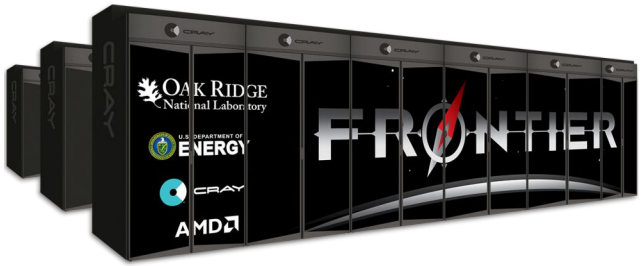
https://uob-hpc.github.io

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



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The Next Platform, Jan 13th 2020: "HPC in 2020: compute engine diversity gets real"
https://www.nextplatform.com/2020/01/13/hpc-in-2020-compute-engine-diversity-gets-real/

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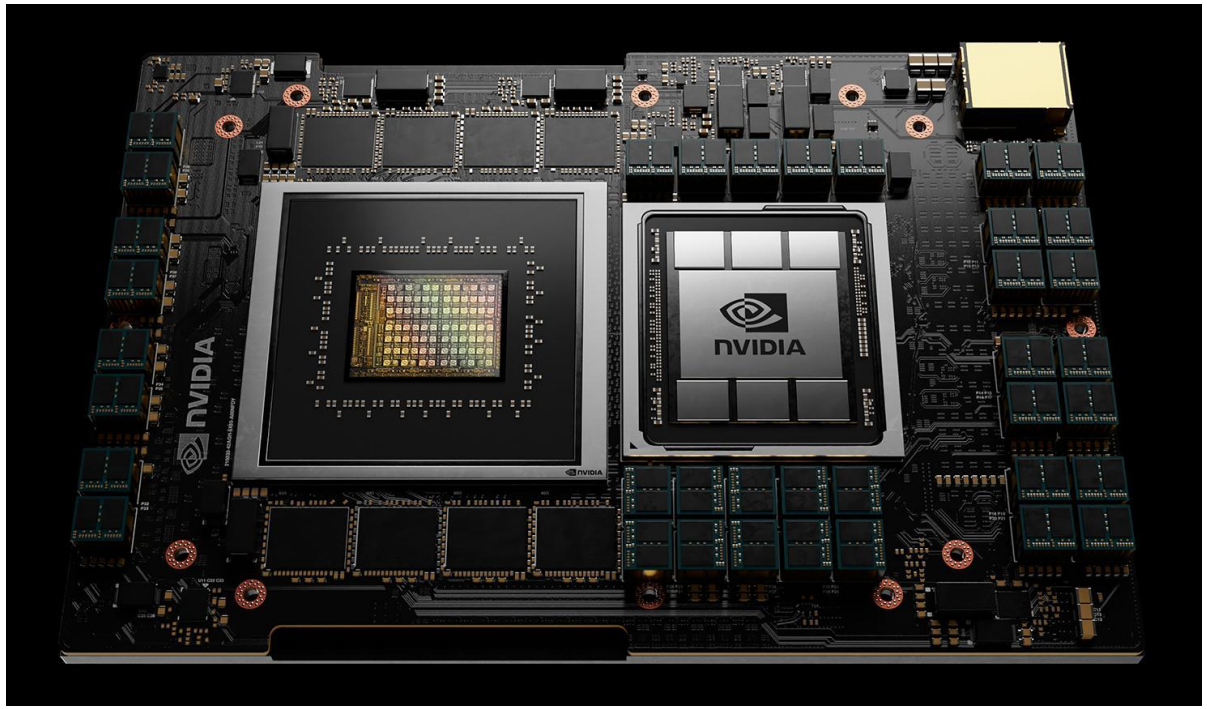
CPUs and GPUs becoming more tightly coupled



- 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

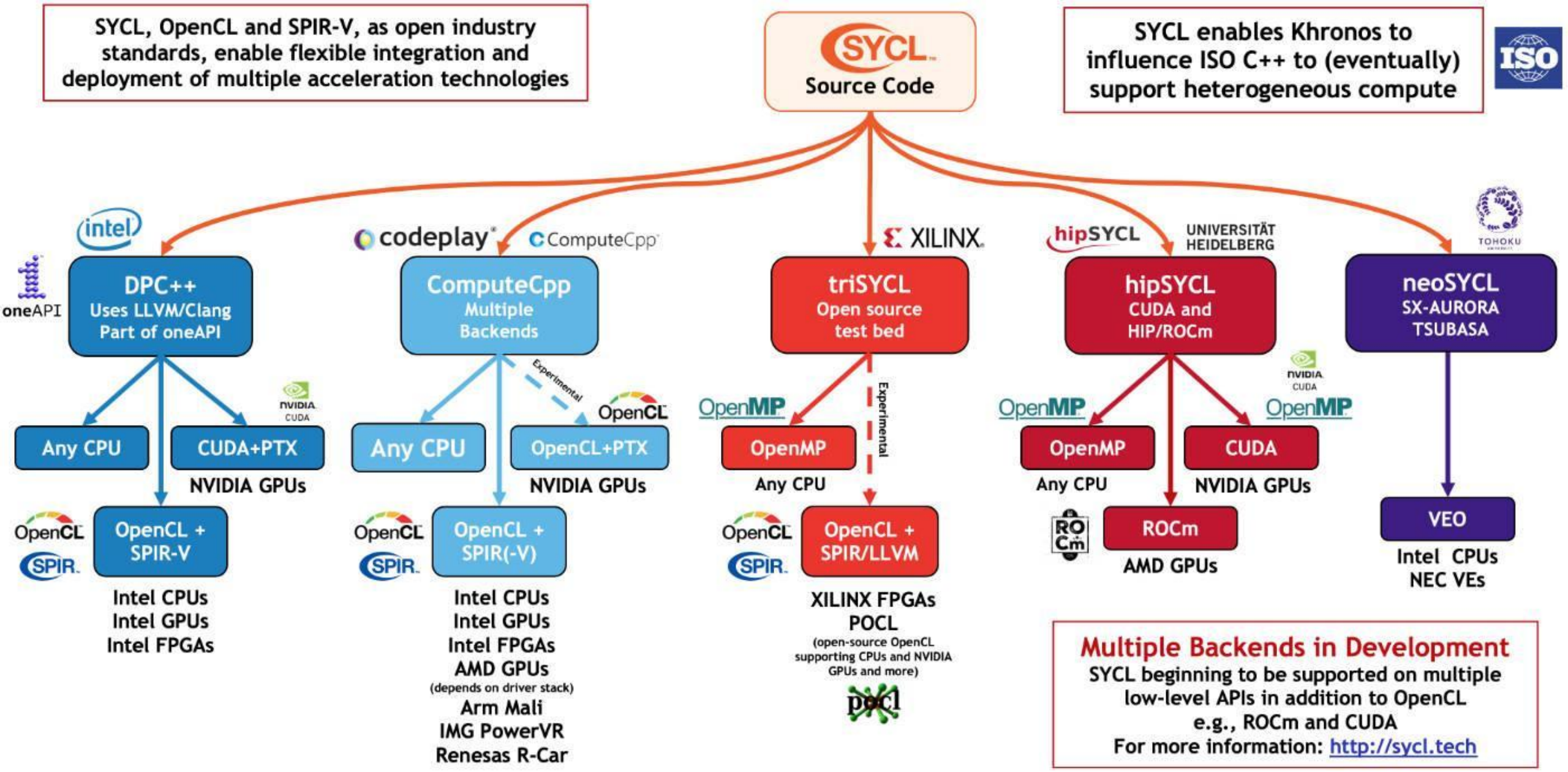
SYCL is a royalty-free, cross-platform abstraction layer that enables code for heterogeneous processors to be written using standard ISO C++ with the host and kernel code for an application contained in the same source file.

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

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

SYCL Source Code

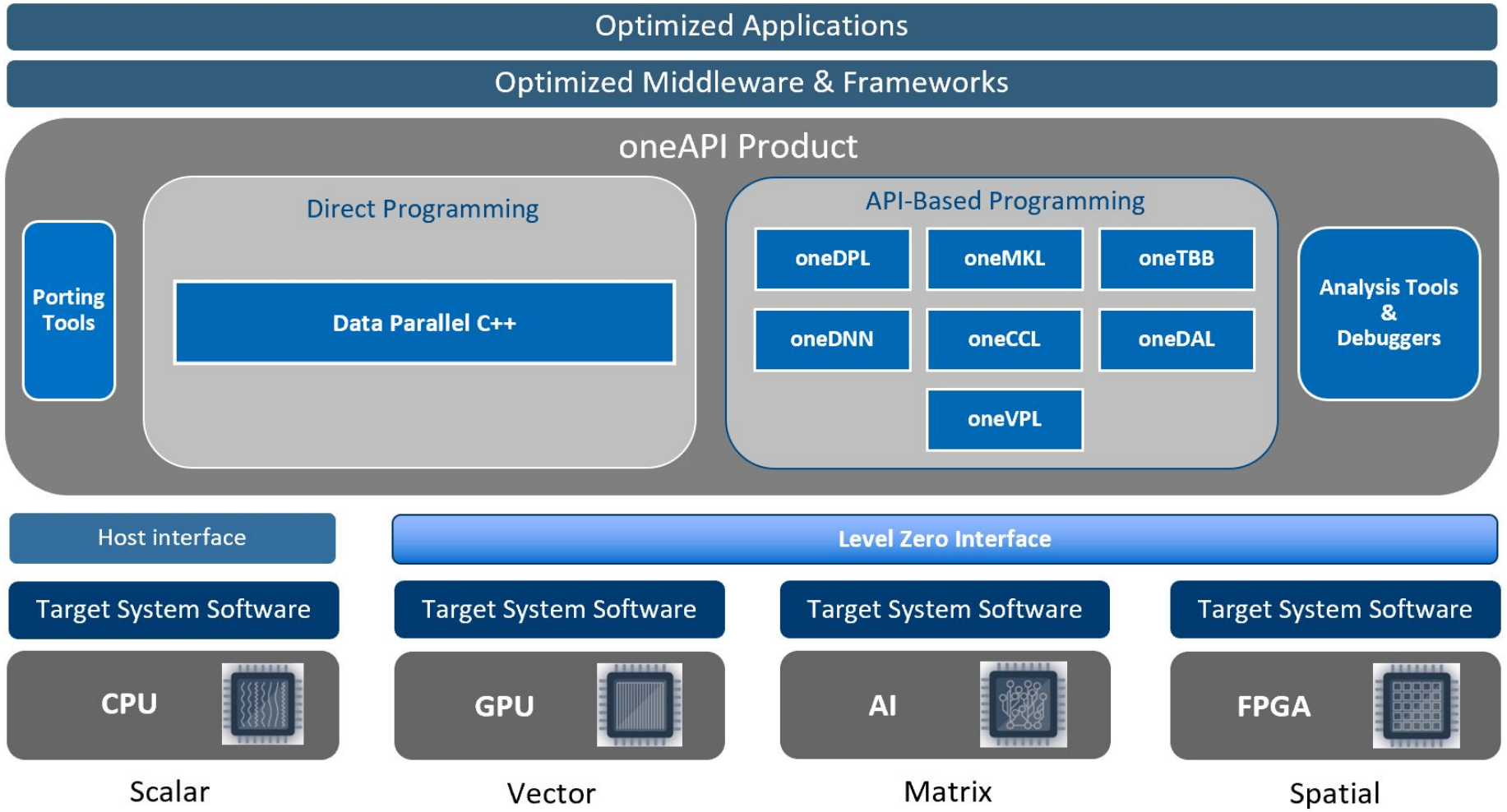
SYCL enables Khronos to influence ISO C++ to (eventually) support heterogeneous compute



Multiple Backends in Development

SYCL beginning to be supported on multiple low-level APIs in addition to OpenCL
e.g., ROCm and CUDA
For more information: http://sycl.tech

Intel's oneAPI is a comprehensive framework for heterogeneous programming



Source: https://spec.oneapi.io/level-zero/latest/core/INTRO.html

EXCALIBUR: THE UK'S EXASCALE READINESS PROGRAM

Met Office

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

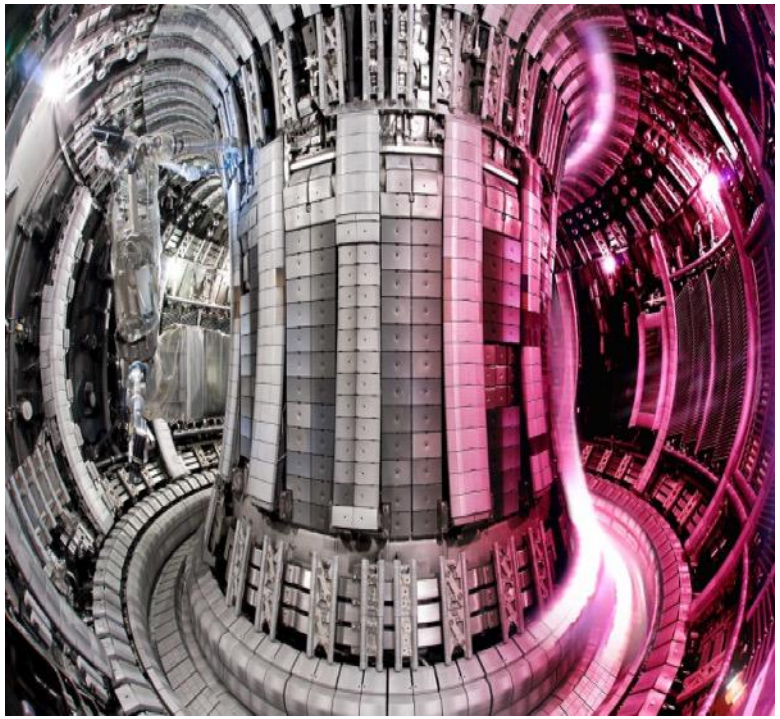


Photo credit: UK Atomic Energy Authority (UKAEA)

ExCALIBUR project-wide benchmarking initiative

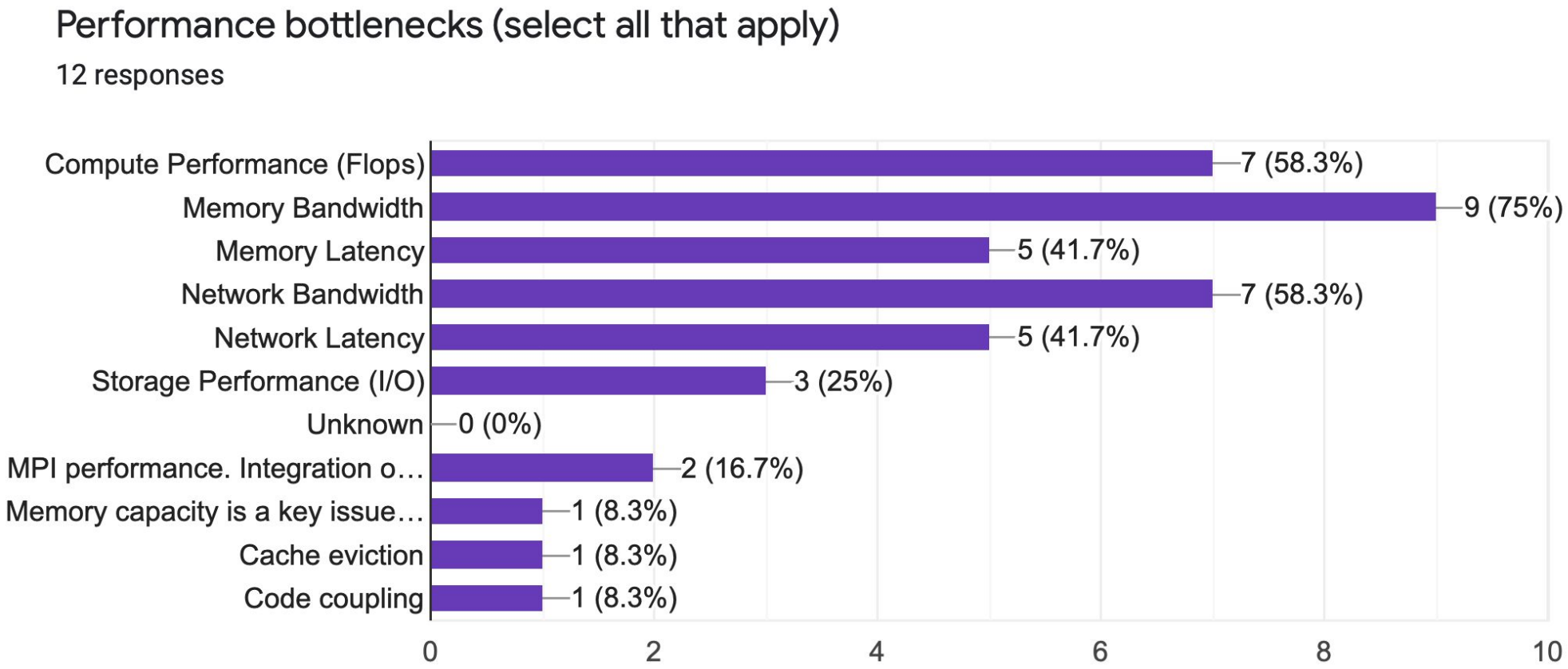
- **Phase 1:** understand ExCALIBUR science drivers and requirements
- **Phase 2:** determine a set of kernels, synthetic benchmarks, and applications, to use as representative codes
  - Re-use as much as possible from ECP, EuroHPC, ARCHER, DiRAC etc
  - Use standard frameworks for build systems and 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

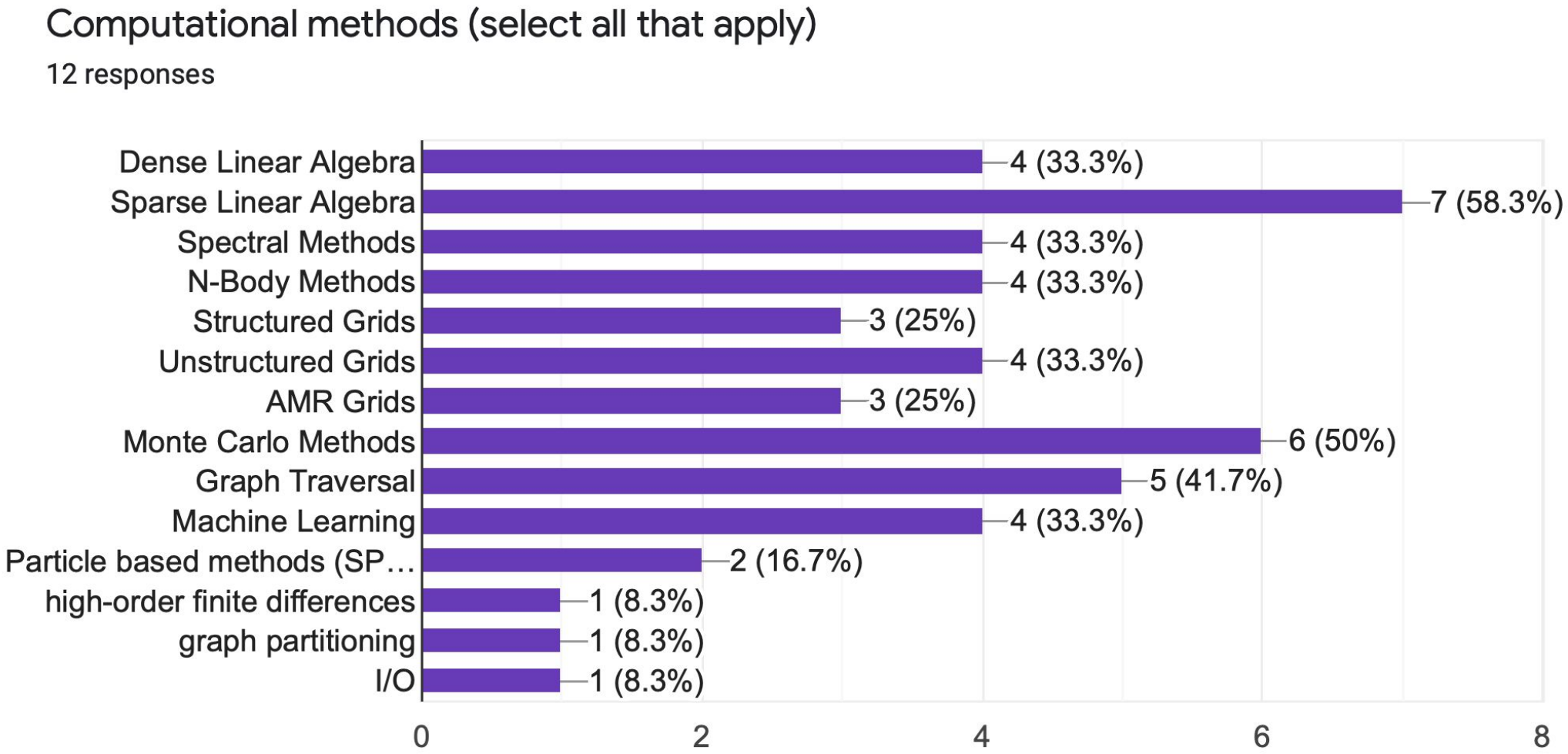
Code (benchmark/mini-app)

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

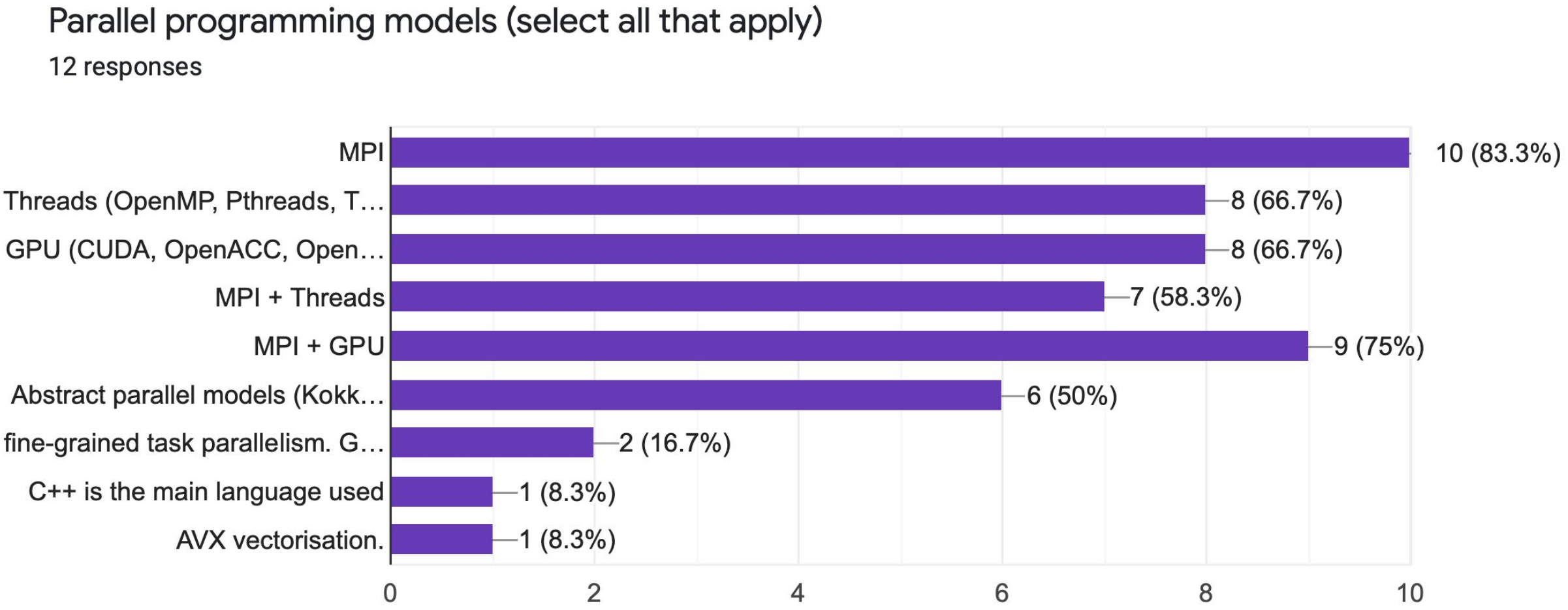
ExCALIBUR project-wide benchmarking initiative



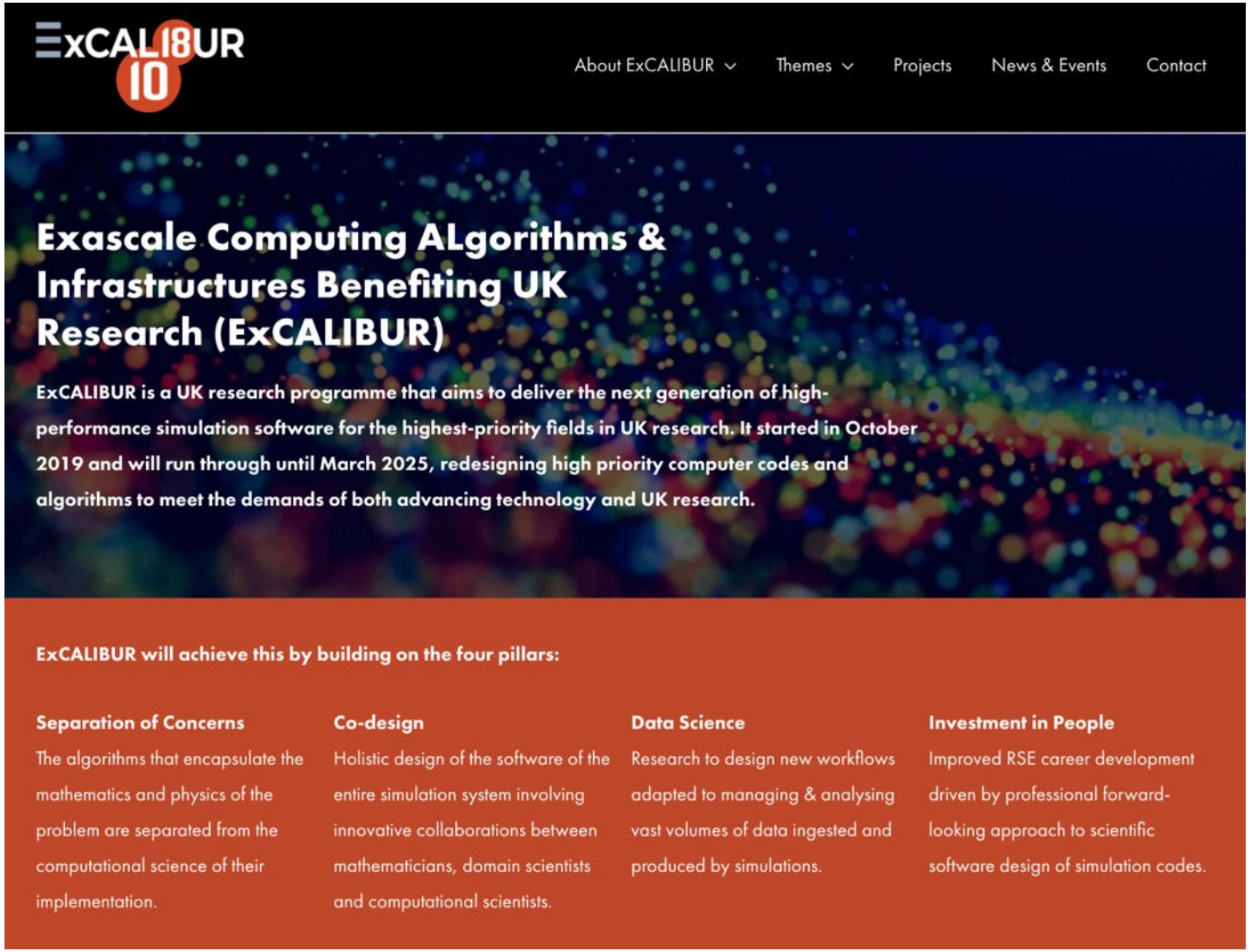
ExCALIBUR project-wide benchmarking initiative



ExCALIBUR project-wide benchmarking initiative



For more about ExCALIBUR…



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https://excalibur.ac.uk

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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/

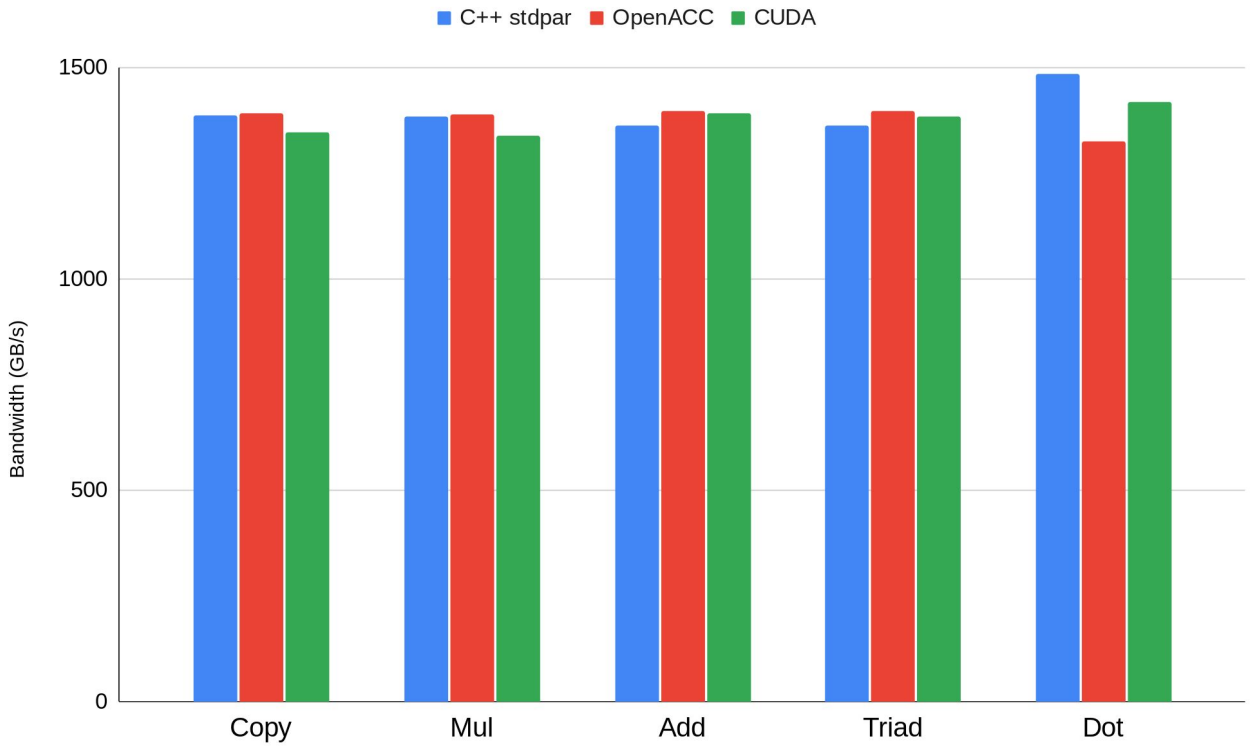
SYCL has company in the parallel C++ space

- 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

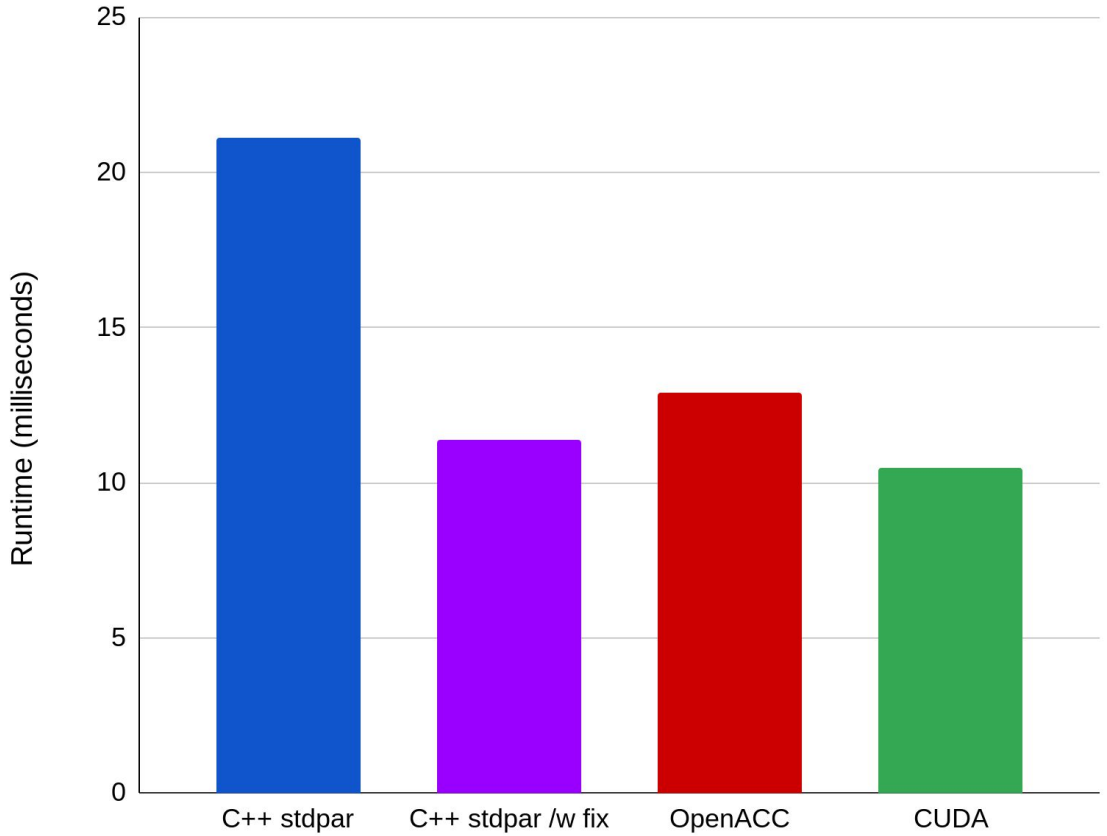
Work by Tom Lin & Tom Deakin

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/

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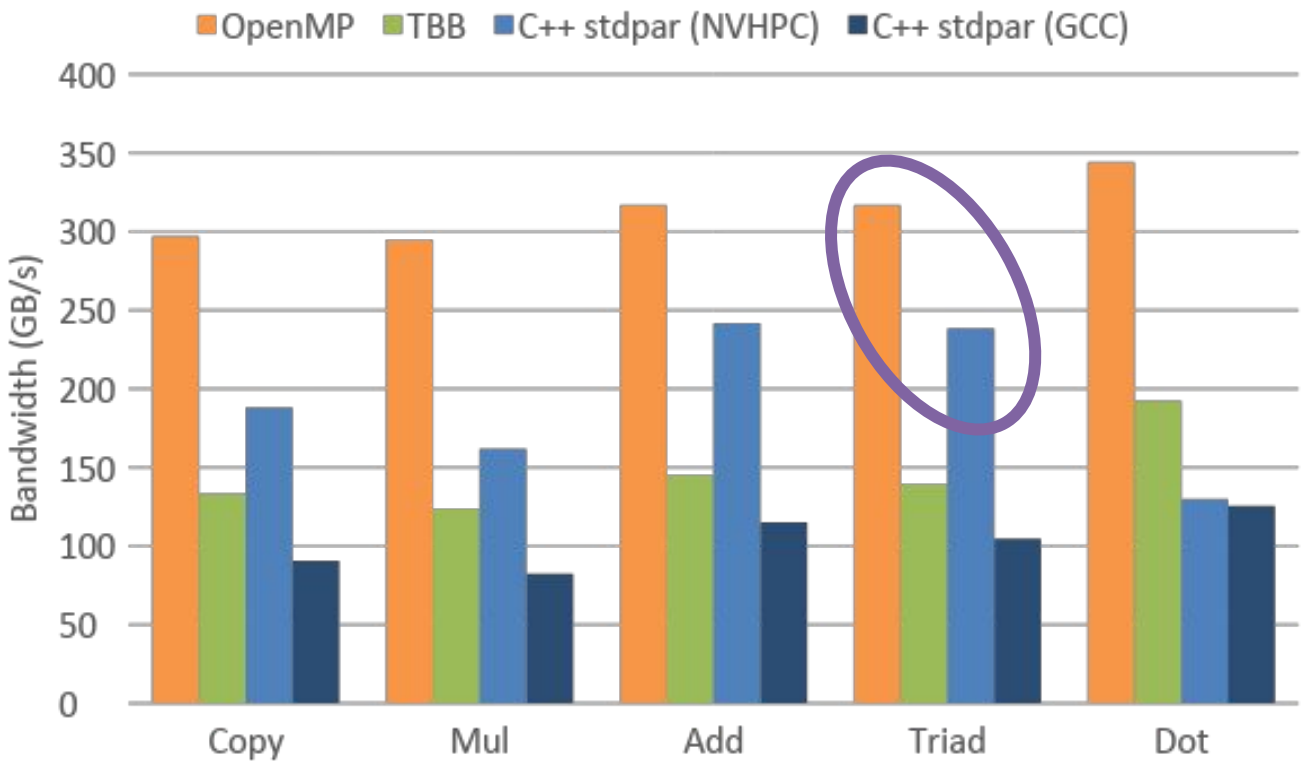
ISO C++ on Icelake Xeon Gold 6338 dual-socket CPU

BabelStream
Higher is better



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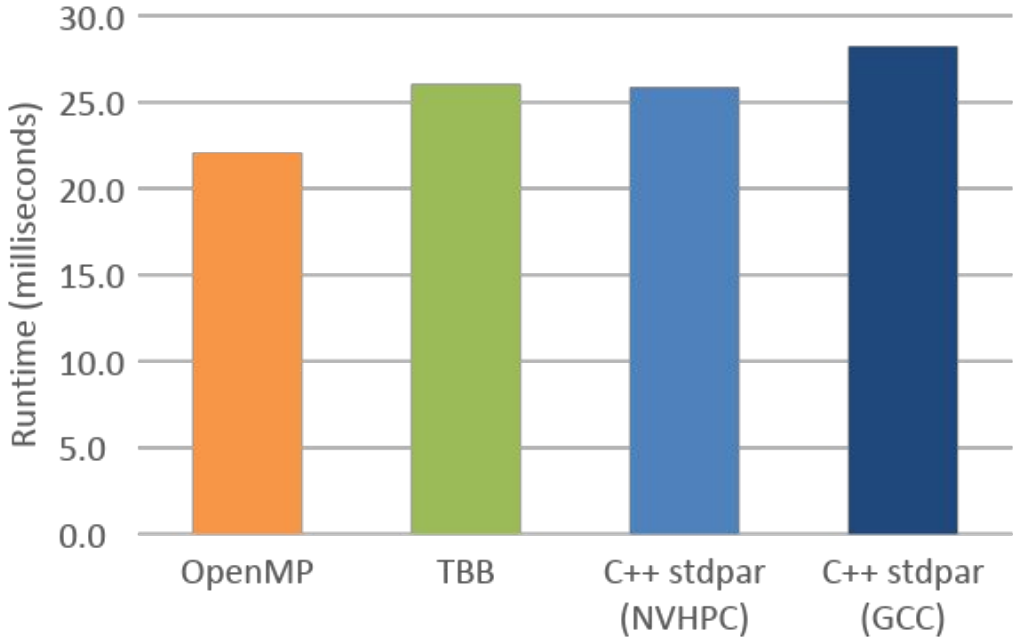

NVHPC gets close to OpenMP performance – except for reductions. GCC uses TBB under the hood.

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

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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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