# **Publishing Statistical Models** — getting the most out of particle physics experiments —

**Sabine Kraml LPSC Grenoble** 

IRN Terascale @ LPC Clermont 22-24 Nov 2021

arXiv:2109.04981

# Introduction

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Primary measurements

Parameters of interest (POIs)

 $p(x, y | \mu, \theta) = p(x | \mu, \theta) p(y | \theta)$ 

auxiliary data

nuisance parameters

Describes the probabilistic dependence of the observable data on the parameters of interest and the nuisance parameters.

When observed data are entered into the stat. model, this becomes the likelihood function.

Probability density of the auxiliary data

The values y are often estimates of corresponding nuisance parameters, and their probability may be, e.g., a Gaussian with a specified standard deviation

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ameters of interest

In recent years, a lot of progress has been made regarding presentation of results, reinterpretation efforts, Open Data, etc.

Publication of the full statistical models is a logical next step to maximise the shelf life and the scientific return of exp. analyses; technical solutions exist to make this feasible.



# 202 Sep 10[hep-ph] arXiv:2109.04981v1

### Publishing statistical models: Getting the most out of particle physics experiments

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September 9, 2021

### Abstract

The statistical models used to derive the results of experimental analyses are of incredible scientific value and are essential information for analysis preservation and reuse. In this paper, we make the scientific case for systematically publishing the full statistical models and discuss the technical developments that make this practical. By means of a variety of physics cases — including parton distribution functions, Higgs boson measurements, effective field theory interpretations, direct searches for new physics, heavy flavor physics, direct dark matter detection, world averages, and beyond the Standard Model global fits — we illustrate how detailed information on the statistical modelling can enhance the short- and long-term impact of experimental results.

### Submission

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## - 2000 First PHYSTAT workshop [CERN 2000-005]

Unanimous agreement that particle physicists should publish likelihood functions, given their fundamental importance in extracting quantitative results from experimental data.

## - 2012 Les Houches Recommendations for the Presentation of LHC Results [arXiv:1203.2489]

**Recommendation 3b:** When feasible, provide a mathematical description of the final likelihood function in which experimental data and parameters are clearly distinguished, [....].

**Recommendation 3c:** Additionally provide a digitized implementation of the likelihood that is consistent with the mathematical description.

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### **ATLAS PUB Note**

ATL-PHYS-PUB-2019-029

21st October 2019



### **Reproducing searches for new physics with the ATLAS experiment through publication of full** statistical likelihoods

The ATLAS Collaboration

The ATLAS Collaboration is starting to publicly provide likelihoods associated with statistical fits used in searches for new physics on HEPData. These likelihoods adhere to a specification first defined by the HistFactory p.d.f. template. This note introduces a JSON schema that fully describes the HistFactory statistical model and is sufficient to reproduce key results from published ATLAS analyses. This is per-se independent of its implementation in ROOT and it can be used to run statistical analysis outside of the ROOT and RooStats/RooFit framework. The first of these likelihoods published on HEPData is from a search for bottom-squark pair production. Using two independent implementations of the model, one in ROOT and one in pure Python, the limits on the bottom-squark mass are reproduced, underscoring the implementation independence and long-term viability of the archived data.



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28 April 2021

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The ATLAS

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# LHC reinterpreters think long-term

**CERN Courier** 

 $\mathscr{L}$ ikelihoods

Made public likelihoods the predominant topic at the Reinterpretation Workshop last February



# Why it matters

w/o proper statistical model, a Gaussian approximation is forced onto the reuse of experimental results

$$\chi^{2}(\mu) = \frac{1}{N_{\text{dat}}} \sum_{ij=1}^{N_{\text{dat}}} \left( \mathcal{O}_{i}^{(\text{th})}(\mu) - \mathcal{O}_{i}^{(\text{exp})} \right) \left( \text{cov}^{-1} \right)_{ij} \left( \mathcal{O}_{j}^{(\text{th})}(\mu) - \mathcal{O}_{j}^{(\text{exp})} \right)$$

## **Issues**:

- Often lack of information on correlations
- Non-positive-definite cov. matrices on HEPData
- Lack of breakdown of correlated systematic sources
- Systematic uncertainties might not be Gaussian
- Different naming for systematic sources complicates  $\bullet$ combining processes
- Correlations between processes often not available

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### **Severely affects many areas:**

- Parton distribution functions
- Effective field theory fits
- Higgs physics
- Heavy flavour physics
- Limits on new particles
- Global averages
- **BSM Global fits**
- DM constraints

. . . . .

Examples discussed in arXiv:2109.04981



# **Some examples**

from the white paper and the hands-on workshop Nov 8-12

see paper and Indico for more

# Higgs Measurements — Limitations of Reconstructed LLHs

# **Example: ATLAS** $H \rightarrow ZZ \rightarrow 4\ell$ [ATLAS 2004.03447]

# **HiggsSignals** implementation

measurements • (12-bin STXS)

- experimental correlations
- theory correlations [2017 Scheme]









# **Jonas Wittbrodt**

**Publication of Statistical Models** Hands-on workshop 8-12 Nov 2021 https://indico.cern.ch/event/1088121/

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EFT fits involve Higgs, top, diboson, etc. data Need to choose which observables to use, to **avoid double-counting** Choices are **neither straightforward nor unique** 

# **Veronica Sanz on EFT fits**

Combination is important: each operator affects many observables beyond the LHC group separation



Ellis, Madigan, Mimasu, VS and You JHEP(21), 2012.02779

Publication of Statistical Models Hands-on workshop 8-12 Nov 2021 https://indico.cern.ch/event/1088121/



### Simple exercise for the white paper: just Higgs, compare single vs combined experimental results



# Veronica Sanz on EFT fits

When considering many observables at once: With a fixed set of cuts we can compute how the EFT coefficients correlate among different observables but lack information on how all these measurements correlate, even within each experiment (lumi, pdfs, jet resolution, ...)

**Signal** and **backgrounds** can both be affected by EFT effects, and background composition changes within the differential distribution whereas typical analyses assume BSM affects signal only.

"It is clear that with more information we would be able to push further these studies; aim is to find a **robust deviation**, which may not have a clear equivalent in one distribution/ individual channel."

> Publication of Statistical Models Hands-on workshop 8-12 Nov 2021 https://indico.cern.ch/event/1088121/





Assess impact in fit by transforming the original covariance matrix into a matrix with the **same** eigenvectors but with clipped eigenvalues below some cut-off: stable PDFs with much lower x<sup>2</sup>

Dataset	$N_{ m dat}$	$Z_{ m orig}$	$\chi^2_{ m orig}$	$\chi^2_{ m reg}$	
ATLAS W, Z 7 TeV CC ( $\mathcal{L} = 4.6 \text{ fb}^{-1}$ )	46	9.01	1.89	0.93	minimal modification of
ATLAS $W$ 8 TeV (*)	22	11.28	3.50	1.15	correlation model, large
CMS dijets 7 TeV	54	4.70	1.81	1.73	impact in fit quality,
ATLAS dijets 7 TeV	90	9.93	2.14	0.92	PDFs stable
CMS 3D dijets 8 TeV $(*)$	122	4.47	1.50	0.92	
		~			-

# **Juan Rojo on PDF fits**

Key component of predictions for particle, nuclear, and astro-particle experiments.

Address fundamental questions in QCD.

Publication of Statistical Models Hands-on workshop 8-12 Nov 2021 https://indico.cern.ch/event/1088121/







**Juan Rojo on PDF fits** 





# **Averages of measurements**

done by, e.g., the Particle Data Group (PDG) or the Heavy Flavor Averaging Group (HFLAV)

- Likelihood is reasonably well defined if a central value with symmetric uncertainties is quoted. In case of asymmetric uncertainties, assumptions have to be made about the shape of the likelihood function.
- If a limit on the parameter is published the situation is even worse. The likelihood function of the measurement is largely undefined.
- Correlations
  - between measurements by different collaborations
  - between measurements by the same collaboration with different methods or datasets

must be known if correct averages are to be produced. This information is often not or only partly available.





# Ways forward

# (Profile) likelihoods: very useful but not sufficient

- In the likelihood, the data is baked in
  - cannot evaluate likelihood on new data
  - cannot sample from the model (pseudo-data, toy MC)
- In profile likelihoods, nuisance parameter are fixed
  - cannot statistically combine profile likelihoods targeting parameters of interest if they share nuisances
  - cannot update constraint terms (auxiliary measurements)
- - risk of introducing dependencies which can result in a loss of information



# Reparametrization in terms of different parameters of interest is not always possible

parametrization in terms of quantities such as masses, cross sections, widths, branching fractions, etc., is often more useful than a parametrization in terms of theory-model (Lagrangian) parameters





# Publish the full statistical model

ideally in a serialized (written to a file) format that is both human-readable and machine-readable with a declarative specification that provides a mathematical definition of the model.

Lots of advantages:

- no loss of information
- full set of systematics
- full structure apparent
- long-term preservation and reuse
- simplified approaches still possible but developed / carried out in public





# **ATLAS took the leap**

... and started to publish plain-text serialisation of HistFactory workspaces in JSON format

Provides background estimates, changes under systematic variations, and observed data counts at the same fidelity as used in the experiment.

	Description	Modification	Constraint Term $c_{\chi}$
constrained	Uncorrelated Shape Correlated Shape Normalisation Unc. MC Stat. Uncertainty Luminosity	$\begin{aligned} \kappa_{scb}(\gamma_b) &= \gamma_b \\ \Delta_{scb}(\alpha) &= f_p \left( \alpha \middle  \Delta_{scb,\alpha=-1}, \Delta_{scb,\alpha=1} \right) \\ \kappa_{scb}(\alpha) &= g_p \left( \alpha \middle  \kappa_{scb,\alpha=-1}, \kappa_{scb,\alpha=1} \right) \\ \kappa_{scb}(\gamma_b) &= \gamma_b \\ \kappa_{scb}(\lambda) &= \lambda \end{aligned}$	$\begin{aligned} \prod_{b} \operatorname{Pois} \left( r_{b} = \sigma_{b}^{-2} \middle  \rho_{b} = \sigma_{b}^{-2} \gamma_{b} \right) \\ \operatorname{Gaus} \left( a = 0 \middle  \alpha, \sigma = 1 \right) \\ \operatorname{Gaus} \left( a = 0 \middle  \alpha, \sigma = 1 \right) \\ \prod_{b} \operatorname{Gaus} \left( a_{\gamma_{b}} = 1 \middle  \gamma_{b}, \delta_{b} \right) \\ \operatorname{Gaus} \left( l = \lambda_{0} \middle  \lambda, \sigma_{\lambda} \right) \end{aligned}$
free	Normalisation Data-driven Shape	$\begin{aligned} \kappa_{scb}(\mu_b) &= \mu_b \\ \kappa_{scb}(\gamma_b) &= \gamma_b \end{aligned}$	

Rate modifications defined in HistFactory for bin b, sample s, channel c.

- Usage: RooFit, **pyhf**
- Target: long-term data/analysis preservation, reinterpretation purposes

### ATL-PHYS-PUB-2019-029

Input
$\sigma_b$
$\Delta_{scb,\alpha=\pm 1}$
$\kappa_{scb,\alpha=\pm 1}$ $\delta_b^2 = \sum_s \delta_{sb}^2$ $\lambda_0, \sigma_\lambda$



Resources

### gz File

Archive of full likelihoods in the HistFactory JSON format described in ATL-PHYS-PUB-2019-029 Provided are 3 statiscal models labeled RegionA RegionB and RegionC respectively each in their own sub-directory. For each model the background-only model is found i the file named 'BkgOnly.json' For each model a set of patches for various signal points is provided

Download

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Likelihood availabl

Input  $\sigma_b$  $\Delta_{scb,\alpha=\pm 1}$  $\kappa_{scb,\alpha=\pm 1}$  $\delta_{h}^{2} = \sum_{s} \delta_{s}^{2}$  $\iota_0, \sigma_\lambda$ 

Search for charginos and neutralinos in all-hadronic final states	SUSY	Accepted by PRD	17-AUG-21	13
4-top xsec measurement	TOPQ	Accepted by JHEP	22-JUN-21	13
Search for gluinos, stops and electroweakinos in RPV models in final states with 1L and many jets	SUSY	Accepted by EPJC	17-JUN-21	13
Search for charginos and neutralinos in final states with 3L and MET	SUSY	Accepted by EPJC	03-JUN-21	13
Measurement of ttZ cross sections in Run 2	TOPQ	Eur. Phys. J. C 81 (2021) 737	23-MAR-21	13
Search for third-generation scalar leptoquarks decaying to a top quark and a tau lepton	EXOT	JHEP 06 (2021) 179	27-JAN-21	13
Search for squarks and gluinos in final states 1L, jets and MET	SUSY	Eur. Phys. J. C 81 (2021) 600	05-JAN-21	13
Search for charginos and neutralinos in RPV models in final states with 3L (or more)	SUSY	Phys. Rev. D 103, (2021) 112003	20-NOV-20	13
Search for displaced leptons	SUSY	Phys. Rev. Lett. 127 (2021) 051802	13-NOV-20	13
Search for squarks and gluinos in final states with 0L, jets and MET	SUSY	JHEP 02 (2021) 143	27-OCT-20	13
Measurement of the ttbar production cross-section in the lepton+jets channel at 13 TeV	TOPQ	Phys. Lett. B 810 (2020) 135797	24-JUN-20	13
Stop pair, long-lived; displaced vertex and displaced muon	SUSY	Phys. Rev. D 102 (2020) 032006	26-MAR-20	13
Chargino-neutralino pair; 3 leptons, weak-scale mass splittings	SUSY	Phys. Rev. D 101 (2020) 072001	18-DEC-19	13
Chargino-neutralino pair, slepton pair; soft leptons	SUSY	Phys. Rev. D 101 (2020) 052005	28-NOV-19	13
Staus; taus	SUSY	Phys. Rev. D 101 (2020) 032009	15-NOV-19	13
Chargino-neutralino pair; Higgs boson in final state, 2 b-jets and 1 lepton	SUSY	Eur. Phys. J. C 80 (2020) 691	19-SEP-19	13
Stop pair, sbottom pair, gluino pair; two same-sign leptons or three leptons	SUSY	JHEP 06 (2020) 46	18-SEP-19	13
Sbottom; b-jets	SUSY	JHEP 12 (2019) 060	08-AUG-19	13

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139 fb <sup>-1</sup>
136 fb <sup>-1</sup>
139 fb <sup>-1</sup>

# Usage in BSM tools





# reinterpretation becomes JSON patching

Illustration from talk by Lukas Heinrich Hands-on workshop 8 Nov 2021



# **Usage in BSM tools**





# reinterpretation becomes JSON patching

SM

Illustration from talk by Lukas Heinrich Hands-on workshop 8 Nov 2021

Interfaced to pyhf since SModelS v1.2.4 (now v2.1) G. Alguero, SK, W. Waltenberger, arXiv:2009.01809



# **Usage in BSM tools**



G. Alguero, J. Araz, B. Fuks, SK,

Functionality available v1.9 onward, paper in progress



# reinterpretation becomes JSON patching

SH

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## ATLAS Run 2 results in SModelS 2.1.0 database

ID	Short Description	$\mathcal{L}$ [fb <sup>-1</sup> ]	$\mathbf{UL}_{\mathrm{obs}}$	UL
ATLAS-SUSY-2015-01 [62]	2 <i>b</i> -jets	3.2	$\checkmark$	
ATLAS-SUSY-2015-02 [63]	$1\ell$ stop	3.2	$\checkmark$	
ATLAS-SUSY-2015-06 [64]	$0\ell+2-6~{ m jets}$	3.2		
ATLAS-SUSY-2015-09 [65]	$\mathrm{jets}+2~\mathrm{SS}~\mathrm{or}\geq 3\ell$	3.2	$\checkmark$	
ATLAS-SUSY-2016-06 [66]	disappearing tracks	36.1		
ATLAS-SUSY-2016-07 [67]	$0\ell+ ext{jets}$	36.1	$\checkmark$	
ATLAS-SUSY-2016-08 [68]	displaced vertices	32.8	$\checkmark$	
ATLAS-SUSY-2016-14 [69]	$2~{ m SS}~{ m or}~3~\ell{ m 's}+{ m jets}$	36.1	$\checkmark$	
ATLAS-SUSY-2016-15 [70]	$0\ell$ stop	36.1	$\checkmark$	
ATLAS-SUSY-2016-16 [71]	$1\ell$ stop	36.1	$\checkmark$	
ATLAS-SUSY-2016-17 [72]	2 OS leptons	36.1	$\checkmark$	
ATLAS-SUSY-2016-19 [73]	$2 \ b ext{-jets} +  au ext{'s}$	36.1	$\checkmark$	
ATLAS-SUSY-2016-24 [74]	$23 \ \ell$ 's, EWino	36.1	$\checkmark$	
ATLAS-SUSY-2016-26 [75]	$\geq 2 c$ -jets	36.1	$\checkmark$	
ATLAS-SUSY-2016-27 [76]	$\mathrm{jets}+\gamma$	36.1	$\checkmark$	
ATLAS-SUSY-2016-28 [77]	2 b-jets	36.1	$\checkmark$	
ATLAS-SUSY-2016-32 [44]	HSCP	31.6	$\checkmark$	<b>↓</b> √
ATLAS-SUSY-2016-33 [78]	2 OSSF $\ell$ 's	36.1	$\checkmark$	
ATLAS-SUSY-2017-01 [79]	WH(bb), EWino	36.1	$\checkmark$	
ATLAS-SUSY-2017-02 [80]	$0\ell +  ext{jets}$	36.1	$\checkmark$	<b>↓</b> √
ATLAS-SUSY-2017-03 [21]	multi- $\ell$ EWino	36.1	$\checkmark$	
ATLAS-SUSY-2018-04 [81]	2 hadronic taus	139.0	$\checkmark$	
ATLAS-SUSY-2018-06 [22]	3 leptons, EWino	139.0	$\checkmark$	<b>↓</b> √
ATLAS-SUSY-2018-10 [17]	$1\ell +  ext{jets}$	139.0	$\checkmark$	
ATLAS-SUSY-2018-12 [19]	$0\ell+\mathrm{jets}$	139.0	$\checkmark$	<b>↓</b> √
ATLAS-SUSY-2018-14 [15]	displaced leptons	139.0		
ATLAS-SUSY-2018-22 [18]	multi-jets	139.0	$\checkmark$	
ATLAS-SUSY-2018-23 [20]	$WH(\gamma\gamma)$ , EWino	139.0	$\checkmark$	<b>↓</b>
ATLAS-SUSY-2018-31 [82]	2b+2H(bb)	139.0	$\checkmark$	
ATLAS-SUSY-2018-32 [59]	2 OS leptons	139.0	$\checkmark$	
ATLAS-SUSY-2019-08 [60]	$1\ell + H(bb),  { m EWino}$	139.0	$\checkmark$	





## Efficiency maps for 17 analyses, 10 with full Run 2 luminosity 4 with full likelihoods (more to come)



Resources

### gz File

Archive of full likelihoods in the HistFactory JSON format described in ATL-PHYS-PUB-2019-029 Provided are 3 statiscal models labeled RegionA RegionB and RegionC respectively each in their own sub-directory. For each model the background-only model is found i the file named 'BkgOnly.json' For each model a set of patches for various signal points is provided

Download



5

1S ises

# ATLAS' bkg-only models in SModelS

NB the signal patches also provided by ATLAS turn out to be highly useful for extracting A×ε maps needed by SModelS



## Statistical combination of signal regions is important → much better agreement with official limits

For signal region combination within a given analysis, a simplified likelihood would be sufficient and much faster. However, eventually we want to do more than that (next slide)















# Looking for dispersed signals

- In 2012.12246: prototype statistical learning algorithm to
  - identify potential dispersed signals in the LHC data
  - fit "proto-models" (new particles, decay modes, signal strengths) to them while remaining compatible with the entirety of LHC results in the SModelS database
- Based on simplified model results  $\rightarrow$  exploits SModelS functionality and database
- Construct a global likelihood as product of likelihoods of approximately uncorrelated analyses
- To determine a global p-value for the SM, we produce "fake" SModelS databases by sampling background models (i.e. setting <#observed>=#expected, sampled within BG uncertainties)

Could also be applied to look for consistent small deviations in SM measurements, EFT interpretation, etc. Correct statistical modelling is crucial







Waltenberger, Lessa, SK, arXiv:2012:12246

# Conclusions

- The available details on the statistical model may heavily affect the short- and long-term impacts of any measurement.
- Use cases are a clear call to action.

An immediate action that can be taken by the community:

publish all the associated RooWorkspaces or

- for binned statistical models based on the HistFactory specification, publish the models in the pyhf JSON format.
- If adopted, will lead to more and higher-quality, science. Huge impact.

Longer-term developments are certainly needed to enhance, streamline, and facilitate the use of published statistical models. However, the publication of the currently available statistical models would already be a watershed development in the field, one we hope the community is ready to embrace.





## From the white paper summary

An immediate action that can be taken by the community:

- (i) publish all the associated RooWorkspaces or
- (ii) for binned statistical models based on the HistFactory specification, publish the models in the pyhf JSON format.

published models user-friendly, efficient, and effective.

one we hope the community is ready to embrace.

- This would provide the impetus for the development of tools to make the use of the
- Longer-term developments are certainly needed to enhance, streamline, and facilitate the use of published statistical models. However, the publication of the currently available statistical models would already be a watershed development in the field,



## Challenges and outstanding issues; cf. white paper sect. 5

- Systematic naming conventions for (nuisance) parameters
   facilitate combinations
- Serialisation of statistical models beyond HistFactory
   e.g., CMS Combine tool
- Strategies and public tools for pruning, simplification and/or partial profiling of the full model when runtime is an issue
   model surveys, global fits
- Systematic use in theory community; extension of fitting procedures and tools that currently assume Gaussian error sources
   → e.g. PDF, EFT fits
- Errors on errors

▶ ...

Exciting developments ahead



# HistFactory/pyhf JSON format

```
"observations": [
                                                             [....]
 "channels": [
                                                                       "data": {
                                                                                                                                                   "data": [
. . . .
                                                                        "hi": 0.997066,
                                                                                                                                                    72
    "name": "SR1cut_cuts",
                                                                        "lo": 1.00293
                                                                                                                                                   "name": "QCR1cut_cuts"
    "samples": [
                                                                      "name": "JET_JER_EffectiveNP_Rest",
                                                                       "type": "normsys"
       "data": [
        1.3658181428909302
                                                                                                                                                    "data": [
                                                                                                                                                     27
      "modifiers": [
                                                                       "data": {
                                                                                                                                                   "name": "QCR2cut_cuts"
                                                                        "hi": 0.998218,
         "data": null,
                                                                        "lo": 1.00178
         "name": "lumi",
         "type": "lumi"
                                                                      "name": "MET_SoftTrk_ResoPara",
                                                                                                                                                    "data":
                                                                       "type": "normsys"
                                                                                                                                                    10
         "data": [
                                                                                                                                                   "name": "SR1cut_cuts"
          0.32472213661884547
                                                                       "data": {
                                                                        "hi": 1.01429,
         "name": "staterror_SR1cut_cuts",
                                                                        "lo": 0.985706
                                                                                                                                                    "data":
         "type": "staterror"
                                                                      "name": "MET_SoftTrk_ResoPerp",
                                                                       "type": "normsys"
                                                                                                                                                    "name": "SR2cut_cuts"
         "data": {
          "hi": 1.02838,
                                                             [....]
          "lo": 0.972354
                                                                                                                                                    "data":
                                                                                                                                                    1099
         "name": "PRW_DATASF",
                                                                                                                                                   1
         "type": "normsys"
                                                                                                                                                   "name": "WCRcut_cuts"
[....]
                                                                                                                                                 "version": "1.0.0"
                                                                       IRN Terascale @ LPC Clermont, 22-24 Nov 2021
```

