# How to measure the W mass with 10 MeV uncertainty

**EP-IT Data Science Seminars** 

16 October 2024, CERN

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#### Introduction

Analysis presented in LPC seminar last month

• Document: [CMS-PAS-SMP-23-002]

First measurement of  $m_{\ensuremath{\mathsf{W}}}$  from CMS

- Most precise at LHC
- In agreement with the SM but in tension with CDF

This seminar will focus on the technical aspects



Use 16.8 fb<sup>-1</sup> pp collision data at  $\sqrt{s}$ =13TeV

Large inclusive W cross section

• 300M data and 4B MC events (4 times MC statistical power)

Largest dataset used for W boson mass analysis

- Opportunity to exploit multi dimensional information
- Challenging data processing

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Much more data available now and in the years to come

 $\rightarrow$  Software developments have to keep up with technical challenges

HL-LHO





The measurement is performed using the muon kinematics only

#### How we measure the W boson mass

Strategy to use large data sample and constrain theory uncertainties in-situ Profile likelihood fit to single muon  $p_T \eta$ , charge distribution

• 2880 bins



## Multiple analyses in one

- Z dilepton  $m_{II}$ ,  $p_T^Z$ - $y^Z$ , W-like
- Unfolding
- Helicity cross section fit
- Generator studies







Precise treatment of uncertainties requires large amount of variations

• O(1000) parameters in single fit

Systematic uncertainties	W-like $m_Z$	$m_{\rm W}$
Muon efficiency	3127	3658
Muon eff. veto	_	531
Muon eff. syst.	343	
Muon eff. stat.	2784	
Nonprompt background	-	387
Prompt background	2	3
Muon momentum scale	338	
L1 prefire	14	
Luminosity	1	
PDF (CT18Z)	60	
Angular coefficients	177	353
W MINNLO <sub>PS</sub> $\mu_{\rm F}$ , $\mu_{\rm R}$	_	176
Z MINNLO <sub>PS</sub> $\mu_{\rm F}$ , $\mu_{\rm R}$	176	
PYTHIA shower $k_{\rm T}$	1	
$p_{\rm T}^{\rm V}$ modeling	22	32
Nonperturbative	4	10
Perturbative	4	8
Theory nuisance parameters	10	
c, b quark mass	4	
Higher-order EW	6	7
Z width	1	
Z mass	1	
W width	_	1
W mass	-	1
$\sin^2 \theta_W$	1	
Total	3750	4859

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#### Requirements

#### Fast analysis turnaround

→ external libraries;
 low level critical parts in c++
 → "smart" parallelism

Our analysis framework

#### Reliable & transparent

- low error rate
- reproducible
- $\rightarrow$  git versioning; continuous integration
  - $\rightarrow$  documentation

Fast development

- flexible
- low barrier to entry
  - easy to maintain
  - $\rightarrow$  customizable

 $\rightarrow$  high level scripts in python



#### Shorten the gap between data and results: NanoAOD

Central supported compact CMS event data format [0,1]

- Flat ROOT TTree
  - Independent of experiment specific software
- High level physics objects
  - ( $p_T$ ,  $\eta$ ,  $\phi$ , ID, ... of muons, electrons, jets, ...)
- ~2kB per event
- Good for ~50% of analyses

D,1]	Data tier	Size (kB)
	RAW	1000
	Gen	<50
Analysis data formats	SIM	1000
	DIGI	3000
	RECO(SIM)	3000
	AOD(SIM)	400
	MiniAOD(SIM)	50
	NanoAOD(SIM)	2



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- ~2kB per event

Easy customization with additional information

• Alternate PDFs, Info for muon track fit, ...

0,1]	Data tier	Size (kB)
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# NanoGEN and NanoLHE

NanoAOD with only then GEN-related branches

- Developed to validate MiNNLO event generator
  - Now centrally supported in CMS
- Producible directly from gridpack
- Lightweight, no detector simulation
- ~0.4kB per event

Large quantities produced

- O(100M) for MiNNLO validation
- O(10B) for EW uncertainties

	Data tier	Size (kB)
	RAW	1000
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	NanoAOD(SIM)	2
	NanoGEN	0.4



Ran on daily basis (>1000 times)

#### HOW LONG CAN YOU WORK ON MAKING A ROUTINE TASK MORE EFFICIENT BEFORE YOU'RE SPENDING MORE TIME THAN YOU SAVE? (ACROSS FIVE YEARS)



Where we started

## High performance computing machines

Custom analysis framework executed locally

- No resubmission of failed jobs/ merging of jobs etc.
- Direct feedback on progress

Run on single high performance machine	_	CERN	MIT/Pisa
<ul> <li>Reading/writing on fast NVMe SSDs</li> </ul>	CPU	2 x EPYC 7702	2 x EPYC 9654
<ul> <li>Local or via network interface 100Gbit/s</li> </ul>	cores	128	192
<ul> <li>Reading from local CERN eos via xrootd</li> </ul>	threads	256	384
<ul> <li>Network interface 100Gbit/s</li> </ul>	memory	1TB	1.5/2TB

Possible upgrade for the future

• EPYC Turin machine with 384 cores/ 768 threads



Select objects, filter events, fill histograms

• Pythonic, declarative, graph-style analysis

```
from ROOT import RDataFrame
df = RDataFrame(dataset);
df2 = df.Filter("x > 0")
            .Define("r2", "x*x + y*y");
rHist = df2.Histo1D("r2");
g = df2.Graph("x","y")
```

- Lazy execution: perform all operations in parallelized single event loop
- Executed on local machine
  - Plan to explore distRDF for multi-node scaling
- See RDF reference, documentation, EP seminar

Many optimizations conducted to ensure good thread scaling

• Now fully integrated in ROOT





Critical parts in c++

• Functions: e.g. check if reco muon has a match to any gen muon

```
bool hasMatchDR2(const float& eta, const float& phi, const Vec_f& vec_eta, const Vec_f& vec_phi, const float dr2 = 0.09) {
  for (unsigned int jvec = 0; jvec < vec_eta.size(); ++jvec) {
    if (deltaR2(eta, phi, vec_eta[jvec], vec_phi[jvec]) < dr2) return true;
    }
    return false;
}</pre>
```

- Compiled at runtime using cling jitting
- And in python

df = df.Filter("wrem::hasMatchDR2(goodMuons\_eta0,goodMuons\_phi0,GenPart\_eta[postfsrMuons],GenPart\_phi[postfsrMuons],0.09)")

- Other examples much more complex but follow same logic
- We also tried Numba, but found less efficient and not more convenient



Critical parts in c++

• Helpers – classes that contain histograms with corrections and functions to apply them: e.g. reweight pileup spectrum in MC to the one in data

```
class pileup_helper {
public:
    pileup_helper(const TH1D &puweights) :
        puweights_(make_shared_TH1<const TH1D>(puweights)) {}
    // returns the pileup weight
    double operator() (float nTrueInt) const {
        return puweights_->GetBinContent(puweights_->FindFixBin(nTrueInt));
    }
private:
    std::shared_ptr<const TH1D> puweights_;
};
```

#### • And in python

helper = ROOT.wrem.pileup\_helper(puweights)

df = df.Define("weight\_pu", pileup\_helper, ["Pileup\_nTrueInt"])

• Other examples much more complex – but follow same logic



#### Critical parts in c++

- Often templated (e.g. for histogram bins)
- Also using Eigen and tensorflow c++ libraries

```
template <std::size t NEtaBins>
class muon_prefiring_helper_stat {
public:
 static constexpr std::size_t NVar = NEtaBins + 1;
 using value_type = Eigen::TensorFixedSize<double, Eigen::Sizes<NVar, 2>>;
 muon_prefiring_helper_stat(const muon_prefiring_helper &other) :
   parameters_(other.parameters()), hotspot_parameters_(other.hotspot_parameters()) {}
 value_type operator() (const Vec_f& eta, const Vec_f& pt, const Vec_f& phi, const Vec_i& charge, const Vec_b& looseId, double nominal_weight = 1.0) const {
       [...]
      return res;
   }
  private:
   std::shared_ptr<const TH2D> parameters_;
   std::shared_ptr<const TH2D> hotspot_parameters_;
 };
```

#### • And in python

helper\_stat = ROOT.wrem.muon\_prefiring\_helper\_stat[netabins](helper)

df = df.Define("weight\_newMuonPrefiringSF", muon\_prefiring\_helper, ["Muon\_correctedEta", "Muon\_correctedPt", "Muon\_correctedPhi", "Muon\_correctedCharge", "Muon\_looseId"])

#### Histograms



Strategy to perform computations on histograms later in analysis chain

- Allows for more flexibility
- E.g. data-driven nonprompt background prediction
- Nominal histogram is 5D

Axis	Bins
$p_{T}^{\mu}$	30
$\eta^{\mu}$	48
qμ	2
l <sub>rel</sub> μ	2
$m_{T}^{W}$	3
All	17,280

#### Histograms



Strategy to perform computations on histograms later in analysis chain

• Allows for more flexibility

<ul> <li>E.g. data-driven nonprompt background prediction</li> </ul>	Avis	Rins
<ul> <li>Nominal histogram is 5D</li> </ul>		
	p <sub>T</sub> µ	30
<ul> <li>Largest histograms with 8D and 20M bins</li> </ul>	η <sup>μ</sup>	48
• For efficiency scale factor 2D smoothed in $p_T$ and $u_T$	$q^{\mu}$	2
<ul> <li>~same histograms for 16 processes</li> </ul>	ا <sub>rel</sub> μ	2
	m⊤ <sup>w</sup>	3
Significant memory consumption	var. η <sup>μ</sup>	48
$\rightarrow$ For largest histogram: 2 5GB	var. q <sup>µ</sup>	2
$\rightarrow$ For all 12CP	eig. vec.	12
	All	19,906,560
	All (w/ flow)	358,400,000

Gets much worse if flow bins can't be disabled (as in root histograms)

#### **Boost histograms**

RDataFrame

Boost Histograms

~1-2 h

Previously: one root histogram copy for each thread

- But large memory consumption was a showstopper
- Long merging time when adding up at the end

Solution: use <a href="mailto:std:atomic<double>">std:atomic<double></a> with c++ <a href="mailto:boost-histograms">boost-histograms</a>

- All threads write in same histogram
- But can't use python binding directly ... (cppyy vs. pybind 11)

Custom copy conversion into python boost histograms

- Arbitrary number of axes
- Configurable underflow/overflow bins
- Convenient (numpy like) indexing/ manipulation

Histograms stored with pickle

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- Using proxies dictionary in .hdf5 to allow lazy loading (code)
- Including meta data (e.g. number of processed events, cross section/luminosity, command, ...)





#### Tensor axes



All systematic uncertainties represented by event weight variations Traditionally one histogram per variation

• e.g. NNPDF provides 101 alternate PDF weights  $\rightarrow$  101 histograms

Better: a single histogram with an additional axis

Even better: fill full array/tensor at once, only do bin lookup once

- Using Eigen tensors
- Arbitrary number of dimensions



Atomic boost histograms and tensor axes implemented in <u>narf</u> submodule

- More details given at ROOT Users Workshop 2022: link
- Not currently integrated in root; similar functionality in RHistogram?
  - Interest also from outside W mass analysis team



256 threads (2 EPYC 7702)

Hist Type	Hist Config	Evt. Loop	Total	CPUEff	RSS
ROOT THnD	10 × 103 × 5D	59m39s	74m05s	0.74	400GB
ROOT THnD	10 × 6D	7m54s	25m09s	0.27	405GB
Boost ("sta")	10 × 6D	7m07s	7m17s	0.90	9GB
Boost ("sta")	$10 \times (5D + 1$ -tensor)	1m54s	2m04s	0.81	9GB
Boost ("sta")	$1 \times (5D + 2$ -tensor)	1m32s	1m42s	0.77	9GB

- Root histograms slowed down by merging step
- Memory much lower with atomic accumulation
- Factor ~4 time reduction with tensor axes due to reduced lookup
- Some additional subtleties related to cash locality

## HDF5 writer



- Purely python based (boost histograms, numpy, ...)
- Flexibility & efficient implementation is essential •
- Perform selections/ accumulations/ other computations on histograms •
  - Signal selection
  - Data-driven nonprompt background estimation
    - Smoothing "on-the-fly" using least squares (code)
  - Modify systematic variations e.g. decorrelating/ combining

Sparse tensor implementation for unfolding

#### Binned profile maximum likelihood fit

Log likelihood from Poisson distributed bin-by-bin event numbers

$$L = \sum_{ibin} \left( -n_{ibin}^{obs} \ln n_{ibin}^{exp} + n_{ibin}^{exp} \right) + \frac{1}{2} \sum_{ksyst} \left( \theta_{ksyst} - \theta_{ksyst}^{0} \right)^{2}$$
$$n_{ibin}^{exp} = \sum_{jproc} \mu_{jproc} n_{ibin,jproc}^{exp} \prod_{ksyst} \kappa_{ibin,jproc,ksyst}^{\theta_{ksyst}}$$

- Gaussian constraint nuisance parameters  $\theta$  for systematic uncertainties
- Signal strength modifier  $\mu$
- Systematic variations in 3D tensor κ

#### **Tensorflow fit**



RooFit via minuit insufficient

- Limited numerical stability and efficiency
  - E.g. can not be parallelized

Tensorflow library with automatic gradient computation via back propagation for minimization:

- Quasi Newton trust region based minimizer to reliably find global minimum
  - Native tensorflow implementation; algorithm based on arXiv:1506.07222
- Fast, numerically accurate, stable
- Parallelized vector processing units and/or multiple threads
- Sparse tensor implementation to minimize memory consumption (if response matrix is close-to-diagonal, e.g. leptonic observables)
- Implemented in <u>combineTF</u>, see also PyHEP 2020: <u>link</u>

#### Tensorflow 2 fit



Re-written in Tensorflow 2:

- More developer-friendly due to eager execution
- Almost feature complete combineTF2 implementation
- More efficient computatoin of hessian and hessian vector products
- Trust-krylov minimizer from SciPy, computing the gradient and hessian-vector product in tensorflow 2
  - I.e. not using quasi-newton methods as in the combineTF1 case

Benchmark using MIT machine		fit	fit + covariance
• CPU: FPYC 9654	CombineTF1 CPU	1m49s	3m48s
	CombineTF2 CPU	34s	47s
• GPU: INVIDIA A30	CombineTF2 GPU	36s	39s

GPU "only" used to calculate the gradient/hessian/hessian-vector-product

## **Continuous integration**

Common framework among all analyzers

- Sharing as much code as possible among different efforts
- Reuse existing code, find/avoid bugs, save time
- Quickly developed with O(10) contributors, now at >500 pull requests (PRs)

However

- Updates often unintentionally affected other parts
  - Framework was constantly broken
- Sometimes not clear where certain changes came from

Solution  $\rightarrow$  GitHub actions: platform for automate developer workflows

- Use continuous integration and deployment (CI/CD) pipeline
- Same tool as used for code development instead of third party integration
- Slim and easily to set up and manage (compared to e.g. Jenkins)





## Github CI workflow

Different analysis chains implemented

- Independent jobs run in parallel, each job contains a set of steps
- Different arguments for plotting/ fitting for good code coverage
- Investigate failed jobs directly in Github actions



## Github CI workflow

Running full analysis chain (code)

1) For each PR on reduced set of files (~1%)



- 2) Scheduled each morning on reduced set of files (~1%) as reference for PR
- 3) Scheduled 3 times a week on (1:1) data:MC files to backtrack changes
  - All output files (e.g. histograms) stored on EOS for later use
  - Separate workflow to delete old files
- 4) Workflow dispatch on (1:1) data:MC files to manually run on chosen branch
  - To test a new feature (e.g. apply new nominal calibration/correction)

In the process of adding code checks

- Run in CI and as pre-commit hooks
- Syntax checks for python, c++, yaml, json files
- Linters: Black, Flake8, isort

**Everything blinded** 

## Github CI infrastructure

Maintained via service account with CMS access and eos area

• <u>Self hosted runners</u> to easy access resources and execute code on the CERN high-performance analysis machine used for this analysis



 Repository with sub modules checked out including large file storage (Ifs) support



Network authentication via Kerberos, key stored in local keytab file

```
    name: setup kerberos

75
76
             run:
               kinit -kt ~/private/.keytab cmsmwbot@CERN.CH
77
               klist -k -t -e ~/private/.keytab
               klist
79
               echo "xrdfs root://eosuser.cern.ch// ls $EOS DIR"
               xrdfs root://eosuser.cern.ch// ls $EOS DIR
81
82
           - name: setup kerberos within singularity image
83
84
             run:
               scripts/ci/run with singularity.sh kinit -kt ~/private/.keytab cmsmwbot@CERN.CH
               scripts/ci/run with singularity.sh klist -k -t -e ~/private/.keytab
               scripts/ci/run with singularity.sh klist
87
               echo "xrdfs root://eoscms.cern.ch// ls $EOS DATA DIR"
               scripts/ci/run with singularity.sh xrdfs root://eoscms.cern.ch// ls $EOS DATA DIR
```

#### Webpage support

Results initially created in local temporary folder

- Copied via xrdcp to CMS protected webpage
- CMS centrally maintained plot browser
- Automatic lumi scaling for using subset of data files



#### Directories

- Archive
- Dispatch
- PR2XX
- PR3XX
- PR4XX
- PR500
- PR501
  - [...]
- PR553
- PR554
- ReferenceRuns
- ScheduledBuilds

#### Webpage support



#### 🐔 / WMassAnalysis / PRValidation

#### Directories

- Archive
- Dispatch
- PR2XX
- PR3XX
- PR4XX
- PR500
- PR501
  - [...]
- PR553
- PR554
- ReferenceRuns
- ScheduledBuilds

Plots for nuisance parameter pulls, constraints, and impacts produce via <u>plotly</u>

- Available in interactive .html
- See all O(1000) nuisances with more digits

Each plot is produced with a .log file

		Script called at 2024-10-01 15:56:53 608388
.log files Check exact event yields		The command was: scripts/plotting/postfitPlots.py '/scratch/dwalter/CombineStudies/test/ZMassDilepton_ptll_yll/fitresults_123456789.root' legCols 1eoscp -f '241001_test'yscale '1.25'
	Chock ovact	Yield information for Stacked processes
	event yields	Process         Yield         Uncertainty           0         \$\gamma\$-induced         1796.97         94.01           1         Z/\$\gamma^{\star}\to\tau\tau\$         1582.57         77.61           2         0ther         1630.27         14.59           3         Z/\$\gamma^{\\star}\to\mu\mu\$         1931915.83         336.74
		Yield information for Unstacked processes
		Process Yield Uncertainty 0 Data 1936925.64 2547.78 1 Inclusive 1936925.64 313.63
		===> Sum unstacked to data is 100.00%
		Meta info from input file AnalysisOutput
	Command chain	r
	used to produce	ι "time": "2024-10-01 15:39:52.107792", "command": "scripts/combine/setupCombine pyi
	the plot	<pre>'/scratch/dwalter/results_histmaker/test/mz_dilepton.hdf5'fitvar 'ptll-yll'lumiScale 100realData -o '/scratch/dwalter/CombineStudies/test'",</pre>
	$\rightarrow$ Look up how	<pre>"args": {     "outfolder": "/scratch/dwalter/CombineStudies/test",     "inputFile": [</pre>
	to run specific scr	ipts ], "postfix": null, "verbose": 3,
		[]
	Git commit hash	"git_hash": "\"4713c27278391e1df49f86834c6d122cff8beba5\"
	Local untracked changes	"git_diff": "diffgit a/scripts/combine/saturatedGOF.py b/scripts/combine/saturatedGOF.py index lb9fb2e9ldf140a8 100644 a/scripts/combine/saturatedGOF.py +++ b/scripts/combine/saturatedGOF.py @@ -15,7 +15,7 @@ tree.GetEntry(0)
	$\rightarrow$ Each plot is reproducible	<pre>fitresult_h5py = combinetf_input.get_fitresult(args.infile.replace(\".root\",\".hdf5\")) meta = ioutils.pickle_load_h5py(fitresult_h5py[\"meta\"]) -nbins = sum([np.product([len(a) for a in info[\"axes\"]]) for info in meta[\"channel_info\"].values()]) +nbins = sum([np.prod([len(a) for a in info[\"axes\"]]) for info in meta[\"channel_info\"].values()]) ndf = nbins - tree.ndofpartial</pre>

#### Many interesting features not discussed today

Other analysis ingredients

- Efficiencies
  - Using tag and probe fits, smoothing of scale factors in 1D/2D
- Helicity cross section corrections & uncertainties
  - Based on Eigen
- Muon calibration
  - Object to event weight variations via CDF transform
- Recoil calibration

...

• Functional fit based on JAX, evaluation with tensorflow lite c++

#### Summary

Increasing amount of data opens new opportunities

• Software developments must be ahead to fully exploit potential

Fast analysis turnaround was essential for this complex measurement

- RDF provides a convenient and efficient library
  - Initially showstoppers observed in scaling
  - Extensive work on critical parts to improve RDF and histogram implementation
- Full analysis runs in ~hours

Challenging collaborative work with increasing number of contributors

- Github CI/CD pipeline has turned out to be extremely useful
- Time savings in PR reviews, spot/avoid bugs, backtrack changes
- Always ensure working implementation for different analyses/ configurations

Many areas identified for further improvements
## Backup

Precision measurements of standard model parameters provide opportunity to over constrain the theory and pose stringent tests



Indirect prediction (~6MeV) more precise than direct measurement (~10MeV) and in tension (CDF)

 $\rightarrow$  Call for more precise measurements

# Lumitools

Automatic computation of integrated luminosity of processed data

- CMS data is organized by fill, run, luminosity block (~24s)
  - Use .csv file containing integrated luminosity information
  - Provided by the CMS BRIL group
- Processed with RDataFrame, read non-ROOT data
- Guarantees consistent luminosity calculation
- Convenient for running on subset of data

Implemented in <u>lumitools</u>

• Could be used standalone

### Histogram benchmark

Hist Type	Hist Config	Evt. Loop	Total	CPUEff	RSS
ROOT THnD	10 × 103 × 5D	59m39s	74m05s	0.74	400GB
ROOT THnD	10 x 6D back	7m54s	25m09s	0.27	405GB
ROOT THnD	$10 \times 6D$ front	13m52s	30m27s	0.42	406GB
Boost ("sta")	10 x 6D back	7m07s	7m17s	0.90	9GB
Boost ("sta")	$10 \times 6D$ front	3m22s	3m33s	0.86	9GB
Boost ("sta")	$10 \times (5D + 1$ -tensor)	1m54s	2m04s	0.81	9GB
Boost ("sta")	$1 \times (5D + 2$ -tensor)	1m32s	1m42s	0.77	9GB

- In the tensor/array weight-case the weights for the different systematic idxs are contiguous in memory by construction
- In the N+1-d histogram case it depends on the array ordering
- TH1/2/3 and boost-histograms have fortran array ordering → systematic idx axis is best at the front
- THn has C array ordering  $\rightarrow$  systematic idx axis is best at the back
- The difference is about a factor of 2 for both root and boost hists (but still > 50% additional gain from tensor filling)
- Largely accounted simply by skipping the extra FDIVs needed for redundant value-to-index conversion for the 5 axes

### QCD multijet background estimation

Estimated from data using extended ABCD method

- Prediction from yields in sideband regions in bins of high relative isolation and low  $m_{\rm T}{}^{\rm W}$
- Prompt background in sideband region subtracted from simulation
  - Repeated for each systematic variation ~O(1000) times
- Evaluated in fine bins in  $p_{T^{\mu}},\,\eta^{\mu},\,q^{\mu}$





## QCD multijet background estimation

Smoothing each sideband region in  $p_{T^{\mu}}$  with exponential "on-the-fly"

- Maintain good statistical properties
- Smoothing in 5 regions, 96 bins for  $\eta^{\mu}\!,\,q^{\mu}$
- Repeated for O(1000) systematic variations
- Robust and efficient calculation required
  - Use polynomial in log space
  - Analytic solutions using least squares

$$f_i(p_{\rm T}) = e^{P_i(p_{\rm T})}$$
$$f_{\rm D}(p_{\rm T}) = e^{\sum_i w_i P_i(p_{\rm T})}$$



- Systematic uncertainties from eigenvector decomposition
- Everything done in ~seconds

More complex procedures tested

• E.g. using integrated Bernstein polynomials with <u>nnls</u> to enforce monotonicity













	Systematic uncertainties	W-like $m_Z$	$m_{\rm W}$
	Muon efficiency	3127	3658
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Precise treatment of uncertainties	Muon eff. stat.	2784	
requires large amount of variations	Nonprompt background	-	387
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	Higher-order EW	6	7
	Z width	1	
	Z mass	1	
	W width	-	1
	W mass	-	1
	$\sin^2 \theta_W$	1	
7	Total	3750	4859













### High performance computing machines

Custom analysis framework executed locally

- No resubmission of failed jobs/ merging of jobs etc.
- Direct feedback on progress

Run on single high performance machine		CERN	MIT/Pisa
<ul> <li>Reading/writing on fast NVMe SSDs</li> </ul>	CPU	2 x EPYC 7702	2 x EPYC 9654
<ul> <li>Local or via network interface 100Gbit/s</li> </ul>	cores	128	192
<ul> <li>Reading from local CERN eos via xrootd</li> </ul>	threads	256	384
<ul> <li>Network interface 100Gbit/s</li> </ul>	memory	1TB	1.5/2TB

Possible upgrade for the future

• EPYC Turin machine with 384 cores/ 768 threads









Histograms	RDataFrame ~1	- <u>2 h</u> Ba Histo	oost ograms
Strategy to perform computations <ul> <li>Allows for more flexibility</li> </ul>	on histograms later in anal	ysis chain	
• E.g. data-driven nonprompt back	ground prediction	Axis	Bins
<ul> <li>Nominal histogram is 5D</li> </ul>		p <sub>T</sub> <sup>µ</sup>	30
J. J		η <sup>μ</sup>	48
		q <sup>µ</sup>	2
		Ι <sub>rel</sub> μ	2
		$m_{T}^{W}$	3
		All	17,280
19			

Histograms	RDataFrame	~1-2 h His	Boost tograms
Strategy to perform computations on hi • Allows for more flexibility	stograms later in a	analysis chain	
E.g. data-driven nonprompt backgroup	na prediction	Axis	Bins
• Nominal histogram is 5D		p⊤ <sup>µ</sup>	30
<ul> <li>Largest histograms with 8D and 20M</li> </ul>	bins	η <sup>μ</sup>	48
<ul> <li>For efficiency scale factor 2D smoot</li> </ul>	q <sup>µ</sup>	2	
<ul> <li>~same histograms for 16 processes</li> </ul>	<ul> <li>~same histograms for 16 processes</li> </ul>		
		m⊤ <sup>w</sup>	3
Significant memory consumption		var. η <sup>μ</sup>	48
$\rightarrow$ For largest histogram: 2 5GB		var. q <sup>µ</sup>	2
> For all: 12CD		eig. vec.	12
$\rightarrow$ FOI all. 13GB		All	19,906,560
		All (w/ flow)	358,400,000
Gets much worse if flow bins can't be d	sabled (as in root	histograms)	
20			



Tensor axes	RDataFrame ~1-2 h Boost Histograms
All systematic uncertainties represented Traditionally one histogram per variatio • e.g. NNPDF provides 101 alternate P	d by event weight variations n DF weights → 101 histograms
<ul><li>Better: a single histogram with an addit</li><li>Even better: fill full array/tensor at once</li><li>Using Eigen tensors</li><li>Arbitrary number of dimensions</li></ul>	ional axis e, only do bin lookup once
<ul> <li>Atomic boost histograms and tensor ax</li> <li>More details given at ROOT Users We</li> <li>Not currently integrated in root; simil</li> <li>Interest also from outside W mass a</li> </ul>	es implemented in <u>narf</u> submodule orkshop 2022: <u>link</u> ar functionality in RHistogram? analysis team
22	

Histogram benchmark		(	RD	ataF	rame	~1-2	h,	B Hist	oost ograms	$\square$		
	40014					、		40		~	16	

256 threads (2 EPYC 7702)

Hist Type	Hist Config	Evt. Loop	Total	CPUEff	RSS
ROOT THnD	$10 \times 103 \times 5D$	59m39s	74m05s	0.74	400GB
ROOT THnD	10 × 6D	7m54s	25m09s	0.27	405GB
Boost ("sta")	10 × 6D	7m07s	7m17s	0.90	9GB
Boost ("sta")	$10 \times (5D + 1$ -tensor)	1m54s	2m04s	0.81	9GB
Boost ("sta")	$1 \times (5D + 2$ -tensor)	1m32s	1m42s	0.77	9GB

• Root histograms slowed down by merging step

• Memory much lower with atomic accumulation

• Factor ~4 time reduction with tensor axes due to reduced lookup

• Some additional subtleties related to cash locality



### Binned profile maximum likelihood fit

Log likelihood from Poisson distributed bin-by-bin event numbers

$$L = \sum_{ibin} \left( -n_{ibin}^{obs} \ln n_{ibin}^{exp} + n_{ibin}^{exp} \right) + \frac{1}{2} \sum_{ksyst} \left( \theta_{ksyst} - \theta_{ksyst}^{0} \right)^{2}$$
$$n_{ibin}^{exp} = \sum_{jproc} \mu_{jproc} n_{ibin,jproc}^{exp} \prod_{ksyst} \kappa_{ibin,jproc,ksyst}^{\theta_{ksyst}}$$

- Gaussian constraint nuisance parameters  $\theta$  for systematic uncertainties
- Signal strength modifier  $\mu$
- Systematic variations in 3D tensor κ

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Tensorflow 2 fit	hdf5 tensor		Tensorflow fit
Re-written in Tensorflow 2		,	/
More developer-friendly due to a	orgerevecution		Fitresults
Almost feature complete combine	eiF2 implementation		
<ul> <li>More efficient computatoin of he</li> </ul>	ssian and hessian vector	products	5
<ul> <li>Trust-krylov minimizer from SciPy product in tensorflow 2</li> </ul>	, computing the gradien	t and hes	sian-vector
• I.e. not using quasi-newton me	thods as in the combineT	F1 case	
		fit	fit + covariance
Benchmark using MIT machine	CombineTE1 CPU	1m49s	3m48s
• CPU: EPYC 9654	CombineTF2 CPU	345	475
• GPU: Nvidia A30	CombineTF2 GPU	36s	39s
GPU "only" used to calculate the gr	adient/hessian/hessian-	vector-pr	oduct
		-	
27			

#### Continuous integration

Common framework among all analyzers

- Sharing as much code as possible among different efforts
- Reuse existing code, find/avoid bugs, save time
- Quickly developed with O(10) contributors, now at >500 pull requests (PRs)

#### However

- Updates often unintentionally affected other parts
  - Framework was constantly broken
- Sometimes not clear where certain changes came from

Solution  $\rightarrow$  GitHub actions: platform for automate developer workflows

- Use continuous integration and deployment (CI/CD) pipeline
- · Same tool as used for code development instead of third party integration
- Slim and easily to set up and manage (compared to e.g. Jenkins)

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#### Github CI workflow

Different analysis chains implemented

- Independent jobs run in parallel, each job contains a set of steps
- Different arguments for plotting/ fitting for good code coverage
- Investigate failed jobs directly in Github actions



#### Github CI workflow

Running full analysis chain (<u>code</u>)

1) For each PR on reduced set of files (~1%)

2) Scheduled each morning on reduced set of files (~1%) as reference for  $\mathsf{PR}$ 

pull\_request: | branches: [ main ]

10

1) 2) 3) 4)

- 3) Scheduled 3 times a week on (1:1) data:MC files to backtrack changes
  - All output files (e.g. histograms) stored on EOS for later use
  - Separate workflow to delete old files
- 4) Workflow dispatch on (1:1) data:MC files to manually run on chosen branch
  - To test a new feature (e.g. apply new nominal calibration/correction)

In the process of adding code checks

- Run in CI and as pre-commit hooks
- Syntax checks for python, c++, yaml, json files
- Linters: <u>Black</u>, <u>Flake8</u>, <u>isort</u>

Everything blinded

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# Webpage support

Results initially created in local temporary folder

- Copied via xrdcp to CMS protected webpage
- CMS centrally maintained plot browser
- Automatic lumi scaling for using subset of data files



#### 🐔 / WMassAnalysis / PRValidation

#### Directories

- Archive • Dispatch
- PR2XX
- PR3XX
- PR4XX
- PR500 • PR501
- [...] • PR553
- PR554
- ReferenceRuns
- ScheduledBuilds



		Consist colled at 2024 10 01 15.55.53 600200				
.log files	The command was: scripts/plotting/postiPlots.py '/scratch/dwalter/CombineStudies/test/ZMassDilepton_ptll_yll/fitresults_123456789.root' legCols 1escop -f '24100_ltest'yscale '1.25'					
	Check exact event yields	Yield information for Stacked processes           Process         Yield Uncertainty           0         \$\gamma^{106.07         94.01           1         Z/\$\gamma^{105.07         94.01           2         Other         1582.57         77.61           2         Other         1630.27         14.59           3         Z/\$\gamma^{\star}\townu\musk         1931915.83         336.74           Yield information for Unstacked processes         Process         Yield Uncertainty           0         Data         1936925.64         2547.78           1         Inclusive         1936925.64         313.63           wwws Sum unstacked to data is 100.00%         100.00%				
		Meta info from input file AnalysisQuitput				
	Command chain used to produce the plot → Look up how to run specific scr	<pre>inter ite ite ite ite ite ite ite ite ite ite</pre>				
	[]					
	Git commit hash	"git_hash": "\"4713c27278391e1df49f86834c6d122cff8beba5\"				
	Local untracked changes	<pre>"git diff": "diffgit a/scripts/combine/saturatedGOF.py b/scripts/combine/saturatedGOF.py index 10Pb2e9. laf140480 100644  a/scripts/combine/saturatedGOF.py +++ b/scripts/combine/saturatedGOF.py @@ -15,7 +15,7 @@ tree.GetEntry(0) fitresult_h5py = combinetf input.get fitresult(args.infile.replace(\".root\",\".hd</pre>				
34	→ Each plot is reproducible	<pre>meta = loutlis.pickle_load_nbpy(tirtesut_hbpy[\"meta\"]) -nbins = sum([np.product[[len(a] for a in info[\"axes\"]]) for info in meta[\"channel_info\"].values()]) +nbins = sum([np.prod([len(a) for a in info[\"axes\"]]) for info in meta[\"channel_info\"].values()]) ndf = nbins - tree.ndofpartial</pre>				
•••						

## Many interesting features not discussed today

Other analysis ingredients

- Efficiencies
  - Using tag and probe fits, smoothing of scale factors in 1D/2D
- Helicity cross section corrections & uncertainties
  - Based on Eigen
- Muon calibration
  - Object to event weight variations via CDF transform
- Recoil calibration
  - Functional fit based on JAX, evaluation with tensorflow lite c++

• ...

### Summary

Increasing amount of data opens new opportunities

• Software developments must be ahead to fully exploit potential

Fast analysis turnaround was essential for this complex measurement

- RDF provides a convenient and efficient library
  - Initially showstoppers observed in scaling
  - Extensive work on critical parts to improve RDF and histogram implementation
- Full analysis runs in ~hours

Challenging collaborative work with increasing number of contributors

- Github CI/CD pipeline has turned out to be extremely useful
- Time savings in PR reviews, spot/avoid bugs, backtrack changes
- Always ensure working implementation for different analyses/ configurations

Many areas identified for further improvements

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# Lumitools

Automatic computation of integrated luminosity of processed data

- CMS data is organized by fill, run, luminosity block (~24s)
  - Use .csv file containing integrated luminosity information
  - Provided by the CMS BRIL group
- Processed with RDataFrame, read non-ROOT data
- Guarantees consistent luminosity calculation
- Convenient for running on subset of data

Implemented in lumitools

• Could be used standalone

### Histogram benchmark

Hist Type	Hist Config	Evt. Loop	Total	CPUEff	RSS
ROOT THnD	10 × 103 × 5D	59m39s	74m05s	0.74	400GB
ROOT THnD	$10 \times 6D$ back	7m54s	25m09s	0.27	405GB
ROOT THnD	$10 \times 6D$ front	13m52s	30m27s	0.42	406GB
Boost ("sta")	$10 \times 6D$ back	7m07s	7m17s	0.90	9GB
Boost ("sta")	$10 \times 6D$ front	3m22s	3m33s	0.86	9GB
Boost ("sta")	$10 \times (5D + 1$ -tensor)	1m54s	2m04s	0.81	9GB
Boost ("sta")	$1 \times (5D + 2$ -tensor)	1m32s	1m42s	0.77	9GB

- In the tensor/array weight-case the weights for the different systematic idxs are contiguous in memory by construction
- In the N+1-d histogram case it depends on the array ordering
- TH1/2/3 and boost-histograms have fortran array ordering  $\rightarrow$  systematic idx axis is best at the front
- THn has C array ordering  $\rightarrow$  systematic idx axis is best at the back
- The difference is about a factor of 2 for both root and boost hists (but still > 50% additional gain from tensor filling)
- Largely accounted simply by skipping the extra FDIVs needed for redundant value-to-index conversion for the 5 axes

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More complex procedures tested

• E.g. using integrated Bernstein polynomials with nnls to enforce monotonicity

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