

ExaTEPP

# The SWIFT-HEP project and UK ~~HPC~~ DRI

23 July 2024

History and context

SWIFT-HEP and ExaTEPP

A few comments on Digital Research Infrastructure

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# UK HEP computing infrastructure

- **GridPP:** Provides the compute, disk, tape needed to operate PP experiments. As well as the software fabric and support needed to run the experiment payloads.
- **IRIS:** set up to bring coherence, collaboration, coordination and sharing across all of STFC (Smaller experiments, astronomy, facilities)
- **DiRAC:** UK high performance computing facility supporting STFC theory users

Physical hardware is only part of the expense. We should remember about the staff effort to support the infrastructure!

## UKRI Digital Research Infrastructure:

- Large investments in AI machines, e.g. Isambard AI (which is useful for AI!)
  - ... but mainly GPU based and so not applicable to HEP production computing
- Not necessarily in sync with the needs from the PP community
- A large HPC may not suit PP requirements

# Timeline and history

	Entity	Scope	2018	2019	2020	2021	2022	2023	2024	2025	2026	2027	2028	2029
Infrastructure	LHC	Global	Run-2	LS2			Run-3			LS3			Run-4	
	WLCG	Global	Global coordination of requirements, resources, policies, networking, security, etc.											
	GridPP	UK	GridPP5			GridPP6			GridPP7			...		
	IRIS-UK	UK	UKTO	IRIS 4yr x £4m			IRIS...							
Experiments	ATLAS-CMS	Global	S&C Conceptual Design			S&C Technical Design			S&C deployment			Operation		
	LHCb	Global	S&C TDR	S&C deployment			Operation and Upgrade 2 preparation							
	DUNE	Global	Protodune	S&C CDR		ProtoDUNE Comp model	DUNE implementation and deployment				Operation			
	Others	Global	Experiments common software infrastructure design and development (neutrino, dark matter, etc)											
Software	HSF	Global	HEP Software Forum: White Paper --> Working Groups --> Community Meetings --->											
	NSF	USA	S2I2	IRIS-HEP					IRIS-HEP (Phase 2)					
	DOE	USA				HEP-CCE				CCE				
	STFC	UK				ECHEP								
	Excalibur	UK				Excalibur		ExaTEPP			??			
	STFC	UK					SWIFTHEP-1			SWIFTHEP-1.5		SWIFT-HEP2		

# Multi-experiment software development

## The UK Particle Physics Technology Advisory Panel (PPTAP) ([link](#)) 2021

[34] Likewise within software and computing the UK has significant leadership in a significant number of important areas, including in exploitation of computing accelerators, exploitation of low power compute units, computing operations, enabling software and computing, reconstruction algorithms, software framework development, development of cross- experiment development tools, use of HPC and development of collision simulation/generation programmes.

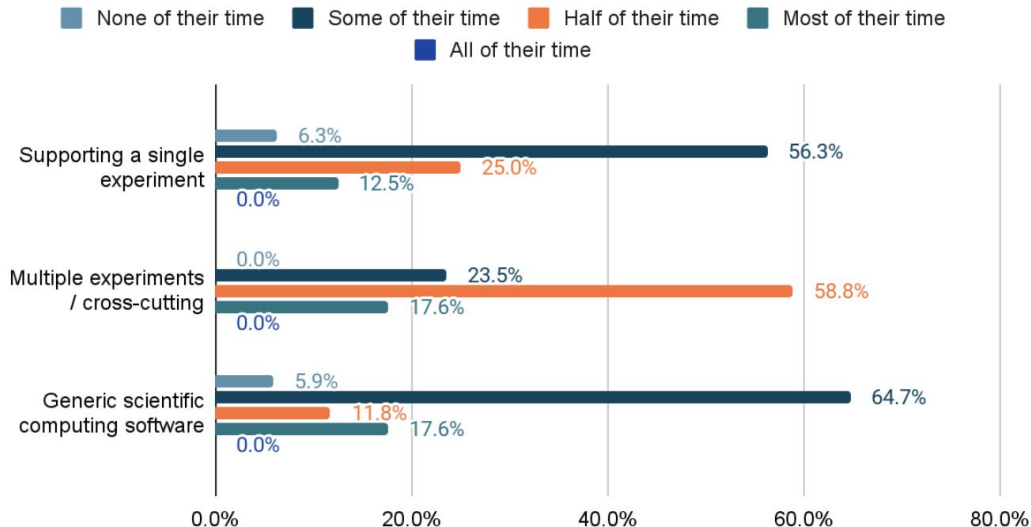
Layer	Domain	Experiment 1	Experiment 2	Experiment 3
6	Physicists	Analysis code	...	...
5	Experiment Physicists programmer and software engineers	Analysis framework. Simulation, Reconstruction, Calibration Code	...	...
4	Experiment Software Engineers	Software Frameworks	...	...
3	Common Software HSF / SWIFT-HEP	Common software components (Data management, Generators, Geant4, Accelerator integration)		
2	GridPP / WLCG	Middleware infrastructure for Distributed Computing		
1	GridPP / WLCG	Physical Hardware		

Moving Software down the stack ↓

# Some results from community surveys

## Particle Physics Technology Advisory Panel (PPTAP) 2021 (RTP= Research Technical Professional)

How should RTPs time be spread?



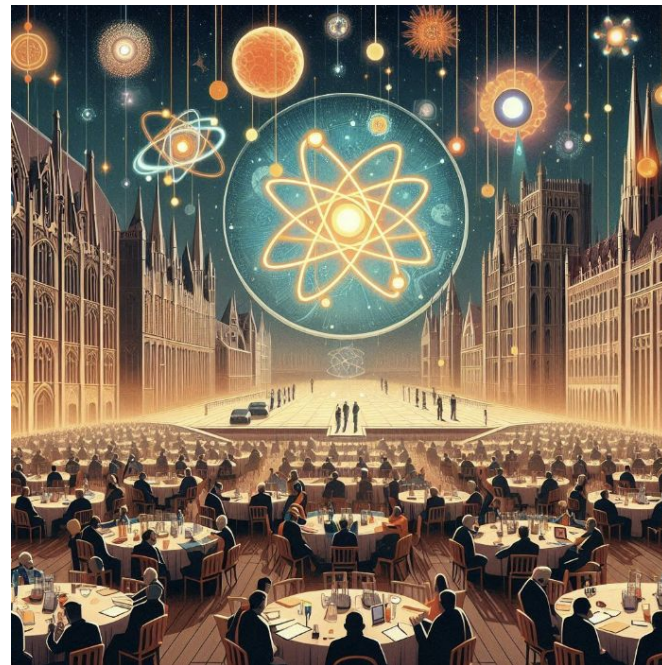
## Particle Physics Advisory Panel (PPAP) 2024

Q: Key infrastructure requirements

Most people said computing resources are adequate

More Research Software Engineers are needed

AI-generated particle physics community meeting



History and context

SWIFT-HEP and ExaTEPP

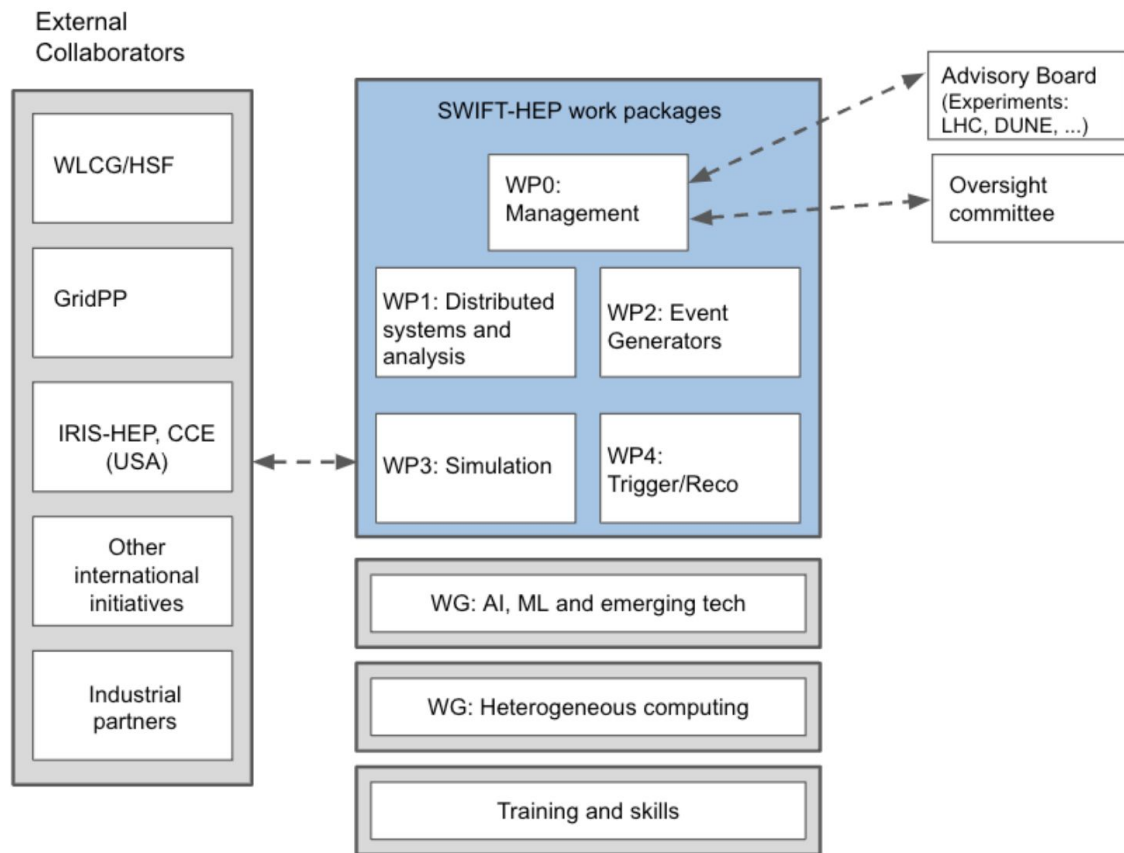
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# Current UK HEP software projects

SWIFT-HEP (5 FTE) Software Infrastructure for HEP	ExaTEPP (3 FTE) Exascale software for PP
Sheffield (PI)	Sheffield (PI)
Bristol	Edinburgh
Imperial College	Swansea
Manchester	Warwick
Warwick	Hartree Centre (Daresbury Lab)
UCL	
Rutherford Lab (PPD and SCD divisions)	

# What does SWIFT-HEP do?



5 FTE. Funded from September 2020 until 2025 (so far) - £2.5M

**Part fund** people at Universities and national Labs to match with other projects

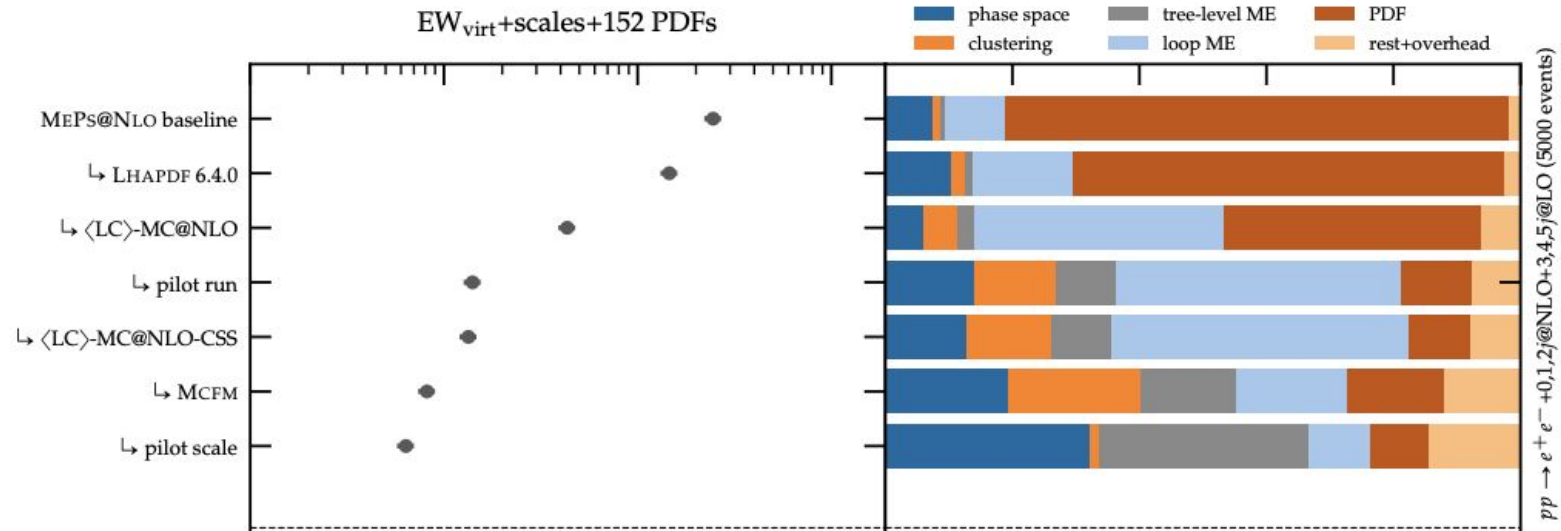
Overall about 10 people funded directly by SWIFT-HEP

Slow ramp up due to recruitment difficulties (especially WP1 and WP4)

# Software improvements. An example from event generators

- Event generators are a key ingredient at the LHC
  - Higher precision generators needed for high precision physics
  - Not just the LHC, also neutrino physics (e.g. Genie)
- Same physics results with less computing ([more info](#))
  - Example from Sherpa (possible thanks to SWIFT-HEP funding)

UCL, Glasgow, Durham  
Chris Gutschow et al,  
[EPJ C82 \(2022\) 12](#)



# Simulation and GPUs (SWIFT-HEP + ExaTEPP)

A significant fraction of WLCG CPU time is spent simulating events  
(and a lot of it is EM showers)

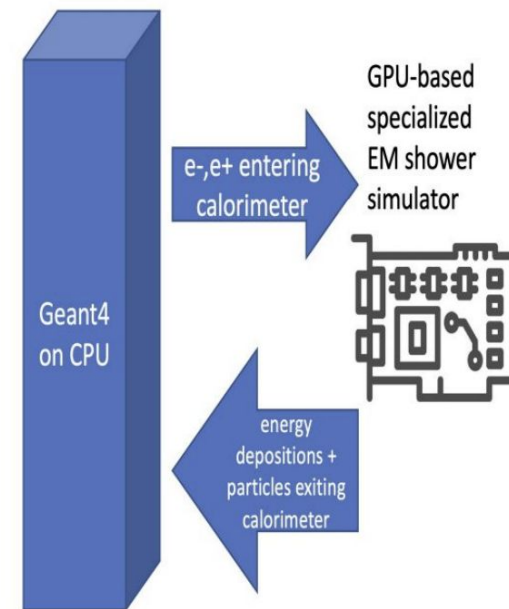
Warwick, Sheffield, Manchester

Great collaboration with **Celeritas** (and AdePT) - **See next talk**  
Development of common interfaces CelerAdePT (Ben Morgan)  
Recent hackathon with Seth and Elliott

## Deliverable:

API, data structures, and workflows for implementing  
GPU-based scoring in AdePT/Celeritas  
Working in collaboration with ATLAS (Hackathon in October)

Work initiated in evaluating Mitsuba for optical photons



# Trigger/Reco work package

Run HLT software on FPGAs (S. Harper et al, mostly for CMS ECAL now) RAL, Warwick, Sussex  
Very early R&D, requires mastering HLS coding

Traccc: integrating the Alpaka framework (S. Martin-Haugh, R. Cross, et al)

Cuda vs Alpaka-cuda are similar

HIP still under development

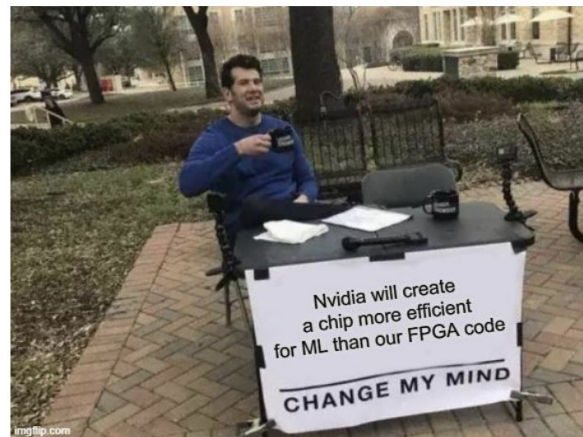
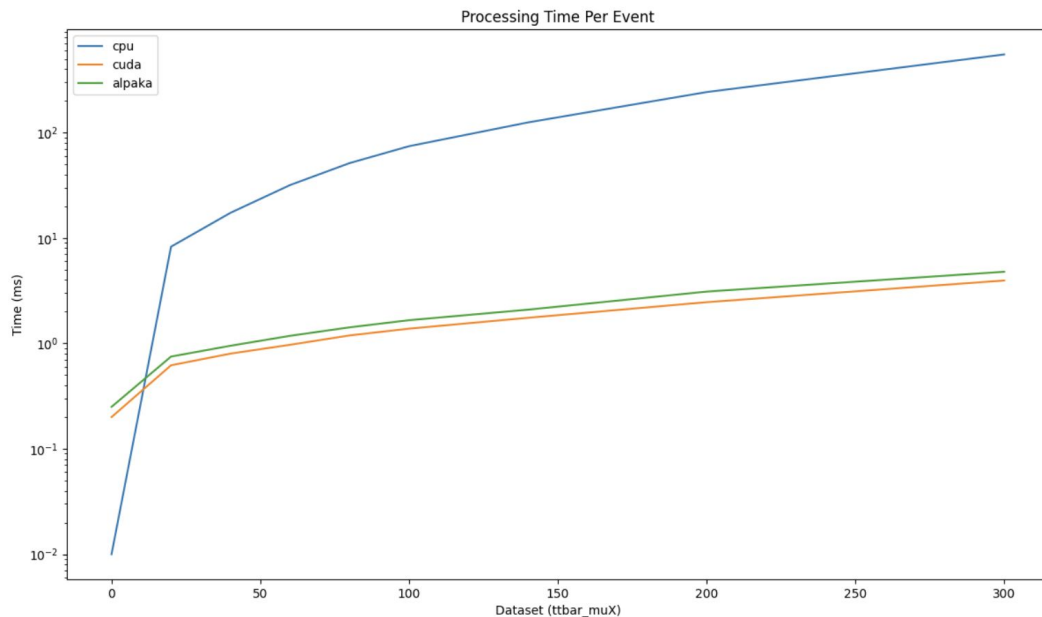
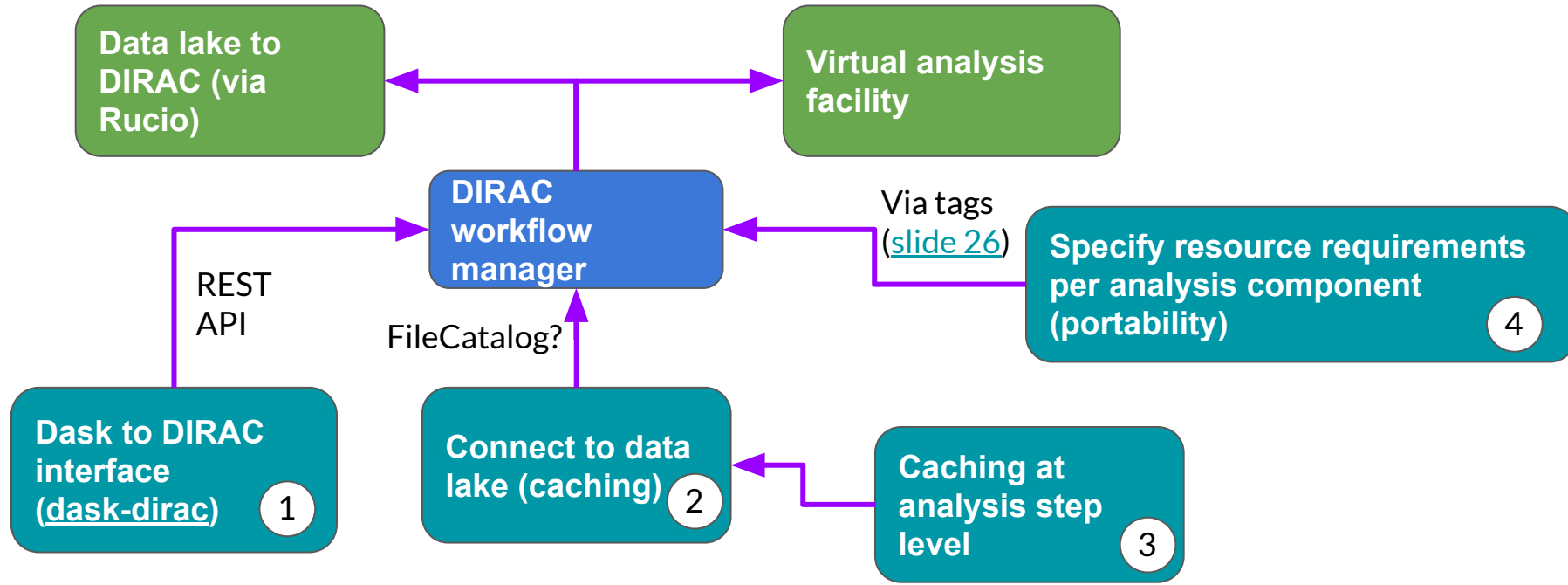


Image from Sam Harper

# Analysis grand challenge on UK infrastructure

Bristol, RAL, Imperial, Brunel

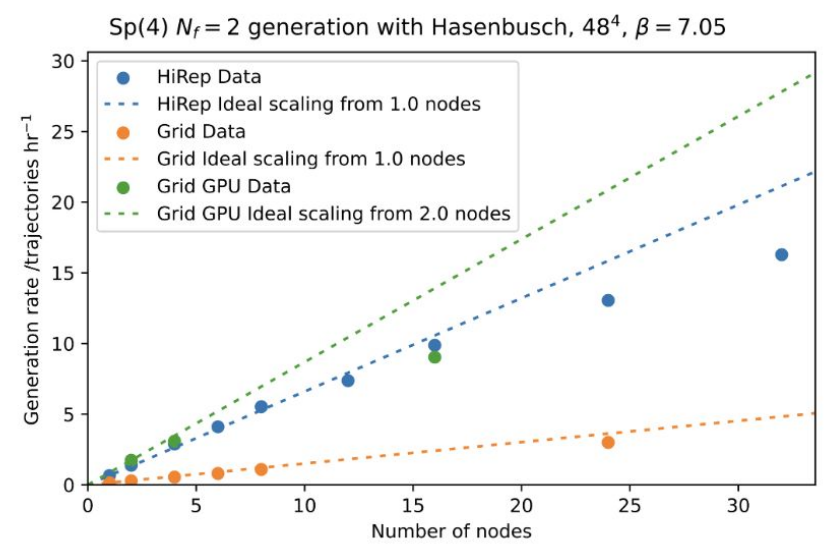
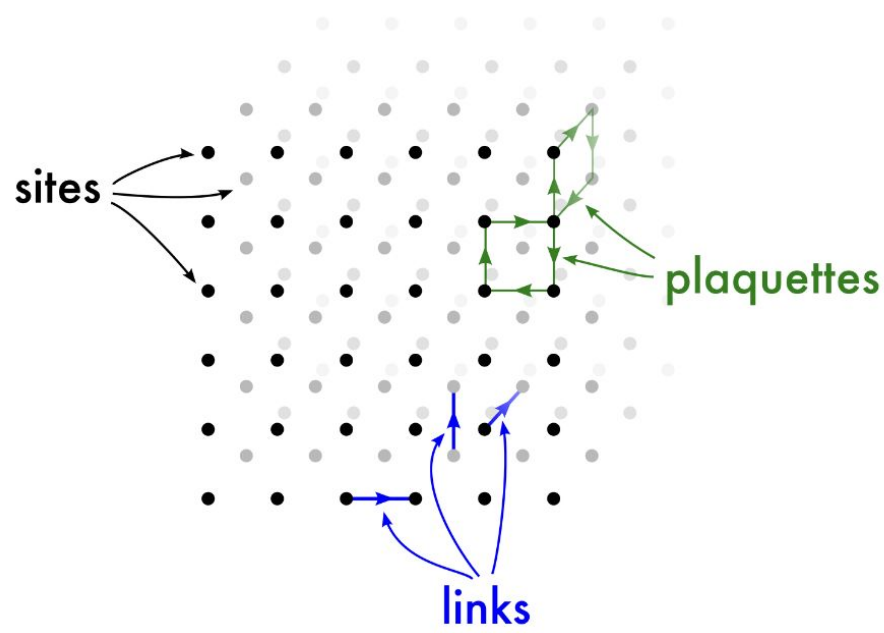


Closest example of what we want to achieve: [Dask-based Distributed Analysis Facility](#) ([kubernetes slides](#))

# ExaTEPP example: Quantum field theory on a lattice

Solve lattice field theories on a 4D lattice of points

Lots of matrix algebra. Large lattices require large GPU calculations across multiple nodes  
(co-design as part of DiRAC)



# The DiRAC HPC Facility

HPC for theoretical astrophysics, cosmology, particle & nuclear physics in the UK

## Memory Intensive “COSMA8” (Durham)



DELL EMC

- 528 TB RAM
- Large-scale cosmological simulations



Atos

## Extreme Scaling “Tursa” (Edinburgh)

- GPU-based system
- Large lattice-QCD simulations

## Data Intensive “Dial” (Leicester)



Hewlett Packard  
Enterprise

- Heterogeneous architecture for complex simulation and modelling workflows



DELL EMC

## Data Intensive “CSD3” (Cambridge)

- Heterogeneous architecture for complex simulation and modelling workflows

Project Office (UCL)



# Ongoing phase. SWIFT-HEP 1.5 (April 2024 - September 2025)

D1.1	SSD storage to accelerate Data Transfer	Month 1-6
D1.2	SSD storage to accelerate Data processing	Month 6-12
D1.3	Benchmarking new workflows on different QoS	Month 6-18
D1.4	Deployment of an analysis facility on GridPP infrastr	Month 6-18
D2.7	Review of performance bottlenecks in EvGen Including interface formats (e.g. LHE, HepMC)	Month 1-4
D2.8	Develop a flexible, efficient and compressed event format and generator interface code release (e.g. HepMC)	Month 4-18
D3.4	Integration of GPU-based EM transport and scoring in ATLAS simulation with performance metrics	Month 1-18
D3.5	API, data structures, and workflows for implementing GPU-based scoring in AdePT/Celeritas	Month 1-18
D3.6	Customisable optical photon propagation with Mitsuba fully integrated in Geant4.	Month 1-18
D4.7	Report on the performance of the ECAL algorithm using HLS language	Month 1-18
D4.8	Full functionality of traccc within ACTS using Alpaka	Month 1-12
D4.9	Prototype developments using SYCL/oneAPI	Month 12-18

# Planning: SWIFT-HEP 2.0 (October 25 to ??)

We submitted a “Statement of Interest” at the end of April (3 pages)

- **3 scenarios:** minimum (5 FTE, 0.6M£/year), core (8 FTE 1M£/year), desired (16 FTE 2M£/year)
- Reviewed by Science Board in June
- We were then asked to define the minimum scenario for 2 years (Oct 2025 - Sep 2027)
- Recommendation to request funding as part of the Digital Research Infrastructure initiative (**DRI**) - See following slides

7 work packages (core/desired), 4 work packages (minimum)

- WP1 Distributed systems and analysis
- WP2 Event generators
- WP3 Simulation of particle interactions with matter
- WP4 Reconstruction algorithms
- WP5 Benchmarking and sustainability
- WP6 Software frameworks for future experiments
- WP7 Artificial intelligence tools and emerging technologies

AI work not very well defined. Starting a working group on AI (kick off in October)

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## DRI THEMES

Interconnected priorities



### DATA INFRASTRUCTURE

Data infrastructure is essential to the research and innovation ecosystem, fundamental to advances in areas such as data science and AI. Data should be findable, accessible, shareable, reproducible and secure.



### LARGE SCALE COMPUTING (LSC)

LSC underpins the research breakthroughs needed to address the key scientific and societal questions of the next five years and beyond through data and compute-intensive research. UKRI seeks to facilitate the use of LSC across all research domains



### SERVICES AND TOOLS

UKRI will work with partners to provide secure and trusted data services for research use of sensitive data (generated through research and from elsewhere) and the tools for researchers, innovators, decision-makers, and ultimately society to benefit.



### SKILLS AND CAREER PATHWAYS

Quality training is necessary to exploit the opportunities presented by DRI. This requires a new approach to engaging, developing and retaining expertise, as well as supporting rewarding, sustainable and flexible career pathways.



### FOUNDATIONAL TOOLS, TECHNIQUES AND PRACTICES

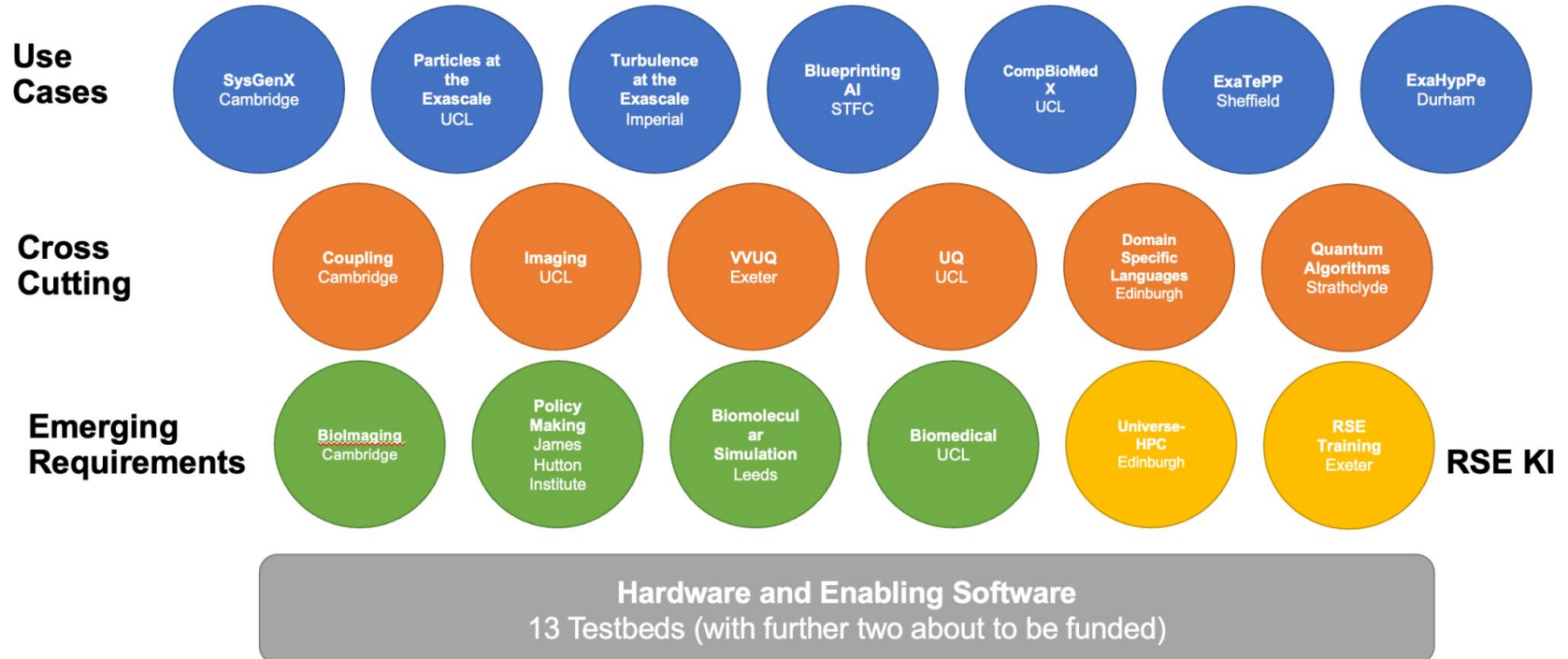
We aim to connect our data, computers, and people by developing essential resources. By establishing and upkeeping a range of foundational tools, UKRI seeks to support the entire UK research and innovation community.

# The ExCALIBUR programme

A UK programme to develop Exascale software algorithms.

(Ending in March 2025, a new programme expected in October 25)

ExaTEPP: Exascale software for Theoretical and Experimental Particle Physics



# Things I would like to learn this week

## New ideas on how to improve the way we organise things

- I like the “all-hands” concept (though it requires parallel sessions)
- Project management and how to monitor deliverables
- How to go from R&D to experiment deployment? Who is in charge?
- ...

## How do you define AI and how to introduce it in HEP workflows?

- In a useful and meaningful way
- In the light of large “AI machines” being commissioned

## HPCs (or large scale computing) and their limitations and usage

- Interaction with other non-HEP communities
- Large HPCs being commissioned in the UK (e.g. IsambardAI in Bristol)

## Approaches to training, skills, career development

# Conclusions and lessons learned

## It's all about people

- Recruiting and retaining staff is the most difficult part of the job
- We can only recruit integer people for longer term (possibly “open ended”)
- People have careers and they have options outside HEP and research
- Research Software Engineers (RSE) pools are a good working model provided we can retain (and fund!) people for longer periods of time

## The distributed model is our way of work

- Mixture of staff at universities, national labs (RAL PPD and SCD)

## Money is always tight. There is no magic money tree

- HEP needs software and computing. This is now loud and clear. (But it's tensioned against other needs!)
- Lot of effort to write proposals, reviews, documents. Better project management?

## “Thou shall use GPUs” (they are the solution to all problems, right?)

## There are other communities out there

- With different problems and ways of working. We need to continue making our case