International Fortran Conference 2020

Interfacing with OpenCL from Modern Fortran for Highly Parallel Workloads

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Presentation Outline

I. Background
II. Focal – A pure Fortran interface library for OpenCL
III. Results and Conclusions

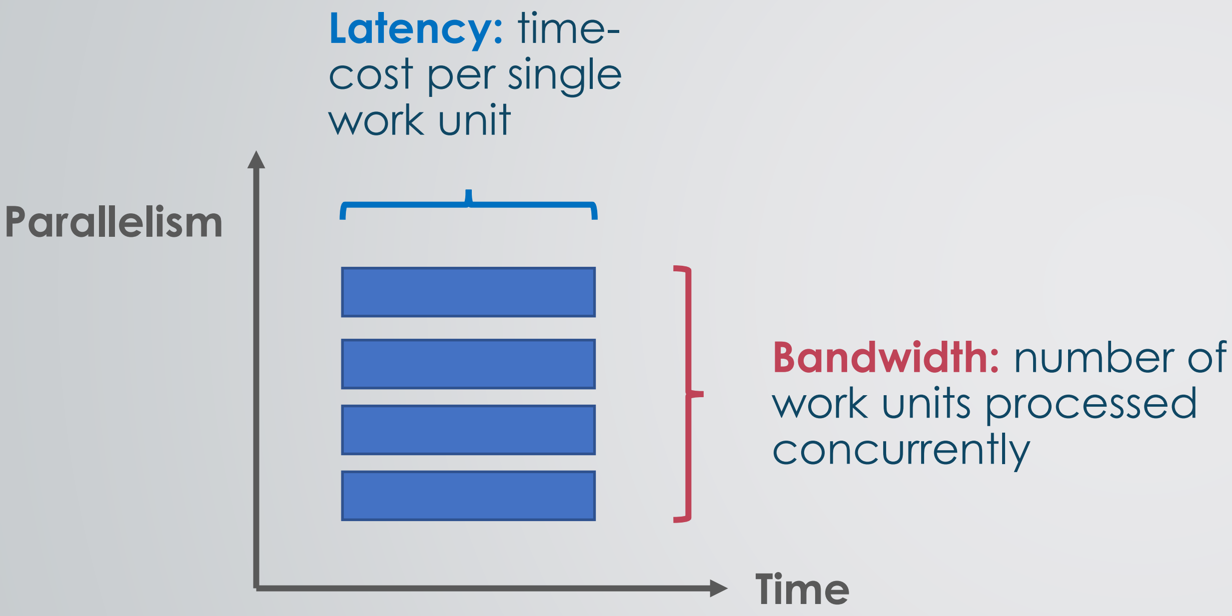
I. Background

Current and future trends in HPC

Programming CPUs vs GPUs

OpenCL overview

Maximising throughput: CPUs vs GPUs



GPUs: maximise bandwidth

- Highly parallel: 1000s of simple cores
- Very high bandwidth memory

$$\textbf{Throughput} = \frac{\textbf{Bandwidth}}{\textbf{Latency}}$$

(amount of work processed per unit time)

CPUs: minimise latency

- Large cache hierarchies (memory latency)
- Instruction pipelining / branch prediction
- Hyper-threading (hide latency)

Programming GPU architectures

Problem type: SIMD

- Running the same instructions on many thousands of different data
- Little or no global synchronisation between threads

Workload: arithmetic intensity

- Maximise the amount of computation and minimise the amount of memory accessed

Memory access: coalesced, structured, direct

- Consecutive threads should access contiguous memory (no striding)
- Hierarchical memory structure

Physically distinct memory space: minimise host-device data transfer

- PCIe bandwidth between GPU and CPU is very slow

Programming models

Languages
- CUDA (NVIDIA)
- HIP (AMD)
- OpenCL (Khronos)
- SYCL (Khronos)
- OneAPI (Intel)

Libraries
- cuBLAS, cuFFT, etc.
- clSPARSE
- Kokkos
- ArrayFire
- RAJA
- Loopy

Domain-specific languages
- PyFR
- OP2
- OPS

Directives
- OpenMP 4.0
- OpenACC

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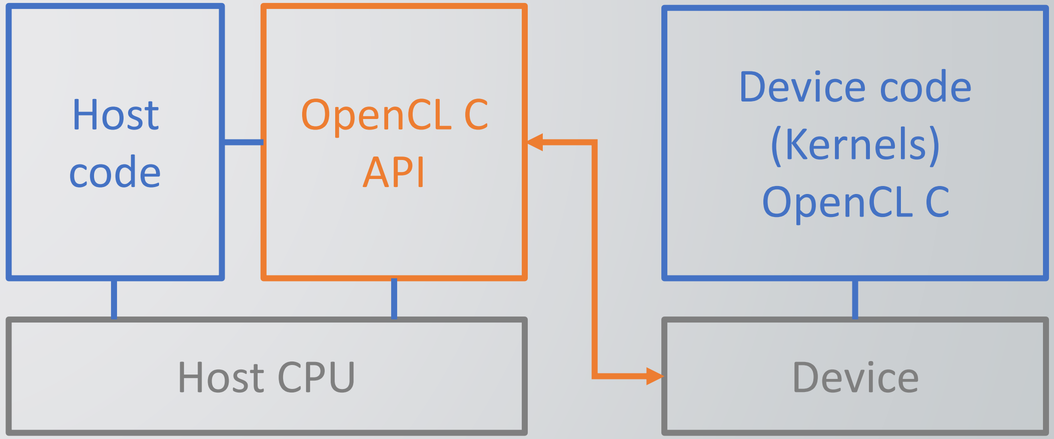
Is C++ becoming the *de facto* language for massive parallelism?

OpenCL

An open cross-platform standard for programming a diverse range of architectures for parallel workloads.

- **Portable:** Intel, AMD, NVIDIA, ARM, Qualcomm
- **Mature:** initial release in 2009
- **Explicit control**
  - Memory management
  - Dependencies
  - Execution & synchronisation



OpenCL & Fortran: Motivation

- OpenCL is an extensive and powerful framework for programming highly parallel workloads
- Low-level C API - bad for domain scientists and engineers:
  - Very verbose: distracts from research problem
  - Pointers aplenty: unsafe, prone to user-error
- Low-level C API – good for developing libraries and abstractions
  - Modern Fortran allows simplification and abstraction of C interfaces

II. The Focal Library

A modern Fortran abstraction library for OpenCL

Focal: An overview

➢ Focal is a modern Fortran abstraction of the OpenCL API

A Pure Fortran Library

- Not a language extension
- Tested with **`gfortran`** and **`ifort`**

Requirements

- Compiler support for **Fortran 2008**
- An OpenCL SDK (*e.g. NVIDIA CUDA SDK*)

Features

- Simple but **explicit syntax** to wrap API calls
- Remove use of C pointers
- Adds level of **type-safety**
- Built-in **error handling** of OpenCL API calls
- Built-in **'debug' mode** for checking correctness
- Built-in routines for collecting and presented **profiling information**

Focal: Using the library

Building

- Requires: F2008 compiler

```
$ make -j
```

```fortran
program test
    use Focal
    implicit none

end program test
```

Using

```
$ $FC -c test.f90 -J/path/to/focal/mod
```

Linking

```
$ $FC *.o -L/path/to/focal/lib -lFocal -lOpenCL
```

By example: initialising OpenCL

```
cl_uint errcode;
cl_platform_id* platform_ids;
cl_device_id* device_ids;
cl_uint num_devices;
cl_uint num_platforms;

// Get number of platforms
errcode = clGetPlatformIDs(0, NULL, &num_platforms);

// Allocate space for platforms
platformIDs = (cl_platform_id *) malloc(sizeof(cl_platform_id)*num_platforms);

// Get platforms
cl_int errcode = clGetPlatformIDs(num_platforms, platformIDs, num_platforms);

// INSERT logic to choose a platform

// Get number of devices
errcode = clGetDeviceIDs( platform_id, CL_DEVICE_TYPE_DEFAULT, 0,
        NULL, &num_devices);

// Allocate space for devices
device_ids = (cl_device_id *) malloc(sizeof(cl_device_id)*num_platforms);

// Get devices
errcode = clGetDeviceIDs( platform_id, CL_DEVICE_TYPE_DEFAULT, num_devices,
        device_ids, num_devices);

// Create an OpenCL context
cl_context context = clCreateContext( NULL, num_devices, device_ids, NULL, NULL, &errcode);
```

Very verbose

- Pointers
- Low-level memory allocation
- Size in bytes
- API error handling (not shown)

By example: initialising OpenCL **with Focal**

Simplified and self-explanatory interface

Pointers replaced with derived types

```
type(fclDevice) :: device
...
device = fclInit(vendor='nvidia,amd',type='gpu',sortBy='cores')

call fclSetDefaultCommandQueue( fclCreateCommandQ(device) )
```

Additional commands allow multi-device and multi-platform initialisation

Initialise device memory

Derived types for device buffers:

```fortran
integer, parameter :: N = 1000000
type(fclDeviceInt32) :: device_int
type(fclDeviceFloat) :: device_float
type(fclDeviceDouble) :: device_dbl
...
call fclInitBuffer(cmdq,device_int,N)  ! Use specific cmdq
call fclInitBuffer(device_float,N)     ! Use default command queue
call fclInitBuffer(device_dbl,N)
```

Derived types in Focal bring a level of type-safety to the OpenCL API

Host-device memory transfers

```fortran
use iso_c_binding, only: c_int32_t, c_float, c_double
integer, parameter :: N = 1000000
type(fclDeviceInt32) :: device_int
type(fclDeviceFloat) :: device_float
type(fclDeviceDouble) :: device_dbl1, device_dbl2

integer(c_int32_t) :: host_int(N)
real(c_float) :: host_float(N)
real(c_double) :: host_dbl(N)
...
device_int = host_int             ! Host to device
host_float = device_float         ! Device to host
device_dbl2 = device_dbl1         ! Host to host
```

- ***Overloaded assignment** for buffer types gives simple syntax for buffer transfer operations.*
- *Only matching types are overloaded: adds **type safety***
- *Supports both blocking and non-blocking transfers*

Device kernels

Host code:

Compile program to obtain a kernel object:

```
type(fclProgram) :: prog
type(fclKernel) :: sumKernel
character(:), allocatable :: kernelSrc
...
call fclSourceFromFile('kernels/sum.cl',kernelSrc)
prog = fclCompileProgram(kernelSrc)
sumKernel = fclGetProgramKernel(prog,'sum')
```

Device code:

A simple OpenCL kernel to add two vectors:

```
kernel void sum(const int N,
                const global float * v1,
                global float * v2){
  int i = get_global_id(0);
  if(i < N) v2[i] += v1[i];
}
```

Host code:

Launch kernel:

```
type(fclDeviceFloat) :: array1, array2
...
sumKernel%global_work_size = [Nelem, 1, 1]
call sumKernel%launch(Nelem,array1,array2)
```

Synchronisation & Dependencies

Wait on host:

Synchronise host and device execution

```
! Wait on default command queue
call fclWait()

! Wait on a specific command queue
call fclWait(cmdq)

! Wait on last kernel launch
call fclWait(fclLastKernelEvent)

! Wait on last transfer on cmdq
call fclWait(cmdq%lastCopyEvent)
```

Set event dependencies:

Event objects allow easy dependencies

```
type(fclCommandQ) :: cmdq
type(fclKernel) :: myKernel
type(fclDeviceFloat) :: deviceArray
type(fclEvent) :: e
...
myKernel%launch(cmdq,deviceArray) ! Launch kernel
e = cmdq%lastKernelEvent

call fclSetDependency(e) ! Data transfer dependent
hostData1 = deviceData1  !  on kernel completion
```

Profiling device operations

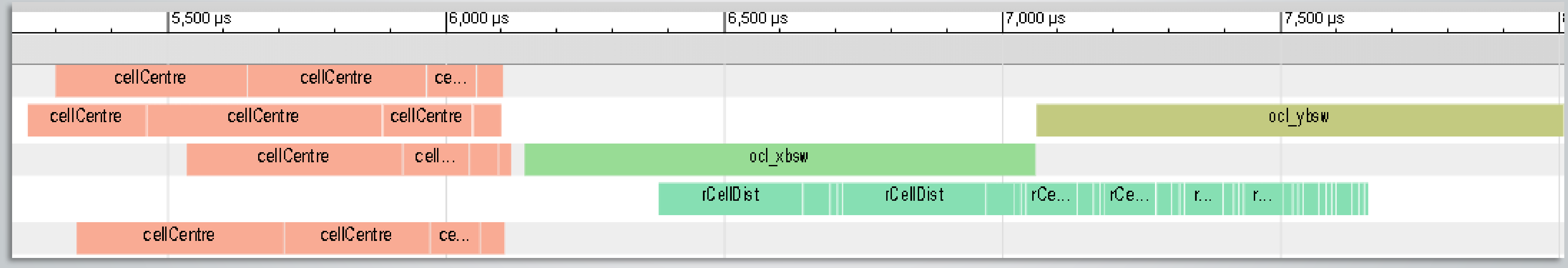
OpenCL has built-in support for **event profiling**

```fortran
type(fclProfiler) :: profiler
...
call fclDumpProfileData(profiler,[unit])

call fclDumpTracingData(profiler, &
                        filename='trace.json')
```

Profile name (Kernel)	No. of events	T_avg (ns)	T_max (ns)	T_min (ns)	Local Mem.	Privat Mem.	PWGS
initialise	1	308750	308750	308750	0	0	32
collide	5000	846595	1527166	735833	0	0	32
boundaryConditions	5000	154161	234083	131333	0	0	32
stream	5000	1067590	1419500	921000	0	0	32
macroVars	50	897174	1104250	802833	0	0	32

ns: nanoseconds, PWGS: Preferred work group size, Mem: Memory in bytes.



Extra details

Fortran submodules

- *Absolute separation of interface & implementation*
- *Fast compilation*
    - *Parallel*
    - *Incremental*
- *Interface parent module can be included as 'header' file*

Documentation

- *Website and user-guide (mkdocs): lkedward.github.io/focal-docs*
- *API reference (FORD): lkedward.github.io/focal*

github.com/LKedward/focal

License MIT

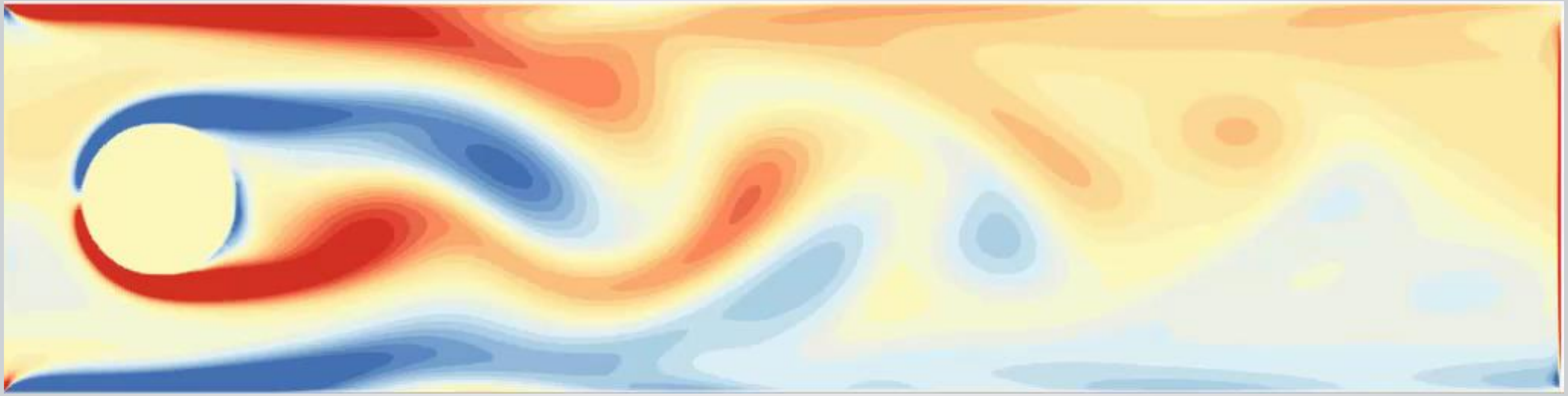
Development

- *Automated tests (Travis): using Intel OpenCL on x86*
- *Code coverage: codecov.io/gh/LKedward/focal*

III. Results & Conclusions

A modern Fortran abstraction library for OpenCL

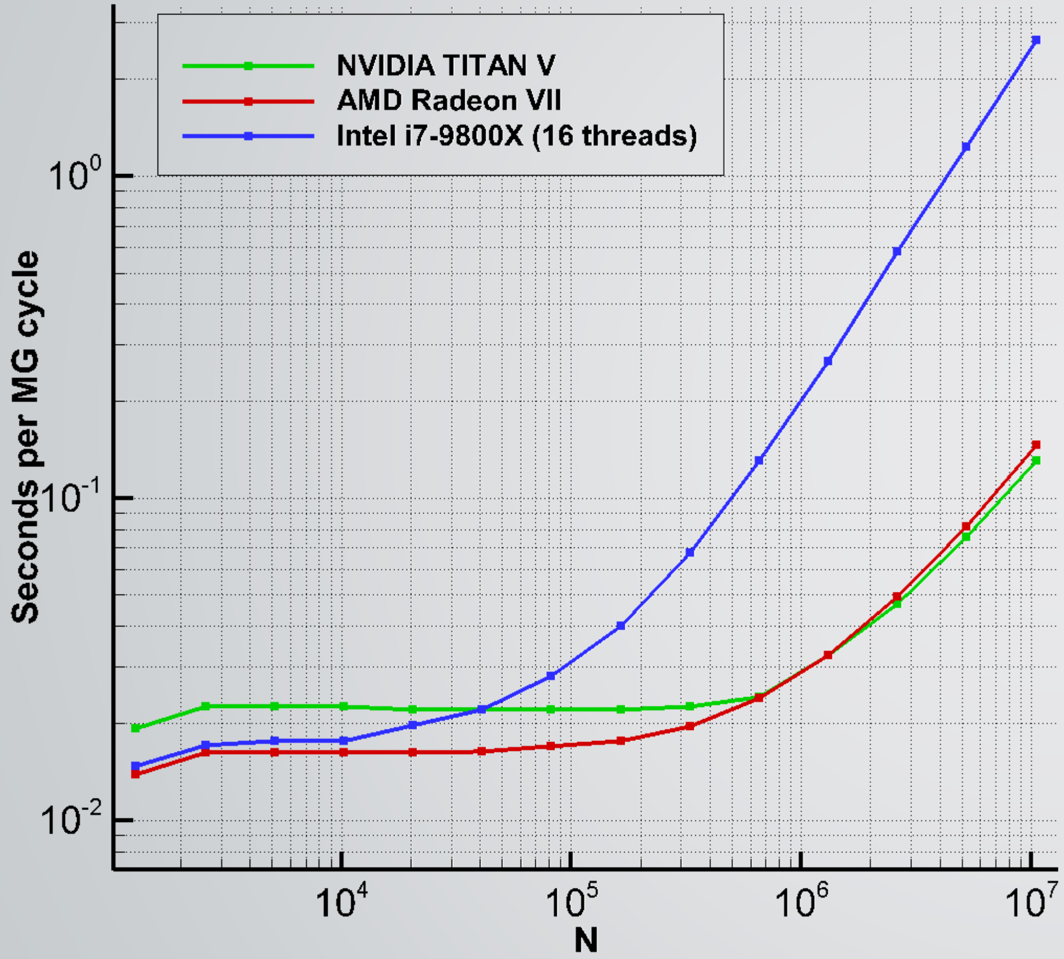
Demonstration: Lattice Boltzmann



github.com/LKedward/lbm2d_ocl

- **128 lines of Fortran code**
- **142 lines of OpenCL kernel code**
- **12x speedup** on Tesla P100 GPU **versus 28 Xeon cores**

Demonstration: Finite Volume Euler



Speedup over Intel CPU (16 threads):

AMD Radeon VII: 18x

NVIDIA Titan V: 20x

Very memory-bound application:

- Various optimisations for maximising arithmetic intensity
- 20% improvement from exploiting work-group shared memory
- Demonstrate mixed-precision solver

Kedward, L. J. and Allen, C. B., "Implementation of a Highly-Parallel Finite Volume Test Bench Code in OpenCL" in AIAA Aviation Forum, June 2020, doi.org/10.2514/6.2020-2923

Summary

- **Portable**
  - Pure standard-conforming Fortran library
  - Only dependency is OpenCL SDK from hardware vendor
  - No vendor/compiler lock-in
  - OpenCL is a mature and portable standard
- **Easy to use**
  - Easy to build and use
  - Simple and explicit syntax
- **Powerful**
  - Supports most features of OpenCL 1.2
  - Allows fine-grain control and optimisation
- **Dual source**
  - Still need to write kernel code in OpenCL C dialect

Ideas for the Future

Fortran already contains the abstractions required to simplify accelerator programming

```fortran
kernel subroutine fluxIntegral(grid,primitives,resid,...)
  type(TGRID), intent(in) :: grid
  type(TPRIM), intent(in) :: primitives
  real(c_double), intent(out) :: resid(:,:)

  real(c_double), address(shared) :: wavespeeds(size(resid,1))
  integer :: i = get_kernel_index(0)

  ...

end subroutine fluxIntegral
```

- Assumed-shape arguments
- Native multi-dimensional arrays
- Custom array bounds
- Derived types/structs in kernels
- Optional kernel arguments
- Work-group shared buffers
- Operator overloading

Acknowledgements

This work was funded by the MENtOR project, a UKVLN project supported by the Engineering and Physical Sciences Research Council (EPSRC) of the UK. Grant reference number EP/S010378/1

EPSRC
Engineering and Physical Sciences Research Council

MENtOR
A UKVLN Project
Methods and Experiments for NOvel Rotorcraft

UK VERTICAL LIFT NETWORK

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Thank you for listening!

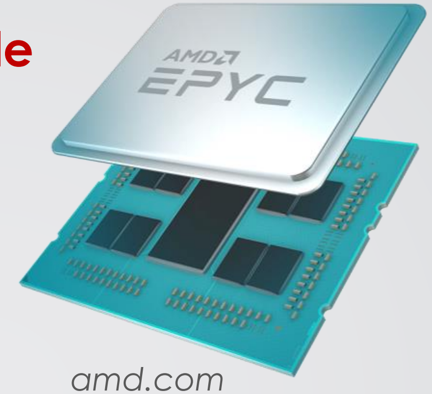
University of BRISTOL

Current and future trends in HPC

Intel.com

Intel 2nd gen. (2019) Xeon scalable

- 56 cores & 112 threads
- Up to 3.80 GHz
- 77MB cache



amd.com

AMD 2nd gen. (2018) EPYC

- 64 cores & 128 threads
- Up to 3.4GHz clock
- 256MB cache
- 30 bn transistors

Fujitsu ARM A64FX many-core processor

- 2.7 TFLOPs
- 8bn transistors
- 48 cores
- 32GB on-chip memory
- 1024GB/s on-chip bandwidth

insidehpc.com

NVIDIA A100 'Ampere' (late 2020)

- 19.5 TFLOPs
- 54bn transistors
- 8192 compute cores
- 1866 GB/s memory bandwidth