

<https://uob-hpc.github.io>

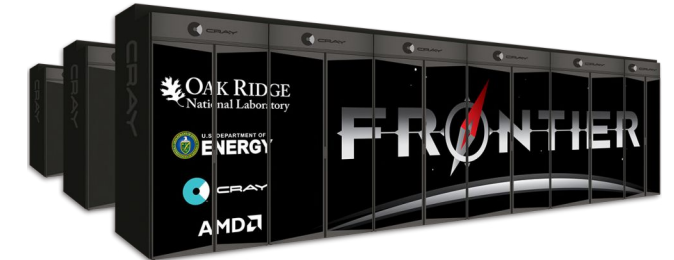
Parallel
programming
models and
SYCL in the UK's
Exascale programs



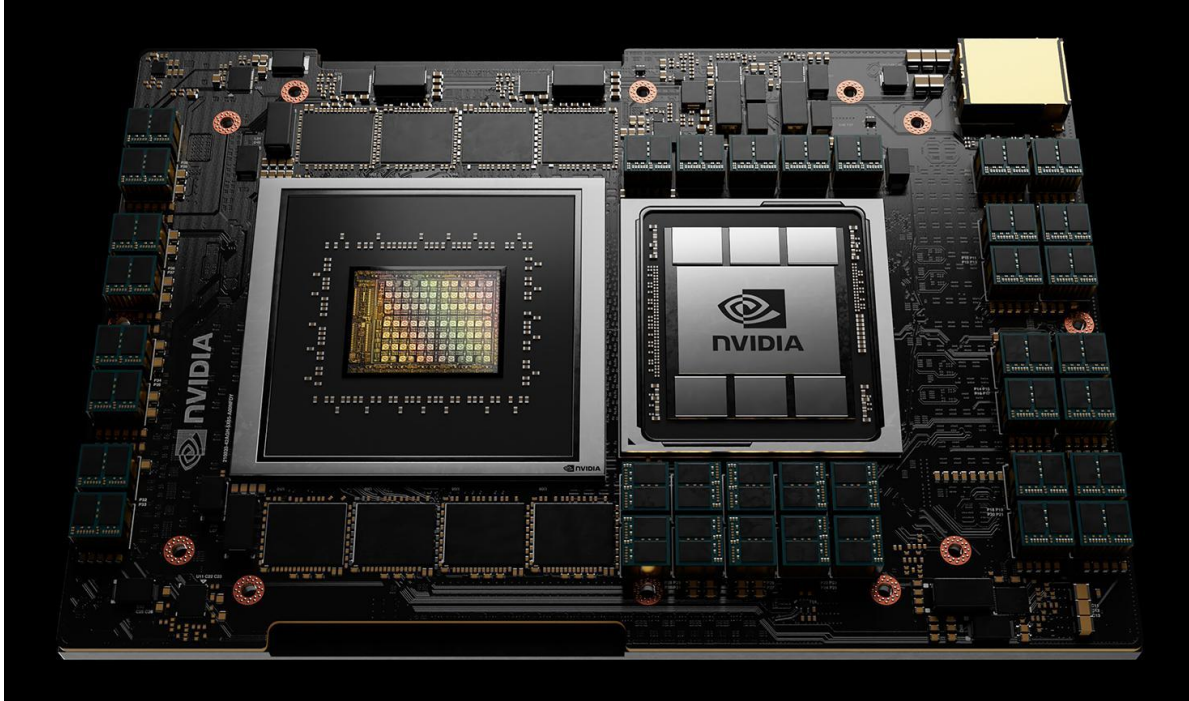
Next-generation supercomputers are largely heterogeneous

The coming generation of Exascale systems will include a diverse range of architectures at massive scale, most (but not all) heterogeneous:

- **Fugaku:** Fujitsu A64FX Arm CPUs
- **Perlmutter:** AMD EYPC CPUs and NVIDIA GPUs
- **Frontier:** AMD EPYC CPUs and Radeon GPUs
- **Aurora:** Intel Xeon CPUs and Xe GPUs
- **El Capitan:** AMD EPYC CPUs and Radeon GPUs



CPUs and GPUs becoming more tightly coupled



- E.g. NVIDIA announced the “**Grace**” Arm CPUs
- 900GB/s interconnect between the CPU and GPU
 - >10x fastest PCIe
- Very high memory bandwidth for a CPU
 - >500GB/s
- Shipping 2023 with the Hopper next-gen GPUs
- Similar arrangements from Intel and AMD

<https://www.nextplatform.com/2021/04/12/nvidia-enters-the-arms-race-with-homegrown-grace-cpus/>

How are we going to program these heterogeneous systems?

- This is where approaches like SYCL and Intel's oneAPI come in

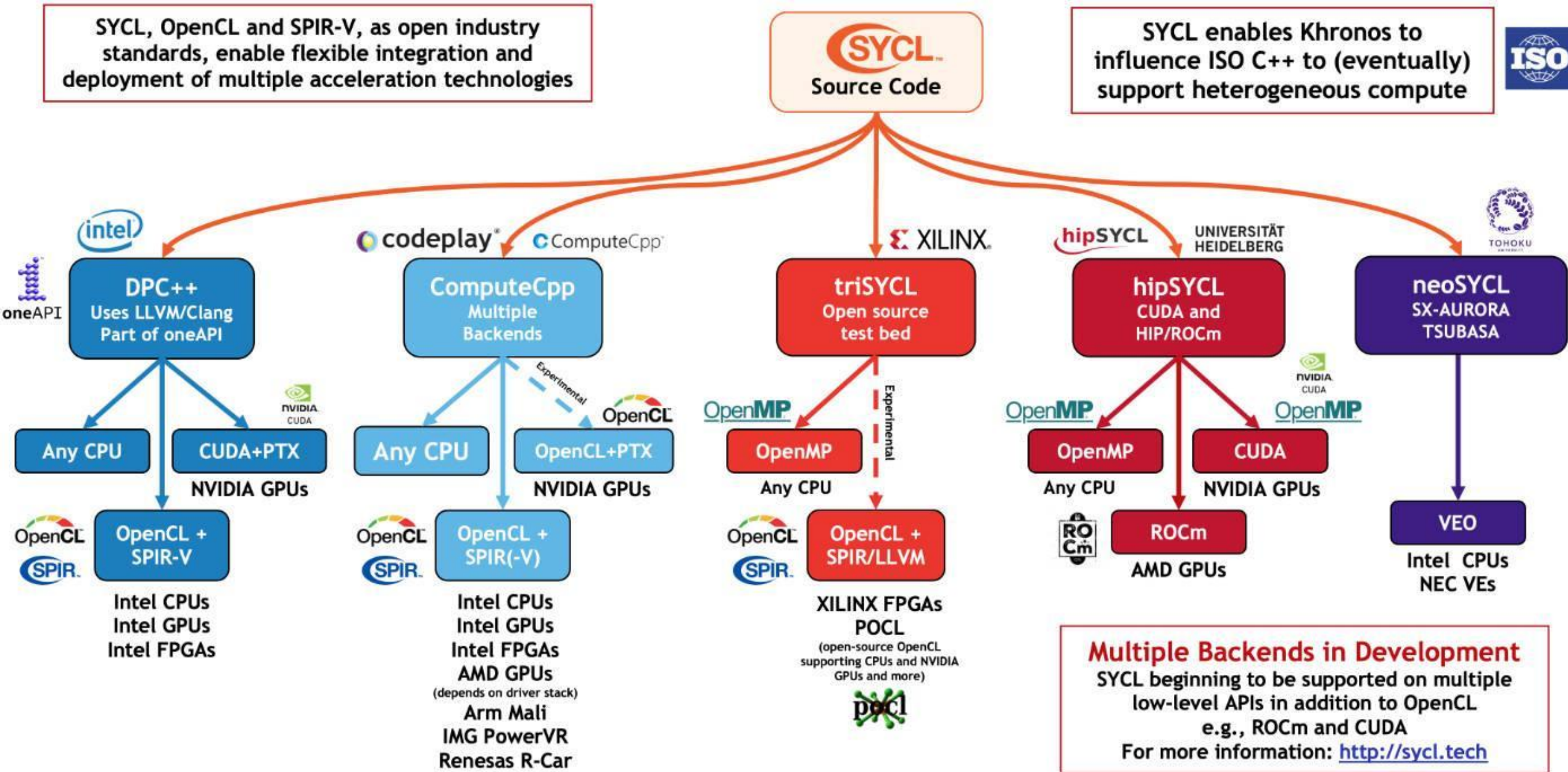


SYCL is a royalty-free, cross-platform abstraction layer that enables code for heterogeneous processors to be written using standard ISO C++ with the host and kernel code for an application contained in the same source file.

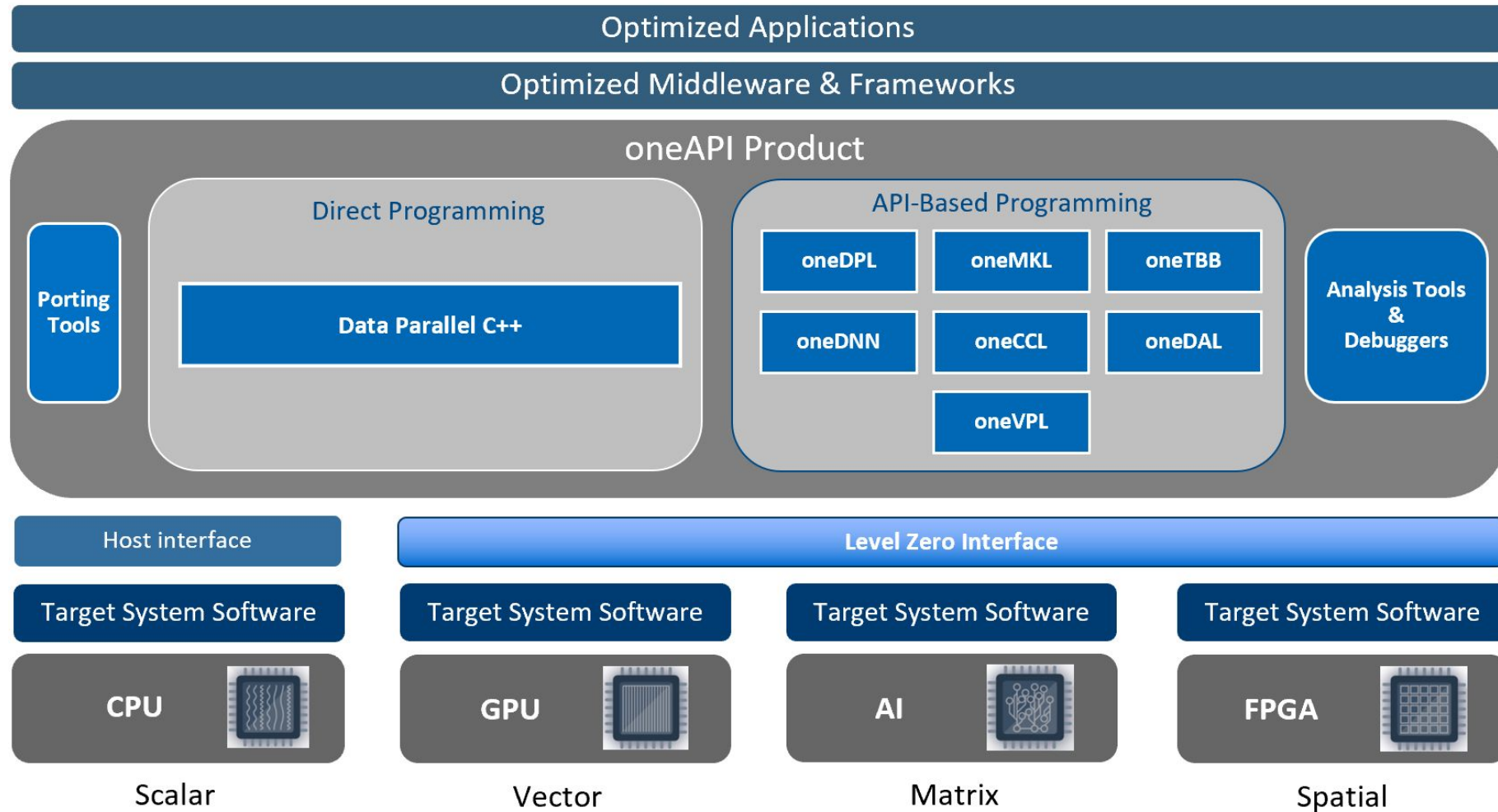
<https://www.khronos.org/sycl/>

SYCL, OpenCL and SPIR-V, as open industry standards, enable flexible integration and deployment of multiple acceleration technologies

SYCL enables Khronos to influence ISO C++ to (eventually) support heterogeneous compute



Intel's oneAPI is a comprehensive framework for heterogeneous programming





**EXCALIBUR
10**

EXCALIBUR: THE UK'S EXASCALE READINESS PROGRAM



**UK Research
and Innovation**



**UK Atomic
Energy
Authority**

ExCALIBUR High Level Overview

- **Exascale Computing Algorithms and Infrastructures Benefiting UK Research**
 - £45.7M from the Strategic Priorities Fund (SPF)
 - Led by UKRI and the Met Office with UKAEA
 - The UK's 5 year Exascale programme
 - Primary focus is on software and algorithms
 - 10% of budget allocated to testbeds exploring novel hardware and enabling software

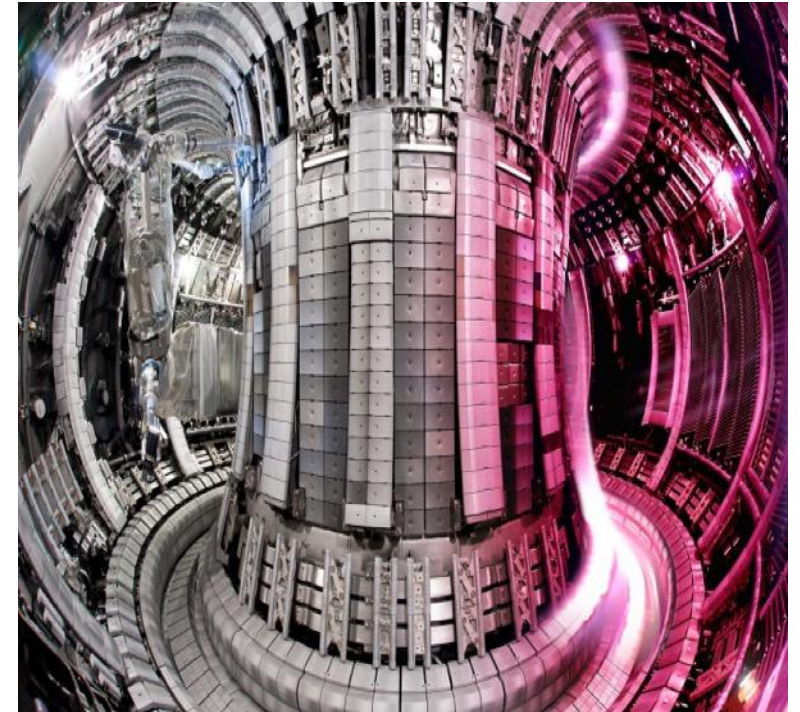


Photo credit: UK Atomic Energy Authority (UKAEA)

ExCALIBUR project-wide benchmarking initiative

- **Phase 1:** understand ExCALIBUR science drivers and requirements
- **Phase 2:** determine a set of kernels, synthetic benchmarks, and applications, to use as representative codes
 - Re-use as much as possible from ECP, EuroHPC, ARCHER, DiRAC etc
 - Use standard frameworks for build systems and benchmarking, such as SPACK, Reframe etc
 - Establish standard build and run scripts
 - Codes selected to be as cross-platform and performance-portable as possible

Identified kernels/mini-apps/benchmarks

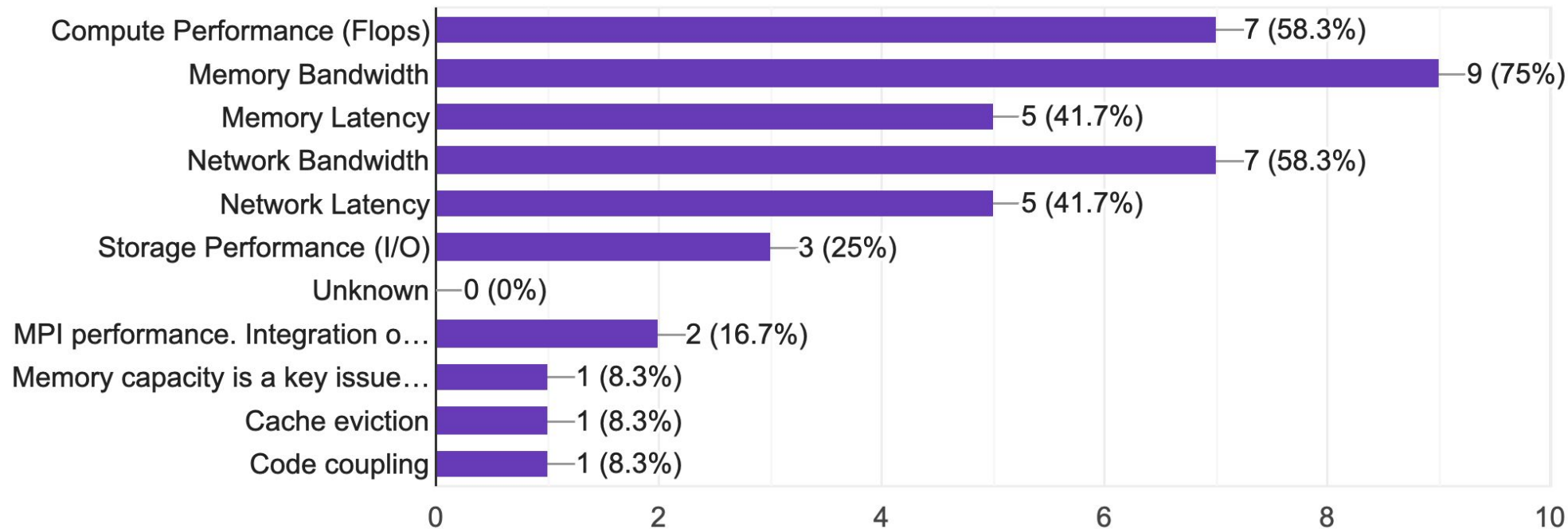
Code (benchmark/mini-app)

- Firedrake (HPGMG)
- NEPTUNE (MiniEPOCH)
- SciML (SciML)
- Xcompact3D (OpenSBLI)
- GRID (Sombrero)
- Unified Model (LFRic)
- ExaHype ()
- SWIFT ()

ExCALIBUR project-wide benchmarking initiative

Performance bottlenecks (select all that apply)

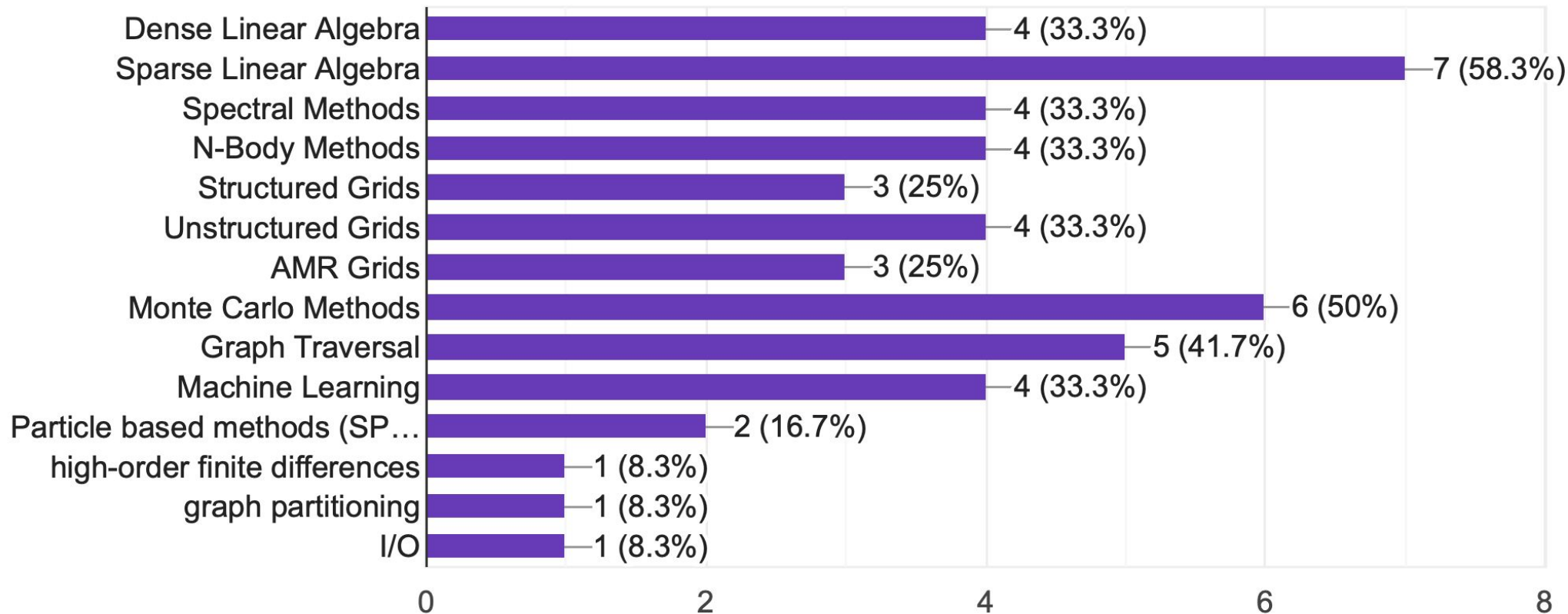
12 responses



ExCALIBUR project-wide benchmarking initiative

Computational methods (select all that apply)

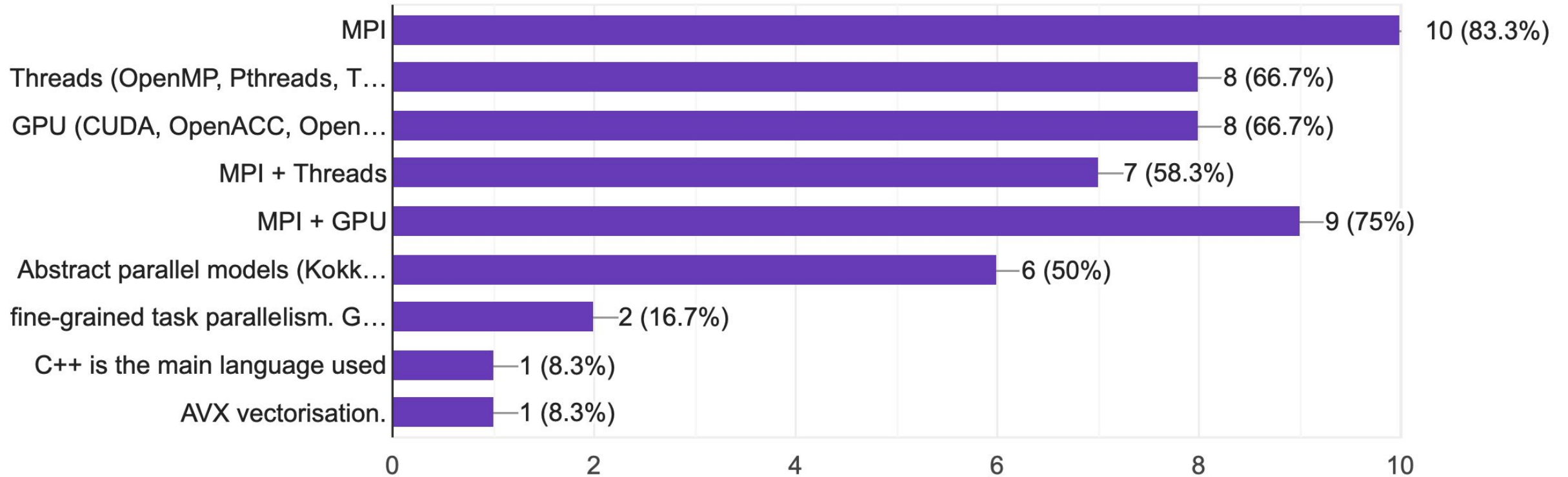
12 responses



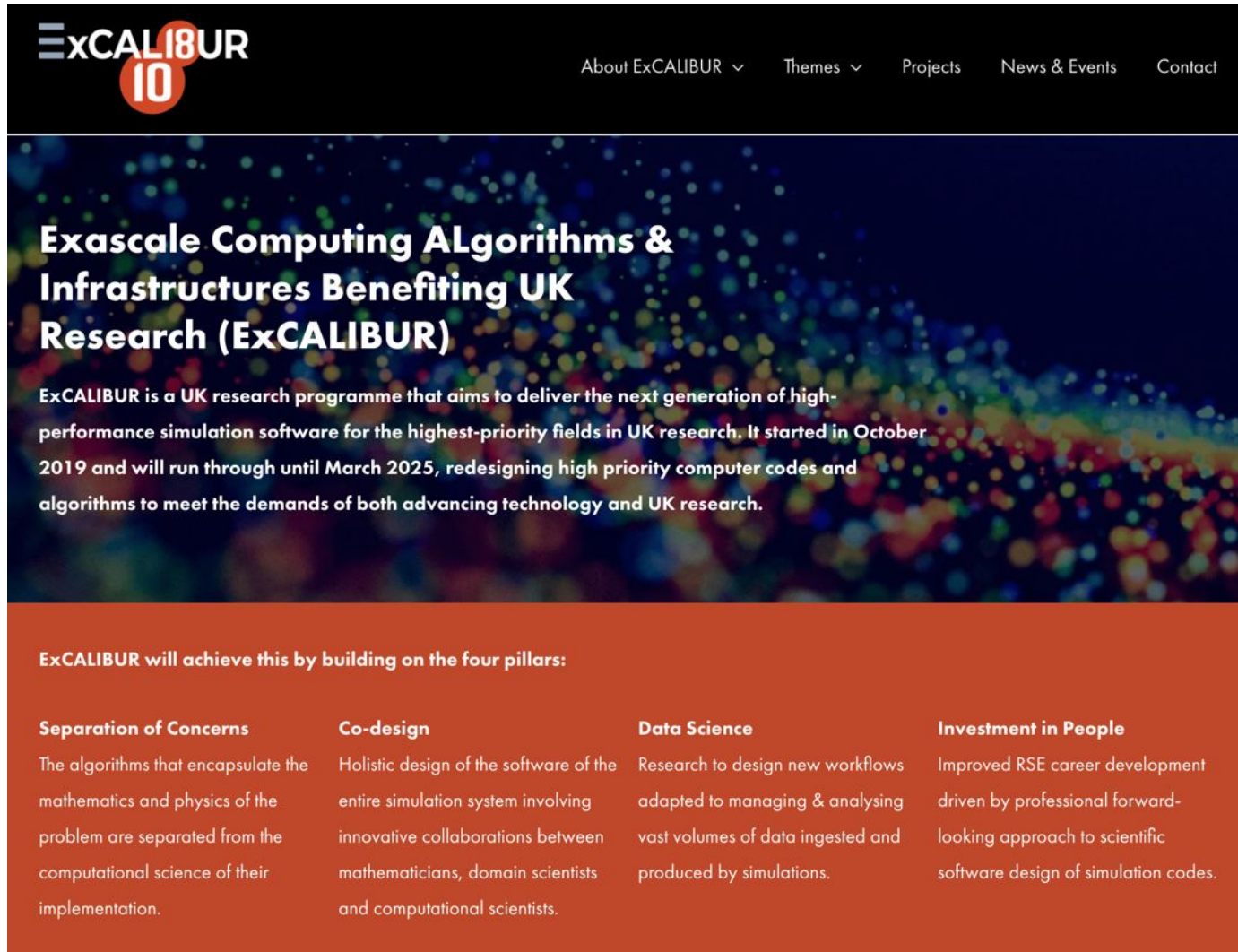
ExCALIBUR project-wide benchmarking initiative

Parallel programming models (select all that apply)

12 responses



For more about ExCALIBUR...

The image is a screenshot of the ExCALIBUR website. At the top, there is a dark navigation bar with the ExCALIBUR logo on the left and a menu on the right containing links for 'About ExCALIBUR', 'Themes', 'Projects', 'News & Events', and 'Contact'. Below the navigation bar is a large hero section with a background image of colorful, glowing particles. The main heading in this section is 'Exascale Computing Algorithms & Infrastructures Benefiting UK Research (ExCALIBUR)'. Below the heading is a paragraph of text describing the program. At the bottom of the hero section, there is a red banner with the text 'ExCALIBUR will achieve this by building on the four pillars:'. Below this banner is a grid of four columns, each representing a pillar: 'Separation of Concerns', 'Co-design', 'Data Science', and 'Investment in People'. Each column contains a brief description of the pillar's focus.

ExCALIBUR
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About ExCALIBUR ▾ Themes ▾ Projects News & Events Contact

Exascale Computing Algorithms & Infrastructures Benefiting UK Research (ExCALIBUR)

ExCALIBUR is a UK research programme that aims to deliver the next generation of high-performance simulation software for the highest-priority fields in UK research. It started in October 2019 and will run through until March 2025, redesigning high priority computer codes and algorithms to meet the demands of both advancing technology and UK research.

ExCALIBUR will achieve this by building on the four pillars:

| Separation of Concerns | Co-design | Data Science | Investment in People |
|--|---|---|--|
| The algorithms that encapsulate the mathematics and physics of the problem are separated from the computational science of their implementation. | Holistic design of the software of the entire simulation system involving innovative collaborations between mathematicians, domain scientists and computational scientists. | Research to design new workflows adapted to managing & analysing vast volumes of data ingested and produced by simulations. | Improved RSE career development driven by professional forward-looking approach to scientific software design of simulation codes. |

SYCL / oneAPI in the UK's Exascale program

- ExCALIBUR's goal is to produce codes that will **work well across a range** of different heterogeneous supercomputers
- **No single parallel programming model** strongly supported across all the CPU/GPU vendors
- **SYCL** is one of the most promising options
 - Strongly supported by Intel
 - Works well on AMD and NVIDIA via 3rd party tools
 - Both open source and commercial

SYCL progress within UK science codes

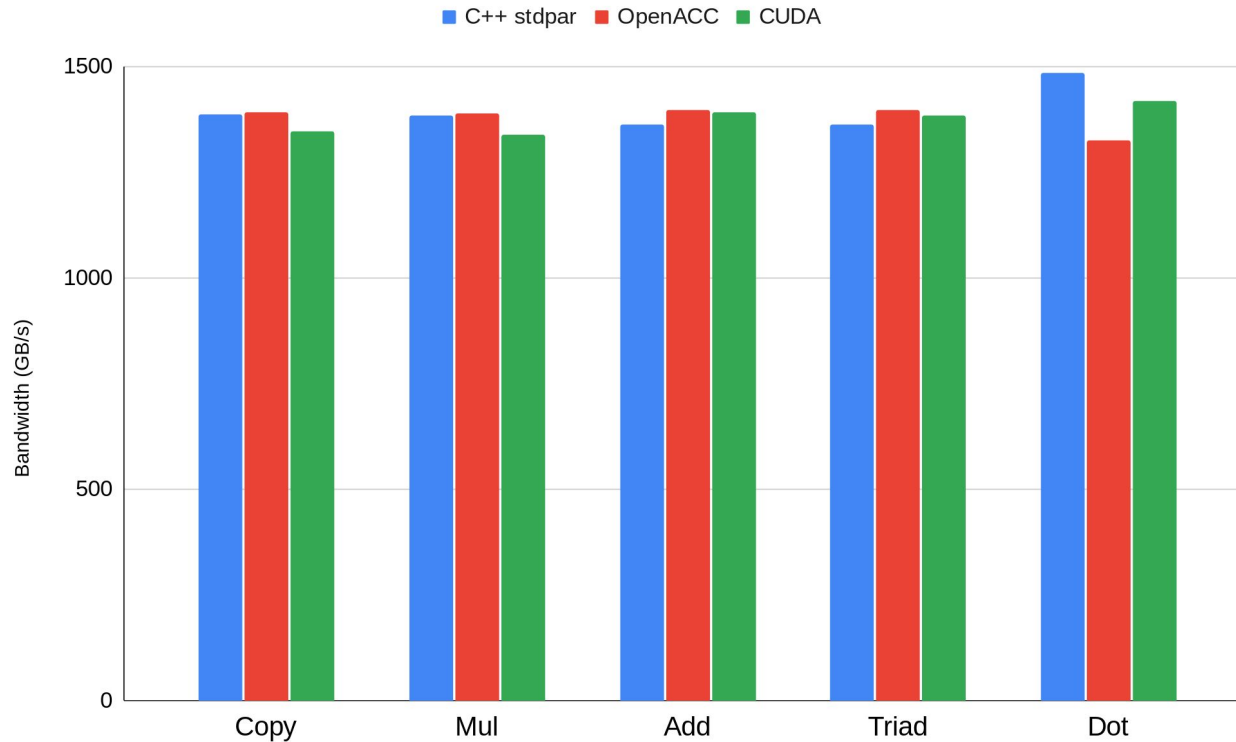
- Certain codes either developed or widely used in the UK, are already being or have been ported to SYCL:
 - GROMACS
 - FEniCS (DolfinX)
 - Psyclone
 - Grid
 - OP2 / MG-CFD
 - BabelStream
 - Over 140 SYCL projects now listed on <https://sycl.tech/projects/>

SYCL has company in the parallel C++ space

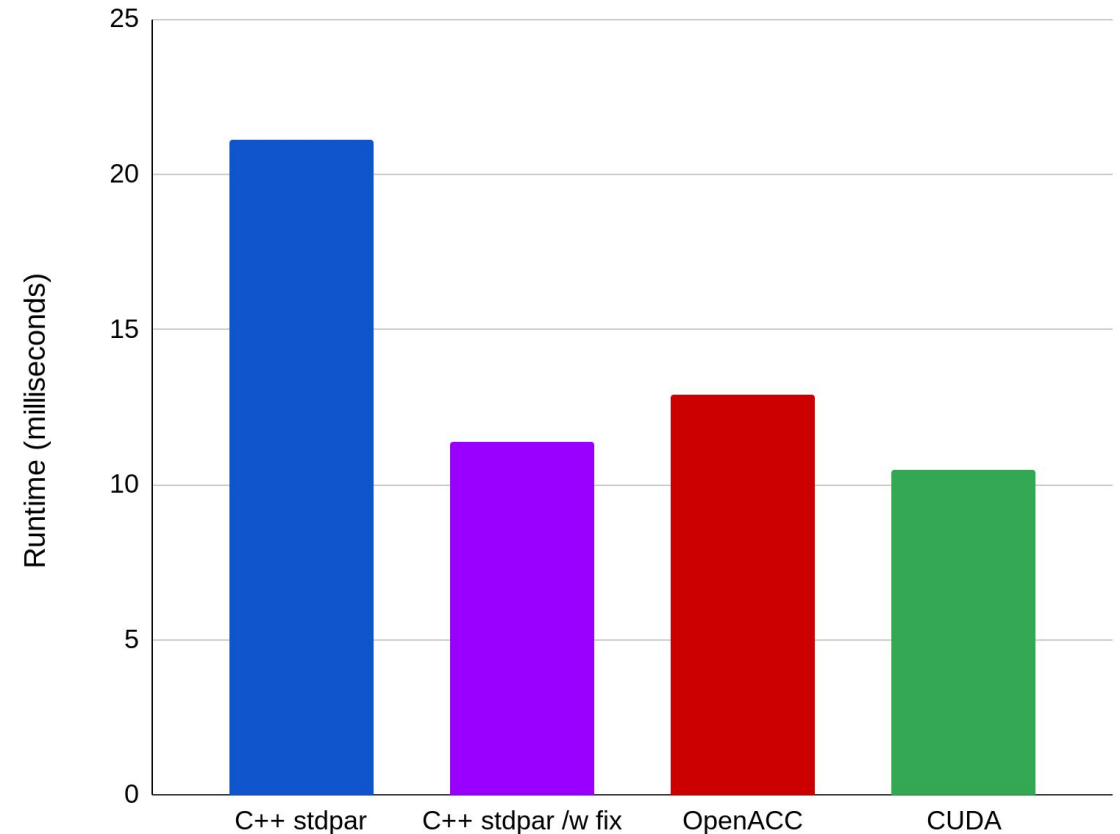
- Others have been exploring how best to expose parallelism within C++ too:
 - **Kokkos** from Sandia
 - **Raja** from Lawrence Livermore
 - **ISO C++** standard parallelism promises to help describe parallel algorithms portably
- All take slightly different approaches in how much they expose
- SYCL offers support for identifying available devices, managing disjoint memories, and directing work to devices – three things ISO C++ doesn't do (at least, not yet)
- SYCL is an open standard, managed by an experienced open standards group, Khronos, and strongly supported by multiple vendors and compiler providers

From GTC: ISO C++ on A100 (40GB) GPU

BabelStream
Higher is better



MiniBUDE
Lower is better

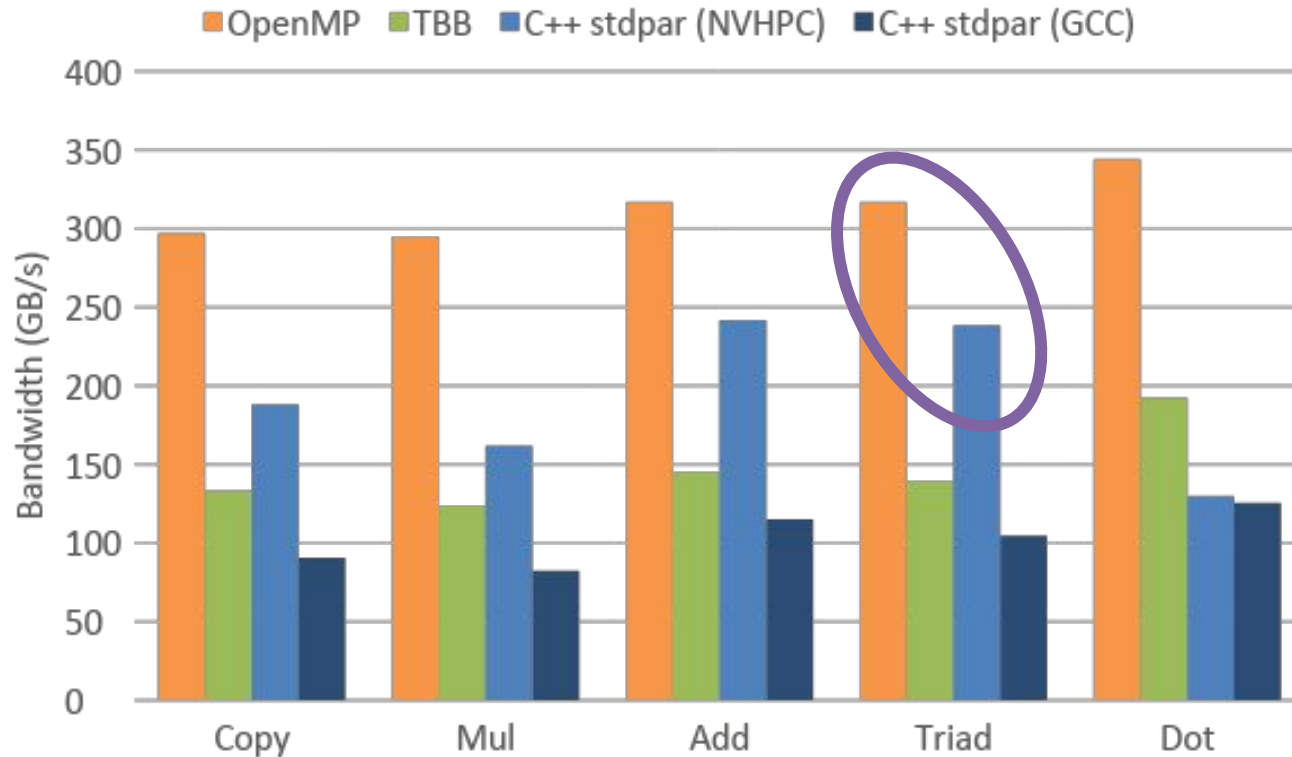


ISO C++ achieving close to performance parity with OpenACC and CUDA for memory bandwidth bound and compute bound codes

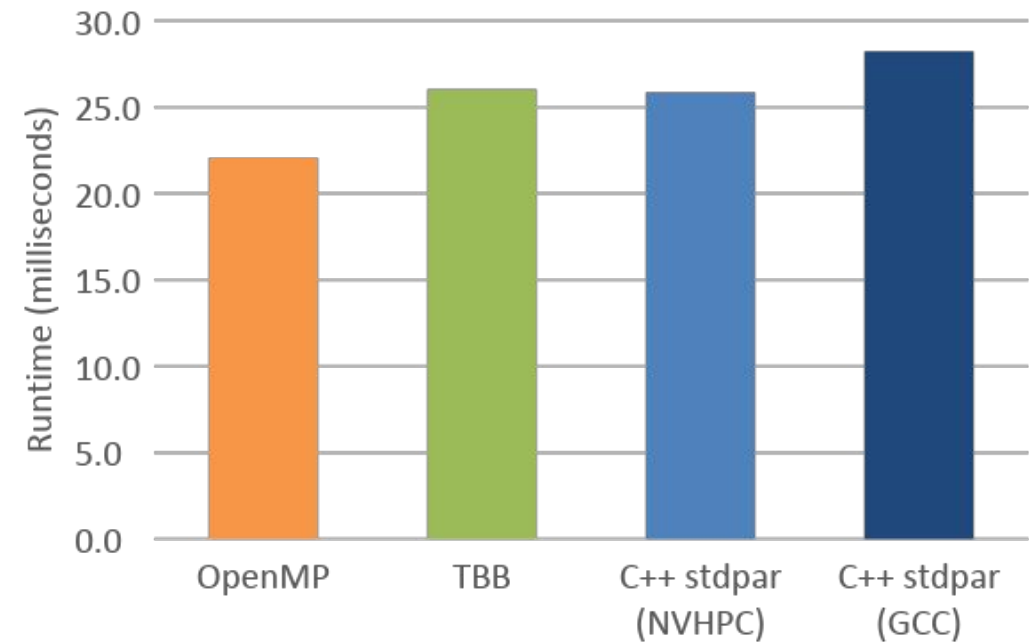
<https://www.nvidia.com/en-us/on-demand/session/gtcspring22-s41618/>

ISO C++ on Icelake Xeon Gold 6338 dual-socket CPU

BabelStream
Higher is better



MiniBUDE
Lower is better



NVHPC gets close to OpenMP performance – except for reductions. GCC uses TBB under the hood.



University of
BRISTOL

<https://www.nvidia.com/en-us/on-demand/session/gtcspring22-s41618/>



Conclusions

- **Exascale** is coming, and the UK's **ExCALIBUR** programme is designed to prepare UK science codes for it
- The hardware space is going to be **varied** and **heterogeneous**
- **SYCL** is of great interest due to level of cross-vendor support and existing ecosystem of compiler providers
- ExCALIBUR is exploring **SYCL as a leading contender** to enable **cross-platform performance portability**

For more information

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