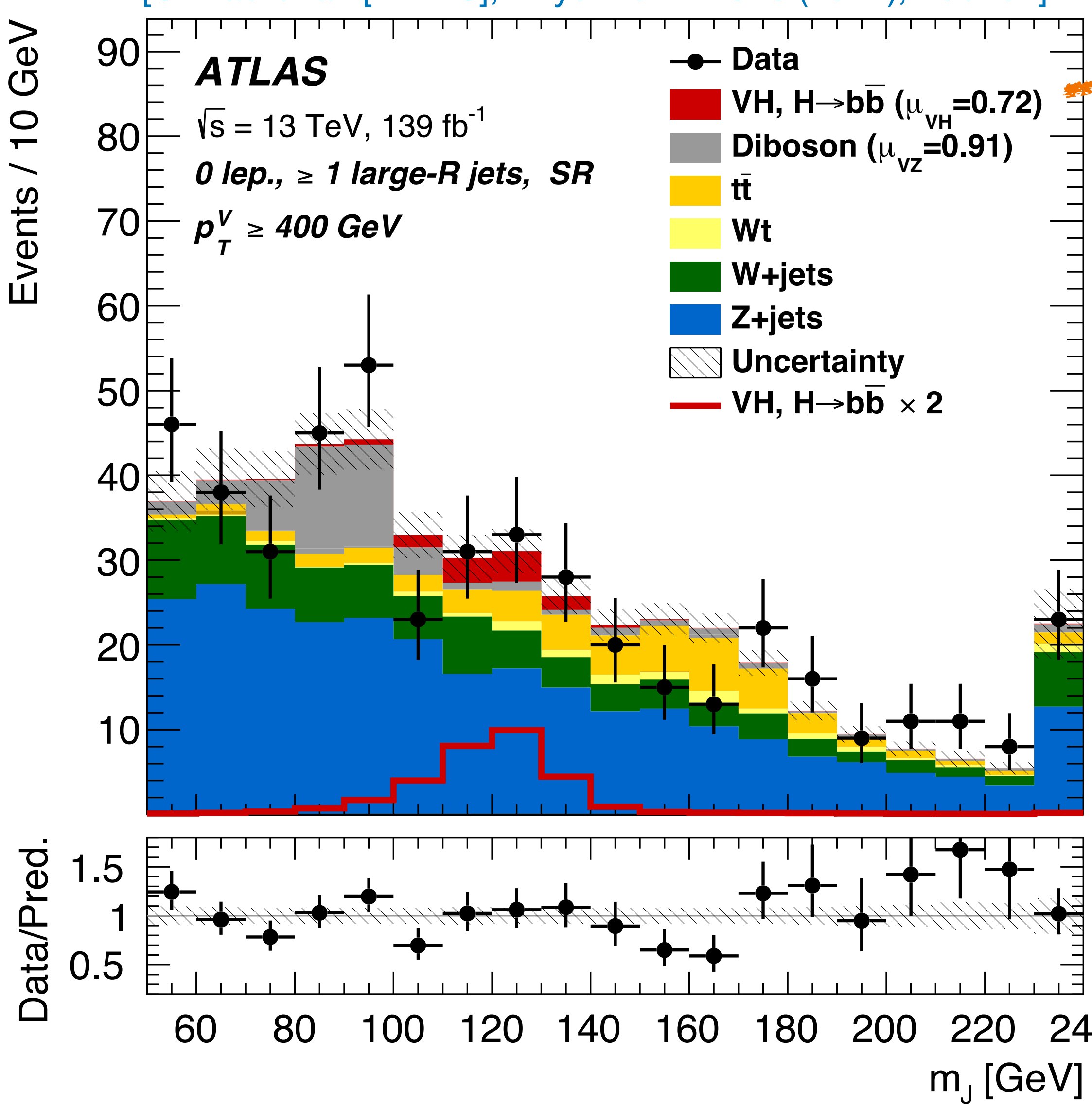


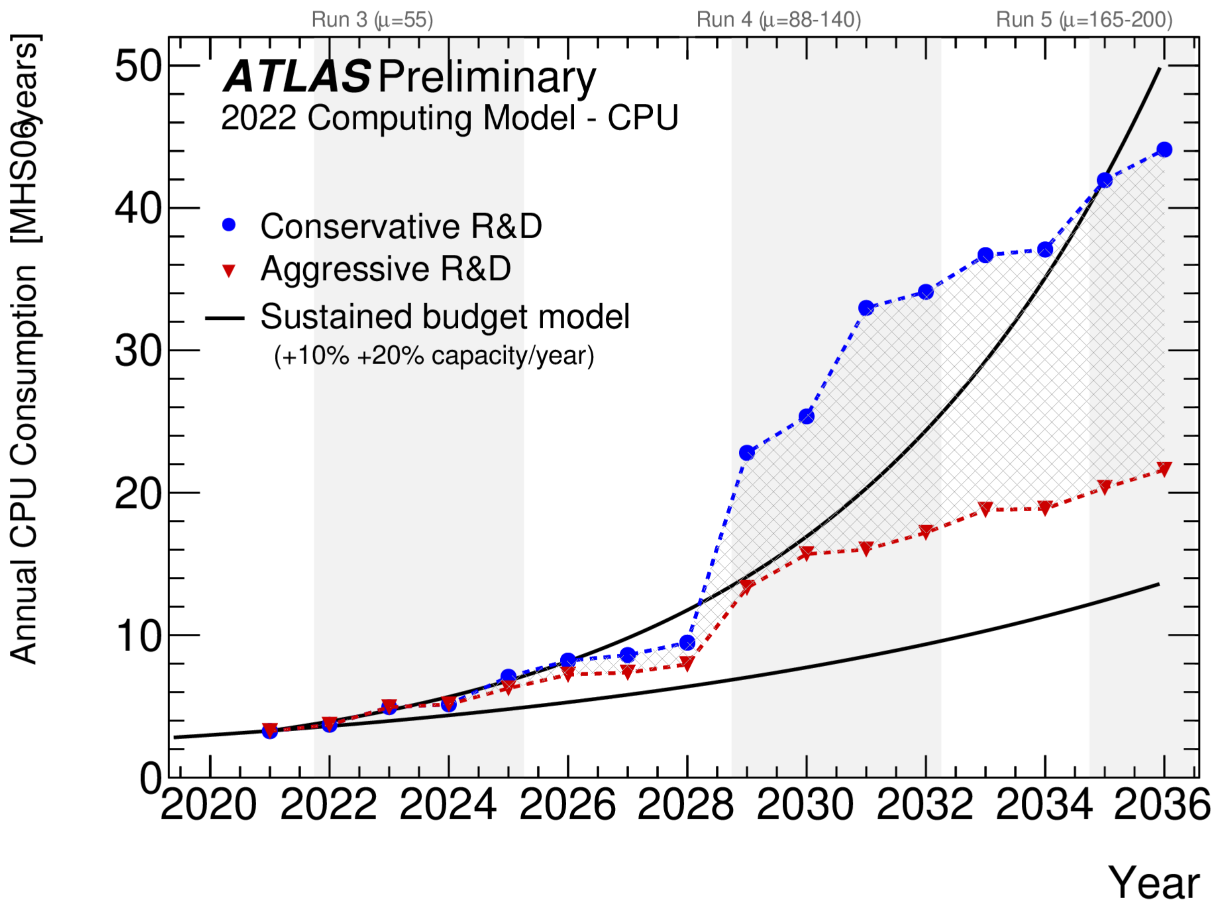
"measured signal yield to that predicted by the Standard Model, is $0.72^{+0.39}_{-0.36}$ "

- results like this need (automated) first-principle forward simulation for all relevant processes
  - accuracy in perturbative expansion: (N)NLO QCD, (N)LO EW, NLL etc.
  - multi-jet predictions
  - quantifiable uncertainties for model parameters, perturbation theory, etc.

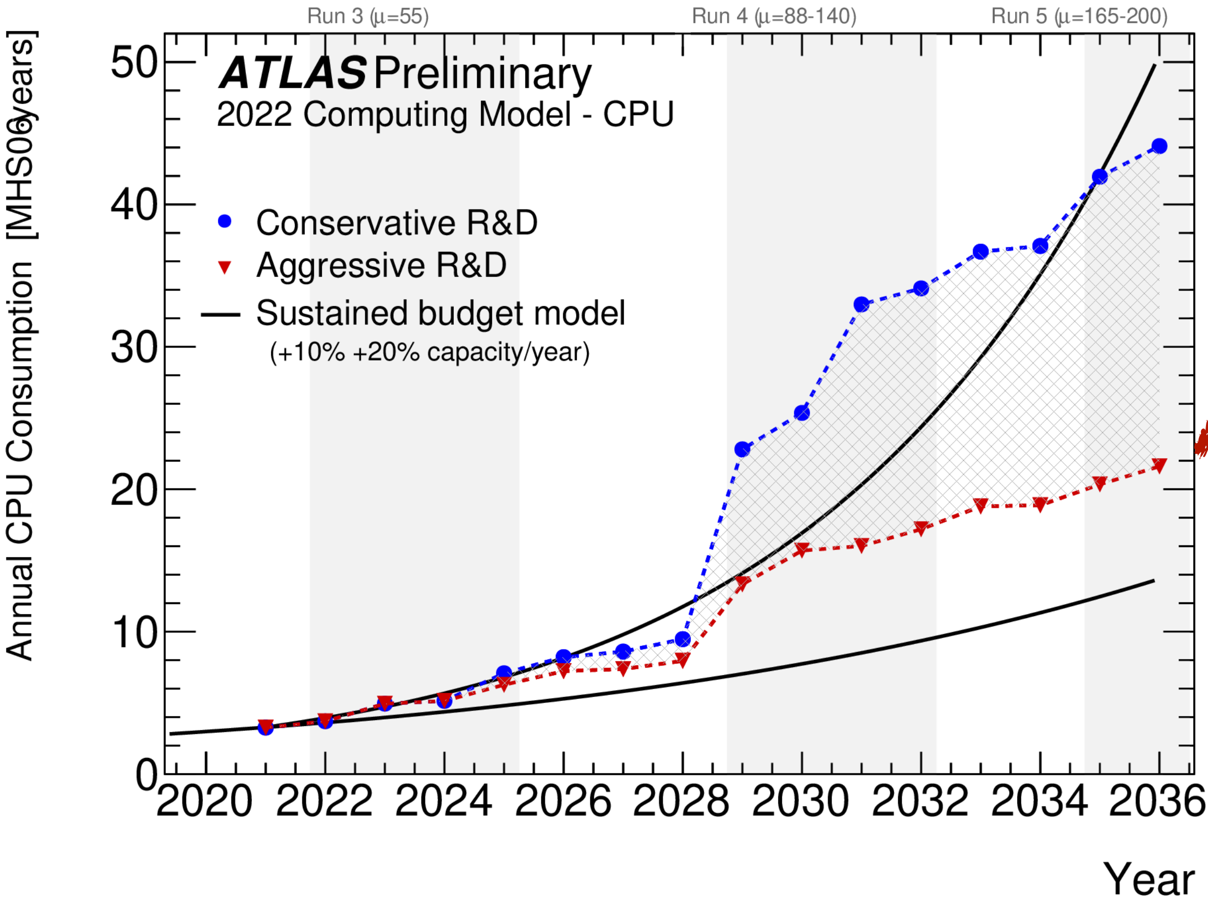
➡ MCEG provide this

➡ but precision simulations are expensive

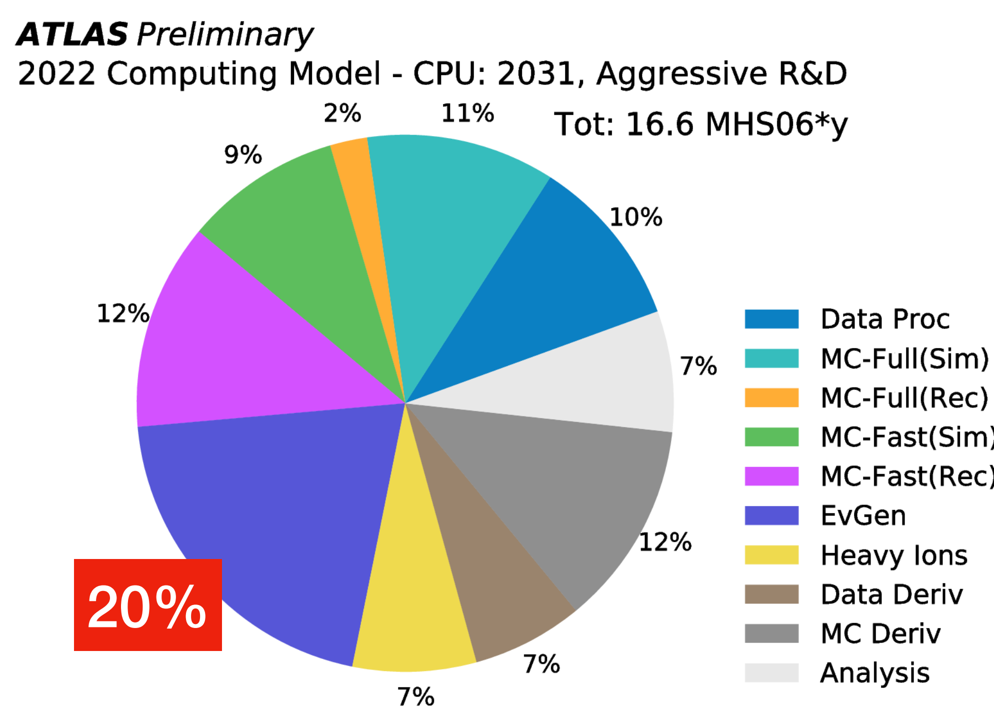
Event generation computing challenge



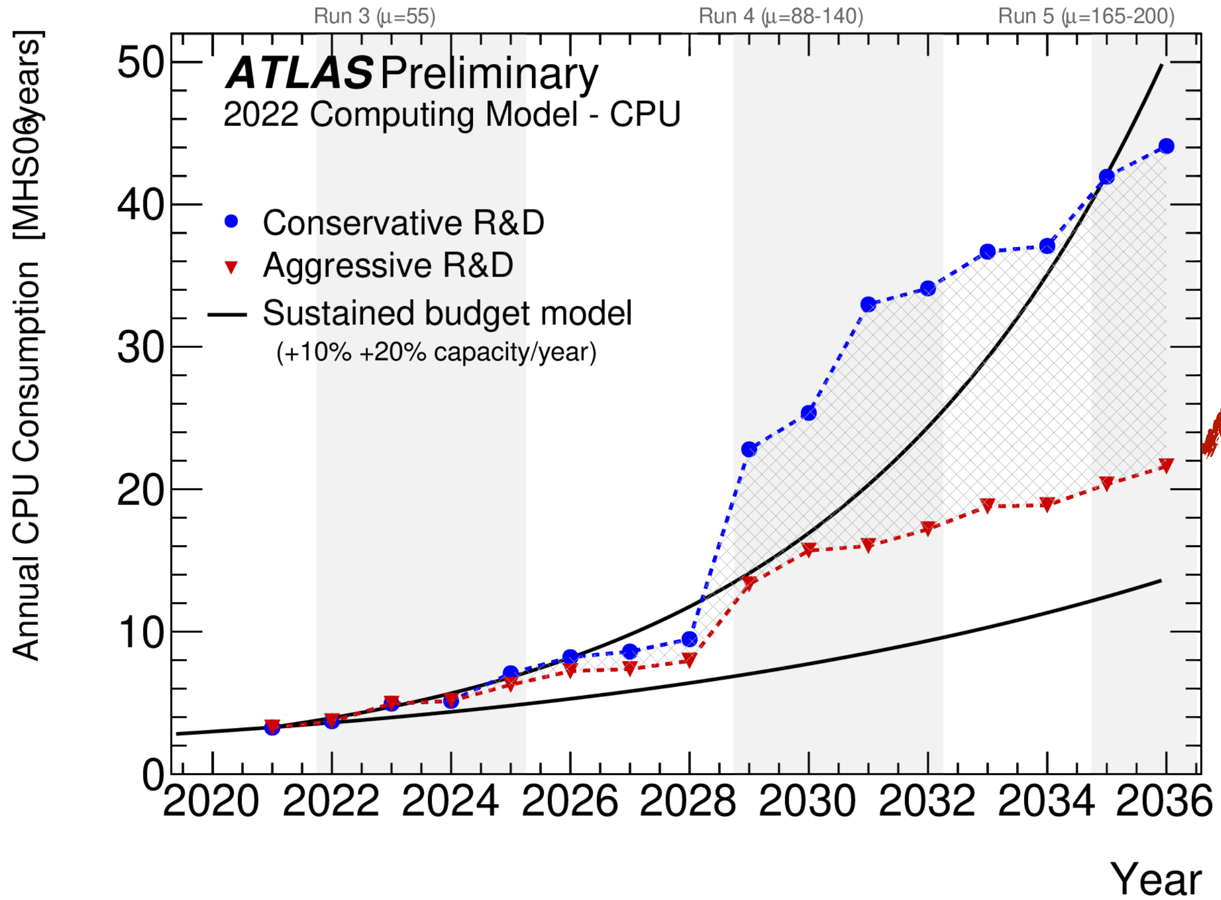
Event generation computing challenge



composed of …



Event generation computing challenge



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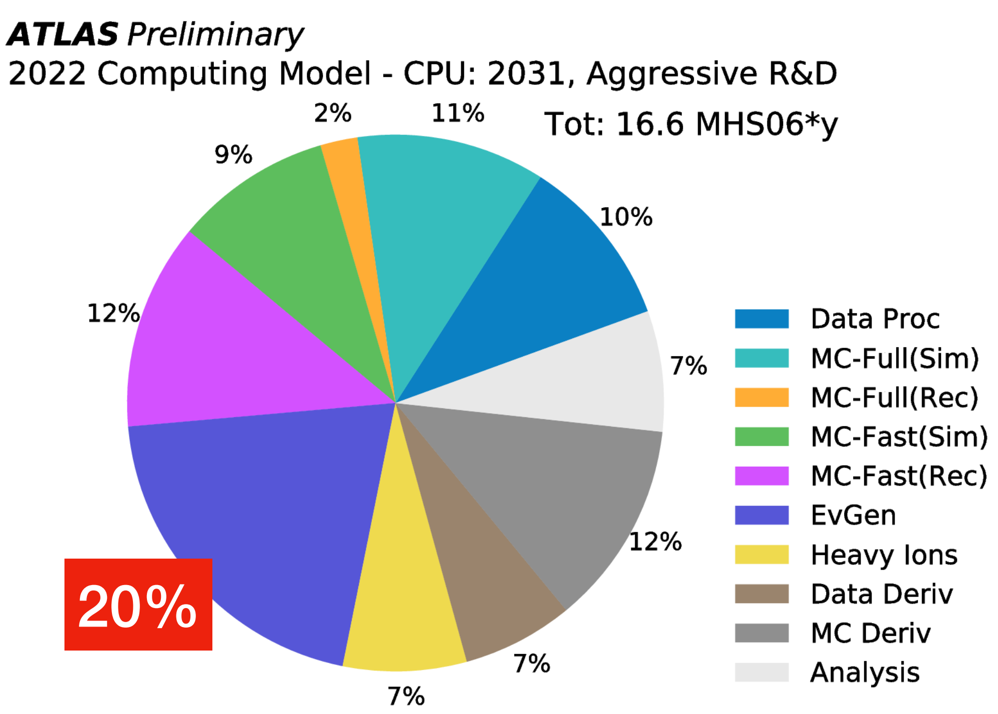
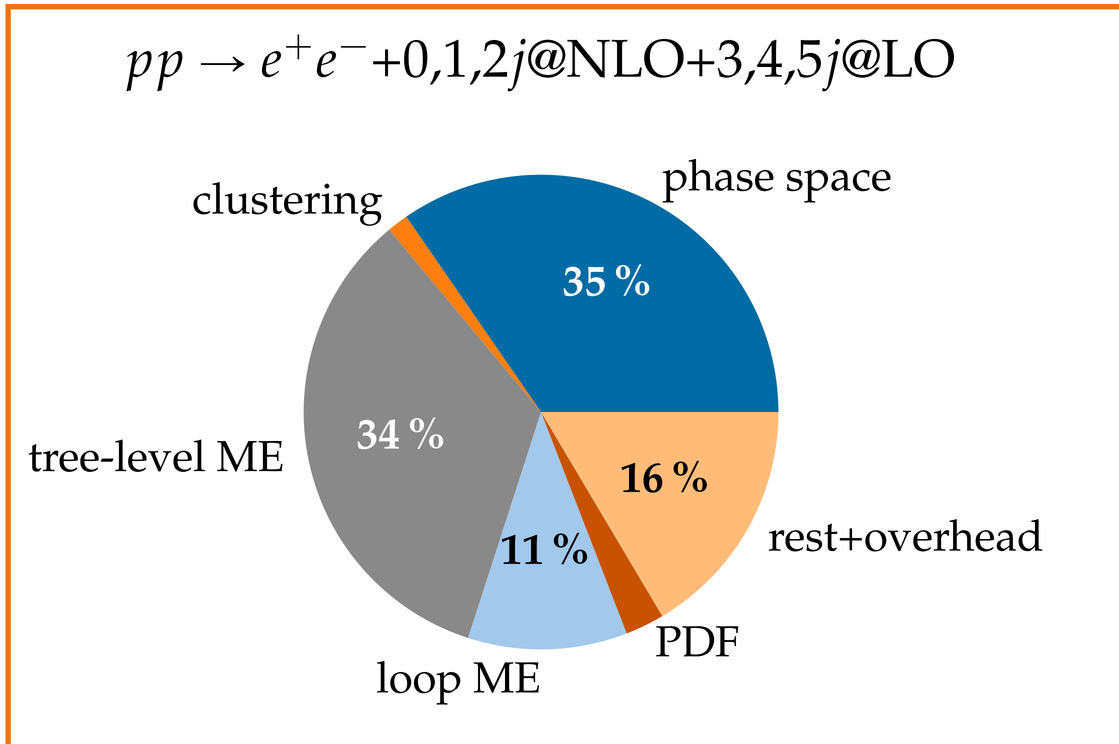


- Run-III & HL-LHC CPU requirements spark renewed interest in efficiency
  [ATLAS HL-LHC Computing CDR, Valassi et al Challenges in MCEG software for HL-LHC arXiv:2004.13687]
- Event Generators is significant consumer of CPU hours
- Beyond addressing this important issue …
  - … faster simulation also enables physics: better accuracy, higher jet multiplicity, etc.

Event Generation Bottlenecks

Our job is to sample this integral:

$$\sigma_{pp\to X_n} = \sum_{ab} \int \mathrm{d}x_a \mathrm{d}x_b \, \mathrm{d}\Phi_n \; f_a(x_a, \mu_F^2) f_b(x_b, \mu_F^2) \, |\mathcal{M}_{ab\to X_n}|^2 \, \Theta_n(p_1, \ldots, p_n)$$



relative CPU time usage for a typical ATLAS V+jets setup with SHERPA

(after series of optimisations which give a ~40x speed-up, thus ticking off one of the major HSF generator WG milestones)

[EB et al. 2209.00843]
[Talk by C. Gutschow]

➡ relevant remaining bottleneck: phase-space & matrix elements $|\mathcal{M}|^2$ (ME)

- better phase-space sampling directly reduces number of ME evaluations

When expensive integrands meet poor sampling efficiencies

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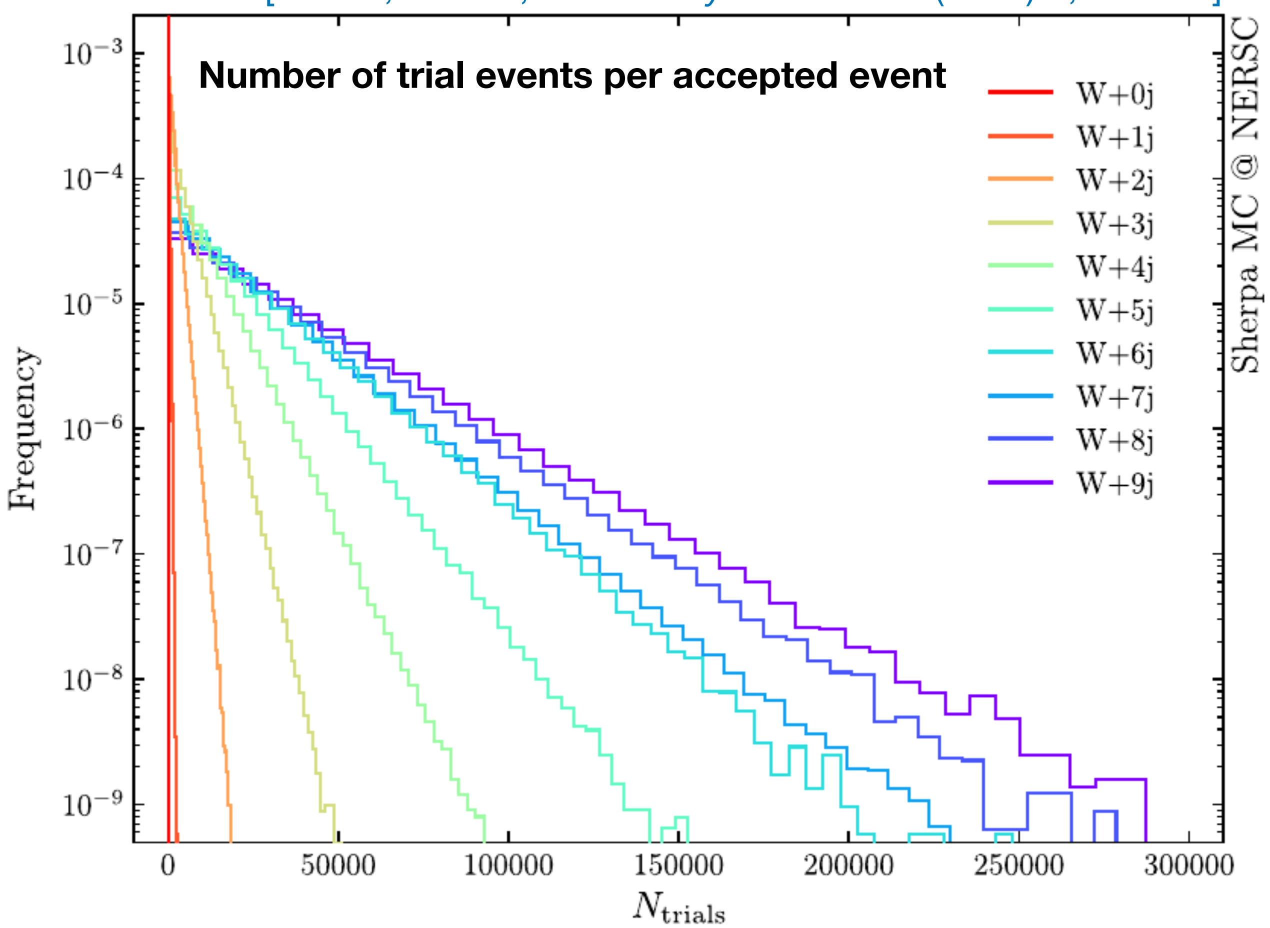
First figure of merit:

$$\epsilon = \frac{1}{\langle N_{\mathrm{trials}} \rangle}$$

(rejection sampling efficiency)

- Low sampling efficiency ϵ, why?
  - multi-modal, wildly fluctuating target distribution $f_a f_b |\mathcal{M}|^2$
  - subject to non-trivial acceptance cuts Θ_n
  - high dimensionality $\dim[\Phi_n] = 3n - 4$
- Good news: Fairly generic sampling/ integration problem

[Höche, Prestel, Schulz *Phys.Rev.D* 100 (2019) 1, 014024]



Can we use ML/NN as a remedy without compromising on precision requirements?

Multi-channel importance sampling

- Consider generic integral over target function $f(x), x \in V \subseteq \mathbb{R}^d$
- Choose variable mapping $y : V \to U \subseteq \mathbb{R}^d$

$$I = \int_V \mathrm{d}^d x\, f(x) = \int_U \mathrm{d}^d y\, \frac{f(x)}{g(x)}\bigg|_{x \equiv x(y)} \quad \text{with} \quad \left|\frac{\partial y(x)}{\partial x}\right| = g(x)$$

↪ reduce variance of MC estimate
through suitable $g(x)$, such that $w = f/g \approx \text{const}\,.$

Second figure of merit:

$$\mathrm{Var} \approx \frac{\langle w^2 \rangle - \langle w \rangle^2}{N}$$

(Monte-Carlo variance)

↪ for multi-modal target use multi-channel $g(x) = \sum_i \beta_i g_i(x)$ with $\sum_i \beta_i = 1$

$$I = \int_V \mathrm{d}^d x\, f(x) = \sum_i \int_V \mathrm{d}^d x\, \beta_i\, g_i(x) \frac{f(x)}{g(x)} = \sum_i \int_{U_i} \mathrm{d}^d y_i\, \beta_i\, \frac{f(x)}{g(x)}\bigg|_{x \equiv x(y_i)}$$

↪ ME generators use physics knowledge about $f_a f_b |\mathcal{M}|^2$ to construct channels, mapping out prominent features/singularities, but not all features are known

We can embed ML into this for additional optimisation of $y(x)$.
But we need to (i) guarantee phase-space coverage and (ii) cheap evaluation.

Neural Importance Sampling (Normalising Flows)

[Bothmann et al., SciPost Phys. 8 (2020) no.4, 069], [Gao et al., Phys. Rev. D 101 (2020) no.7, 076002]

- Further generic optimisation of random number mapping entering phase-space channels $g(x)$

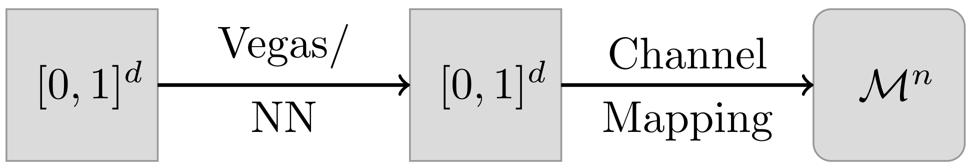
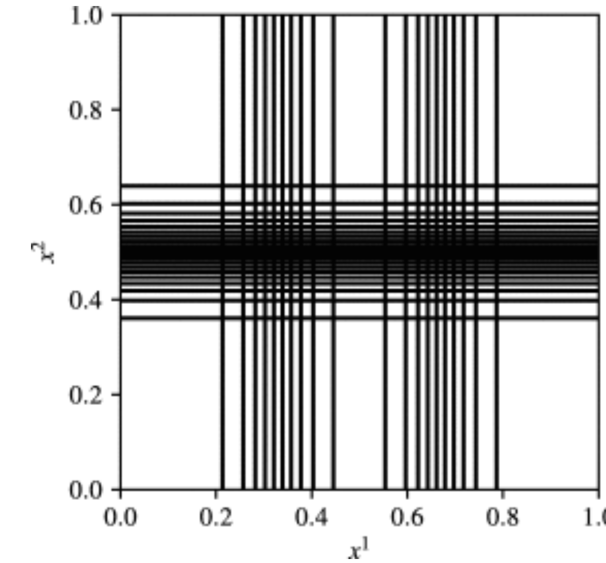


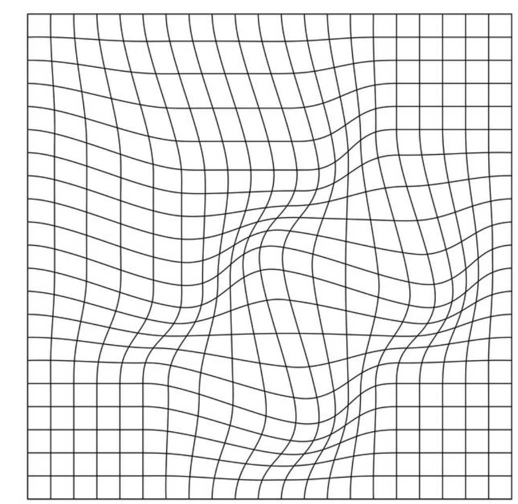
Illustration: Linear VEGAS grid



- Chain of bijective maps, called coupling layers ℓ

$$\left.\begin{array}{lll} x^A & \rightarrow & y^A := x^A \\ x^B & \rightarrow & y^B := C\left(x^B; m(x^A)\right) \end{array}\right\} \; J = \left| \begin{pmatrix} \mathrm{diag}(1) & 0 \\ \frac{\partial C}{\partial m}\frac{\partial m}{\partial x_A} & \frac{\partial C}{\partial x_B} \end{pmatrix} \right| = \left| \frac{\partial C}{\partial x_B} \right|$$

Illustration: Nonlinear NIS grid

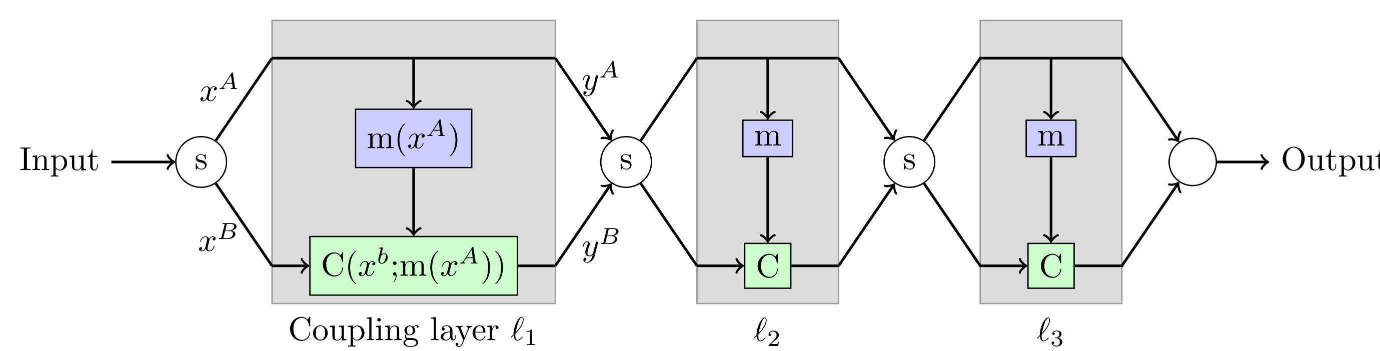


- C invertible+separable yields cheap Jacobian ~ $\mathcal{O}(d)$

- m arbitrary function → use DNN

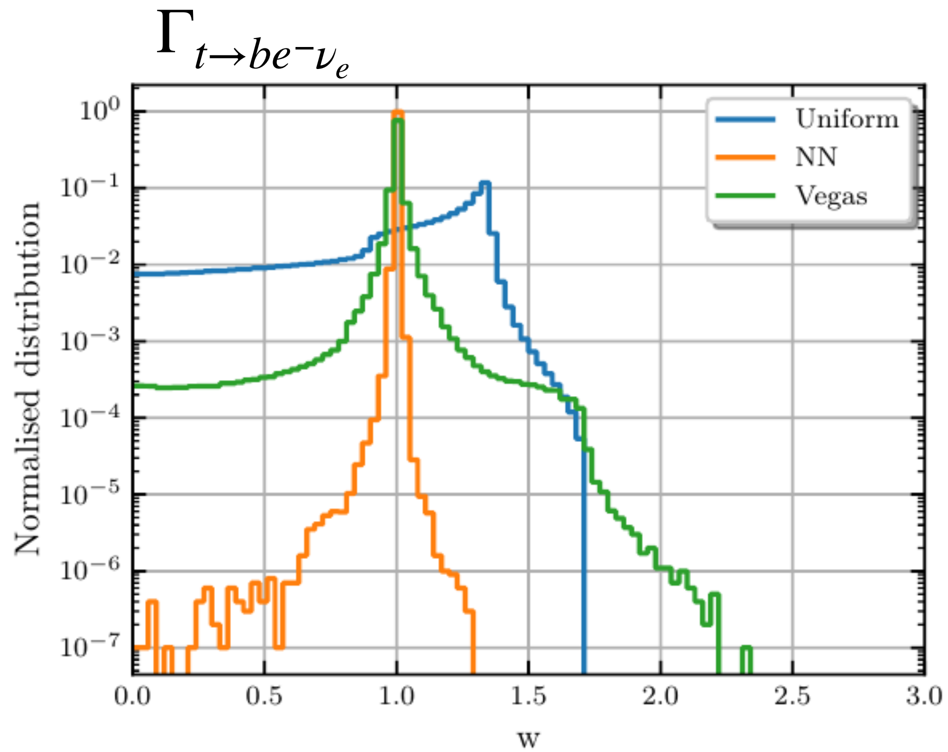
- C piecewise quadratic → „Neural Importance Sampling"
  first applied to ray tracing in 3D scenes
  [Müller et al. arXiv:1808.03856]

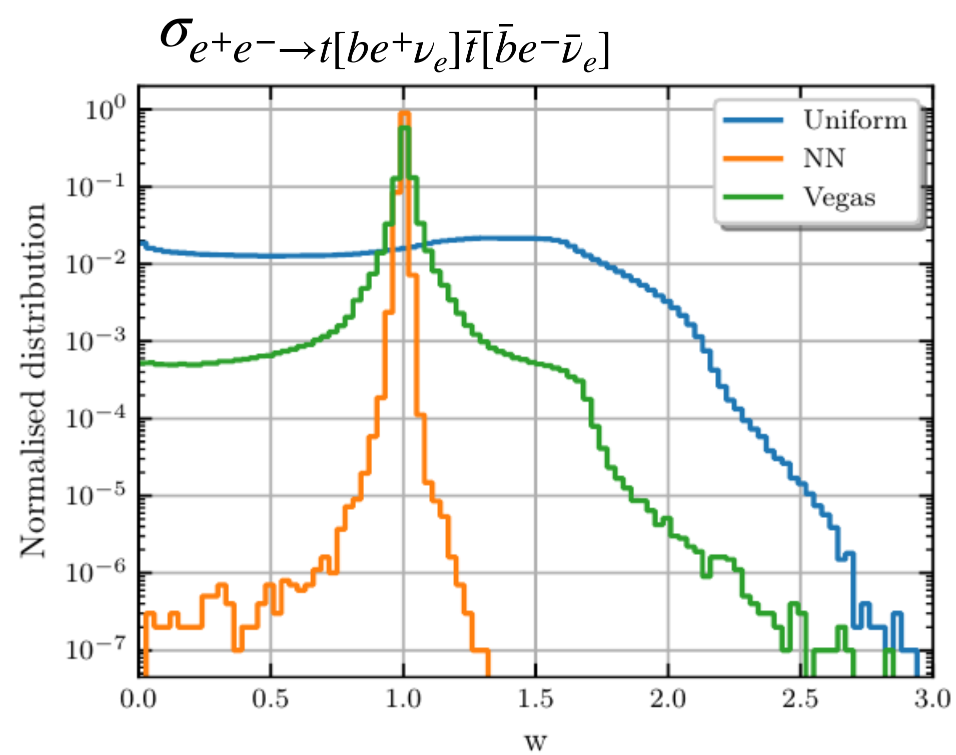
- very expressive+cheap non-linear variable transformations (non-factorisable!)



Neural Importance Sampling – Results

remember: aim for $w = f/g \approx 1$, i.e. peaked distribution of w





	top decays		top-pair production		$gg \to 3g$		$gg \to 4g$	
Sample	ϵ_{uw}	E_N [GeV]	ϵ_{uw}	E_N [fb]	ϵ_{uw}	E_N [fb]	ϵ_{uw}	E_N [fb]
Uniform	59 %	0.1679(2)	35 %	1.5254(8)	3.0 %	24806(55)	2.7 %	9869(20)
Vegas	50 %	0.16782(4)	40 %	1.5251(1)	27.7 %	24813(23)	31.8 %	9868(10)
NN	84 %	0.167865(5)	78 %	1.52531(2)	64.3 %	24847(21)	48.9 %	9859(10)

- Smaller impact for more complicated (multi-channel) processes, similar in [Gao et al., Phys. Rev. D 101 (2020) no.7, 076002]
- GPU evaluation of MEs desirable for efficient training cf. talks by M. Knobbe, R. Wang and A. Valassi
- Alternative to ML-*assisted* phase space sampling: directly learn target distribution using autoregressive flows, GANs, VAEs [Stienen and Verheyen SciPost Phys. **10**, 038 (2021)], [Butter, Plehn and Winterhalder, SciPost Phys. **7** (6), 075 (2019)], [Sipio et al. JHEP **08**, 110 (2019)], [Otten et al. Nature Commun. **12** (1), 2985 (2021)], [Choi and Lim, J. Korean Phys. Soc. **78** (6), 482 (2021)]
    - if no surjectivity guarantee → might miss tails of distributions and get small bias in overall integration result

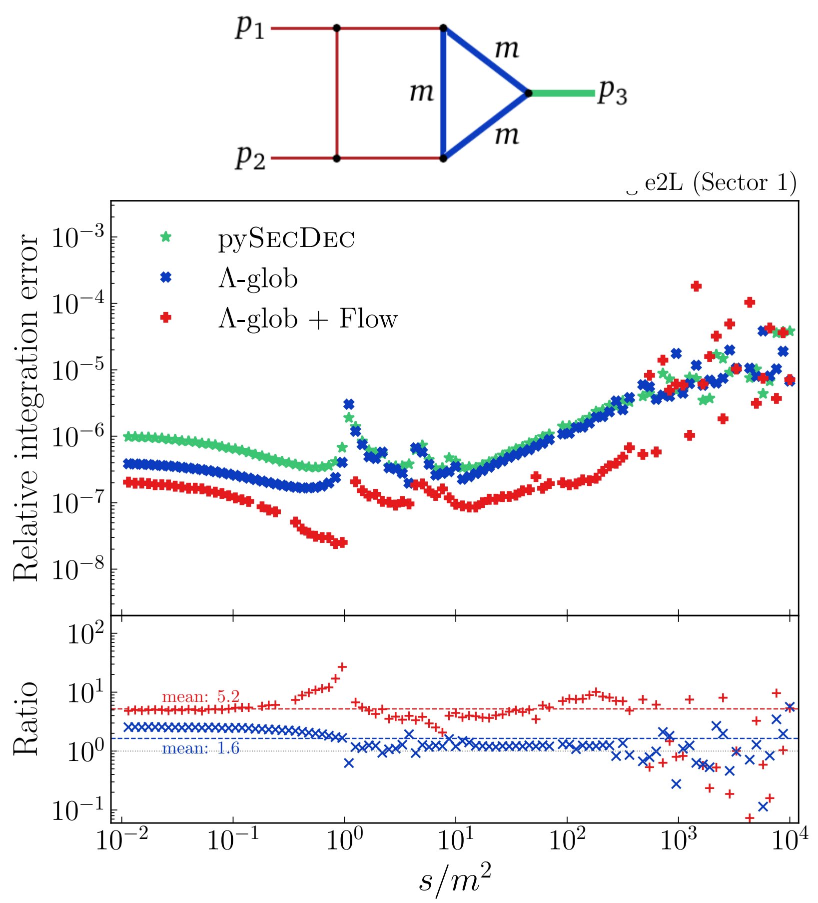
Neural Importance Sampling – Spin-Offs

Aim: Improve numerical evaluation of integral over Feynman parameters in multi-loop diagrams.

Method: Use Neural Importance Sampling to improve sampling

2-loop, one massive

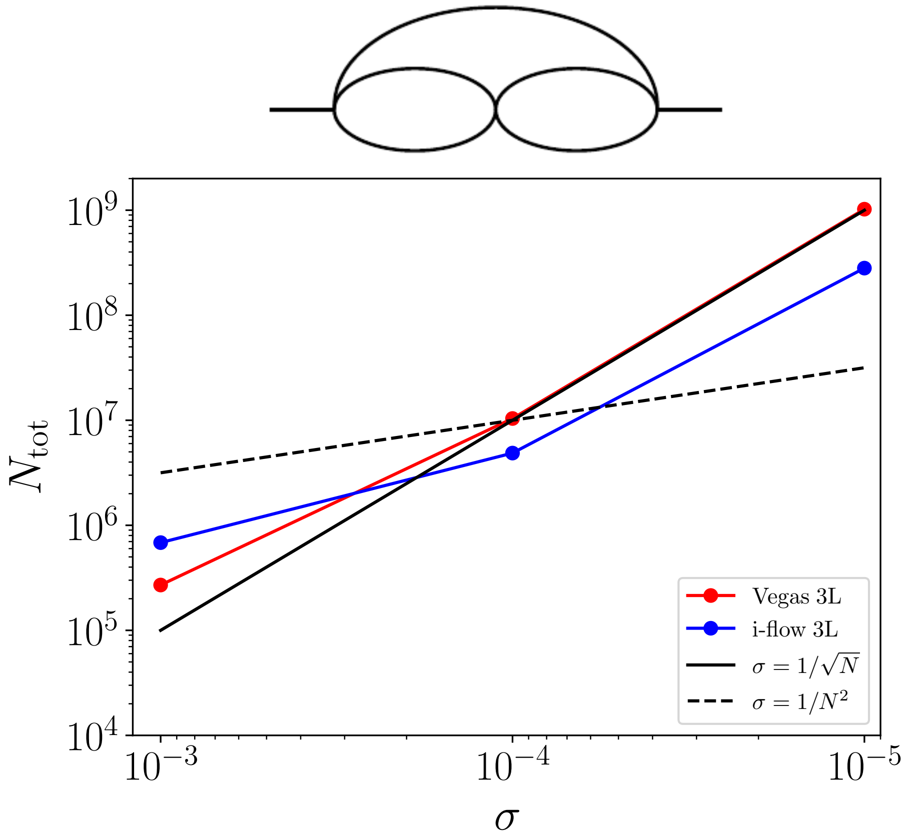
[Winterhalder et al., "Targeting multi-loop integrals with neural networks", arXiv:2112.09145 [hep-ph]]



- 6 dimensions
- Achieve reduction of numerical uncertainties by 2–10x

1,2,3-loop binary dynamics in GR

[Jinno, Kälin, Liu and Rubira: "Machine Learning Post-Minkowskian Integrals", arXiv:2209.01091 [hep-th]]



- 9 dimensions
- training phase included here
- Achieve precision target with less evaluations compared to VEGAS 2–3x

NN integration of multi-loop integrals
[Talk by D. Maître]

Related: application of Normalising Flows in Lattice Field Theory
[Talk by A. Singha]

More on integrating loops
[Plenary Talk by S. Badger, Talks by E. de Doncker, A. Butter]

Exploring Phase Space with Nested Sampling

[Yallup, Janßen, Schumann and Handley, Eur. Phys. J. C 82 (2022), 8]

- Transfer Bayesian inference algorithm to our sampling problem
  - applications in cosmology, statistical thermodynamics, material science
  - wide range of existing tools, e.g. `PolyChord` [Handley, Hobson and Lasenby]
- Consider uniform prior, posteriori matching target distribution
- aim: optimise rejection sampling efficiency ϵ, example $gg \to ng$:

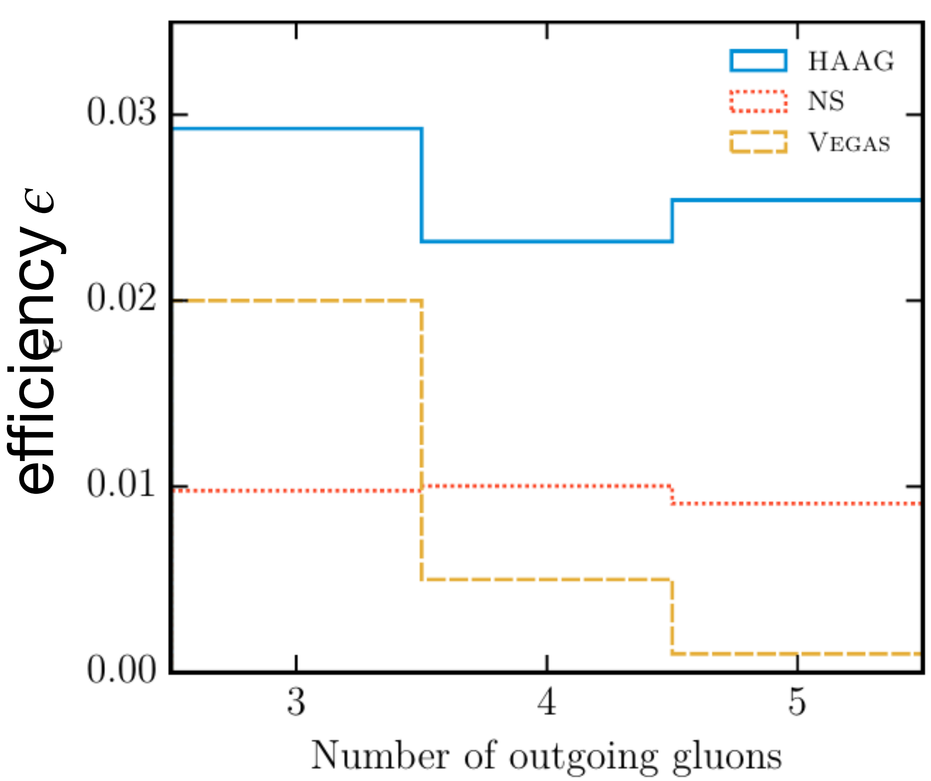
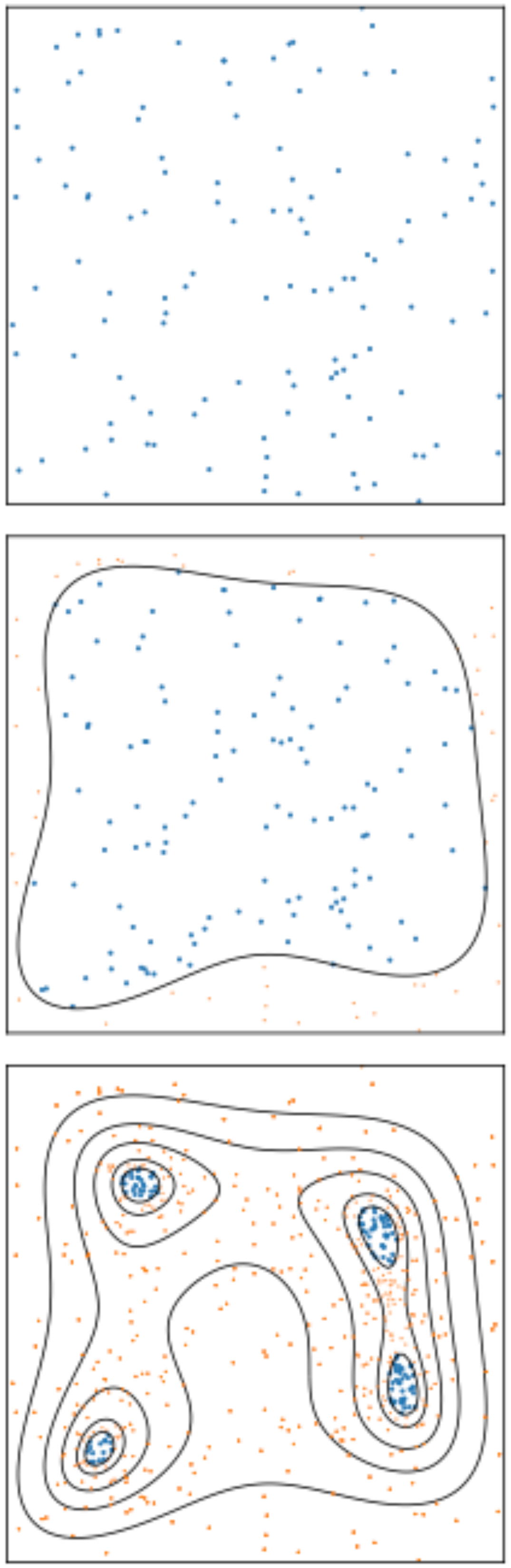
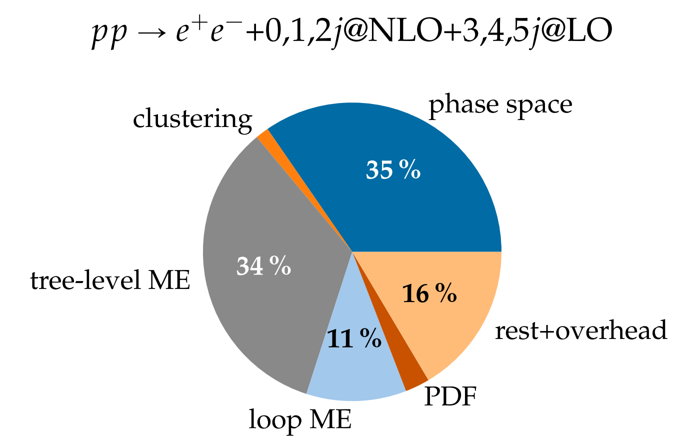


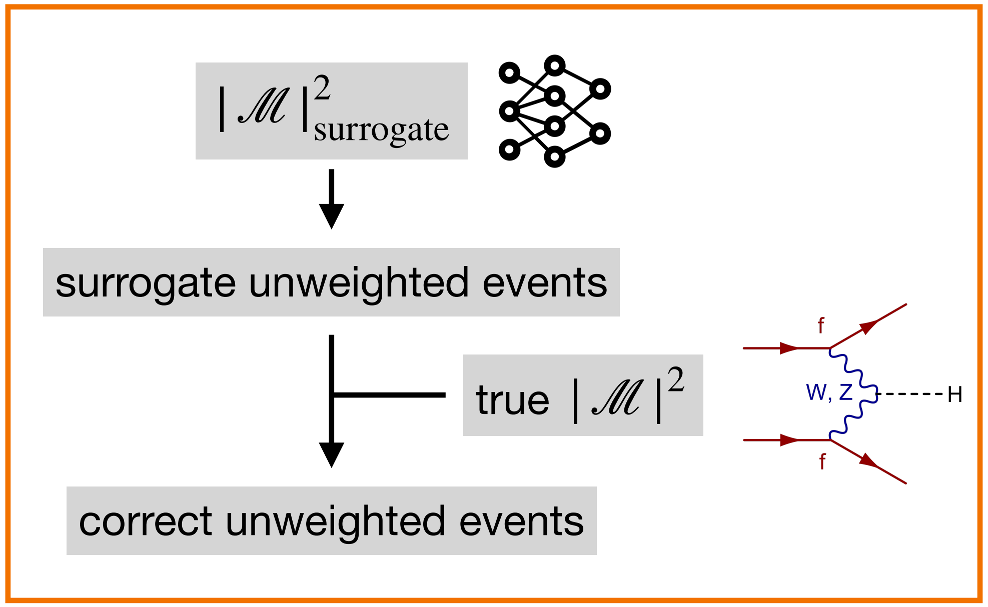
Illustration of Algorithm:

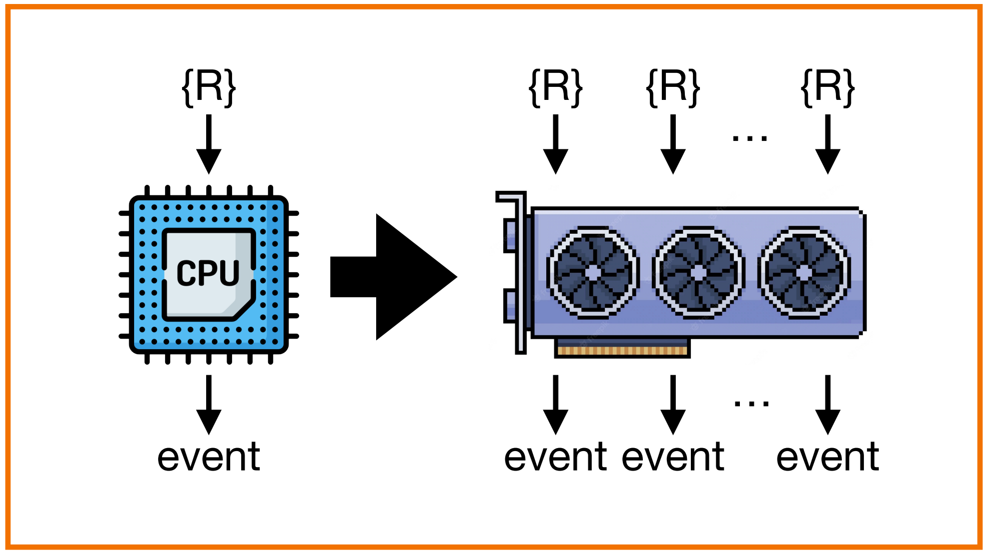


Active research on alternative approaches

- live with low phase-space efficiency, but make $|\mathcal{M}|^2$ evaluation much faster
  - surrogate unweighting
    [Danziger et al. 2109.11964], [Talk by T. Janßen]
    - use integrand emulator for trial events
    - correct accepted events later to exact result by 2nd rejection step
    - emulation must be close to the real thing, but failure to do so only reduces gain factor
    - proof-of-concept: simple DNN gives effective gain factors between 2 and 10
    - provides use case for more sophisticated ME emulators
      [Maître and Truong, JHEP 11 (2021), 066], [Aylett-Bullock, Badger and Moodie, JHEP 08 (2021), 066], [Badger et al., arXiv:2206.14831 [hep-ph]], [Janßen, Maître, Schumann, Siegert and Truong, tbp soon]
  - Accelerated $|\mathcal{M}|^2$: GPU, Vector Engines, …
    - madgraph4gpu
      [Talk by A. Valassi]
    - BlockGen
      [Talks by M. Knobbe, T. Childers]







Conclusions

- The Problem
  - LHC physics programme & computing demands efficient event generation, for signal and background processes
  - Main event generator bottleneck identified:
    - Expensive (N)NLO ME and many-jets LO ME evaluations
    - Combined with inefficient phase-space sampling
- Solutions (active & explorative research!)
  - Development and implementation of novel sampling algorithms
    Neural Importance Sampling, Nested Sampling, …
  - Beyond toy examples, traditional approaches not so easy to beat
  - Many more ideas (see previous slide)
    surrogate NN models, faster (GPU-accelerated) ME, …
- Interdisplinary relevance
  for range of integration/sampling problems
  - Cross talk to many other fields
    ML, Lattice FT, cosmo, industry, …