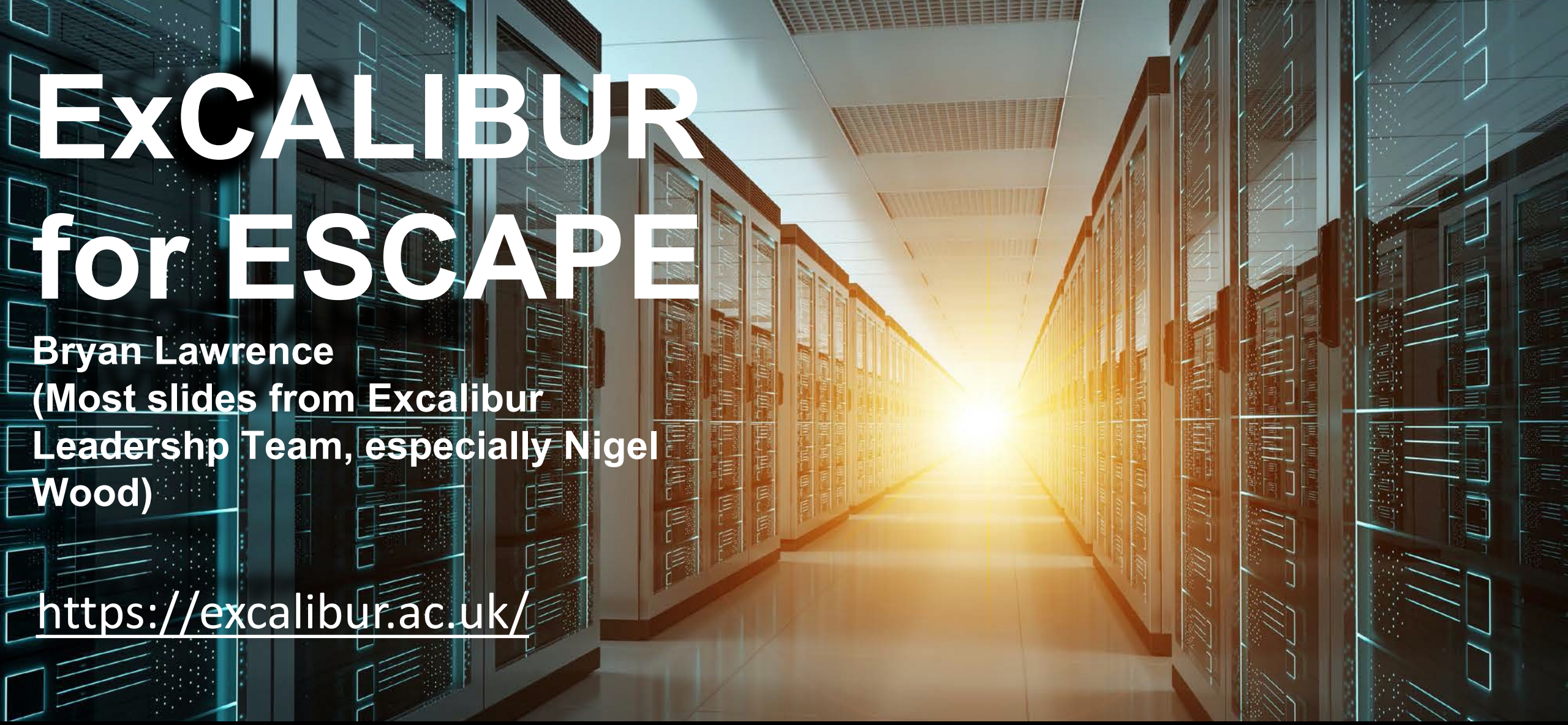
ExCALIBUR for ESCAPE

Bryan Lawrence
(Most slides from Excalibur Leadershp Team, especially Nigel Wood)

https://excalibur.ac.uk/



ExCALIBUR 10 Met Office UKRI UK Research and Innovation UK Atomic Energy Authority

Our challenge

Why Exascale?

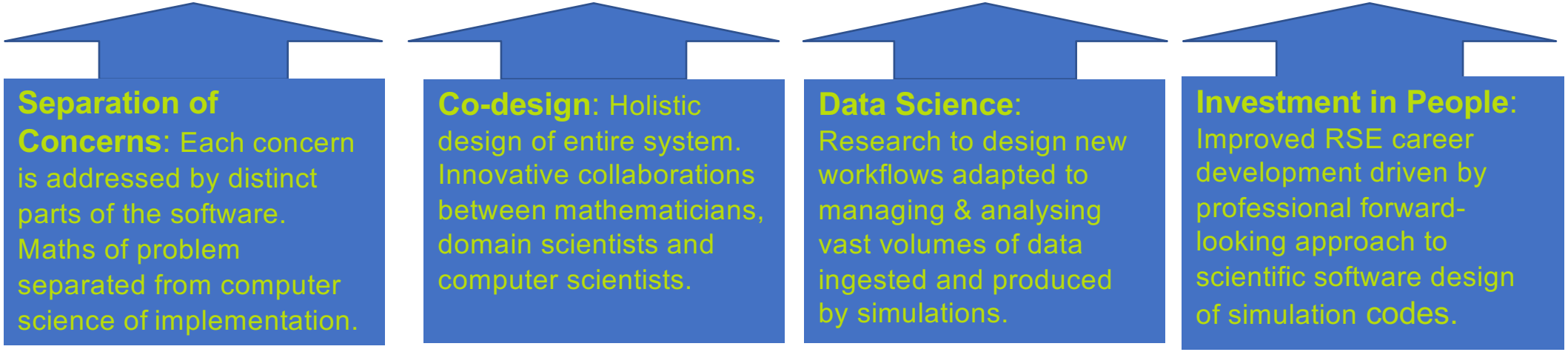
- Currently the Met Office simulates the world's weather at 10 km intervals
- To complete the 7 day forecast in 1 hour needs a petascale machine (16 Pflops) (currently using 19,000 cores)

- To get to 5 km means 2x2 more cells and a 2 times smaller interval in time
  - **O(10)** increase in compute power & data
- To get to 1 km means 10x10 more cells and a 10 times smaller interval in time
  - **O(1000)** increase in compute power & data

Harnessing Exascale Computing

Exascale Computing ALgorithms & Infrastructures for the Benefit of UK Research (ExCALIBUR)

- 5 year programme
- Delivery partners: Met Office (PSREs) + EPSRC (UKRI)
- ***Aiming to redesign high priority simulation codes and algorithms to fully harness the power of future supercomputers, keeping UK research and development at the forefront of high-performance simulation science***



UKRI SPF Wave 2: Met Office, UKAEA, EPSRC, STFC, NERC, MRC

Programme Delivery

RSE Knowledge Integration (~£750k, yrs 1-5)

UKRI

High Priority Use Cases (~£26m, yrs 1-5)

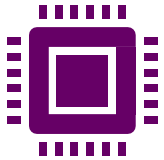
UKRI Met Office

Emerging Requirements for High Performance Algorithms (~£3m, yrs 2-3)

UKRI

Cross-cutting Research (~£10m, yrs 2-5)

UKRI Met Office



Hardware and Enabling Software (~£4.5m yrs 1-5)

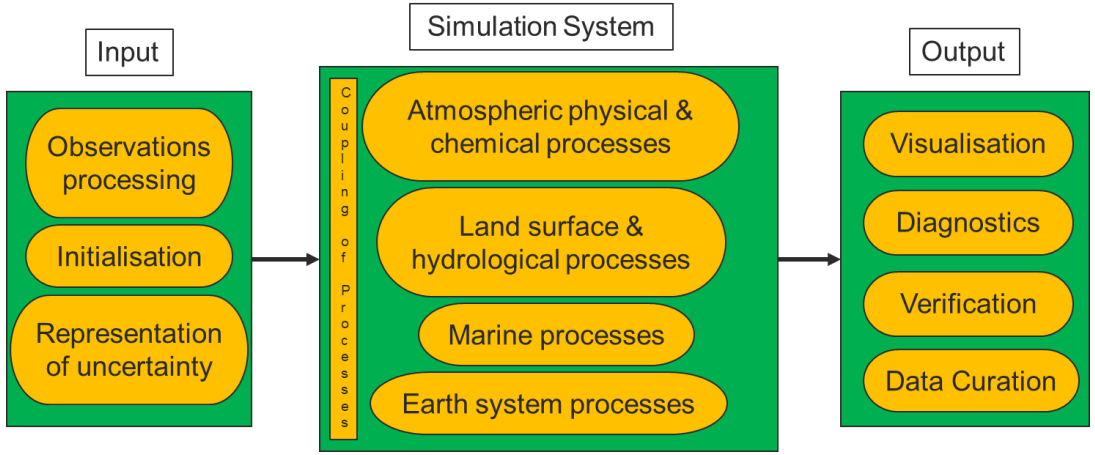
UKRI

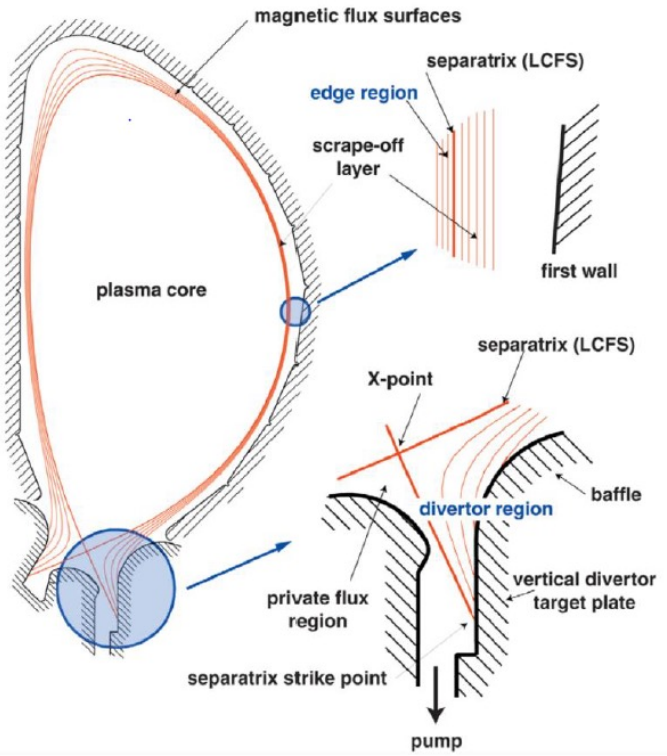
Use Cases

PSRE

- **Weather & Climate Prediction System**
  - ➢ **10 activities**

- **Fusion Modelling**
  - ➢ **8 activities**





Component Model Co-Design

Met Office Work Package 1

Activity	Duration	Aim	Delivery
UK Chemistry & Aerosol (UKCA) model Design	June 2020 – March 2022	Significant improvement in UKCA performance and flexibility on current and anticipated supercomputer architectures	Commissioned
Marine Systems (NEMO) design	June 2020- March 2022	Agree a strategy for the application of the separation to the whole of NEMO and subsequently explore the potential to apply the approach to NEMO –like code bases.	Commissioned
Atmospheric Model data layout and memory access design	October 2019 – July 2021	The dynamical core of the new atmospheric model will speed up the model completion time and deliver the ability to use different precision parts and make optimal use of the new processor architecture.	Met Office
Atmospheric observation pre-processing and assimilation	October 2019 – March 2021	To deliver a new framework for processing observations that is more flexible in being able to exploit new observations types and deployable across different architectures.	Met Office
Marine Systems (WAVEWATCH III) design	April 2020 – April 2022	To research and develop modifications to the wave model that will provide step change in its flexibility and capability by enabling it to exploit shared memory architectures.	Met Office
Verification system components design, integration and testing	April 2020 – September 2023	To deliver a new model evaluation and operational verification suites fit for the UK's weather and climate prediction system for the next ~20 years.	Met Office

System Co-Design

Met Office Work Package 2

Activity	Duration	Aim	Delivery
Design and implementation of new weather and climate diagnostic system	October 2019 – March 2021	To deliver a more user friendly modelling system, enabling scientists to efficiently and flexibly interact with data from the new modelling system.	Met Office
Spatial decoupling of dynamics, physics and chemistry	April 2020 – September 2022	To deliver a step change in modelling capability that will open up a huge range of configuration and optimisation options, benefitting the entire range of modelling systems.	Met Office
Coupling multiple components as a single executable	October 2020 – November 2021	To deliver the option of a new paradigm within the UK's weather and climate prediction system for coupling together the ocean and atmosphere modelling components.	Met Office
Framework for application input configuration and validation	April 2021 – June 2022	To design and develop a flexible framework to constrain the configuration of the inputs to applications using different code bases as part of a larger complex next-generation system.	Met Office

Use Cases

UKRI – Design and Development Working Groups

- ELEMENT - Exascale Mesh Network
- Materials And Molecular Modelling Exascale Design And Development Working Group
- Gen X: ExCALIBUR working group on Exascale continuum mechanics through code generation
- Exascale Computing for System-Level Engineering: Design, Optimisation and Resilience.
- Massively Parallel Particle Hydrodynamics for Engineering and Astrophysics
- Benchmarking for AI for Science at Exascale (BASE).
- Lattice Field Theory at the Exascale Frontier
- ExaClaw: Clawpack-enabled ExaHyPE for heterogeneous hardware
- ExCALIBUR-HEP (= High Energy Physics)
- Turbulent Flow Simulations at the Exascale: Application to Wind Energy and Green Aviation

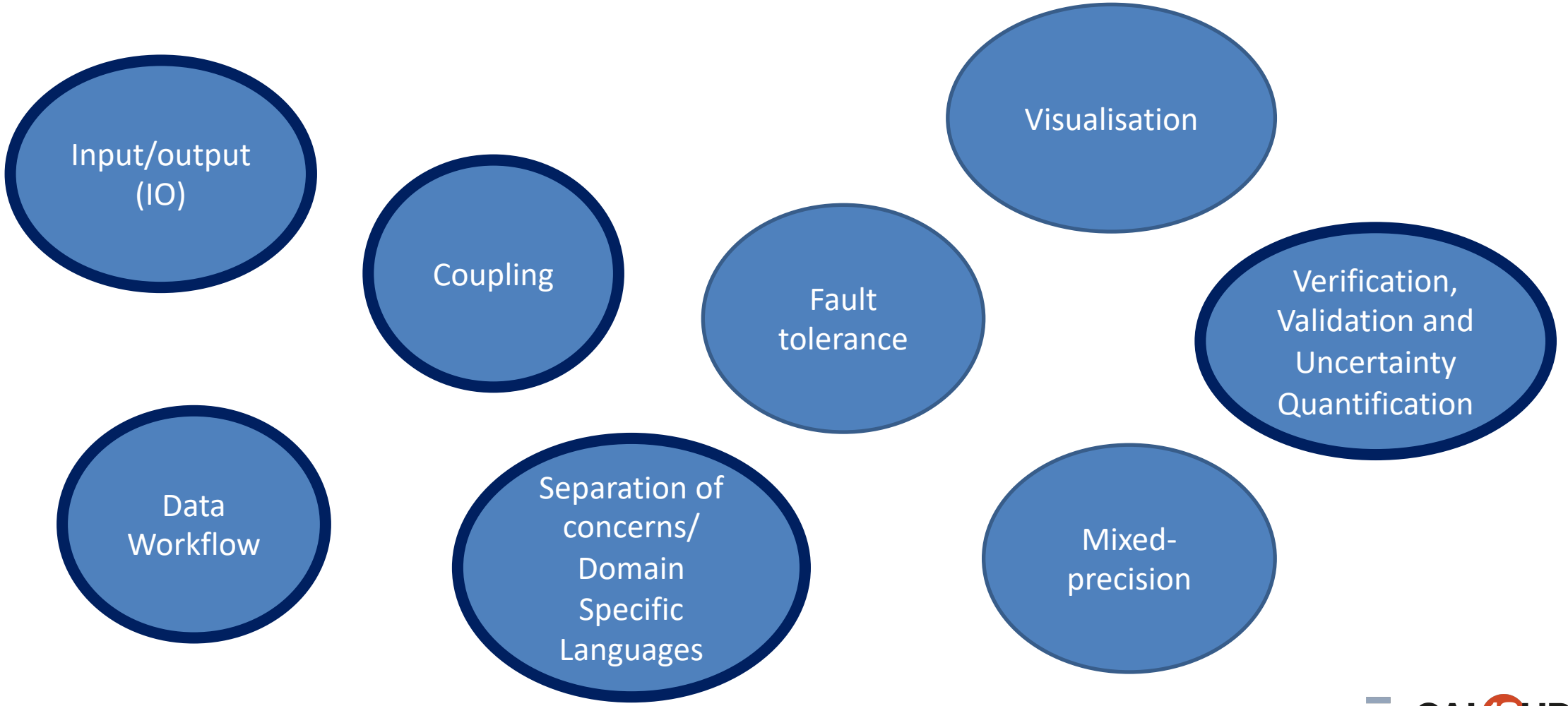
Cross-cutting approach

- Co-ordinated approach addressing known technology/infrastructure issue
- Resolution will lead to significant progress across range of exascale software development challenges
- Apply to multiple Use Cases
- Utilise the lessons learnt from the use cases and design and development working groups to address common issues that impact scientific code under development for use at exascale
- Needs to include contributors from beyond the Use Cases – should be domain agnostic (within remit of ExCALIBUR)
- ExCALIBUR two cross-cutting work packages:

    1. **Common approaches and solutions**
    2. **Potential disruptors**

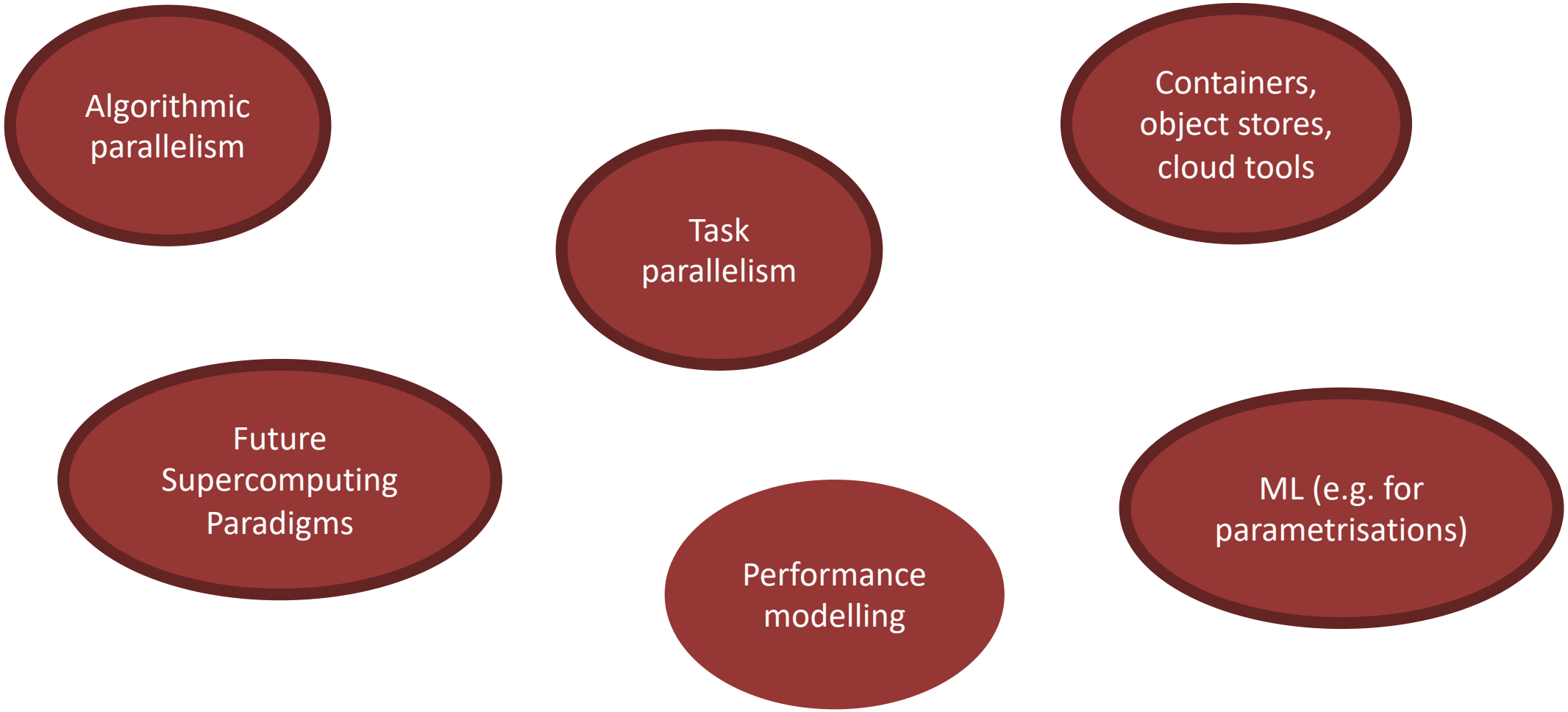
Cross-Cutting Work Package 1

Common Approaches and Solutions – topics (most just starting)



Cross-Cutting Work Package 2

Potential disruptors – topics (Most just starting)



Cross-Cutting: I/O Storage and Middleware

ExCALIData (ExCALIWork, and ExCALIStore – PI Lawrence)

Seven Work Packages; Six distinct activities

1. (WP-I1) Storage Interfaces; Atomic Datasets distributed across storage

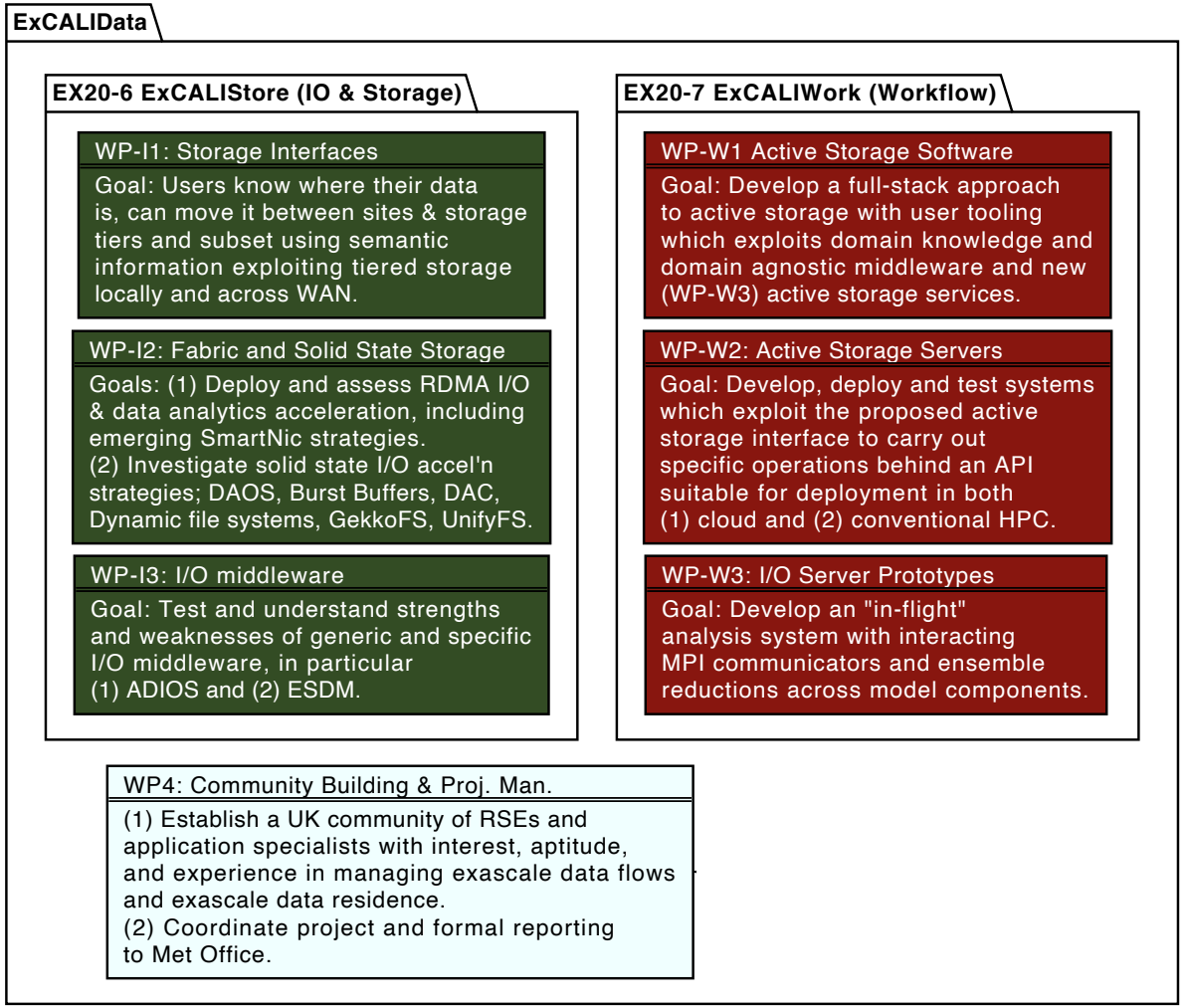
2.(WP-I2) Fabric and Solid State Storage; Understanding technology options

3.(WP-I3) Comparing middleware, generic and discipline specific.

4.(WP-W1 and WP-W2) Active Storage in the DASK software stack (W1) and storage (W2)

5.(WP-W3) Extending I/O server functionality

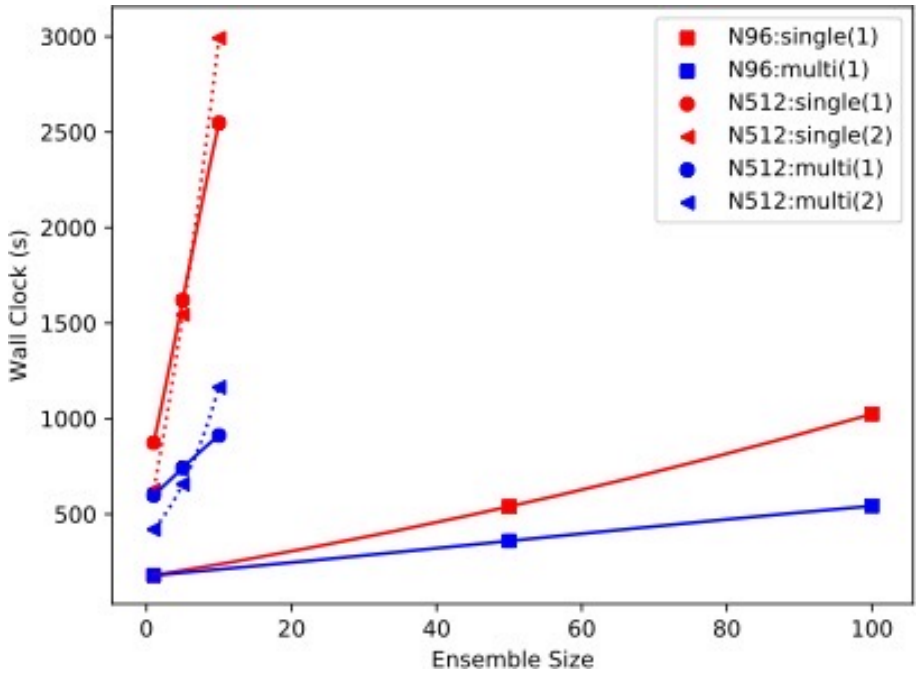
6.(WP4) Community Building

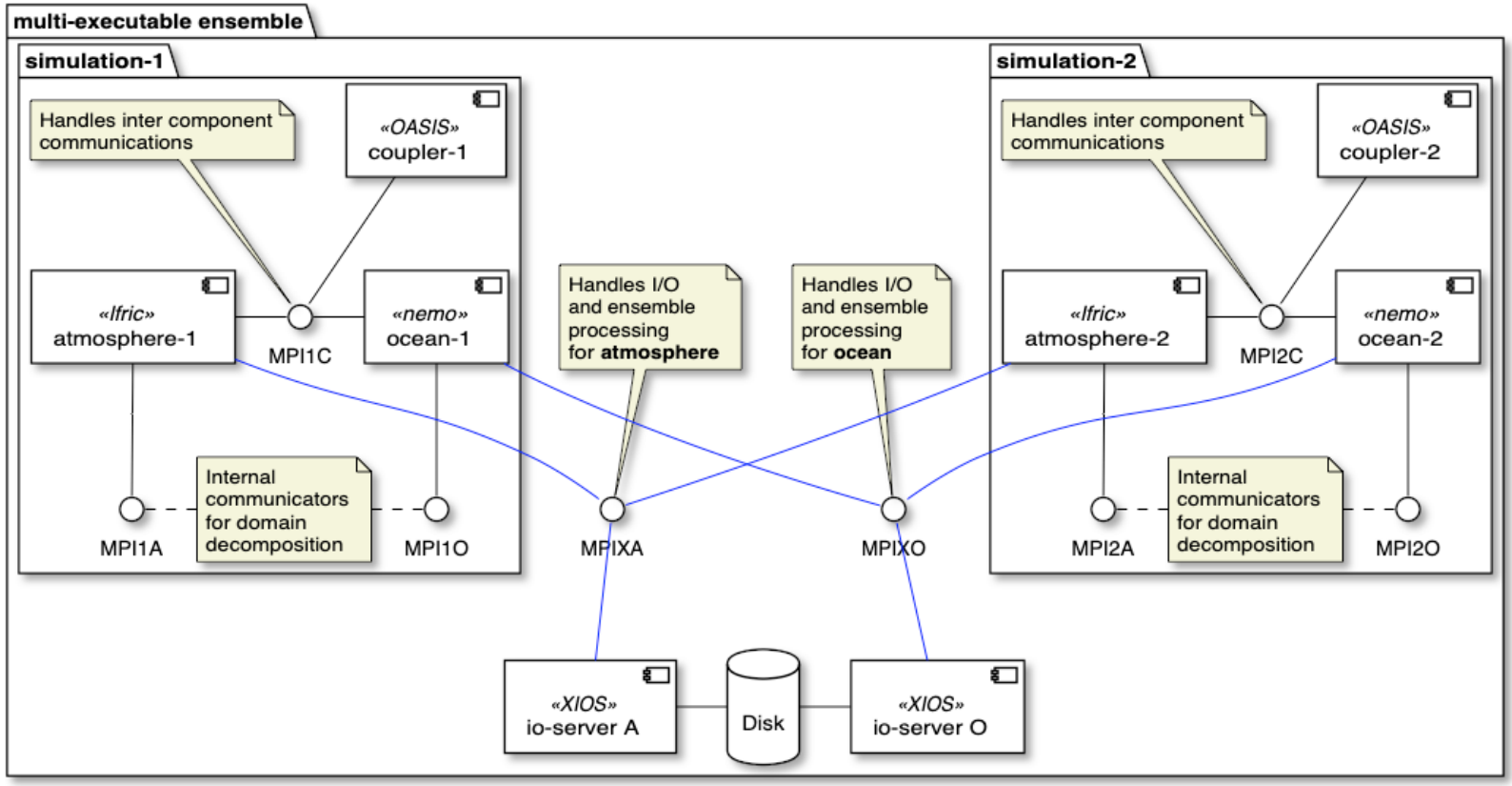


University of Reading · University of Cambridge · StackHPC Ltd · ddn · National Centre for Atmospheric Science, Natural Environment Research Council · ExCALIBUR IO

ExCALIWOrk – Building on ESiWACE

WP- W3 I/O Server Prototypes





Ensemble processing for atmosphere only to be extended for coupled models.
Making use of enhanced XIOS (and new ensemble operators?)

ExCALIDATA – Building on ESiWACE

WPI-I3 I/O Middleware

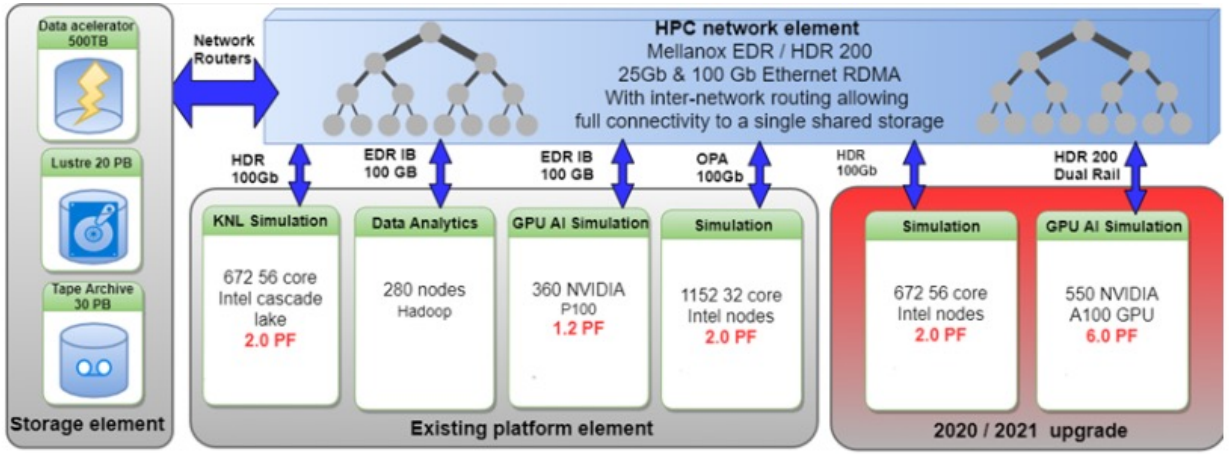
ADIOS2 is generic cross-domain I/O middleware being developed in the US exascale programme. The main objective is to facilitate fast I/O for massively parallel jobs in a heterogeneous storage environment. ADIOS also provides some coupling functionality.

ESDM is I/O middleware developed for application in earth system modelling. It is specifically developed for fast I/O in weather and climate applications.

The objective of this work package is to compare and contrast the ease of use of this middleware in weather and climate and fusion use cases.

- There will be a close relationship between this and WP-W3 where the XIOS sub-system is being used, and we will compare and contrast all three. (XIOS has other capabilities, but we will also look at the ease-of-use and performance in “I/O middleware” mode.)

Exploiting the ExCALIBUR Hardware and Software Enabling Platforms, including the Cambridge Solid State Testbed



Also WP – I2 Fabric and Burst Buffer Configurations

Summary and Schedule

Somewhat behind this schedule for obvious reasons, but catching up

ExCALIBUR Pillars

Separation of Concerns:
Maths of problem separated from computer science of implementation.

Co-design:
Holistic, collaborative design of entire system by mathematicians, domain scientists and computer scientists.

Data Science:
Research new workflows to manage & analyse vast volumes of simulation data.

Investing in People:
Interdisciplinary RSE career development driven by forward-looking scientific software design.