DUNE OA using GUNDAM **GUNDAM Oscillation Analysis Tools**



<u>Ciro Riccio</u> on behalf of Tristan Doyle, Vlada Yevarouskaya and Clark McGrew DUNE LBL meeting August, 19th 2024





The GUNDAM group

Adrien Blanchet (CERN)

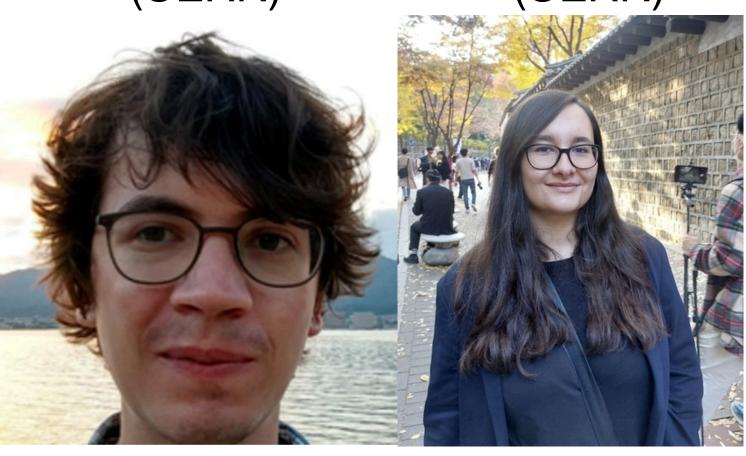


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Margherita Buizza Avanzini (LLR)



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What is GUNDAM?

- GUNDAM, which stand for Generalized and Unified Neutrino Data Analysis Methods, is an analysis tool developed in the context of the upgrade of the off-axis near detector of T2K
- It is a synthesis of two tools used in the T2K cross-section and OA WGs (<u>xsLLhFitter</u>) and BANFF)
- Its goal is to explore a likelihood function that can be defined by using a set of YAML/JSON configuration files
- Code structure designed for handling different analyses and as much as possible analysis independent
- Code optimized for both CPUs and GPUs
 - 10s 100s Hz depending on the analysis, system and if using CPUs only or GPUs • Example: analysis with ~4000 sample bins and ~600 parameters few hours (~3d
 - previous generation tool)
- Collaborative code developed on <u>GitHub</u> under same GPL as ROOT







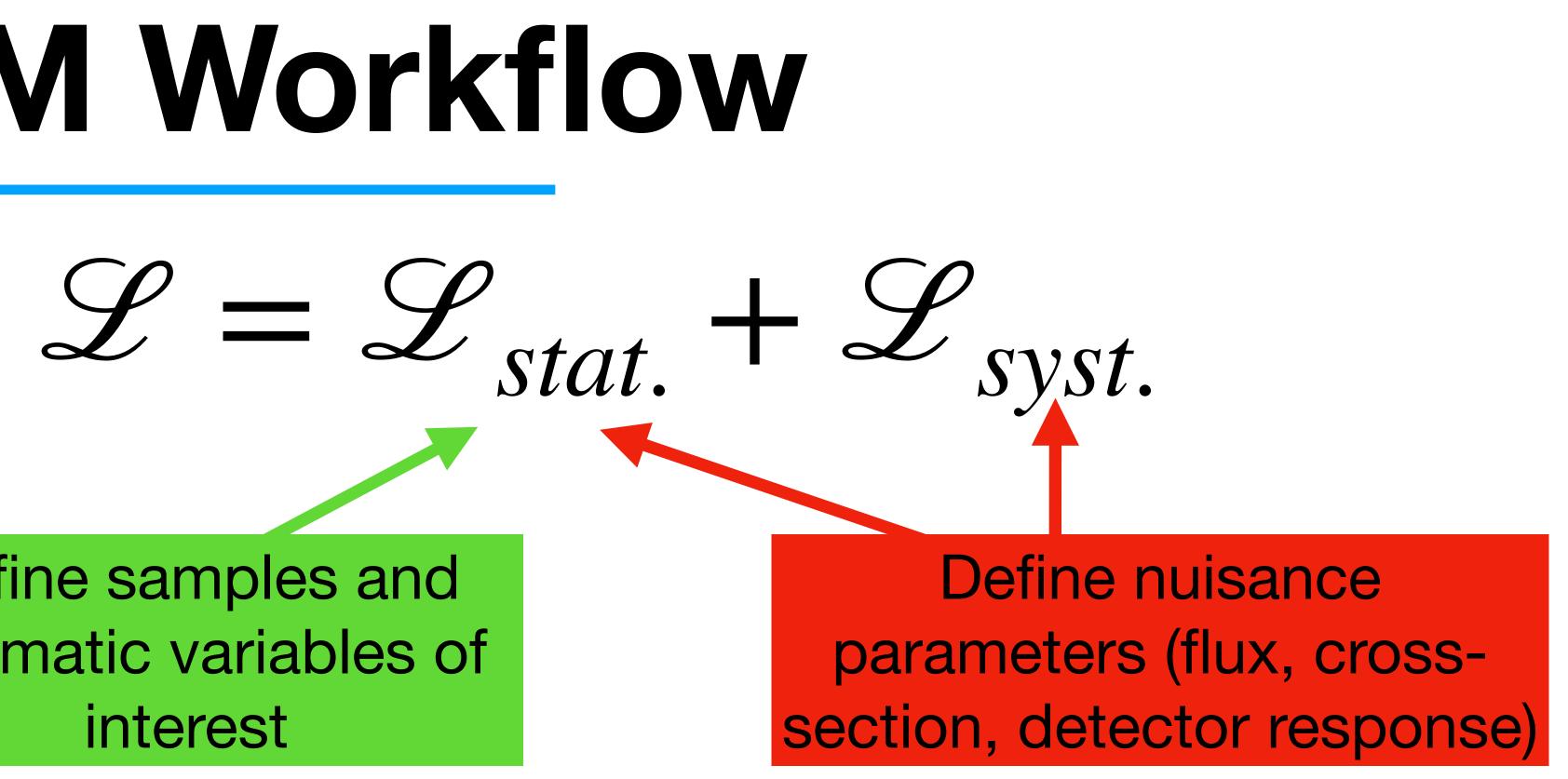
GUNDAM Workflow

Goal: explore the likelihood

> Define samples and kinematic variables of interest

> > Choose minimization (MINUIT, GSL) or likelihood sampling (MCMC) algorithm

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Output analysis results





Config examples

mainConfig.yaml

1	outputFolder: "./output"
2	minGundamVersion: 1.8.4
3	
4	
5	fitterEngineConfig:
6	
7	engineType: minimizer
8	<pre>minimizerConfig: "./inputs/fitter/configMinimizer.yaml"</pre>
9	
10	propagatorConfig:
11	
12	llhStatFunction: "BarlowBeestonLLH"
13	#llhStatFunction: "PoissonLLH"
14	
15	<pre>dataSetList: "./inputs/datasets/configDatasets.yaml</pre>
16	fitSampleSetConfig: "./inputs/samples/configSamples.yaml"
17	<pre>parameterSetListConfig: "./inputs/parameters/configParSet.yaml</pre>
18	<pre>plotGeneratorConfig: "./inputs/output/configPlotGenerator.y</pre>
19	<pre>scanConfig: "./inputs/output/configScan.yaml"</pre>

Note: illustrative only examples



aml"

Convenient to break this is several files but doesn't have to be



Engine configuration

mainConfig.yaml

1	outputFolder: "./output"	
2	minGundamVersion: 1.8.4	
3		
4		
5	fitterEngineConfig:	
6		
7	engineType: minimizer	
8	<pre>minimizerConfig: "./inputs</pre>	s/fitter/configMinimizer.yaml"
9		
10	propagatorConfig:	
11		
12	llhStatFunction: "Barlow	wBeestonLLH"
13	#llhStatFunction: "Poiss	sonLLH"
14		
15	dataSetList:	"./inputs/datasets/configDatasets.yaml"
16	fitSampleSetConfig:	"./inputs/samples/configSamples.yaml"
17	<pre>parameterSetListConfig:</pre>	"./inputs/parameters/configParSet.yaml"
18	plotGeneratorConfig:	"./inputs/output/configPlotGenerator.yaml"
19	scanConfig:	"./inputs/output/configScan.yaml"

Note: illustrative only examples

```
# https://root.cern.ch/doc/master/NumericalMinimization_8C.html
 type: "RootMinimizer"
 minimizer: "Minuit2"
 algorithm: "Migrad"
 #algorithm: "Combined"
 #algorithm: "Simplex"
#algorithm: "Fumili2"
 #minimizer: "Fumili"
#minimizer: "GSLMultiMin"
#algorithm: "ConjugateFR"
#algorithm: "ConjugatePR"
#algorithm: "BFGS"
 #algorithm: "BFGS2"
#algorithm: "SteepestDescent"
 #minimizer: "GSLMultiFit"
#minimizer: "GSLSimAn"
#minimizer: "Genetic"
enableSimplexBeforeMinimize: true # help Migrad to find the right spot
simplexMaxFcnCalls: 20000 # end SIMPLEX algo after this amount regardless of EDM
simplexToleranceLoose: 10000 # using EDM from fitter times this number -> less precise but should converge faster
simplexStrategy: 1
errors: "Hesse"
#errors: "Minos"
enablePostFitErrorFit: true
# https://root.cern.ch/download/minuit.pdf
print_level: 1 # 2 will print the giant gradient matrix...
# Migrad: The default tolerance is 0.1, and the minimization will stop
# when the estimated vertical distance to the minimum (EDM) is less
# than 0.001*[tolerance]*UP (see SET ERR).
# UP:
# Minuit defines parameter errors as the change in parameter value required
# to change the function value by UP. Normally, for chisquared fits
# UP=1, and for negative log likelihood, UP=0.5
tolerance: 1E-2
strategy: 1
max_iter: 100000
 max_fcn: 1E9
# useNormalizedFitSpace: when true, every parameter is rescaled such as the
 # prior mean value is set to 0 and the prior sigma is set to 1. This option
 # can help Minuit to converge while some parameter may have very different scales.
 # default: true
```

```
useNormalizedFitSpace: true
```





Engine configuration

mainConfig.yaml

1	outputFolder: "./output"	
2	minGundamVersion: 1.8.4	
3		
4		
5	fitterEngineConfig:	
6	mcmc	
7	engineType: minimizer	configMCMC.yaml
8	<pre>minimizerConfig: "./inputs</pre>	s/fitter/ configMinimizer.yaml "
9		
10	propagatorConfig:	
11		
12 13	llhStatFunction: "Barlow	wBeestonLLH"
13	#llhStatFunction: "Poiss	sonLLH"
14 15		
15	dataSetList:	"./inputs/datasets/configDatasets.yaml"
16	fitSampleSetConfig:	"./inputs/samples/configSamples.yaml"
17 18	<pre>parameterSetListConfig:</pre>	"./inputs/parameters/configParSet.yaml"
18	plotGeneratorConfig:	"./inputs/output/configPlotGenerator.yaml"
19	scanConfig:	"./inputs/output/configScan.yaml"

Note: illustrative only examples





Likelihood definition

mainConfig.yaml



Note: illustrative only examples

Different test statistics implemented in the core code



Dataset definition

mainConfig.yaml

1	outputFolder: "./output"		
2	minGundamVersion: 1.8.4		
3			
4			
5	fitterEngineConfig:		
6			
7	engineType: minimizer		
8	<pre>minimizerConfig: "./inputs/fitter/configMinimizer.yaml"</pre>		
9			
10	propagatorConfig:		
11			
12	llhStatFunction: "BarlowBeestonLLH"		
13	#llhStatFunction: "PoissonLLH"		
14			
15	<pre>dataSetList: "./inputs/datasets/configDatasets.yaml"</pre>		
16	fitSampleSetConfig: "./inputs/samples/configSamples.yaml"		
17	<pre>parameterSetListConfig: "./inputs/parameters/configParSet.yaml"</pre>		
18	<pre>plotGeneratorConfig: "./inputs/output/configPlotGenerator.ya</pre>		
19	<pre>scanConfig: "./inputs/output/configScan.yaml"</pre>		

Note: illustrative only examples

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Dataset definitions - name: "DUNE-FD" 5 isEnabled: true 6 selectedDataEntry: "data" 8 9 10 mc: # MC tree 11 MC format: event-by-12 tree: "mc_event_tree" 13 # MC file path event MC reweighed to filePathList: 14 fit data histograms - "mc-inputfile.root" 15 # selection cuts 16 selectionCutFormula: "passedEvent && Enu > 2" 17 # nominal weight 18 19 nominalWeightFormula: - "correctionWeight*POTWeight" 20 # variables dictionary 21 variableDict: 22 - { name: "Var1", expr: "RecoVar1" } 23 24 data: 25 # data files 26 aml" tree: "data_event_tree" 27 # data file path 28 filePathList: 29 30 - "data-inputfile.root"

variable dictionary

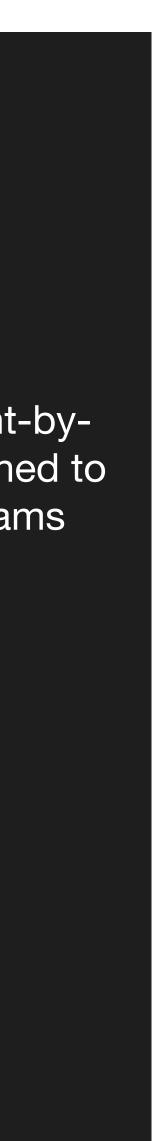
variableDict:

31

32

33

- { name: "Var1", expr: "RecoVar1" }





Samples definition

mainConfig.yaml

1	outputFolder: "./output"	
2	minGundamVersion: 1.8.4	
3		
4		
5	fitterEngineConfig:	
6		
7	engineType: minimizer	
8	minimizerConfig: "./inputs	s/fitter/configMinimizer.yaml"
9		
10	propagatorConfig:	
11		
12	llhStatFunction: "Barlow	wBeestonLLH"
13	#llhStatFunction: "Poiss	sonLLH"
14		
15	dataSetList:	"./inputs/datasets/configDatasets.yaml"
16	fitSampleSetConfig:	"./inputs/samples/configSamples.yaml"
17	<pre>parameterSetListConfig:</pre>	"./inputs/parameters/configParSet.yaml"
18	plotGeneratorConfig:	"./inputs/output/configPlotGenerator.yaml"
19	scanConfig:	"./inputs/output/configScan.yaml"

Note: illustrative only examples

Any number of samples



1	variables: Var1Low Var1Up Var2Low Va	r2Up
2	03-11	
3	0312	
4	0323	
5	0345	
6	0367	
7	0378	
8	03910	
9	0 3 11 12	
10	0 3 13 14	
11	0 3 15 16	
12	0 3 17 18	
13	0 3 19 20	

Bin in any number of dimension



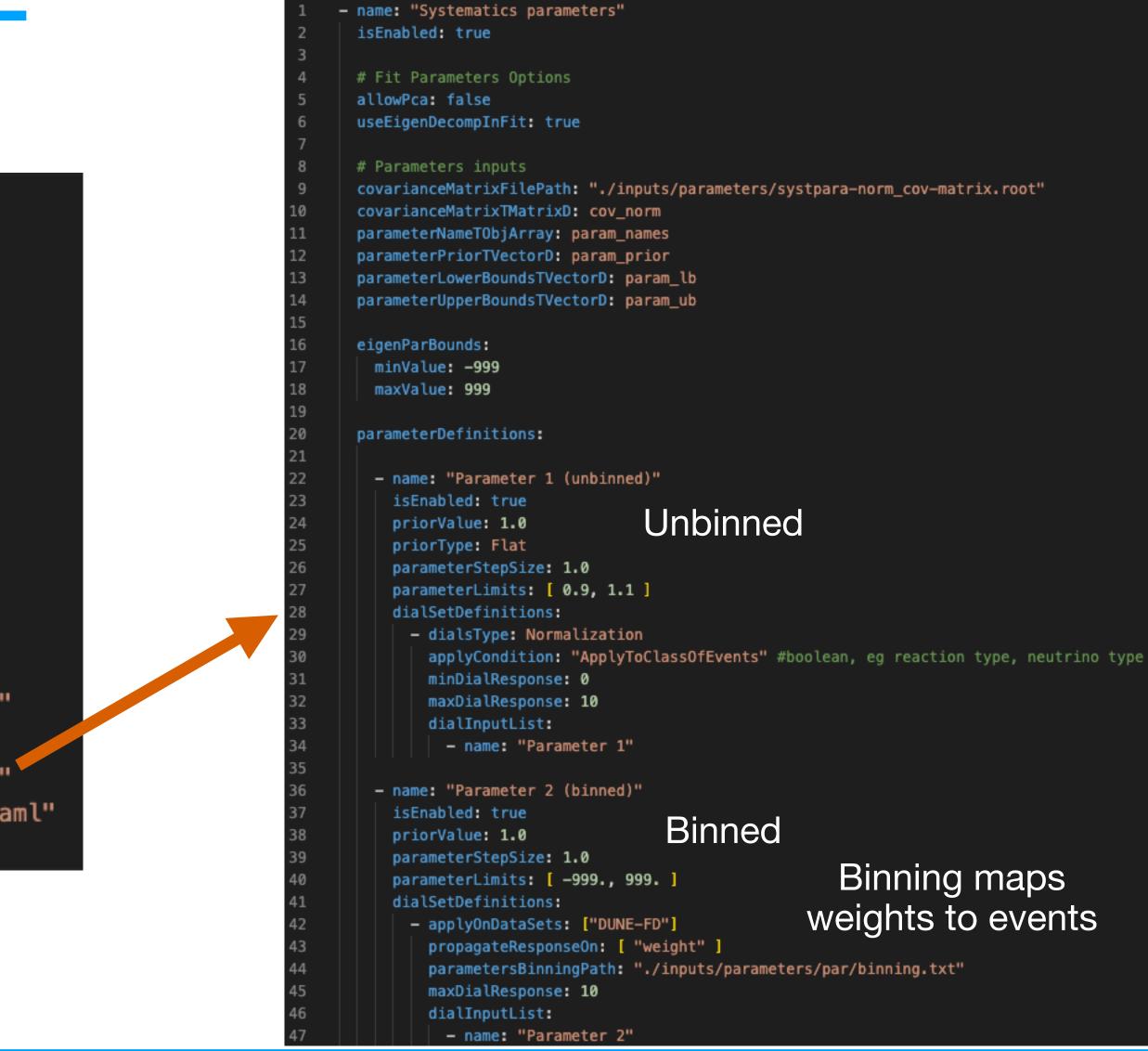


Parameter set: normalization

mainConfig.yaml

1	outputFolder: "./output"	
2	minGundamVersion: 1.8.4	
3		
4		
5	fitterEngineConfig:	
6		
7	engineType: minimizer	
8	<pre>minimizerConfig: "./inputs/fitter/configMinimizer.yaml"</pre>	
9		
10	propagatorConfig:	
11		
12	llhStatFunction: "BarlowBeestonLLH"	
13	#llhStatFunction: "PoissonLLH"	
14		
15	<pre>dataSetList: "./inputs/datasets/configDatasets.yaml</pre>	
16	<pre>fitSampleSetConfig: "./inputs/samples/configSamples.yaml"</pre>	
17	<pre>parameterSetListConfig: "./inputs/parameters/configParSet.yaml</pre>	
18	<pre>plotGeneratorConfig: "./inputs/output/configPlotGenerator.y</pre>	
19	<pre>scanConfig: "./inputs/output/configScan.yaml"</pre>	

Note: illustrative only examples





Parameter set: response function

mainConfig.yaml

1	outputFolder: "./output"		
2	minGundamVersion: 1.8.4		
3			
4			
5	fitterEngineConfig:		
6			
7	engineType: minimizer		
8	<pre>minimizerConfig: "./inputs/fitter/configMinimizer.yaml"</pre>		
9			
10	propagatorConfig:		
11			
12	llhStatFunction: "BarlowBeestonLLH"		
13	#llhStatFunction: "PoissonLLH"		
14			
15	dataSetList: "./inputs/datasets/configDatasets.yaml		
16	fitSampleSetConfig: "./inputs/samples/configSamples.yaml"		
17	<pre>parameterSetListConfig: "./inputs/parameters/configParSet.yaml</pre>		
18	<pre>plotGeneratorConfig: "./inputs/output/configPlotGenerator.y</pre>		
19	<pre>scanConfig: "./inputs/output/configScan.yaml"</pre>		

Note: illustrative only examples

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57	- name: "Systematics parameters (response function)"
58	isEnabled: true
59	
60	# Parameters inputs
61	<pre>covarianceMatrixFilePath: "./inputs/parameters/systpara-dials_cov-matrix.root</pre>
62	covarianceMatrixTMatrixD: cov
63	parameterNameTObjArray: param_names
64	parameterPriorTVectorD: param_prior
65	parameterLowerBoundsTVectorD: param_lb
66	parameterUpperBoundsTVectorD: param_ub
67	
68	parameterDefinitions:
69	
70	<pre>- name: "Parameter 1 (unbinned)"</pre>
71	isEnabled: true dialSetDefinitions: Unbinned
72	dialSetDefinitions:
73	- dialsType: Spline
74	<pre>dialSubType: "not-a-knot,monotonic" #"catmull-rom (or pixar)", "akima"</pre>
75	applyOnDataSets: ["DUNE-FD"]
76	dialLeafName: "Para1Graph" # TObjArray
77	minDialResponse: 0
/8	maxDialResponse: 10
79	
80	<pre>- name: "Parameter 2 (binned)"</pre>
81	isEnabled: true
82	dialSetDefinitions: Binned
83	- dialsType: Graph
84	dialSubType: "light"
85	applyOnDataSets: ["DUNE-FD"]
86	applyCondition: "ApplyToClassOfEvents" #boolean, eg reaction type, ne
87	dialLeafName: "Para2Graph" # TObjArray
88	<pre>binningFilePath: "./inputs/parameters/binning.txt"</pre>
89	minDialResponse: 0
90	maxDialResponse: 10

Binning maps response functions to events













Multi-parameter dials

mainConfig.yaml

1	outputFolder: "./output"	
2	minGundamVersion: 1.8.4	
3		
4		
5	fitterEngineConfig:	
6		
7	engineType: minimizer	
8	<pre>minimizerConfig: "./input</pre>	s/fitter/configMinimizer.yaml"
9		
10	propagatorConfig:	
11		
12	llhStatFunction: "Barlo	wBeestonLLH"
13	#llhStatFunction: "Pois	sonLLH"
14		
15	dataSetList:	"./inputs/datasets/configDatasets.yaml
16	fitSampleSetConfig:	"./inputs/samples/configSamples.yaml"
17	parameterSetListConfig:	"./inputs/parameters/configParSet.yaml
18	plotGeneratorConfig:	"./inputs/output/configPlotGenerator.y
19	scanConfig:	"./inputs/output/configScan.yaml"

Note: illustrative only examples

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92 -	name: "Multi parameter dials"
93	isEnabled: false
94	
95	# Parameters inputs
96	<pre>covarianceMatrixFilePath: "./inputs/parameters/multipar-dials_cov-matrix.root'</pre>
97	covarianceMatrixTMatrixD: cov
98	
99	parameterDefinitions:
100	- name: "Parameter 1"
101	isEnabled: true
102	priorValue: 0
103	parameterLimits: [-1, 1]
104	
105	<pre>- name: "Parameter 2"</pre>
106	isEnabled: true
107	isFixed: false
108	priorValue: 0
109	parameterLimits: [-1, 1]
110	
111	dialSetDefinitions:
112	- dialType: Surface
113	dialSubType: Bicubic
114	printDialsSummary: true
115	minDialResponse: 0
116	
117	dialInputList:
118	<pre>- name: "Parameter 1" # x[0]</pre>
119	<pre>- name: "Parameter 2" # x[1]</pre>



1



Tabulated dials

mainConfig.yaml

1	outputFolder: "./output"	
2	minGundamVersion: 1.8.4	
3		
4		
5	fitterEngineConfig:	
6		
7	engineType: minimizer	
8	<pre>minimizerConfig: "./input</pre>	s/fitter/configMinimizer.yaml"
9		
10	propagatorConfig:	
11		
12	llhStatFunction: "Barlo	wBeestonLLH"
13	#llhStatFunction: "Pois	sonLLH"
14		
15	dataSetList:	"./inputs/datasets/configDatasets.yaml
16	fitSampleSetConfig:	"./inputs/samples/configSamples.yaml"
17	parameterSetListConfig:	"./inputs/parameters/configParSet.yaml
18	plotGeneratorConfig:	"./inputs/output/configPlotGenerator.y
19	scanConfig:	"./inputs/output/configScan.yaml"

Note: illustrative only examples

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Note: External pre-compiled C++ libraries which belong to the inputs, not the code of GUNDAM itself





Applications

Applications

\sim src

- Generation gundamCalcXsec.cxx
- Generation gundamConfigCompare.cxx
- Generation gundamConfigUnfolder.cxx
- Generation gundamFitCompare.cxx
- General gundamFitReader.cxx
- GundamFitter.cxx
- Ge gundamInputZipper.cxx
- General gundamPlotExtractor.cxx

[GundamGreetings]: -	
[GundamGreetings]: W	Welcome to GUNDAM m
[GundamGreetings]: -	
[gundamFitter.cxx]:	> gundamFitter is
[gundamFitter.cxx]:	> guildum recor ro
[gundamFitter.cxx]:	> It takes a set o
[gundamFitter.cxx]:	> and initialize t
[gundamFitter.cxx]:	> Once ready, the
[gundamFitter.cxx]:	> produce a set of
[gundamFitter.cxx]:	Usage:
[gundamFitter.cxx]:	Main
[gundamFitter.cxx]:	<pre>configFile {-c,c</pre>
[gundamFitter.cxx]:	nbThreads {-t,nb
[gundamFitter.cxx]:	outputFilePath {-o
[gundamFitter.cxx]:	outputDir {out-d
[gundamFitter.cxx]:	randomSeed {-s,s
[gundamFitter.cxx]:	useDataEntry {us
	• • •
[gundamFitter.cxx]:	useDataConfig {u
[gundamFitter.cxx]:	injectParameterCon
[gundamFitter.cxx]:	appendix {append
[gundamFitter.cxx]:	Trigg
[gundamFitter.cxx]:	dry-run {dry-run
[gundamFitter.cxx]:	asimov {-a,asimo
[gundamFitter.cxx]:	enablePca {pca,-
[gundamFitter.cxx]:	skipHesse {skip-
[gundamFitter.cxx]:	<pre>skipSimplex {ski</pre>
[gundamFitter.cxx]:	generateOneSigmaP1
[gundamFitter.cxx]:	lightOutputMode {-
[gundamFitter.cxx]:	noDialCache {no-
[gundamFitter.cxx]:	ignoreVersionCheck
[gundamFitter.cxx]:	scanParameters {
[gundamFitter.cxx]:	scanLine {scan-l
[gundamFitter.cxx]:	<pre>toyFit {toy}: Ru</pre>
[gundamFitter.cxx]:	Runti
[gundamFitter.cxx]:	<pre>kickMc {kick-mc}</pre>
[gundamFitter.cxx]:	debugVerbose {de
[gundamFitter.cxx]:	usingCacheManager
[gundamFitter.cxx]:	usingGpu {gpu}:
[gundamFitter.cxx]:	forceDirect {cpu
[gundamFitter.cxx]:	overrides {-0,ov
[gundamFitter.cxx]:	overrideFiles {-of

ain fitter the main interface for the fitter. of inputs through config files and command line argument, he fitter engine. fitter minimize the likelihood function and plot saved in the output ROOT file. options config-file}: Specify path to the fitter config file (expected: 1 value) -threads}: Specify nb of parallel threads (expected: 1 value) ,--out-file}: Specify the output file (expected: 1 value) dir}: Specify the output directory (expected: 1 value) eed}: Set random seed (expected: 1 value) e-data-entry}: Overrides "selectedDataEntry" in dataSet config. Second arg is to select a given dataset (expected: use-data-config}: Add a data entry to the data set definition and use it for the fit (expected: 1 value) ofig {--inject-parameters}: Inject parameters defined in the provided config file (expected: 1 value) ix}: Add appendix to the output file name (expected: 1 value) er options — ,-d}: Perform the full sequence of initialization, but don't do the actual fit. (trigger) v}: Use MC dataset to fill the data histograms (trigger) -enable-pca}: Enable principle component analysis for eigen decomposed parameter sets (trigger) hesse}: Don't perform postfit error evaluation (trigger) ip-simplex}: Don't run SIMPLEX before the actual fit (trigger) .ots {--one-sigma}: Generate one sigma plots (trigger) -light-mode}: Disable plot generation (trigger) -dial-cache}: Disable cache handling for dial eval (trigger) {--ignore-version}: Don't check GUNDAM version with config request (trigger) -scan}: Enable parameter scan before and after the fit (can provide nSteps) (optional: 1 value) ine}: Provide par injector files: start and end point or only end point (start will be prefit) (optional: 2 values. un a toy fit (optional arg to provide toy index) (optional: 1 value) 🗲 me/debug options : Amount to push the starting parameters away from their prior values (default: 0) (optional: 1 value) bug}: Enable debug verbose (can provide verbose level arg) (optional: 1 value) {--cache-manager}: Toggle the usage of the CacheManager (i.e. the GPU) [empty, 'on', or 'off'] Use GPU parallelization (trigger) u}: Force direct calculation of weights (for debugging) (trigger) verride}: Add a config override [e.g. /fitterEngineConfig/engineType=mcmc) (expected: N values) ,--override-files}: Provide config files that will override keys (expected: N values)

Example: gundamFitter –c mainConfig.yaml –t 16 ––cache–manager –s 123 ––toy 1 –of configOverride.yaml



Documentation

- Short outline:
 - A general introduction
 - Installation guide
 - How to set up the configuration files with examples
 - Meaning of the entries of a configuration file
 - How to use the different applications
- Work in progress (almost by definition)

I don't need to read the documentation I can make it work !!!

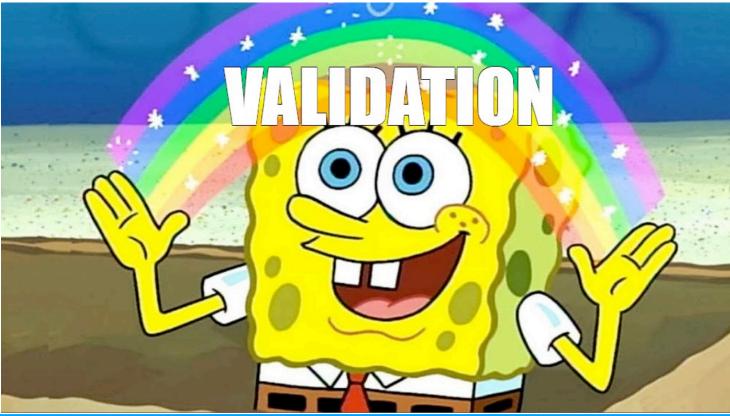






Testing and Validation

- Tests workflow implemented for a continuous validation
- testing with specialized script (running mock analysis and checking expectations)
- We have two type of tests running: unit tests with GoogleTest and executable Executable testing with specialized script can be divided in:
 - Fast: always run and used during continuous integration (eg. few-parameter fit)
 - Regular: quick tests that are not used for CI, but should be run locally before any PR (eg. response functions interpolation)
 - Extended: slower tests (eg. MCMC)
 - Slow: long validation tests (eg. more complex fit)
- Always looking for missing tests!!!











GUNDAM Oscillation Analysis Tools

- Oscillation probability calculation
 - Already using <u>Prob3++</u> but other libraries can be used
- OA functionality to be implemented:
 - Frequentist analysis, ie profiling:
 - Constant $\Delta \chi^2$ (fast fit), $\Delta \chi^2$ with FC, etc.
 - Bayesian analysis
 - Marginalization with MCMC
- Would like to test what has developed so far and continue
 - Wei Shi (SBU) pointed us toward inputs at this link used for DUNE PRISM
 - Guidance on the latest inputs DUNE-LBL WG is using would help us setting up our config files and add features to the code base if needed









Conclusions

- GUNDAM is a versatile, fully configurable and high-performance tool that can analyze high-dimensional models and binning
- Used for T2K OA-ND and cross-section analyses, but also ICARUS Collaborators are using it for a cross-section analysis
- Can contribute to DUNE LBL in many ways:
 - LBL and LBL+atm sensitivities
 - DUNE PRISM and "classical" ND sensitivities
 - Cross-section analyses (future)
 - Many other analyses
- GUNDAM Oscillation Analysis Tools work ongoing and we exploring the interests of other groups and individuals



Backup

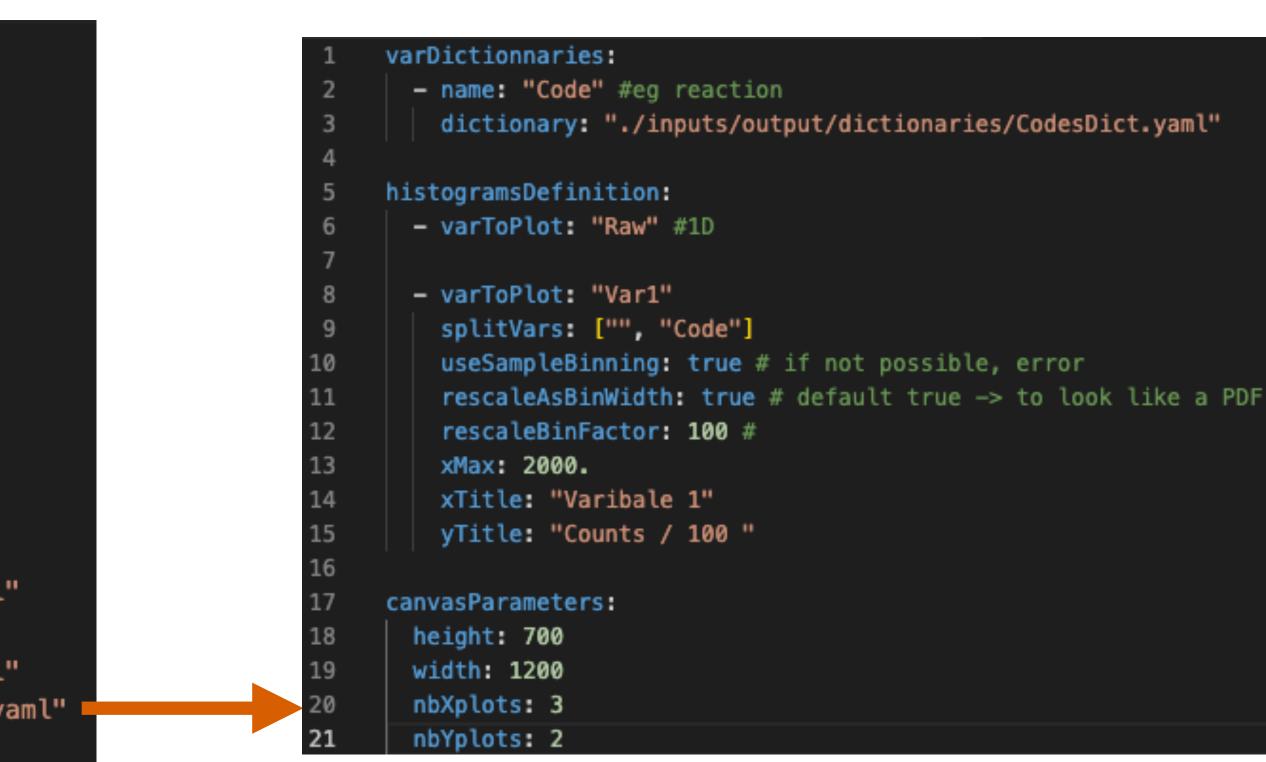


Plot generator

mainConfig.yaml

1	outputFolder: "./output"	
2	minGundamVersion: 1.8.4	
3		
4		
5	fitterEngineConfig:	
6		
7	engineType: minimizer	
8	<pre>minimizerConfig: "./input</pre>	s/fitter/configMinimizer.yaml"
9		
10 11 12 13 14 15	propagatorConfig:	
11		
12	llhStatFunction: "Barlo	wBeestonLLH"
13	#llhStatFunction: "Pois	sonLLH"
14		
15	dataSetList:	"./inputs/datasets/configDatasets.yaml
16	fitSampleSetConfig:	"./inputs/samples/configSamples.yaml"
17	<pre>parameterSetListConfig:</pre>	"./inputs/parameters/configParSet.yaml
18	plotGeneratorConfig:	"./inputs/output/configPlotGenerator.y
19	scanConfig:	"./inputs/output/configScan.yaml"

Note: illustrative only examples





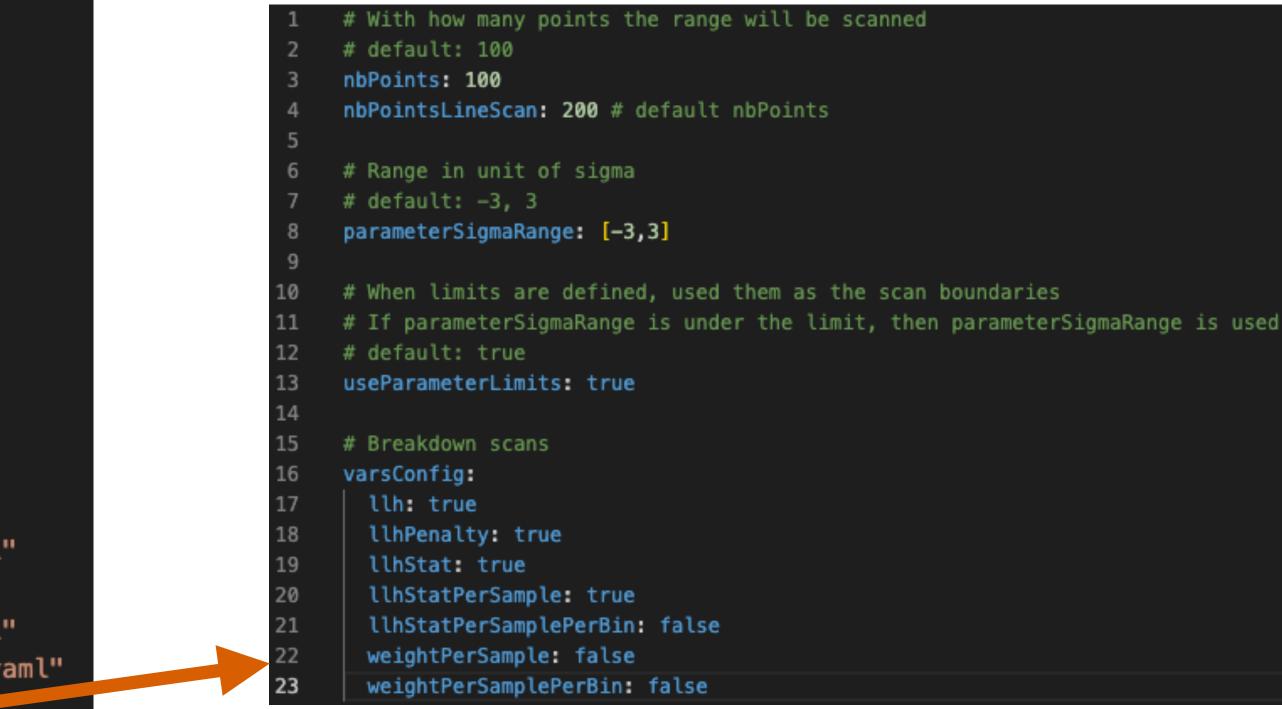


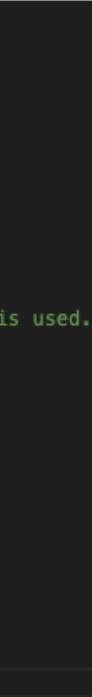
Likelihood scanning

mainConfig.yaml

1	outputFolder: "./output"		
2	minGundamVersion: 1.8.4		
3			
4			
5	fitterEngineConfig:		
6			
7	engineType: minimizer		
8	<pre>minimizerConfig: "./inputs/fitter/configMinimizer.yaml"</pre>		
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14			
15	dataSetList: "./inputs/datasets/configDatasets.yaml		
16	<pre>fitSampleSetConfig: "./inputs/samples/configSamples.yaml"</pre>		
17	<pre>parameterSetListConfig: "./inputs/parameters/configParSet.yaml</pre>		
18	<pre>plotGeneratorConfig: "./inputs/output/configPlotGenerator.y</pre>		
19	<pre>scanConfig: "./inputs/output/configScan.yaml"</pre>		

Note: illustrative only examples







Development policy

- For internal development an issue should be opened and it should happen in a dedicated branch with a descriptive name of the feature. We recommend the following tags:
 - fix/myFix: to address specific issues with the code
 - feature/myFeature: to add specific feature
 - doc/myDoc: for documentation additions
 - experimental/myBranch: for idea developments
- Change description (commit messages and PR) must be explicit and limited to a single issue
- Create a PR and merge after review and Cl is successfully completed External developers are encouraged following the same procedure as above (might fork the code)

