



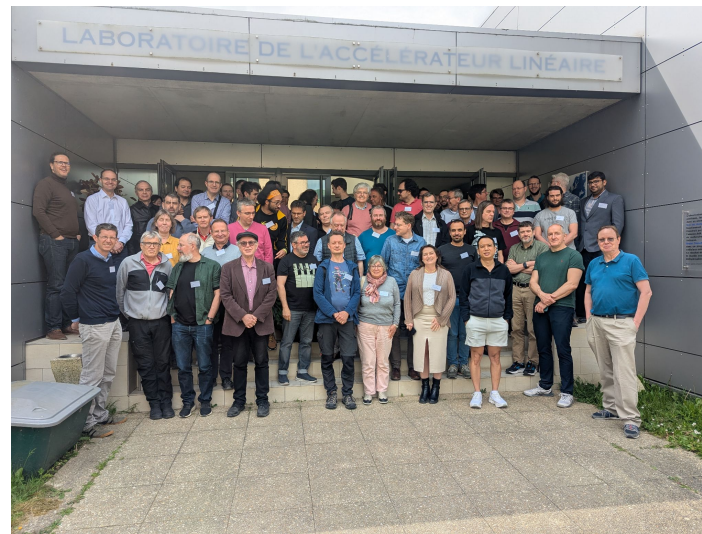
# Community Software and Software Sustainability

Graeme Stewart (CERN)

PUNCH Lunch Seminar, 26 June 2025

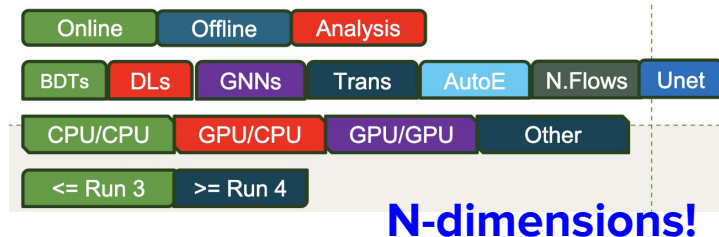
# WLCG/HSF Workshop in Orsay

- Worldwide LHC Computing Grid and HEP Software Foundation workshop
  - Tradition now to bring together the distributed computing and the HEP software communities
- Latest workshop was in May 2025, at IJCLab in Orsay
  - Covering many aspects of computing and Software, including...
    - **AI and heterogeneous resources**
    - **Common software**
    - WLCG facilities
    - Analysis at HL-LHC
    - WLCG operations
    - **Sustainability**
- I will give an overview here of the **bold** topics



# AI Overview

- AI has been disruptive, highly beneficial and very broadly applicable
  - Cheaper: ultra fast high-fidelity simulation
  - Better: x100 improvement in background rejection
  - New: anomaly detection with auto-encoders
  - It also has, and is, moving very fast
    - New techniques come all the time
    - Areas of applicability expand
  - AI will impact our computing resources
    - Need to prepare for this
    - Providing the correct resources and (grid) accounting for them

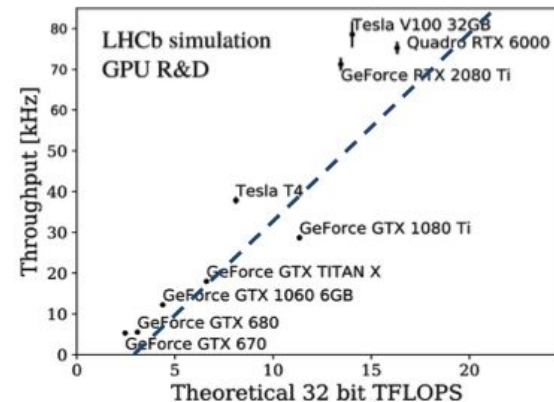


- ◆ **1<sup>st</sup> axis: application domain**
  - ◆ **Online, offline, analysis**
- ◆ **2<sup>nd</sup> axis: AI technology**
  - ◆ **GNNs, GANs, Fully connected, ...**
- ◆ **3<sup>rd</sup> axis: resource domain**
  - ◆ **Training: laptop, server, GPU, many servers and GPUs**
  - ◆ **Inference: laptop, WLCG nodes, GPUs, FPGA, ...**
- ◆ **4<sup>th</sup> axis: experiment**
- ◆ **5<sup>th</sup> axis: when?**

To be followed up in the “Heterogeneous architectures in WLCG” workshop Dec 3-5

# Heterogeneous computing

- What computing that we do on CPUs could be envisioned on GPUs in 5 or 10 years?
  - We have some outstanding examples of success: ALICE TPC reconstruction, LHCb Allen L1 trigger
- What could be next?
  - Event generation
  - Detector simulation
- KPI: event throughput per unit cost
- Heterogeneous computing is challenging and needs training
  - Not too much interest from students in C++/legacy codes
    - **Long time to train people, struggle to retain**
  - Can we live with single/reduced precision?
    - NGT - Openlab "Optimising Floating Point Precision" [Workshop next week](#)
  - Not many experts in our field (CUDA, Alpaka, ...)
  - Distill experience and expertise in languages, compilers, platforms, etc.

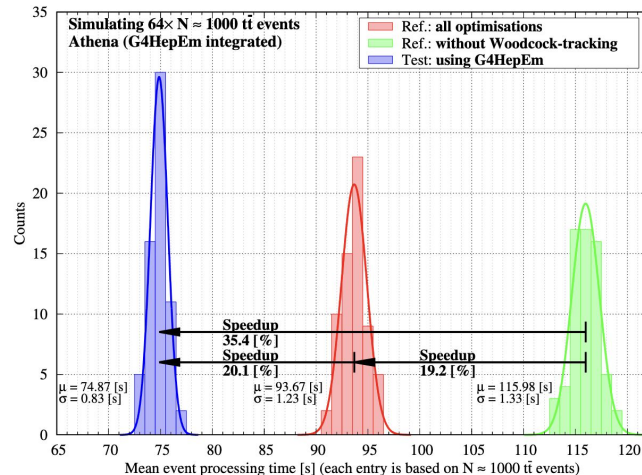
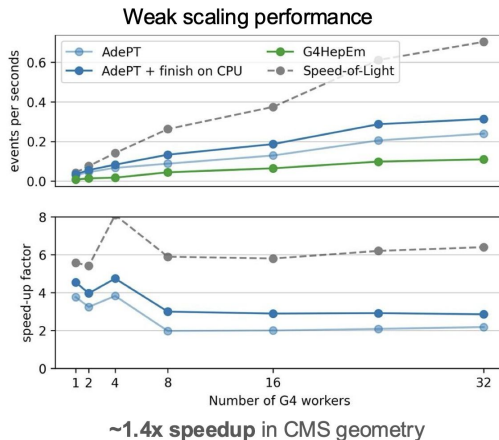


To be followed up in the “Heterogeneous architectures in WLCG” workshop Dec 3-5

# Common software - Simulation with G4HepEm, AdePT

Accelerate HEP simulations of electrons, positrons and photons:

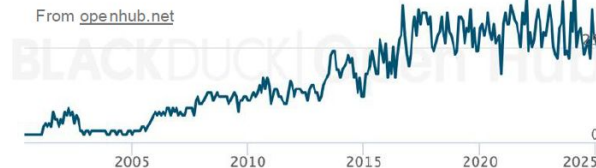
- G4HepEm: specialized tracking for  $e^-$ ,  $e^+$ , and  $\gamma$  on **CPU**
  - Provides a significant (20%) speedup for the Run 4 ATLAS/CMS detector simulations
- AdePT: offloading electromagnetic showers to **GPU**
  - Still very much R&D, some promising indications of speed-ups, but not proven yet in full use cases
  - Geometry bottleneck (VecGeom) is being worked on



# Common software - ROOT and RooFIT

- **2025 Programme of Work** proceeding well
- Steady increase in number of issues closed over the past year
- **1st stable RNTuple format released in 6.34.00**
- New histograms under development towards a thread-safe & fast class (for ROOT7)
- RFile will replace TFile (WIP)
- A lot of work on interoperability (SOFIE, for ML)
- **Python ecosystem seeing a lot of attention**
- Histograms to honour Scikit-HEP's proposed UHI protocol
- **Many significant performance enhancements in RooFit - for CPUs and GPUs**
- E.g., Automatic Differentiation available via Clad

Already >50 unique contributors in 2025!



Per unit time:  $N_{\text{contributors}} \approx 1.5 \times N_{\text{Core Dev FTEs}}$

All contribution counts for ROOT!

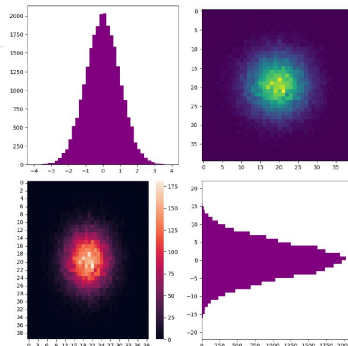


UHI and ROOT: 2D

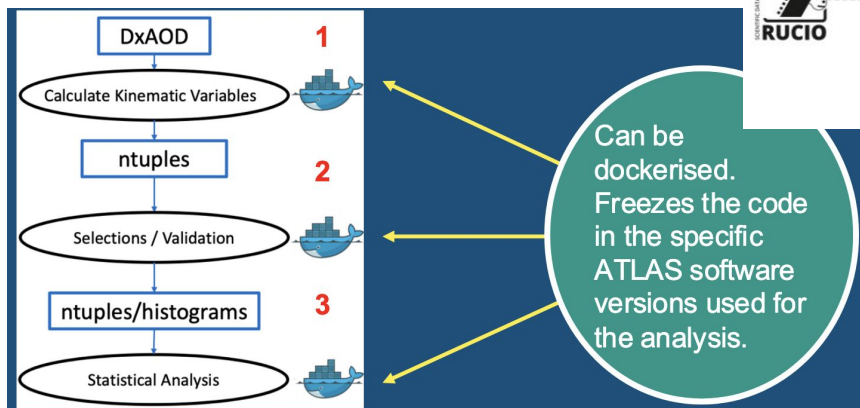
```
1 import ROOT
2 from ROOT.uhi import sum
3 import numpy as np
4 import matplotlib.pyplot as plt
5 import mplhep as hep
6 import seaborn as sns
7
8 h2 = ROOT.TH2F("h2", "", 40, -4, 4, 40, -20, 20)
9
10 for i in range(25000):
11     px, py = np.random.normal(0, 1, 2)
12     h2.Fill(px, 5 * py)
13
14 projh2X = h2[:,sum, :]
15 projh2Y = h2[:, :sum]
16
17 fig, axes = plt.subplots(2, 2, figsize=(9, 9))
18
19 axes[0, 1].imshow(h2.values(), interpolation='nearest')
20
21 sns.heatmap(h2.values(), ax=axes[1, 0])
22
23 hep.histplot(projh2X, ax=axes[0, 0], histtype='fill', color='purple')
24
25 hep.histplot(projh2Y, ax=axes[1, 1], histtype='fill', color='purple', orientation='horizontal')
26
27 plt.tight_layout()
28 plt.show()
```

Yet another example of Python tools and ROOT interoperability!

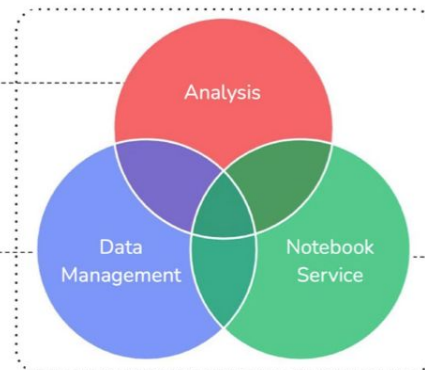
Coming next: we are experimenting with new approaches, input is welcome!



# Common software - Virtual Research Env. user experience



reana



Authentication and  
authorization  
infrastructure (AAI)



- ✓ Available at the click of a button
- ✓ Data persistence
- ✓ No account restrictions
- ✓ Change easily the software stack
- ✗ Access >200 cores
- ✗ Access to batch
- ✗ Access to GPUs
- ✓ Integration with Data Lake tech.
- ✓ Integration with REANA

```
Code Blame Executable File · 74 lines (67 loc) · 2.81 KB Code 55%
1 stages:
2 - name: SVJEventSelectionStep1_mc16a
3 dependencies: [init]
4 scheduler:
5 scheduler_type: singlestep-stage
6 parameters:
7   AT_config_file: 'config_files/config_mc16a.txt'
8   dxaod_file_mc16a: {step: init, output: dxaod_file_mc16a}
9   prw_file_mc16a: {step: init, output: prw_file_mc16a}
10  tdp_file_path: {step: init, output: tdp_file_path}
11  output_step1: '{workdir}/output_step1'
12  step: {${ref: 'specs/steps.yml#/SVJEventSelectionStep1_mc16a'}}
13
14 - name: SVJEventSelectionStep1_mc16d
15 dependencies: [init]
16 scheduler:
17 scheduler_type: singlestep-stage
18 parameters:
19   AT_config_file: 'config_files/config_mc16d.txt'
20   dxaod_file_mc16d: {step: init, output: dxaod_file_mc16d}
21   prw_file_mc16d: {step: init, output: prw_file_mc16d}
22   tdp_file_path: {step: init, output: tdp_file_path}
23   output_step1: '{workdir}/output_step1'
24   step: {${ref: 'specs/steps.yml#/SVJEventSelectionStep1_mc16d'}}
25
26 - name: SVJEventSelectionStep1_mc16e
27 dependencies: [init]
```

- Good experience using the CERN VRE and rerunning an ATLAS analysis
  - Containerised workflow steps key

# Sustainable Software

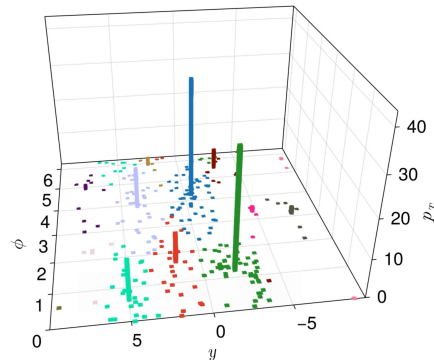
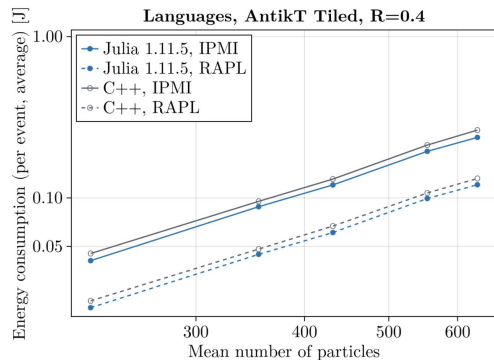
What do we mean by sustainable?

- Efficient Code (for machines)
  - Energy consumption to do a calculation should be as low as possible
  - Worldwide data centre power consumption is about 1.5%, but rising fast
    - Computing for LHC has a significant environmental footprint, which we want to minimise
- Sustainable Code (for humans)
  - Code needs to be maintained for decades
    - Experiment lifetimes are long
    - Preservation lifetimes for results are even longer
  - Code needs to be easy as possible to understand and maintain
  - Concentrate on our problems, reuse as much as possible

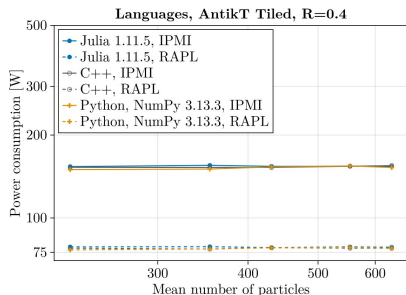


# Sustainable software - Julia

- Jet reconstruction is a good “Goldilocks” problem to study
- Sequential jet reconstruction implemented natively in Julia
  - Tested alongside C++ and Python
- Excellent ergonomics in Julia
  - Expressive, compact code
  - Array operations and broadcast
  - Code composes very well
  - Macros allow spot optimisation



Julia can be faster (=use less energy) than C++ due to superior use of SIMD - many ergonomic/ecosystem advantages



CPU's use ~the same energy at 100%, irrespective of code source

```
@inbounds dij_min = dij[1]
@turbo for here in 2:n
    newmin = dij[here] < dij_min
    best = newmin ? here : best
    dij_min = newmin ? dij[here] : dij_min
end
```

# Sustainable software: EVERSE Project

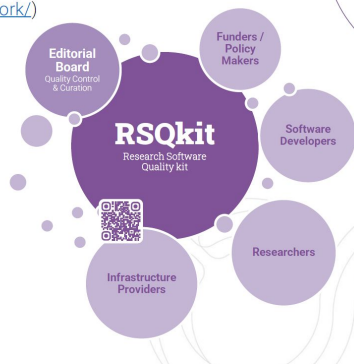
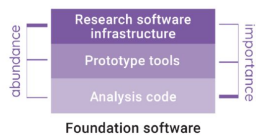
Engagement with 5 European Science Clusters ESCAPE covers HEP, plus Life Science, Environmental, Social, Photon and Neutron

## Establishing a Community

How to contribute to, and engage with EVERSE

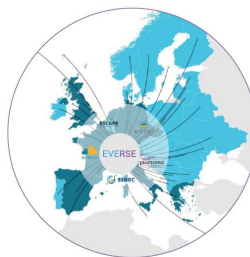
### Elements of EVERSE

- The Network (<https://everse.software/network/>)
- RSQkit (<https://everse.software/RSQKit/>)
- Software Reference model
- Training
- Recognition framework



### Join Us

Any individual or organization that agrees with our vision statement is welcome to join the network



## EVERSE

Paving the way towards a European **V**irtual Institute for **R**esearch **S**oftware **E**xcellence

EVERSE aims to create a framework for research software and code excellence, collaboratively designed and championed by the research communities, in pursuit of building a European network of Research Software Quality and setting the foundations of a future Virtual Institute for Research Software Excellence

- ✓ ensure research software curation, quality, preservation and adoption of best practices, by the Communities, for the Communities, build on collaboration with the five EOSC Science Clusters
- ✓ adopt a three-tier model for research software, i.e., analysis code, prototype tools and research software infrastructure, which captures the varying complexity of research software and its development, and can be used as a basis for research software excellence

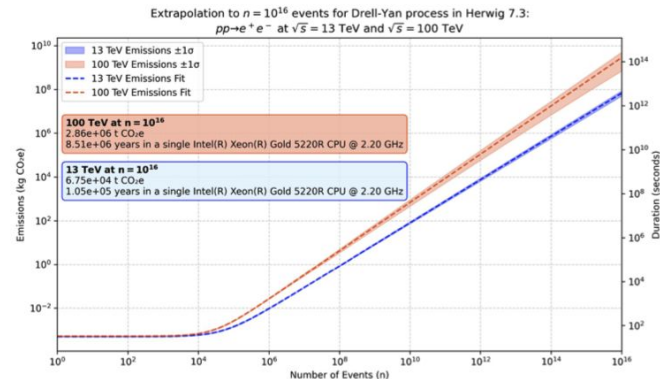
Other developers and software are essential components of our strategy to promote sustainable software practices

The screenshot shows the RSQKit website. The top navigation bar includes links for 'About', 'Get involved', 'Contact us', and social media icons for Bluesky, LinkedIn, and GitHub. A search bar is also present. The left sidebar contains a menu with 'Research software', 'Research software quality', 'Research clusters & infrastructures', 'Research Software Stories', 'Your role', and 'Your tasks' (which is highlighted). The main content area is titled 'Your tasks' and contains a list of tasks with brief descriptions: 'Choosing languages, tools & infrastructures', 'Organising software projects', 'Using version control', 'Reproducible software environments', 'Writing readable code', 'Code review', 'Testing software', 'Task automation using GitHub Actions', 'Licensing software', 'Citing software', 'Software identifiers', and 'Documenting software'. Below this, there are several task cards with icons and titles: 'Your tasks: Choosing languages, tools & infrastructures', 'Your tasks: Citing software', 'Your tasks: Continuous Integration and Continuous Delivery/Deployment', 'Your tasks: Creating a good README', 'Your tasks: Documenting software', 'Your tasks: Documenting software using "Read The Docs"', 'Your tasks: Improving environmental sustainability', 'Your tasks: Licensing software', and 'Your tasks: Organising software projects'.

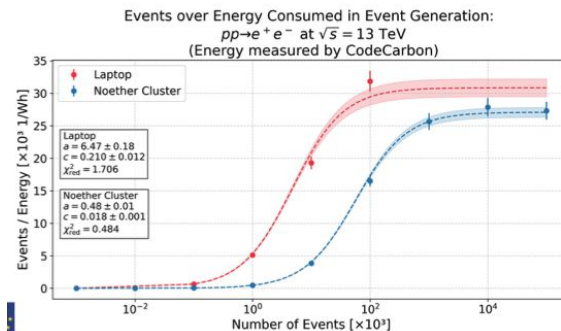
# Green Software - Generator Benchmarks

- Goal is to understand the energy cost of computing at University of Manchester
- Drell-Yan events simulated in Herwig 7.3
  - Energy consumption grows linearly with number of events
- CO<sup>2</sup> Emissions vary widely per country
- Lifecycle environmental impact is very complicated
  - Vendor numbers are not standardised
  - Difficult to get estimates for modern equipment
  - Idea is to grow expertise in the community on understanding these impacts
    - Improve policies to lower impact

- Extrapolation to LHC scales ( $10^{16}$  events)
  - LHC (13 TeV):  $6.75 \times 10^4$  t CO<sub>2</sub>e
  - FCC (100 TeV):  $2.86 \times 10^6$  t CO<sub>2</sub>e



Significant CO<sub>2</sub> emissions at LHC scale workloads



Laptops are efficient for small workloads!

# Outlook and next steps



- Software's importance can hardly be overstated!
- Software projects are making great strides towards HL-LHC
  - AI is becoming ubiquitous
  - Heterogeneous computing is hard, but there are successes and promising R&D
- HSF's mission is to help us to get to better, more sustainable and efficient software in the field
  - Will work closely with projects like EVERSE to define indicators and support tools that do that
  - VREs helping also with reproducibility
- Understanding sustainable software can be improved
  - Develop expertise in assessing the impacts of our software
  - Leverage important trends towards usability and efficiency (Eduardo's talk on Scikit-HEP)
  - Improve the community's understanding and level of skills (Michel's talk on training)

**The HSF is bottom up - we want to hear your ideas and suggestions too!**

Mailing List: [hsf-forum@googlegroups.com](mailto:hsf-forum@googlegroups.com); Website: <https://hepsoftwarefoundation.org>; Contact: [hsf-steering@googlegroups.com](mailto:hsf-steering@googlegroups.com)<sup>12</sup>