Maximising Sustainability of Isambard AI Exascale Supercomputing Platform, from Data Centre to Compute Nodes

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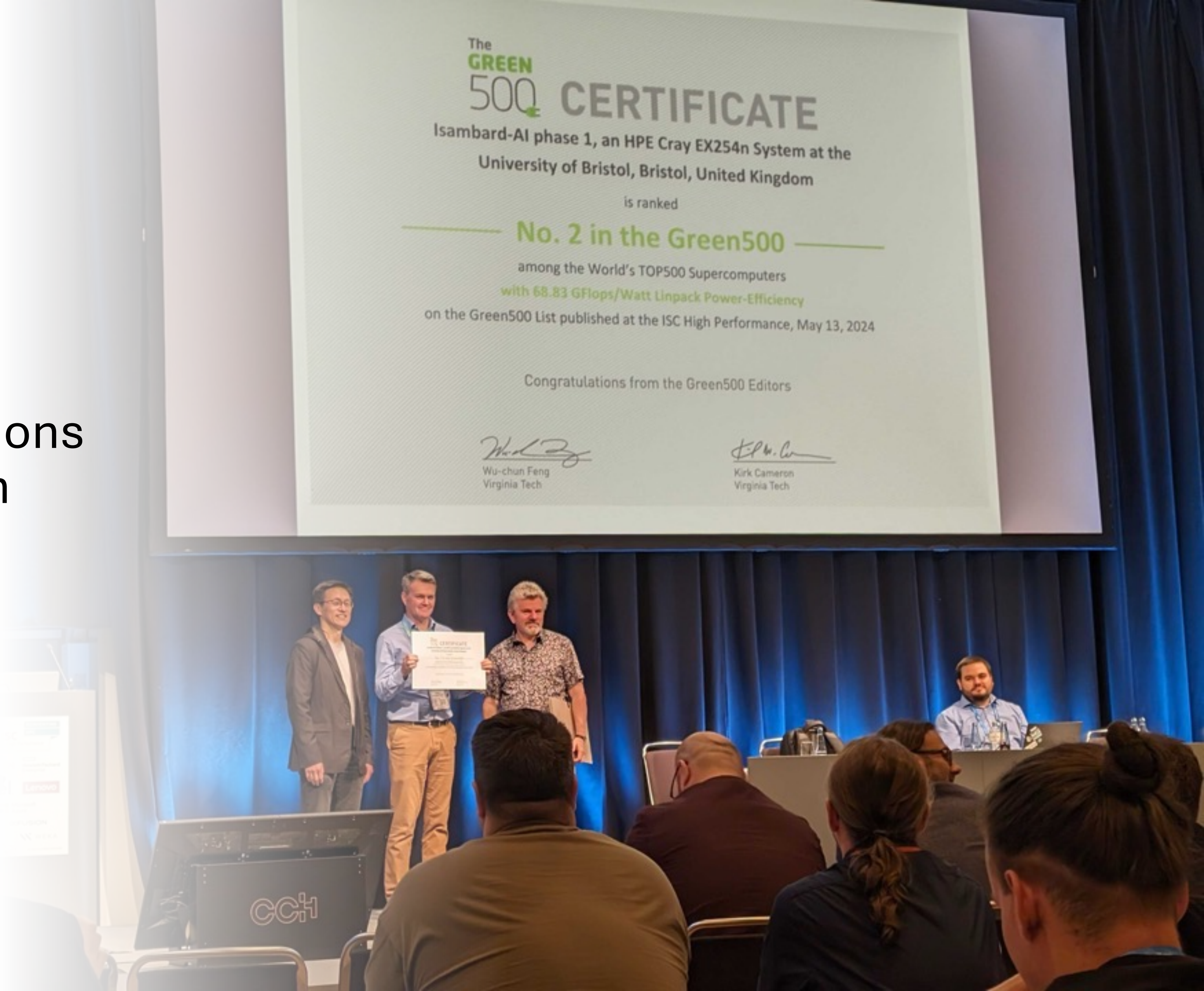
University of Bristol, UK

ExaComm 2024
May 16, 2024
Hamburg, Germany

Outline

- Background and timeline
- Design specifications for an AI Research Resource (AI RR)
  - Sustainability
  - Performance
  - Accessibility
- Next steps



The GREEN 500 CERTIFICATE

Isambard-AI phase 1, an HPE Cray EX254n System at the University of Bristol, Bristol, United Kingdom

is ranked

No. 2 in the Green500

among the World's TOP500 Supercomputers

with 68.83 GFlops/Watt Linpack Power-Efficiency

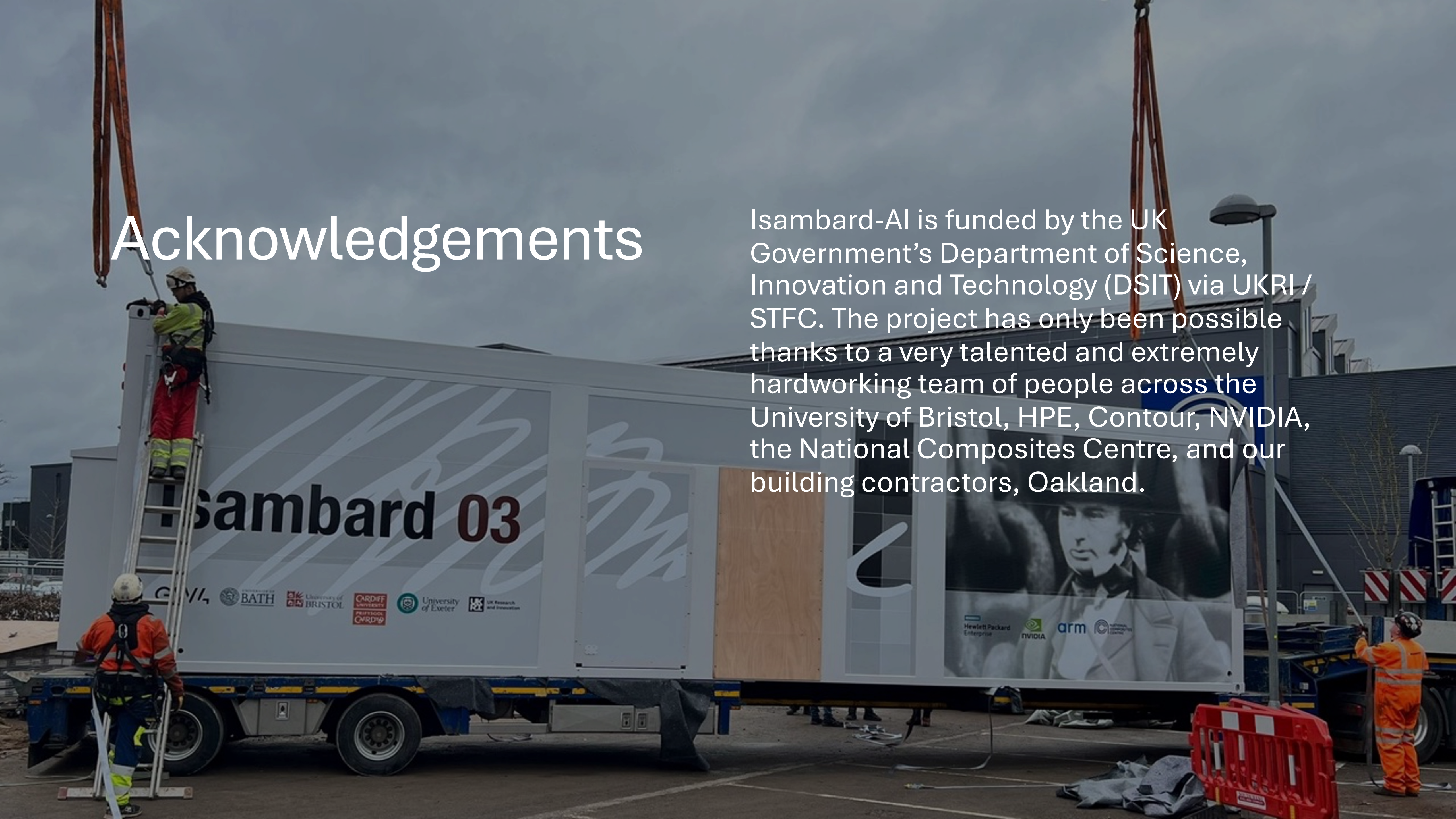
on the Green500 List published at the ISC High Performance, May 13, 2024

Congratulations from the Green500 Editors

Wu-chun Feng
Virginia Tech

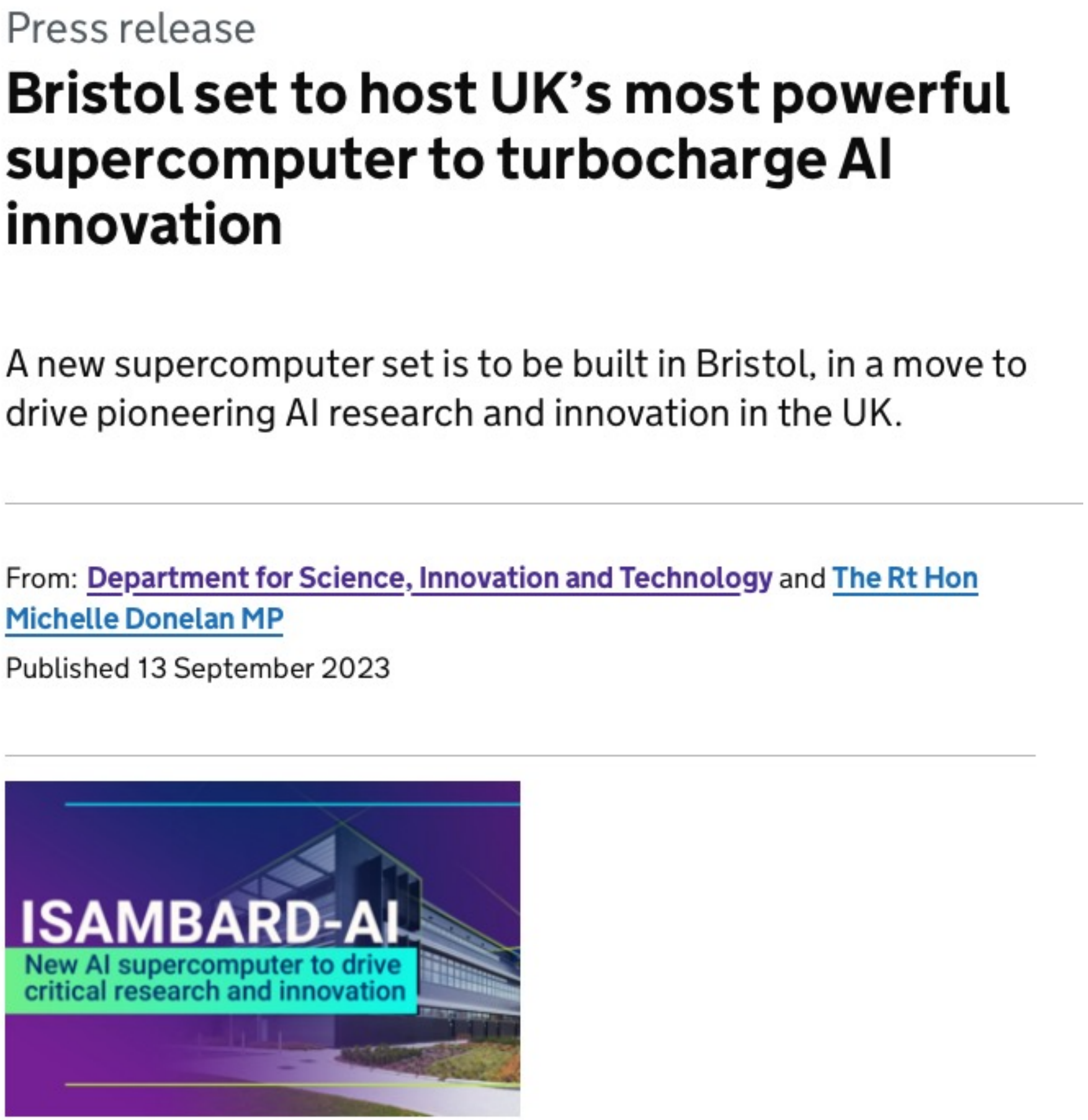
Kirk Cameron
Virginia Tech

University of BRISTOL



Acknowledgements

Isambard-AI is funded by the UK Government’s Department of Science, Innovation and Technology (DSIT) via UKRI / STFC. The project has only been possible thanks to a very talented and extremely hardworking team of people across the University of Bristol, HPE, Contour, NVIDIA, the National Composites Centre, and our building contractors, Oakland.



Press release

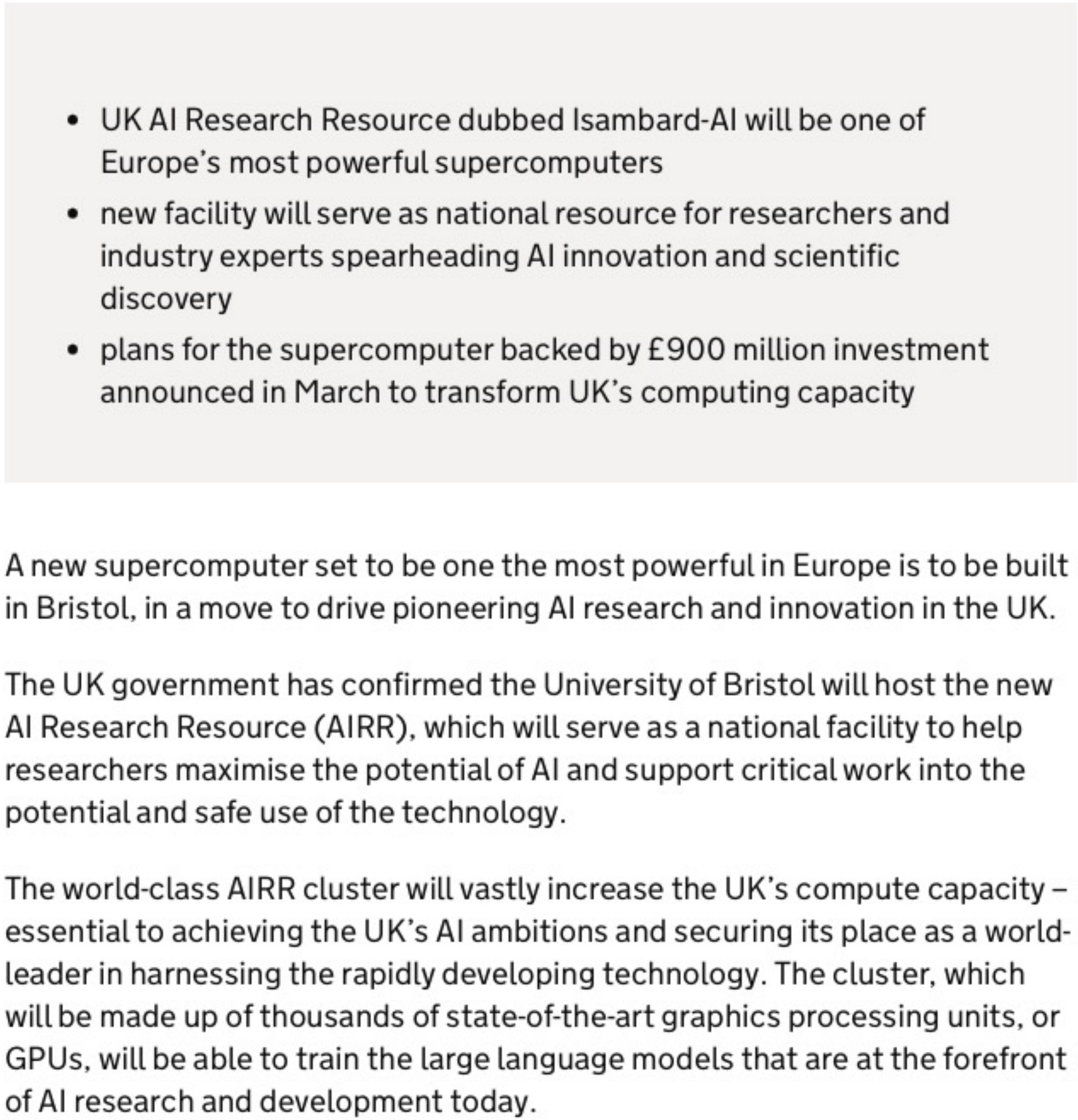
Bristol set to host UK’s most powerful supercomputer to turbocharge AI innovation

A new supercomputer set is to be built in Bristol, in a move to drive pioneering AI research and innovation in the UK.

From: Department for Science, Innovation and Technology and The Rt Hon Michelle Donelan MP

Published 13 September 2023

ISAMBARD-AI
New AI supercomputer to drive critical research and innovation



- UK AI Research Resource dubbed Isambard-AI will be one of Europe’s most powerful supercomputers
- new facility will serve as national resource for researchers and industry experts spearheading AI innovation and scientific discovery
- plans for the supercomputer backed by £900 million investment announced in March to transform UK’s computing capacity

A new supercomputer set to be one the most powerful in Europe is to be built in Bristol, in a move to drive pioneering AI research and innovation in the UK.

The UK government has confirmed the University of Bristol will host the new AI Research Resource (AIRR), which will serve as a national facility to help researchers maximise the potential of AI and support critical work into the potential and safe use of the technology.

The world-class AIRR cluster will vastly increase the UK’s compute capacity – essential to achieving the UK’s AI ambitions and securing its place as a world-leader in harnessing the rapidly developing technology. The cluster, which will be made up of thousands of state-of-the-art graphics processing units, or GPUs, will be able to train the large language models that are at the forefront of AI research and development today.

https://www.gov.uk/government/news/bristol-set-to-host-uks-most-powerful-supercomputer-to-turbocharge-ai-innovation

2016–July 2023

(ARM based Isambard 1, 2) Isambard 3 in 2023/4 (no data centre and Isambard PI Simon MS with a non-dedicated GW4 team)

Aug. 2023

UK govt feedback on Bristol’s Isambard-AI proposal

Sep.–Oct. 2023

Isambard-AI procurement

Nov. 2023

AI Safety Summit

Dec. 2023

Isambard hiring started

Mar. 2024

Modular data centre (POD) and Isambard-AI phase 1 installed + a new team in ~3 months

Apr. 2024

Service configuration and hardening for AI users

May 2024

Running AI and HPC applications

microsoft
/Phi-3-mini-128k-instruct
huggingface.co

```
"Who is Isambard?"
running on Isambard-AI
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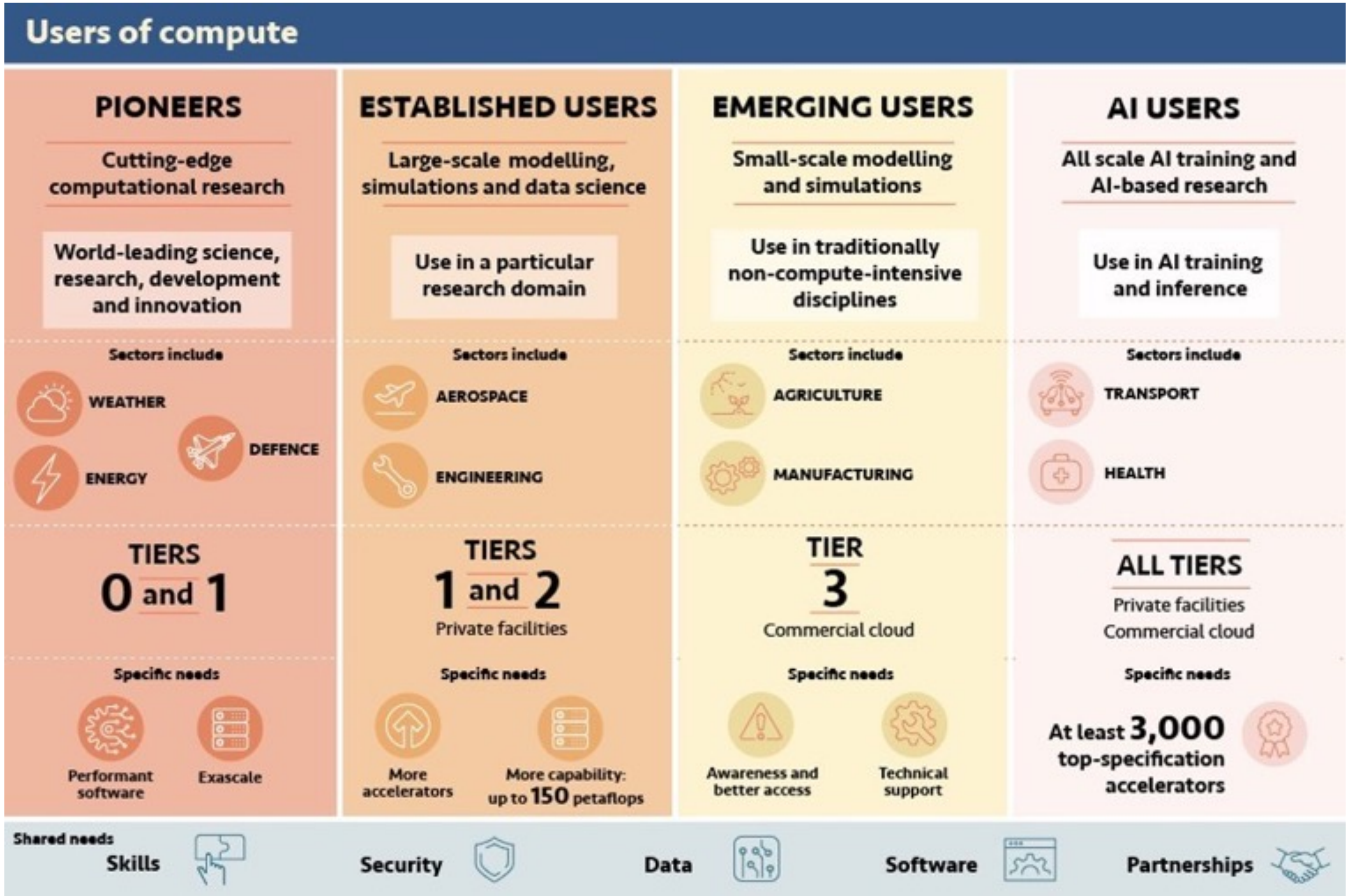
Design Specifications for AI Research Resource (RR)



Users of compute

PIONEERS	ESTABLISHED USERS	EMERGING USERS	AI USERS
Cutting-edge computational research	Large-scale modelling, simulations and data science	Small-scale modelling and simulations	All scale AI training and AI-based research
World-leading science, research, development and innovation	Use in a particular research domain	Use in traditionally non-compute-intensive disciplines	Use in AI training and inference
Sectors include WEATHER DEFENCE ENERGY	Sectors include AEROSPACE ENGINEERING	Sectors include AGRICULTURE MANUFACTURING	Sectors include TRANSPORT HEALTH
TIERS 0 and 1	TIERS 1 and 2 Private facilities	TIER 3 Commercial cloud	ALL TIERS Private facilities Commercial cloud
Specific needs Performant software Exascale	Specific needs More accelerators More capability: up to 150 petaflops	Specific needs Awareness and better access Technical support	Specific needs At least 3,000 top-specification accelerators

Shared needs: Skills, Security, Data, Software, Partnerships

Accessible to all users

Sustainable AI supercomputing

Accessible to all sectors

Performance for all tiers

Sustainable AI RR program

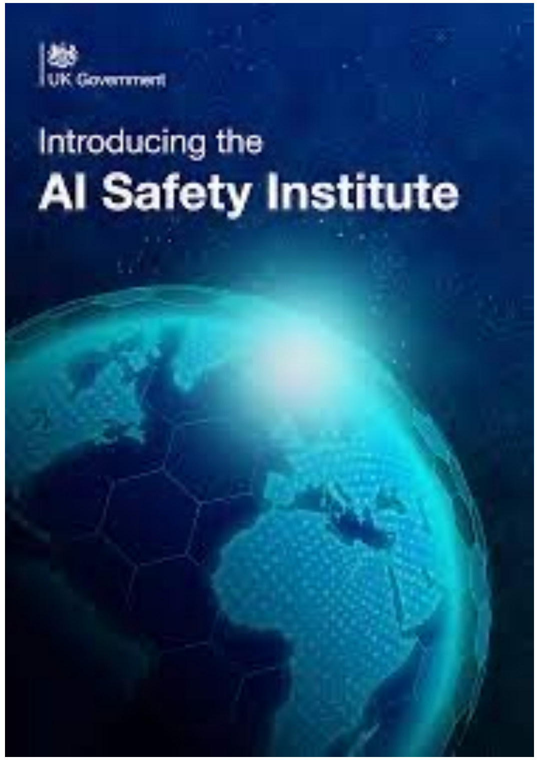
References: Independent Review of The Future of Compute: Final report and recommendations, March 2023; National AI Strategy - AI Action Plan, July 2022; £300 million to launch first phase of new AI Research Resource

What is Isambard-AI for?

- UKRI-funded AI research in the UK, e.g.:
  - Training large language models
  - Large-scale inference
  - Foundational AI research
  - AI safety and understanding
  - Hybrid AI + simulation workflows
  - Machine learning
- Research on Isambard-AI must have a strong AI component
- Accommodate GPU jobs at any scale
  - Interactivity via JupyterHub—single to 100s of GPUs
  - Long running jobs for large-scale training—10s to 1000s of GPUs

UKRI UK Research and Innovation

Department for Science, Innovation, & Technology


UK Government

Introducing the

AI Safety Institute

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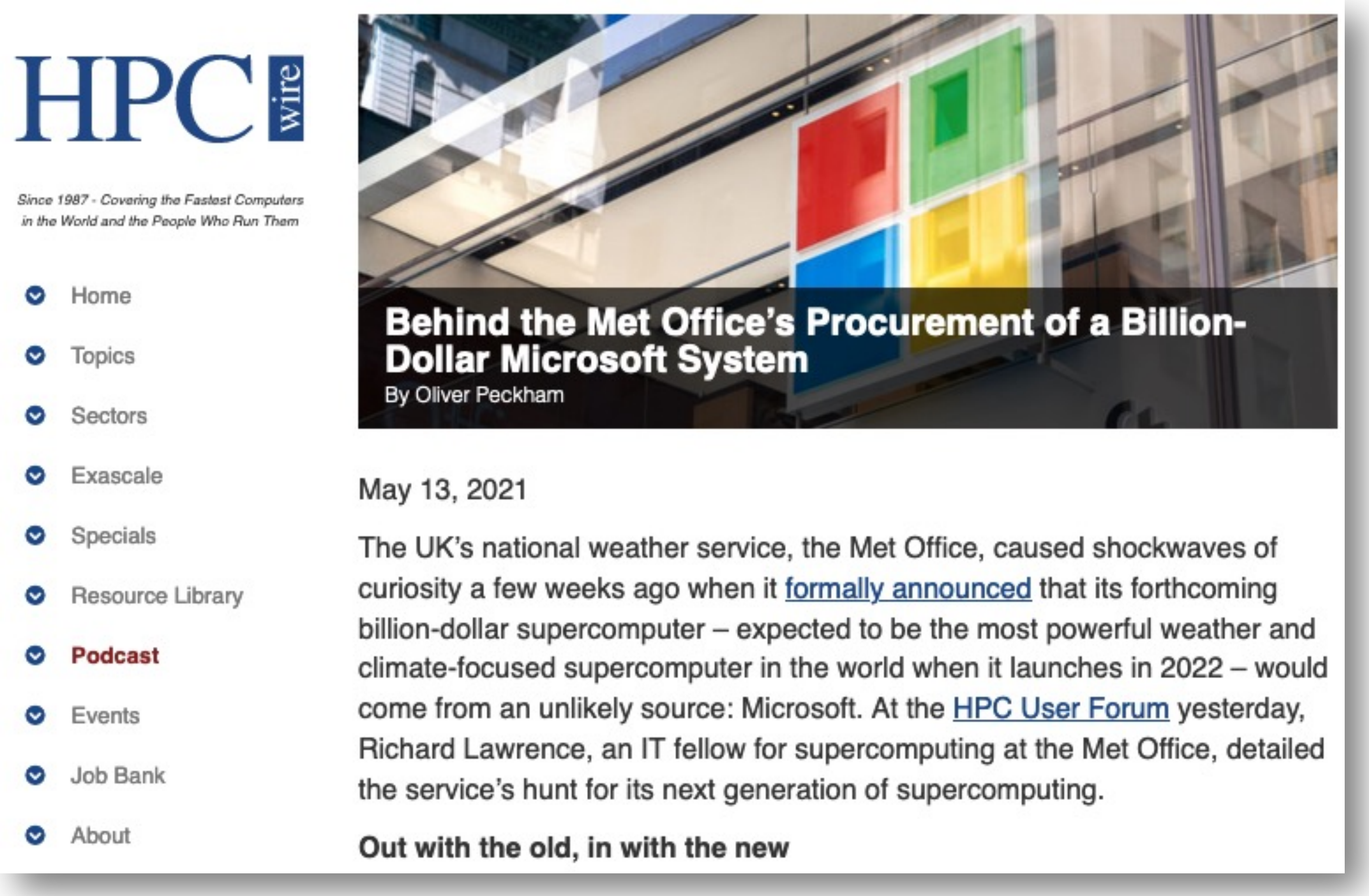
Sustainability as a Key Design Principle

- Optimisation targets
  - PUE = Power Usage Effectiveness
    - Target <1.1
  - CUE = Carbon Usage Effectiveness
    - Non-fossil fuel sources
  - Plan for heat reuse for nearby buildings and local district heat circuit in future
- Aligning with university of Bristol Net Zero and sustainability targets for 2030
  - Categorising emissions
    - Scope 1 (~0%), 2 (90%) and 3 (10%)—based on an average UK data of 0.2123 kg CO2/kWh (IEA 2022 data)
  - Recycling 90% of components at the end of life in the UK

Isambard 1, 2 & 3 – Leading ARM for HPC since 2016 as a UK national tier-2 resource

- Isambard 1 and 2 hosted at the UK Met Office data centre
- Options considered:
  - Renting space in a DC—£££ plus not available for hundreds of KW DLC cabinets like Cray HPE XE
  - Building new-–time and ££££
- Solution—containersied data centre or MDC


HPC wire
Since 1987 - Covering the Fastest Computers in the World and the People Who Run Them
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Behind the Met Office's Procurement of a Billion-Dollar Microsoft System

By Oliver Peckham

May 13, 2021

The UK's national weather service, the Met Office, caused shockwaves of curiosity a few weeks ago when it formally announced that its forthcoming billion-dollar supercomputer – expected to be the most powerful weather and climate-focused supercomputer in the world when it launches in 2022 – would come from an unlikely source: Microsoft. At the HPC User Forum yesterday, Richard Lawrence, an IT fellow for supercomputing at the Met Office, detailed the service's hunt for its next generation of supercomputing.

Out with the old, in with the new

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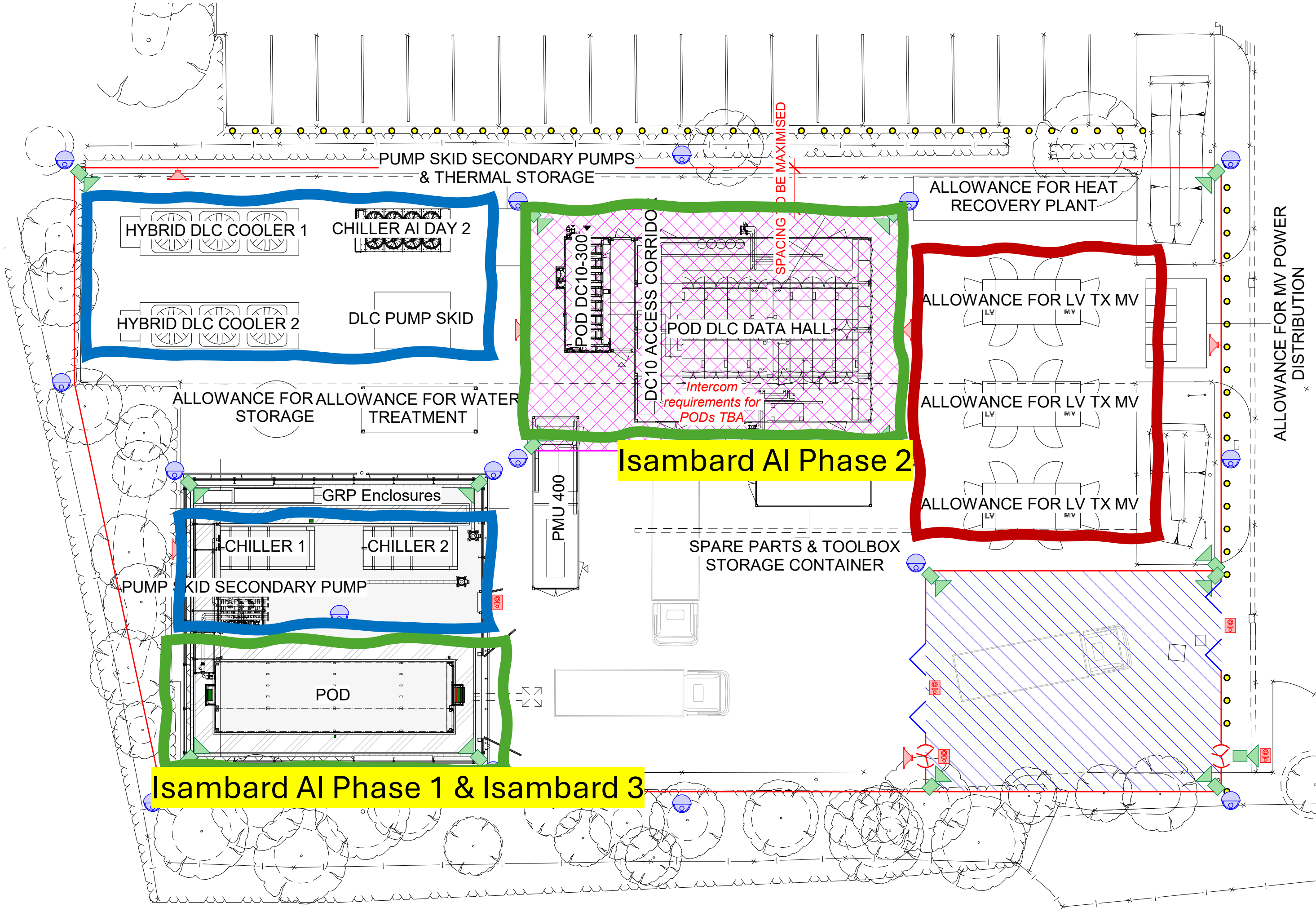
What is an MDC

- Modular, self-contained & agile
  - Described as Lego blocks—designed and tuned for functional and performance specifications e.g. high availability, security, etc.
  - Everything from all IT (compute, network & storage), power (UPS, batteries) and cooling can be included as self-contained units
- Efficient and flexible deployments
  - Typically built and commissioned in months
  - Accommodates different environmental conditions
    - On-site integration options
    - Offsite integration options
- Sustainable
  - Holistic, fine-grain telemetry via DCIM
  - Upgradable, refreshable, recyclable with a lifespan on 10-15 years

The Isambard Site (Isambard AI phase 1 & 2, and Isambard 3)



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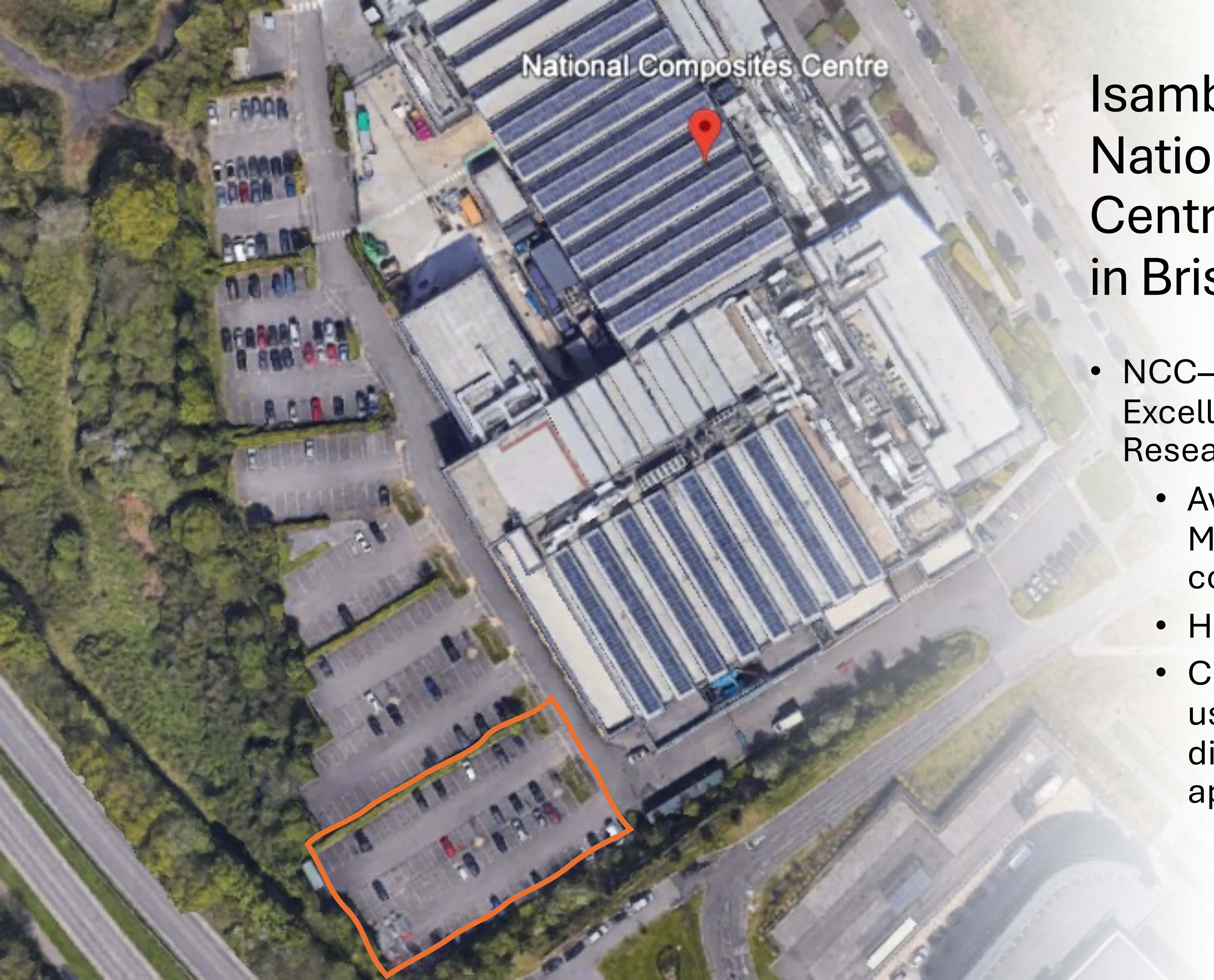


Isambard Site – National Composite Centre (NCC) Facility in Bristol

- NCC—UK's Centre of Excellence for Composites Research and Development
  - Availability of power (~10 MW), networking and cooling
  - Heat reuse options
  - Co-location with industrial user community that has a digitalisation first approach

Physical Space Constraints at NCC

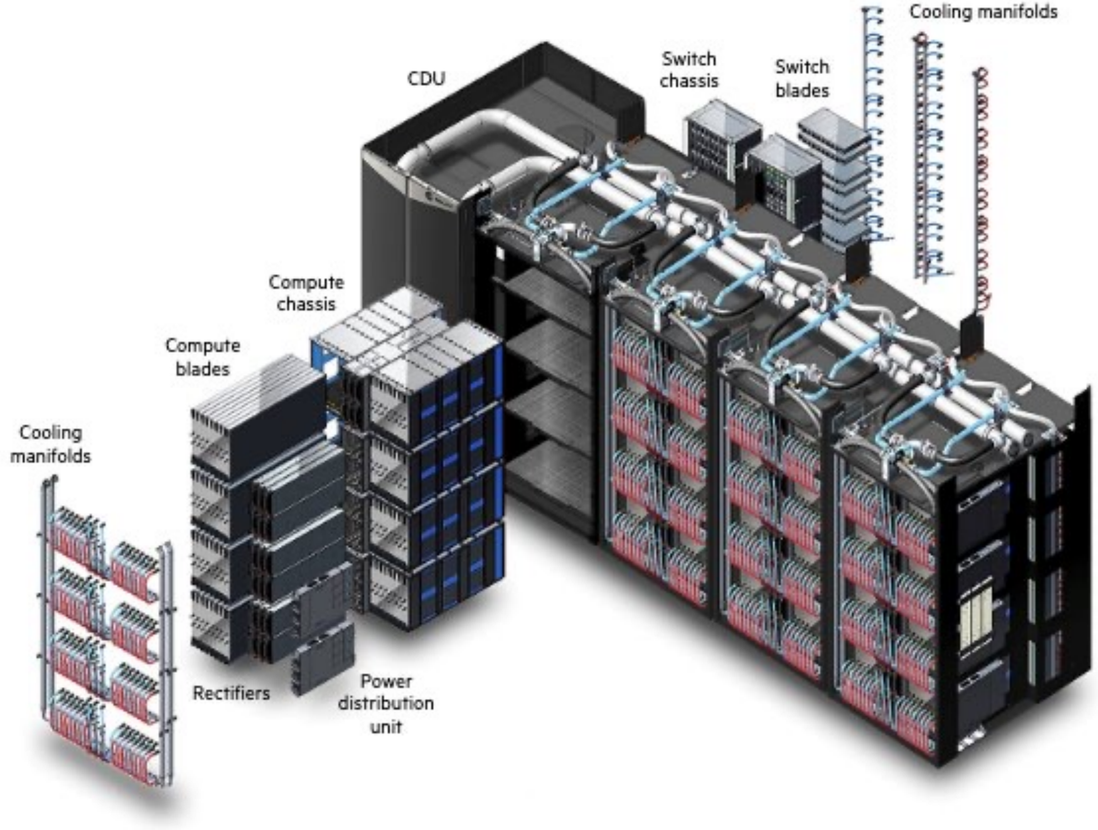
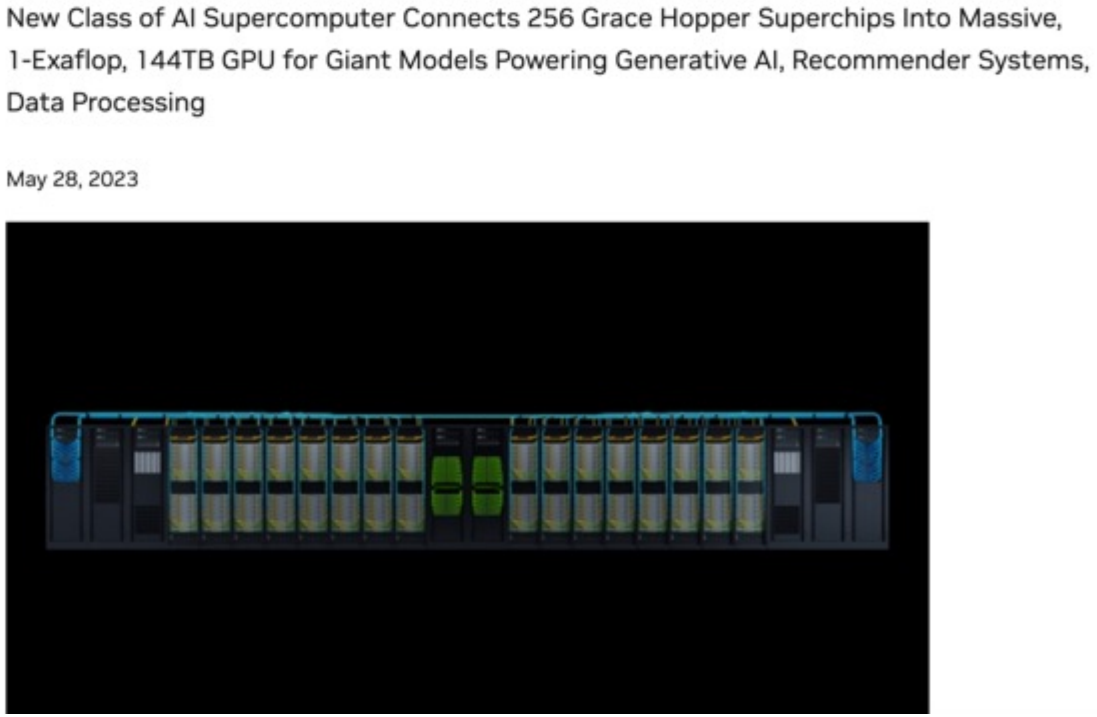


FIGURE 1. HPE Cray EX cabinet exploded view

~5,300 GPUs in **12 EX4000 cabinets**



New Class of AI Supercomputer Connects 256 Grace Hopper Superchips Into Massive, 1-Exaflop, 144TB GPU for Giant Models Powering Generative AI, Recommender Systems, Data Processing

May 28, 2023

DGX SuperPOD with **256 GPUs in 16 cabinets**

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HPE EX Series DLC and Nvidia GH 200

- HPE EX solution
  - Direct liquid cooling for high performance computing and networking
- 4-way Nvidia GHr superchip
  - NVLink-C2C also only uses 1.3 picojoules/bit transferred—5x more energy efficient than PCIe Gen 5

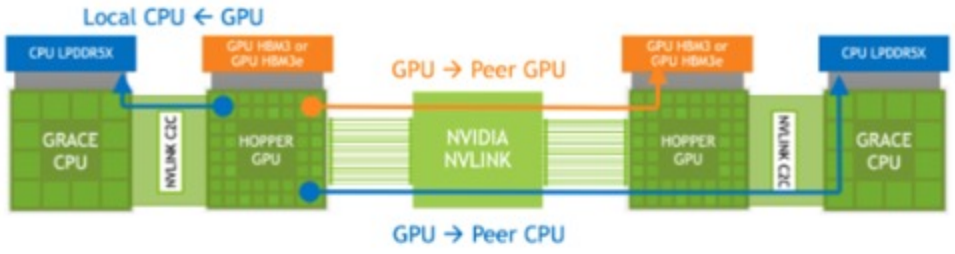

Figure 5. Memory Accesses across NVLink-connected Grace Hopper Superchips

Source: NVIDIA Grace Hopper Superchip Architecture Whitepaper

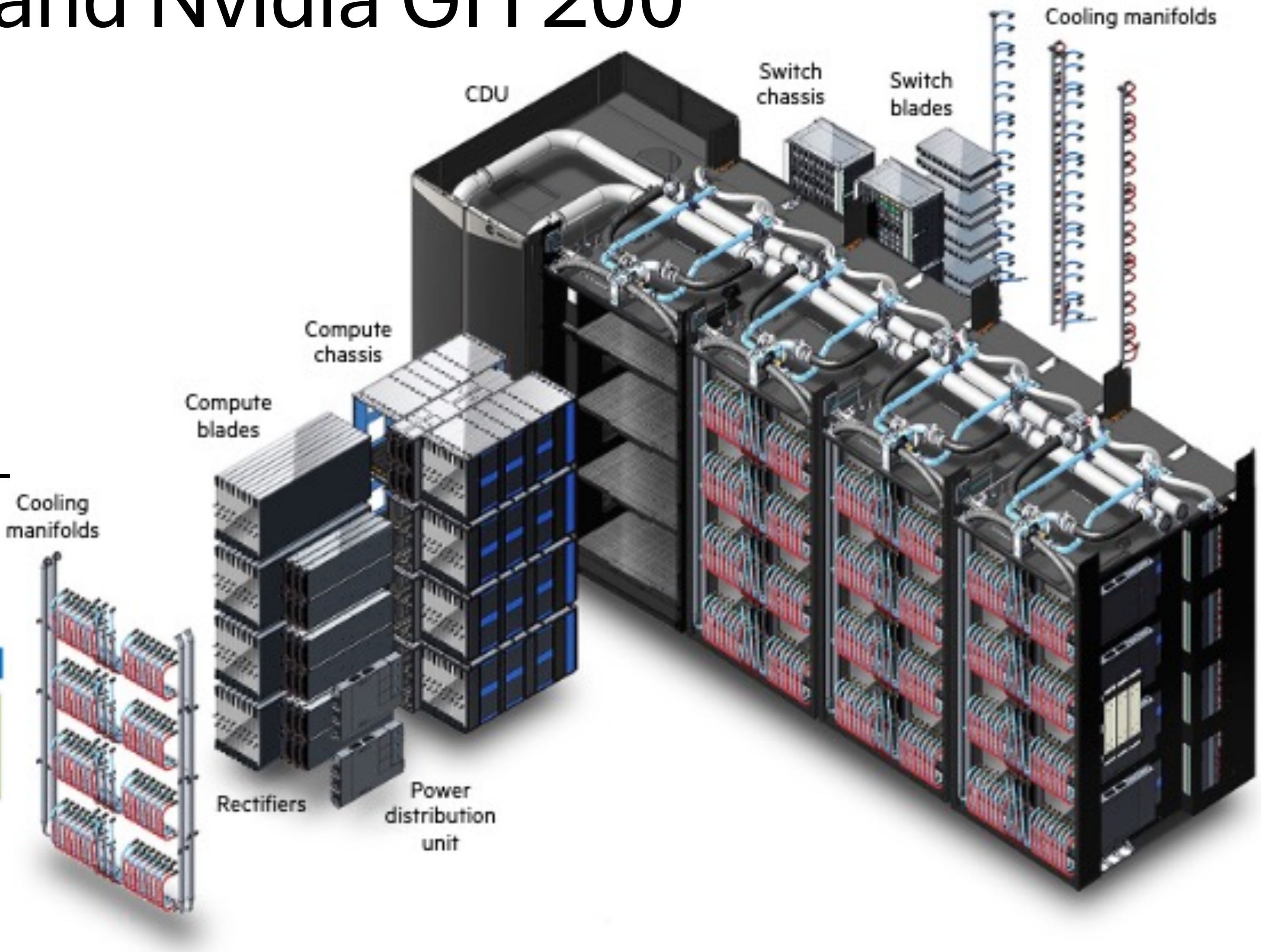

FIGURE 1. HPE Cray EX cabinet exploded view

Source: HPE CRAY EX Liquid-Cooled Cabinet for Large Scale Systems brochure

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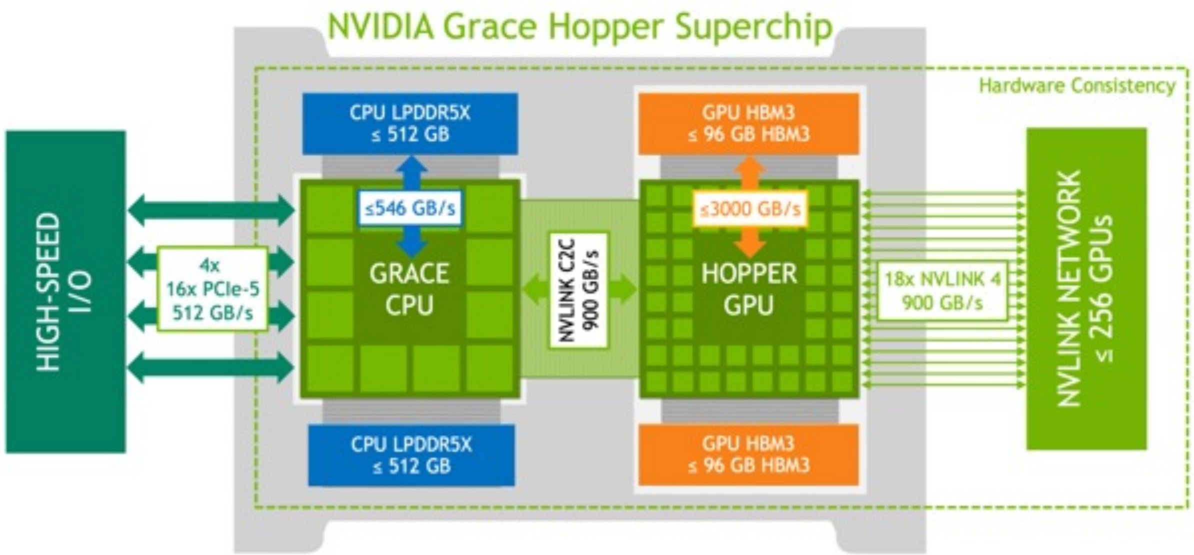
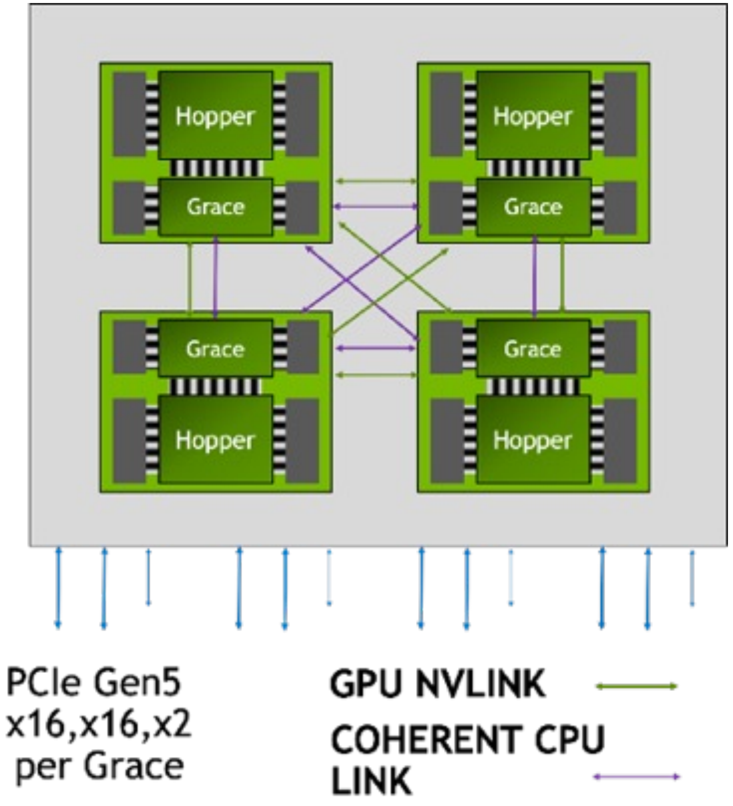
Grace-Hopper Superchip & HPE EX Compute Blade



Source: NVIDIA Grace Hopper Superchip Architecture Whitepaper



Source: HPE EX4000 Grace-Hopper blade

4 x Grace ARM CPUs
288 cores
512 GB Memory

4 x Hopper GPUs
~260 64-bit Tflops, ~16k 8-bit Tflops
384 GB High Bandwidth Memory

896 GB Memory Total
NVLink-C2C = 900 GB/s

Isambard AI node = 4 x GH200
Injection bandwidth = 4 x 200 Gbps

Memory Architecture of GH 200

A boon for developers and users

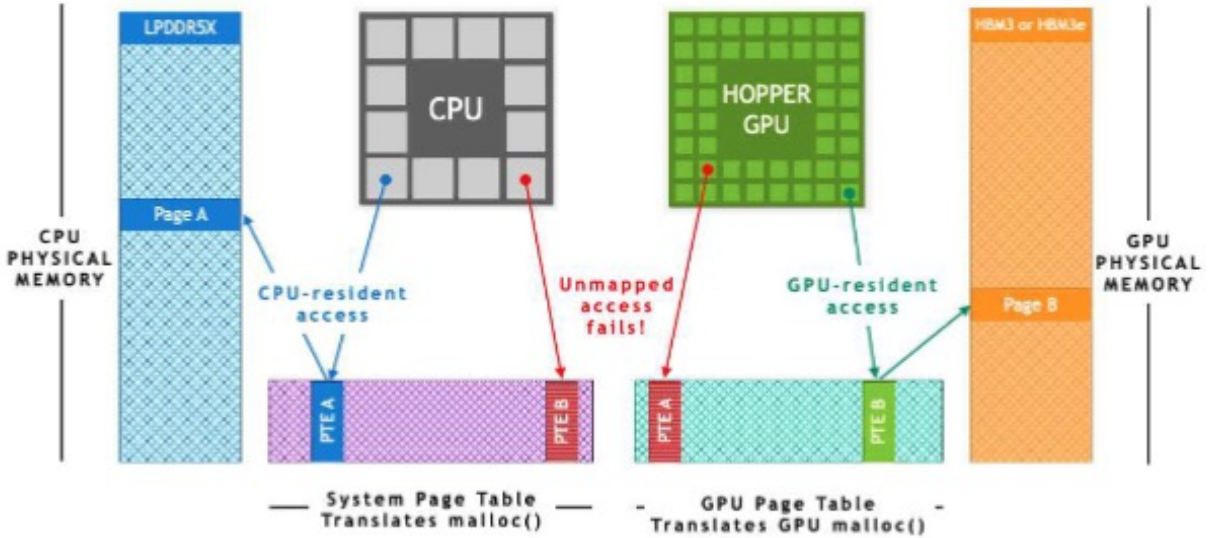


Figure 7. NVIDIA Hopper System with Disjoint Page Tables

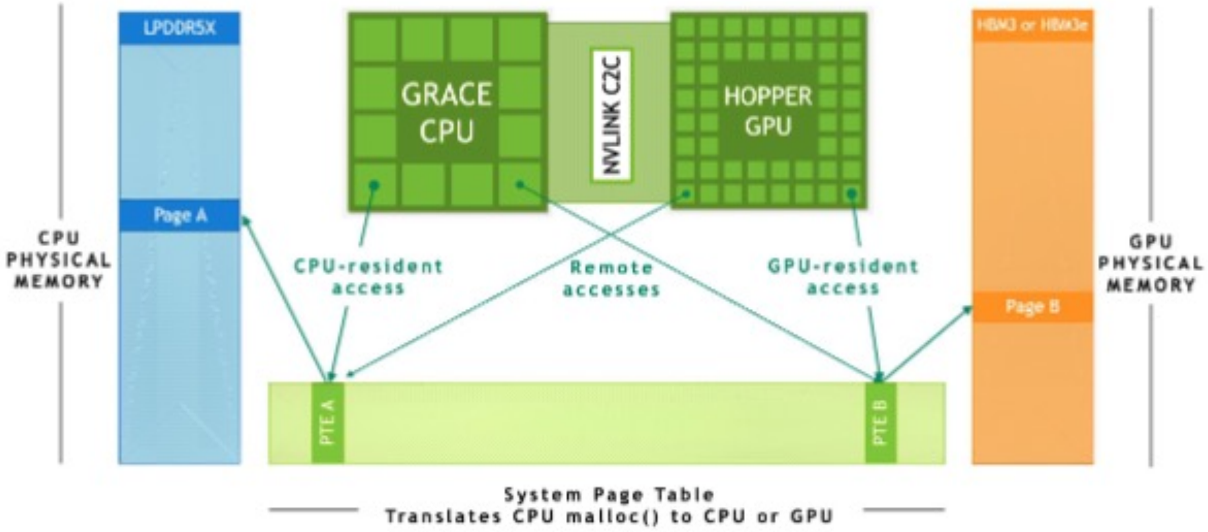


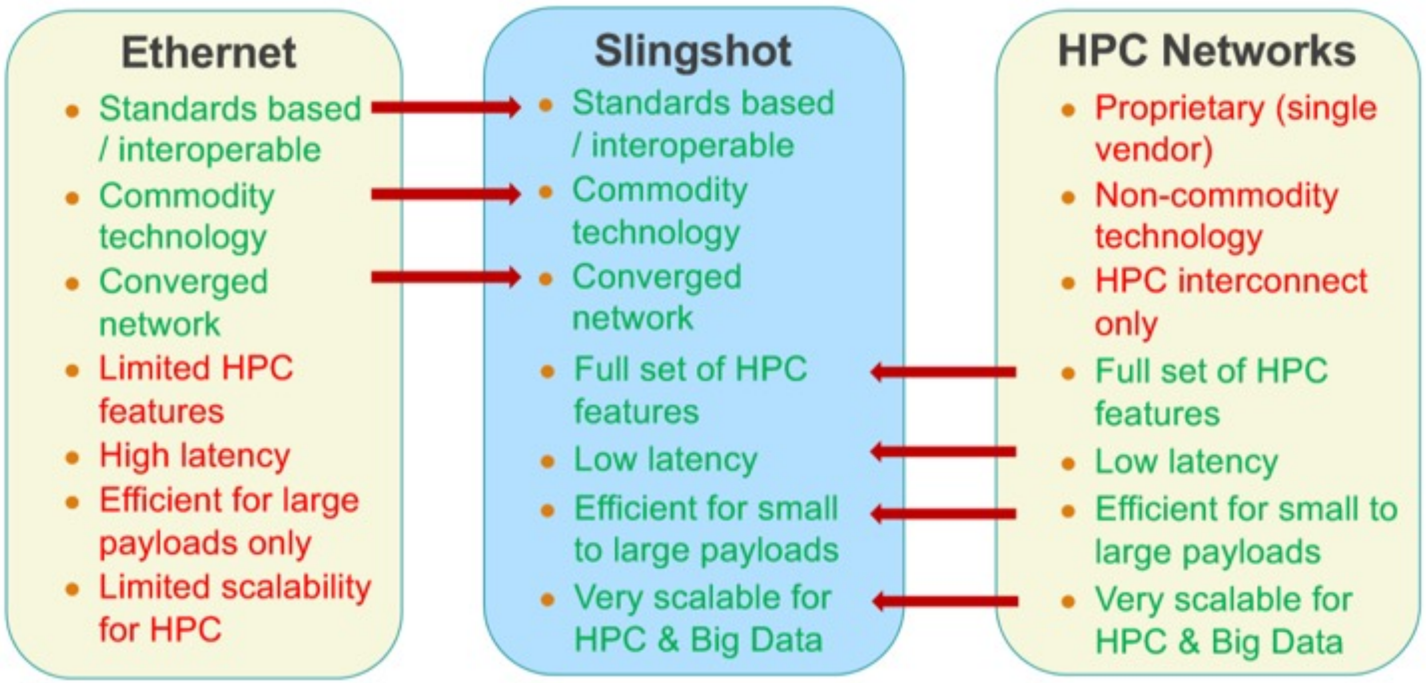
Figure 8. ATS in an NVIDIA Grace Hopper Superchip System

Source: NVIDIA Grace Hopper Superchip Architecture Whitepaper

In PCIe-connected x86+Hopper systems, the CPU and the GPU have independent per process page tables, and system allocated memory is not directly accessible from the GPU

Address Translation Service (ATS) enables the CPU and GPU to share a single per-process page table, enabling all CPU and GPU threads to access all system-allocated memory

HPE SlingShot High Speed Interconnect for AI & HPC



Ethernet

- Standards based / interoperable
- Commodity technology
- Converged network
- Limited HPC features
- High latency
- Efficient for large payloads only
- Limited scalability for HPC

Slingshot

- Standards based / interoperable
- Commodity technology
- Converged network
- Full set of HPC features
- Low latency
- Efficient for small to large payloads
- Very scalable for HPC & Big Data

HPC Networks

- Proprietary (single vendor)
- Non-commodity technology
- HPC interconnect only
- Full set of HPC features
- Low latency
- Efficient for small to large payloads
- Very scalable for HPC & Big Data

Source: https://www.nextplatform.com/2019/08/16/how-cray-makes-ethernet-suited-for-hpc-and-ai-with-slingshot/

Liquid cooled interconnect (sustainability & scalability)
Example with 16-switch group
2 switches per chassis for single injection to 32 compute nodes (8 compute blades)
6 switches per cabinet for single injection to 256 compute nodes (64 compute blades)

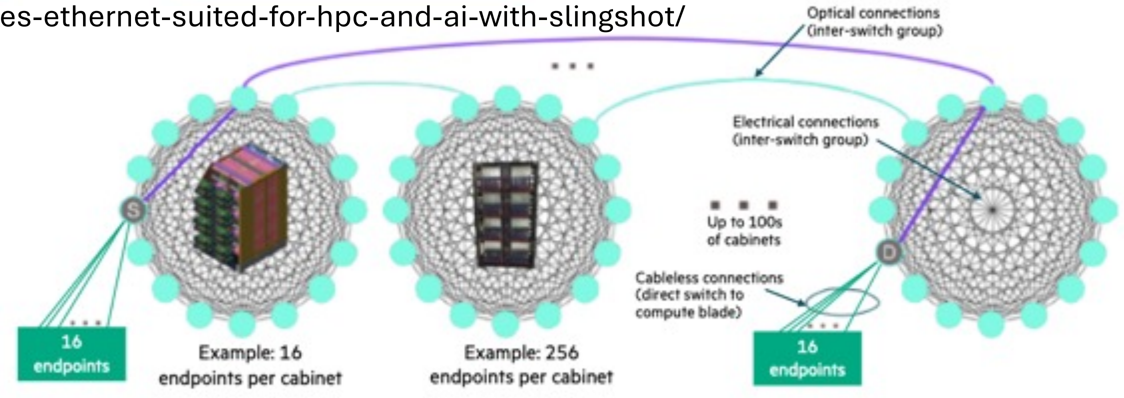

Optical connections (inter-switch group)
Electrical connections (inter-switch group)
Up to 100s of cabinets
Cableless connections (direct switch to compute blade)
S
D
16 endpoints
Example: 16 endpoints per cabinet
Example: 256 endpoints per cabinet
16 endpoints

FIGURE 7. Example of Dragonfly topology in HPE Slingshot switches

Source: HPE CRAY EX Liquid-Cooled Cabinet for Large Scale Systems brochure

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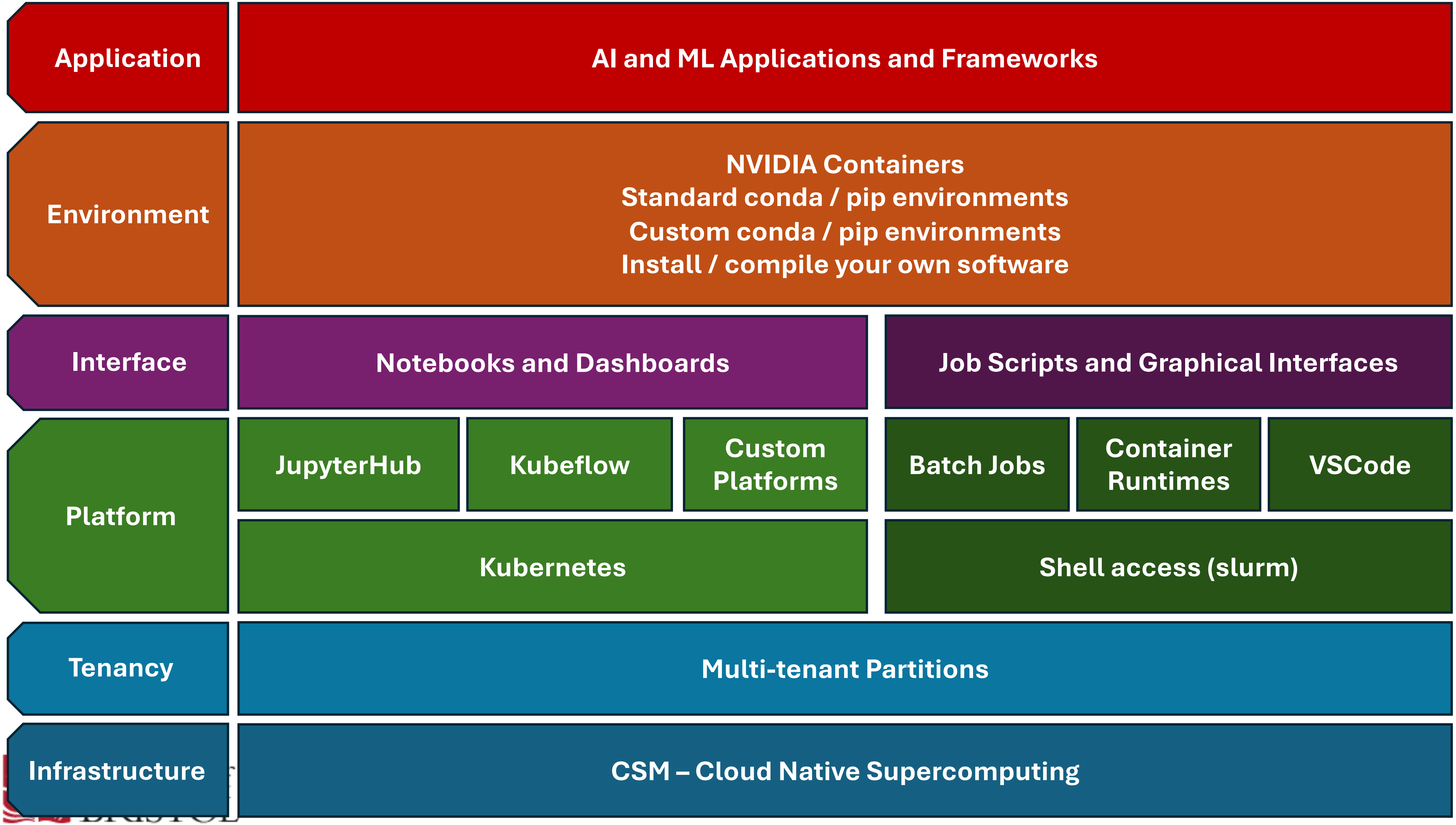


Application

AI and ML Applications and Frameworks

Environment

NVIDIA Containers
Standard conda / pip environments
Custom conda / pip environments
Install / compile your own software

Interface

Notebooks and Dashboards

Job Scripts and Graphical Interfaces

Platform

JupyterHub

Kubeflow

Custom Platforms

Batch Jobs

Container Runtimes

VSCode

Kubernetes

Shell access (slurm)

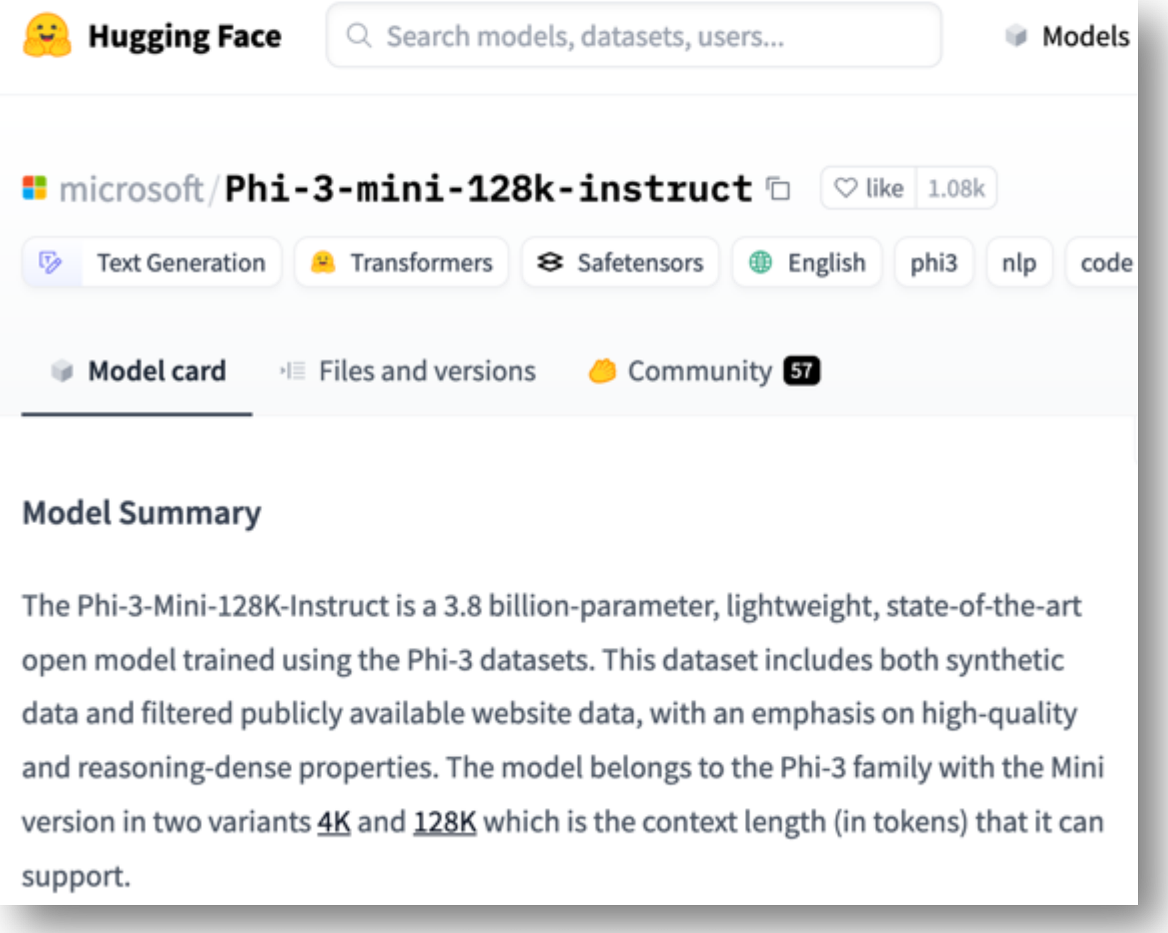
Tenancy

Multi-tenant Partitions

Infrastructure

CSM – Cloud Native Supercomputing

Isambard-AI >> Who is Isambard?



Model Summary

The Phi-3-Mini-128K-Instruct is a 3.8 billion-parameter, lightweight, state-of-the-art open model trained using the Phi-3 datasets. This dataset includes both synthetic data and filtered publicly available website data, with an emphasis on high-quality and reasoning-dense properties. The model belongs to the Phi-3 family with the Mini version in two variants 4K and 128K which is the context length (in tokens) that it can support.

```
Isambard Kingdom Brunel was a renowned
British engineer and architect who
lived from April 9, 1806, to September
15, 1859. He is best known for his
significant contributions to the
development of the United Kingdom's
infrastructure during the Industrial
Revolution. Brunel designed and built
numerous important structures,
including the Great Western Railway,
which connected London to the west of
England and Wales. He also designed
several iconic bridges, tunnels, and
ships, such as the SS Great Britain,
the first iron-hulled, screw propelled
ship. Brunel's innovative designs and
engineering feats have left a lasting
legacy in the field of engineering.
```

Phi-3 Mini installed on pytorch through, pip, using cuda 11.8 on GH200 GPU, using ~7GB of HBM3.

Contact Wahab Kawafi a.kawafi@bristol.ac.uk for details

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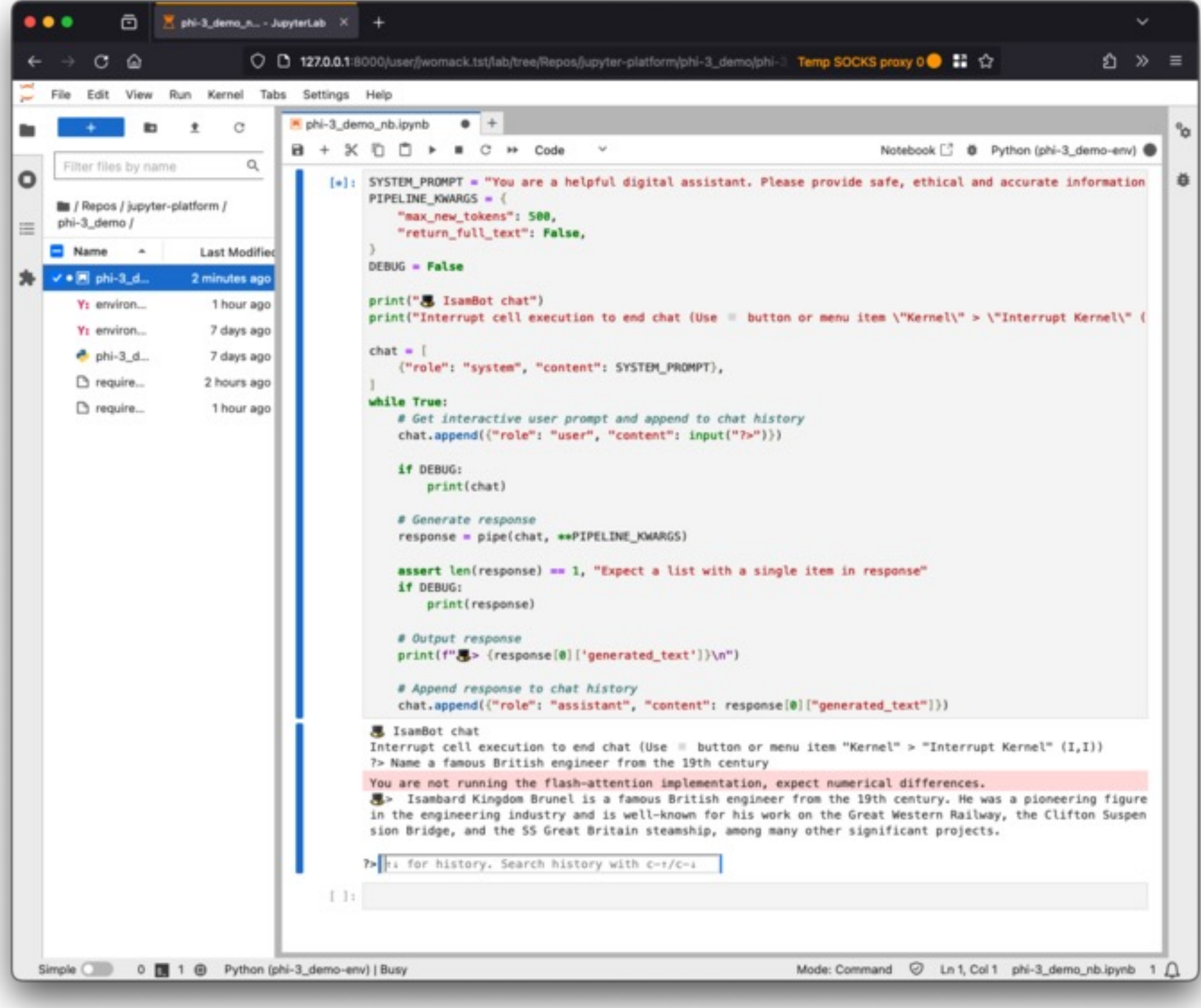
IsamBot running in a Jupyter notebook on Isambard-AI (spawned by JupyterHub on a rCN)



```
[*]: SYSTEM_PROMPT = "You are a helpful digital assistant. Please provide safe, ethical and accurate information
     PIPELINE_KWARGS = {
         "max_new_tokens": 500,
         "return_full_text": False,
     }
     DEBUG = False

     print("🎩 IsamBot chat")
     print("Interrupt cell execution to end chat (Use ■ button or menu item \"Kernel\" > \"Interrupt Kernel\" (

     chat = [
         {"role": "system", "content": SYSTEM_PROMPT},
     ]
     while True:
         # Get interactive user prompt and append to chat history
         chat.append({"role": "user", "content": input("?>")})

         if DEBUG:
             print(chat)

         # Generate response
         response = pipe(chat, **PIPELINE_KWARGS)

         assert len(response) == 1, "Expect a list with a single item in response"
         if DEBUG:
             print(response)

         # Output response
         print(f"🎩> {response[0]['generated_text']}\n")

         # Append response to chat history
         chat.append({"role": "assistant", "content": response[0]["generated_text"]})
```

```
🎩 IsamBot chat
Interrupt cell execution to end chat (Use ■ button or menu item "Kernel" > "Interrupt Kernel" (I,I))
?> Name a famous British engineer from the 19th century
You are not running the flash-attention implementation, expect numerical differences.
🎩>  Isambard Kingdom Brunel is a famous British engineer from the 19th century. He was a pioneering figure
in the engineering industry and is well-known for his work on the Great Western Railway, the Clifton Suspen
sion Bridge, and the SS Great Britain steamship, among many other significant projects.

?> ↑↓ for history. Search history with c-↑/c-↓
```

```
[ ]:
```

Contact James Womack
j.c.womack@bristol.ac.uk
for details

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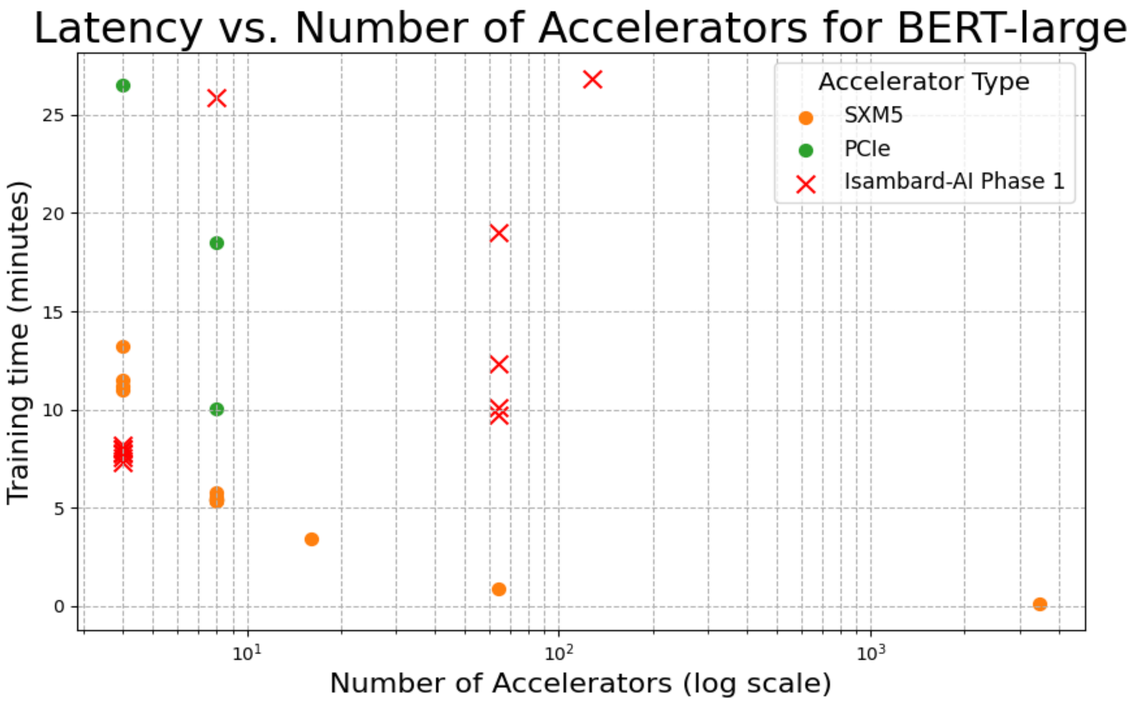
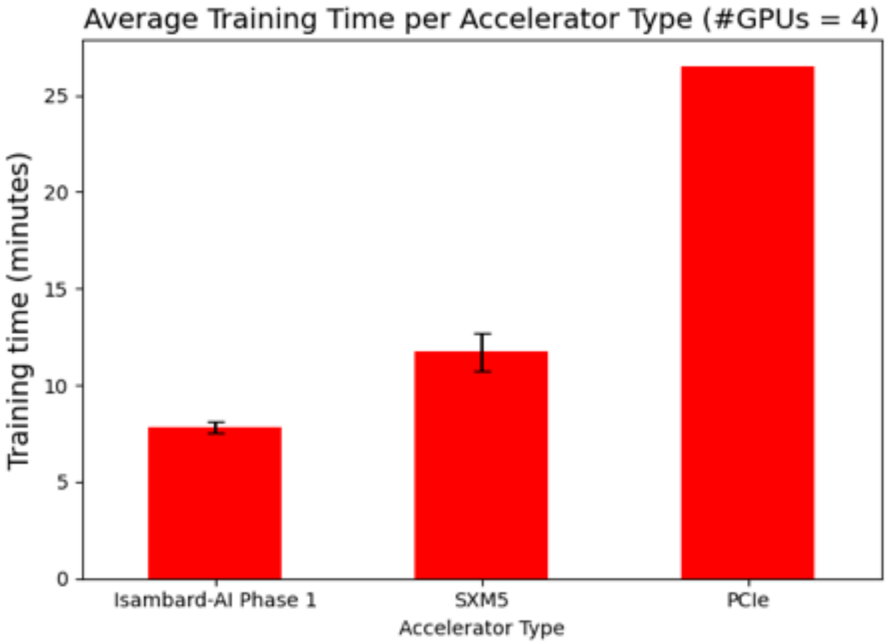
MLPerf Training Early Results (Bert-Large)

https://mlcommons.org/benchmarks/training/

Contact Wahab Kawafi for details:
a.kawafi@bristol.ac.uk





With Slingshot 2.1, libfabric 1.15.2.0 and GPU RDMA enabled. Promising single node results, but more fine tuning required to scale.

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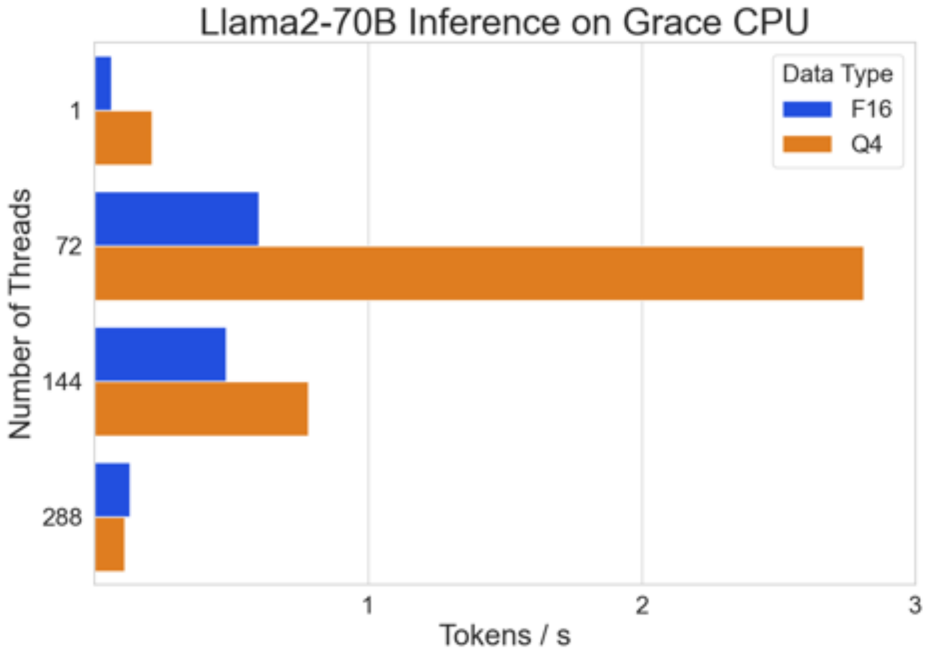
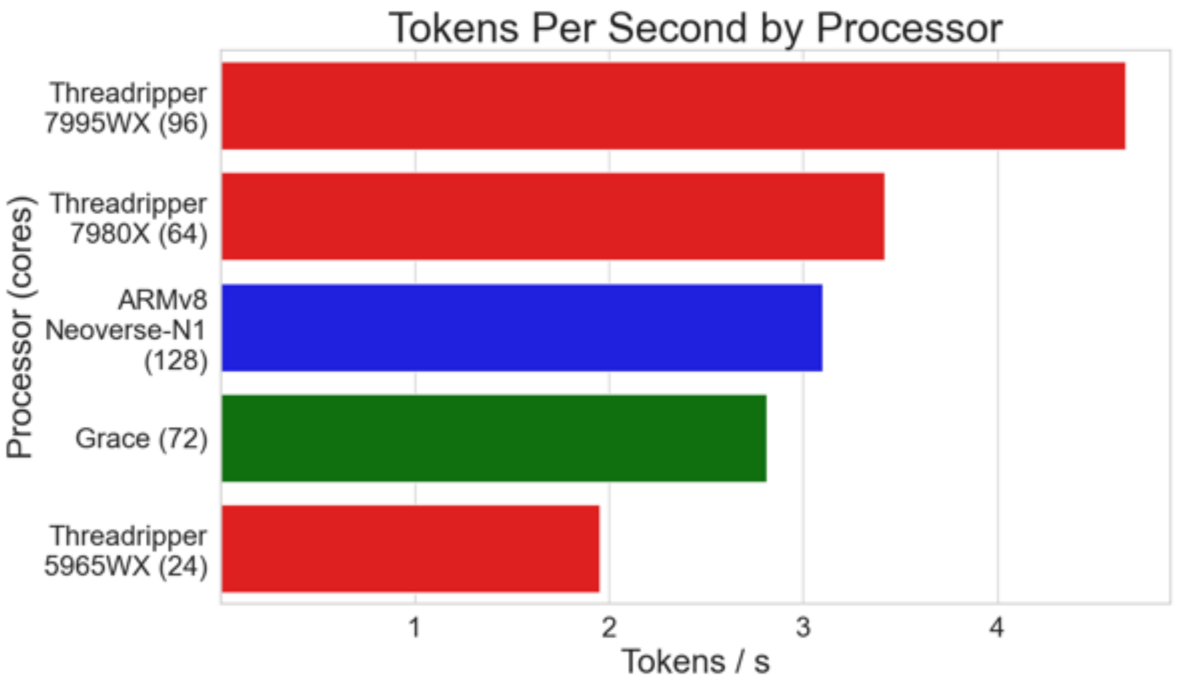
llama.cpp Benchmark Early Results

LLM inference on CPU
https://github.com/ggerganov/llama.cpp
OpenBenchmarking

Contact Wahab Kawafi for details:
a.kawafi@bristol.ac.uk





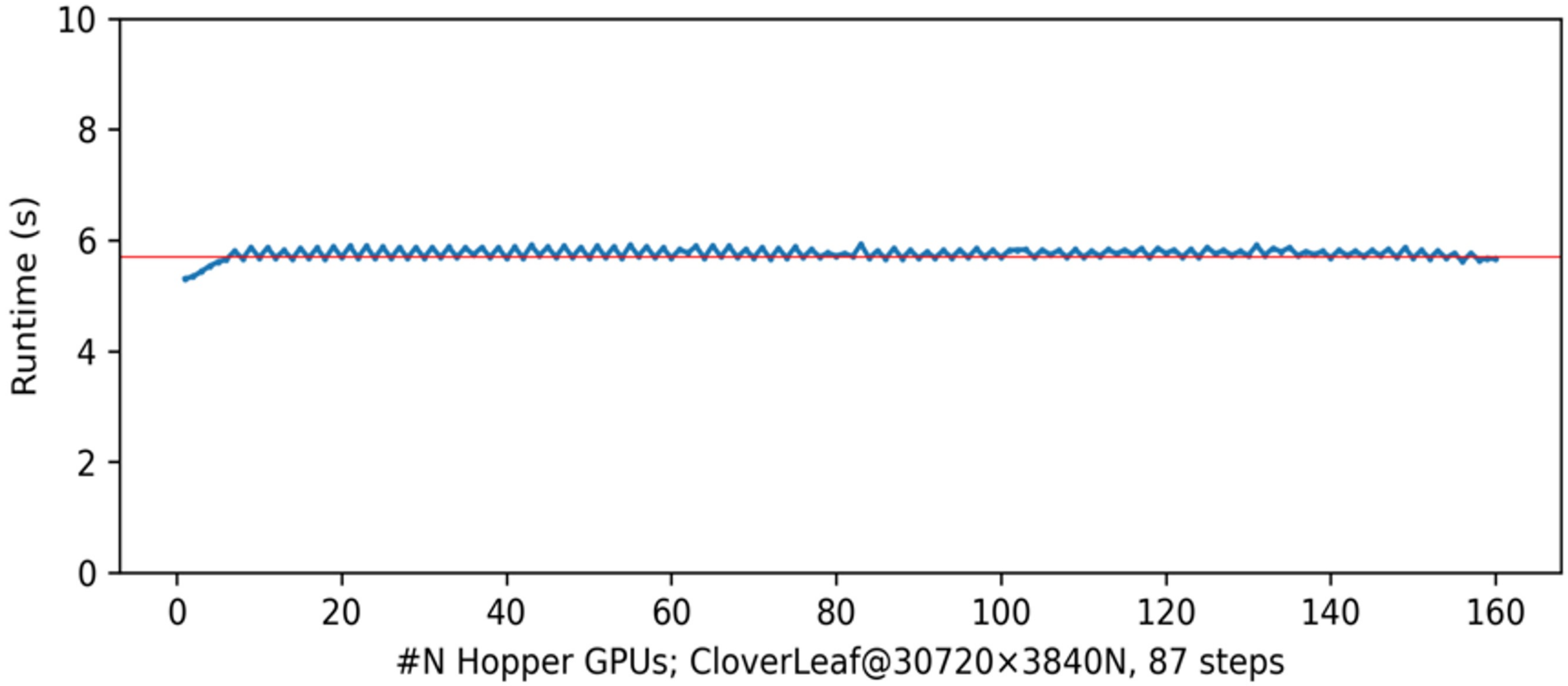
Early results. Grace GH200 CPUs have promising results to complement inference on LLMs (70B) even with a relatively low thread count per socket.

CloverLeaf Benchmark Early Results

https://github.com/UoB-HPC/CloverLeaf

Part of SPEChpc2021, primarily mem-BW, structured grid, stencil pattern, we use the CUDA port

Contact Tom Lin for details: wl14928@bristol.ac.uk



Weak scaling up to almost the entire machine of 160 GPUs (2x4 GPUs are on login node)
Similar results for TeaLeaf (part of SPEChpc2021) primarily mem-BW, MPI collectives, SpMV

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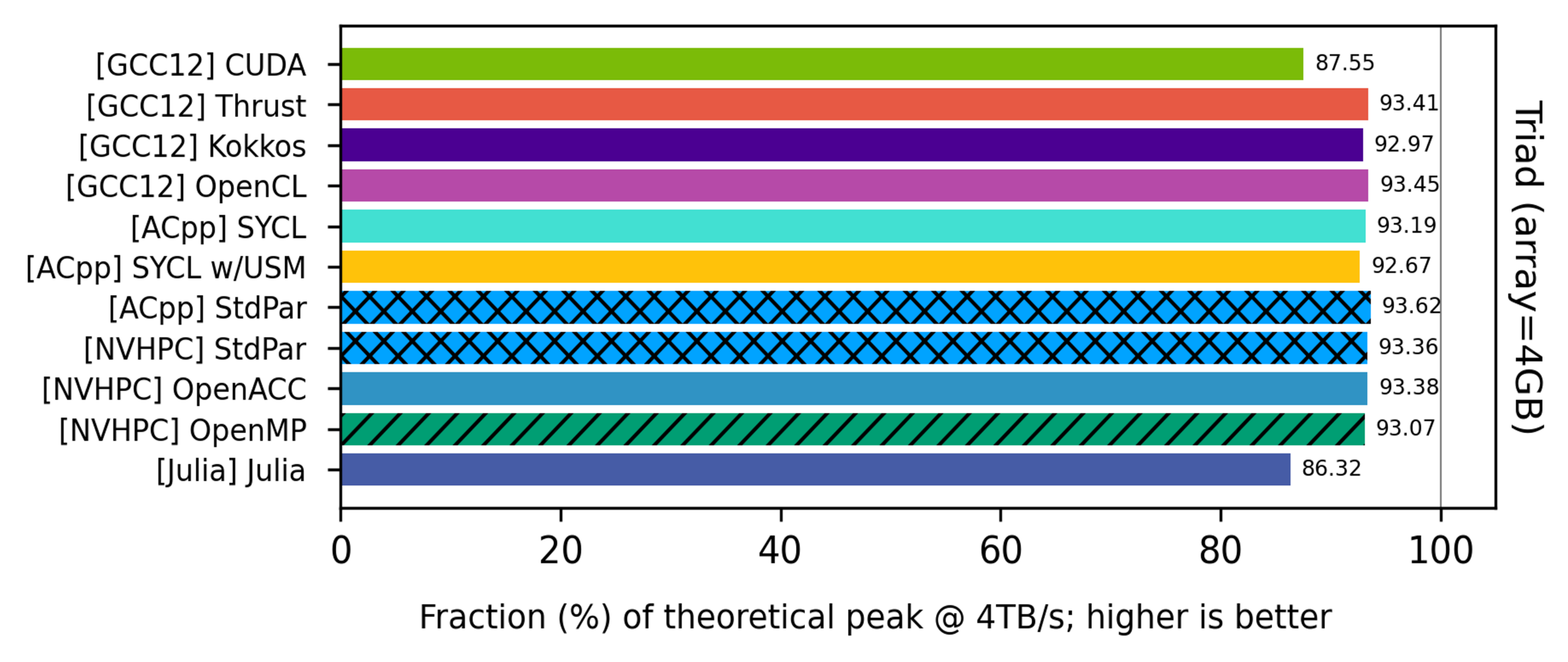
PE and Memory Bandwidth Benchmarking

https://github.com/UoB-HPC/BabelStream

Contact Tom Lin for details: wl14928@bristol.ac.uk



CUDA, Thrust, Kokkos, OpenCL, SYCL (via AdaptiveCpp), StdPar, OpenACC, Julia, OpenMP targets
Some of the compilers (GCC, Acpp, Clang) are built from source and everything worked as expected

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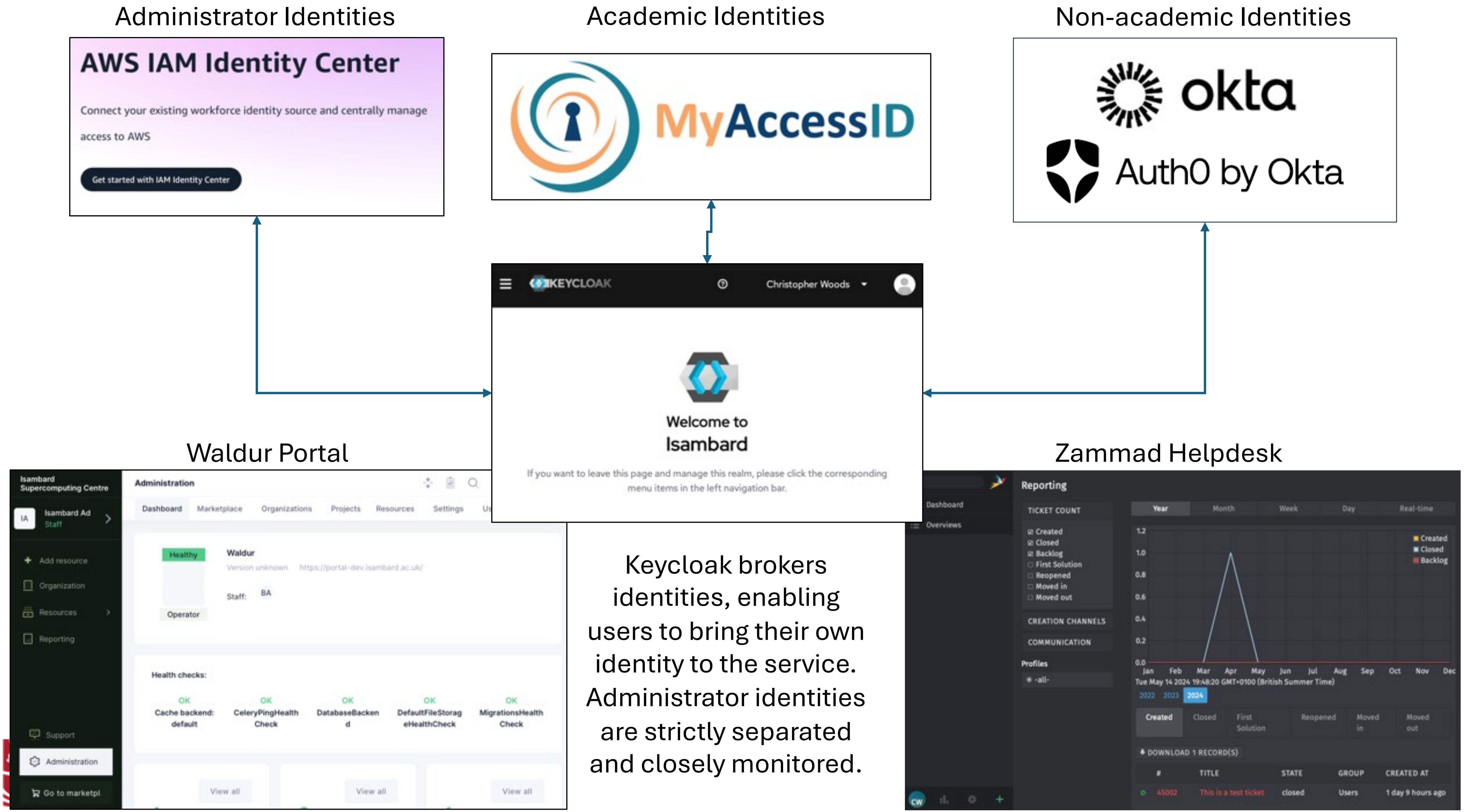
Lowering Access Barriers via IAM and Single Sign-On (SSO)

- OIDC single-sign on – bring your own high-level trust identity with federated academic & research credentials
  - Security via multi-factor authentication (MFA) for web & ssh
  - Okta a preferred option for govt public cloud AI users
- Self-service, cloud-native user and project management portal (single pane of glass for accessing all services plus accounting, reporting and audit trails)
- Waldur: single source of user truth
  - Provides Authorisation via OIDC
  - Manages projects, groups and roles
  - HTTPS (Connects to Waldur via standard OIDC)
  - An SSH key signing CA gets authorisation from Waldur (via OIDC)—Signs a short-lived SSH certificate



Administrator Identities

AWS IAM Identity Center

Connect your existing workforce identity source and centrally manage access to AWS

Academic Identities

MyAccessID

Non-academic Identities

okta

Auth0 by Okta

Welcome to Isambard

If you want to leave this page and manage this realm, please click the corresponding menu items in the left navigation bar.

Waldur Portal

Healthy

Waldur

Version unknown https://portal-dev.isambard.ac.uk/

Staff: BA

Operator

Health checks:

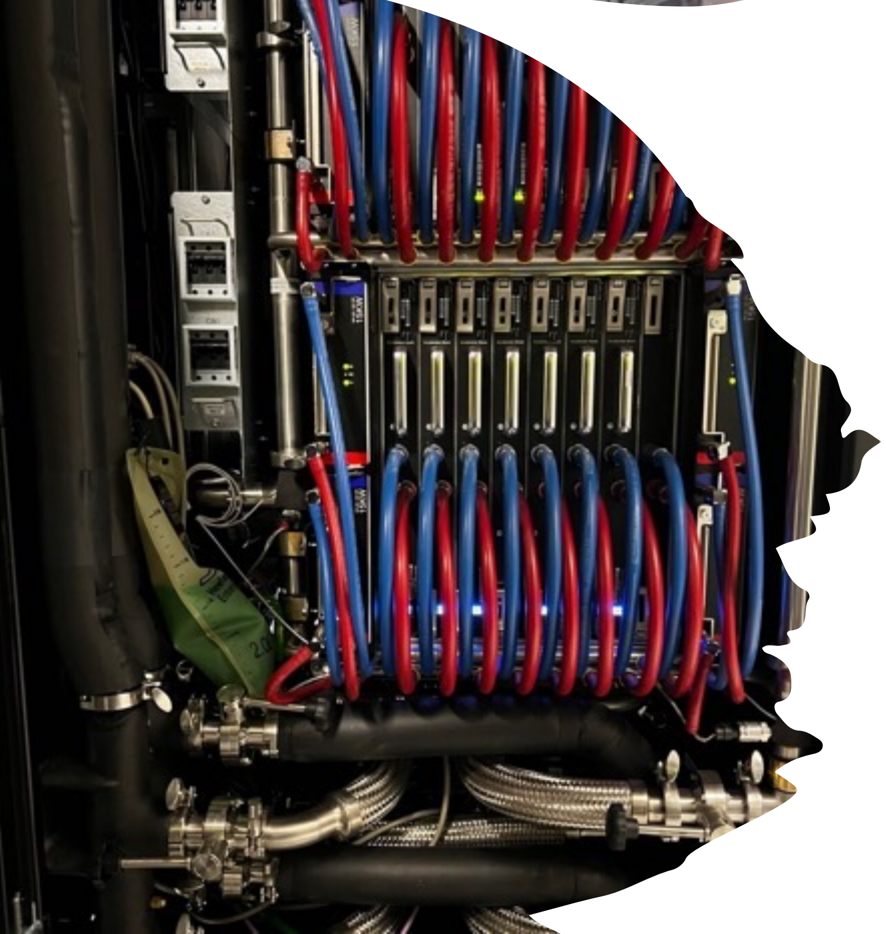
OK	OK	OK	OK	OK
Cache backend: default	CeleryPingHealthCheck	DatabaseBackend	DefaultFileStorageHealthCheck	MigrationsHealthCheck

Keycloak brokers identities, enabling users to bring their own identity to the service. Administrator identities are strictly separated and closely monitored.

Zammad Helpdesk

Tue May 14 2024 19:48:20 GMT+0100 (British Summer Time)

#	TITLE	STATE	GROUP	CREATED AT
45002	This is a test ticket	closed	Users	1 day 9 hours ago



Isambard-AI Firsts

- First HPE Cray EX DLC inside an MDC/POD
- First deployment and power-up < 2 weeks
- First combined DLC (EX2500) for Grace-Hopper Superchip and air-cooled Proliant XD2000 Grace-Grace Superchip

Scaling out in two phases

Phase 1 (~0.7 8-bit AI Exaflops)

Arrived in March 2024 – in Isambard 3 MDC
Piloting, on-boarding and staging services

1 x DLC EX2500 cabinet

21 blades (4-way Grace-Hopper)

42 nodes

168 GH superchips

12,096 Neoverse V2 Armv9 CPU cores

168 Hopper GPUs

21.5 TB CPU memory

16.1 TB high bandwidth GPU memory

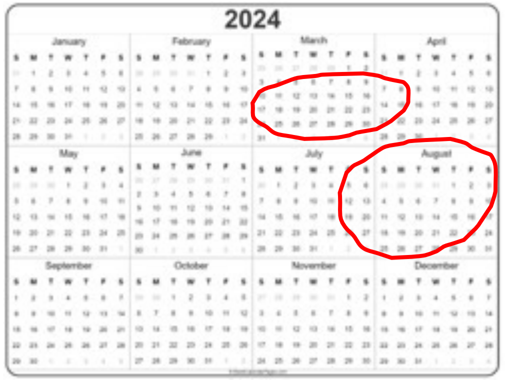
37.6 TB total memory

AI high performance storage

~1 PB all-flash ClusterStor Lustre

Phase 2 (~21 8-bit AI Exaflops)

Arriving Summer 2024 – new Isambard-AI MDC
Delivery of AI services



12 x DLC EX4000 cabinets

660 blades (4-way Grace-Hopper)

1,320 nodes

5,280 GH superchips

380,160 Neoverse V2 Armv9 CPU cores

5,280 Hopper GPUs

675 TB CPU memory

506 TB high bandwidth GPU memory

1.18 PB total memory

AI high performance storage

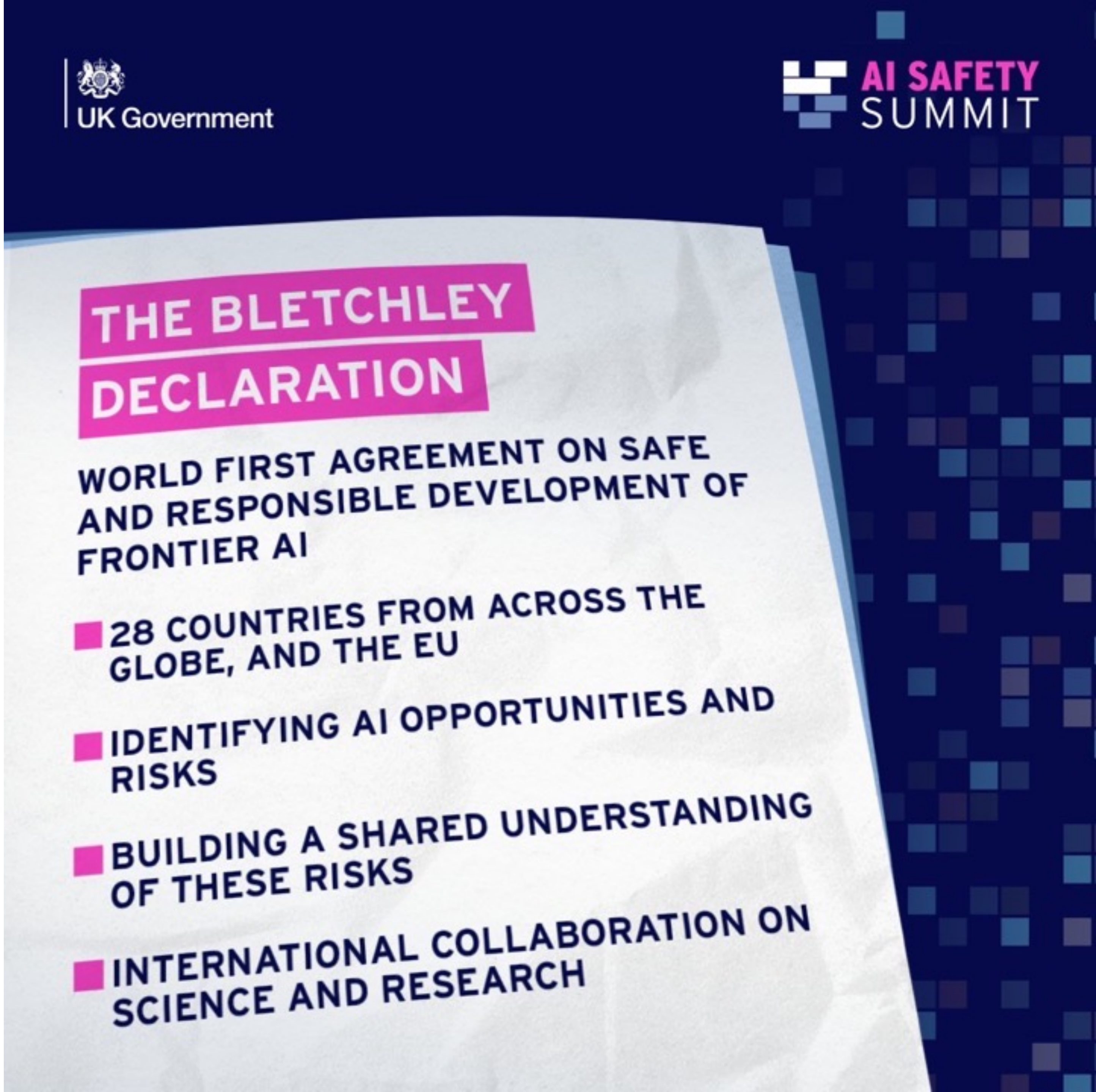
~27 PB all-flash storage!

(~20 PB Lustre, ~7 PB software defined VAST)

University of BRISTOL

Thank you

Stay tuned!



UK Government

AI SAFETY SUMMIT

THE BLETCHLEY DECLARATION

WORLD FIRST AGREEMENT ON SAFE AND RESPONSIBLE DEVELOPMENT OF FRONTIER AI

- 28 COUNTRIES FROM ACROSS THE GLOBE, AND THE EU
- IDENTIFYING AI OPPORTUNITIES AND RISKS
- BUILDING A SHARED UNDERSTANDING OF THESE RISKS
- INTERNATIONAL COLLABORATION ON SCIENCE AND RESEARCH