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JuliaHEP 2023 Workshop

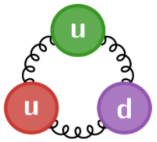
Summary

6–9 Nov 2023

ECAP (Erlangen Centre for Astroparticle Physics)

Ianna Osborne

HSF
HEP Software Foundation



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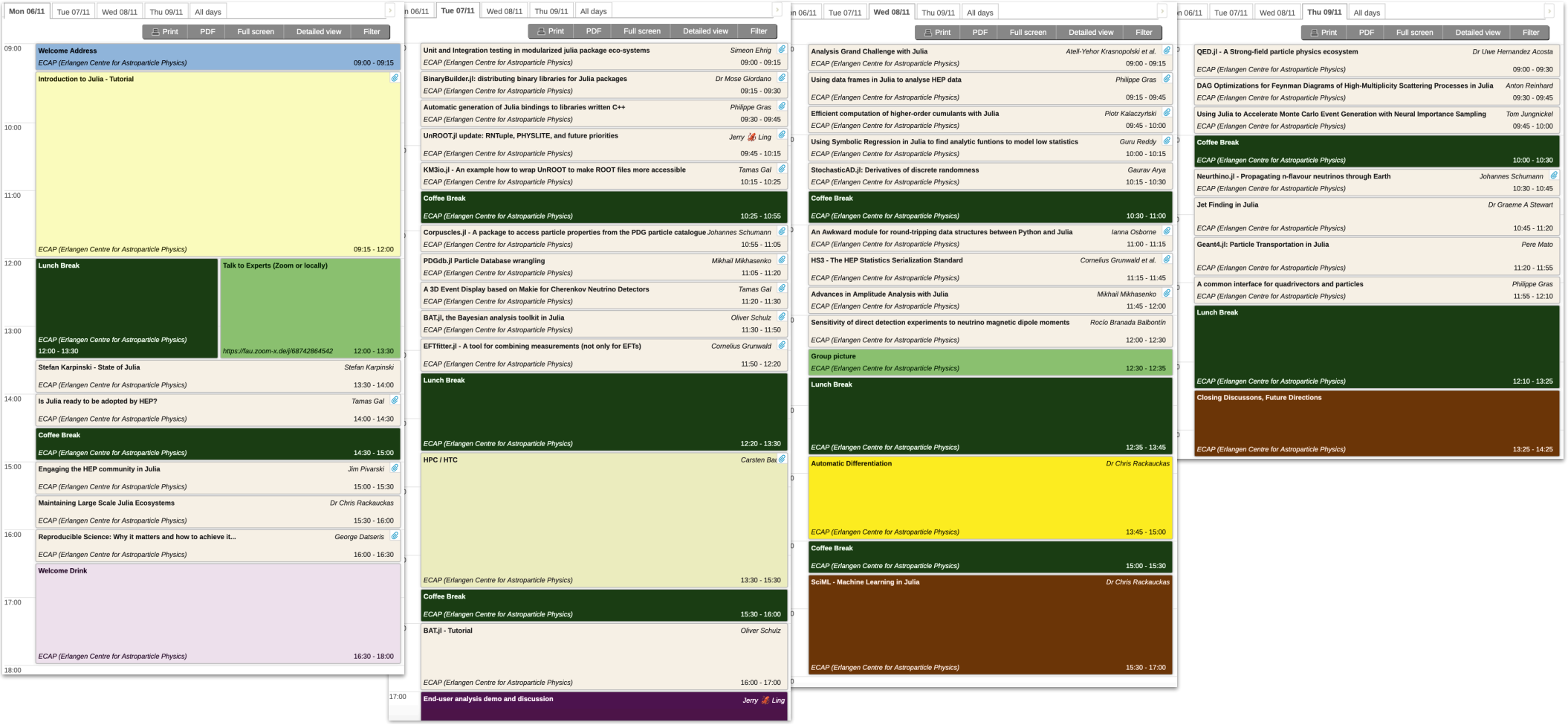
Workshop Agenda



Mon 06/11 | Tue 07/11 | Wed 08/11 | Thu 09/11 | All days

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09:00
- **Welcome Address** — ECAP (Erlangen Centre for Astroparticle Physics) 09:00 - 09:15
- **Introduction to Julia - Tutorial** — ECAP (Erlangen Centre for Astroparticle Physics) 09:15 - 12:00

10:00

11:00

12:00
- **Lunch Break** — ECAP (Erlangen Centre for Astroparticle Physics) 12:00 - 13:30
- **Talk to Experts (Zoom or locally)** — https://lau.zoom-x.de/j/68742864542 12:00 - 13:30

13:00
- **Stefan Karpinski - State of Julia** *Stefan Karpinski* — ECAP (Erlangen Centre for Astroparticle Physics) 13:30 - 14:00

14:00
- **Is Julia ready to be adopted by HEP?** *Tamas Gal* — ECAP (Erlangen Centre for Astroparticle Physics) 14:00 - 14:30
- **Coffee Break** — ECAP (Erlangen Centre for Astroparticle Physics) 14:30 - 15:00

15:00
- **Engaging the HEP community in Julia** *Jim Pivarski* — ECAP (Erlangen Centre for Astroparticle Physics) 15:00 - 15:30
- **Maintaining Large Scale Julia Ecosystems** *Dr Chris Rackauckas* — ECAP (Erlangen Centre for Astroparticle Physics) 15:30 - 16:00

16:00
- **Reproducible Science: Why it matters and how to achieve it...** *George Datseris* — ECAP (Erlangen Centre for Astroparticle Physics) 16:00 - 16:30
- **Welcome Drink** — ECAP (Erlangen Centre for Astroparticle Physics) 16:30 - 18:00

17:00

18:00

Mon 06/11 | Tue 07/11 | Wed 08/11 | Thu 09/11 | All days

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- **Unit and Integration testing in modularized julia package eco-systems** *Simeon Ehrig* — ECAP (Erlangen Centre for Astroparticle Physics) 09:00 - 09:15
- **BinaryBuilder.jl: distributing binary libraries for Julia packages** *Dr Mose Giordano* — ECAP (Erlangen Centre for Astroparticle Physics) 09:15 - 09:30
- **Automatic generation of Julia bindings to libraries written C++** *Philippe Gras* — ECAP (Erlangen Centre for Astroparticle Physics) 09:30 - 09:45
- **UnROOT.jl update: RNTuple, PHYSLITE, and future priorities** *Jerry Ling* — ECAP (Erlangen Centre for Astroparticle Physics) 09:45 - 10:15
- **KM3io.jl - An example how to wrap UnROOT to make ROOT files more accessible** *Tamas Gal* — ECAP (Erlangen Centre for Astroparticle Physics) 10:15 - 10:25
- **Coffee Break** — ECAP (Erlangen Centre for Astroparticle Physics) 10:25 - 10:55
- **Corpuscles.jl - A package to access particle properties from the PDG particle catalogue** *Johannes Schumann* — ECAP (Erlangen Centre for Astroparticle Physics) 10:55 - 11:05
- **PDGdb.jl Particle Database wrangling** *Mikhail Mikhasenko* — ECAP (Erlangen Centre for Astroparticle Physics) 11:05 - 11:20
- **A 3D Event Display based on Makie for Cherenkov Neutrino Detectors** *Tamas Gal* — ECAP (Erlangen Centre for Astroparticle Physics) 11:20 - 11:30
- **BAT.jl, the Bayesian analysis toolkit in Julia** *Oliver Schulz* — ECAP (Erlangen Centre for Astroparticle Physics) 11:30 - 11:50
- **EFTfitter.jl - A tool for combining measurements (not only for EFTs)** *Cornelius Grunwald* — ECAP (Erlangen Centre for Astroparticle Physics) 11:50 - 12:20
- **Lunch Break** — ECAP (Erlangen Centre for Astroparticle Physics) 12:20 - 13:30
- **HPC / HTC** *Carsten Ba* — ECAP (Erlangen Centre for Astroparticle Physics) 13:30 - 15:30
- **Coffee Break** — ECAP (Erlangen Centre for Astroparticle Physics) 15:30 - 16:00
- **BAT.jl - Tutorial** *Oliver Schulz* — ECAP (Erlangen Centre for Astroparticle Physics) 16:00 - 17:00
- **End-user analysis demo and discussion** *Jerry Ling*

Mon 06/11 | Tue 07/11 | Wed 08/11 | Thu 09/11 | All days

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- **Analysis Grand Challenge with Julia** *Atell-Yehor Krasnopolski et al.* — ECAP (Erlangen Centre for Astroparticle Physics) 09:00 - 09:15
- **Using data frames in Julia to analyse HEP data** *Philippe Gras* — ECAP (Erlangen Centre for Astroparticle Physics) 09:15 - 09:45
- **Efficient computation of higher-order cumulants with Julia** *Piotr Kalaczyński* — ECAP (Erlangen Centre for Astroparticle Physics) 09:45 - 10:00
- **Using Symbolic Regression in Julia to find analytic funtions to model low statistics** *Guru Reddy* — ECAP (Erlangen Centre for Astroparticle Physics) 10:00 - 10:15
- **StochasticAD.jl: Derivatives of discrete randomness** *Gaurav Arya* — ECAP (Erlangen Centre for Astroparticle Physics) 10:15 - 10:30
- **Coffee Break** — ECAP (Erlangen Centre for Astroparticle Physics) 10:30 - 11:00
- **An Awkward module for round-tripping data structures between Python and Julia** *Ianna Osborne* — ECAP (Erlangen Centre for Astroparticle Physics) 11:00 - 11:15
- **HS3 - The HEP Statistics Serialization Standard** *Cornelius Grunwald et al.* — ECAP (Erlangen Centre for Astroparticle Physics) 11:15 - 11:45
- **Advances in Amplitude Analysis with Julia** *Mikhail Mikhasenko* — ECAP (Erlangen Centre for Astroparticle Physics) 11:45 - 12:00
- **Sensitivity of direct detection experiments to neutrino magnetic dipole moments** *Rocío Branada Balbontín* — ECAP (Erlangen Centre for Astroparticle Physics) 12:00 - 12:30
- **Group picture** — ECAP (Erlangen Centre for Astroparticle Physics) 12:30 - 12:35
- **Lunch Break** — ECAP (Erlangen Centre for Astroparticle Physics) 12:35 - 13:45
- **Automatic Differentiation** *Dr Chris Rackauckas* — ECAP (Erlangen Centre for Astroparticle Physics) 13:45 - 15:00
- **Coffee Break** — ECAP (Erlangen Centre for Astroparticle Physics) 15:00 - 15:30
- **SciML - Machine Learning in Julia** *Dr Chris Rackauckas* — ECAP (Erlangen Centre for Astroparticle Physics) 15:30 - 17:00

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- **QED.jl - A Strong-field particle physics ecosystem** *Dr Uwe Hernandez Acosta* — ECAP (Erlangen Centre for Astroparticle Physics) 09:00 - 09:30
- **DAG Optimizations for Feynman Diagrams of High-Multiplicity Scattering Processes in Julia** *Anton Reinhard* — ECAP (Erlangen Centre for Astroparticle Physics) 09:30 - 09:45
- **Using Julia to Accelerate Monte Carlo Event Generation with Neural Importance Sampling** *Tom Jungnickel* — ECAP (Erlangen Centre for Astroparticle Physics) 09:45 - 10:00
- **Coffee Break** — ECAP (Erlangen Centre for Astroparticle Physics) 10:00 - 10:30
- **Neurthino.jl - Propagating n-flavour neutrinos through Earth** *Johannes Schumann* — ECAP (Erlangen Centre for Astroparticle Physics) 10:30 - 10:45
- **Jet Finding in Julia** *Dr Graeme A Stewart* — ECAP (Erlangen Centre for Astroparticle Physics) 10:45 - 11:20
- **Geant4.jl: Particle Transportation in Julia** *Pere Mato* — ECAP (Erlangen Centre for Astroparticle Physics) 11:20 - 11:55
- **A common interface for quadrivectors and particles** *Philippe Gras* — ECAP (Erlangen Centre for Astroparticle Physics) 11:55 - 12:10
- **Lunch Break** — ECAP (Erlangen Centre for Astroparticle Physics) 12:10 - 13:25
- **Closing Discussons, Future Directions** — ECAP (Erlangen Centre for Astroparticle Physics) 13:25 - 14:25

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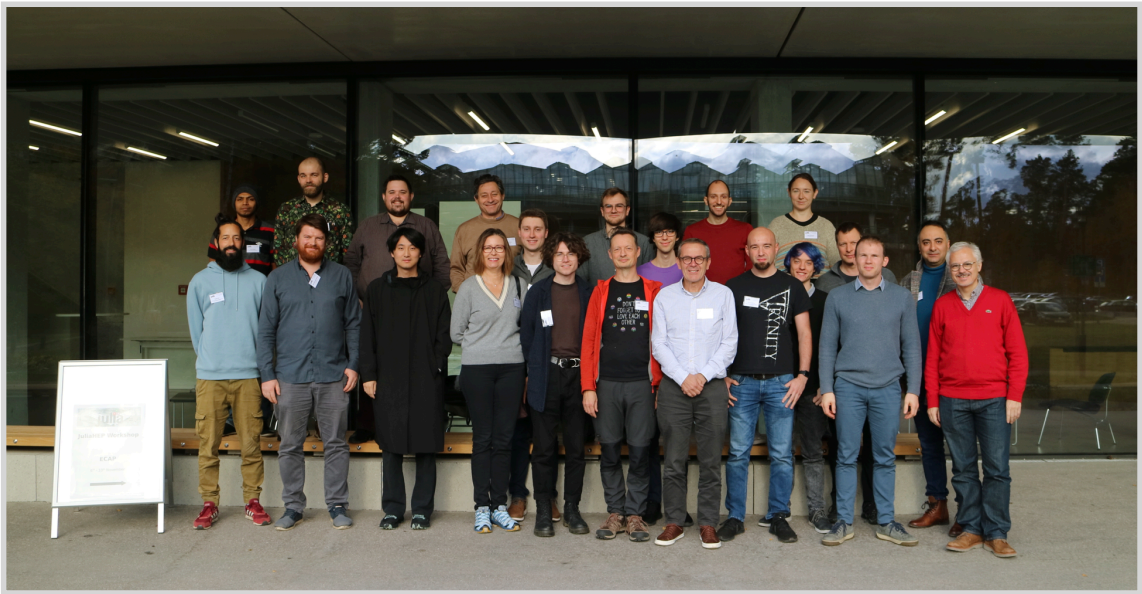
Workshop Key Themes

- Day 1 (Nov 6):
  - Welcome and Julia Tutorial
  - Insights from **Stefan Karpinski** on the State of Julia
  - Exploring Julia's Potential in High Energy Physics Computing
- Day 2 (Nov 7):
  - Testing, Binary Building, and Julia Bindings
  - Updates on UnROOT.jl and Package Showcases
  - HPC/HTC and End-User Analysis Tutorial
- Day 3 (Nov 8):
  - Grand Challenge, Data Frames, and Visualization in Julia
  - Reproducible Science and **Julia in Differentiation**
  - Focus on **Scientific Machine Learning** (SciML)
- Day 4 (Nov 9):
  - Particle Physics Ecosystem in Julia
  - Optimization Strategies and Monte Carlo Event Generation
  - Neutrino Propagation, Jet Finding, and Geant4.jl

over 200 participants registered
~ 60 attending each day



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Exploring Julia's Potential in HEP

julia

FAU Friedrich-Alexander-Universität Erlangen-Nürnberg

ECAP ERLANGEN CENTRE FOR ASTROPARTICLE PHYSICS

Is Julia ready to be adopted by HEP?

JuliaHEP 2023 - ECAP
06. - 09. November 2023

Tamas Gal – Erlangen Centre for Astroparticle Physics

https://indico.cern.ch/event/1292759/contributions/5614633/

Philippe Gras (IRFU, CEA, Université Paris-Saclay, Gif-sur-Yvette, France), **Pere Mato** (CERN, Switzerland), **Jerry Ling** (Harvard University), **Oliver Schulz** (TU Dormund, Germany), **Uwe Hernandez Acosta** (CASUS, Görlitz, Germany), **Graeme A Stewart** (CERN, Switzerland)

Interfacing legacy code

- Many high-quality, **mature libraries** for numerical computing written in C and Fortran were developed and optimised over **the past decades**
- Julia supports **native call** (without any glue code) **into C and Fortran** libraries (via the built-in `ccall()` function)
- **C++** wrapping available via external packages like **CxxWrap.jl**
- **Zero-overhead Python** wrapping (**PyCall.jl**)
- An honorable mention for a **fully wrapped HEP** software
  - **Geant4.jl** (fully wrapped using CxxWrap.jl) Join the talk from Pere Mato on Thursday at 11:20: https://indico.cern.ch/event/1292759/contributions/5613048/
  - https://github.com/JuliaHEP/Geant4.jl

12

Summary

- We think that the **two-language problem needs** more attention and a **fundamentally different approach than** creating more and more **Python extensions and libraries**
- **Julia** is an **excellent language for scientific computing** with **high potential for HEP**
- **HEP specific needs** are very **well covered** by Julia
- **Code sharing** and **extending** foreign packages **are a no-brainer**, thanks to the package distribution system and the **multiple dispatch** design
- **Distributed and parallel computing** are first-class citizens in Julia
- Join the **JuliaHEP GitHub** organisation: https://github.com/JuliaHEP

18

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Engaging the HEP community in Julia

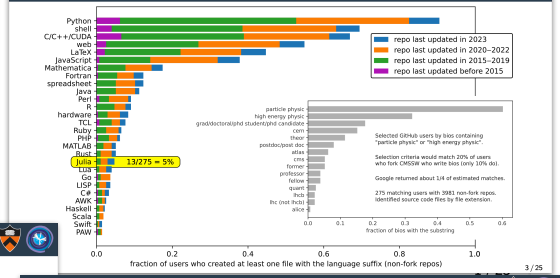
Jim Pivarski

As we've seen, Julia is a perfect fit for HEP, technologically.

- It allows for an exploratory phase, in which the data analyst focuses on *what* to compute, rather than how it will be accelerated.
- It allows the exploratory code to be tweaked to scale up to large datasets.

There is a *gradual path* from brainstorming to optimized code, not a rewrite.

State of language use by particle physicists as of last Friday



3 / 25

Julia is not yet "adopted" in HEP, but it is getting more attention than any other rival to C++ and Python.

From here, it could continue to rise in prominence or end up passing as a fad. *This is a critical time.*

Conclusions

We need stronger connections between HEP analysis tools in Python and HEP analysis tools in Julia.

- StatsBase.Histogram/FHist.jl generalization that is interchangeable with scikit-hep/boost-histogram, scikit-hep/hist?
- LorentzVectors.jl or LorentzVectorHEP.jl: interop with scikit-hep/vector?
- Corpuscles.jl: share data with scikit-hep/particle?
- IMinuit.jl √
- zfit, pyhf, cabinetry, Coffea, etc.?

Encourage Python users to use Julia *with* their Python/C++ code!
(Otherwise, they won't use it at all.)

25 / 25

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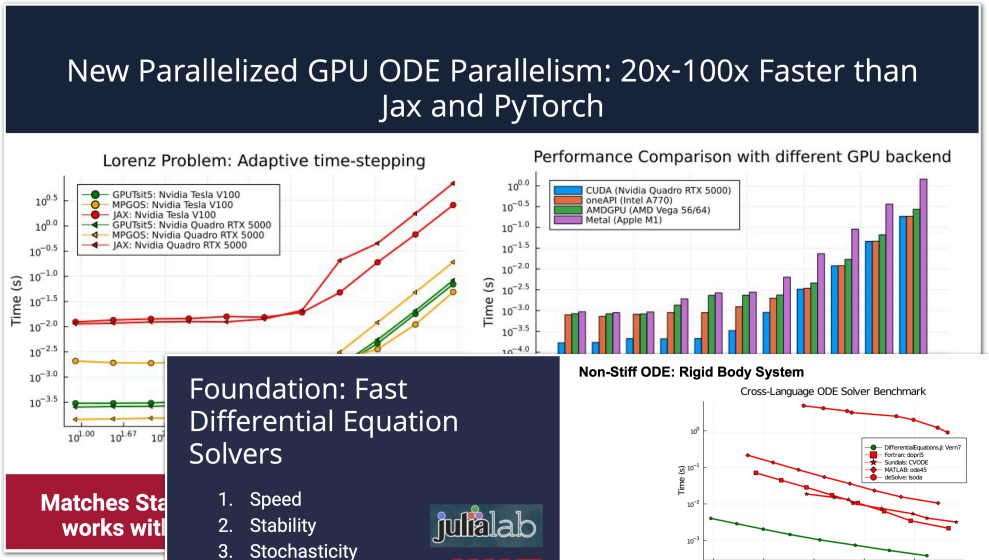
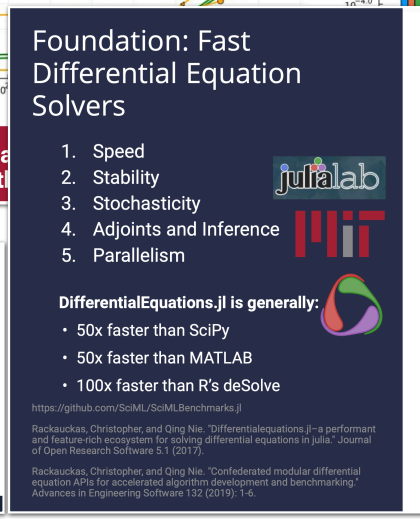
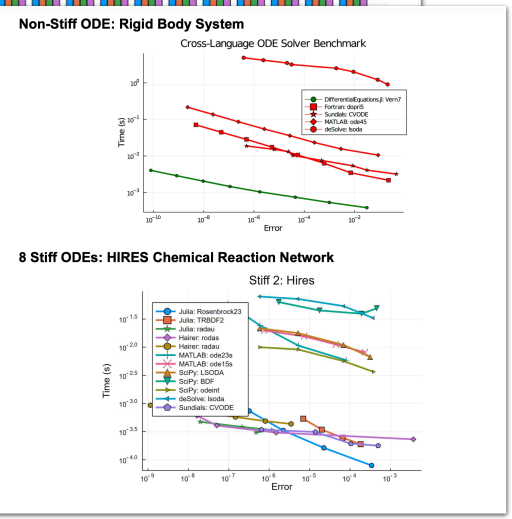
Maintaining Large Scale Julia Ecosystems

- Discussion on the challenges and strategies for sustaining large-scale Julia ecosystems

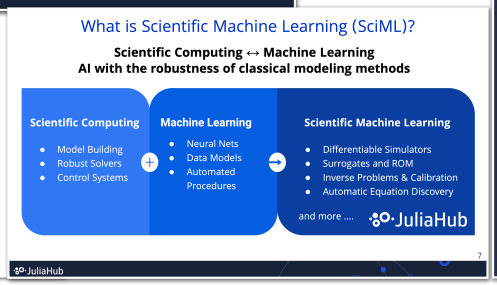






Building an ecosystem is a large project over many years. In this talk I'll share

- **Opinions**: built with time and experience
- **Practice**: some Julia-specific tips for improving maintainability
- **Tools**: you cannot do it all by yourself



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Testing, Building, Integration

Unit and Integration testing in modularized Julia package eco-systems

CASUS CENTER FOR ADVANCED SYSTEMS UNDERSTANDING

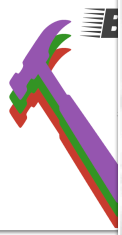
Simeon Ehrig

www.casus.science

HZDR · TECHNISCHE UNIVERSITÄT DRESDEN · CBG · UFZ HELMHOLTZ · Universytet Wrocławski · Federal Ministry of Education and Research · SACHSEN

BinaryBuilder.jl

Distributing binary libraries for Julia packages



Mosè Giordano @ Julia HEP 2023

BinaryBuilder.jl — Summary

- Helps you cross-compile binaries for a large number of systems
- Automatically catches portability issues, and in many cases correct them
- Its integration with Pkg and Artifacts system provides an end-to-end solution for building and deploying binaries for public packages

Further reading:

- BinaryBuilder website: https://binarybuilder.org
- BinaryBuilder recipes: https://github.com/JuliaPackaging/Yggdrasil
- JLL packages: https://github.com/JuliaBinaryWrappers

Lessons Learned

- Start implementing (automatic) testing as early as possible
- Think about your development workflow
- Develop your CI pipeline incrementally
- Prepare yourself that your CI concept has gaps

Update: The algorithm for searching for package dependencies becomes a separate package: https://github.com/QEDjl-project/IntegrationTests.jl

Julia-HEP workshop 2023, Nov 6-9, 2023

Automatic generation of Julia bindings to libraries written C++

Philippe Gras

IRFU, CEA, Université Paris-Saclay, France

Nov 6-9, 2023

cea irfu

Summary

- Prototype developed to test automatic generation of Julia bindings for C++ based on CxxWrap.
- It demonstrates the feasibility of such automation.
- Well advanced. More development needed to leverage the prototype to a production tool with full support of C++ templates.
- Used to provide a Julia interface to Geant4! See Pere Mato's Talk on Thursday.

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Analysis Grand Challenge

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UNI WÜ

julia

Julia for AGC

Atell-Yehor Krasnopolski
IRIS-HEP Fellow
Universität Würzburg

Jerry Ling
Harvard University

Alexander Held
UWM

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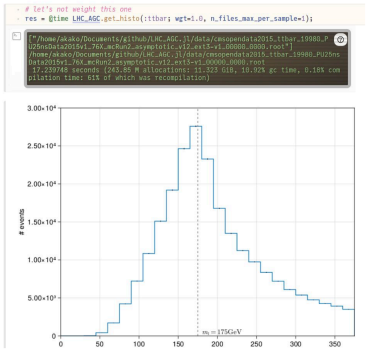
10



Atell-Yehor Krasnopolski *Julia for AGC*

UnROOT.jl Past, Now, Future

Jerry Ling[1] Tamás Gál[2]

Nov. 07, 2023

[1]Harvard Univseristy/ATLAS

Future 2: Quality of Life in Analysis

Over the 2023 summer, Alex Held and I supervised an IrisHEP Fellow project — Analysis Grand Challenge in Julia(LHC_AGC.jl)[8].

Atell and I realized that, although we wrote less boilerplate in Julia, it's far from perfect. Obvious wish list: declarative systematics branches, automatic histogram variations, built-in cutflow etc.

Discussion: What's a composable interface without a performance hit? What "package" should these live in?

[8]See Atell-Yehor Krasnopolski's talk

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Data Analysis

technische universität dortmund

EFTfitter.jl - A tool for combining & interpreting measurements

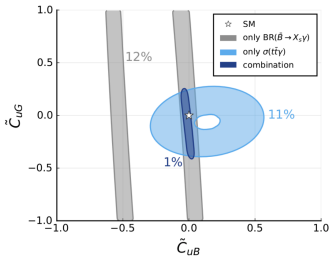
(not only for EFTs)

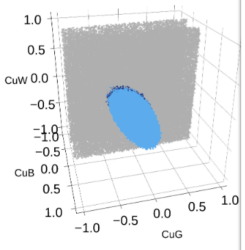
Cornelius Grunwald
TU Dortmund University

Julia HEP Workshop 2023
November 7th, 2023

What is EFTfitter ?

Tool to **constrain free model parameters** by **combining** multiple **measurements** (having **uncertainties** & **correlations**) of different **observables** and **comparing to** model **predictions**!





EPJC 80 (2020) 2, 136 [arXiv: 1909.13632]

What is EFTfitter ?

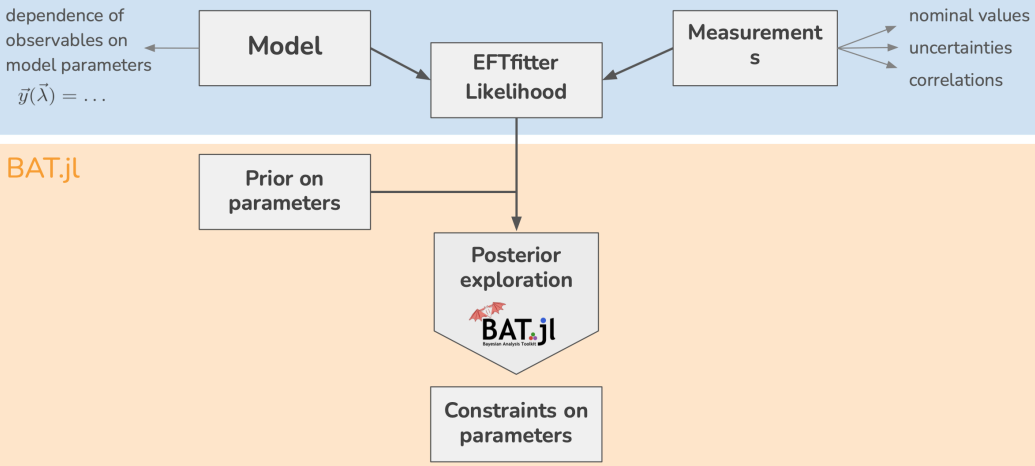
- tool for the statistical combination & interpretation of measurements
- well suited for EFT interpretations, but not restricted to this field of applications

What it does:

- combines measurements of the same or of different observables
- uses a Bayesian approach for inference on model parameters & uncertainty propagation
- provides access to the full posterior distribution of the model parameters (via BAT.jl)
- emphasis on correct statistical treatment of uncertainties & correlations
- allows the implementation of user-defined (EFT) models & the formulation of physical constraints on observables and model parameters

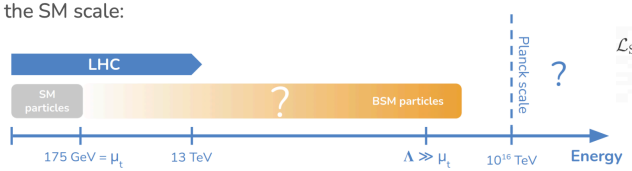
➡ basically: a user-friendly interface to BAT.jl for a specific kind of likelihood

EFTfitter.jl



Why is it called EFTfitter ?

Effective Field Theory (EFT): effective extension of the SM Lagrangian for energies much higher than the SM scale:

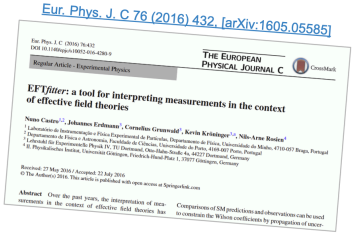


$$\mathcal{L}_{\text{SMEFT}} = \mathcal{L}_{\text{SM}} + \underbrace{\frac{1}{\Lambda^2}\sum_i C_i^{(6)} O_i^{(6)}}_{\text{BSM physics}} + \ldots$$

Λ : energy scale
O_i : higher dimensional operators
C_i : Wilson coefficients

- released the "EFTfitter" package in 2016, based on the C++ version of BAT
- targeted to be used in HEP for EFT interpretations
- EFTfitter.jl: rewrite of EFTfitter in Julia
- still for EFT use cases, but tool is also much more generally applicable

Eur. Phys. J. C 76 (2016) 432, [arXiv:1605.05585]



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Data Analysis

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The Bayesian Analysis Toolkit (BAT)

Oliver Schulz
on behalf of the BAT team

MAX-PLANCK-GESELLSCHAFT
Max-Planck-Institut für Physik (Werner-Heisenberg-Institut)
BAT BAYESIAN ANALYSIS TOOLKIT

oschulz@mpp.mpg.de

Conclusions and Outlook

- BAT concept: user brings domain knowledge and likelihood, BAT provides sampling, integration and visualization
- BAT.jl v3.x releases will gradually add more "measure language" in API:

$$\int_B \alpha_b(A)\,\mathrm{d}\,\bar{\beta} = P(A \times B) = \int_A \beta_a(B)\,\mathrm{d}\,\bar{\alpha}$$

$$\alpha_b(A) = \int_A \frac{\mathrm{d}\,\beta_a}{\mathrm{d}\,\bar{\beta}}(b)\mathrm{d}\,\bar{\alpha}(a)\,, \quad \bar{\beta}(B) = \int_{\mathcal{A}} \beta_a(B)\,\mathrm{d}\,\bar{\alpha}$$

- In progress: Switch from tuning MCMC proposals to tuning space transformations
- Next sampler (we hope): Dynamic space transformations via RQS normalizing flows during algorithm tuning
- ToDo: Add SciMAL optimization and integration algorithms

Using data frames in Julia to analyse HEP data

Enrico Guiraud[1], **Philippe Gras**[2]
Nov 5-6, 23

[1]Princeton University, USA
[2]CEA/IRFU - Saclay, France

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Corpuscles.jl in a nutshell

Corpuscles.jl

- Native Julia package
- Uses same CSV table like SciKit-HEP particle
  → Official catalog slightly modified/fixed
- Mainly based on info encoded to PDGID
  → PDGdb.jl seems to provide a lot more additional info: e.g. decays and branching ratios ...
- Values are given using `Unitful.jl`

PDGdb.jl

Wrangling the Particle Data Base

Mikhail Mikhasenko
Ruhr University Bochum

Erlangen, 7/11/2023

The PDG is on the track to make the databases available. **Decays properties are accessible!**
MySQL is the internal format; new releases will be in the same form.

We get to deal with the historic records.
not-clean: physics-aware **processing** and **cleaning** is needed.
not-consistent: feedback to the PDG is appreciated. Collected in [Issues]

Cleaned and shaped DB can be exported e.g. to Corpuscles.jl, scikit-hep/particle

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HS^3 - A serialization standard for statistical models in high energy physics

Cornelius Grunwald[1], Robin Pelkner[1]

Many people involved: Carsten Burgard, Oliver Schulz, Mikhail Mikhasenko, Jerry Ling, Lukas Heinrich, Alexander Held, Wouter Verkerke, Jonas Eschle, Lorenzo Moneta, Matthew Feickert, Louis Moureaux, Tomas Dado, and many others

JuliaHEP Workshop 2023 - 08.11.2023

[1] TU Dortmund University

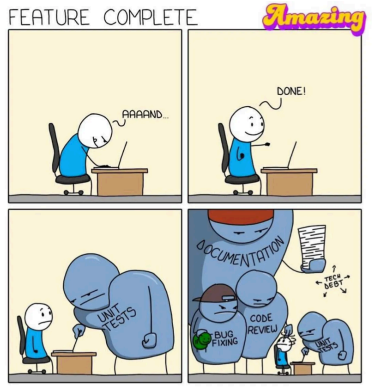
technische universität dortmund

Julia Prototype Implementation

technische universität dortmund

- WIP HS^3 implementation, still ongoing
- most functionalities for **reading** HS^3 are there
- currently: focusing on **reproducing physics results**
  - ATLAS Higgs discovery workspaces
  - Master thesis deadline in 2 weeks

⇒ code currently more optimized for reproducing physics results rather than for a ready-to-be-used package



- still needed: code clean-up, extension, performance improvements, tests, ...
- but: **proof of concept** implementation already shows feasibility of the approach

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Reproducible Science

Why it matters and how to achieve it...

Scientific project reproducibility

PUBLISH REPRODUCIBLE PAPERS,
END THE CYCLE OF DESPAIR

How I make a 100% reproducible project

1. Initialize a DrWatson project and add all packages I foresee using
2. Open three columns in my IDE: source, script, console
3. Start doing the analysis on middle column, the script, which uses DrWatson
4. Functionality of general purpose goes to the source file after creation in script
5. Periodically the code base is reorganized to more script and source files
6. When ready to publish:
   - Make one script per paper figure or table that needs numbers
   - Publish the entire code repository (+ README, Project.toml, Manifest.toml) on GitHub
   - Assign a DOI to the GitHub repo via Zenodo.org. Then, cite the DOI in the paper!
   - Example: Minimal recipes for global cloudiness (latest paper with code base)

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HPC / HTC

High-Performance Computing / High Throughput Computing

PADERBORN UNIVERSITY

Paderborn Center for Parallel Computing

Julia for High-Performance Computing (HPC)

Carsten Bauer

November 7, 2023 @ ECAP
JuliaHEP Workshop

NATIONALES HOCHLEISTUNGS RECHNEN

Summary

- **Julia can be a great option for HPC!**
  - serial and parallel performance on-par with Fortran/C/C++
  - portability and high-productivity
  - new opportunities, e.g. interactive HPC
- **New challenges**
  - workflow / interactivity at scale, Julia depot, system binaries, …
- **"Early adoption" cost**
  - Julia for HPC is a niche
  - lack of support, tooling, …

The Julia for HPC community is small but vibrant. Join us!

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Tutorials

from a beginner to an expert

- Introduction to Julia by Graeme A Stewart, Samuel Skipsey
- HPC / HTC by Carsten Bauer
- BAT.jl - Tutorial by Oliver Schulz
- Amplitude Analysis with Julia by Mikhail Mikasenko
- Automatic Differentiation by Dr Chris Rackauckas
- SciML - Machine Learning in Julia by Dr Chris Rackauckas
  - Julia's SciML
  - 18.337 - Parallel Computing and Scientific Machine Learning

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Workshop Summary

Discussion: JuilaHEP 2023 Workshop

- Interoperation with existing software
- Data analysis
- Julia libraries for HEP
  - Identified needs include LorentzVector interfaces, PDG data, histograms, and plotting support
  - Suggestion to provide recipes for popular plotting libraries like Plots.jl, Makie.jl, and PGFPlots
- ML in HEP
- HPC in HEP
- Workflows in Julia
  - Exploration of workflow tools (e.g., Snakemake equivalent) and xyzpy equivalent
  - Consideration of GPU data analysis workflows and potential challenges
- Documentation & training
  - Emphasis on tutorials hosted on JuliaHEP and HSF websites, including a JuliaHEP primer
  - Monthly community calls and plans for the next workshop at CERN, potentially with a hackathon

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Overall Impact

- Discussions on Julia's role in the future of High Energy Physics
- Several development projects identified
- Workshop served as a vibrant platform for knowledge exchange, showcasing Julia in HEP and envisioning its continued growth