



*fast*NLO Toolkit

Daniel Britzger, **Klaus Rabbertz**, Georg Sieber, Fred Stober, Markus Wobisch
(DESY, KIT * 3, Louisiana Tech University)

in cooperation with

Enrico Bothmann, Steffen Schumann
(Uni Göttingen)



Part 1

fastNLO v2 & Toolkit Development



From v1.4 to v2.1

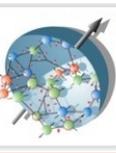


- ✓ 1. Cross-checked old v1.4 versus new v2.1 tables
- ✓ 2. Converted existing v1.4 tables to new format
- ✓ 3. Cross-checked new table reader code in C++ vs. Fortran
- ✓ 4. Public release of table reader code as autotools tarball:
 - ➔ First release 14.02.2012: fastNLO_reader 2.1.0-1062
- ✓ 5. Transformed C++ reader code into linkable library
 - ➔ Latest release 14.02.2014: fastNLO_reader 2.1.0-1689
- ✓ **Installation:**
 - ➔ **Requirements: LHAPDF5 or 6**
 - ➔ `./configure --prefix=/path/to/install/directory [--with-lhapdf=/path]`
 - ➔ `fnlo-tk-config` available to list config info and compiler/linker options
- ✓ 6. Implemented new functionalities ...

LHAPDF, M. Whalley et al., hep-ph/0508110,
LHAPDF6, A. Buckley et al., arXiv:1405.1067.



Use of alternative α_s evolutions



✓ LHAPDF5/6

✓ CRunDec 08/2012

➔ included in fastNLO

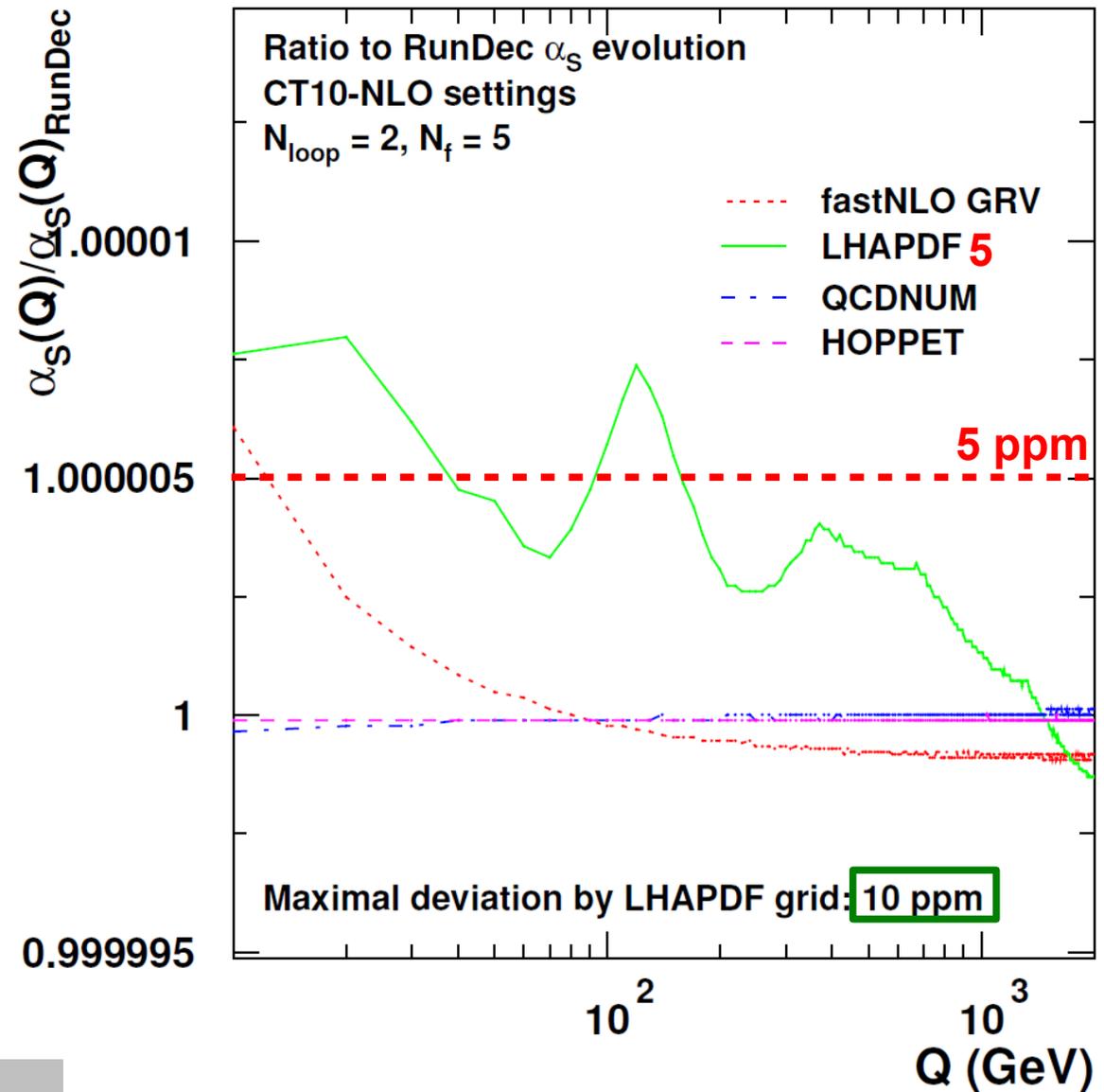
✓ QCDNUM v17-00-06

➔ ... [--with-qcdnum=/path/...]

➔ Makefiles adapted, need -fPIC on x86_64 systems

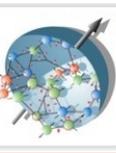
✓ HOPPET v1.1.5

➔ ... [--with-hoppet=/path/...]

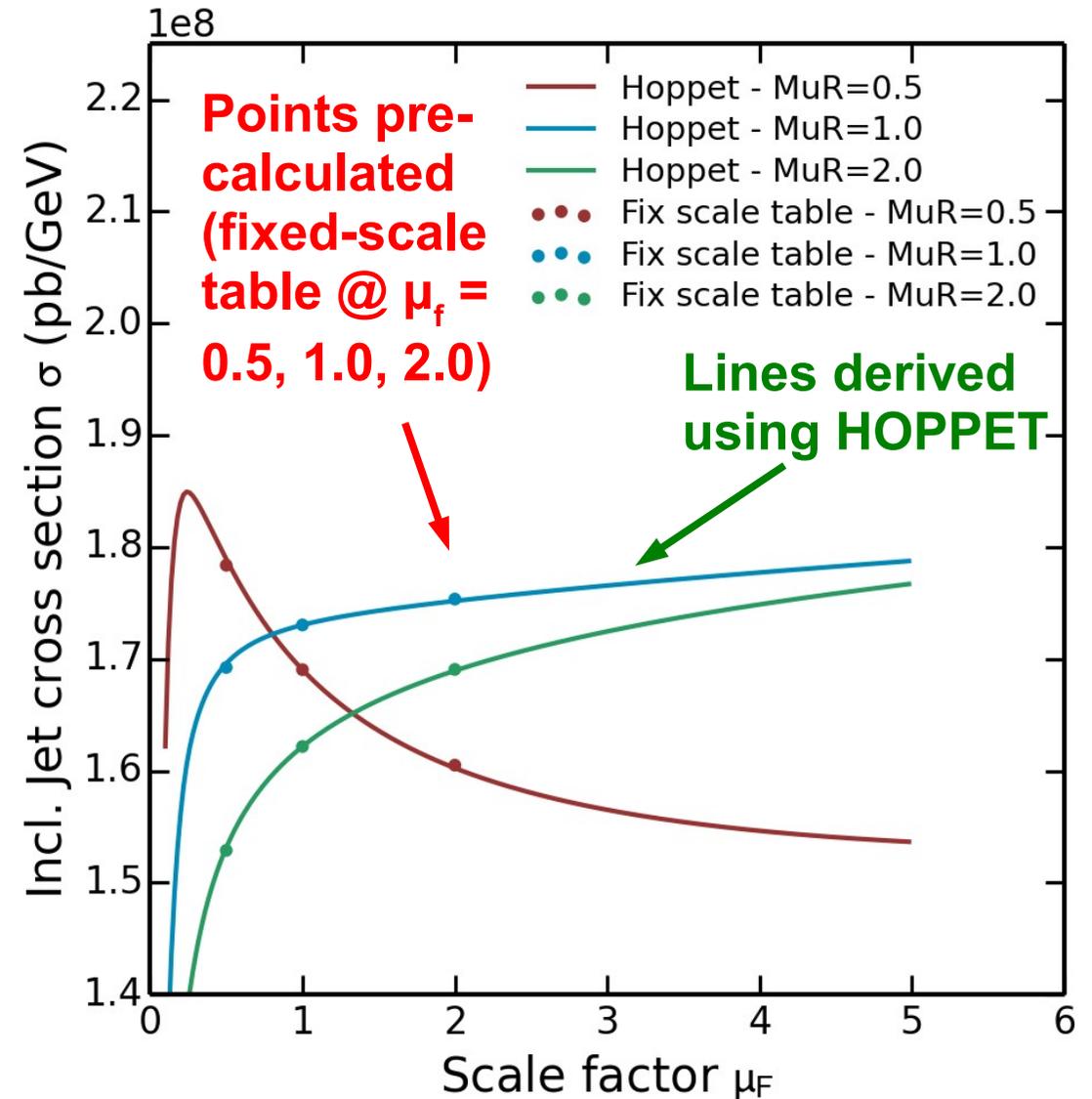


RunDec, B. Schmidt, M. Steinhauser, CPC183, 2012;
K. Chetyrkin, J. Kühn, M. Steinhauser, CPC133, 2000.
QCDNUM, M. Botje, CPC182, 2011.
HOPPET, G. Salam, J. Rojo, CPC180, 2009.

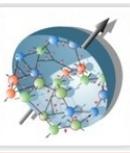
Use of HOPPET for μ_f variation



- ✓ fastNLO v1.4 used extra tables for μ_f variation with fixed scale factors
 - straightforward also @ NNLO
 - avoids additional integrations
 - increases table size
- ✓ In fastNLO v2.3 can also use HOPPET for μ_f variation
 - Same method as used in APPLgrid
 - continuous curve



APPLgrid, T. Carli et al., EPJC 66 (2010) 503.



- Problem

- Scale variations become more difficult in NNLO than in NLO

- Current available implementations for NLO calculations

Renormalization scale variations

- Scale variations applying RGE
 - Use LO matrix elements times $n\beta_0\ln(c_r)$
- Flexible-scale implementation
 - Store scale-independent weights:

[fastNLO, APPLgrid]

[fastNLO]

Factorization scale variations

- Calculate LO DGLAP splitting functions using HOPPET
- Store coefficients for desired scale factors
- Flexible-scale implementation

[APPLgrid, fastNLO]

[fastNLO]

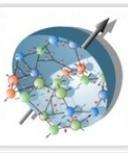
[fastNLO]

- Scale variations for NNLO calculations

- renormalization scale variations become more complicated
- NLO splitting functions are needed for factorization scale variations e.g. with HOPPET
 - Calculations become slower again => Not desired for fast repeated calculations



Flexible-scale tables



- Storage of scale-independent weights enable full scale flexibility also in NNLO

→ Additional logs in NNLO

$$\omega(\mu_R, \mu_F) = \underbrace{\omega_0 + \log(\mu_R^2)\omega_R + \log(\mu_F^2)\omega_F}_{\text{log's for NLO}} + \underbrace{\log^2(\mu_R^2)\omega_{RR} + \log^2(\mu_F^2)\omega_{FF} + \log(\mu_R^2)\log(\mu_F^2)\omega_{RF}}_{\text{additional log's in NNLO}}$$

→ Store weights: $\omega_0, \omega_R, \omega_F, \omega_{RR}, \omega_{FF}, \omega_{RF}$ for order α_s^{n+2} contributions

- Advantages

- Renormalization and factorization scale can be varied *independently* and by *any* factor
 - No time-consuming ‘re-calculation’ of splitting functions in NLO necessary
- Only small increase in amount of stored coefficients

- fastNLO implementation

- Two different observables can be used for the scales
 - e.g.: H_T and $p_{T,max}$
 - or e.g.: p_T and $|y|$
 - ...
- Any function of those two observables can be used for calculating scales

‘Flexible-scale concept’: Best choice for performant NNLO calculations



Flexible-scale tables in DIS



fastnlo @ HepForge

Tables from recent H1 multi-jet study use $\sqrt{Q^2}$ and p_T

Use of this method in fastNLO dates back to 2011 when going from v1.4 to v2.1. Useful for DIS, now also for pp, e.g. with scales M_Z and p_{T_Z} .

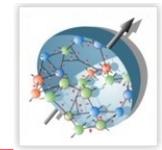
Note: All HERA tables are flexible-scale tables ==> The C++ reader versions must be used.

HERA: ep @ sqrt(s) = 319 GeV

fnh5001_I1301218	H1 inclusive jet HERA-II (kt and anti-kt); LO, NLO inSPIRE no HepData yet	no RIVET analysis available
fnh5002_I1301218	H1 dijet HERA-II (kt and anti-kt); LO, NLO inSPIRE no HepData yet	no RIVET analysis available
fnh5003kt_I1301218	H1 dijet HERA-II (kt); LO, NLO inSPIRE no HepData yet	no RIVET analysis available
fnh5003ak_I1301218	H1 dijet HERA-II (anti-kt); LO, NLO inSPIRE no HepData yet	no RIVET analysis available
fnh4002_I875006	ZEUS inclusive dijet HERA-I+II (kt); LO, NLO inSPIRE no HepData (Note: This table only works with the new fastnlo_toolkit reader, but not yet with the old fastnlo_reader.)	no RIVET analysis available
fnh5201_I838435	H1 inclusive jets at low Q^2 HERA-I (kt); LO, NLO inSPIRE no HepData (Note: This table only works with the new fastnlo_toolkit reader, but not yet with the old fastnlo_reader.)	no RIVET analysis available
fnh5401_I818707	H1 inclusive jets at high Q^2 HERA-I (kt); LO, NLO inSPIRE no HepData, only normalized x section publ. (Note: This table only works with the new fastnlo_toolkit reader, but not yet with the old fastnlo_reader.)	no RIVET analysis available
fnh5101_I753951	H1 inclusive jets HERA-I (kt); LO, NLO inSPIRE HepData (Note: This table only works with the new fastnlo_toolkit reader, but not yet with the old fastnlo_reader.)	no RIVET analysis available
fnh4401_I724050	ZEUS inclusive jets HERA-I (kt); LO, NLO inSPIRE HepData (Note: This table only works with the new fastnlo_toolkit reader, but not yet with the old fastnlo_reader.)	no RIVET analysis available
HERA: ep @ sqrt(s) = 300 GeV		
fnh4301_I593409	ZEUS inclusive jets HERA (kt); LO, NLO inSPIRE HepData (Note: This table only works with the new fastnlo_toolkit reader, but not yet with the old fastnlo_reader.)	no RIVET analysis available



Demo plot using Python extension

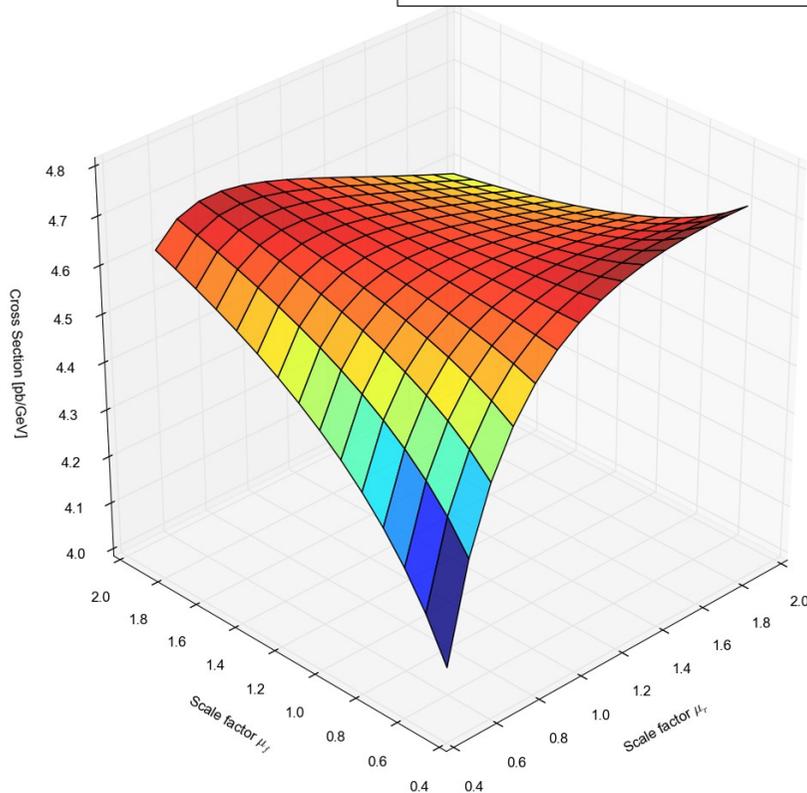


✓ Python extension available

➔ ... [--enable-pyext]

✓ Easy example plotting 2D scale dependence:

• CMS 1 TeV $\leq M_{JJ} < 1.23$ TeV, $2 \leq |y_{max}| < 2.5$, $\mu = p_{T,12}$



```
#!/usr/bin/env python2
```

```
from fastnlo import fastNLOLHAPDF
```

```
import matplotlib
import matplotlib.pyplot as plt
from matplotlib import cm
from mpl_toolkits.mplot3d import axes3d
import numpy as np
```

```
fnlo = fastNLOLHAPDF('fnlortable.tab')
fnlo.SetLHAPDFFilename('CT10nlo.LHgrid')
fnlo.SetLHAPDFMember(0)
```

```
mufs = np.arange(0.1, 1.5, 0.10)
murs = np.arange(0.1, 1.5, 0.10)
xs = np.zeros((mufs.size, murs.size))
```

```
for i, muf in enumerate(mufs):
    for j, mur in enumerate(murs):
        fnlo.SetScaleFactorsMuRMuF(mur, muf)
        fnlo.CalcCrossSection()
        xs[i][j] = np.array(fnlo.GetCrossSection())[0]
```

```
fig = plt.figure(figsize=(13,13))
```

... plotting details

```
ax.set_ylabel('Scale factor  $\mu_F$ ')
ax.set_xlabel('Scale factor  $\mu_R$ ')
ax.set_zlabel('Cross Section [pb/GeV]')
plt.show()
```

... plotting details

Setup Python with fastNLO

Select table, PDF & mem.

Define μ_r , μ_f ranges

Loop over μ_r , μ_f

Plot



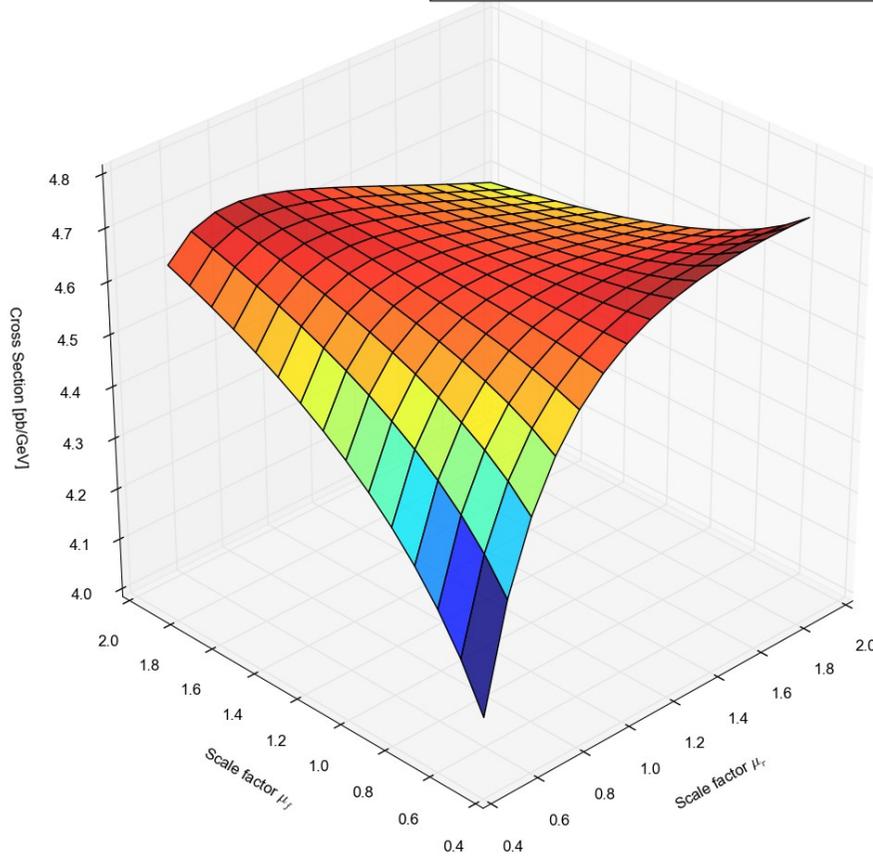
Extra slide: CMS dijet mass



Central scale: $\mu = \langle p_{T,1,2} \rangle$

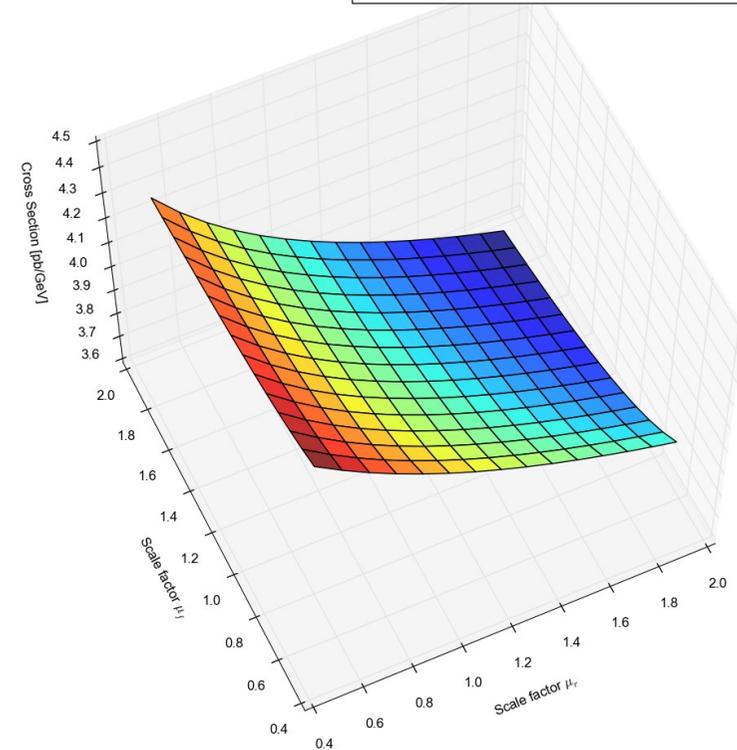
Outer $|y_{\max}|$ bin!

- CMS $1 \text{ TeV} \leq M_{JJ} < 1.23 \text{ TeV}$, $2 \leq |y_{\max}| < 2.5$, $\mu = p_{T,1,2}$



Central scale: $\mu = M_{JJ}/2$

- CMS $1 \text{ TeV} \leq M_{JJ} < 1.23 \text{ TeV}$, $2 \leq |y_{\max}| < 2.5$, $\mu = M_{JJ}/2$



Derived from one fastNLO flexible-scale table



Extra slide: ATLAS dijet mass



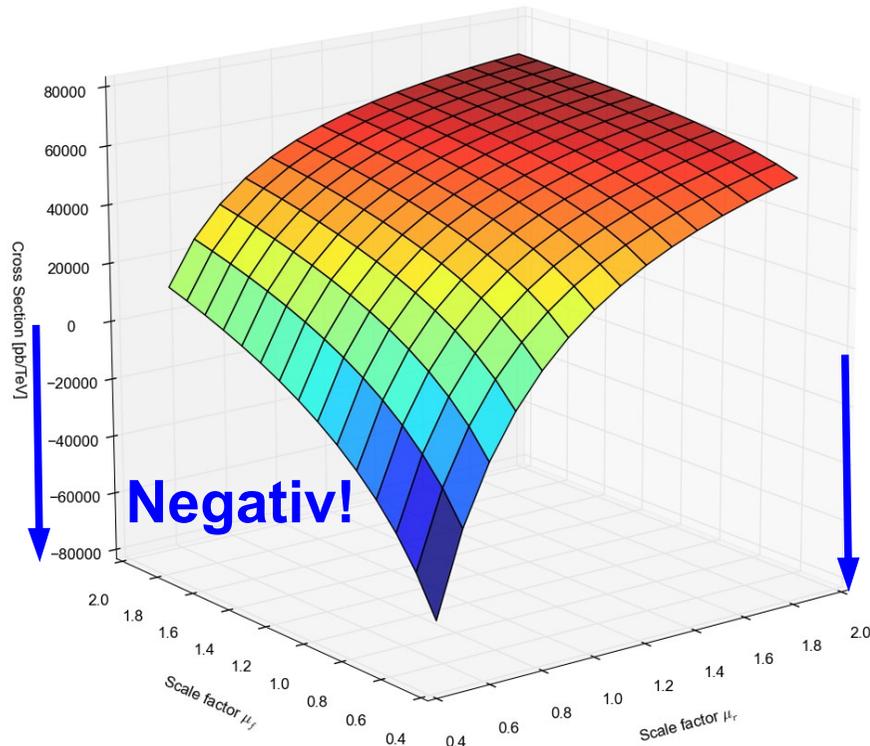
Central scale: $\mu = pT_{\max}$

Outer y^* bin!

• ATLAS $1.18 \text{ TeV} \leq M_{jj} < 1.31 \text{ TeV}$, $3.0 \leq y^* < 3.5$, $\mu = pT_{\max}$

+80k

-80k

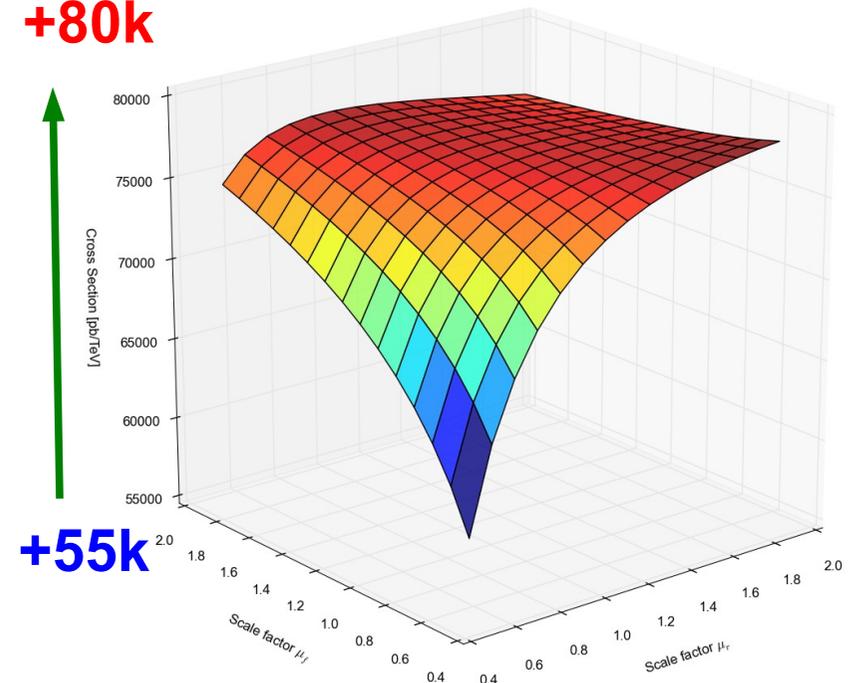


Central scale: $\mu = pT_{\max} \cdot \exp(0.3 y^*)$

• ATLAS $1.18 \text{ TeV} \leq M_{jj} < 1.31 \text{ TeV}$, $3.0 \leq y^* < 3.5$, $\mu = pT_{\max} \cdot \exp(0.3 y^*)$

+80k

+55k



Derived from one fastNLO flexible-scale table

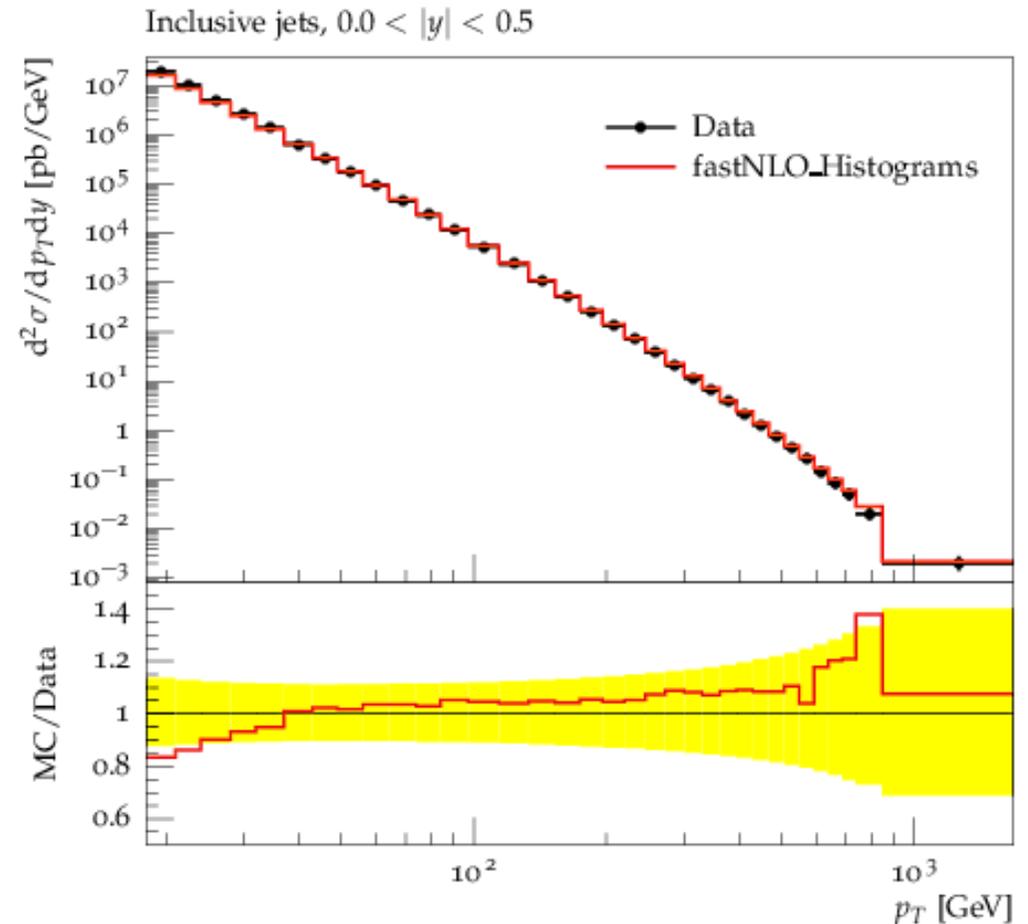


Use with Rivet 2 & YODA Format



Summer student project of
Stefanos Tyros (with Peter Skands):

- ✓ Provide YODA formatted output for fastNLO tables
 - `fnlo-tk-yodaout fnlortable.tab`
- ✓ Compare with data (or MC) histograms using Rivet
 - `rivet-mkhtml fnlortable.yoda`
 - `browser plots/index.html`
- ✓ Can provide e.g. NLO plots to mcplots.cern.ch
- ✓ Test inclusion of fastNLO in GENSER successful



It is very desirable to have the RIVET analyses from the experiments!

RIVET, A. Buckley et al., CPC184 (2013),
rivet.hepforge.org, yoda.hepforge.org.



Re-factoring v2.1 into Toolkit

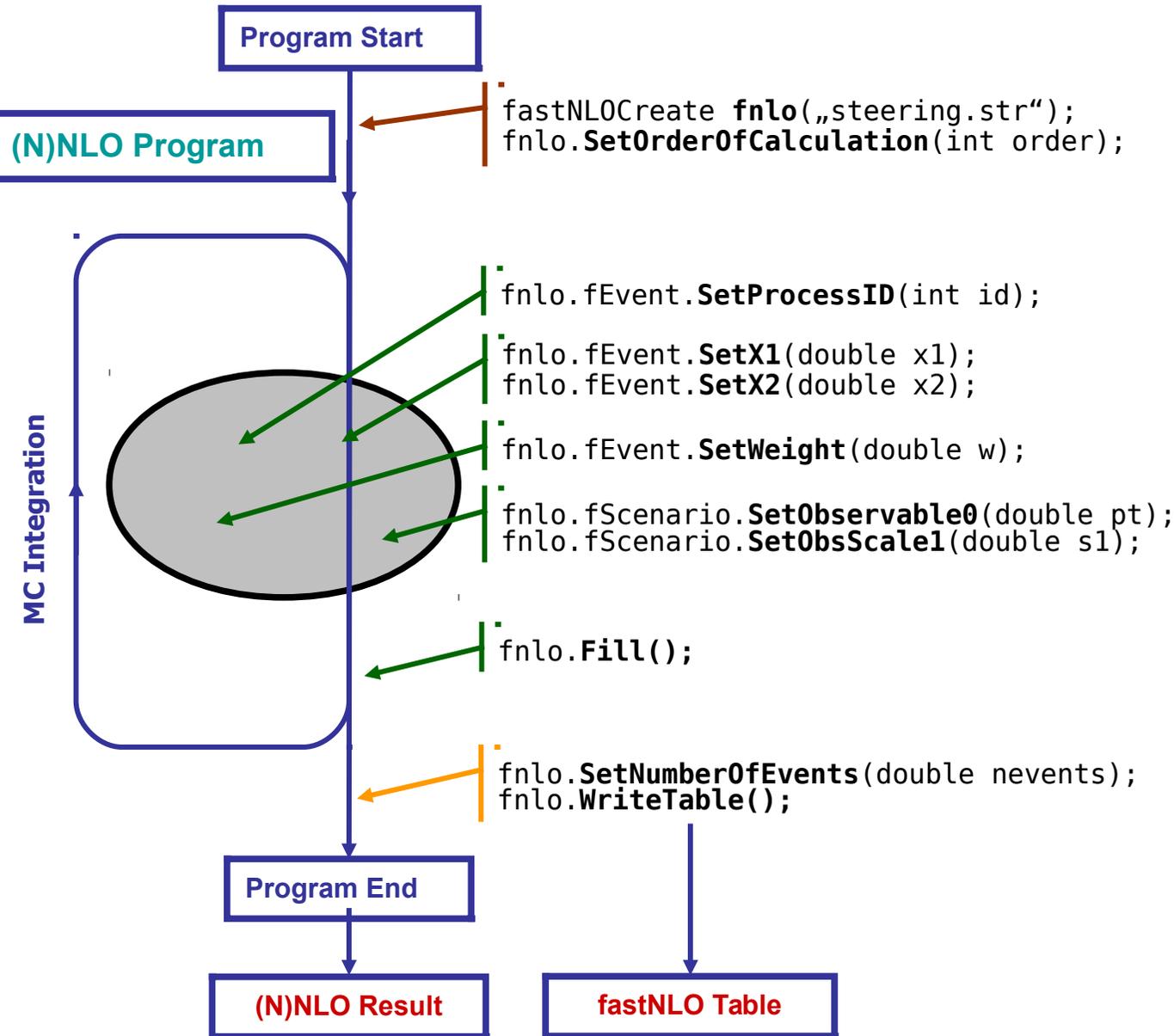
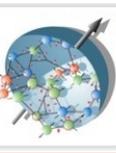


- ✓ **1. Code split into:**
 - ✓ **Toolkit library for creating & evaluating interpolation grids**
 - ➔ Independent of any generator
 - ➔ First pre-release 17.07.2014: fastnlo_toolkit 2.3.1pre-1854
 - ✓ **Specific helper interfaces, if required, to N(N)LO programs**
 - ➔ e.g. to use with NLOJet++: fastnlo_interface_nlojet 2.3.1pre-1855
- ✓ **2. Checked backwards compatibility with v2.1**
- ✓ **3. Facilitated use with extensible steering files**
- ✓ **4. Interface other theory programs ...**

NLOJet++, Z.Nagy,
PRD68 2003, PRL88 2002



Simple example for use of Toolkit



Initialize fastNLO class(es)

Pass the process specific variables during the 'event loop' to fastNLO

- Order does not matter
- Many other convenient implementations possible

Pass all information to fastNLO

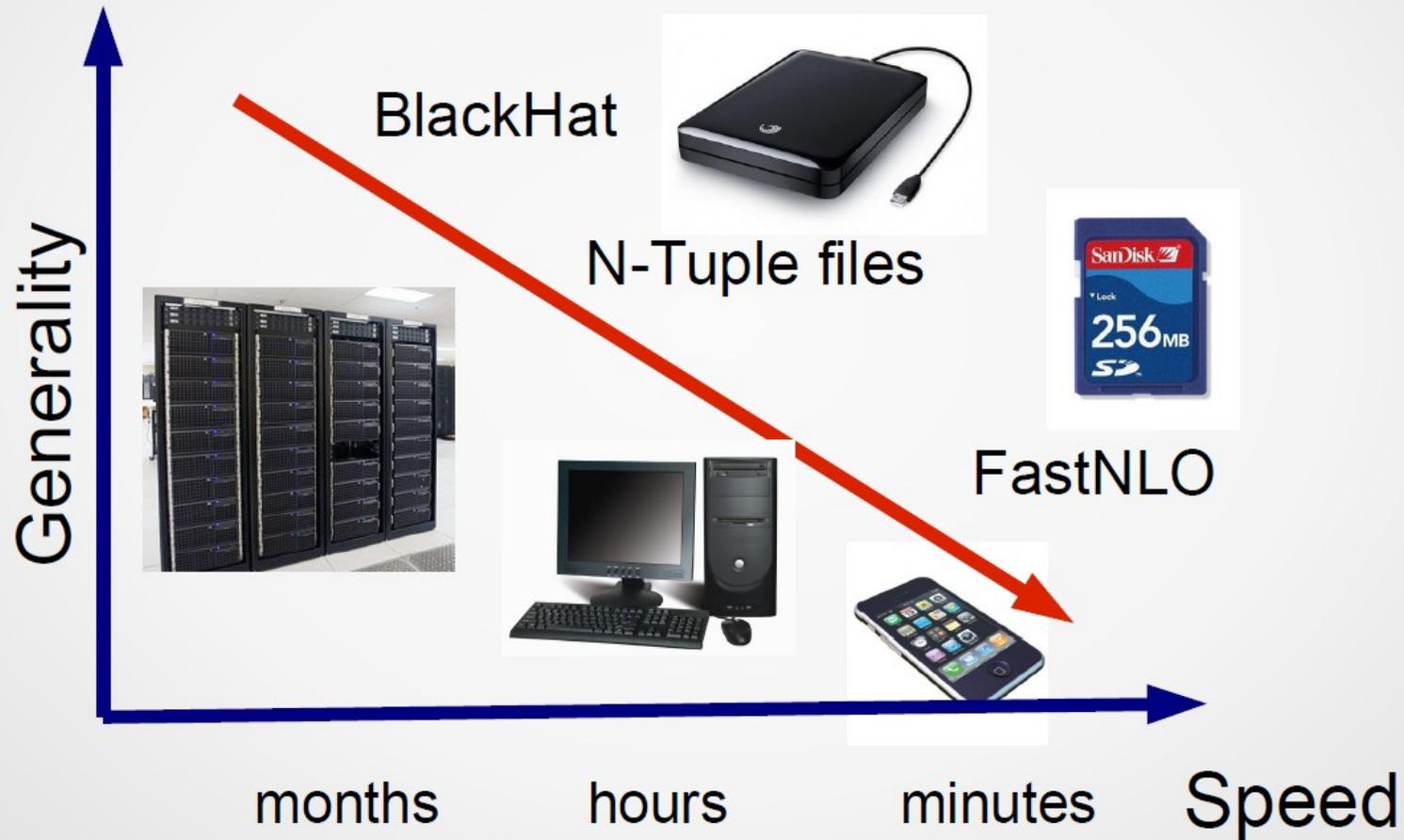
Set normalization of the MC integration and write table

Minimum implementation: 11 lines of code

Convenient implementation of fastNLO into any (N)NLO program possible!



Speed vs Generality

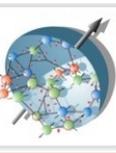


Slide from Daniel Maitre

Loops and Legs 2014, Weimar, 1th May



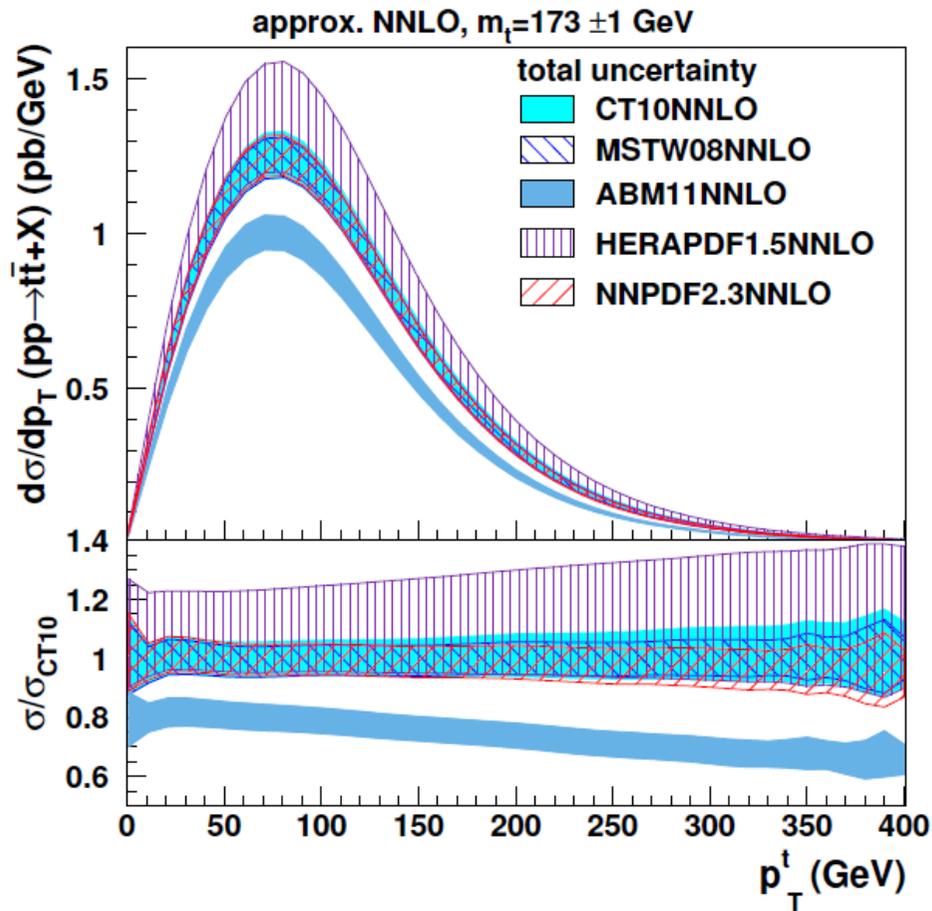
Use with DiffTop



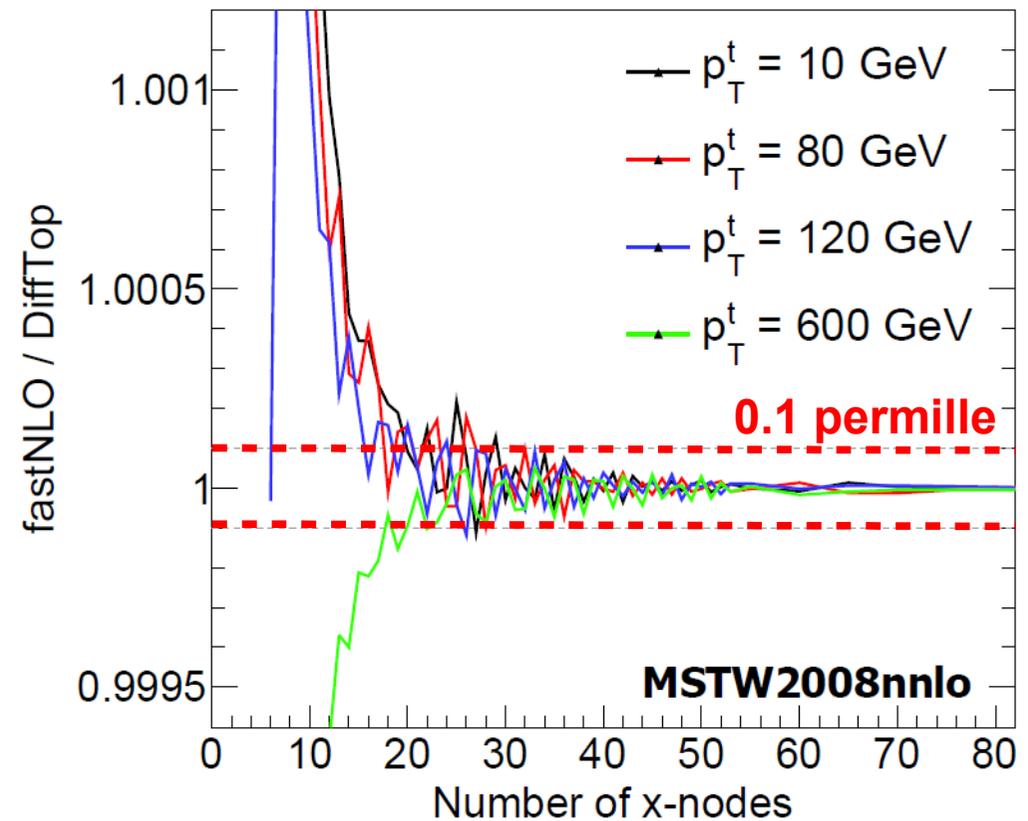
Differential $t\bar{t}$ in approx. NNLO:
 $d\sigma/dp_T, d\sigma/dy$

Precision study of fastNLO tables over
DiffTop standalone vs. no. of x nodes

(total uncertainty: quadr. sum of PDF, scale, α_s, m_t variations)



Interpolation precision NNLO



786 repeated calculations needed
including (separate) variation of m_t

DiffTop, M. Guzzi et al.,
JHEP01, 2015.

Perfect agreement for probed x-range of
 $2 \cdot 10^{-3} < x < 1$



Part 2

New: Interface **to Sherpa via MCgrid**

in collaboration with
Enrico Bothmann & Steffen Schumann



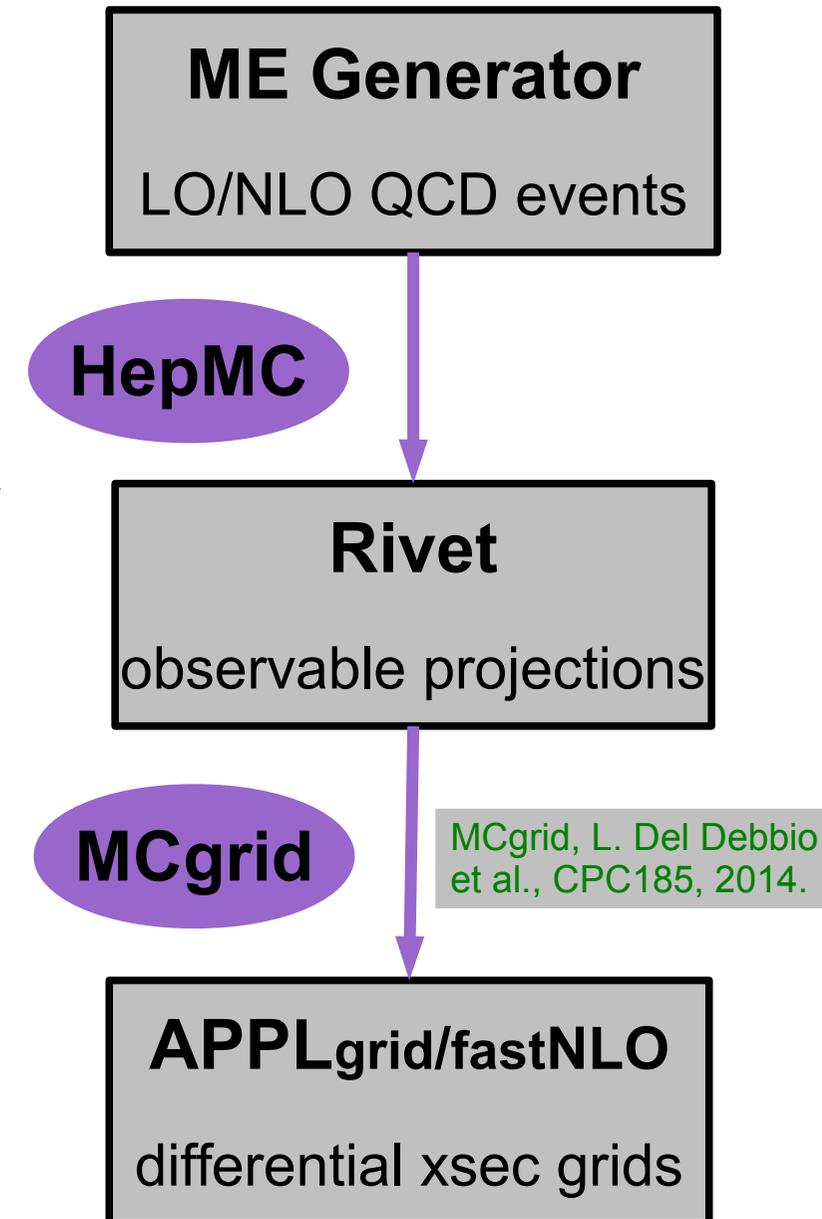
Use with Sherpa & MCgrid



✓ fastNLO Toolkit access implemented:

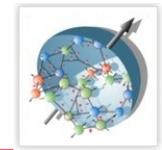
- ➔ Events generated with Sherpa 2.1.1
- ➔ Two analyses from Rivet 2.2.0 tested
- ➔ MCgrid 2.0 for cross section projection into grids (**to be released**)
- ➔ Same toolkit functions accessed either via direct calls from MCgrid-enabled Rivet analysis or via steering file
- ➔ Usable with large number of processes available via Sherpa and one-loop generators like BlackHat, GoSam, OpenLoops, NJET, ...

Sherpa, T. Gleisberg et al., JHEP02, 2004; JHEP02, 2009.
BlackHat, C.F. Berger et al., PRD78, 2008.
GoSam, G. Cullen et al., EPJC72, 2012.
OpenLoops, F. Cascioli et al., PRL108, 2012.
NJET, S. Badger et al., CPC184, 2013.
...





Snippets of Rivet+MCgrid analysis



```

#include "Rivet/Analysis.hh"
#include "mcgrid/mcgrid.hh"
...
namespace Rivet {

  /// CDF Z boson rapidity modified to generate grid files
  class MCgrid_CDF_2009_S8383952 : public Analysis {
  public:

    ...
    using namespace MCgrid;
    Histo1DPtr _hist_yZ; // Rivet histogram
    gridPtr _grid_yZ; // Corresponding grid

    // Init phase
    subprocessConfig subproc("DY-ppbar.str", BEAM_PROTON, BEAM_ANTIPROTON);
    fastNLOGridArch arch(50, 1, "Lagrange", "OneNode", "sqrtlog10", "linear");
    fastNLOConfig config(0, subproc, arch, 1960.0);
    _hist_yZ = bookHisto1D(2, 1, 1); // Book Rivet
    _grid_yZ = bookGrid(_hist_yZ, histoDir(), config); // Book MCgrid/fastNLO

    // Analyse phase
    PDFHandler::HandleEvent(event, histoDir()); // Update subprocess statistics
    _hist_yZ->fill(yZ, weight); // Fill Rivet
    _grid_yZ->fill(yZ, event); // Fill MCgrid/fastNLO

    // Finalise phase
    scale(_hist_yZ, normalisation); // Scale Rivet
    _grid_yZ->scale(normalisation); // Scale MCgrid/fastNLO
    PDFHandler::CheckOutAnalysis(histoDir()); // Finalise
  };
}

```

Setup Rivet with MCgrid

Basic scheme very similar with APPLgrid, differences in steering & functionalities.



```
subprocessConfig subproc("DY-ppbar.str", BEAM_PROTON, BEAM_ANTIPROTON);
fastNLOGridArch arch(50, 1, "Lagrange", "OneNode", "sqrtlog10", "linear");
fastNLOConfig config(0, subproc, arch, 1960.0);
```

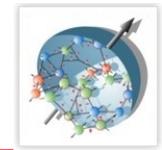
Book & config grid and histos

Fill events in event loop.

Final check out, normalize, write table.



Drell-Yan @ Tevatron



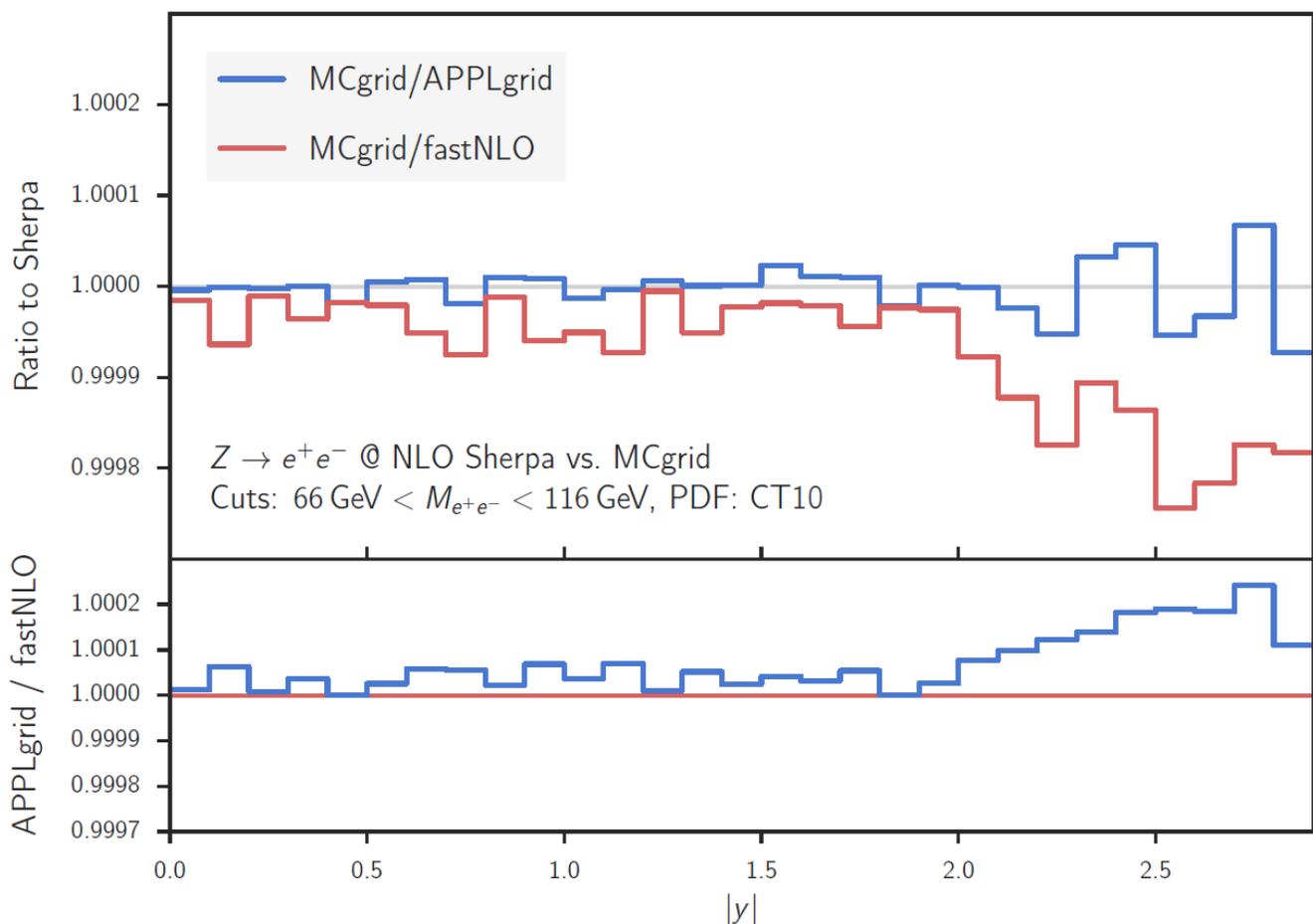
Drell-Yan Z rapidity:

➤ 1M (phase space)/10M (fill) events

➤ Interpolation in x only

➤ **No optimizations performed for either fastNLO or APPLgrid**

Drell-Yan @ Tevatron 1.96 TeV



**Agreement between
interpolations
and to Sherpa at
sub-permille level!**

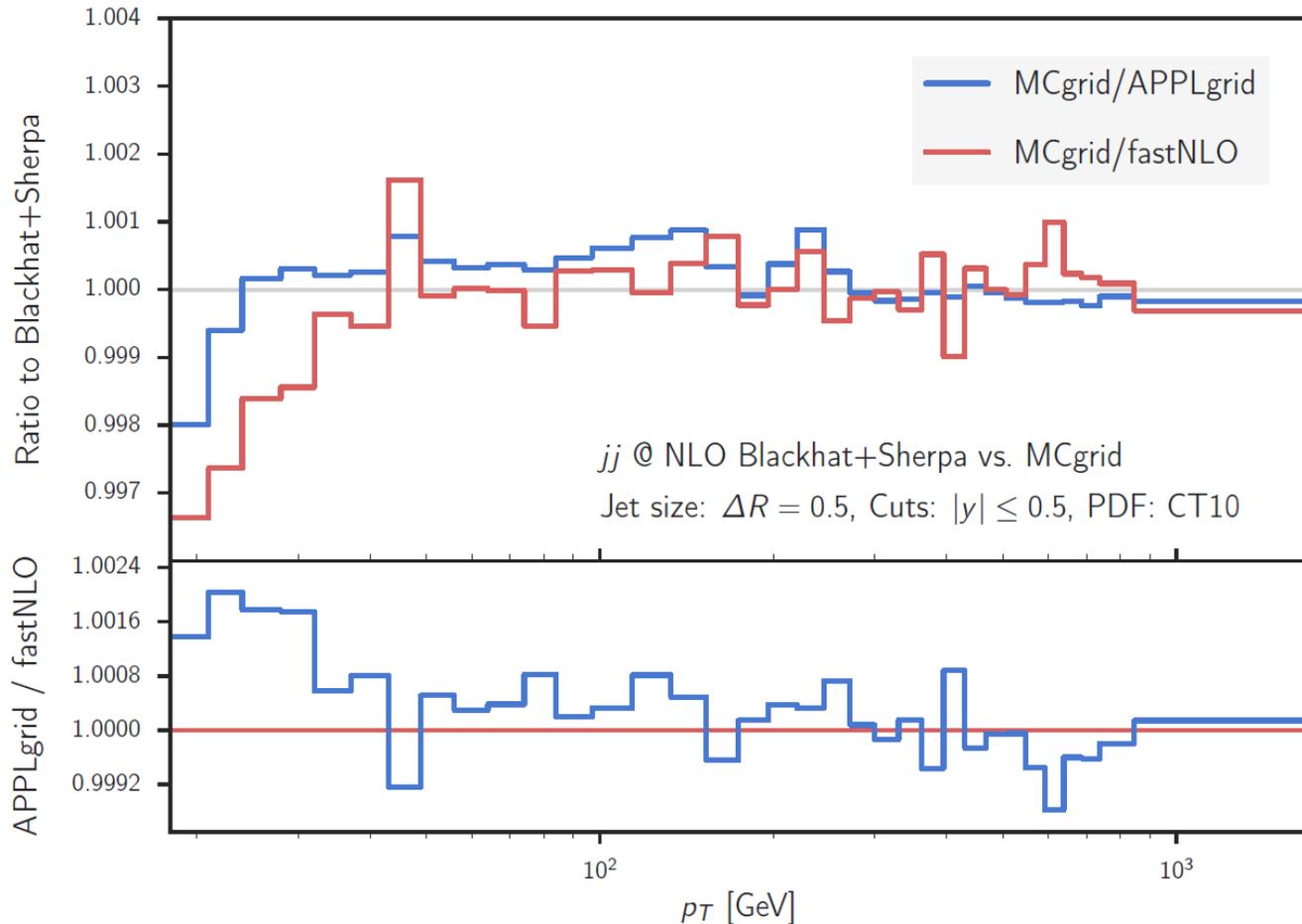


Jet pT distribution:

- 10M (phase space)/10M (fill) events
- Interpolation in x and scales
- No optimizations for either fastNLO or APPLgrid

Updated versions of fastNLO Toolkit and MCgrid to be released soon.

Inclusive Jets @ LHC 7 TeV



Agreement between interpolations and to BlackHat+Sherpa at permille level!



- The toolkit provides simple access to full capability of creating, filling, reading, and evaluating fast interpolation tables in the fastNLO format
- A simplified interface to NLOJet++ is publically available as well
- Uses flexible-scale table format, well-suited for NNLO
- Tested at (approx.) NNLO with DiffTop and by BlackHat
==> well prepared for i.a. jets at NNLO :-)
- Other theory programs can be/have been interfaced
- Demonstrated new application with MCgrid and Sherpa
- New release of the fastNLO Toolkit imminent
- Will be synchronized with new release of MCgrid
- Work in progress with Herwig++/Matchbox
- Work on inclusion of statistical uncertainty of calculation within table
- and last but not least ...



Table production initiative



✓ Started large-scale table production as stress test on computing centers as private cloud providers

➤ Uses Karlsruhe generic grid submission tool grid-control and HTCondor & OpenStack

✓ Test production at Xmas:

➤ 800 virtualised CPUs

➤ 13000 jobs

➤ 95000 h of CPU time

➤ 10^{12} events

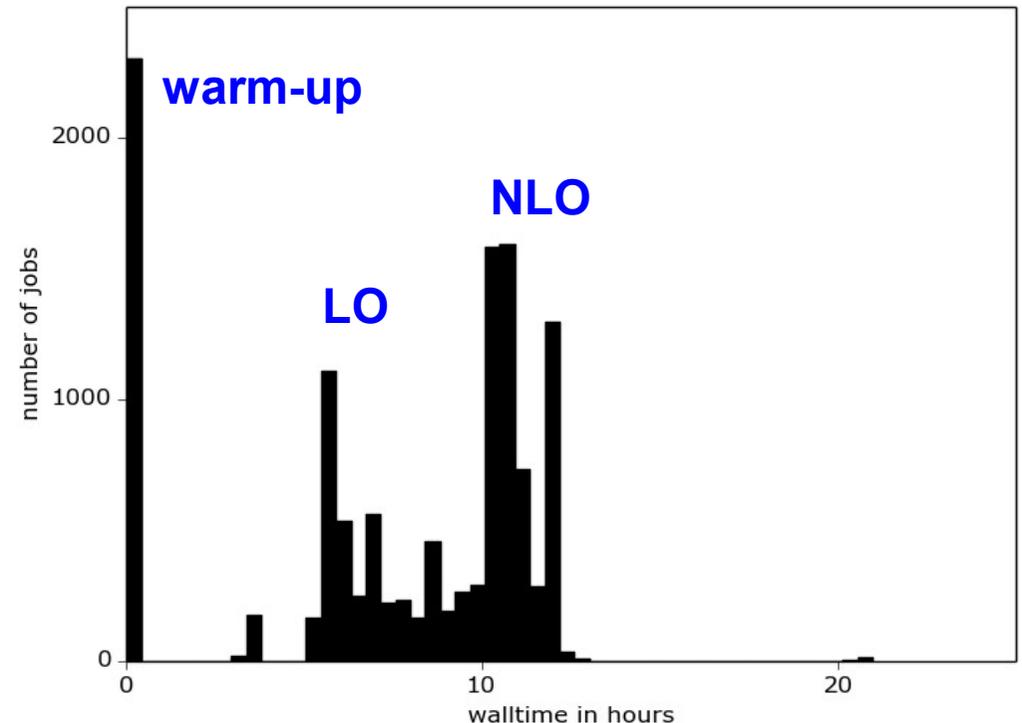
➤ 13 fastNLO tables

✓ Anything on your wishlist?

Many thanks to the Computing Centre of the University Freiburg for providing the bwForCluster test system!

Summary of job timings

walltime per job distribution



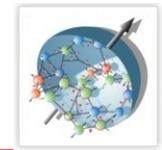


Backup Slides





Excerpt of steering.str



```

ScenarioName fnl2342b_I902309_v23_flex          # Name and describe scenario
ScenarioDescription {
  "d2sigma-jet_dpT_dy_[pb_GeV]"
...
JetAlgo          2          # fastjet jet algorithm: 0,1,2=kT,CA,anti-kT
Rjet             0.5       # Jet size parameter: Required for all jets
ptjmin          18.       # Minimal jet pT
yjmin           0.0       # Minimal jet rapidity
yjmax           3.0       # Maximal jet rapidity
... extensible
LeadingOrder     2          # Number of jets for the L0 process
DifferentialDimension 2      # Dimensionality of binning
DimensionLabels {
  "|y|"          # Labels (symbol and unit) for dimensions
  "pT_[GeV]"     # Defines the observables to be calculated!
}
FlexibleScaleTable true     # Create table fully flexible in mu_f
ScaleDescriptionScale1 "pT_jet_[GeV]" # This defines the scale to be used
ScaleDescriptionScale2 "pT_max_[GeV]" # Specify 2nd scale name and unit

DoubleDifferentialBinning {{
  1stDimLo  1stDimUp  "----- Array of bin-grid for 2nd dimension -----"
  0.0       0.5       18.   21.   24.   28.   32.   37.   43.   49.   56. ...
...
}}

```

Running any other scenario can be as simple as adapting some kinematical cuts & binning, often not even a recompile necessary!

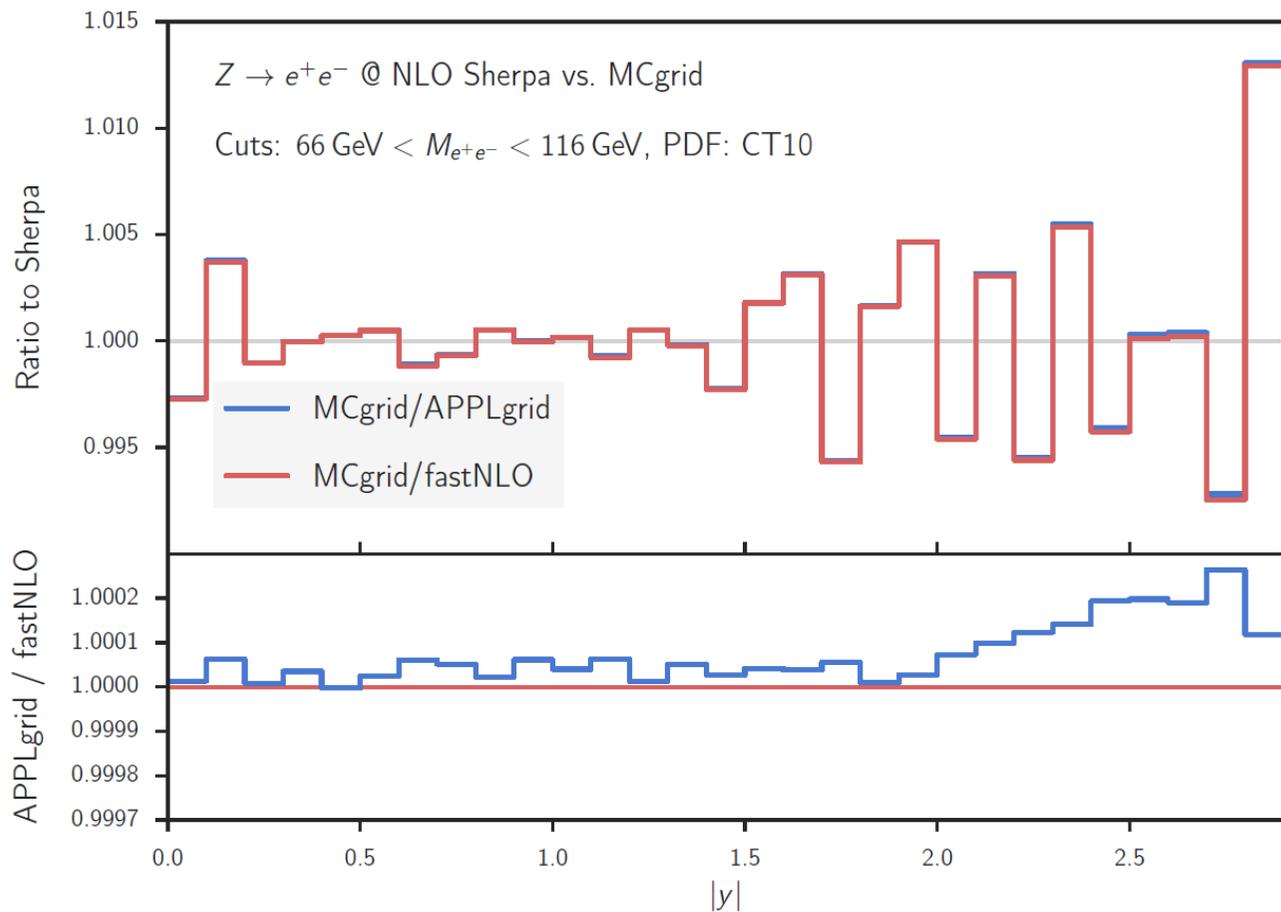


DY with reduced flavour-basis



- ✓ Store identical subprocesses into same “process bin” instead of full 121 flavour basis
- Dramatic reduction in required storage space!

Drell-Yan @ Tevatron 1.96 TeV



✗ But not exactly an apple-to-apple comparison anymore

➤ Statistical variations visible between exclusive Sherpa events and interpolated results

✓ Anyway still ok at sub-percent level