

## Science of the second s

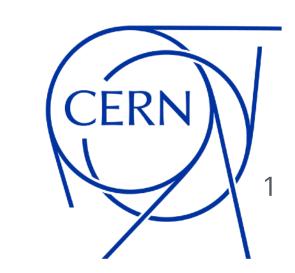
# HSF, JENA, EVERSE and other European Inputs towards sustainable HEP Software

## HEP-CCE AHM

Graeme Stewart, CERN EP-SFT (Particular thanks to Torre Wenaus, Caterina Doglioni, Stefan Roiser, Sanje Fenkart for material)







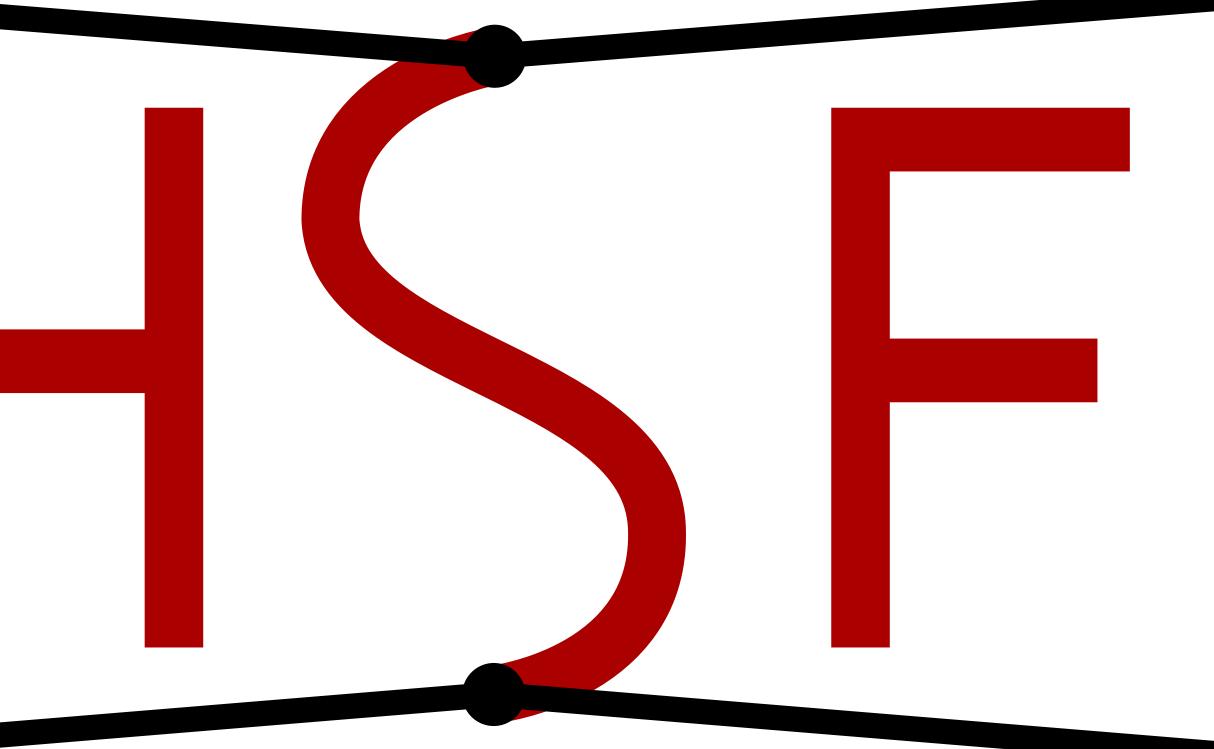
2024-07-23

## Overview

- HEP Software Foundation
- JENA and SPECTRUM
- Software Sustainability
- EVERSE
- Conclusions for Collaboration

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## HSF



## HEP Software Foundation

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## HEP Software Foundation Happy Birthday HSF, we are 10 years old!

- Motivations today are very much the same as we had a decade ago
  - Changing hardware landscape making efficient software more difficult to implement
    - Today multi-core processing is very well established in all experiments
    - Accelerator programming has advanced significantly
  - An exciting physics programme ahead, e.g., High-Luminosity LHC, but this will put tremendous pressure on software and computing
  - We need to train a new generation of software experts
    - And still give them recognition and a career path
    - RSEs are a new model from the same era



• Event complexity and rate will jump, physics precision is growing across the board - but the budget is ~fixed

• Try to avoid duplicated solutions and multiple rediscoveries of the same things, given the severe lack of experts





## DESY Workshop

- We celebrated our birthday at DESY, Joint <u>WLCG-HSF Workshop</u> in May
- Good time to look back at our accomplishments
  - <u>Community White Paper</u> (CWP) process that mapped out the roadmap towards HL-LHC
  - Provided a voice for software and its importance in high-level strategic discussions
    - LHCC, European Strategy Update, Snowmass, P5, ECFA, JENA, ...
  - Advice on practical matters such as licensing and tooling
  - Input from experts on GeantV, GPUs, DUNE frameworks
  - Plus community forums, from working groups in topical areas to, e.g., Compute and Accelerator Forum
  - Reference implementation for conditions databases
  - Google Summer of Code
  - HSF Training Initiatives with close to 3000 students trained new <u>Training Centre online</u>



The activity of the HSF has helped create a positive atmosphere where more software projects are successfully funded: IRIS-HEP, SWIFT-HEP, HEP-CCE, ErUM-Data-Hub

This is very different from 10 years ago!



## But how can we do better.?

- We asked the question about how we could be even more effective in the next years
  - How can we sustain, grow and prioritise?
  - Strengthening our connections to the community, to projects and the experiments
- Reorient the HSF organising team to a <u>Steering Group</u>
  - Take more executive oversight of the HSF
    - Though not discouraging our do-ocratic nature!
  - Very open to new members who would like to contribute to steering the HSF
- MCnet, ...)

• In the process of setting up an Advisory Group, primarily from the experiments (LHC, DUNE, Belle II, EIC/ePIC,

• More regular way to gather external feedback on the HSF's activities and how these are helping the community





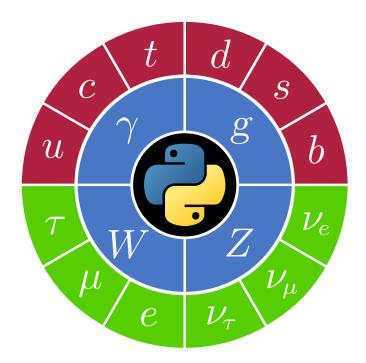
## Working Groups, Activities, Seminars

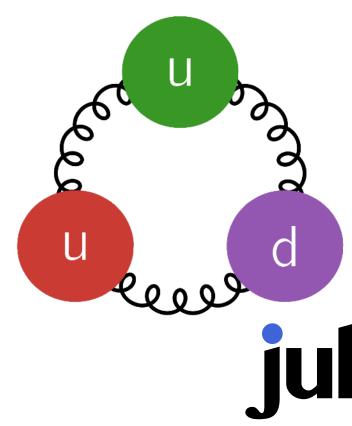
- After the CWP we setup a number of Working Groups
  - e.g., Simulation, Reconstruction, Event Generators, Data Analysis
- These have been quite successful, but more as forums for discussions than places where work is actually organised
  - We decided that in many cases these groups would be better described as activity forums
  - Contribute to a new **HSF Seminar Series** 
    - Regular time slot (Wednesdays 16h30 CE(S)T/CERN time)
    - Alternating with the Compute and Accelerator Forum
      - e.g., planning a meeting on 4D tracking at the LHC experiments
  - Notwithstanding that there will still be focused non-seminar activities/meetings, e.g., the generator group would like to organise some discussions on the evolution of HepMC3

# Tools, Languages, Training, ...

- Other HSF areas really are helping to organise work, or doing it themselves
  - Language evolution has been a successful activity
    - PyHEP was a success to organise both coherent discussions between developers, as well as didactic and outreach events for physicists
      - PyHEP online workshops <u>most recent edition 1-4 July</u>
      - <u>PyHEP.dev</u> (2nd edition) will be in Aachen, 26-30 August
    - JuliaHEP helping marshall activity related to exploring Julia for high-energy physics
      - Next JuliaHEP workshop at CERN, 30 September 4 October
    - Training Group very active in organising <u>regular training events</u> for HEP
      - Core software skills, Python analysis and CI/CD are very popular
      - Contributions to the training programme always welcome material or helping to teach
      - Pre-CHEP workshop on <u>Training in HEP</u>, 19-20 October

HSF helped these activities achieve a certain critical mass beyond their funding (if they had any)









## Community Software

- At the workshop we had a great series of topics promoted and developed by the community
  - Particularly strong series of talks from the generators teams
    - Nice to have the neutrino experiments discussing their needs and how they align/contrast with respect to HEP
  - Also talks on tracking (ACTS), simulation (Gaussino), L1 triggers (Allen)
  - And community software projects like SciKit-HEP, ROOT, HSF India, Key4hep, Phoenix
- Shows a great strength of the HSF as a forum for the community to share knowledge and discuss common approaches and solutions
- Our "do-ocracy" approach has been a success
  - Thanks to the efforts put in by a large number of people

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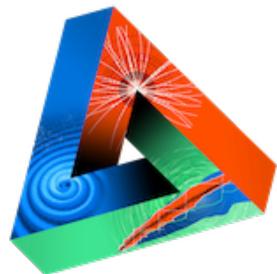
## Software Projects

- The HSF itself didn't become the home of software projects
  - A few projects were very closely aligned (prmon, phoenix, harvester)
  - We did not control funding (deliberately!) and development services evolved greatly (GitHub and GitHub actions)
- We propose to revisit the idea of HSF supported projects
  - So that the HSF can **endorse projects** as recognition of their role in the community
    - Considering a differentiated way to do this, depending on the criteria fulfilled (open development model, usage in the community, etc.)
  - Projects always retain full control of their development and management
- We are also happy to arrange for expert reviews or to help work towards reference implementations and white papers for common software solutions





# JENA and SPECTRUM







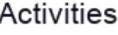


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## JENA Computing Initiative

- JENA: Joint ECFA NuPECC APPEC
  - ECFA European Committee for Future Accelerators
  - NuPPEC Nuclear Physics European Consortium
  - APPEC AstroParticle Physics European Consortium
- Three major scientific communities working together on science and infrastructure themes of common interest
- JENA Symposia in 2022 in Madrid
  - Plenary presentations and the closed sessions discussed computing
  - Funding agency representatives identified an increased need for discussions on the strategy and implementation of European federated computing at future large-scale research facilities

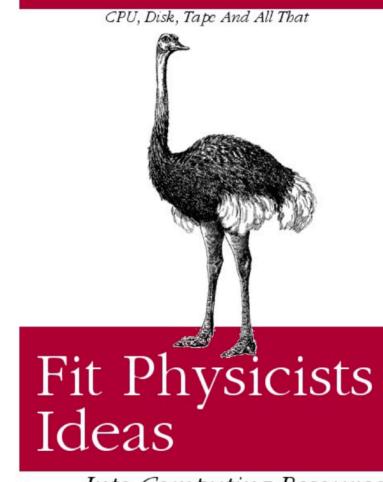






# JENA Computing Workshop

- We started this process organising a <u>computing workshop</u> in Bologna, June 2023
  - Reviewed the major challenges for each field
    - Particle Physics
      - High Luminosity LHC enormous stress on software and computing from higher trigger rates and higher pileup
    - Nuclear Physics
      - GSI-FAIR experiments will increase data rate and computing needs
      - Need to support many experiments, including small ones
      - Try to make the software and the computing as common a problem as possible with common solutions (example: FAIR-ALICE collaboration)
    - Astro(patricle) Physics
      - Observatory model running and upcoming projects with data piped into existing computer centres
      - Need to generalise access and interfaces to give scientists access to data products and alerts
      - Vera Rubin, SKA very high data rates



Into Computing Resources

O RLY





## Known Challenges

- Hardware evolution continues with manufacturers adapting to smaller scales
  - Chiplet architectures and 3D lithography
- Heterogeneity is inevitable
  - Many software challenges arise from this to make algorithmic changes and implement efficient solutions
- Significant European investment in HPCs (see Maria's talk)

  - Has to integrate into our established distributed model
- Machine Learning (AI) increasingly important in workflows
  - Resource implications not yet really well understood
    - Hope is for higher fidelity and reduced costs for inference cf. other methods
    - But how much training will be required?



• We need to engage and find common ground to allow HPCs to be more effectively used by data intensive sciences



## Computing Initiative Working Groups

- HPCs
  - Augmenting the computing capacity available and facilitating the federation with existing data facilities
- Software and Heterogeneous Architectures
  - Find common solutions to using heterogeneous architectures, lowering the costs of computing and addressing sustainability
- Federated Data Management, Virtual Research Environments, FAIR Principles and Open Data
  - Managed by the ESCAPE Consortium, strengthen data management synergies and how workflows interact with FAIR principles
- Machine Learning and Artificial Intelligence
  - Quantify the resource needs and to define the interfaces and services that are needed by physicists to run ML workloads
- Training, Dissemination, Education
  - Leverage the experience in the HSF training initiative and find common ground with other sciences; explore how to develop a curriculum with universities

#### Goal is to write a whitepaper, drafted for November 2024, to be finalised at the next JENA Symposium



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## Software and Heterogeneous Architectures

- We have surveyed the *prior art* material from all three communities
  - Now in the process of synthesising these inputs into summary documents
- Meanwhile we have been preparing a **survey** that looks at different aspects of software and computing in the community
- We have done this in conjunction with the SPECTRUM project
  - Strategic Research, Innovation and Deployment Agenda (SRIDA) and a Technical Blueprint for a European compute and data continuum
    - Concentrating on HEP and Radio Astronomy
- JENA/SPECTRUM Survey (Announcement)
  - Answers from all international partners also very welcome!
  - The overall survey is pretty huge, but answering the questions on software and training should take < 15 minutes



## Sustainable Software



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## FAIR Software

# FIVE ENDORSE RECOMMENDATIONS FOR FAIR SOFTWARE

- Public repository with version control
- A licence
- Code is catalogued
- Enable citations
- Use a software quality checklist

https://fair-software.eu/

### FAIR Principles for Research Software https://doi.org/10.15497/RDA00068

The FAIR4RS Principles are:

#### F: Software, and its associated metadata, is easy for both humans and machines to find.

F1. Software is assigned a globally unique and persistent identifier.

- F1.1. Components of the software representing levels of granularity are assigned distinct identifiers.
- F1.2. Different versions of the software are assigned distinct identifiers.
- F2. Software is described with rich metadata.
- F3. Metadata clearly and explicitly include the identifier of the software they describe.

F4. Metadata are FAIR, searchable and indexable.

#### A: Software, and its metadata, is retrievable via standardized protocols.

A1. Software is retrievable by its identifier using a standardized communications protocol.

- A1.1. The protocol is open, free, and universally implementable.
- A1.2. The protocol allows for an authentication and authorization procedure, where necessary.
- A2. Metadata are accessible, even when the software is no longer available.

## I: Software interoperates with other software by exchanging data and/or metadata, and/or through interaction via application programming interfaces (APIs), described through standards.

Software reads, writes and exchanges data in a way that meets domain-relevant community standards.
Software includes qualified references to other objects.

#### R: Software is both usable (can be executed) and reusable (can be understood, modified, built upon, or incorporated into other software).

R1. Software is described with a plurality of accurate and relevant attributes.

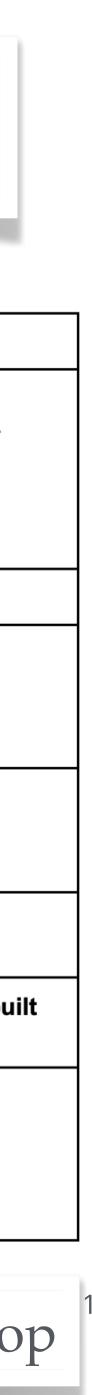
- R1.1. Software is given a clear and accessible license.
- R1.2. Software is associated with detailed provenance.

R2. Software includes qualified references to other software.

R3. Software meets domain-relevant community standards.

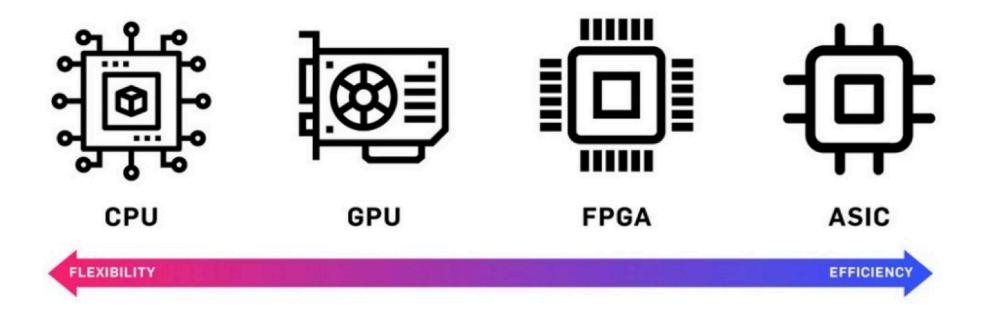
Table 1: The FAIR Principles for Research Software

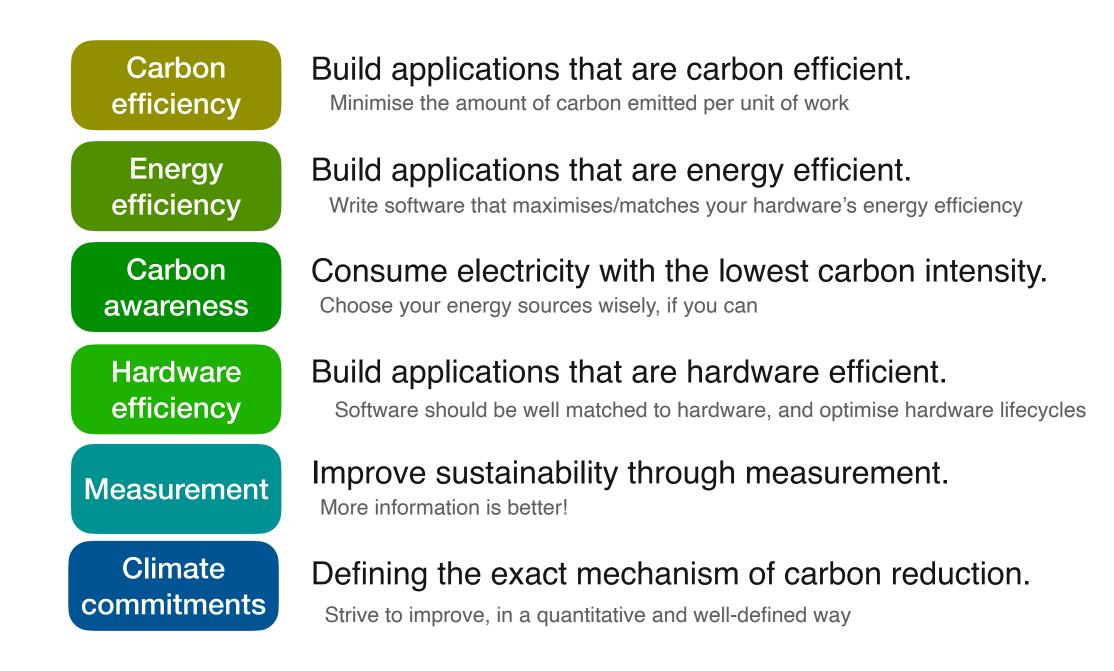
#### Software Sustainability - IRIS-HEP Blueprint Workshop



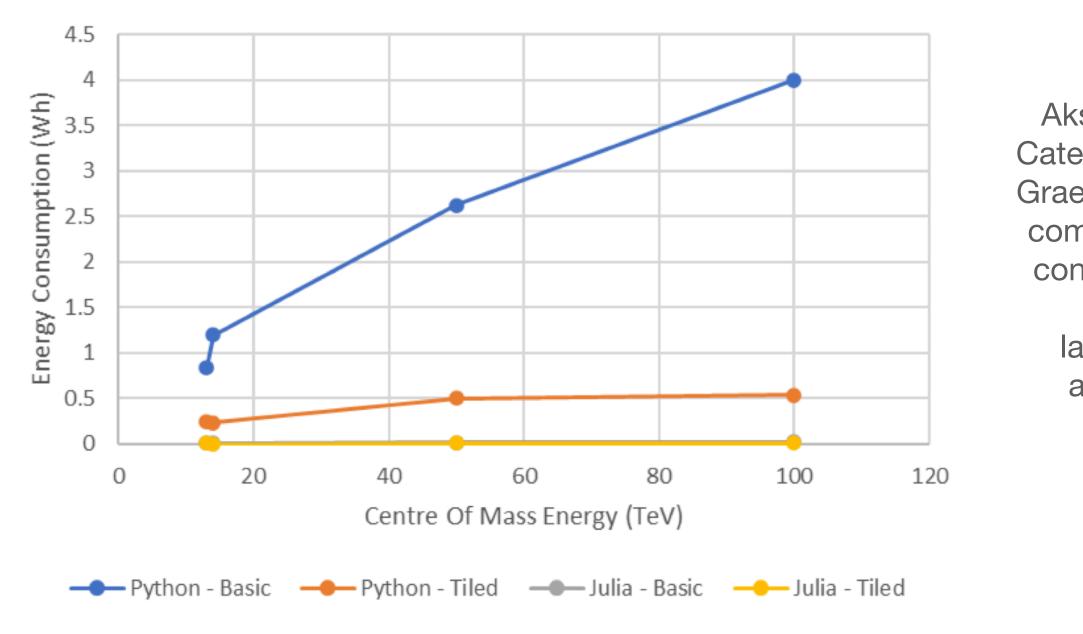
## Green Software

- From <u>https://</u> learn.greensoftware.foundation/
- Concrete example from SwiftHEP where x50 improvements were gained in ATLAS's use of the Sherpa event generator's multi-leg NLO calculations
  - Also supported in HEP-CCE!

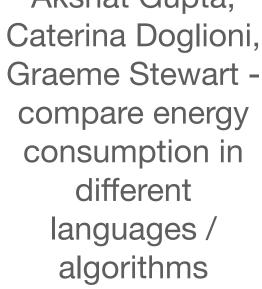


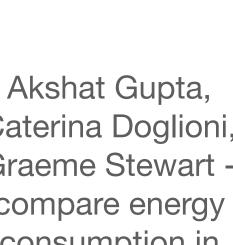


#### Energy Consumption at different Centre of Mass Energies



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## FVFRSF

# COSC C EVERSE





## HVHRSH

• EVERSE Project is 3 year EU funded project, €8M



- Started 1 March 2024
- Cloud
- Aims to
  - Create a framework for research software and code excellence
  - Build a network for software quality, based on existing community standards
  - Lay the foundations for a future virtual institute for research software quality

# **MARCE OF CONTROL OF C**



#### • Build on the software quality aims of the five science clusters in the European Open Science





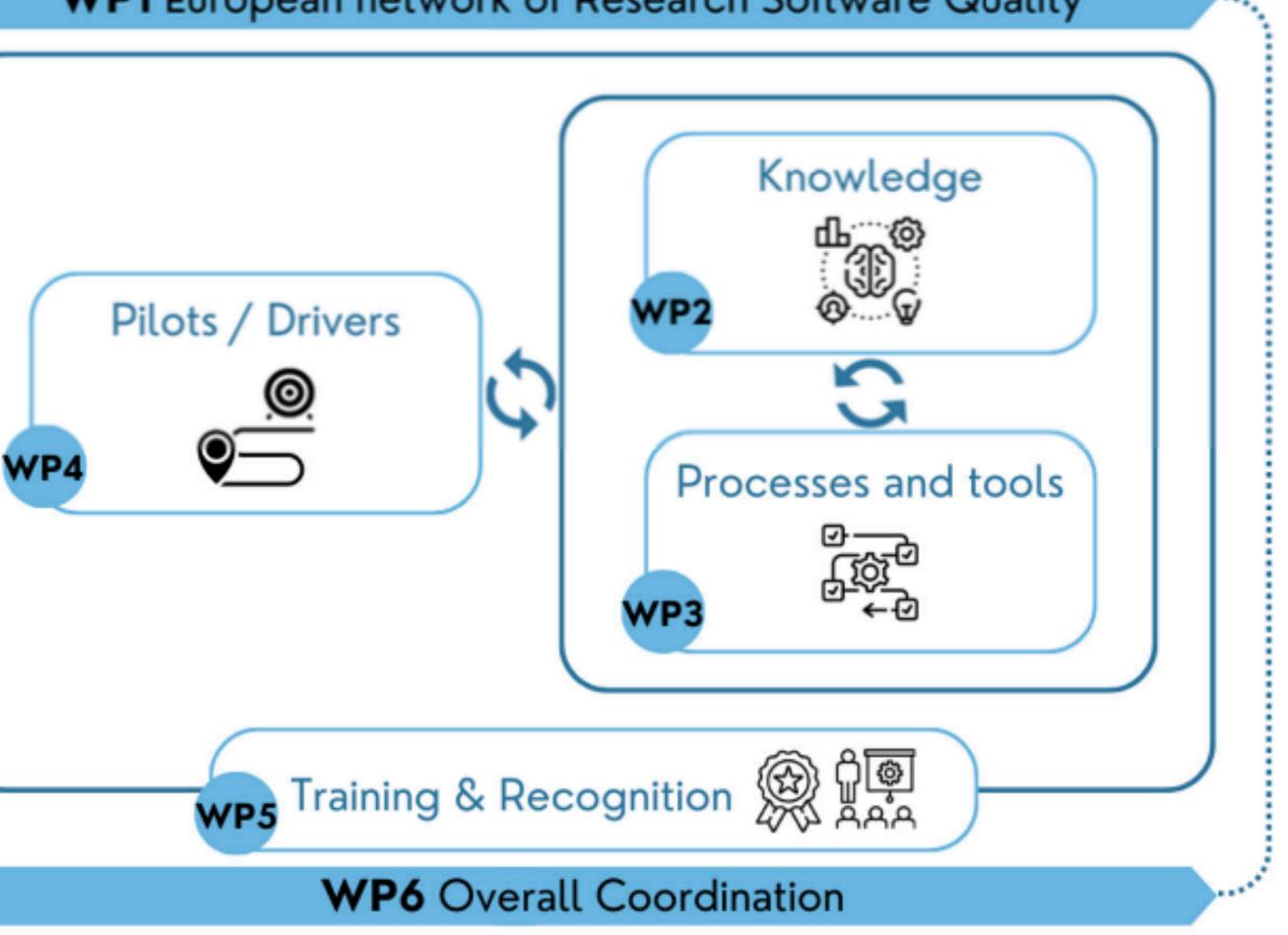


## EVERSE Organisation

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- Significant HEP connections
  - WP1 Graeme Stewart
  - WP3 Thomas Vuillaume
  - WP4 Caterina Doglioni
  - WP5 Stefan Roiser

#### WP1 European network of Research Software Quality



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## EVERSE Activities

- The core activities:
  - Assess current best practices by researchers and make those accessible via the EVERSE "RSQkit"
    - The RSQkit is a meta-repository of documentation, practices, and examples (content still in flow)
    - Prototype for a different purpose/field: <u>RDMKit</u> (from Elixir)
- *Link tools and services* into common pipelines or frameworks for software quality and integrate them into the tools developed by the EOSC clusters
  - Guiding principles are FAIRness and Open Science
- Exercise these concepts via the science clusters' use cases, e.g. these are some of the HEP/ESCAPE use cases:
  - Analysis code for high throughput data from the LHC based on "xAODAnaHelpers" [talk]
  - Prototyping of machine learning tools for data compression [talk]
  - Software infrastructure for the tracking of charged particles based on "ACTS" [talk]

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## EVERSE Network

- Establish a community of practice in the quality of research software
- European based, but an international context
  - Provide standard and documented practices around tools and training for software developers
  - Define the meaning and principles of software quality for the research domain
  - Enhanced recognition for software developers contributing to research activities
- Value
  - EOSC Association expert group on software
  - Help shape software quality practices
  - Define the key aspects around recognition for research software activities
- Currently we are discussing with early adopters to help us shape the network
  - Contact <u>Graeme</u> and <u>Sanje</u> if you are interested to join



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## Conclusions

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## Conclusions for Collaboration

- Software and computing in high-energy physics remains as challenging as ever
  - A critical part of our science exploitation, with HL-LHC coming soon
- The landscape of large scale data intensive sciences is also growing
- <u>HEP Software Foundation</u> has helped our community exchange information, advocate for software at high levels and take practical steps to improve our software
  - We want to continue to work with all partners to keep doing that
  - We are utterly reliant on members of our community contributing to the HSF to do that!
- Broader European initiatives, such as JENA Computing, help align the interests of HEP with other sciences
  - Speak with a common voice to funding agencies and facilities
  - The <u>JENA/SPECTRUM survey</u> is a chance for many people to contribute their view
- EVERSE project works more broadly towards software quality criteria, training and recognition

### In all of these areas possibilities to work usefully with HEP-CCE exist!

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## Stay in Touch

- HSF: <u>hsf-steering@googlegroups.com</u>
  - If you are not signed up to the HSF forum mailing list, please subscribe
- JENA: jena-computing-wp2-software@cern.ch
  - Or mail to Graeme Stewart, Paul Laycock and Adrien Matta (chairs)
- SPECTRUM: <u>community@spectrumproject.eu</u>
- ESCAPE: <u>everse-contact@lists.certh.gr</u>
  - Or contact Graeme Stewart, Stefan Roiser or Caterina Doglioni (HEP WP leaders)

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