Monte Carlo event generation

'Fun-amentals' – part II

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Lectures and tutorials on Monte Carlo event generation

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Me in one minute…

Full professor at Sorbonne Université

- Teaching
  - ➙ Physics (all levels), mathematical methods, numerical techniques, *etc.*
  - ➙ Popular science: blogging, high-schoolers, science camps, *etc.*

- Research in theoretical HEP
  - ➙ Perturbative QCD (higher order calculations, QCD resummation)
  - ➙ BSM phenomenology (SUSY, compositeness, DM, SMEFT, extended symmetries)
  - ➙ Collider physics
  - ➙ Tools and methods for HEP (FeynRules, UFO, MadAnalysis 5, Resummino, *etc.*)
  - ➙ More information on this link

Outline

1. A comprehensive approach for Monte Carlo simulations

2. Implementing models into Monte Carlo event generators

3. From models to hard-scattering events

4. Summary

MC simulations and their role

Towards the characterisation of new physics

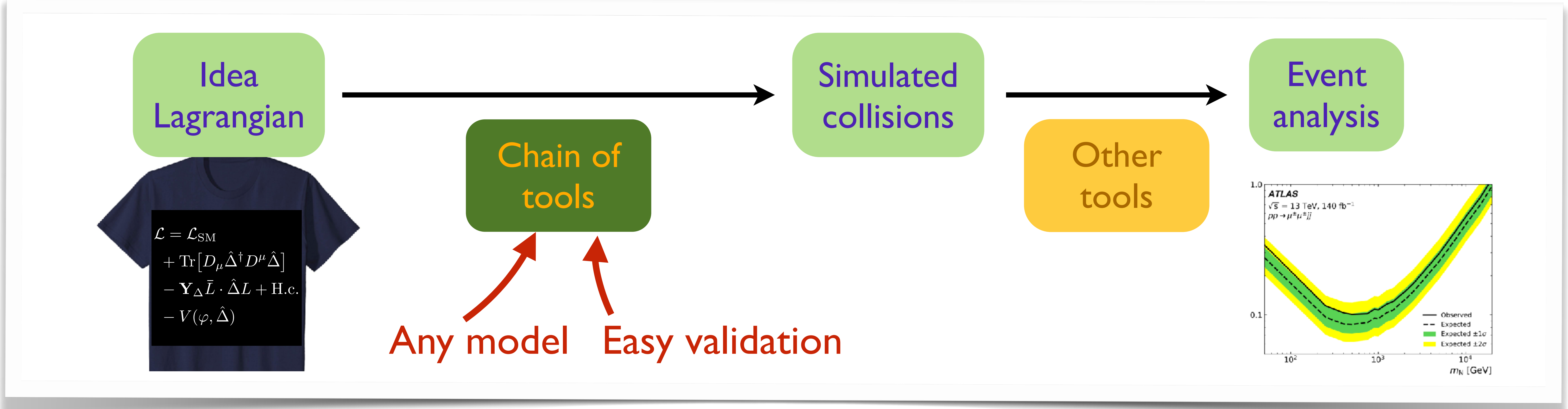
- About the nature of an observation
  - ➙ Fitting and (re)interpreting deviations
  - ➙ Prospective collider studies of varied signals
- Final words on the nature of any potential BSM
  - ➙ Accurate measurements
  - ➙ Precise predictions mandatory (also for the SM)

Monte Carlo tools ≡ key role at each step

- Prospective collider studies (*a priori* preparation)
  - ➙ Study of BSM signals in light of SM backgrounds
- Reinterpretation of existing results (*a posteriori* reactions)
  - ➙ LHC recasting in new contexts

Monte Carlo simulations standard today

- 20 − 25 years of developments ➙ LO simulations ≡ bread and butter
- Simulations at NLO (at least QCD) easily achieved


Idea
Lagrangian
$\mathcal{L} = \mathcal{L}_{\rm SM}$
$+ {\rm Tr}[D_\mu \hat\Delta^\dagger D^\mu \hat\Delta]$
$- \mathbf{Y}_\Delta \bar L \cdot \hat\Delta L + {\rm H.c.}$
$- V(\varphi, \hat\Delta)$
Chain of tools
Any model
Easy validation
Simulated collisions
Other tools
Event analysis
ATLAS
$\sqrt{s}$ = 13 TeV, 140 fb^{-1}
$pp \to \mu^\pm\mu^\pm jj$
1.0
0.1
10^2
10^3
10^4
m_N [GeV]
Observed
Expected
Expected ±1σ
Expected ±2σ

The ‘Chacal’ model – compositeness and dark matter

Modelling composite theories with dark matter and partial compositeness

- Top mass achieved from mixing with vector-like partners
  ➙ bottom quark massless

$$Q^0_{L,R} = \begin{pmatrix} T^0_{L,R} \\ B^0_{L,R} \end{pmatrix} \quad \text{and} \quad \tilde{T}^0_{L,R}$$

- A scalar dark matter candidate *X*

- Quite simple Lagrangian:
  ➙ Yukawa couplings *y* between the partners and the Higgs **Φ**
  ➙ Mass mixings **Δ** [origin not relevant]
  ➙ Yukawa couplings *λ* between *X*, the partners and the SM

$$\begin{aligned}\mathcal{L}_{\rm BSM} = & -M_Q\overline{Q^0_L}Q^0_R - M_{\tilde{T}}\overline{\widetilde{T}^0_L}\widetilde{T}^0_R - \frac{1}{2}M_X X^2 \\ & -\Big(y^*(\overline{Q^0_L}\cdot\Phi^\dagger)\widetilde{T^0_R} + \Delta_L\overline{q^0_L}Q^0_R + \Delta_R\overline{t^0_R}\widetilde{T}^0_L + \text{H.c.}\Big) \\ & + \Big(\hat{\lambda}_{\mathbf{Q}}\ \overline{Q^0_R}\ q^0_L X + \hat{\lambda}_{\mathbf{T}}\ \overline{\tilde{T}^0_L}\ t^0_R X + \text{H.c.}\Big)\end{aligned}$$

Simplified model

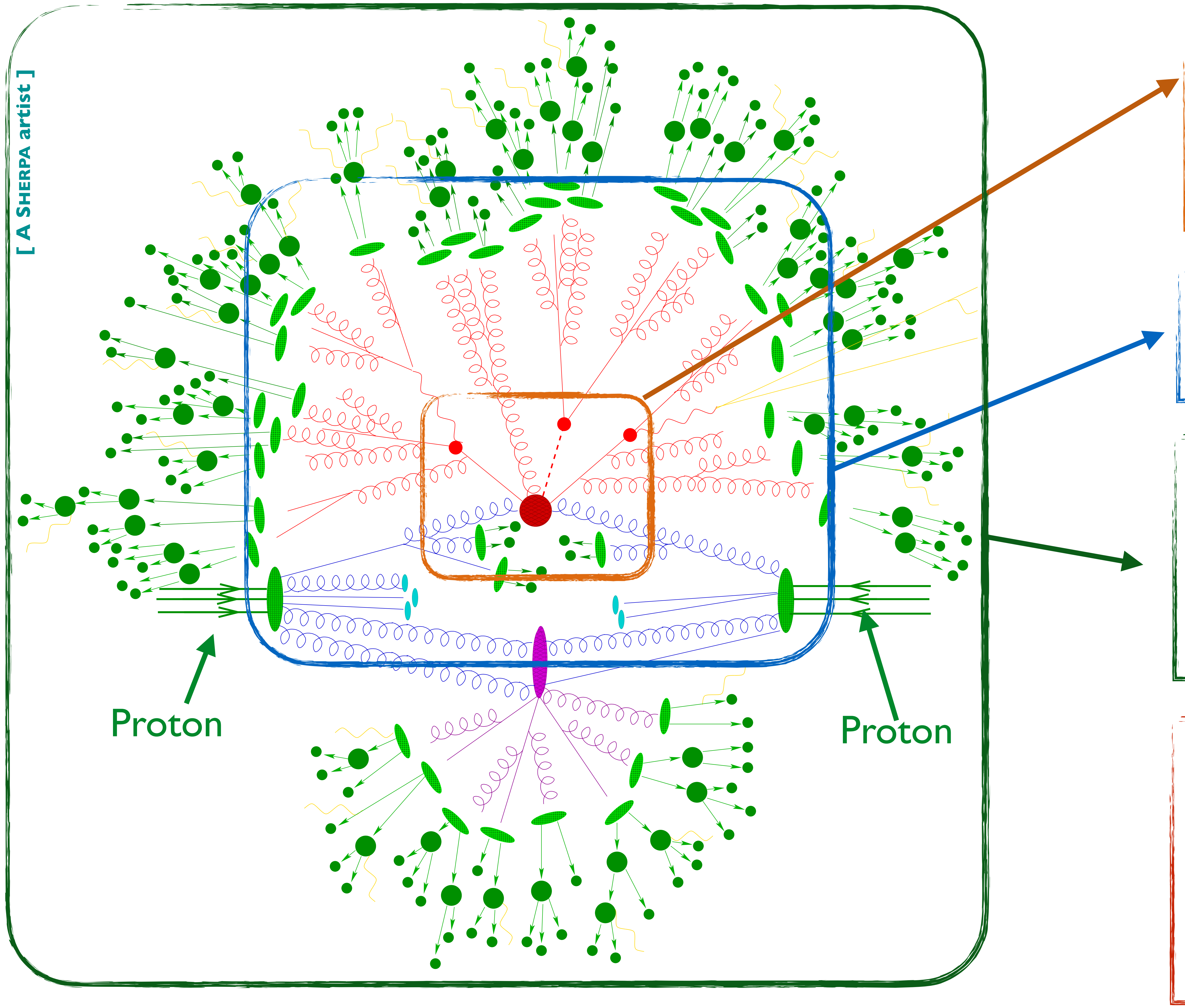
- 3 mediators and 1 dark matter (mass eigenstates ≡ gauge eigenstates)

$$T_{L,R}\,, \quad \tilde{T}_{L,R}\,, \quad B_{L,R} \quad \text{and} \quad X$$

- Lagrangian ➙ Free parameters: 4 masses and 2 couplings

$$\begin{aligned}\mathcal{L}_{\rm BSM} = \mathcal{L}_{\rm kin} - M_T\overline{T}\ T - M_B\overline{B}\ B - M_{\tilde{T}}\overline{\tilde{T}}\ \tilde{T} - \frac{1}{2}M_X X^2 \\ + \Big(\lambda_Q\big[\ \overline{T_R}\ t_L + \overline{B_R}\ b_L\ \big]X + \lambda_T\ \overline{\tilde{T}_L}\ t_R\ X + \text{H.c.}\Big)\end{aligned}$$

Deciphering a proton collision



Hard process (0.1 − 1 TeV scale)

- Depends on the model (SM/BSM)
- Perturbative calculations
- Core of this talk

Parton showering (1 − 100 GeV)

- Universal (QCD)

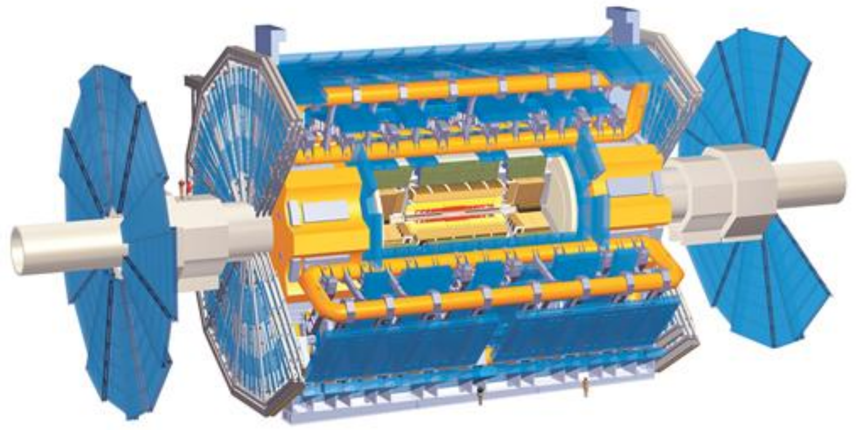
Hadronisation (sub-GeV)

- Model-based, universal

Underlying event (sub-GeV)

- Model-based, non-universal

Detector simulation (sub-MeV)

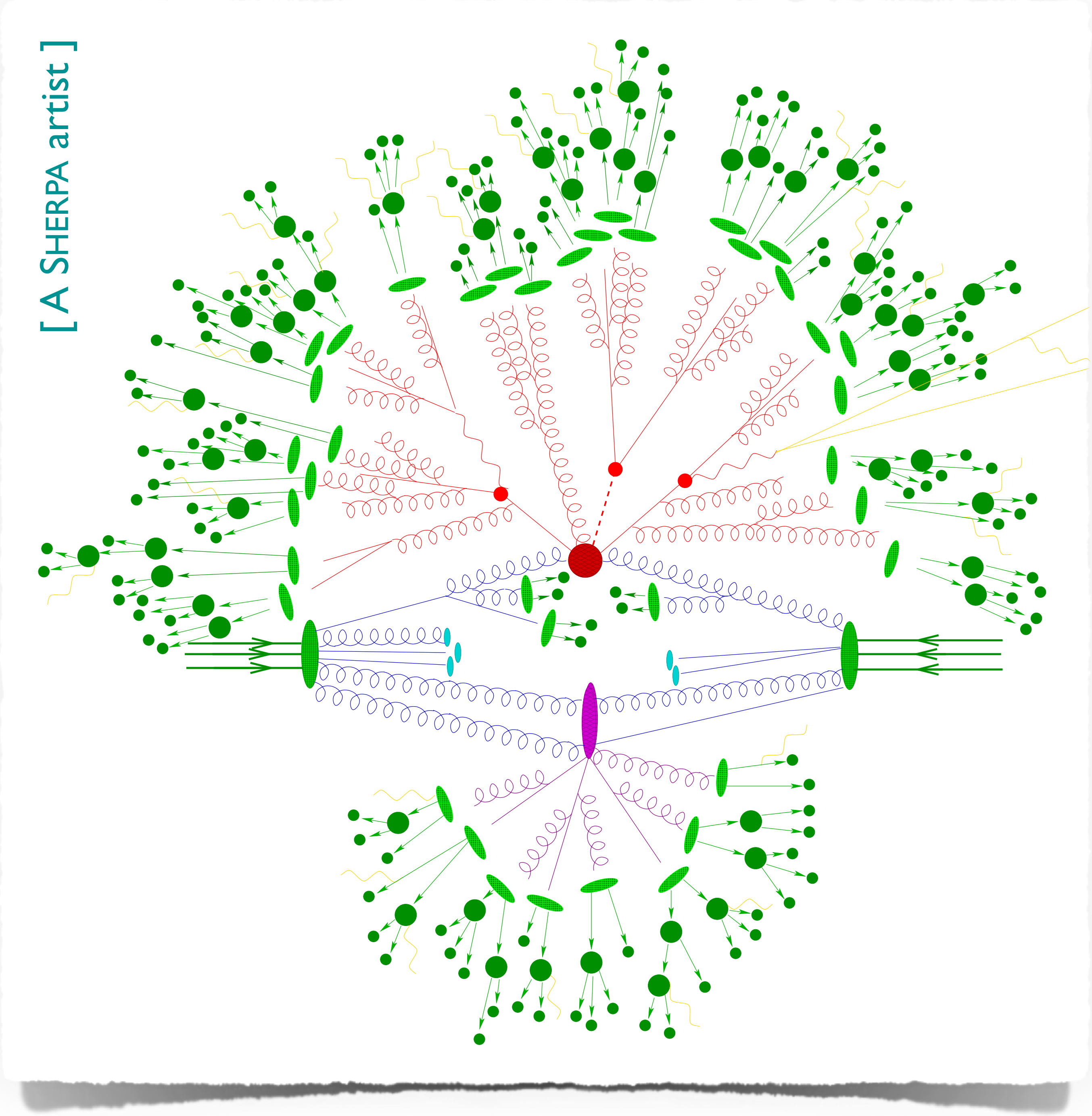


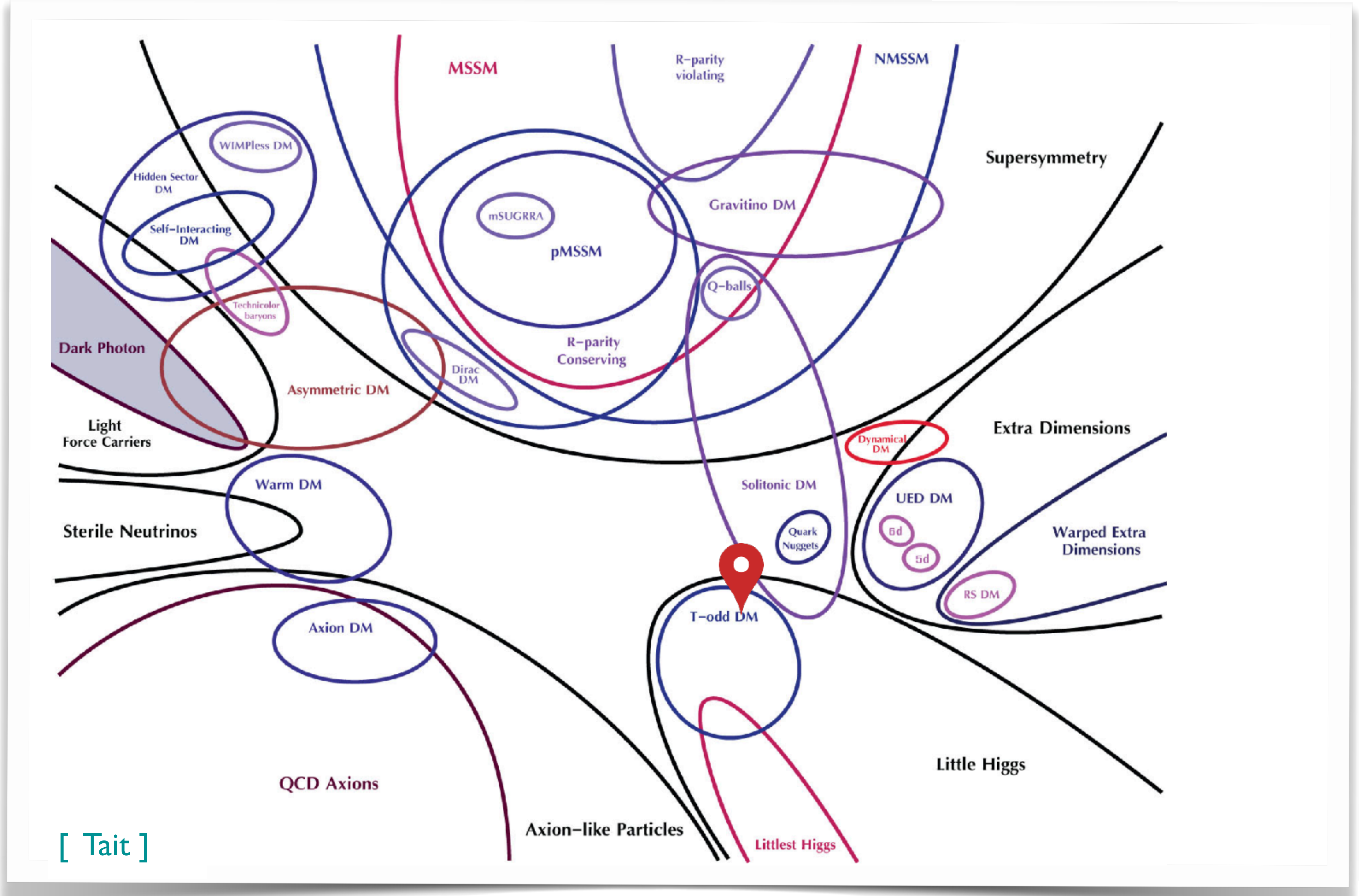
MC simulations for proton collisions

Multi-scale problem ➙ factorisation

- TeV scale: hard scattering (new physics?)
- Down to $\Lambda_{\rm QCD}$: QCD environment
- Down to sub-MeV: interactions with a detector
- Tools and methods for each step

  ➙ to be explored in this school


[A SHERPA artist]



[Tait]

SM simulations under good control

- Relevant LHC processes: known with a very good precision
- Further improvements expected in the next few years

Different challenges for new physics

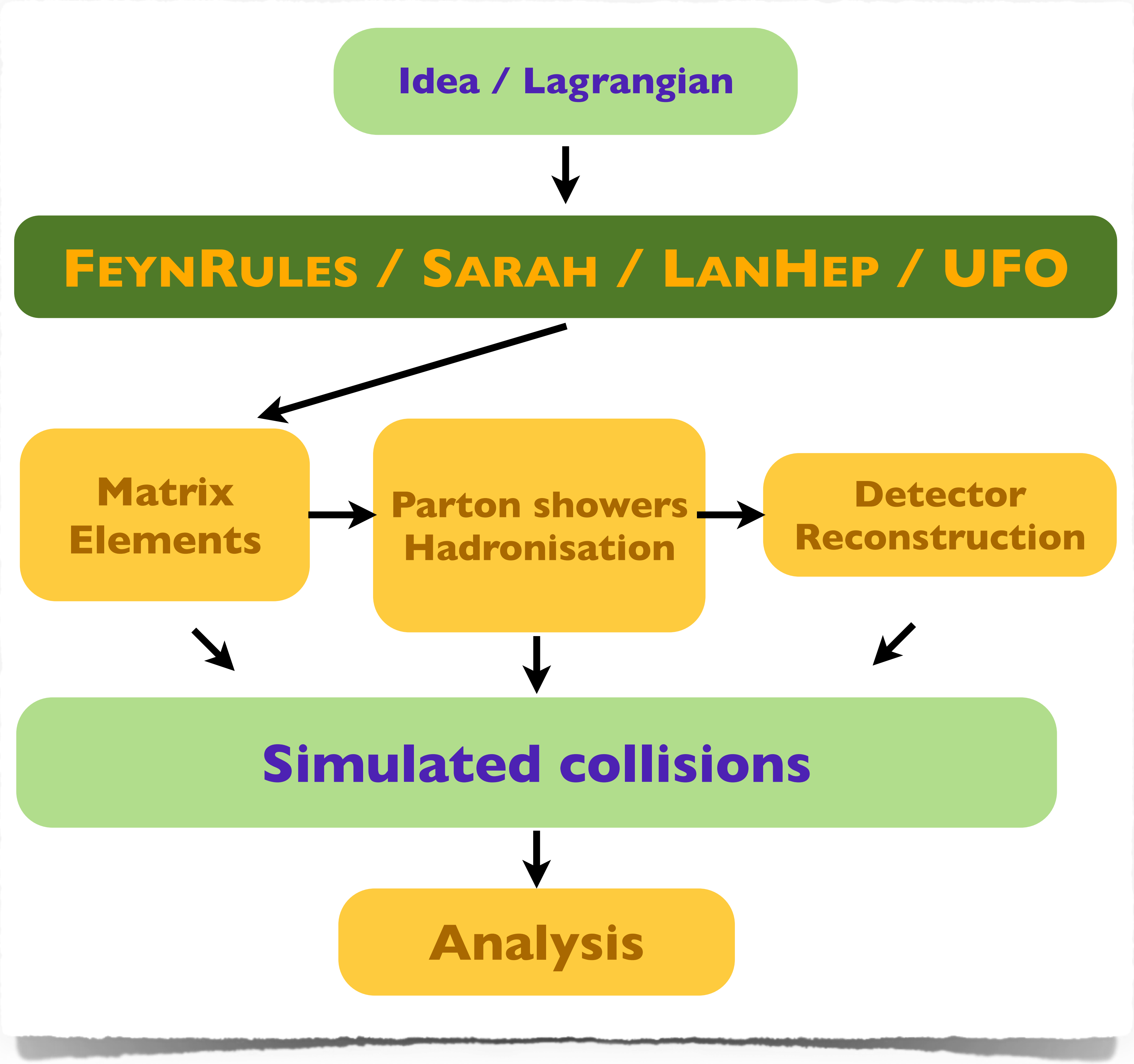
- No sign of new physics

  ➙ no leading candidate theory
- Plethora of models to consider

  ➙ many implementations required

Connecting ideas to simulations…

[Christensen, de Aquino, Degrande, Duhr, BF, Herquet, Maltoni & Schumann (EPJC`11)]



Idea / Lagrangian

FeynRules / Sarah / LanHep / UFO

Matrix Elements

Parton showers Hadronisation

Detector Reconstruction

Simulated collisions

Analysis

- Model building → FeynRules, LanHep, Sarah UFO
- Hard scattering
  - ⋆ Feynman diagram and amplitude generation
  - ⋆ Monte Carlo integration
  - ⋆ Event generation

  → CalcHep, Herwig++, MG5_aMC, Sherpa, Whizard, …
- QCD environment
  - ⋆ Parton showering
  - ⋆ Hadronisation
  - ⋆ Underlying event

  → Herwig, Pythia, Sherpa
- Detector simulation
  - ⋆ Simulation of the detector response
  - ⋆ Object reconstruction

  → Delphes Rivet / MadAnalysis 5 – SFS
- Event analysis
  - ⋆ Signal/background analysis
  - ⋆ LHC recasting

  → Rivet / MadAnalysis 5

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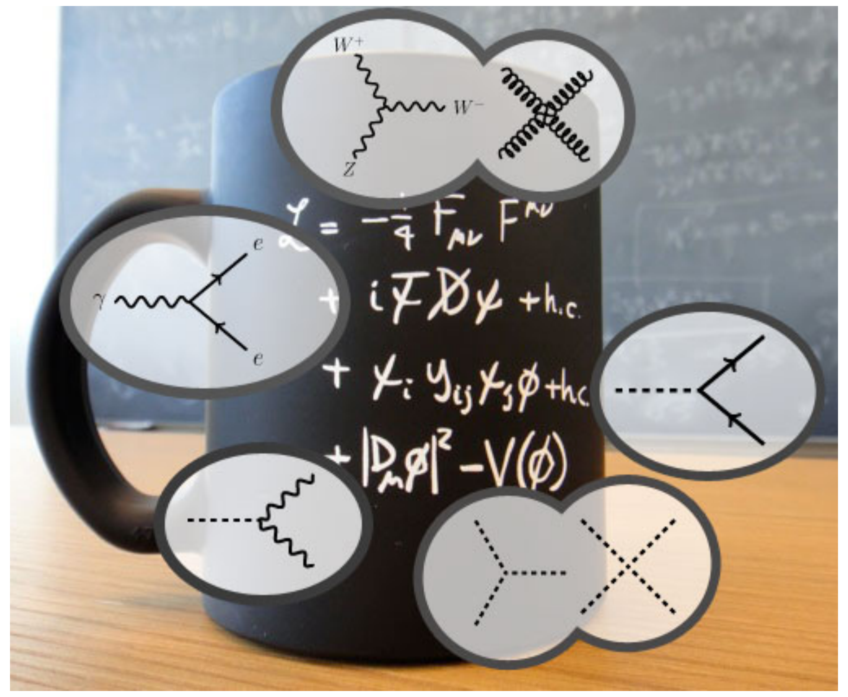
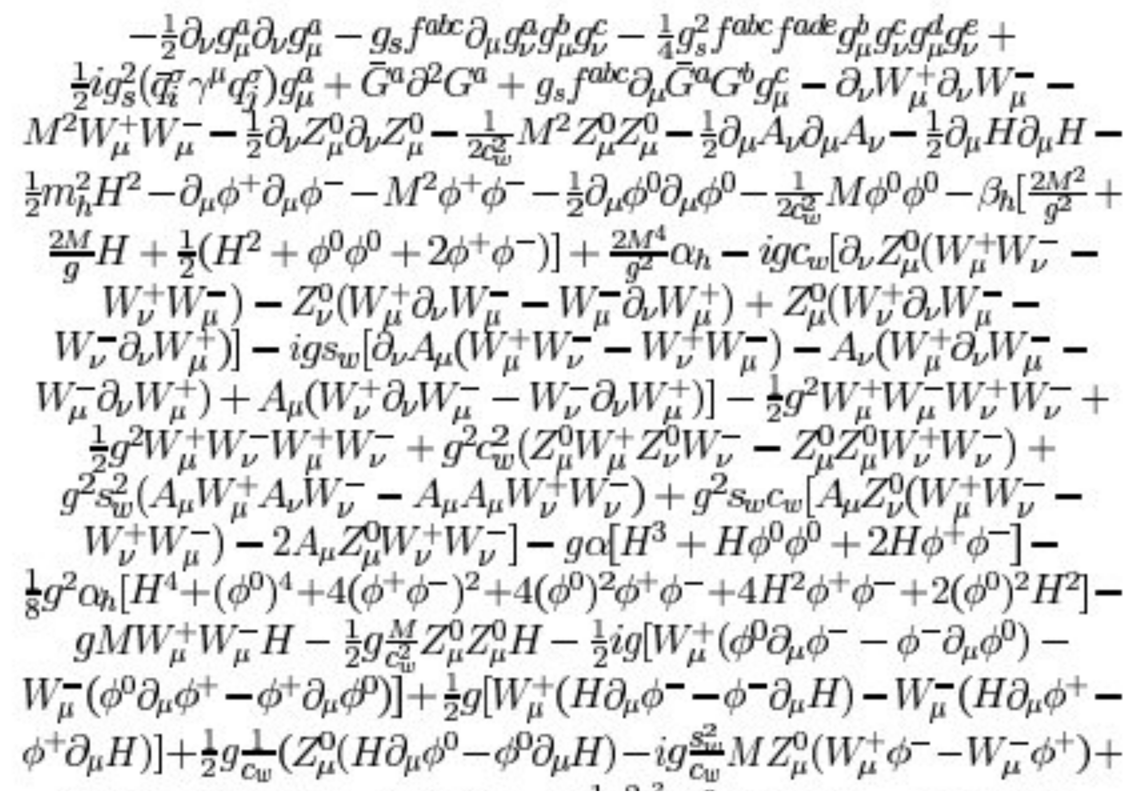
The role of the Lagrangian



$\mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu}$
$+ i\bar{\psi} \not{D} \psi + h.c.$
$+ \bar{\psi}_i y_{ij} \psi_j \phi + h.c.$
$+ |D_\mu \phi|^2 - V(\phi)$



$$
\begin{aligned}
&-\tfrac{1}{2}\partial_\nu g^a_\mu \partial_\nu g^a_\mu - g_s f^{abc}\partial_\mu g^a_\nu g^b_\mu g^c_\nu - \tfrac{1}{4} g_s^2 f^{abc} f^{ade} g^b_\mu g^c_\nu g^d_\mu g^e_\nu + \\
&\tfrac{1}{2} i g_s^2 (\bar{q}^\sigma_i \gamma^\mu q^\sigma_j) g^a_\mu + \bar{G}^a \partial^2 G^a + g_s f^{abc} \partial_\mu \bar{G}^a G^b g^c_\mu - \partial_\nu W^+_\mu \partial_\nu W^-_\mu - \\
&M^2 W^+_\mu W^-_\mu - \tfrac{1}{2}\partial_\nu Z^0_\mu \partial_\nu Z^0_\mu - \tfrac{1}{2c_w^2} M^2 Z^0_\mu Z^0_\mu - \tfrac{1}{2}\partial_\mu A_\nu \partial_\mu A_\nu - \tfrac{1}{2}\partial_\mu H \partial_\mu H - \\
&\tfrac{1}{2} m_h^2 H^2 - \partial_\mu \phi^+ \partial_\mu \phi^- - M^2 \phi^+ \phi^- - \tfrac{1}{2}\partial_\mu \phi^0 \partial_\mu \phi^0 - \tfrac{1}{2c_w^2} M \phi^0 \phi^0 - \beta_h [\tfrac{2M^2}{g^2} + \\
&\tfrac{2M}{g} H + \tfrac{1}{2}(H^2 + \phi^0 \phi^0 + 2\phi^+ \phi^-)] + \tfrac{2M^4}{g^2}\alpha_h - i g c_w [\partial_\nu Z^0_\mu (W^+_\mu W^-_\nu - \\
&W^+_\nu W^-_\mu) - Z^0_\nu (W^+_\mu \partial_\nu W^-_\mu - W^-_\mu \partial_\nu W^+_\mu) + Z^0_\mu (W^+_\nu \partial_\nu W^-_\mu - \\
&W^-_\nu \partial_\nu W^+_\mu)] - i g s_w [\partial_\nu A_\mu (W^+_\mu W^-_\nu - W^+_\nu W^-_\mu) - A_\nu (W^+_\mu \partial_\nu W^-_\mu - \\
&W^-_\mu \partial_\nu W^+_\mu) + A_\mu (W^+_\nu \partial_\nu W^-_\mu - W^-_\nu \partial_\nu W^+_\mu)] - \tfrac{1}{2} g^2 W^+_\mu W^-_\mu W^+_\nu W^-_\nu + \\
&\tfrac{1}{2} g^2 W^+_\mu W^-_\nu W^+_\mu W^-_\nu + g^2 c_w^2 (Z^0_\mu W^+_\mu Z^0_\nu W^-_\nu - Z^0_\mu Z^0_\mu W^+_\nu W^-_\nu) + \\
&g^2 s_w^2 (A_\mu W^+_\mu A_\nu W^-_\nu - A_\mu A_\mu W^+_\nu W^-_\nu) + g^2 s_w c_w [A_\mu Z^0_\nu (W^+_\mu W^-_\nu - \\
&W^+_\nu W^-_\mu) - 2 A_\mu Z^0_\mu W^+_\nu W^-_\nu] - g\alpha [H^3 + H\phi^0\phi^0 + 2H\phi^+\phi^-] - \\
&\tfrac{1}{8} g^2 \alpha_h [H^4 + (\phi^0)^4 + 4(\phi^+\phi^-)^2 + 4(\phi^0)^2 \phi^+\phi^- + 4H^2\phi^+\phi^- + 2(\phi^0)^2 H^2] - \\
&g M W^+_\mu W^-_\mu H - \tfrac{1}{2} g \tfrac{M}{c_w^2} Z^0_\mu Z^0_\mu H - \tfrac{1}{2} i g [W^+_\mu (\phi^0 \partial_\mu \phi^- - \phi^- \partial_\mu \phi^0) - \\
&W^-_\mu (\phi^0 \partial_\mu \phi^+ - \phi^+ \partial_\mu \phi^0)] + \tfrac{1}{2} g [W^+_\mu (H \partial_\mu \phi^- - \phi^- \partial_\mu H) - W^-_\mu (H \partial_\mu \phi^+ - \\
&\phi^+ \partial_\mu H)] + \tfrac{1}{2} g \tfrac{1}{c_w} (Z^0_\mu (H \partial_\mu \phi^0 - \phi^0 \partial_\mu H) - i g \tfrac{s_w^2}{c_w} M Z^0_\mu (W^+_\mu \phi^- - W^-_\mu \phi^+) +
\end{aligned}
$$

Implementation of a new physics model in an MC programme

- Definition: particles, parameters and vertices (≡ Lagrangian)
  - ➙ translated in some programming language
- Tedious, time-consuming, error prone
- Beware of restrictions/conventions

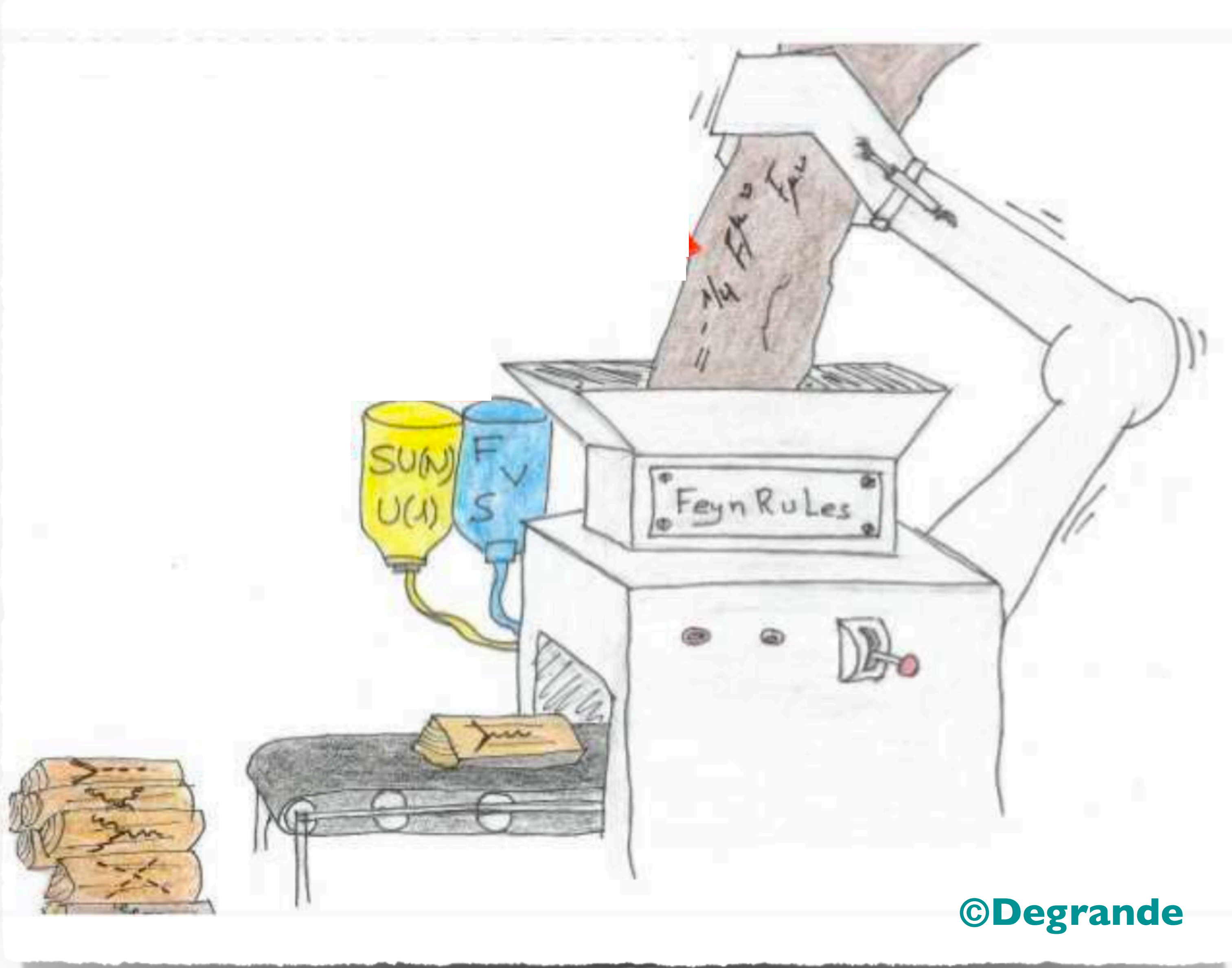
⋆Highly redundant (each tool, each model)

⋆No-brainer tasks (from Feynman rules to codes)

Systematisation
Automation

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

©Degrande



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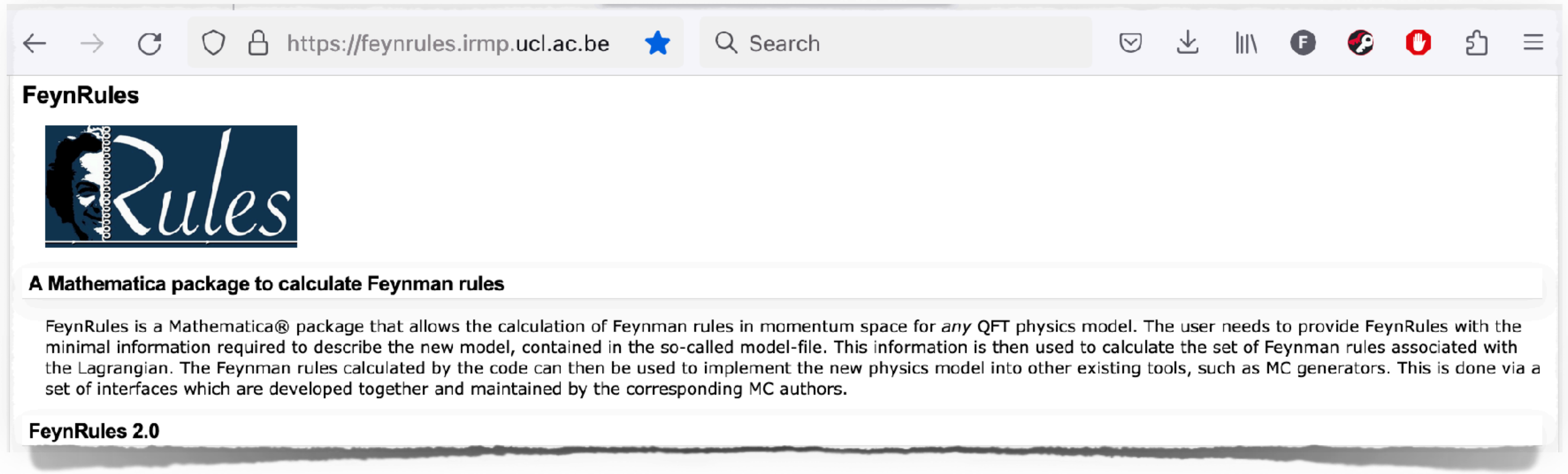
Connecting Lagrangians with HEP software

The FEYNRULES platform (since 2009)

- Working environment: MATHEMATICA
  - ⋆ Flexibility, symbolic manipulations, easy implementation of new methods, *etc.*
  - ⋆ Many plugins (superspace, spectrum, decays, NLO, *etc.*)
- Interfaces to many MC tools
  - ⋆ Dedicated interfaces (CALCHEP, FEYNARTS)
  - ⋆ Generic interface: UFOs (MG5_AMC, HERWIG, SHERPA, WHIZARD, …)
- Very few limitations on models
  - ⋆ Higher-dimensional operators supported
  - ⋆ Spins (up to 2); colour structures (1, 3, 6, 8)



FeynRules

A Mathematica package to calculate Feynman rules

FeynRules is a Mathematica® package that allows the calculation of Feynman rules in momentum space for *any* QFT physics model. The user needs to provide FeynRules with the minimal information required to describe the new model, contained in the so-called model-file. This information is then used to calculate the set of Feynman rules associated with the Lagrangian. The Feynman rules calculated by the code can then be used to implement the new physics model into other existing tools, such as MC generators. This is done via a set of interfaces which are developed together and maintained by the corresponding MC authors.

FeynRules 2.0

[Christensen & Duhr (CPC '09)]
[Alloul, Christensen, Degrande, Duhr & BF (CPC'14)]

Other packages

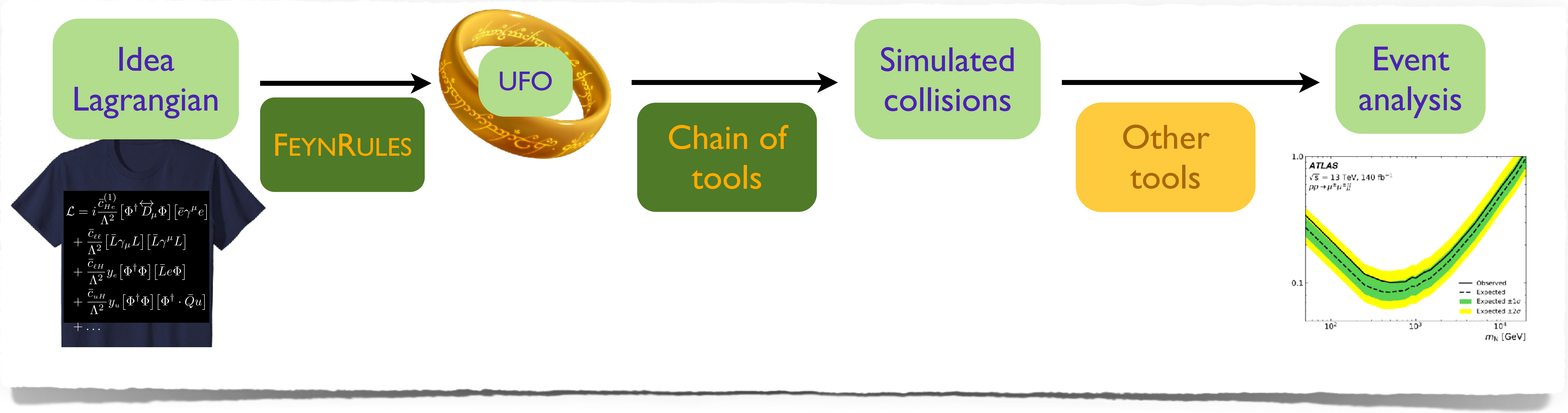
- LANHEP (since 1997) [Semenov (CPC'98); Semenov (CPC'16)]
  - ⋆ Working environment: C
  - ⋆ Initially restricted to CALCHEP/COMPHEP
  - ⋆ Later interfaced to FEYNARTS/UFOs
- The SARAH package (since 2010) [Staub (CPC'10); Staub (CPC'14)]
  - ⋆ Working environment: MATHEMATICA
  - ⋆ Spectrum generator, indirect constraints
  - ⋆ Interfaced to many tools (CALCHEP, FEYNARTS, UFO, WHIZARD)

Interfacing Lagrangians and event generators

Linking a Lagrangian to a Monte Carlo tool

- Derivation of the model's Feynman rules (vertices, particle content, *etc.*)
  ➙ role of FEYNRULES
- Interface of FEYNRULES to event generators
  - ⋆ Removal of vertices not compliant with the tool (colour and Lorentz structures)
  - ⋆ Translation to a specific format and programming language

- The UFO − one format to rule them all
  - ⋆ Too many interfaces not efficient (maintenance, versioning, *etc.*)
  - ⋆ Design of a unique intermediate layer


Idea Lagrangian

FEYNRULES

UFO

Chain of tools

Simulated collisions

Other tools

Event analysis

$\mathcal{L} = i\frac{\bar{c}^{(1)}_{He}}{\Lambda^2}[\Phi^\dagger \overleftrightarrow{D}_\mu \Phi][\bar{e}\gamma^\mu e]$
$+ \frac{\bar{c}_{\ell\ell}}{\Lambda^2}[\bar{L}\gamma_\mu L][\bar{L}\gamma^\mu L]$
$+ \frac{\bar{c}_{\ell H}}{\Lambda^2} y_e [\Phi^\dagger\Phi][\bar{L}e\Phi]$
$+ \frac{\bar{c}_{uH}}{\Lambda^2} y_u [\Phi^\dagger\Phi][\Phi^\dagger \cdot \bar{Q}u]$
$+ \ldots$
ATLAS
$\sqrt{s}$ = 13 TeV, 140 fb^{-1}
$pp \to \mu^\pm\mu^\pm jj$
1.0
0.1
10^2
10^3
10^4
m_N [GeV]
Observed
Expected
Expected ±1σ
Expected ±2σ

The Universal FeynRules Output

[Degrande et al. (CPC ’12)]
[Darmé et al. (EPJC`24)]

The UFO in a nutshell

- UFO ≡ Universal FeynRules output ➙ Universal Feynman Output
  - ⋆ Universal as not tied to any specific programme
- Set of Python files to be linked to any code with full information
  - ⋆ Generic colour and Lorentz structures
  - ⋆ Restrictions on acceptable colour/Lorentz structures enforced at the software level

Initially designed as the MG5aMC model format, UFOs now standard

FeynRules SaRAH LanHEP

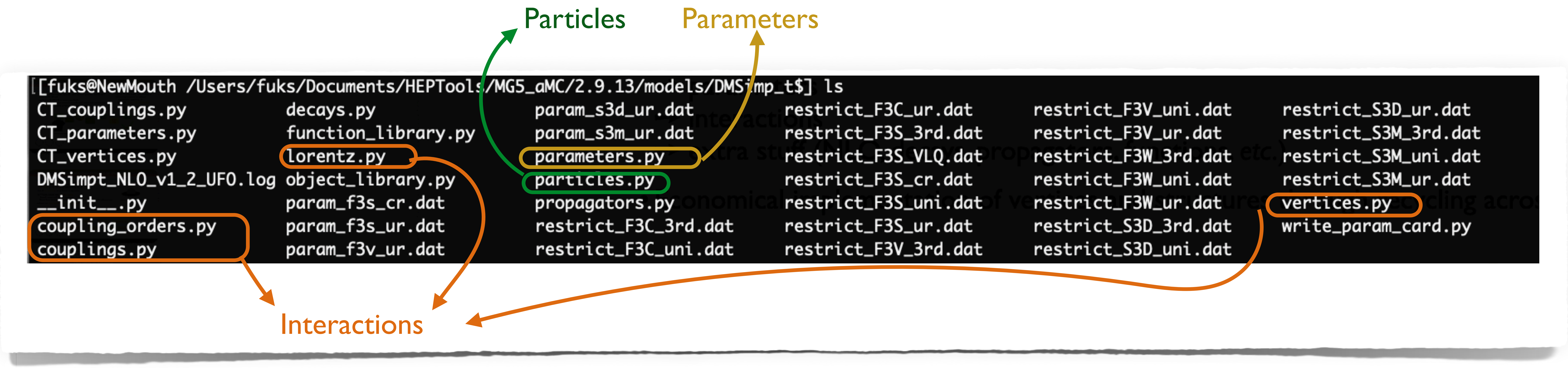
Achilles Comix Contur GoSam Herwig 7 MadAnalysis 5

MadDM MadGraph5_aMC@NLO Recola Sherpa Whizard

The UFO in practice

The UFO ≡ set of PYTHON files

- Factorisation of the information in mandatory and optional files
  - ➙ particles
  - ➙ parameters
  - ➙ interactions
  - ➙ extra stuff (NLO, decays, propagators, functions, *etc.*)
- Economical implementation of vertices and structures through recycling across the model



```
[fuks@NewMouth /Users/fuks/Documents/HEPTools/MG5_aMC/2.9.13/models/DMSimp_t$] ls
CT_couplings.py          decays.py                param_s3d_ur.dat         restrict_F3C_ur.dat      restrict_F3V_uni.dat     restrict_S3D_ur.dat
CT_parameters.py         function_library.py      param_s3m_ur.dat         restrict_F3S_3rd.dat     restrict_F3V_ur.dat      restrict_S3M_3rd.dat
CT_vertices.py           lorentz.py               parameters.py            restrict_F3S_VLQ.dat     restrict_F3W_3rd.dat     restrict_S3M_uni.dat
DMSimpt_NLO_v1_2_UFO.log object_library.py        particles.py             restrict_F3S_cr.dat      restrict_F3W_uni.dat     restrict_S3M_ur.dat
__init__.py              param_f3s_cr.dat         propagators.py           restrict_F3S_uni.dat     restrict_F3W_ur.dat      vertices.py
coupling_orders.py       param_f3s_ur.dat         restrict_F3C_3rd.dat     restrict_F3S_ur.dat      restrict_S3D_3rd.dat     write_param_card.py
couplings.py             param_f3v_ur.dat         restrict_F3C_uni.dat     restrict_F3V_3rd.dat     restrict_S3D_uni.dat
```

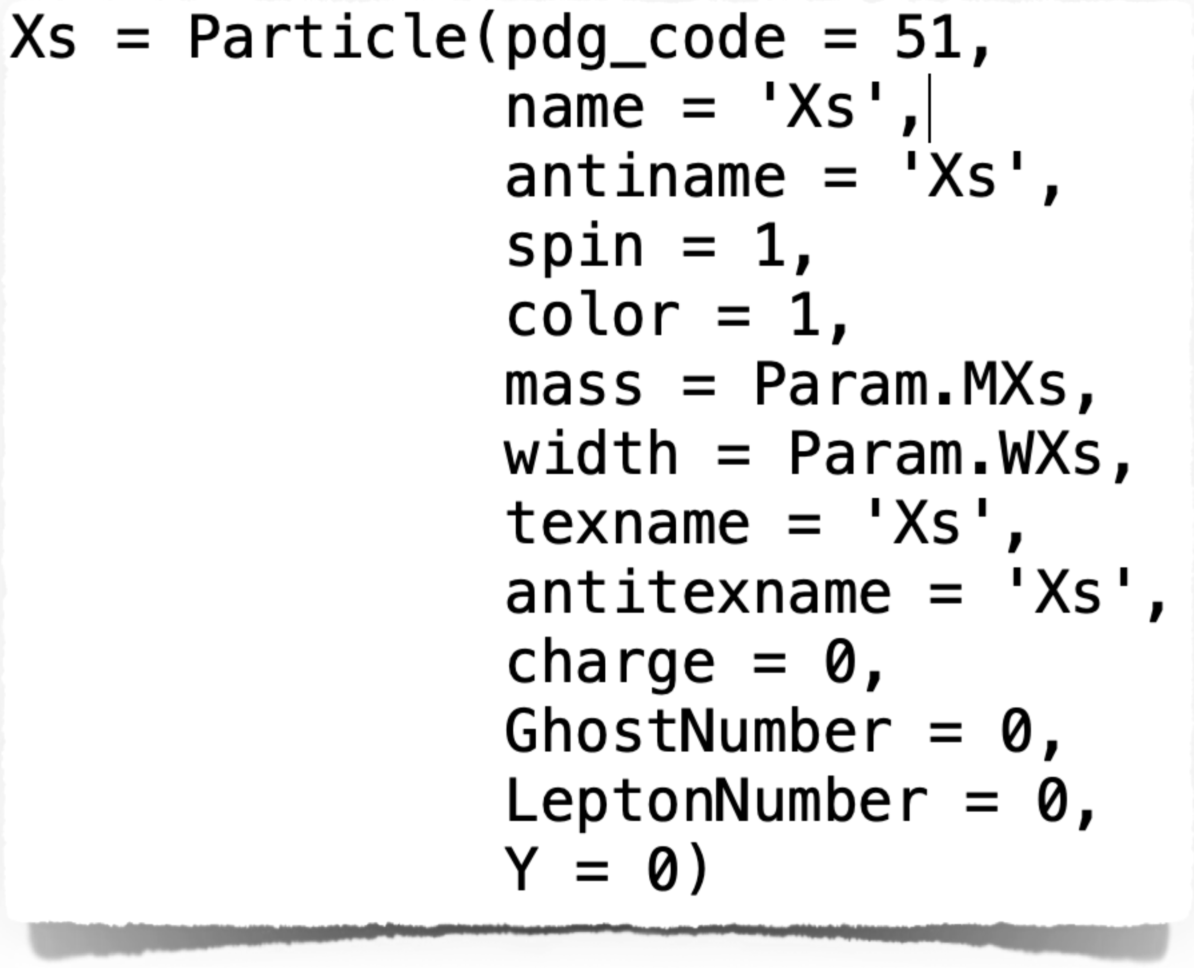
Restrictions: from a general model to a less general one

- Start from the very general DMSIMPt model, and use the F3S_VLQ restriction
  https://cernbox.cern.ch/s/P4CjOKNIfZv56aD

The UFO: particles & parameters

Particles ≡ instances of the particle class

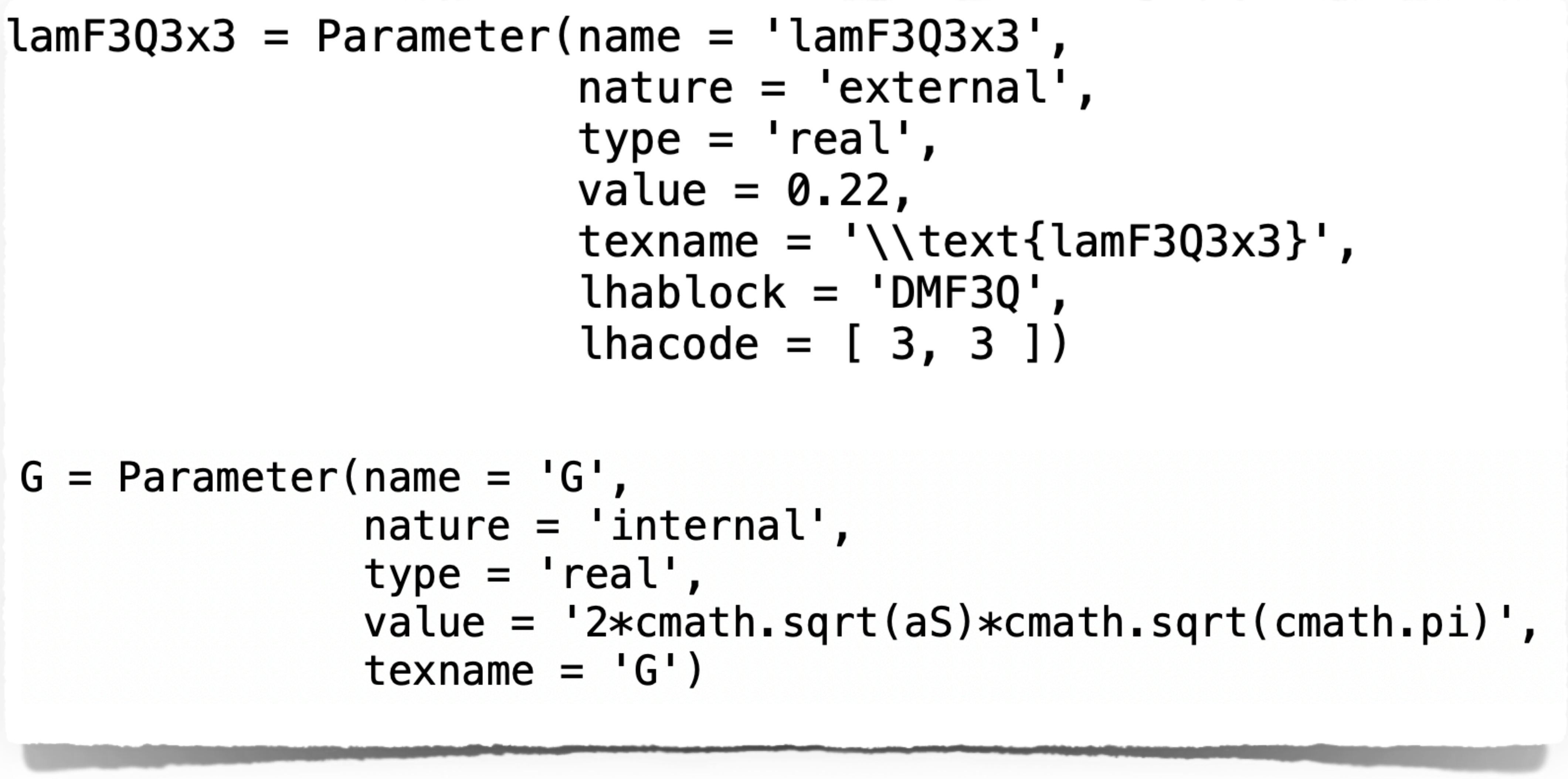
- Attributes: spin, colour representation, mass, width, *etc*.
- Antiparticles automatically derived



```
Xs = Particle(pdg_code = 51,
              name = 'Xs',
              antiname = 'Xs',
              spin = 1,
              color = 1,
              mass = Param.MXs,
              width = Param.WXs,
              texname = 'Xs',
              antitexname = 'Xs',
              charge = 0,
              GhostNumber = 0,
              LeptonNumber = 0,
              Y = 0)
```

Parameters ≡ instances of the parameter class

- External parameters: Les Houches-like structure
- PYTHON-compliant formula for the internal parameters



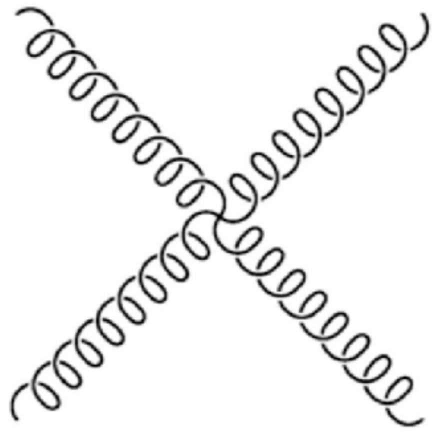
```
lamF3Q3x3 = Parameter(name = 'lamF3Q3x3',
                      nature = 'external',
                      type = 'real',
                      value = 0.22,
                      texname = '\\text{lamF3Q3x3}',
                      lhablock = 'DMF3Q',
                      lhacode = [ 3, 3 ])


G = Parameter(name = 'G',
              nature = 'internal',
              type = 'real',
              value = '2*cmath.sqrt(aS)*cmath.sqrt(cmath.pi)',
              texname = 'G')
```

The UFO: strategy for interactions

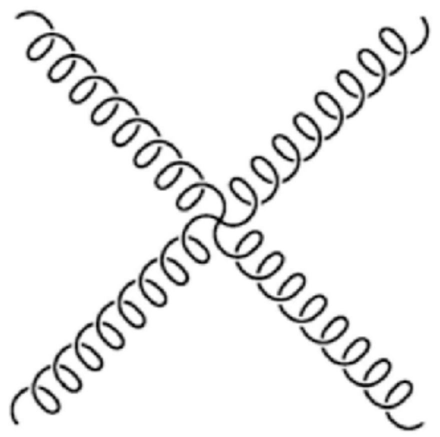
Decomposition in a spin x colour basis (coupling strengths ≡ coordinates)

- Example: the quartic gluon vertex



$$\begin{aligned} & i g_s^2\, f^{a_1a_2b} f^{ba_3a_4} \left(\eta^{\mu_1\mu_4}\eta^{\mu_2\mu_3} - \eta^{\mu_1\mu_3}\eta^{\mu_2\mu_4}\right) \\ & + i g_s^2\, f^{a_1a_3b} f^{ba_2a_4} \left(\eta^{\mu_1\mu_4}\eta^{\mu_2\mu_3} - \eta^{\mu_1\mu_2}\eta^{\mu_3\mu_4}\right) \\ & + i g_s^2\, f^{a_1a_4b} f^{ba_2a_3} \left(\eta^{\mu_1\mu_3}\eta^{\mu_2\mu_4} - \eta^{\mu_1\mu_2}\eta^{\mu_3\mu_4}\right) \end{aligned}$$

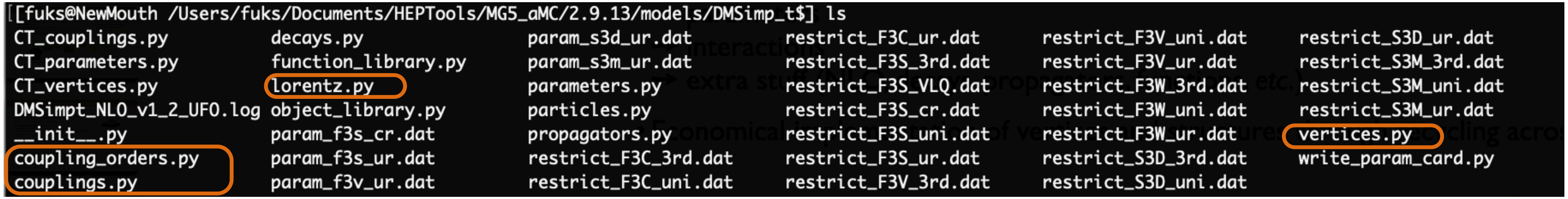
- UFO version



$$\left(f^{a_1a_2b} f^{ba_3a_4},\ f^{a_1a_3b} f^{ba_2a_4}, f^{a_1a_4b} f^{ba_2a_3}\right) \times \begin{pmatrix} i g_s^2 & 0 & 0 \\ 0 & i g_s^2 & 0 \\ 0 & 0 & i g_s^2 \end{pmatrix} \begin{pmatrix} \eta^{\mu_1\mu_4}\eta^{\mu_2\mu_3} - \eta^{\mu_1\mu_3}\eta^{\mu_2\mu_4} \\ \eta^{\mu_1\mu_4}\eta^{\mu_2\mu_3} - \eta^{\mu_1\mu_2}\eta^{\mu_3\mu_4} \\ \eta^{\mu_1\mu_3}\eta^{\mu_2\mu_4} - \eta^{\mu_1\mu_2}\eta^{\mu_3\mu_4} \end{pmatrix}$$

- ⋆ 3 elements for the colour basis
- ⋆ 3 elements for the spin (Lorentz structure) basis
- ⋆ 9 coordinates (6 are zero, only 1 encoded)

Information split across several files



```
[[fuks@NewMouth /Users/fuks/Documents/HEPTools/MG5_aMC/2.9.13/models/DMSimp_t$] ls
CT_couplings.py          decays.py             param_s3d_ur.dat       restrict_F3C_ur.dat    restrict_F3V_uni.dat   restrict_S3D_ur.dat
CT_parameters.py         function_library.py   param_s3m_ur.dat       restrict_F3S_3rd.dat   restrict_F3V_ur.dat    restrict_S3M_3rd.dat
CT_vertices.py           lorentz.py            parameters.py          restrict_F3S_VLQ.dat   restrict_F3W_3rd.dat   restrict_S3M_uni.dat
DMSimpt_NLO_v1_2_UFO.log object_library.py     particles.py           restrict_F3S_cr.dat    restrict_F3W_uni.dat   restrict_S3M_ur.dat
__init__.py              param_f3s_cr.dat      propagators.py         restrict_F3S_uni.dat   restrict_F3W_ur.dat    vertices.py
coupling_orders.py       param_f3s_ur.dat      restrict_F3C_3rd.dat   restrict_F3S_ur.dat    restrict_S3D_3rd.dat   write_param_card.py
couplings.py             param_f3v_ur.dat      restrict_F3C_uni.dat   restrict_F3V_3rd.dat   restrict_S3D_uni.dat
```

To-do:

- ⋆Check the content of the downloaded model
- ⋆Open a few files

Outline

1. A comprehensive approach for Monte Carlo simulations

2. Implementing models into Monte Carlo event generators

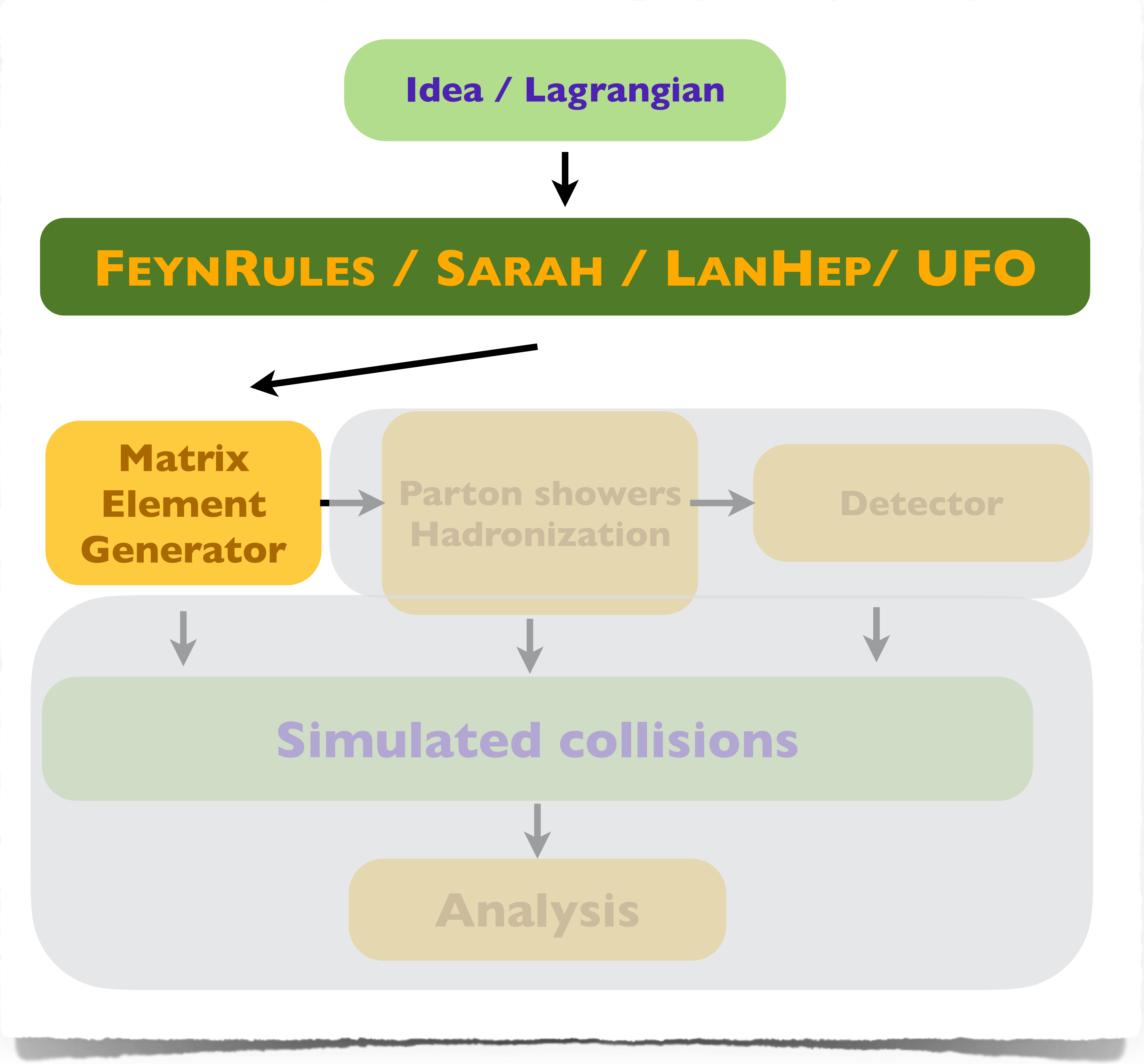
3. **From models to hard-scattering events**

4. Summary

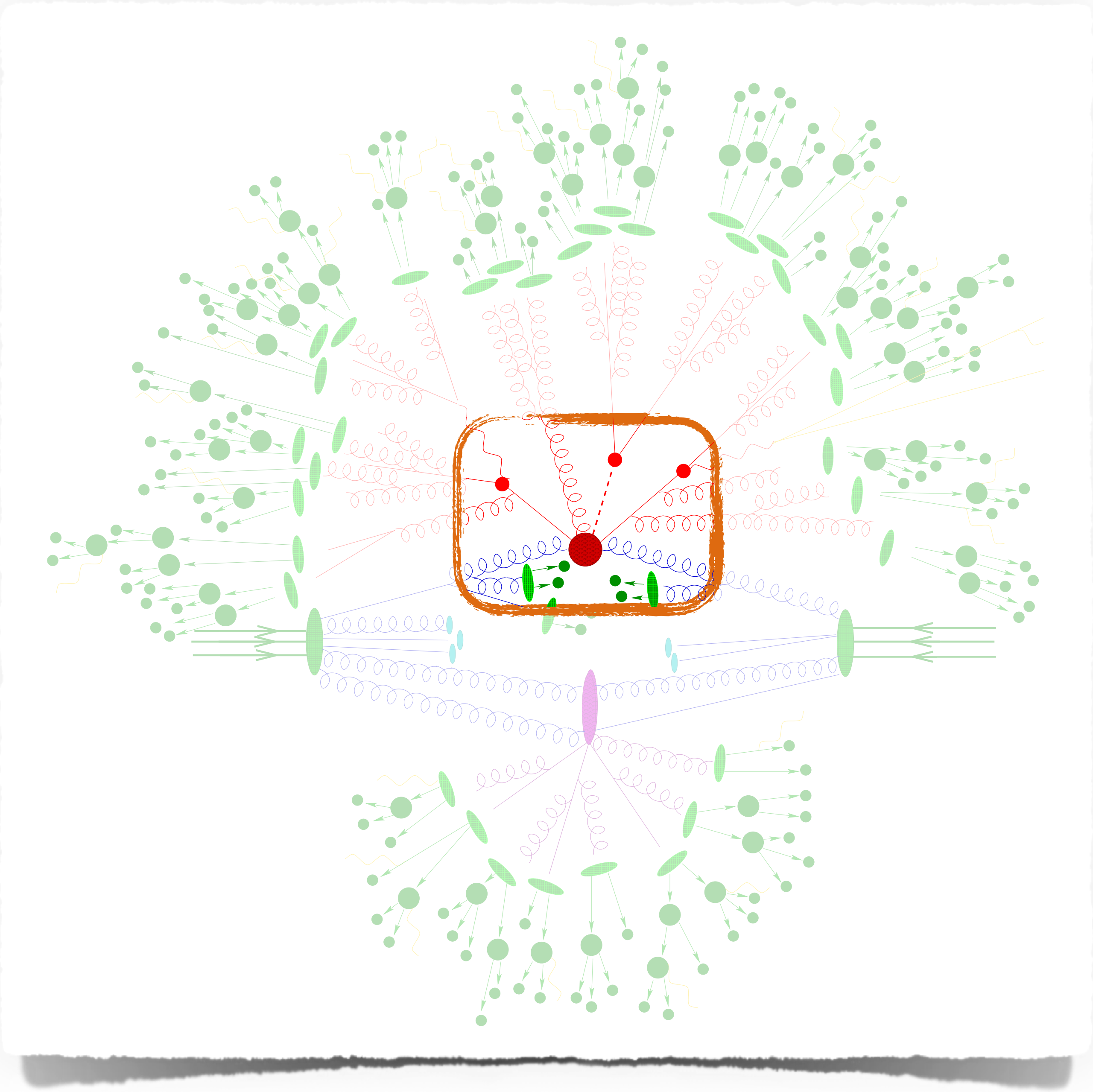
Connecting ideas to simulations…

[Christensen, de Aquino, Degrande, Duhr, BF, Herquet, Maltoni & Schumann (EPJC`11)]

Connecting ideas to simulations (and cross section calculations)



- Model building → FeynRules & UFOs
- Hard scattering → MadGraph5_aMC@NLO
  - ⋆ Feynman diagram and amplitude generation
  - ⋆ Monte Carlo integration
  - ⋆ Event generation

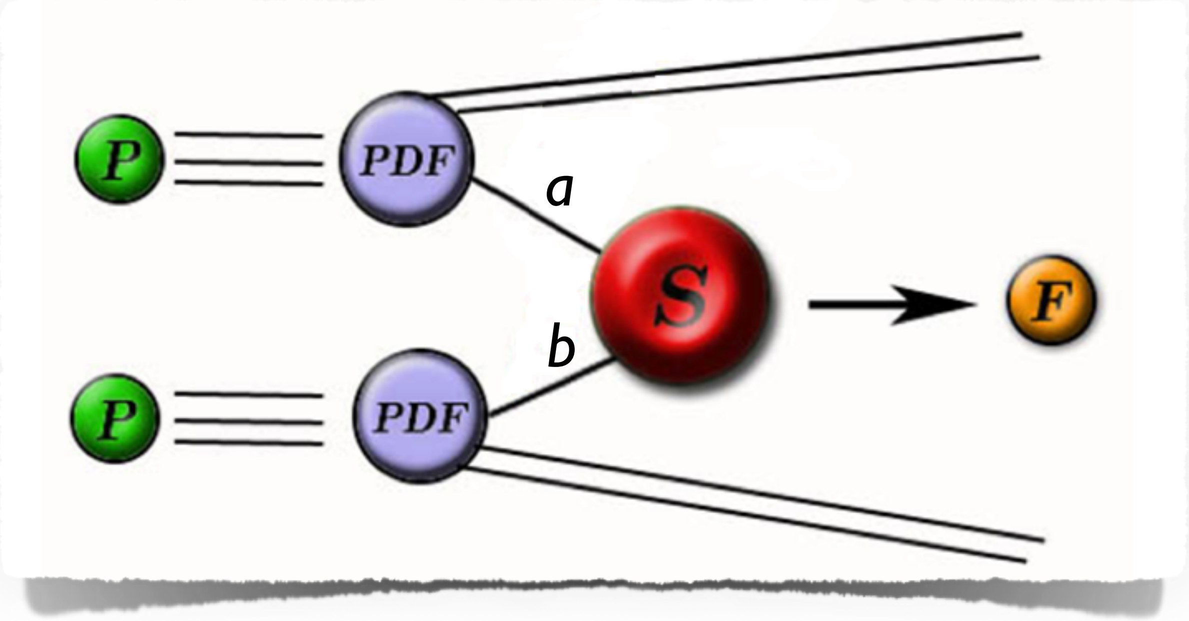


Goals:
→ cross section calculations
→ event generation

Feynman diagrams

QCD 101: predictions at the LHC

Distribution of an observable ω: the QCD factorisation theorem



$$\frac{\mathrm{d}\sigma}{\mathrm{d}\omega} = \sum_{ab}\int \mathrm{d}x_a\,\mathrm{d}x_b\,\mathbf{f}_{a/p_1}(x_a;\mu_F)\,\mathbf{f}_{b/p_2}(x_b;\mu_F)\,\frac{\mathrm{d}\sigma_{ab}}{\mathrm{d}\omega}(\ldots,\mu_F)$$

- Long distance physics: the parton densities
- Short distance physics: the differential parton cross section $\mathrm{d}\sigma_{ab}$
- Separation of both regimes through the factorisation scale μ_F
  - ⋆ Choice of the scale → theoretical uncertainties
- Sum over all final state configurations and all options for the initial state
  - ⋆ Phase space integration of the matrix element
    - → Highly-dimensional integral (*3n-2* integrals ≡ *n*-body final state)
    - → Phase space structure ≡ analytical calculations hopeless

3 ingredients for cross section calculations

- Parton densities
- Matrix element
- Numerical Integration

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\omega} = \sum_{a,b}\int \mathrm{d}x_a\,\mathrm{d}x_b\,\mathrm{d}\Phi_n\;f_{a/p}(x_a;\mu_F)\;f_{b/p}(x_b;\mu_F)\;\frac{1}{2s}\overline{|\mathcal{M}|}^2(s;\mu_F,\mu_R)\;\mathcal{O}_\omega(\Phi_n)$$

Parton densities

Long distance physics: parton densities

- Relation of protons to their quark and gluon content
- Dependence on the momentum fraction x of the parton in the proton
- Dependence on a scale *Q* ➙ new physics at large scale

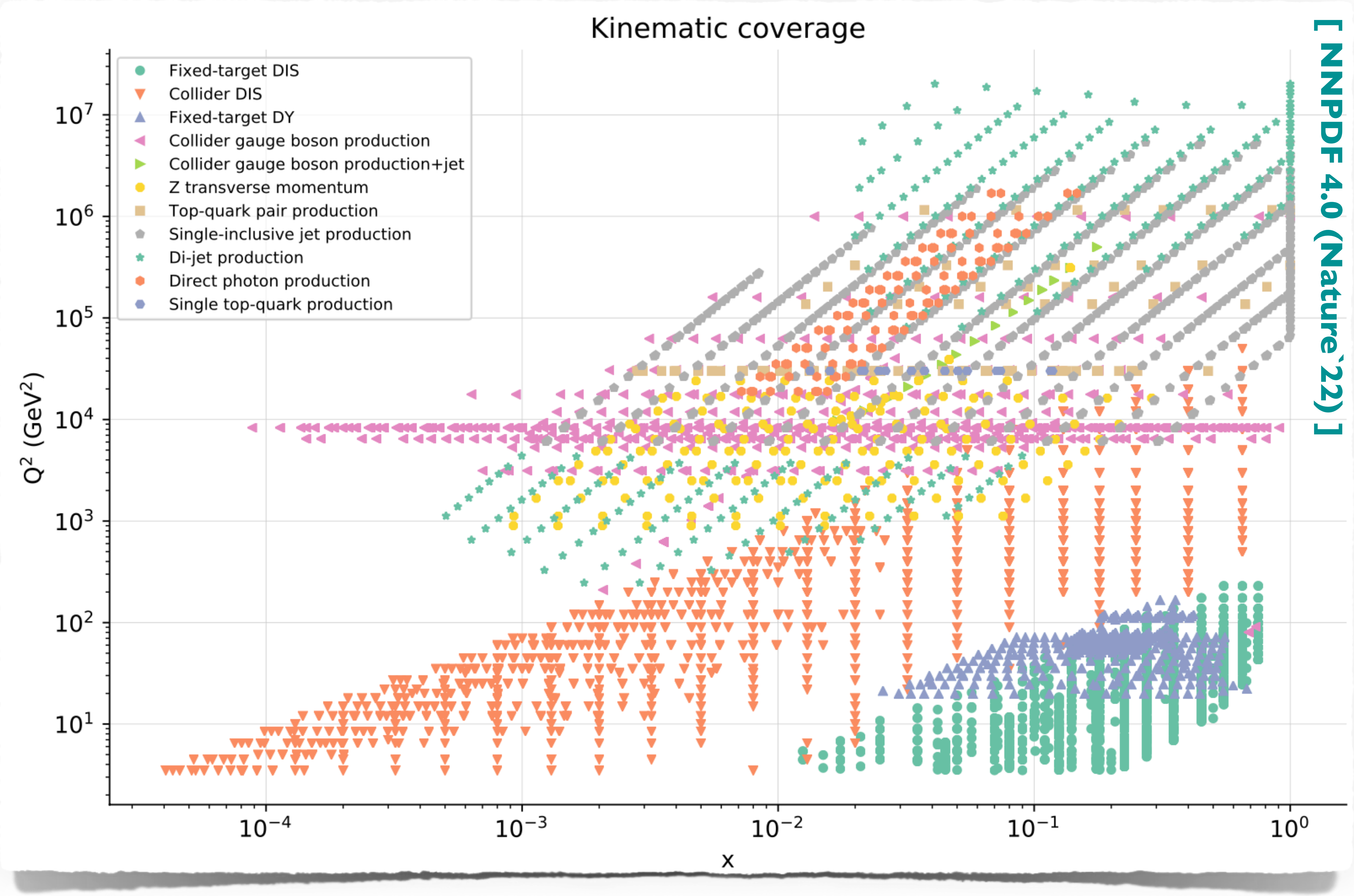
In practice

- Fitted from experimental data [in some regime *(x,Q)*]
- Evolution driven by QCD (DGLAP/BFKL)

➙ PDFs for any *(x, Q)* obtained from the fit

PDF ⇔ dominant initial-states

- Huge gluon luminosity at small *x* (LHC)
- Large valence luminosity at large *x* (LHC)



[NNPDF 4.0 (Nature`22)]

PDF set recommended in the tutorial: NNPDF 4.0

- Installation of LHAPDF (https://lhapdf.hepforge.org/downloads/)
- Download of the set 331900 (*NNPDF40_lo_as_01180*) on https://lhapdf.hepforge.org/pdfsets

  ➙ Copy of the files in the LHAPDF shared folder
- To add the end of the '*info*' file:

```
AlphaS_FlavorScheme: variable
AlphaS_NumFlavors: variable
```

Partonic cross sections

Short distance physics: the partonic cross section

- Calculated order by order in perturbative QCD: $d\sigma = d\sigma^{(0)} + \alpha_s\, d\sigma^{(1)} + \ldots$
  - ⋆ Perturbative series: coupling ≡ expansion parameter
  - ⋆ More orders included ➙ more precise predictions
  - ⋆ Truncation of the series and α_s ➙ theoretical uncertainties [renormalisation and factorisation scales]

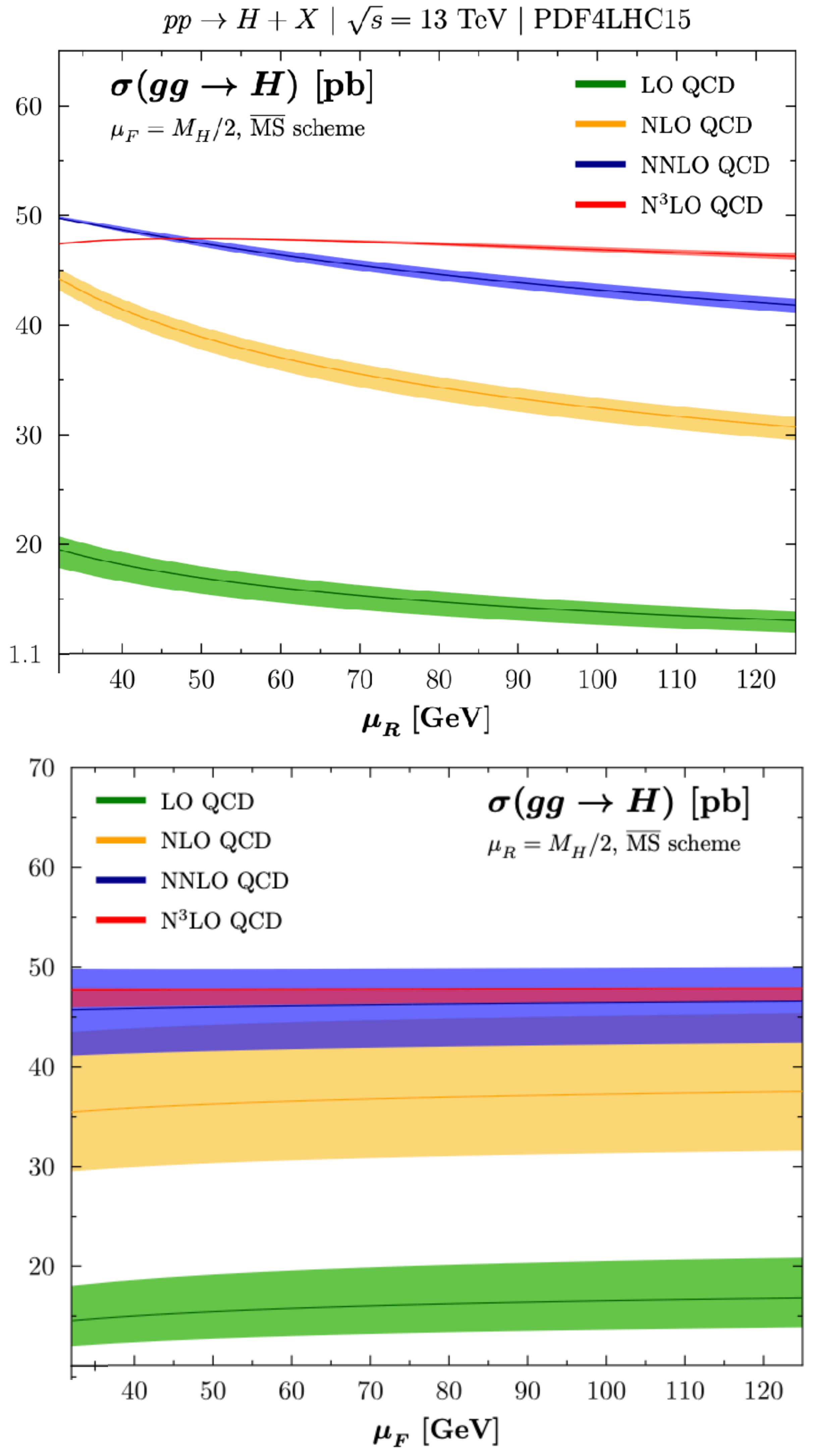
Predictions at leading order (LO)

- Uncertainties mainly on the normalisation (total cross section)
  ➙ reduction of the uncertainties through NLO/NNLO corrections
- Good enough for shapes (at least after using multiparton merging)

Goal of the lecture / tutorial:

- LO cross sections calculations and event generation
- Usage of MG5aMC@NLO (version 2.9.18)
  ➙ Use the DOCKER image
- In the MG5 installation folder: `./bin/mg5aMC`

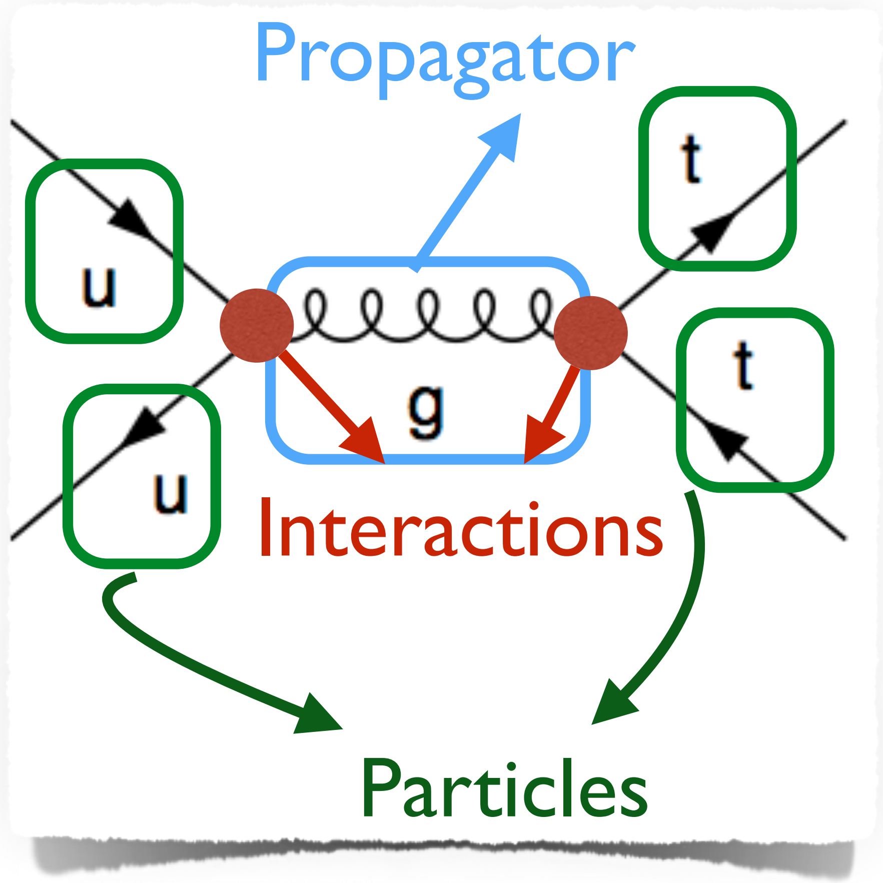
[Baglio, Duhr, Mistlberger & Szafron (JHEP`22)]



Feynman diagram calculations

Matrix elements computed from Feynman diagrams (amplitudes)

- Drawing of all diagrams for a given process
- Extraction of the amplitude from the Feynman rules



A master-level example (HEP students): top-antitop production from quarks

- One single diagram

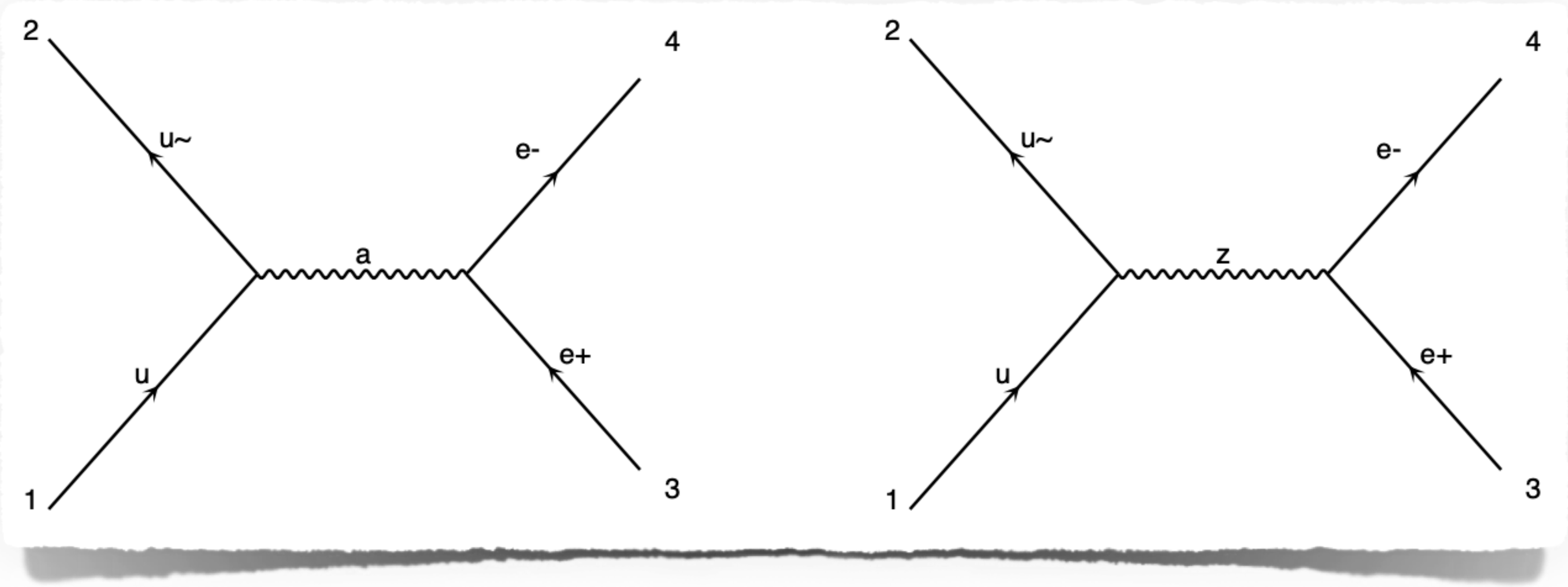
$$i\mathcal{M} = i\underline{g_s^2}\,\Big[\boxed{\bar{v}_2}\,\underline{\gamma^\mu}\,\boxed{u_1}\Big]\,\boxed{\frac{\eta_{\mu\nu}}{s}}\,\Big[\boxed{\bar{u}_3}\,\underline{\gamma^\nu}\,\boxed{v_4}\Big]\,\underline{T^a_{c_2c_1}T^a_{c_3c_4}}$$

- Squaring with the conjugate amplitude
- Algebraic calculation (colour and Lorentz structures)
- Sum/average over the external states

$$\begin{aligned}\overline{|\mathcal{M}|^2} &= \frac{1}{36}\frac{2g_s^4}{s^2}\mathrm{Tr}\Big[\not{p}_1\gamma^\mu\not{p}_2\gamma^\nu\Big]\Big[\not{p}_3\gamma_\mu\not{p}_4\gamma_\nu\Big]\\ &= \frac{16g_s^4}{9s^2}\Big[(p_1\cdot p_3)(p_2\cdot p_4)+(p_1\cdot p_4)(p_2\cdot p_3)\Big]\end{aligned}$$

Standard calculation followed by an efficient phase space integration (compact integrand)

- Drell-Yan process

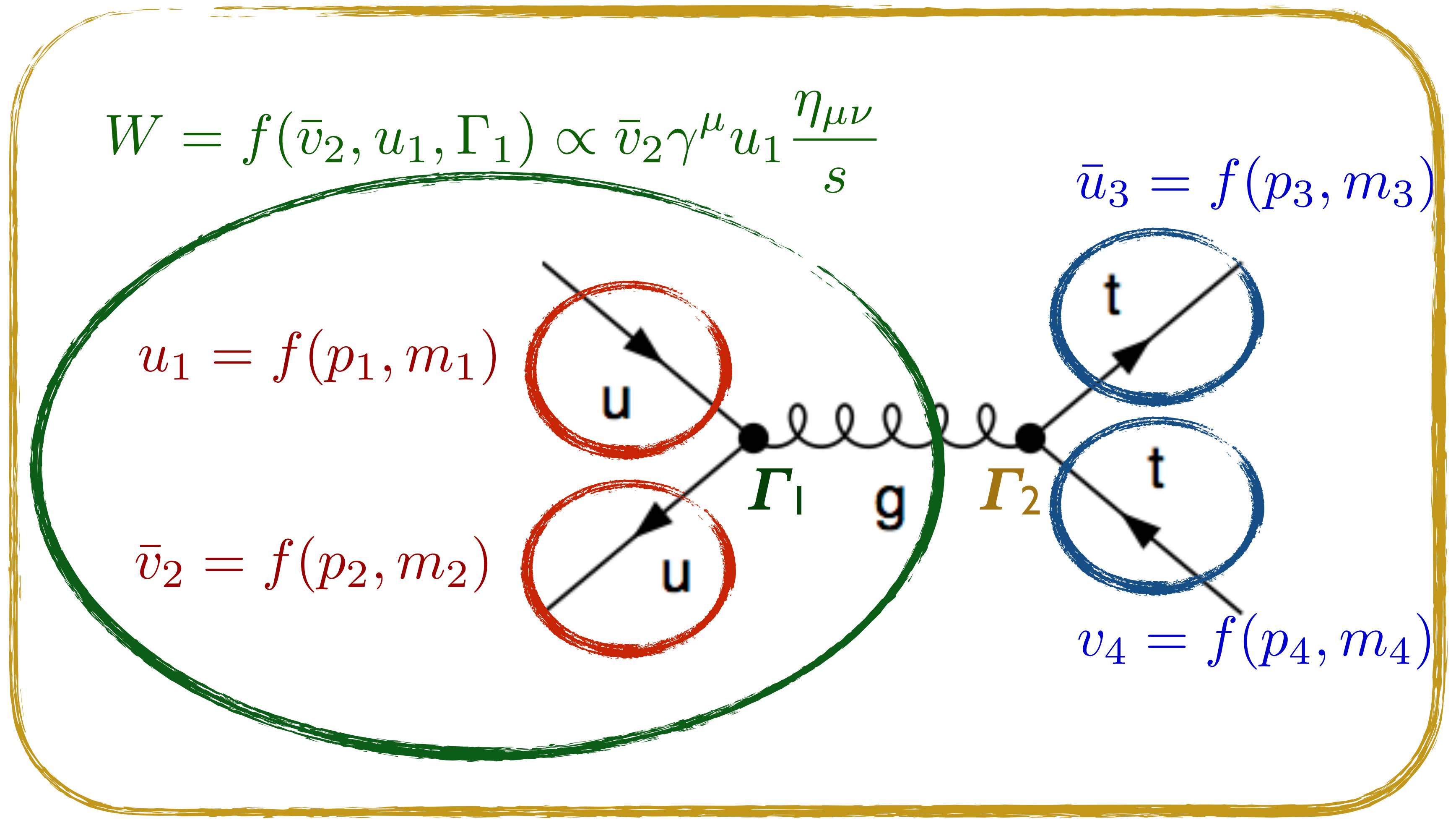


- To compute: $|M|^2 = |M_\gamma|^2 + |M_Z|^2 + 2\Re\{M_\gamma^* M_Z\}$
- The number of diagrams increases with the number of final-state particles
  ➙ Complexity as N^2
- Any 2-to-4 calculation and beyond ≡ a problem

Helicity amplitudes

Principle

- Evaluation of the amplitude for fixed external helicities



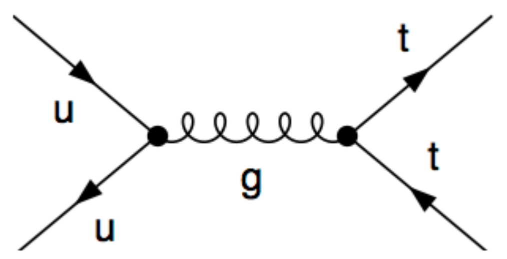
$W = f(\bar{v}_2, u_1, \Gamma_1) \propto \bar{v}_2 \gamma^\mu u_1 \frac{\eta_{\mu\nu}}{s}$
$\bar{u}_3 = f(p_3, m_3)$
$u_1 = f(p_1, m_1)$
u
t
Γ_1
g
Γ_2
t
$\bar{v}_2 = f(p_2, m_2)$
u
$v_4 = f(p_4, m_4)$

$i\mathcal{M} = f(\bar{u}_3, v_4, W, \Gamma_2)$

1. External incoming particles (numbers)
   ➙ For fixed helicity and momentum
2. Wave function of the gluon propagator
3. External outgoing particles
4. Full amplitude (complex number)

- Add all amplitudes ➙ single complex number
- Squaring
- Sum/average over the external states

The building blocks ≡ so-called HELAS functions



$u_1 = f(p_1, m_1)$

$\bar{v}_2 = f(p_2, m_2)$

$\bar{u}_3 = f(p_3, m_3)$

$v_4 = f(p_4, m_4)$

$W = f(\bar{v}_2, u_1, \Gamma_1)$

$i\mathcal{M} = f(\bar{u}_3, v_4, W, \Gamma_2)$

- HELAS ≡ HELicity Amplitude Subroutine
- One routine / Lorentz structure (Γ_i)
  - ⋆ SM [Murayama, Watanabe & Hagiwara (KEK-91-11)]
  - ⋆ MSSM [Cho, Hagiwara, Kanzaki, Plehn, Rainwater & Stelzer (PRD`06)]
  - ⋆ HEFT [Frederix (2007)]
  - ⋆ Spin 2 [Hagiwara, Kanzaki, Li &Mawatari (EPJC`08)]
  - ⋆ Spin 3/2 [Mawatari & Takaesu (EPJC`11)]
  - ⋆ Everything (ALOHA) [de Aquino, Link, Maltoni, Mattelaer & Stelzer (CPC`12)]

Comparison

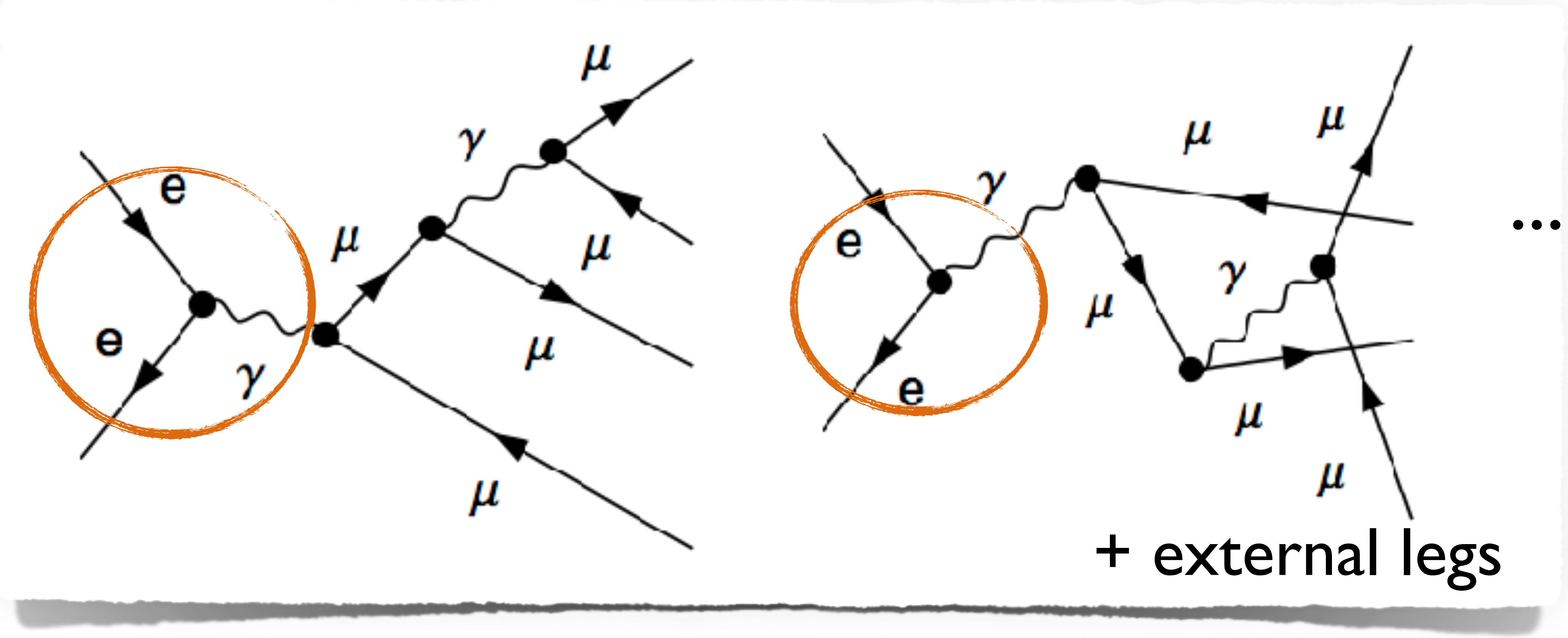
	For *M* diagrams	For *N* particles	2 →6 example
Analytical	M^2	$(N!)^2$	10^9
Helicity	M	$N!\,2^N$	10^7

Still a problem…
Can we do better ?

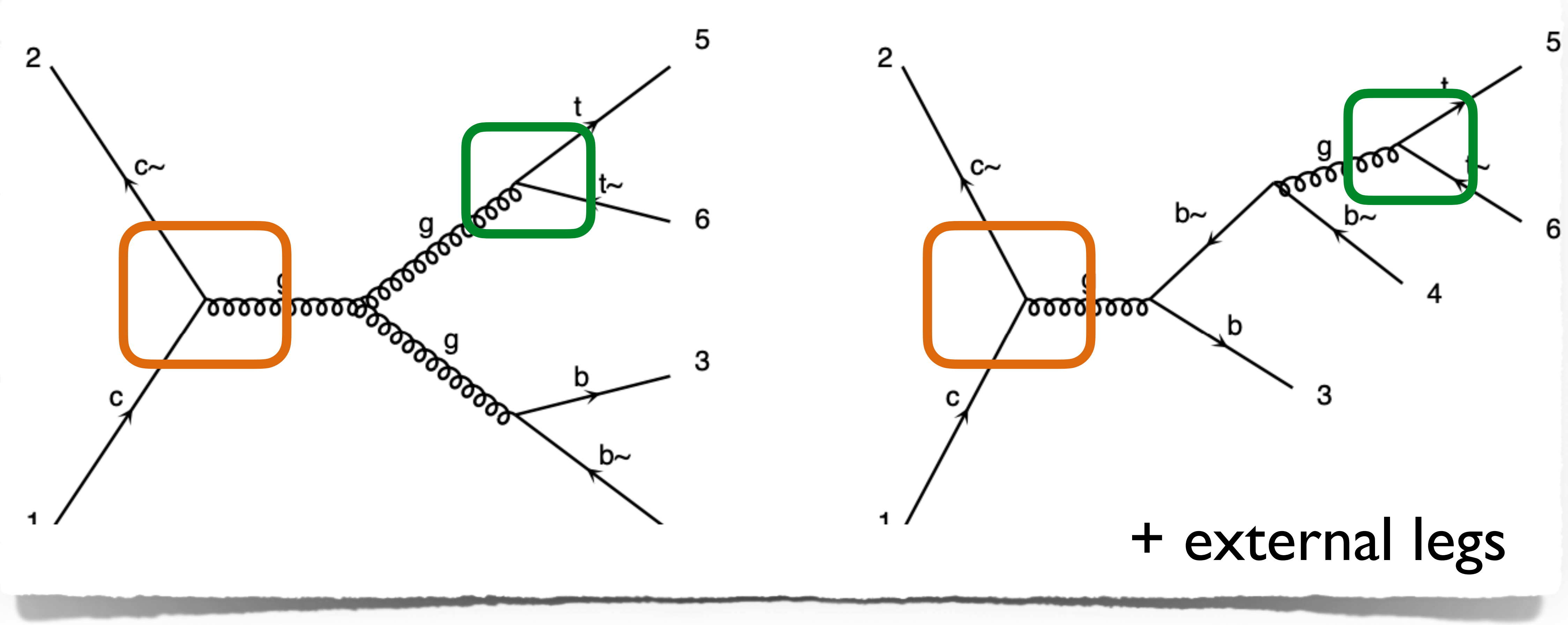
Recycling

Recycling: reusing pieces from one diagram to another

- Not recalculating what is already calculated



+ external legs



+ external legs

- Significative gain in computing time

	For *M* diagrams	For *N* particles	2 →6 example
Analytical	M^2	$(N!)^2$	10^9
Helicity	M	$N!\ 2^N$	10^7
Recycling	M	$(N-1)!\ 2^{N-1}$	$5\text{x}10^5$

Other potential optimisation methods

- Recursion relations, 5D wave functions, *etc.*
- Several new optimisations in MG5aMC (*e.g.* helicity recycling)

[Mattelaer & Ostrolenk (EPJC`21)]

Now this may numerically work!

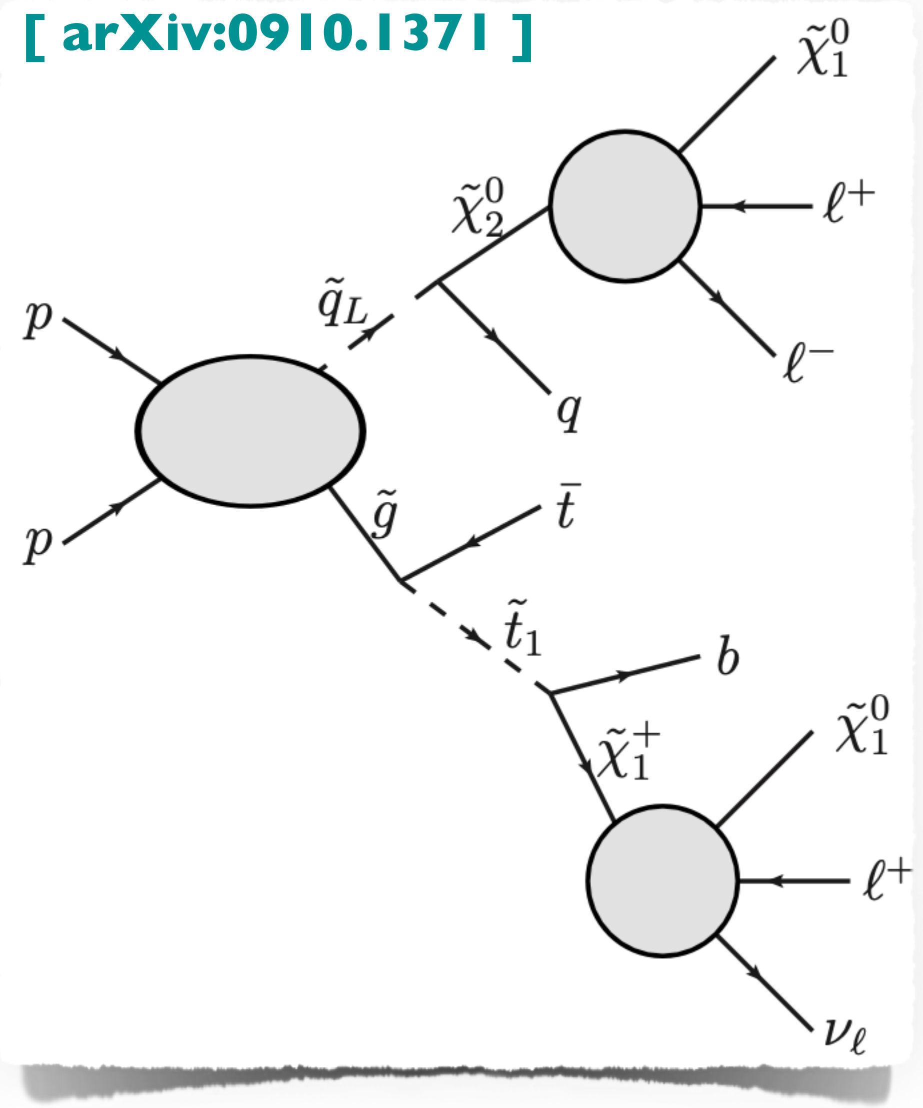
Heavy particle decays

BSM models ➙ new unstable states

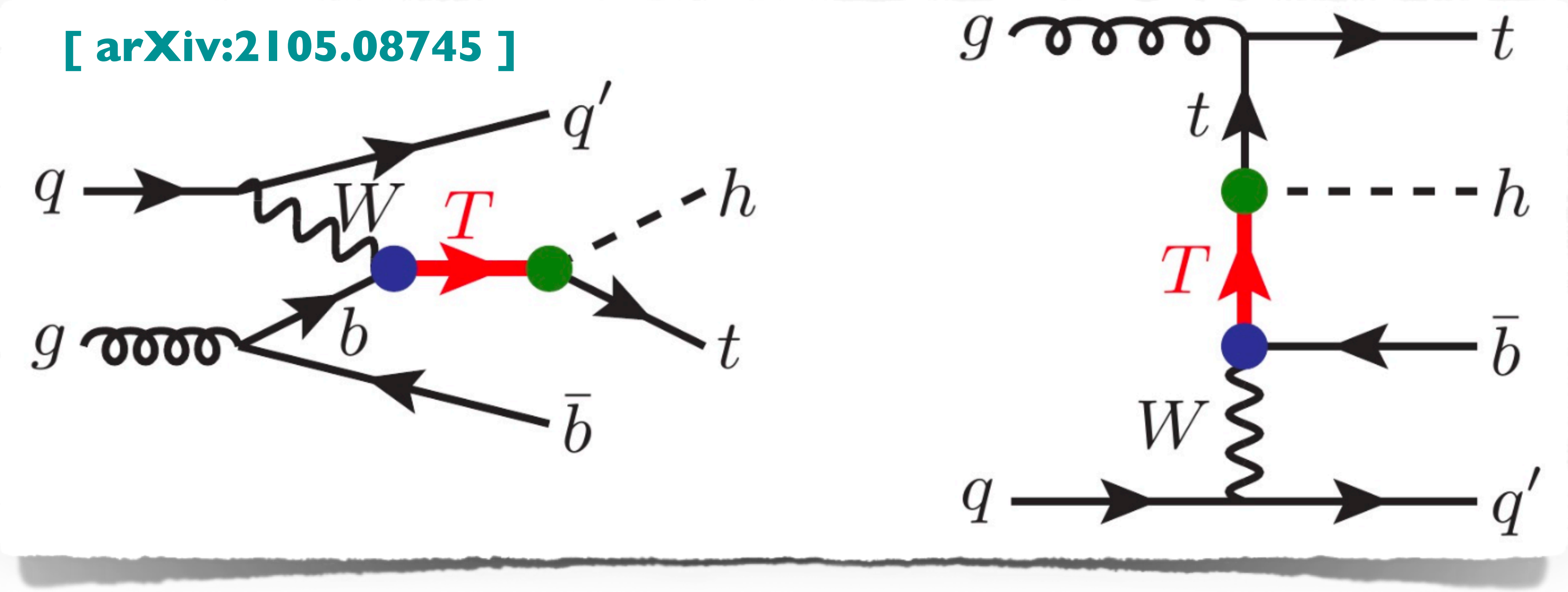
- Example 1: supersymmetry
  - ⋆ Usually pair-produced
  - ⋆ Cascade-decaying into each other
  - ⋆ The lightest new state stable (*cf.* dark matter)
- Example 2: composite top partners
  - ⋆ Single or pair produced
  - ⋆ Decays to SM states
- Large state multiplicity
  - ➙ computationally challenging

$$pp \to \tilde{\chi}_1^0 \ell^+ \ell^- j \ \bar{t} b \tilde{\chi}_1^0 \ell^+ \ell^-$$

$$pp \to t h \bar{b} j$$



[arXiv:0910.1371]



[arXiv:2105.08745]

2-to-*N* matrix-element generation possible

- Issue with the computing time (*cf.* final-state multiplicity)
  - ➙ no technical limitation (in principle)
- Diagrams with intermediate resonances dominate
  - ➙ Factorisation of the production from the decay
  - ➙ Off-shell effects neglected

- Automated in MG5aMC
- Crucial for VLQ pair production (and decay)

Factorisation of production and decay made easy

Simplification of the calculation: production and decay processes factorised

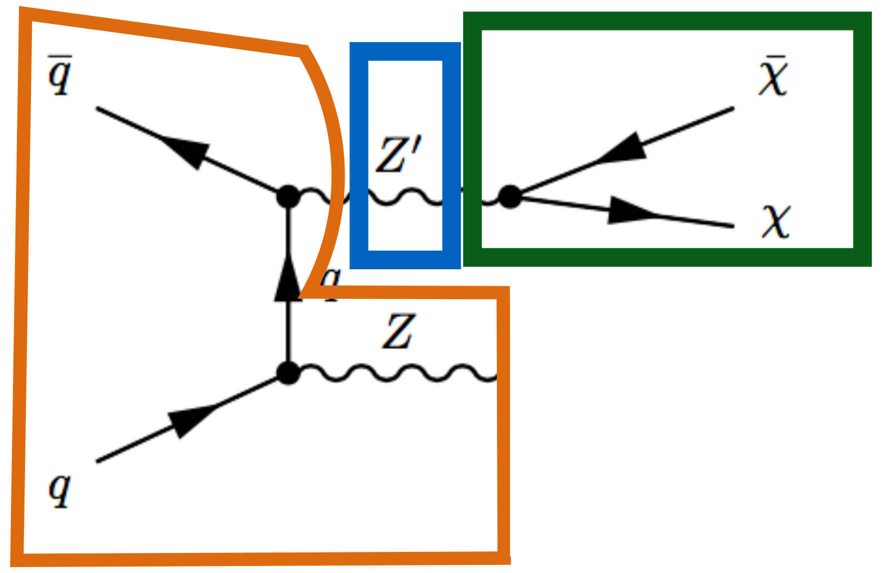
- Propagators ≡ sums of products of external wave functions
- Example for a vector resonance:

$$\mathcal{M} = j_1^\mu \left[\eta_{\mu\nu} - \frac{p_\mu p_\nu}{p^2}\right] j_2^\nu = \sum_\lambda \boxed{j_1^\mu \varepsilon^*_\mu(\lambda)}\ \boxed{j_2^\nu \varepsilon_\nu(\lambda)}$$

Propagation

Production of the resonance

Decay of the resonance



- Off-shell effects lost (as a result of the factorisation)
  - ⋆ Resonance mass smearing: partial recovery [Frixione, Laenen, Motylinski, Webber (JHEP ’07)]

Including spin correlations in the MG5aMC framework

$$\mathcal{M} = \sum_\lambda j_1^\mu \varepsilon^*_\mu(\lambda)\ j_2^\nu \varepsilon_\nu(\lambda)$$

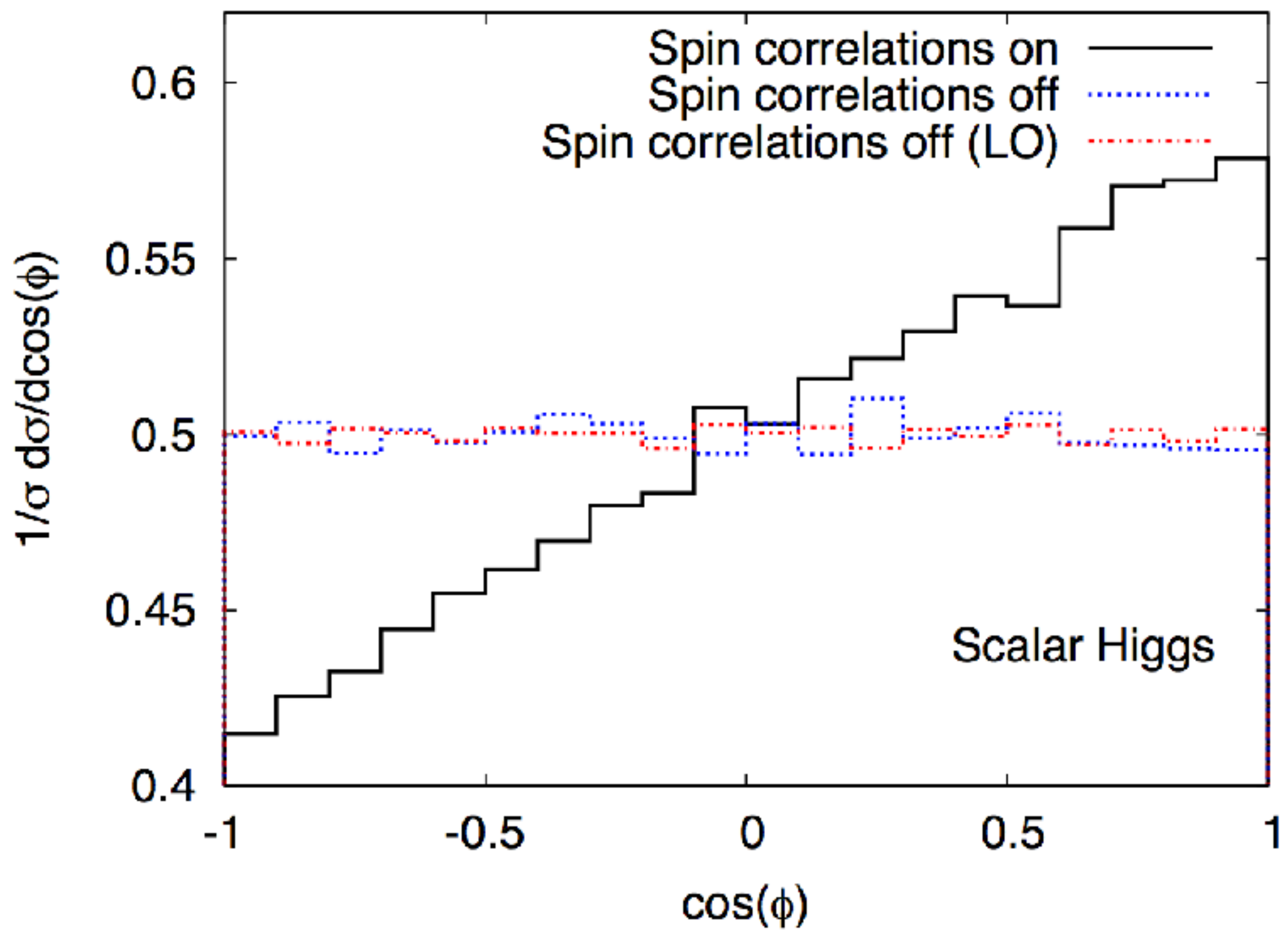
- Re-weighting from decay matrix element (MADSPIN)

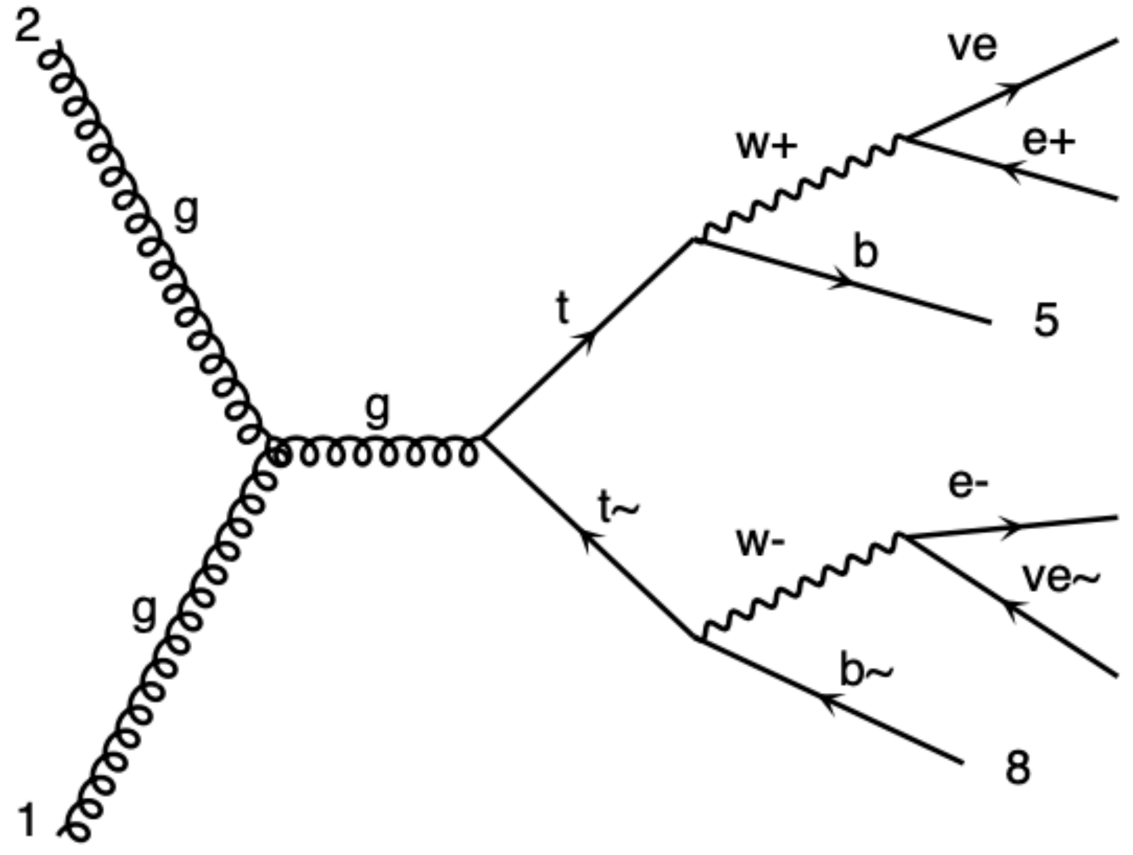
  [Artoisenet, Frederix, Mattelaer & Rietkerk (JHEP ’13)]

Importance of correctly-handled decays

Two examples (dependent of the observable)

Angle between the leptons in the respective mother top rest frames

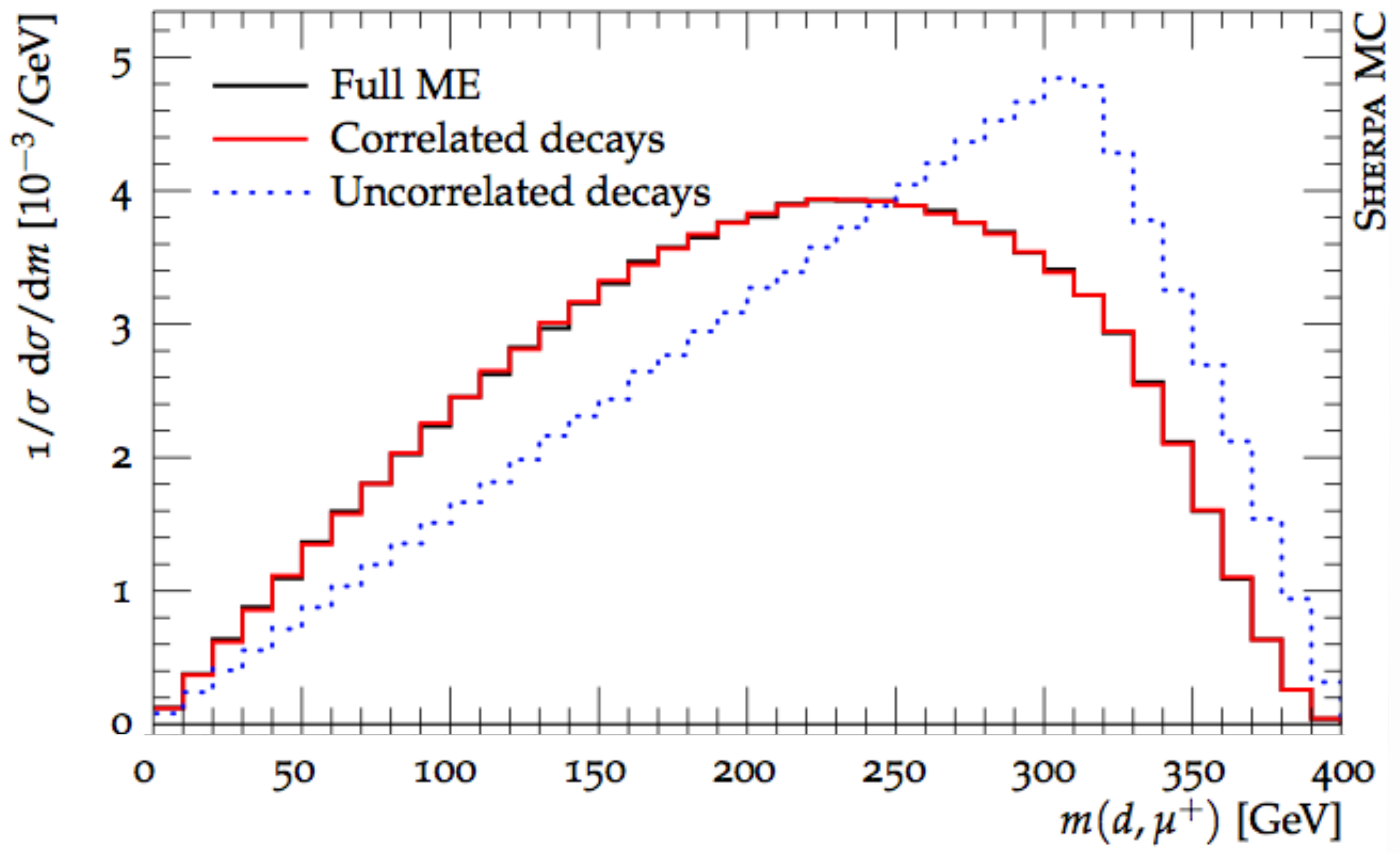




MG5aMC ⊕ MadSpin: $t\bar{t}$H production @ (N)LOQCD
[LHC8, dileptonic tt decay]

[Artoisenet, Frederix, Mattelaer & Rietkerk (JHEP '13)]

Invariant mass between decay products originating from different cascade steps



Sherpa @ LO[LHC8]

$pp \to \tilde{u}\tilde{u}^\dagger$

$\tilde{u} \to d\tilde{\chi}_1^+ \to d\chi_1^0 W^+ \to d\chi_1^0\mu^+\nu_\mu$

$\tilde{u}^\dagger \to \ldots \to \bar{u}e^+e^-\tilde{\chi}_1^0$

[Höche, Kuttimalai, Schumann & Siegert (EPJC'15)]

[Höche, Kuttimalai, Schumann & Siegert (EPJC'15)]

Phase space integration

Observable calculations

The QCD factorisation theorem

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\omega} = \sum_{a,b} \int \mathrm{d}x_a \, \mathrm{d}x_b \, \mathrm{d}\Phi_n \; f_{a/p}(x_a;\mu_F) \; f_{b/p}(x_b;\mu_F) \; \frac{1}{2s} \overline{|\mathcal{M}|}^2(s;\mu_F,\mu_R) \; \mathcal{O}_\omega(\Phi_n)$$

- Any observable ➝ integral calculation needed
- The phase space
  ➝ highly-dimensional integral (*3n-2* integrals ≡ *n*-body final state)
  ➝ complex structure ≡ analytical calculations hopeless

- The integrand is a very peaked function (propagators)
  ➝ Need for general and flexible numerical methods
- Bonus: integration one thing, events another!

Numerical integration − methods

- Standard methods like trapezium/Simpson very good in 4dims, not in D-dims
  ➝ Trapezium: precision in $1/N^{2/d}$
  ➝ Simpson: precision in $1/N^{4/d}$
- Monte Carlo integration saves the day
  ➝ Precision in $1/\sqrt{N}$

Monte Carlo integration: the method

The one-dimensional example: evaluate the integral *I*

$$I = \int_a^b \mathrm{d}x\ f(x)$$

1. Determine $f_{max} > f(x)\ \forall\ x \in [a,b]$

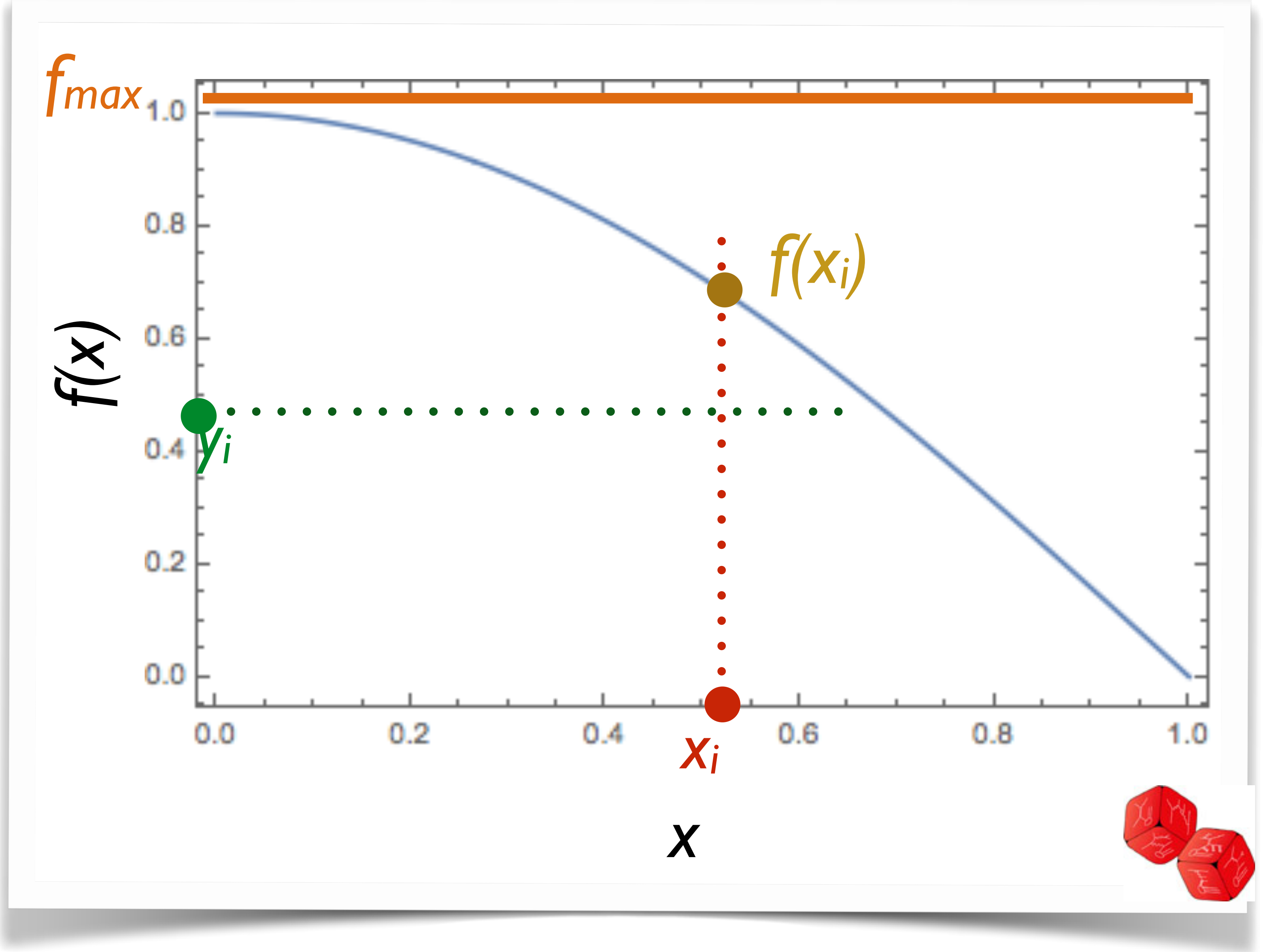
2. At a given step *i*,
   - ⋆ pick a random point $x_i \in [a,b]$
   - ⋆ pick a random number $y_i < f_{max}$

3. Compare with $f(x_i)$
   - ⋆ If $y_i > f(x_i)$: reject the point
   - ⋆ If $y_i < f(x_i)$: accept the point

4. Evaluate the integral

$$I_N = \frac{N_\text{accepted}}{N_\text{total}}\ \mathcal{V}$$

integration volume



Monte Carlo integration: the error

The mean value theorem

- If *f(x)* is continuous:

$$\exists\xi \in [a,b] : I = \int_a^b \mathrm{d}x\ f(x) = (b-a)f(\xi) = (b-a)\langle f\rangle$$

- We can approximate $\langle f\rangle$ by an averaged sum

$$I = \int_a^b \mathrm{d}x\ f(x)\ \approx I_N = \frac{b-a}{N}\sum_{n=1}^{N} f(x_n)$$

★ $\langle f\rangle$ ≡ sampling the integrand at random points

★ MC method: random choice of points

The error on the integral ≡ the variance

- Independent of the number of dimensions
- Minimisable

$$V = (b-a)\int_a^b \mathrm{d}x\ f^2(x) - I^2\ \approx V_N = \frac{(b-a)^2}{N}\sum_{n=1}^{N} f^2(x_n) - I_N^2$$

Result

$$I = I_N \pm \sqrt{\frac{V_N}{N}}$$

- Error easy to estimate and independent of the number of dimensions
- Improvement possible by minimising V_N (ideal case: *f(x)* = *cst* ⇔ *V*=V_N=*0*)

➙ Change of variables to flatten the integrand

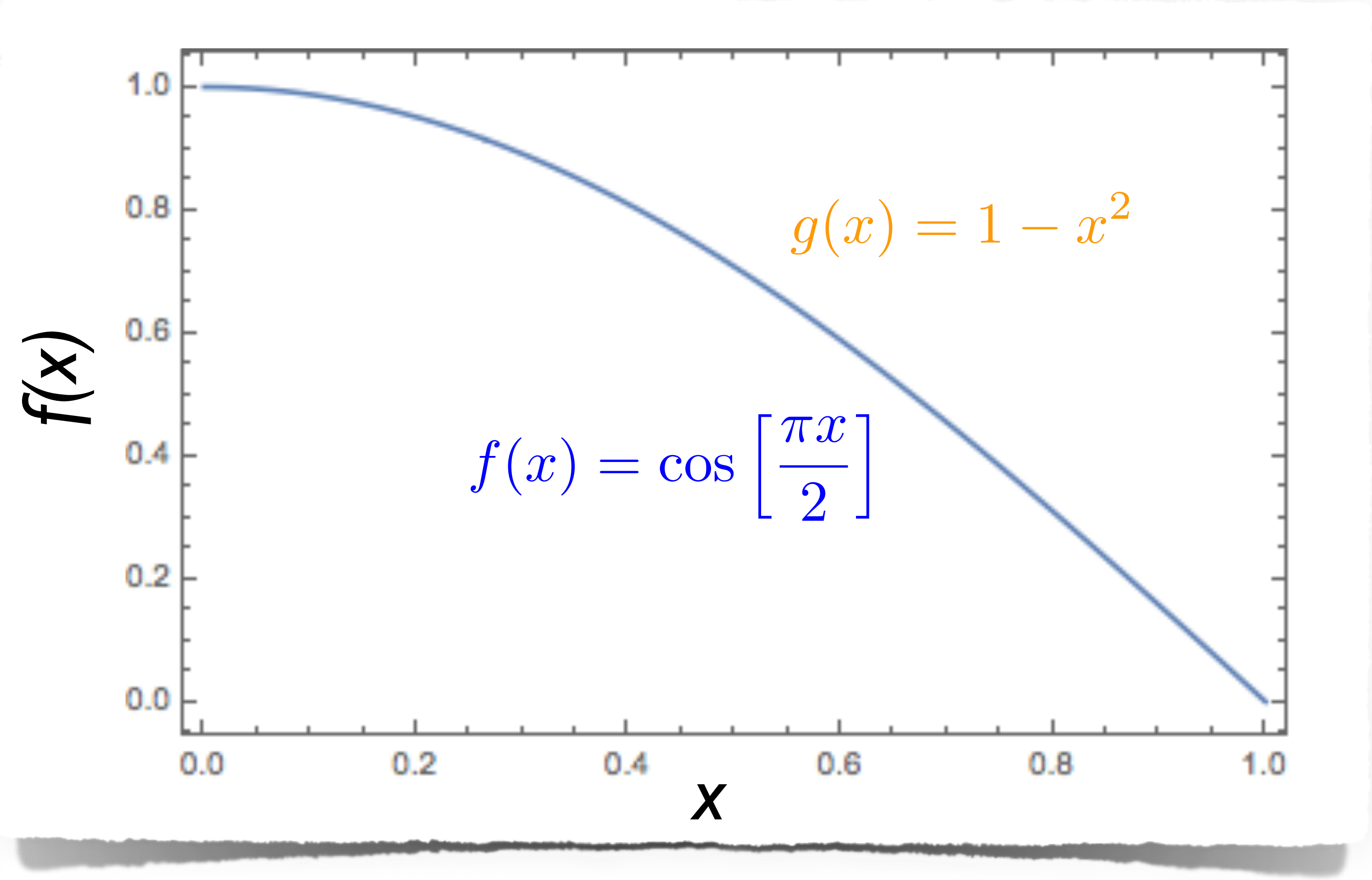
Importance sampling: a practical example

Integral to calculate

$$I = \int_0^1 \mathrm{d}x \ \cos\left[\frac{\pi x}{2}\right] = \frac{2}{\pi} \approx 0.6366$$

$$I_N = 0.637 \pm \frac{0.307}{\sqrt{N}}$$

- Convergence slow
- Precision ⇒ large N
- Strength: scalability with N_{dim}



Clever change of variable ➙ reduction of the variance

- The ratio *f(x)/g(x)* ≃ *1* (ideal case)

$$I = \int_0^1 \mathrm{d}x \ (1-x^2) \frac{\cos\left[\frac{\pi x}{2}\right]}{1-x^2} = \int_{\xi_1}^{\xi_2} \mathrm{d}\xi \ \boxed{\frac{\cos\left[\frac{\pi x(\xi)}{2}\right]}{1-x(\xi)^2}} \simeq 1 \quad \text{with} \quad \xi = x - \frac{1}{3}x^3$$

$$I_N = 0.637 \pm \frac{0.031}{\sqrt{N}}$$

➙ Faster convergence

Phase space parametrisation crucial

- Better convergence

Importance sampling in action

The one-dimensional example: evaluate the integral *I*

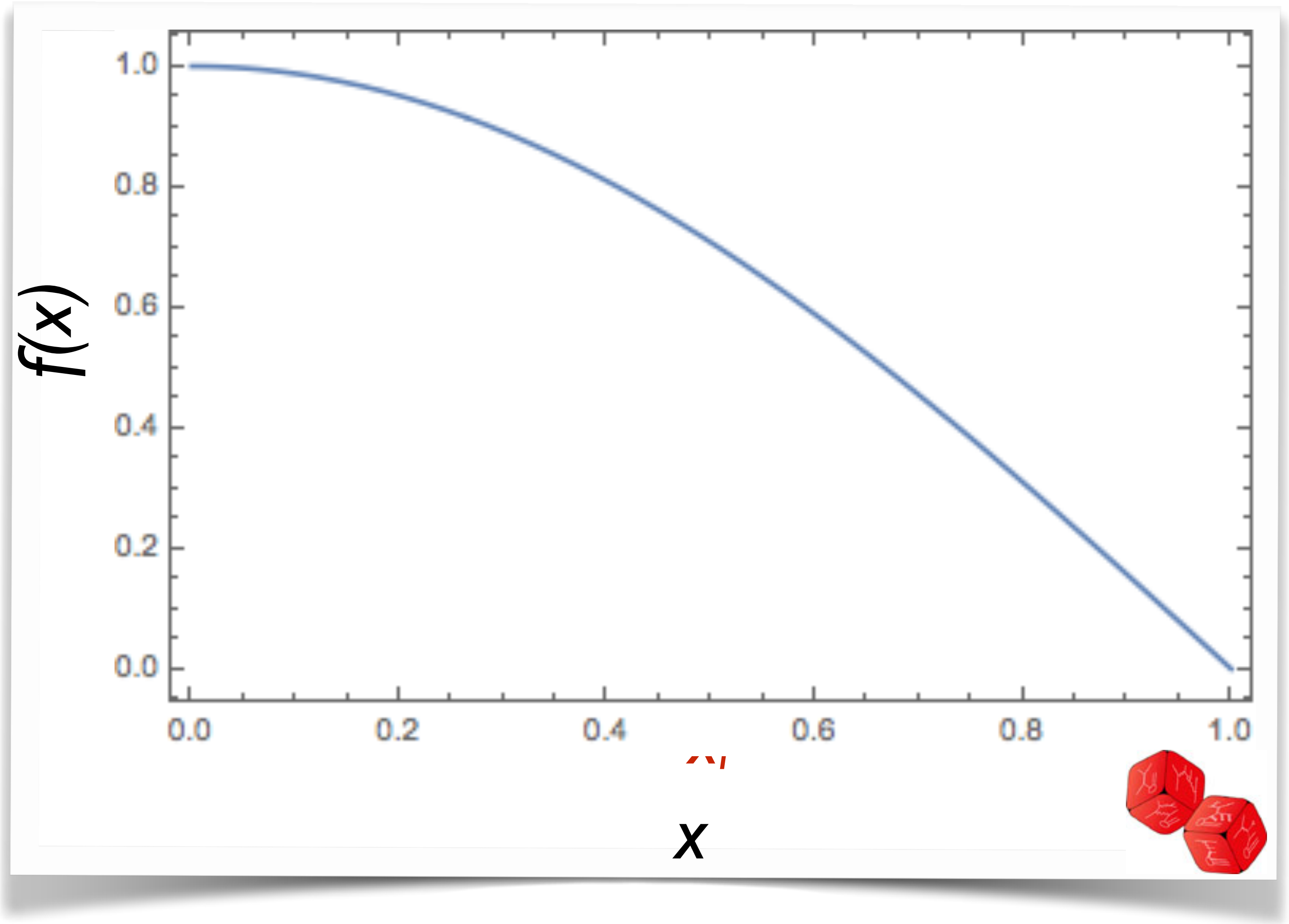
$$I = \int_a^b \mathrm{d}x \; f(x)$$

1. Find *g(x) so that g(x)* > *f(x)* ∀ *x* ∈ *[a,b]*

2. At a given step *i*,
   - ⋆ pick a random point x_i distributed as *g(x)*
   - ⋆ pick a random number $y_i < g(x_i)$

3. Compare with $f(x_i)$
   - ⋆ If $y_i > f(x_i)$: reject the point
   - ⋆ If $y_i < f(x_i)$: accept the point

4. Evaluate the integral $I_N = \dfrac{N_{\mathrm{accepted}}}{N_{\mathrm{total}}} \, \mathcal{V}$



More points are sampled where the function is the largest

Problem of a peaked integrand

The QCD factorisation theorem

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\omega} = \sum_{a,b} \int \mathrm{d}x_a\ \mathrm{d}x_b\ \mathrm{d}\Phi_n\ f_{a/p}(x_a;\mu_F)\ f_{b/p}(x_b;\mu_F)\ \frac{1}{2s}\overline{|\mathcal{M}|}^2(s;\mu_F,\mu_R)\ \mathcal{O}_\omega(\Phi_n)$$

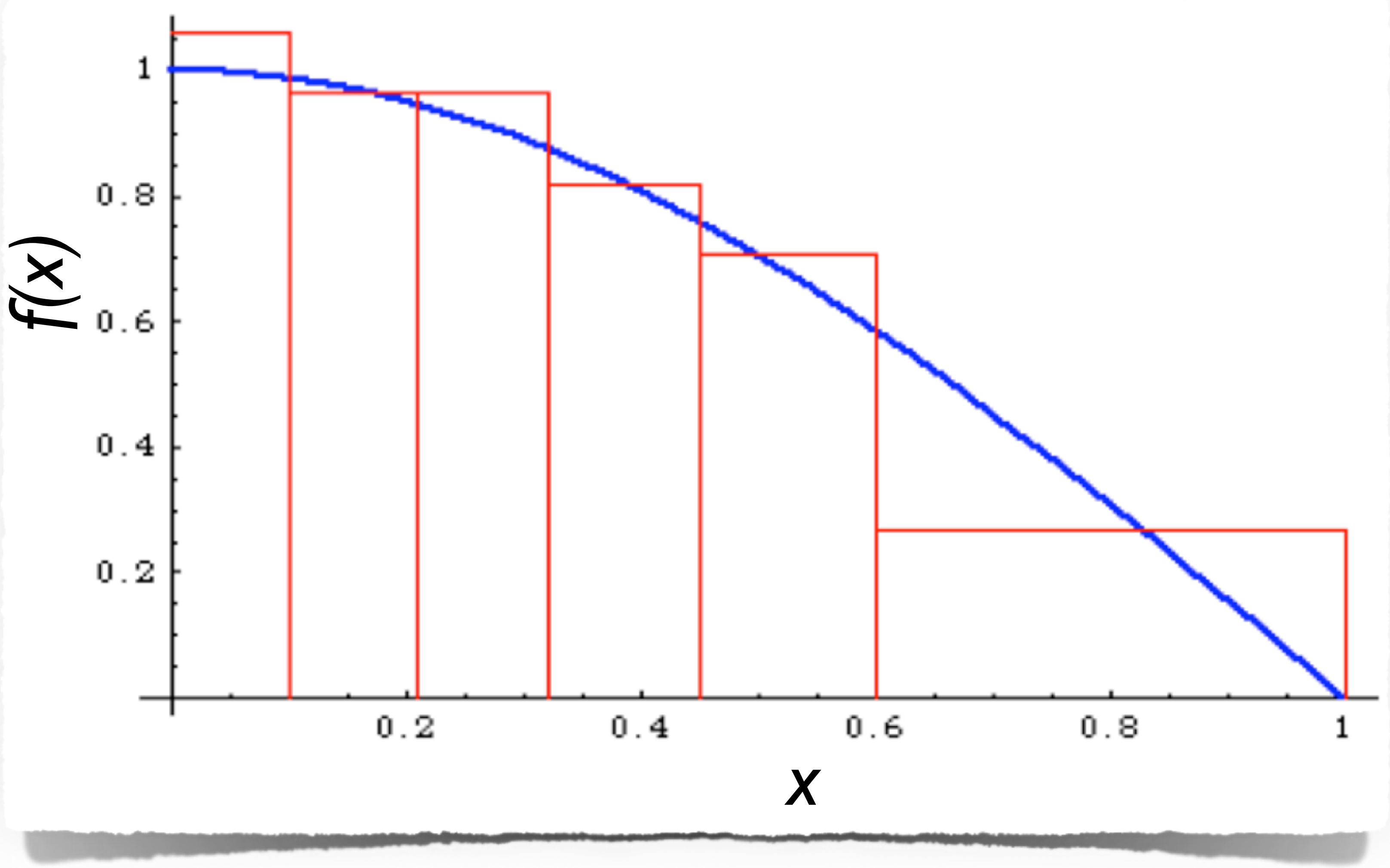
- For each point, we have a weight given by $f_{a/p}(x_a;\mu_F)\ f_{b/p}(x_b;\mu_F)\ \frac{1}{2s}\overline{|\mathcal{M}|}^2(s;\mu_F,\mu_R)$
- Interpretation: each sampled momentum configuration ➝ a weight

Problem: a peaked integral is peaked (➝ propagators)

- Random phase space points: very little chance to contribute
  ➝ Few points carry the bulk of the integral
- Flattening the integrand ≡ change of variables (importance sampling)
  ➝ Knowledge about the integrand (to find the supremum function)

Construction of an approximative function of the integrand

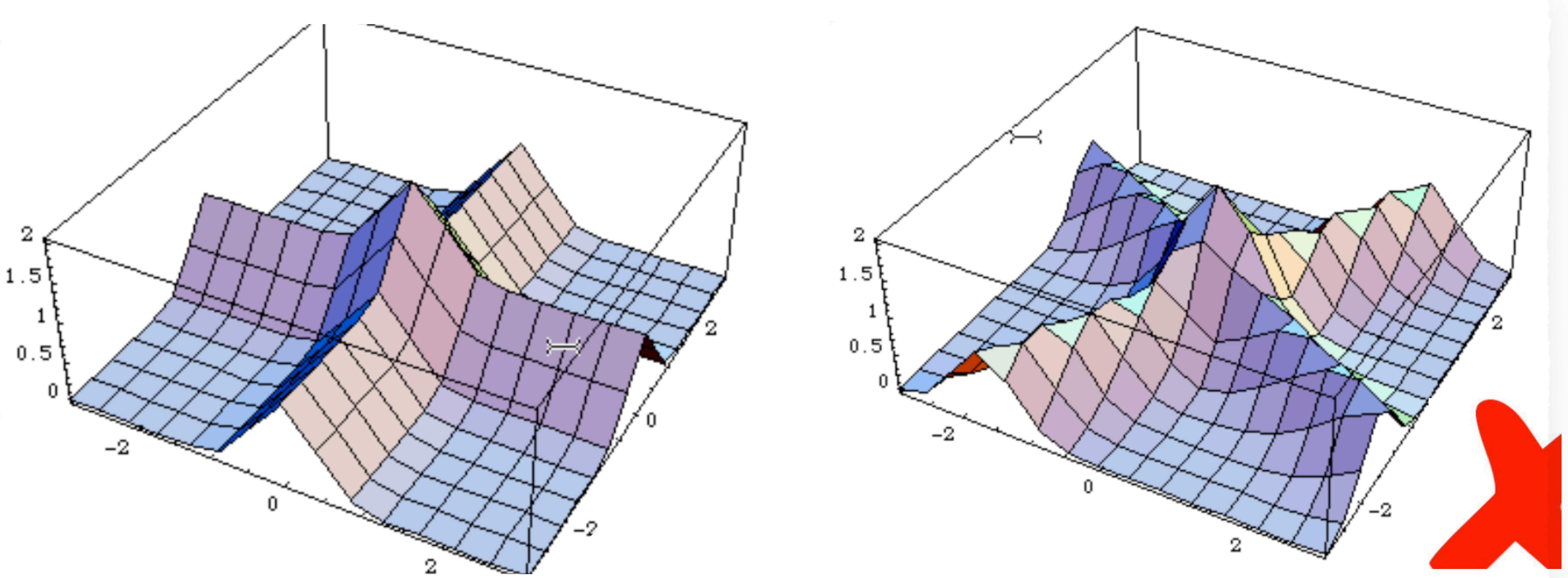
- Division of the integration domain in sub-domains (variable bin-size)
  - ⋆ Adjustment: identical variance in each bin
    ➝ Many bins where the function is large
  - ⋆ Minimisation of the overall variance
- More bins where the integrand fluctuates more
  - ⋆ The binned function ≡ approximation $g(x)$ of the integrand



The VEGAS algorithm

MG5aMC → the VEGAS algorithm

- Relies on 1D integration
- Projections on the various axes to align the integrand
  → Factorisation of integration variable by variable
- Adaptive sampling → points in '*interesting*' domains
- Finding a good rotation crucial
  → Rarely the case
  → Multi-channeling



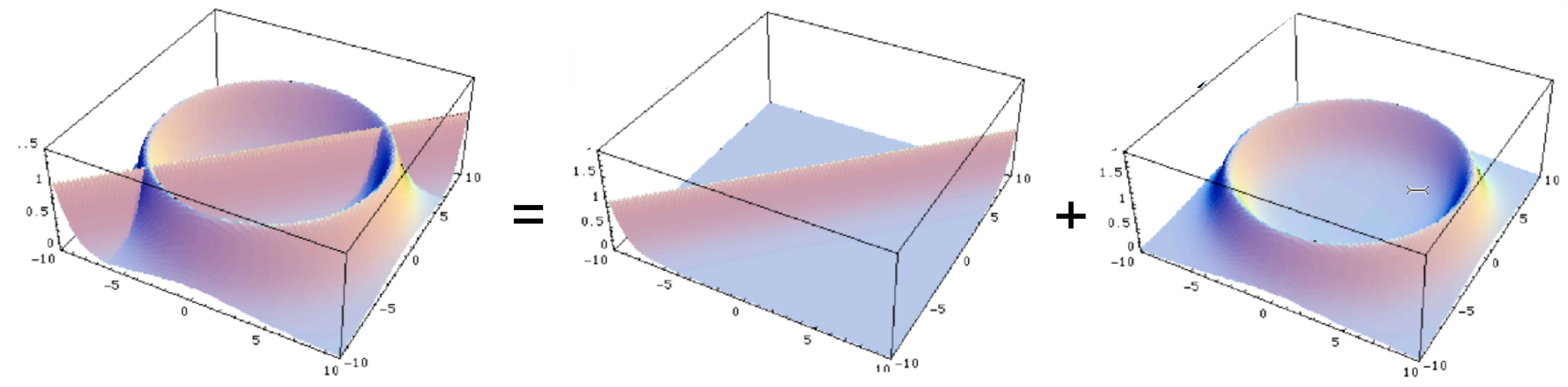
integrand well aligned

rotation needed

Multi-channeling

- One rotation per channel

$$g(x) = \sum_{\text{channels}} \alpha_i g_i(x) \quad \text{with} \quad \sum_{\text{channels}} \alpha_i = 1$$



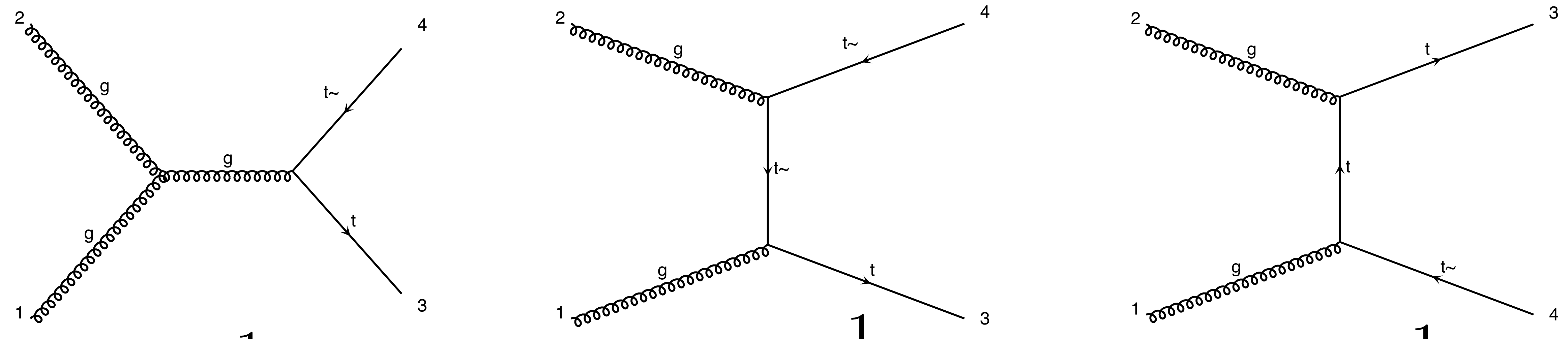
- Each g_i takes care of one single peak of the integrand

$$I = \int \mathrm{d}x \; f(x) = \int \mathrm{d}x \underbrace{\overset{\simeq I}{\boxed{\frac{f(x)}{g(x)}}}}_{\text{importance sampling}} g(x) = \underbrace{\sum_i \alpha_i \int \mathrm{d}x \; \frac{f(x)}{g(x)} g_i(x)}_{\text{multi-channeling}}$$

⋆ Knowledge of the matrix element

Multi-channel integration: an example

Top-antitop production: 3 diagrams



$$\mathcal{A}_s \propto \frac{1}{s} \qquad \mathcal{A}_t \propto \frac{1}{t-m_t^2} \qquad \mathcal{A}_u \propto \frac{1}{u-m_t^2}$$

$$g(x) = \sum_{\text{channels}} \alpha_i g_i(x)$$

- Three different pole structures

$$I = \int \mathrm{d}\Phi_2 \, \left|\mathcal{A}_s+\mathcal{A}_t+\mathcal{A}_u\right|^2 = \sum_{i=s,t,u} \int \mathrm{d}\Phi_2 \, \frac{\overset{g_i(\Phi)}{\left|\mathcal{A}_i\right|^2}}{\underbrace{\left|\mathcal{A}_s\right|^2+\left|\mathcal{A}_t\right|^2+\left|\mathcal{A}_u\right|^2}_{g(\Phi)}} \underbrace{\left|\mathcal{A}_s+\mathcal{A}_t+\mathcal{A}_u\right|^2}_{f(\Phi)}$$

⋆ *f(Φ) / g(Φ) ≃ 1*

→ integration easy

→ Integration of one single diagram at a time (pole structure known)

⋆ Multi-channeling on the basis of the different diagrams

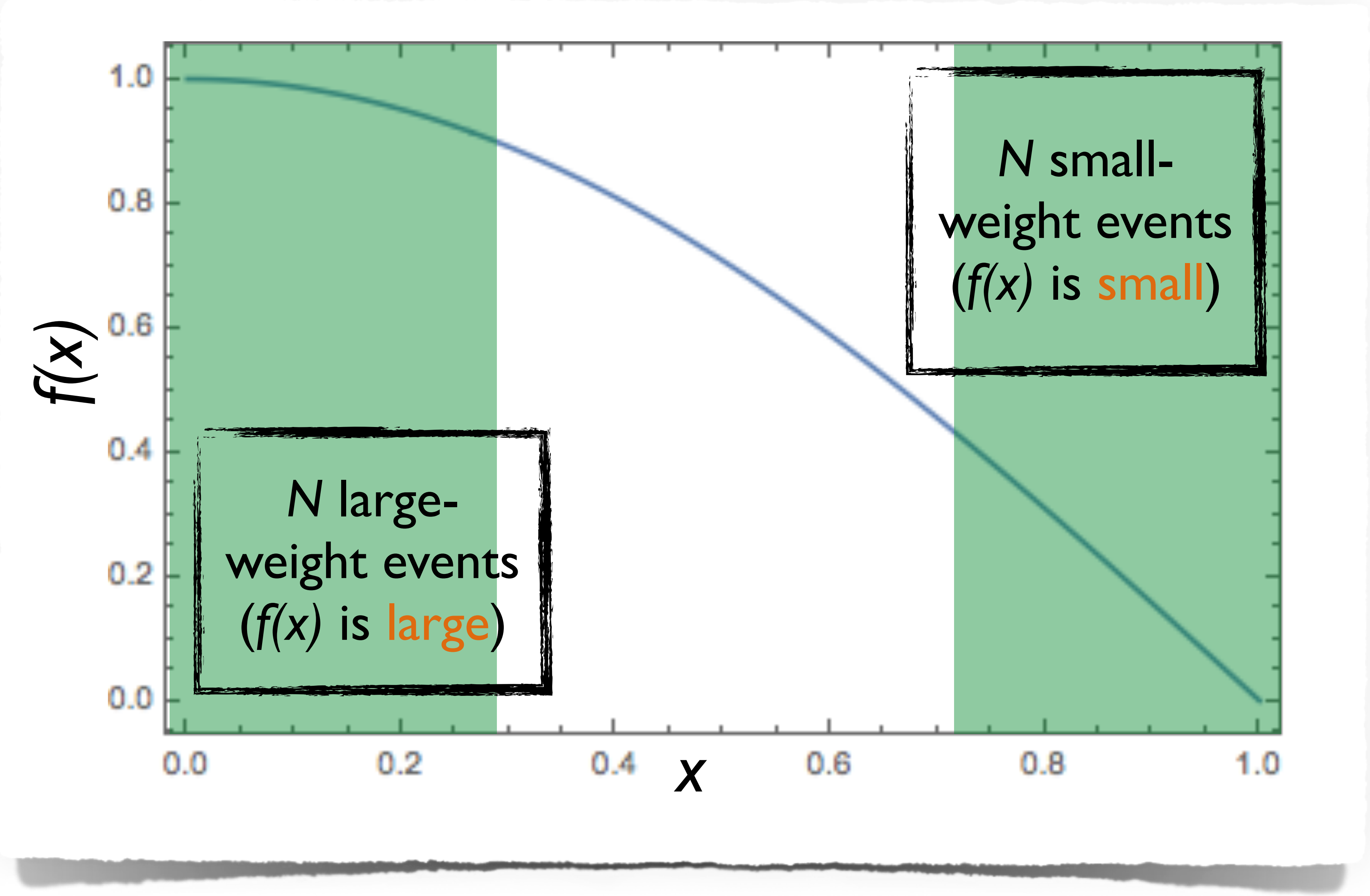
Event generation

Weighted and unweighted events

Accepted points ➙ event generation

- One point ≡ one event
- Integrand value ≡ event weight
- Not all events are equal

Weighted events



N small-weight events (*f*(*x*) is small)

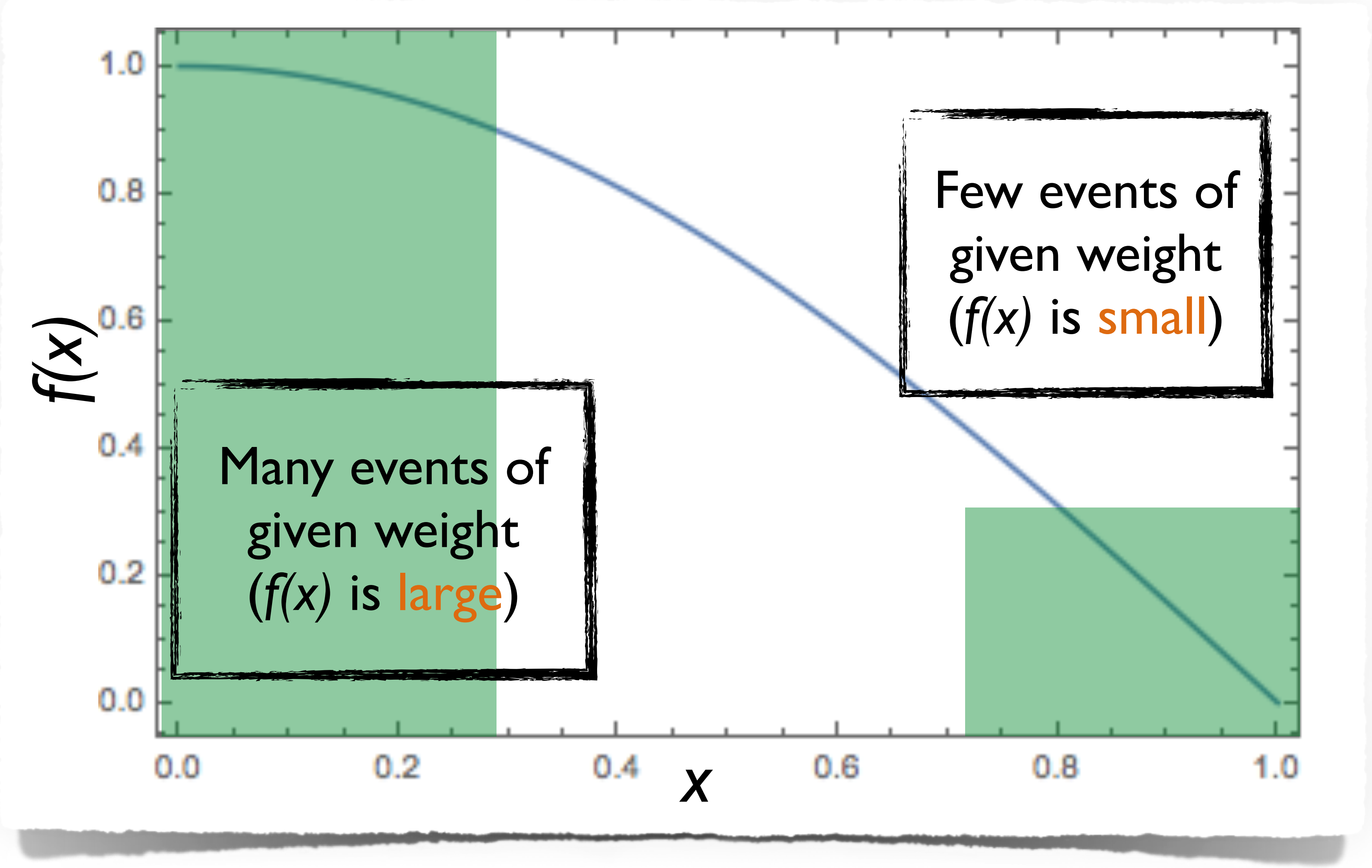
N large-weight events (*f*(*x*) is large)

Enforcing equal-weight events

- Distributed as occurring in nature
- All events are equal
- Weight value: recovering the total rate

➙ $\langle\omega\rangle = \sigma_{tot}/N_{events}$

Unweighted events



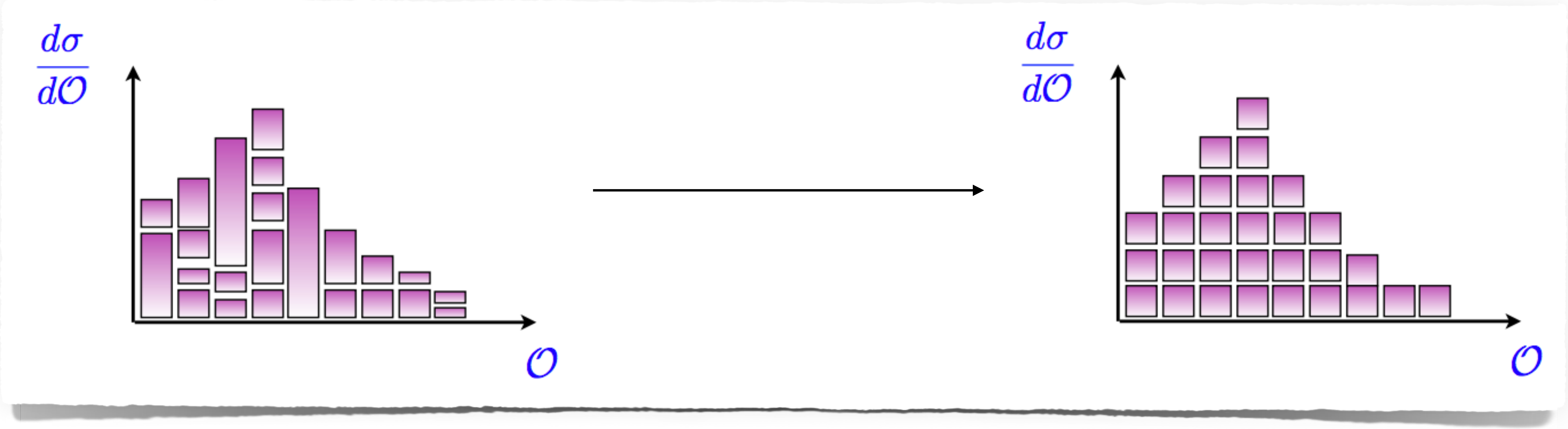
Few events of given weight (*f*(*x*) is small)

Many events of given weight (*f*(*x*) is large)

Unweighted events in practice

Principle of unweighting

- Determination of a threshold during the integration phase $\omega_{\max}$
- Determination of the average weight $\langle\omega\rangle = \sigma_{tot}/N_{events}$
- Accept/reject: acceptation with a probability $\omega(\Phi)$ / ω_{max}
- Each event is assigned the weight $\langle\omega\rangle$


$\frac{d\sigma}{d\mathcal{O}}$
$\mathcal{O}$
$\frac{d\sigma}{d\mathcal{O}}$
$\mathcal{O}$

Requirements

- Integrand bounded from above ($\omega_{\max}$ must exist)
- Integrand positive-definite (bypassable)

Outline

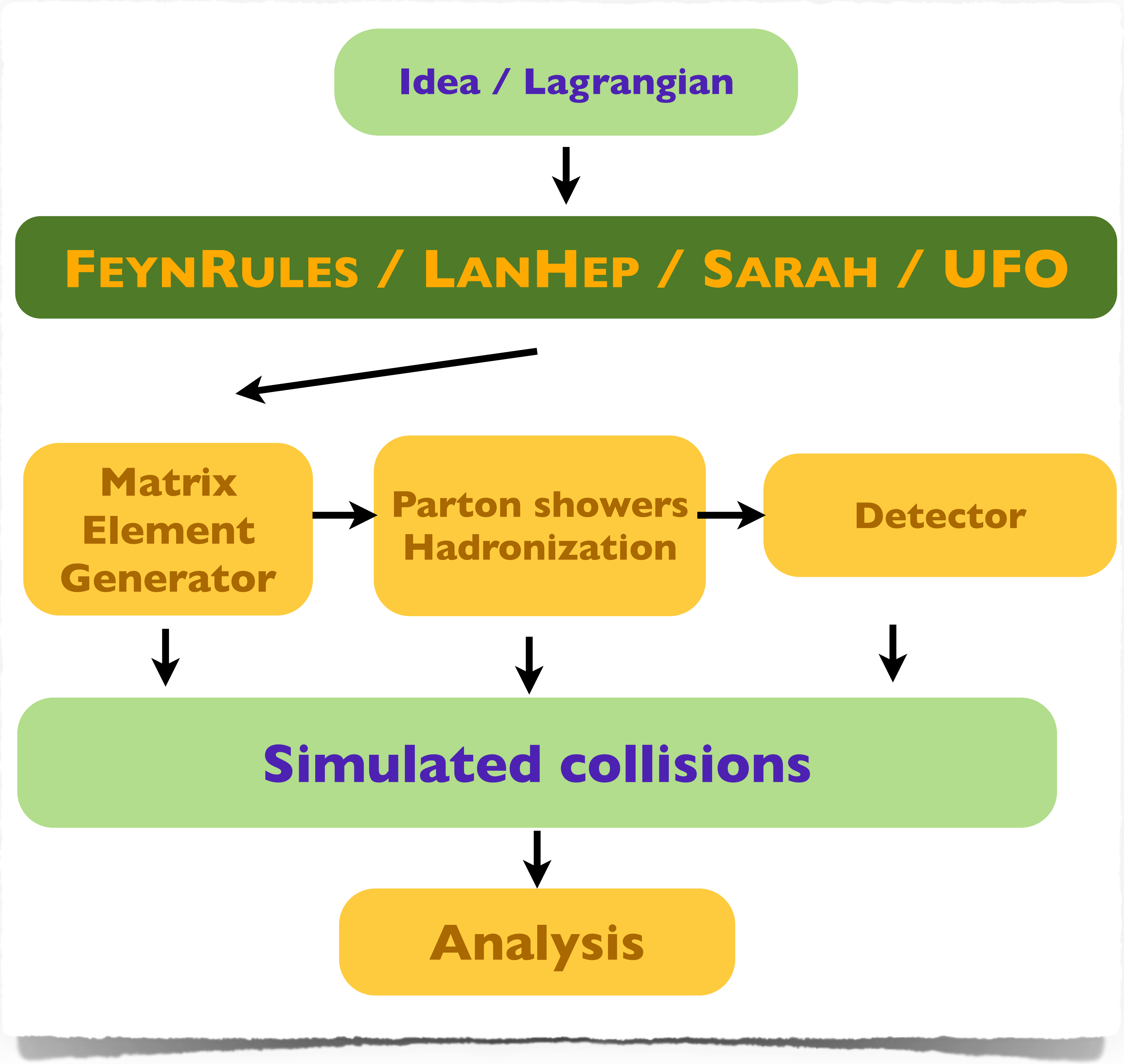
1. A comprehensive approach for Monte Carlo simulations

2. Implementing models into Monte Carlo event generators

3. From models to hard-scattering events

4. **Summary**

Summary



Event simulation is a complex process

- Factorised it into separate parts
- Event simulation performed step-by-step

This lecture: 1st parts of the chain

- Connecting models (Lagrangians) to tools
- Generation of matrix elements
- Heavy particle decays
- Cross section calculations
- Event generation

Next steps

- QCD environment: parton showering, hadronisation
- Detector simulation
- Signal analysis
- Comparison with data / phenomenological study