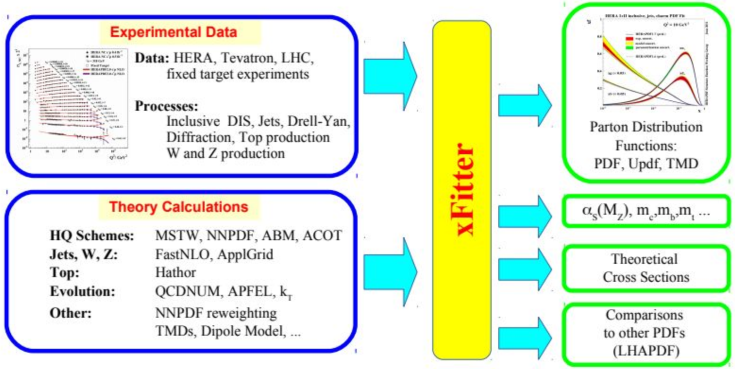
xFitter: introduction and software status

S. Glazov, xFitter workshop,
Orsay, 9 Mar 2022

Last workshop: DESY Feb 26-28th, 2020

- Two years since the last workshop
- First face to face meeting for a long time.
- Many developments in between

xFitter overview



Experimental Data

Data: HERA, Tevatron, LHC,
fixed target experiments

Processes:
Inclusive DIS, Jets, Drell-Yan,
Diffraction, Top production
W and Z production

Theory Calculations

HQ Schemes:	MSTW, NNPDF, ABM, ACOT
Jets, W, Z:	FastNLO, ApplGrid
Top:	Hathor
Evolution:	QCDNUM, APFEL, k_T
Other:	NNPDF reweighting TMDs, Dipole Model, ...

xFitter

Parton Distribution Functions:
PDF, Updf, TMD

$\alpha_S(M_Z)$, m_c,m_b,m_t ...

Theoretical Cross Sections

Comparisons to other PDFs (LHAPDF)

- xFitter is a QCD analysis tool
- Combines experimental data and theory with the focus on parton distribution function determination and other QCD parameters
- xFitter is supported by developers team, with a loose governance, consisting of experimentalists and theorists, with emphasis on phenomenology.
- xFitter developers continue software development of the package, support existing code, and also perform various analyses that are published as a team or as individual authors.

xFitter organization

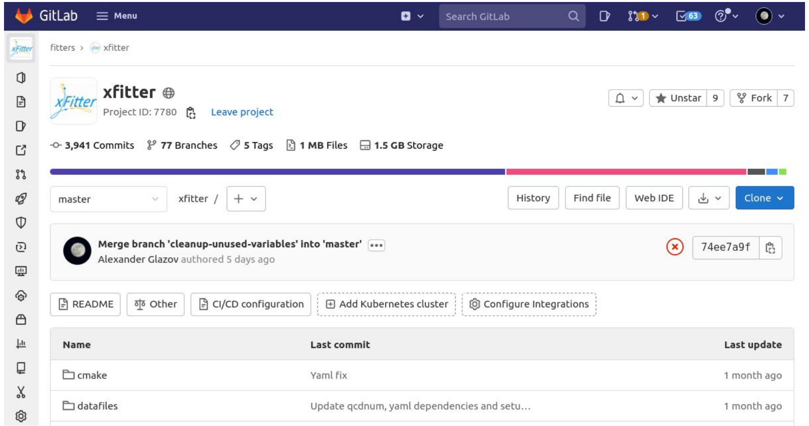
- xFitter developments are coordinated at biweekly xFitter developers' meetings (Wed 3pm CET/CEST).
- Communications occur using xfitter-devel@desy.de mailing list (ask me if you want to subscribe)
- No formal "spokesperson" position
- Everybody welcome to join, however for signing developers' papers a proof of contribution to the project is required.
- Software librarian is currently vacant, after Sasha Zenaiev left the project.

We had more strict governance model in the past, the current loose one seem to work
Ok, but it is open for a change

xFitter software overview

- Two supported “fortran-dominated” releases with a nuclear fork, downloadable from https://www.xfitter.org/xFitter/xFitter/DownloadPage
  - 2.0.0 Frozen frog
  - 2.0.1 Old Fashioned (mostly fixes for 2.0.0)
  - **2.0.1N Nuclear Daiquiri**
- Several analyses used 2.1.0-release candidate, the code is tagged and can be found at gitlab https://gitlab.cern.ch/fitters/xfitter/-/tags/master_before_PionCeres_merge
- Almost ready to be released as 2.2.0 “master” branch on gitlab repository which contains several major updates.
- We are likely to follow with 2.2.1 (bug fix) and 2.3.0 (further restructure) this year

xFitter code organization: gitlab and jira



fitters › xfitter

xfitter

Project ID: 7780 Leave project

Unstar 9 Fork 7

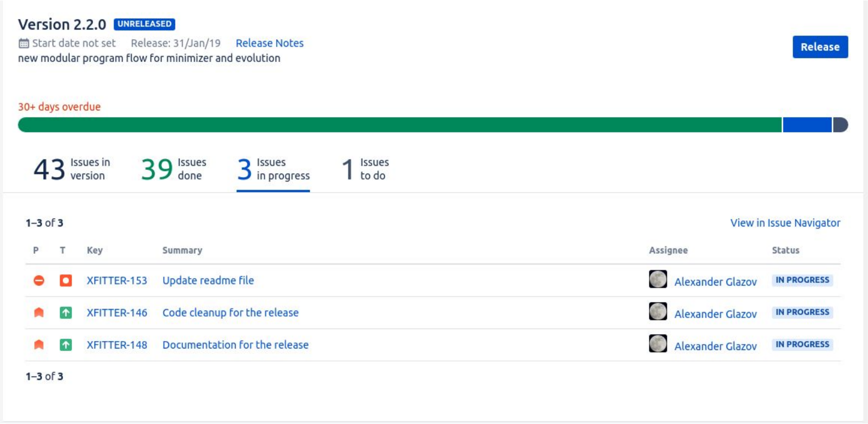
3,941 Commits 77 Branches 5 Tags 1 MB Files 1.5 GB Storage

master xfitter / + History Find file Web IDE Clone

Merge branch 'cleanup-unused-variables' into 'master'
Alexander Glazov authored 5 days ago
74ee7a9f

README Other CI/CD configuration Add Kubernetes cluster Configure Integrations

Name	Last commit	Last update
cmake	Yaml fix	1 month ago
datafiles	Update qcdnum, yaml dependencies and setu…	1 month ago



Version 2.2.0 UNRELEASED

Start date not set Release: 31/Jan/19 Release Notes

new modular program flow for minimizer and evolution

Release

30+ days overdue

43 Issues in version 39 Issues done 3 Issues in progress 1 Issues to do

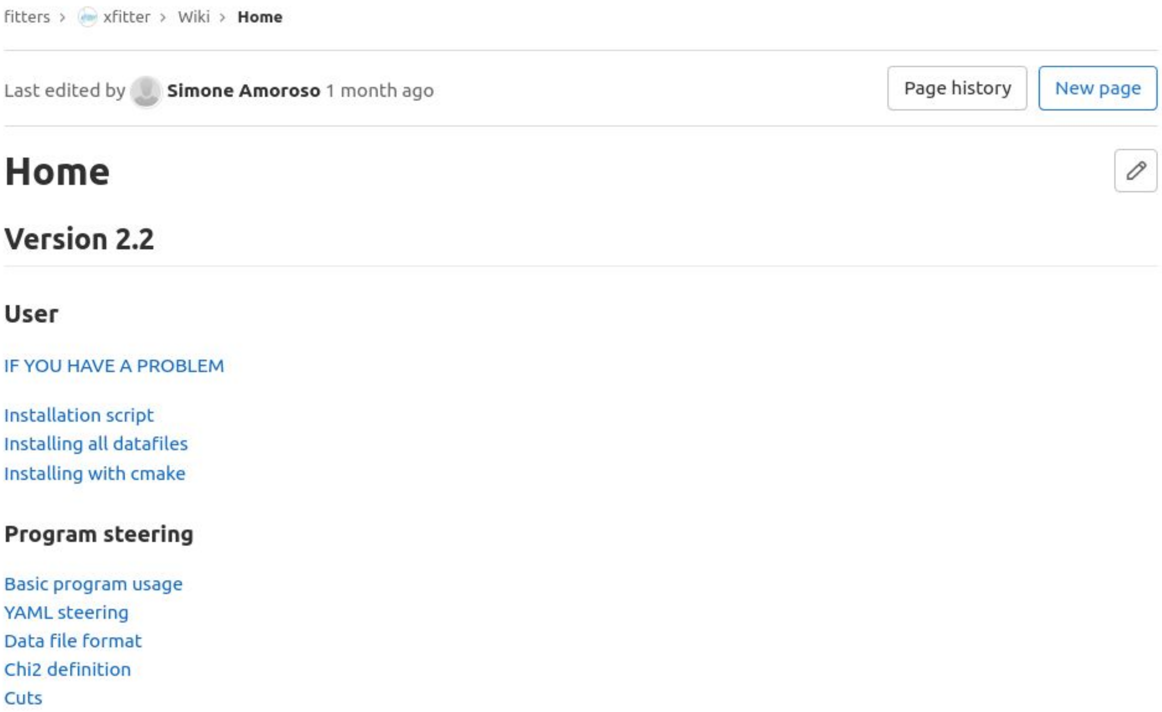
1–3 of 3 View in Issue Navigator

P	T	Key	Summary	Assignee	Status
		XFITTER-153	Update readme file	Alexander Glazov	IN PROGRESS
		XFITTER-146	Code cleanup for the release	Alexander Glazov	IN PROGRESS
		XFITTER-148	Documentation for the release	Alexander Glazov	IN PROGRESS

1–3 of 3

xFitter uses CERN services for the code https://gitlab.cern.ch/fitters/xfitter and issue tracking https://its.cern.ch/jira/projects/XFITTER . A CERN account is required for pull requests/ticket issue.

xFitter documentation: gitlab wiki



fitters › xfitter › Wiki › **Home**

Last edited by **Simone Amoroso** 1 month ago

Home

Version 2.2

User

IF YOU HAVE A PROBLEM

Installation script
Installing all datafiles
Installing with cmake

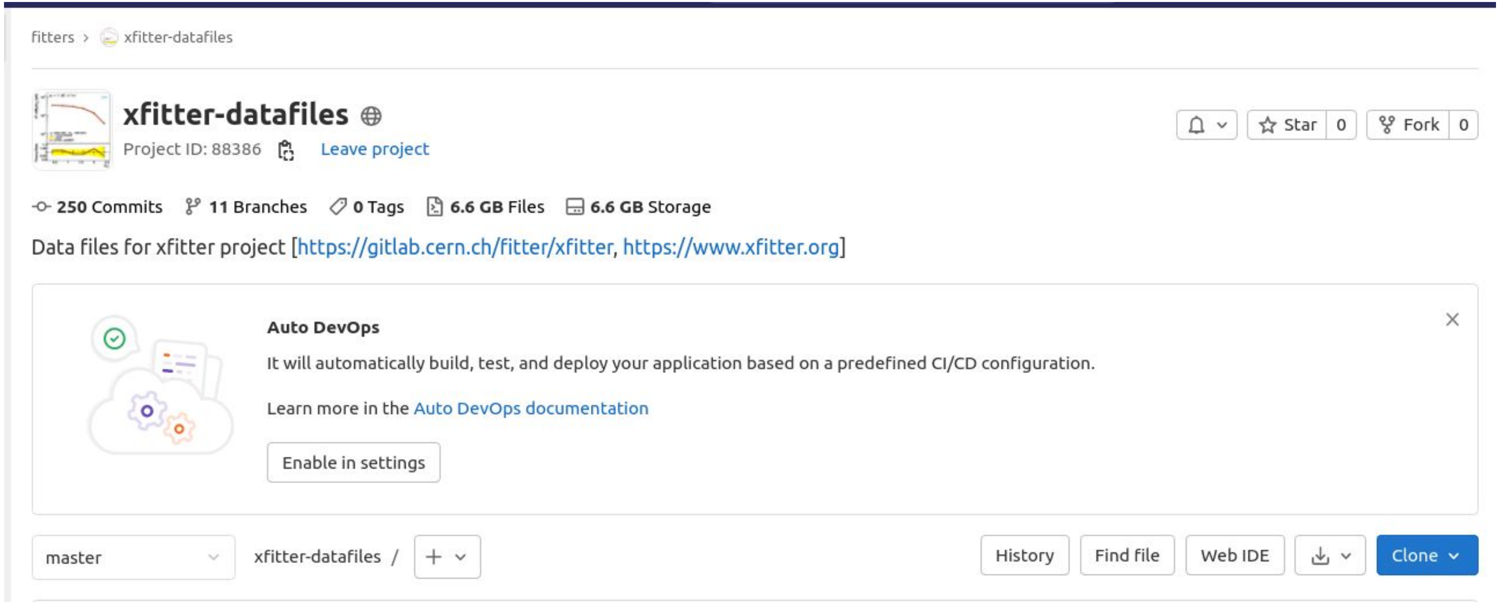
Program steering

Basic program usage
YAML steering
Data file format
Chi2 definition
Cuts

Software documentation is moved to gitlab wiki https://gitlab.cern.ch/fitters/xfitter/-/wikis/home which is significantly improved in preparation for the 2.2.0 release.

Please check the wiki before asking questions, and try to improve it.

xFitter data access: gitlab



xfitter-datafiles

Project ID: 88386 Leave project

250 Commits 11 Branches 0 Tags 6.6 GB Files 6.6 GB Storage

Data files for xfitter project [https://gitlab.cern.ch/fitter/xfitter, https://www.xfitter.org]

Auto DevOps

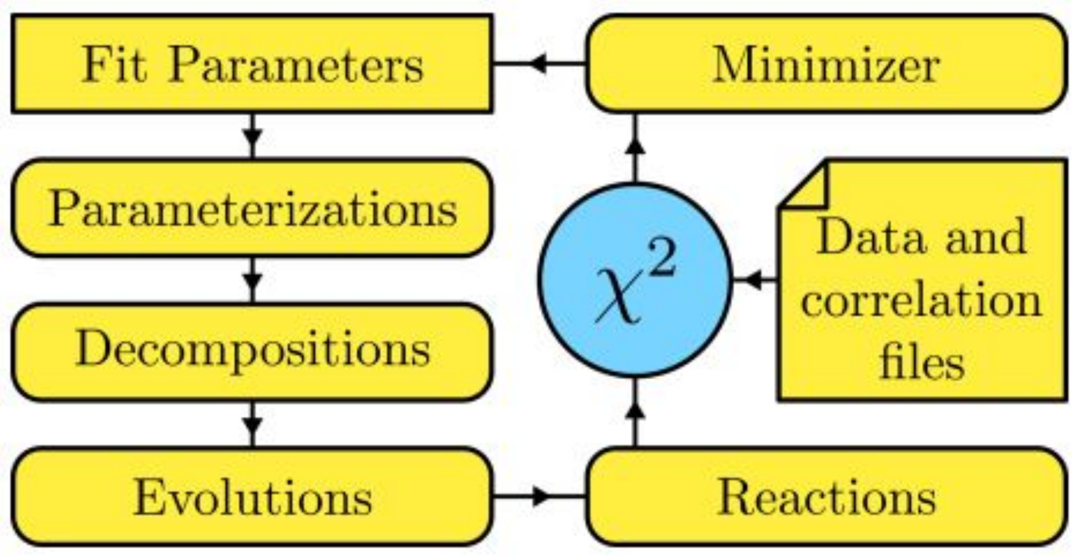
It will automatically build, test, and deploy your application based on a predefined CI/CD configuration.

Learn more in the Auto DevOps documentation

Enable in settings

- Data access is now arranged via https://gitlab.cern.ch/fitters/xfitter-datafiles
- At the moment keep two versions of data files: compatible with 2.2.0 (“-thexp.dat”) and with 2.0.0.

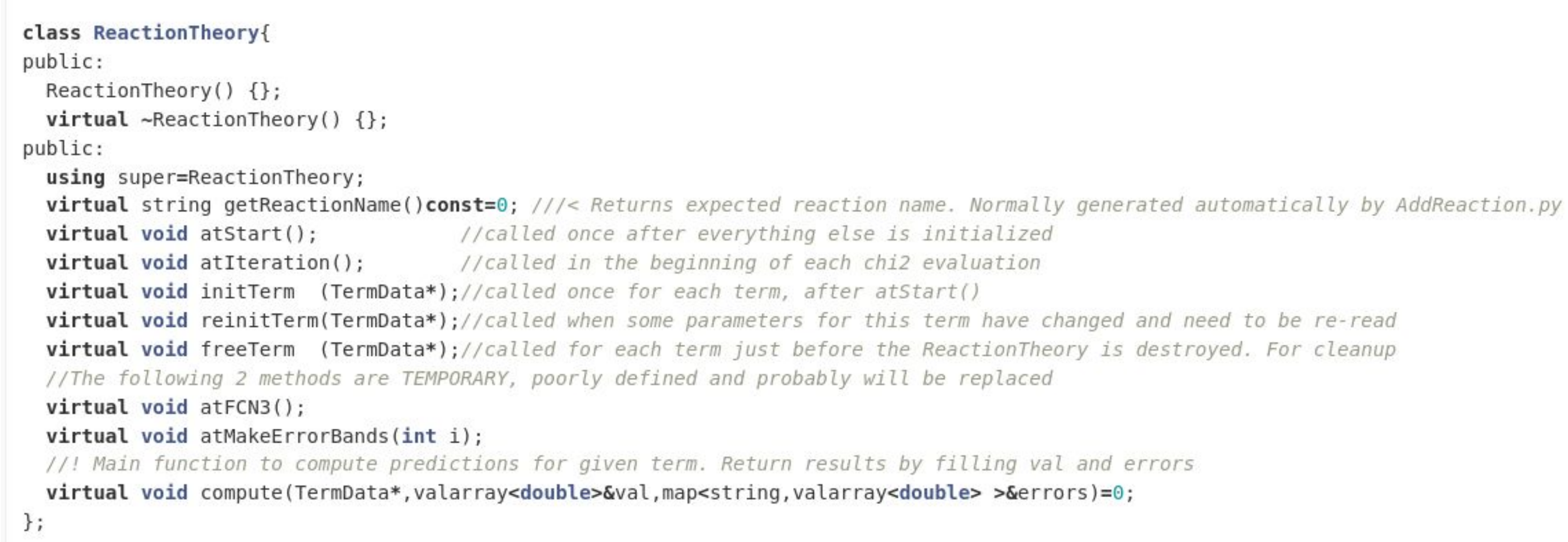
xFitter release 2.2.0



- Significant changes in the internal structure
- Re-written interfaces to minimizers, PDF parameterisation, decomposition, evolution and theory reactions
- Large changes in the user interface
- Data handling, format and chi2 calculation remain largely the same (but there are changes)

From talk by Ivan Novikov

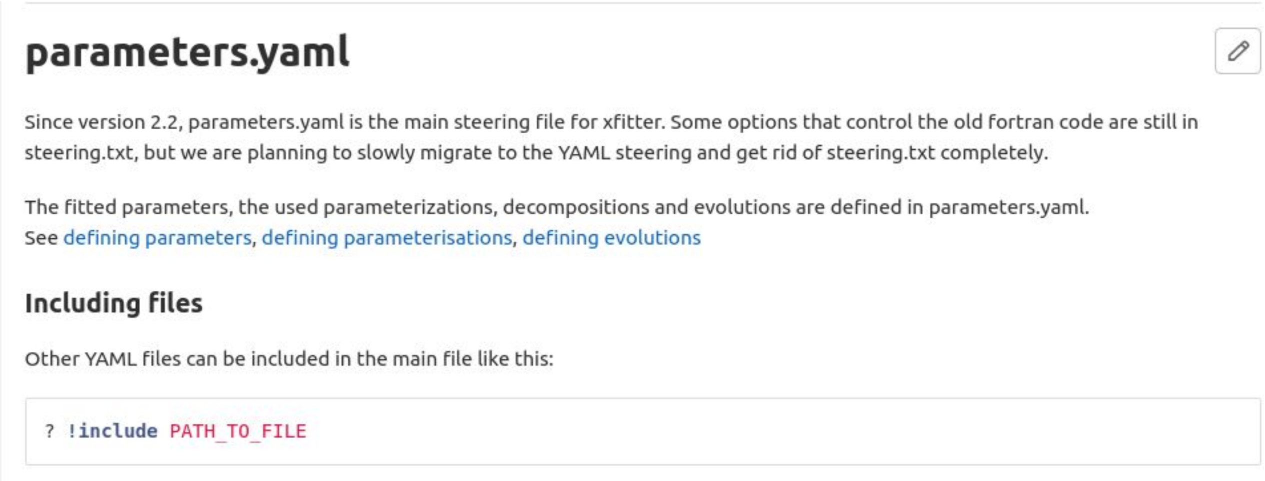
New reaction interface



```
class ReactionTheory{
public:
  ReactionTheory() {};
  virtual ~ReactionTheory() {};
public:
  using super=ReactionTheory;
  virtual string getReactionName()const=0; ///< Returns expected reaction name. Normally generated automatically by AddReaction.py
  virtual void atStart();            //called once after everything else is initialized
  virtual void atIteration();        //called in the beginning of each chi2 evaluation
  virtual void initTerm  (TermData*);//called once for each term, after atStart()
  virtual void reinitTerm(TermData*);//called when some parameters for this term have changed and need to be re-read
  virtual void freeTerm  (TermData*);//called for each term just before the ReactionTheory is destroyed. For cleanup
  //The following 2 methods are TEMPORARY, poorly defined and probably will be replaced
  virtual void atFCN3();
  virtual void atMakeErrorBands(int i);
  //! Main function to compute predictions for given term. Return results by filling val and errors
  virtual void compute(TermData*,valarray<double>&val,map<string,valarray<double> >&errors)=0;
};
```

- All theory predictions inherit from ReactionTheory class.
- Design is to have single instance of the class which handles multiple datafiles

Updates of the program control



parameters.yaml

Since version 2.2, parameters.yaml is the main steering file for xfitter. Some options that control the old fortran code are still in steering.txt, but we are planning to slowly migrate to the YAML steering and get rid of steering.txt completely.

The fitted parameters, the used parameterizations, decompositions and evolutions are defined in parameters.yaml.
See defining parameters, defining parameterisations, defining evolutions

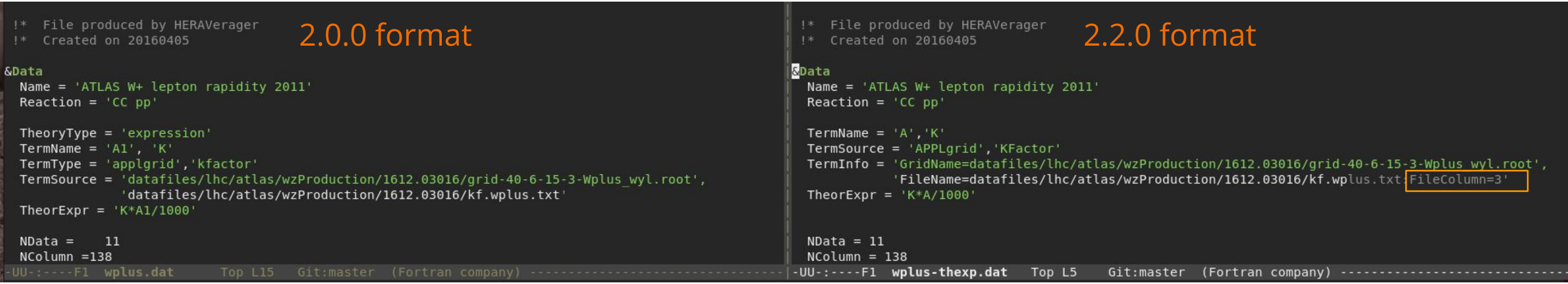
Including files

Other YAML files can be included in the main file like this:

```
? !include PATH_TO_FILE
```

- Major changes in the way xFitter is steered
- Most of the parameters are moved to **parameters.yaml** file with only few options controlled by **steering.txt** namelists.
- The only namelists read from **steering.txt** are &InFiles, &InCorr, &CovarToNuisance, &xFitter (and only chi2 part of it), &Output, and &Cuts, the plan is to drop it altogether with version 2.3.0

Data format changes



2.0.0 format

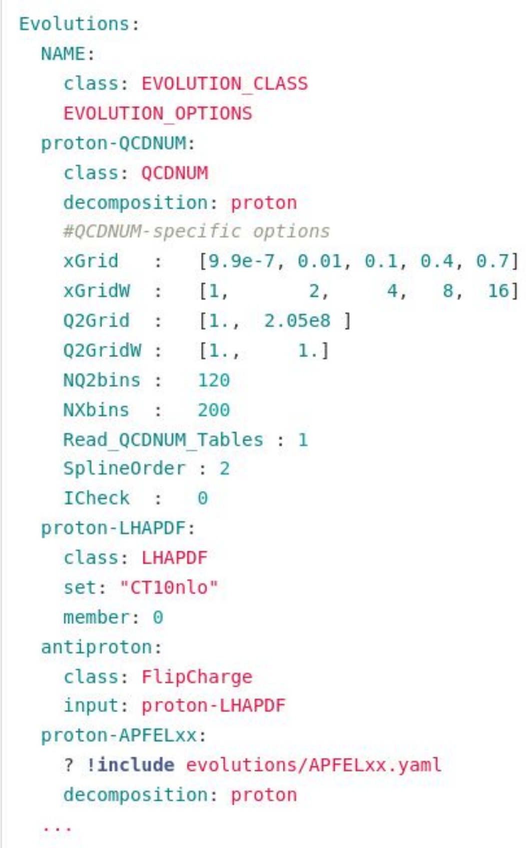
```
!*  File produced by HERAVerager
!*  Created on 20160405

&Data
  Name = 'ATLAS W+ lepton rapidity 2011'
  Reaction = 'CC pp'

  TheoryType = 'expression'
  TermName = 'A1', 'K'
  TermType = 'applgrid','kfactor'
  TermSource = 'datafiles/lhc/atlas/wzProduction/1612.03016/grid-40-6-15-3-Wplus_wyl.root',
               'datafiles/lhc/atlas/wzProduction/1612.03016/kf.wplus.txt'
  TheorExpr = 'K*A1/1000'

  NData =     11
  NColumn =138
-UU-:----F1  wplus.dat      Top L15    Git:master  (Fortran company) ---------------------------------
```

2.2.0 format

```
!*  File produced by HERAVerager
!*  Created on 20160405

&Data
  Name = 'ATLAS W+ lepton rapidity 2011'
  Reaction = 'CC pp'

  TermName = 'A','K'
  TermSource = 'APPLgrid','KFactor'
  TermInfo = 'GridName=datafiles/lhc/atlas/wzProduction/1612.03016/grid-40-6-15-3-Wplus_wyl.root',
             'FileName=datafiles/lhc/atlas/wzProduction/1612.03016/kf.wplus.txt:FileColumn=3'
  TheorExpr = 'K*A/1000'


  NData = 11
  NColumn = 138
-UU-:----F1  wplus-thexp.dat    Top L5     Git:master  (Fortran company) ----------------------------
```

- Data format remains largely the same, main changes in the description of the theory.
- TheoryType, Reaction, TermType parameters become optional (“Reaction” is still used for cuts)
- There is a change of the kFactor table format: becomes more flexible, but also not compatible.
- Dataset parameters can are given in TermInfo, they can be also modified in the

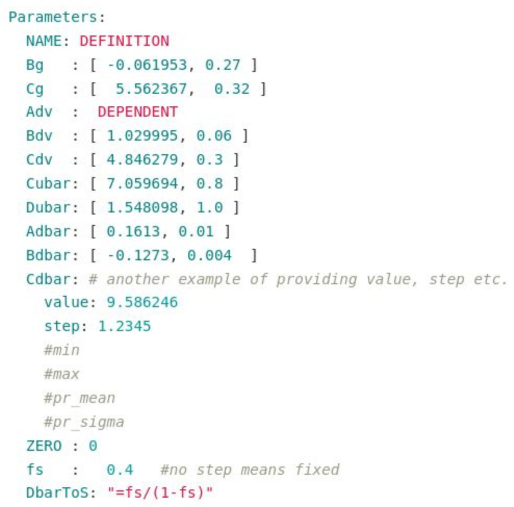
Flexible evolution bindings



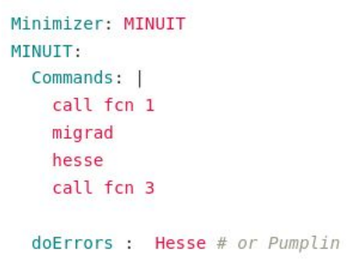
```
Evolutions:
  NAME:
    class: EVOLUTION_CLASS
    EVOLUTION_OPTIONS
  proton-QCDNUM:
    class: QCDNUM
    decomposition: proton
    #QCDNUM-specific options
    xGrid   :   [9.9e-7, 0.01, 0.1, 0.4, 0.7]
    xGridW  :   [1,       2,      4,   8,  16]
    Q2Grid  :   [1.,  2.05e8 ]
    Q2GridW :   [1.,     1.]
    NQ2bins :   120
    NXbins  :   200
    Read_QCDNUM_Tables : 1
    SplineOrder : 2
    ICheck  :   0
  proton-LHAPDF:
    class: LHAPDF
    set: "CT10nlo"
    member: 0
  antiproton:
    class: FlipCharge
    input: proton-LHAPDF
  proton-APFELxx:
    ? !include evolutions/APFELxx.yaml
    decomposition: proton
  ...
```

- Similar to **ReactionTheory**, evolution codes are based on a **BaseEvolution** class
- Evolutions provide computations of the PDFs, α_S, and other parameters based on **PDFdecomposition,** external input, or other evolutions.
- xFitter job can have several or no evolutions (for reactions such as TensorPomeron)
- The extended flexibility simplifies fits involving combination of several targets, e.g. pp, ppbar, pPb, etc.

Changes in the minimizer



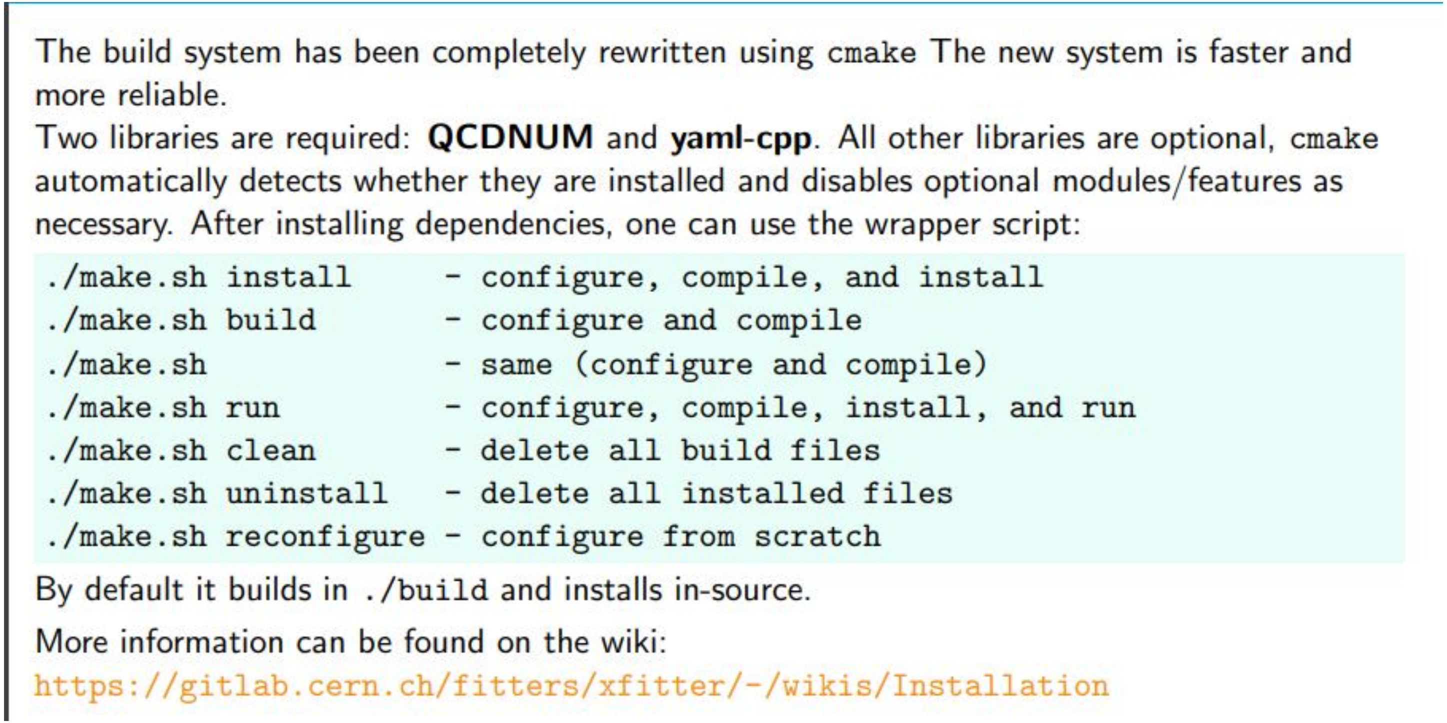
```
Parameters:
  NAME: DEFINITION
  Bg   : [ -0.061953, 0.27 ]
  Cg   : [  5.562367,  0.32 ]
  Adv  :  DEPENDENT
  Bdv  : [ 1.029995, 0.06 ]
  Cdv  : [ 4.846279, 0.3 ]
  Cubar: [ 7.059694, 0.8 ]
  Dubar: [ 1.548098, 1.0 ]
  Adbar: [ 0.1613, 0.01 ]
  Bdbar: [ -0.1273, 0.004  ]
  Cdbar: # another example of providing value, step etc.
    value: 9.586246
    step: 1.2345
    #min
    #max
    #pr_mean
    #pr_sigma
  ZERO : 0
  fs   :   0.4   #no step means fixed
  DbarToS: "=fs/(1-fs)"
```



```
Minimizer: MINUIT
MINUIT:
  Commands: |
    call fcn 1
    migrad
    hesse
    call fcn 3

  doErrors :  Hesse # or Pumplin
```

- Parameters are now specified in **parameters.yaml** file, with the syntax loosely following the one from minuit
- Parameters can be also provided as functions of other parameters
- Parameters are then controlled by minimizers, two of which are interfaced: fortran Minuit and CERES.
- More strict checks of the convergence compared to previous versions

From autotools to cmake



The build system has been completely rewritten using cmake The new system is faster and more reliable.
Two libraries are required: **QCDNUM** and **yaml-cpp**. All other libraries are optional, cmake automatically detects whether they are installed and disables optional modules/features as necessary. After installing dependencies, one can use the wrapper script:

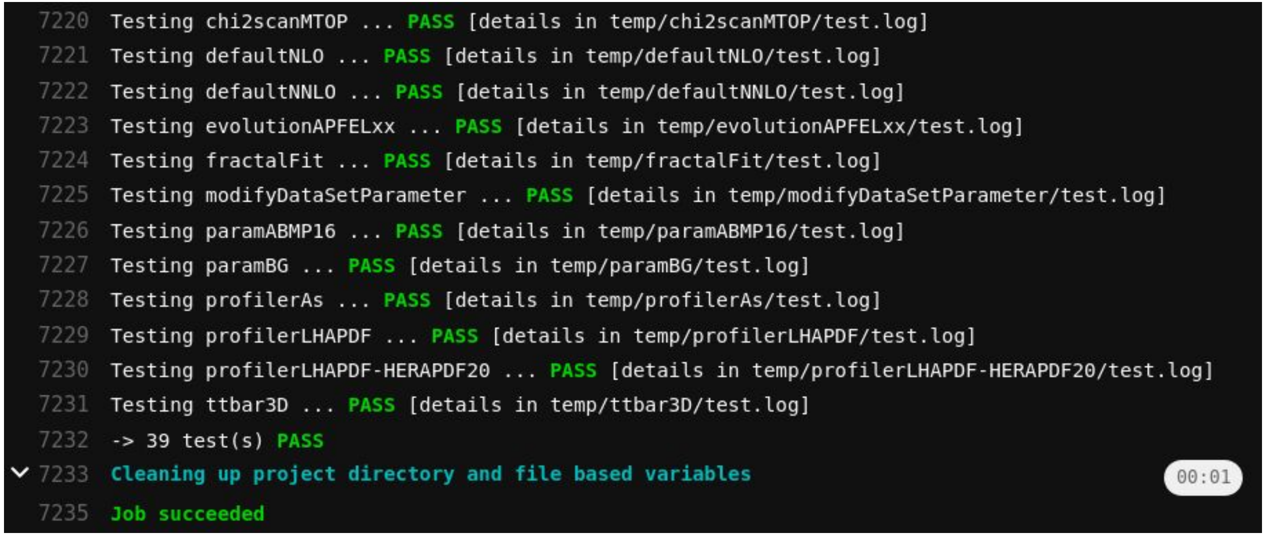
```
./make.sh install     - configure, compile, and install
./make.sh build       - configure and compile
./make.sh             - same (configure and compile)
./make.sh run         - configure, compile, install, and run
./make.sh clean       - delete all build files
./make.sh uninstall   - delete all installed files
./make.sh reconfigure - configure from scratch
```

By default it builds in ./build and installs in-source.

More information can be found on the wiki:
https://gitlab.cern.ch/fitters/xfitter/-/wikis/Installation

(from Ivan’s slides https://indico.desy.de/event/25055/contributions/55814/attachments/36157/45265/status-master_1.pdf)

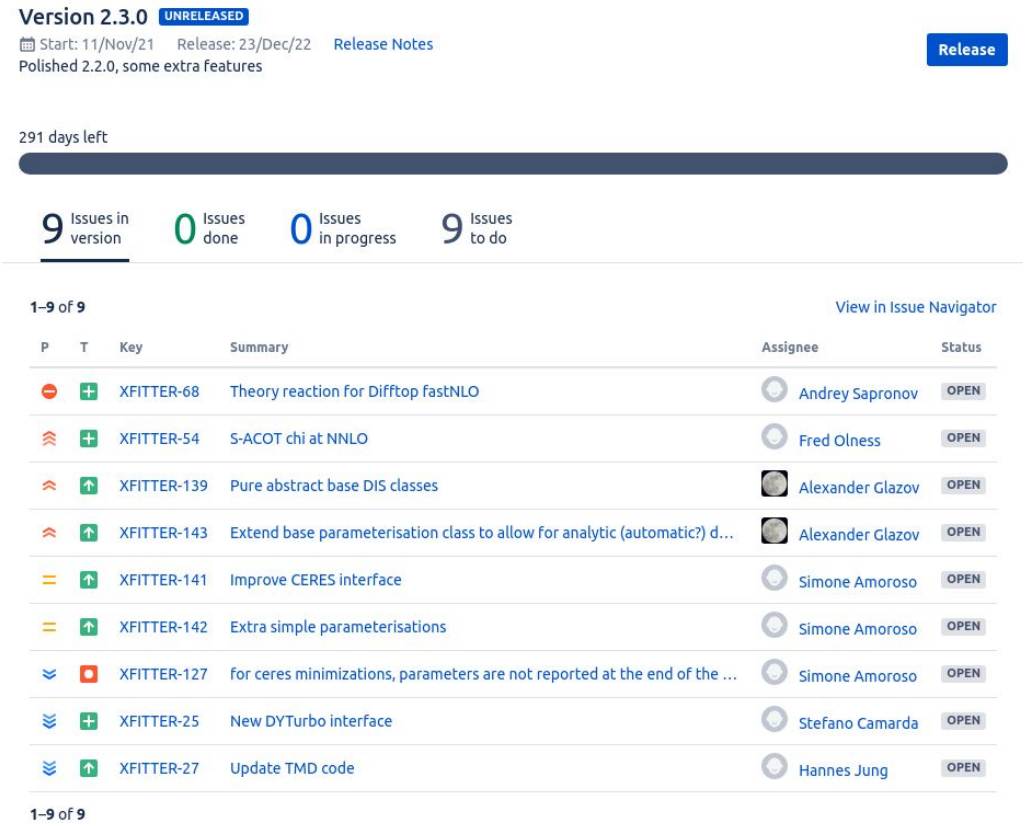
Improved validation



```
Testing chi2scanMTOP ... PASS [details in temp/chi2scanMTOP/test.log]
Testing defaultNLO ... PASS [details in temp/defaultNLO/test.log]
Testing defaultNNLO ... PASS [details in temp/defaultNNLO/test.log]
Testing evolutionAPFELxx ... PASS [details in temp/evolutionAPFELxx/test.log]
Testing fractalFit ... PASS [details in temp/fractalFit/test.log]
Testing modifyDataSetParameter ... PASS [details in temp/modifyDataSetParameter/test.log]
Testing paramABMP16 ... PASS [details in temp/paramABMP16/test.log]
Testing paramBG ... PASS [details in temp/paramBG/test.log]
Testing profilerAs ... PASS [details in temp/profilerAs/test.log]
Testing profilerLHAPDF ... PASS [details in temp/profilerLHAPDF/test.log]
Testing profilerLHAPDF-HERAPDF20 ... PASS [details in temp/profilerLHAPDF-HERAPDF20/test.log]
Testing ttbar3D ... PASS [details in temp/ttbar3D/test.log]
-> 39 test(s) PASS
Cleaning up project directory and file based variables                                  00:01
Job succeeded
```

- Automatic validation of all pull requests / nightly builds
- Tests with minimal and full installation, including all dependences
- Most of functionality covered, plans to extend further.

Release strategy



Version 2.3.0 UNRELEASED

Start: 11/Nov/21 Release: 23/Dec/22 Release Notes

Polished 2.2.0, some extra features

291 days left

9 Issues in version | 0 Issues done | 0 Issues in progress | 9 Issues to do

1–9 of 9

P	T	Key	Summary	Assignee	Status
⊖	⊞	XFITTER-68	Theory reaction for Difftop fastNLO	Andrey Sapronov	OPEN
⇈	⊞	XFITTER-54	S-ACOT chi at NNLO	Fred Olness	OPEN
⌃	⬆	XFITTER-139	Pure abstract base DIS classes	Alexander Glazov	OPEN
⌃	⬆	XFITTER-143	Extend base parameterisation class to allow for analytic (automatic?) d...	Alexander Glazov	OPEN
=	⬆	XFITTER-141	Improve CERES interface	Simone Amoroso	OPEN
=	⬆	XFITTER-142	Extra simple parameterisations	Simone Amoroso	OPEN
⌄	■	XFITTER-127	for ceres minimizations, parameters are not reported at the end of the ...	Simone Amoroso	OPEN
⇊	⊞	XFITTER-25	New DYTurbo interface	Stefano Camarda	OPEN
⇊	⬆	XFITTER-27	Update TMD code	Hannes Jung	OPEN

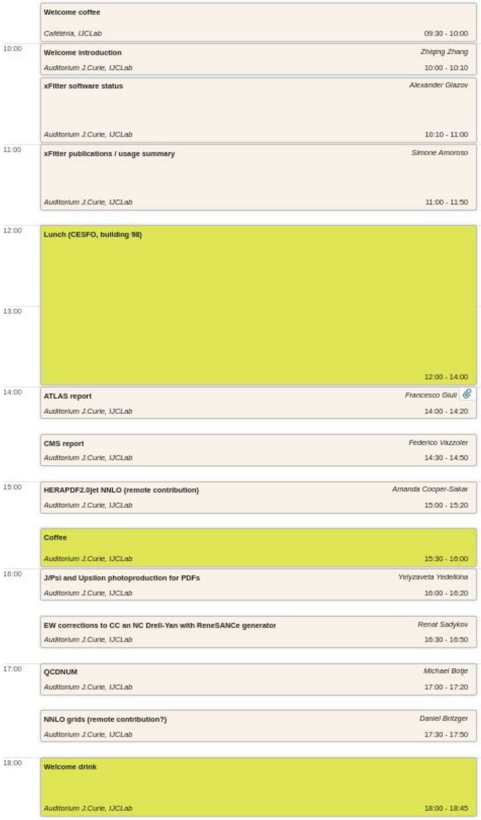
1–9 of 9

- 2.2.0 should be released at the workshop or shortly after
- 2.2.1 will target issues discovered with 2.2.0
- Few items moved from 2.2.0 to 2.3.0
- Further changes are to be discussed, including major update of data interface and chi2 computation.

Workshop goals

- Discuss xFitter software developments, finalize release 2.2.0, decide on 2.3.0
- Discuss xFitter developers’ team ongoing and potential future analyses.
- Finalize Snowmass contribution

Workshop agenda



Welcome coffee
Cafétéria, IJCLab 09:30 - 10:00

Welcome introduction *Zhiqing Zhang*
Auditorium J.Curie, IJCLab 10:00 - 10:10

xFitter software status *Alexander Glazov*
Auditorium J.Curie, IJCLab 10:10 - 11:00

xFitter publications / usage summary *Simone Amoroso*
Auditorium J.Curie, IJCLab 11:00 - 11:50

Lunch (CESFO, building 98)
12:00 - 14:00

ATLAS report *Francesco Giuli*
Auditorium J.Curie, IJCLab 14:00 - 14:20

CMS report *Federico Vazzoler*
Auditorium J.Curie, IJCLab 14:30 - 14:50

HERAPDF2.0jet NNLO (remote contribution) *Amanda Cooper-Sakar*
Auditorium J.Curie, IJCLab 15:00 - 15:20

Coffee
Auditorium J.Curie, IJCLab 15:30 - 16:00

J/Psi and Upsilon photoproduction for PDFs *Yelyzaveta Yedelkina*
Auditorium J.Curie, IJCLab 16:00 - 16:20

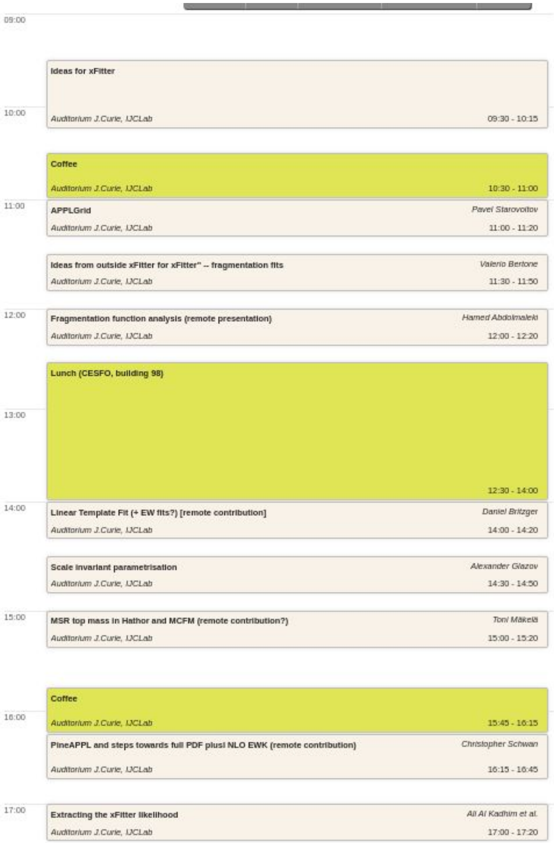
EW corrections to CC an NC Drell-Yan with ReneSANCe generator *Renat Sadykov*
Auditorium J.Curie, IJCLab 16:30 - 16:50

QCDNUM *Michael Botje*
Auditorium J.Curie, IJCLab 17:00 - 17:20

NNLO grids (remote contribution?) *Daniel Britzger*
Auditorium J.Curie, IJCLab 17:30 - 17:50

Welcome drink
Auditorium J.Curie, IJCLab 18:00 - 18:45

Status and user's reports



Ideas for xFitter
Auditorium J.Curie, IJCLab 09:30 - 10:15

Coffee
Auditorium J.Curie, IJCLab 10:30 - 11:00

APPLGrid *Pavel Starovoitov*
Auditorium J.Curie, IJCLab 11:00 - 11:20

Ideas from outside xFitter for xFitter" -- fragmentation fits *Valerio Bertone*
Auditorium J.Curie, IJCLab 11:30 - 11:50

Fragmentation function analysis (remote presentation) *Hamed Abdolmaleki*
Auditorium J.Curie, IJCLab 12:00 - 12:20

Lunch (CESFO, building 98)
12:30 - 14:00

Linear Template Fit (+ EW fits?) [remote contribution] *Daniel Britzger*
Auditorium J.Curie, IJCLab 14:00 - 14:20

Scale invariant parametrisation *Alexander Glazov*
Auditorium J.Curie, IJCLab 14:30 - 14:50

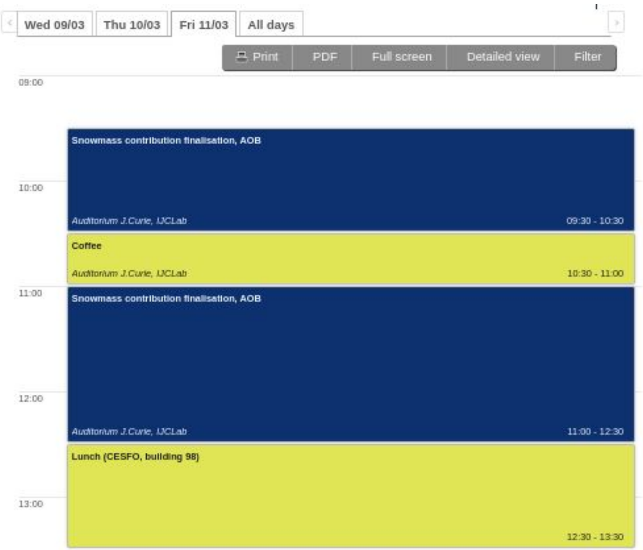
MSR top mass in Hathor and MCFM (remote contribution?) *Toni Mäkelä*
Auditorium J.Curie, IJCLab 15:00 - 15:20

Coffee
Auditorium J.Curie, IJCLab 15:45 - 16:15

PineAPPL and steps towards full PDF plusl NLO EWK (remote contribution) *Christopher Schwan*
Auditorium J.Curie, IJCLab 16:15 - 16:45

Extracting the xFitter likelihood *Ali Al Kadhim et al.*
Auditorium J.Curie, IJCLab 17:00 - 17:20

Ideas for future



Snowmass contribution finalisation, AOB
Auditorium J.Curie, IJCLab 09:30 - 10:30

Coffee
Auditorium J.Curie, IJCLab 10:30 - 11:00

Snowmass contribution finalisation, AOB
Auditorium J.Curie, IJCLab 11:00 - 12:30

Lunch (CESFO, building 98)
12:30 - 13:30

Snowmass paper and AOB