

# FULL STEAM AHEAD

3<sup>RD</sup> ISAMBARD HACKATHON - ONLINE  
MARCH 23RD & 24TH 2021

Begins at 09:30 UTC

arm

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Engineering and  
Physical Sciences  
Research Council



SCAN ME

# *The 3<sup>rd</sup> Isambard Hackathon*

## *“Full Steam Ahead!”*

Prof Simon McIntosh-Smith  
University of Bristol & GW4, UK  
[@simonmcs](https://twitter.com/simonmcs)



# This is an invitation-only event

- Remember the hardware and software is all new and therefore we're expecting/*intending* to find issues
- Before releasing any information from the hackathon,  
**please check with me**
  - Our license arrangement for the Fujitsu compiler requires us to get permission from them before any information can be made public in any form

# Why explore Arm-based supercomputers?

- The architecture development is driven by the ***fast-growing mobile computing space***
- Multiple vendors of Arm-CPUs:
  - Fujitsu, AWS, Qualcomm, Apple, NVIDIA, SiPearl, Marvell, ...
  - Greater **competition**
  - More **choice**
  - Rapid **innovations**, e.g. in vector instruction set

# 'Isambard', a Tier 2 HPC service from GW4

## Named in honour of Isambard Kingdom Brunel



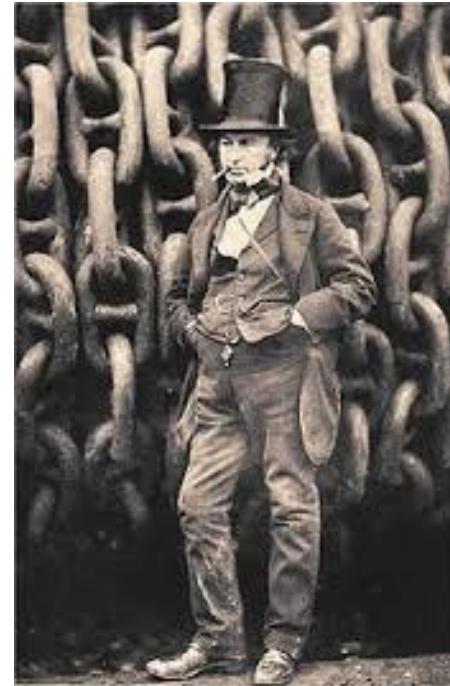
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I.K.Brunel 1804-1859

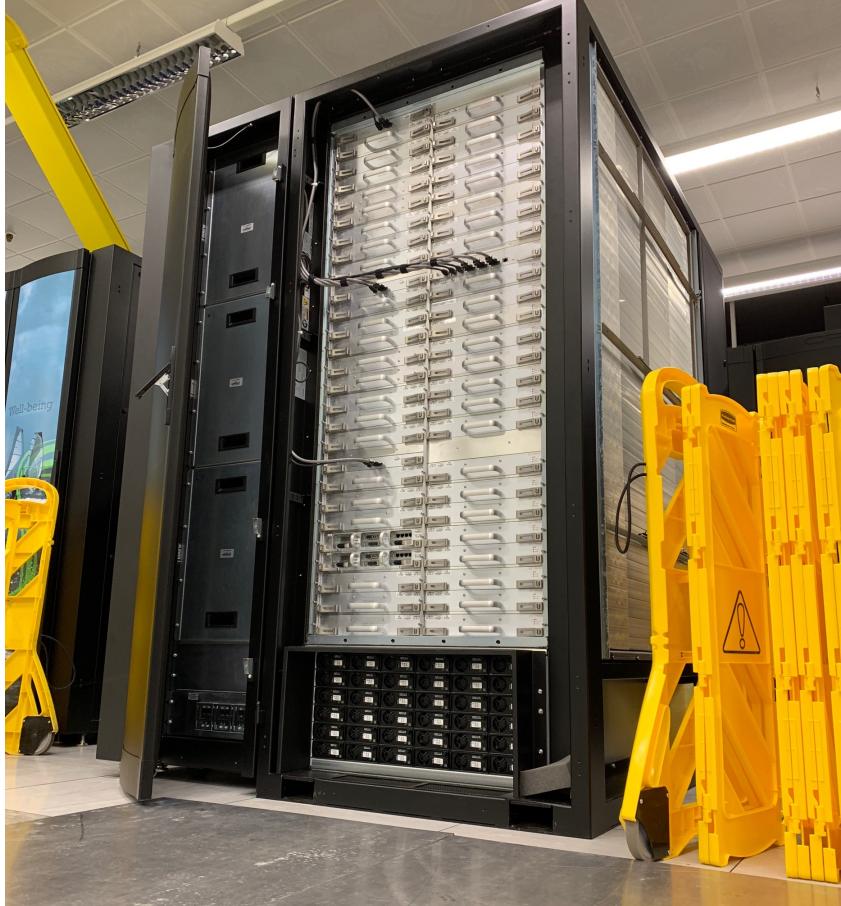
GW4

# The UK's HPC service ecosystem is intentionally diverse



# Isambard 2

- Isambard 1 was the 1st production Arm-based HPC service
- 21,504 Armv8 cores (336n x 2s x 32c)
  - Marvell ThunderX2 32core @ 2.5GHz
- Cray XC50 ‘Scout’ form factor
- High-speed Aries interconnect
- Cray HPC optimised software stack
- >500 registered users



Isambard

# A64fx in Isambard 2

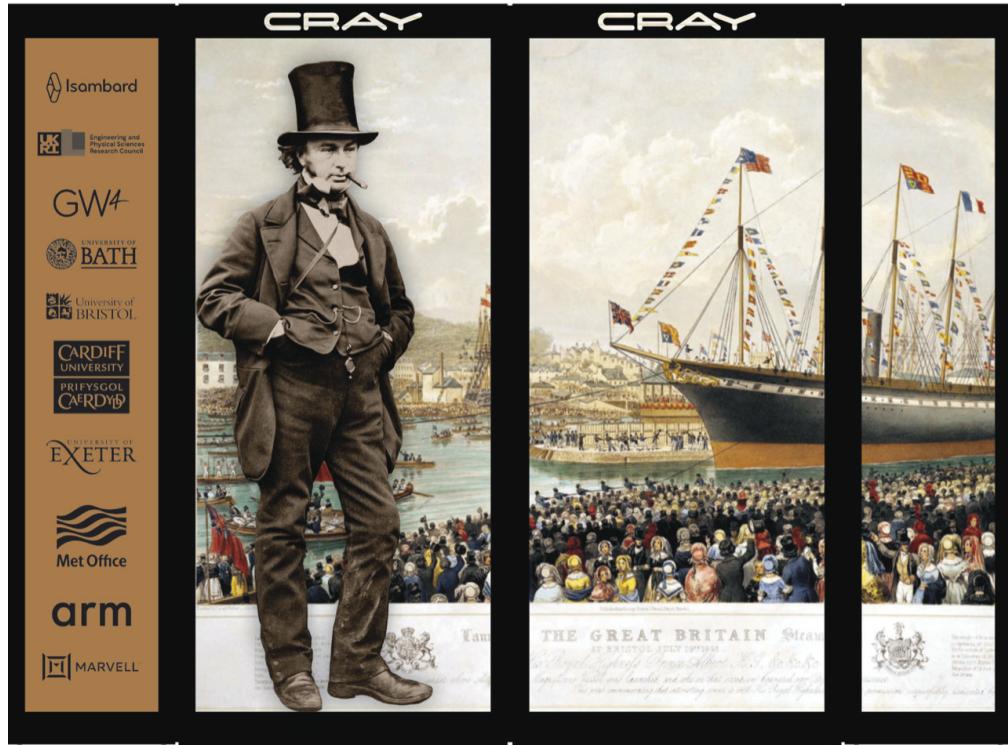
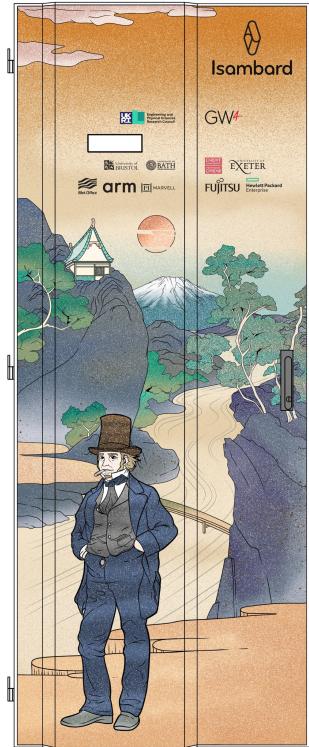
- Fujitsu A64fx Cray/HPE Apollo 80
- 72 nodes, 3456 cores, IB interconnect
- 48 cores per node @ 1.8GHz
- ~800GB/s STREAM bandwidth to 32GB of HBM2 per node
- Cray software stack
- Compilers:
  - Cray, Fujitsu, Arm, GNU



Isambard



# Isambard 2 artwork



# Previous Isambard hackathons

- The **Isambard** project's focus has been on the most heavily used codes on Archer:
  - **VASP**, **CASTEP**, **GROMACS**, **CP2K**, **UM**, HYDRA, **NAMD**, **Oasis**, **SBLI**, **NEMO**
  - Note: 8 of these 10 codes are written in FORTRAN
- Additional important codes for project partners:
  - **OpenFOAM**, **OpenIFS**, WRF, CASINO, LAMMPS, ...
- **RED** = codes at the first hackathon, **BLUE** = codes at the second hackathon



**EPSRC**



**RAISING STEAM**  
1<sup>ST</sup> ISAMBARD HACKATHON - BRISTOL  
NOVEMBER 2ND & 3RD 2017

**arm**



**CRAY**  
THE SUPERCOMPUTER COMPANY



**ETH Zürich**



**EPSRC**



2ND ISAMBARD HACKATHON-BRISTOL  
MARCH 19TH & 20TH 2018

**arm**



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# Isambard progress to date

- Isambard 1 funded in 2016 (£3.1M)
  - 8 early access nodes delivered mid October 2017
  - Full TX2 system of 10,000 cores delivered Spring 2018
- Isambard 2 funded in 2020 (£4.6M):
  - Doubled size of TX2 system to 21,000 cores in Aug 2020
  - Updated MACS system: added AMD Rome, Intel Cascade Lakes, NVIDIA Volta, soon also Milan, Ice Lake, Mi100 and A100
  - **Added A64fx Apollo 80 system**



**ETH** Zürich



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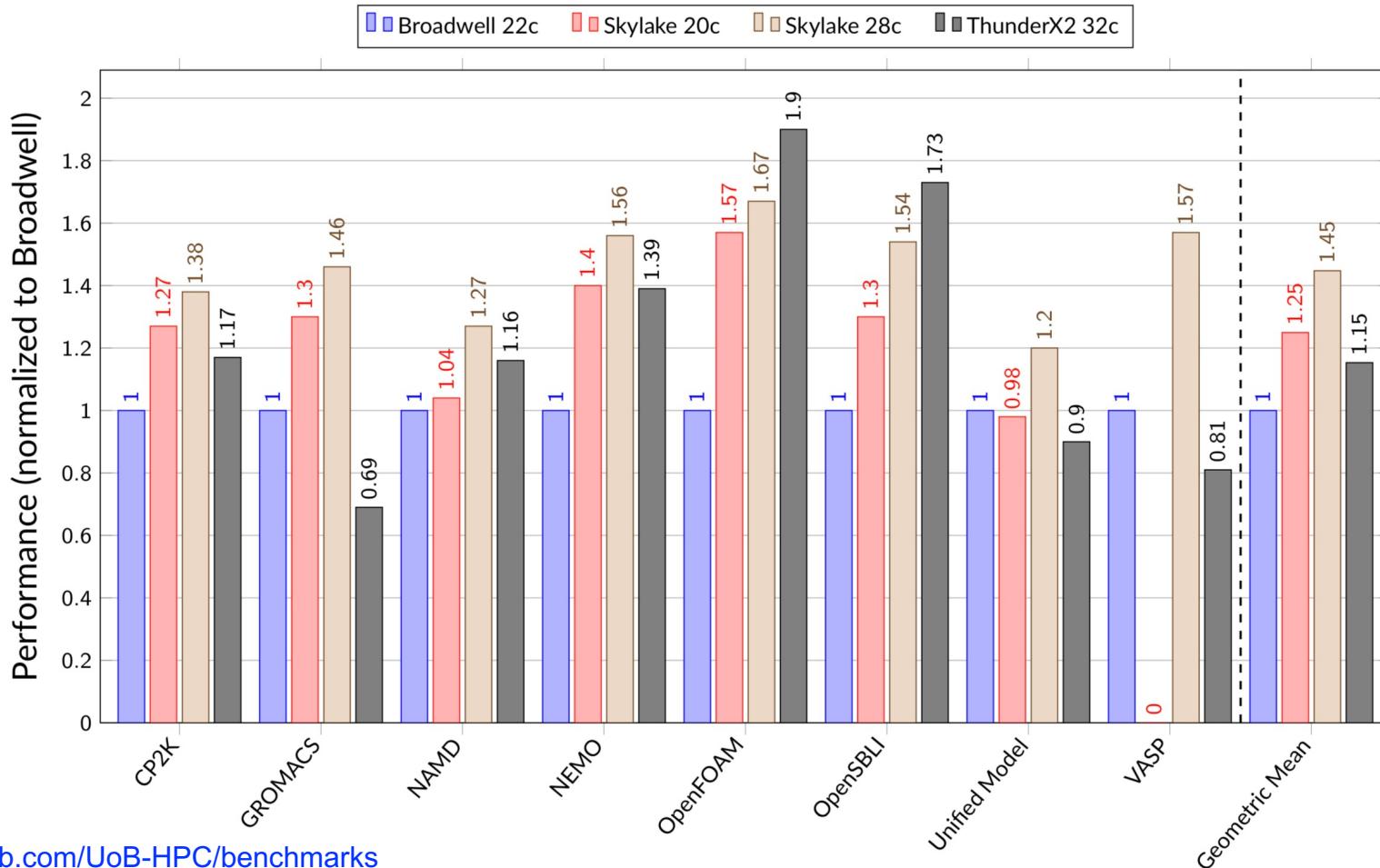
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# Isambard 1 results following the hackathons



# Best compilers by code for each platform

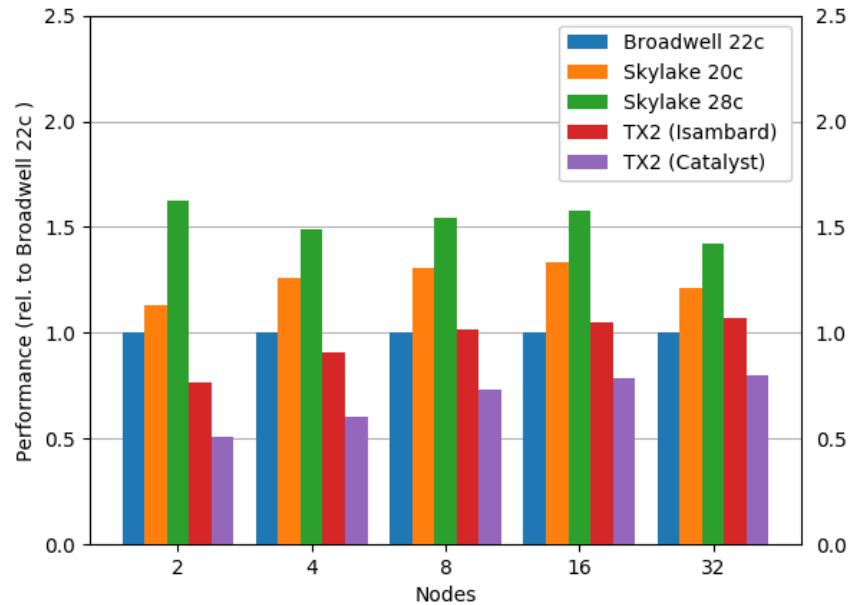
Benchmark	ThunderX2	Broadwell	Skylake	Xeon Phi
STREAM	GCC 8	Intel 18	Intel 18	Intel 18
CloverLeaf	CCE 8.7	Intel 18	Intel 18	Intel 18
TeaLeaf	GCC 7	Intel 18	Intel 18	Intel 18
SNAP	CCE 8.6	Intel 18	Intel 18	Intel 18
Neutral	GCC 8	Intel 18	Intel 18	Intel 18
CP2K	GCC 8	GCC 7	GCC 7	—
GROMACS	GCC 7	GCC 7	GCC 7	—
NAMD	Arm 18.2	GCC 7	Intel 18	—
NEMO	CCE 8.7	CCE 8.7	CCE 8.7	—
OpenFOAM	GCC 7	GCC 7	GCC 7	—
OpenSBLI	CCE 8.7	Intel 18	Intel 18	—
UM	CCE 8.6	CCE 8.5	CCE 8.6	—
VASP	CCE 8.7	Intel 17	Intel 17	—

## Comparison of compilers on Arm

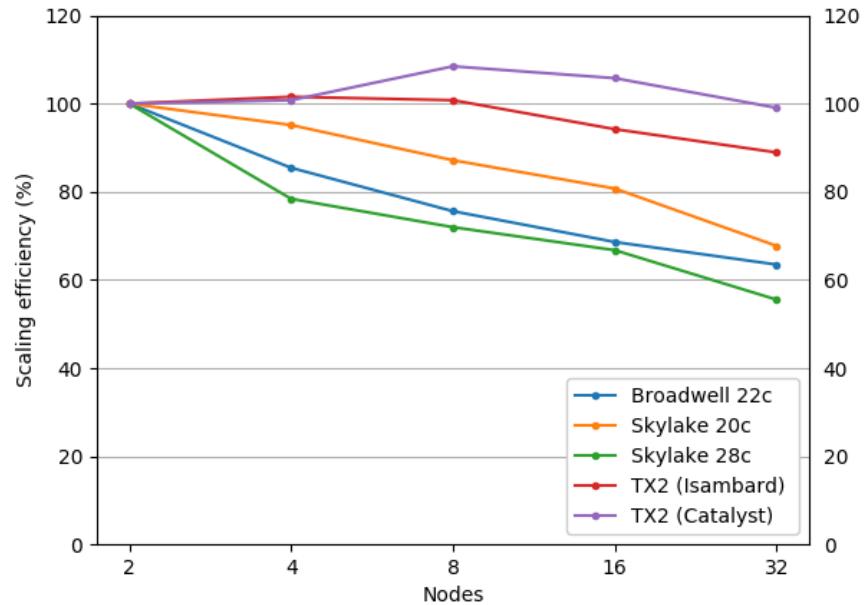
	GCC 7	GCC 8	Arm 18.3	CCE 8.7
STREAM	99%	100%	99%	98%
CloverLeaf	93%	94%	95%	100%
TeaLeaf	100%	95%	95%	99%
SNAP	82%	86%	100%	100%
Neutral	98%	100%	92%	83%
CP2K	98%	100%	BUILD	CRASH
GROMACS	99%	100%	89%	CRASH
NAMD	83%	CRASH	100%	BUILD
OpenFOAM	100%	BUILD	96%	BUILD

Performance normalised to the best for each code (row)

# GROMACS (42 million atoms, ARCHER benchmark)

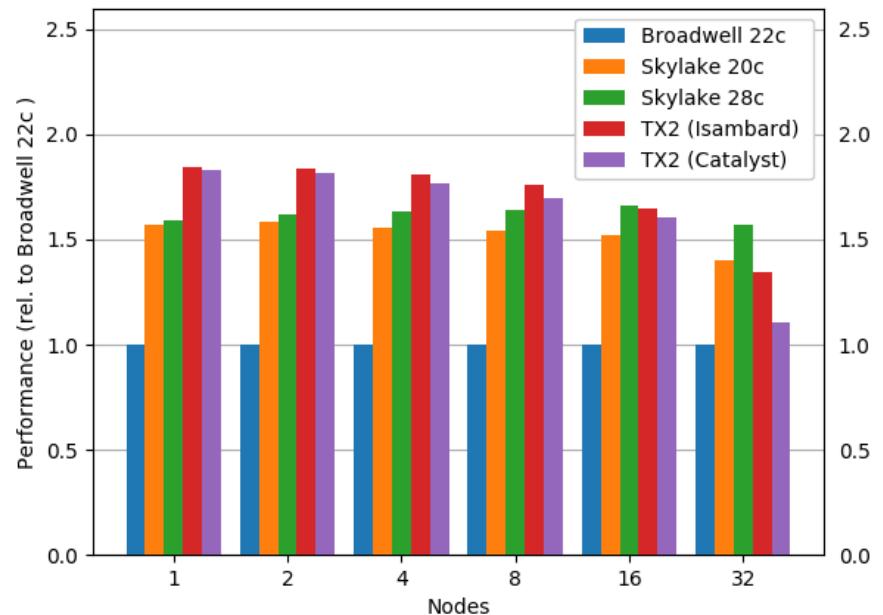


Relative performance

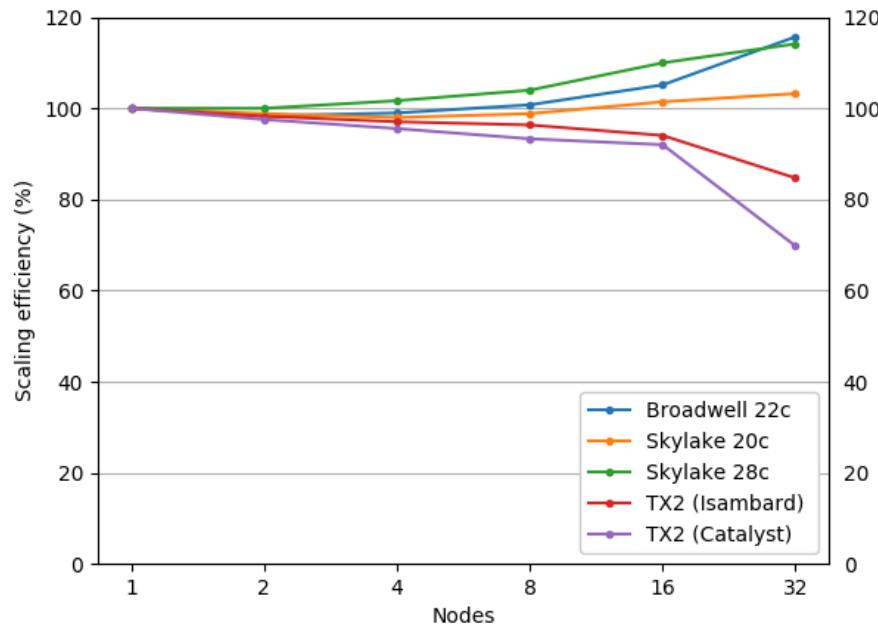


Parallel efficiency

# OpenFOAM (RANS DrivAer, ~64 million cells)



## Relative performance



## Parallel efficiency

# Main Isambard results papers

McIntosh-Smith, Simon, James Price, Tom Deakin, and Andrei Poenaru. "A performance analysis of the first generation of HPC-optimized Arm processors." *Concurrency and Computation: Practice and Experience* 31, no. 16 (2019): e5110.

<https://doi.org/10.1002/cpe.5110>

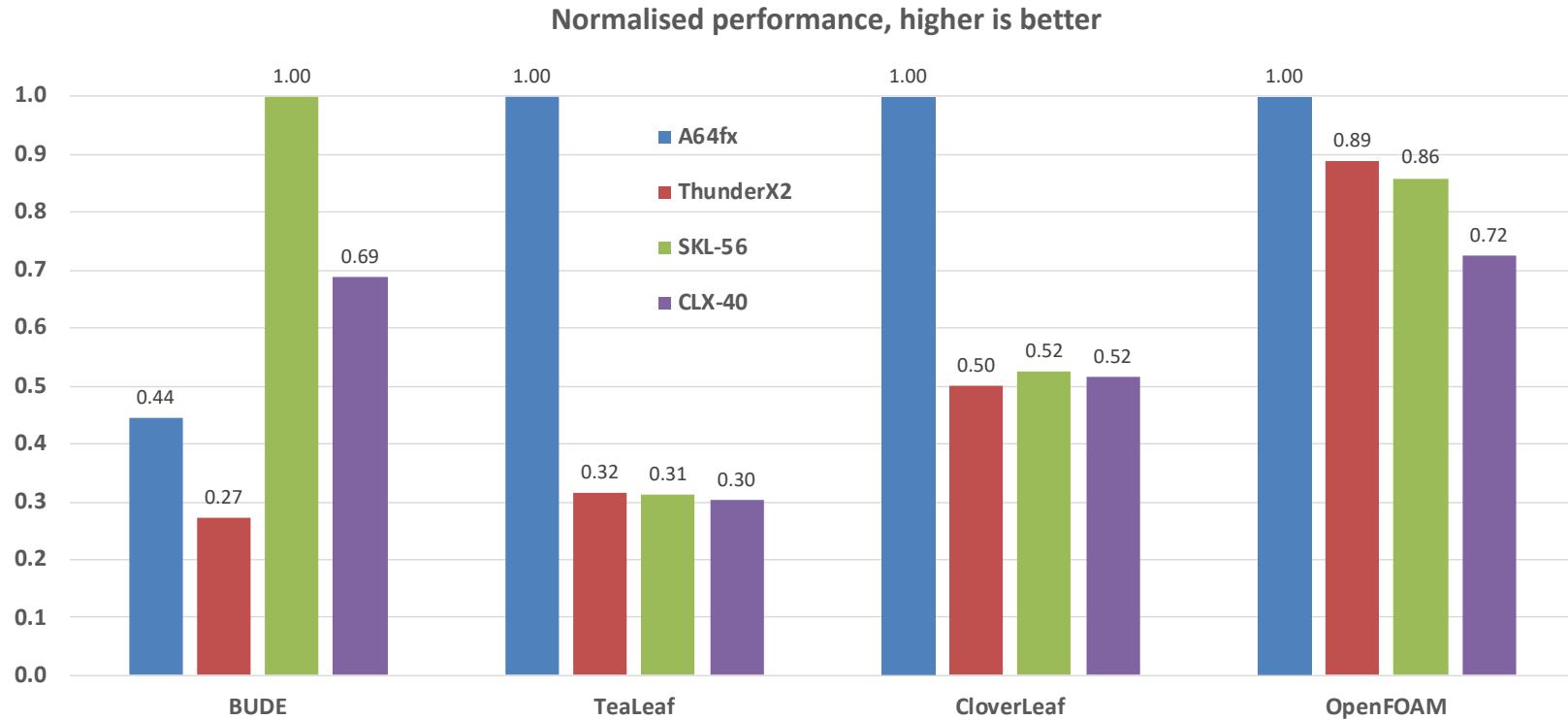
McIntosh-Smith, Simon, James Price, Andrei Poenaru, and Tom Deakin. "Benchmarking the first generation of production quality Arm-based supercomputers." *Concurrency and Computation: Practice and Experience* 32, no. 20 (2020): e5569.

<https://doi.org/10.1002/cpe.5569>

**Build and run scripts:**

<https://github.com/UoB-HPC/benchmarks>

# Early A64fx results look promising on Isambard 2



Slow BUDE results due to compiler issue, currently under investigation.  
Expect ~2x faster for A64fx.

# Virtual Event 101

- Please be VOCAL! If you have a technical issue or start to fall behind **let us know!**



- Please speak up! And please mute when not speaking
- The training parts of the hackathon **are** being recorded, so please be careful while sharing your screen. We won't record the hands-on sessions though
- Hands-on activities will use **Slack** for chats, **Zoom breakout rooms** are available for discussion and screen sharing
- Join the [Isambard Hackathon workspace](#) and open the [#a64fx channel](#)
  - Workspace: [https://join.slack.com/t/isambard-hackathons/shared\\_invite/zt-ngmn6tmb-Tu5wLDnoLKgzzvOcfkC2~bg](https://join.slack.com/t/isambard-hackathons/shared_invite/zt-ngmn6tmb-Tu5wLDnoLKgzzvOcfkC2~bg)
  - Channel: <https://isambard-hackathons.slack.com/archives/C01RZUPFEM6>
- Upgrade zoom! **Version 5.4.0 or later** is required to use the breakout rooms
  - <https://support.zoom.us/hc/en-us/articles/201362233-Upgrade-update-to-the-latest-version>

# Hackathon goals

- **Short term:**
  - Early attempts at porting to A64fx
  - Find issues with compilers, libraries etc
  - Produce exciting A64fx performance results to use at CUG and ISC this summer
- **Medium term:**
  - Accelerate the maturity of the Arm HPC software stack for SVE: Cray's CCE, Arm Clang/LLVM, GNU, Fujitsu et al

# Process for the hackathon

1. Do an initial port of the code to A64fx. Measure and record a performance baseline
  - Please post initial results in Slack, including details such as compiler and version, which flags used etc
  - You can also compare the A64fx results with an Isambard TX2 dual socket node, and with any of the systems in the Isambard MACS, e.g. Broadwell, Cascade Lakes, Rome etc.
2. Measure and record the final performance you achieve by the end of the hackathon
  - Also post these in Slack
  - We'll use these results to build the spreadsheet/graphs for ISC etc.
3. Generate feedback and performance / feature bug reports for all the software tools – compilers, libraries etc.

# Agenda

## Tuesday

- **09:30-10:00:** Welcome and hackathon info (Prof. Simon McIntosh-Smith, Isambard PI)
- **10:00-11:30:** An introduction to the A64fx architecture and software tools (Phil Ridley, Arm)
- **11:30-11:45:** Break
- **11:45-12:45:** The A64fx software environment on the HPE Apollo 80 (John Levesque, HPE)
- **12:45-14:00:** Lunch
- **14:00-17:00:** Hands-on hackathon, supported by GW4, Arm and Cray/HPE staff

## Wednesday

- **09:30-11:00:** Review of Tuesday's session and hackathon continuation
- **11:00-11:30:** Break
- **11:30-13:00:** Hands-on hackathon
- **13:00-14:00:** Lunch
- **14:00-16:30:** Hands-on hackathon
- **16:30:** Hackathon wrap-up and next steps.

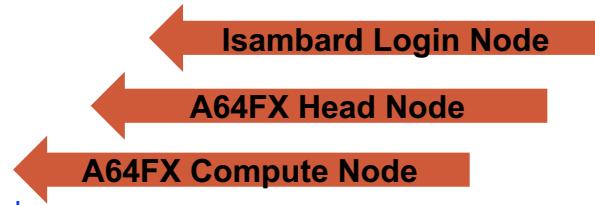
# Accessing Isambard 2

- Three-step login

```
ssh br-trainXX@isambard.gw4.ac.uk
```

```
ssh gw4a64fxlogin01
```

```
qsub -I
```



- User guide <https://gw4-isambard.github.io/docs/user-guide/A64FX.html>

- Quick evaluation of the compilers

```
source ~brx-pridley/doesitvec/isambard-doesitvec.bashrc  
cd doesitvec  
.run
```

- Load environment modules and prepare training materials

```
source ~brx-pridley/arm-sve-tools/isambard-COMP.bashrc
```

Replace **COMP** with one of **arm, cray, fujitsu or gcc**.

- Training materials:

- \$HOME/arm-sve-tools/06\_A64FX/01\_fmla
- \$HOME/arm-sve-tools/06\_A64FX/02\_stream

- Toolchains: Cray, Arm, GNU and Fujitsu

# Important links

**Account:** <https://gw4-isambard.github.io/docs/user-guide/requestaccount.html>

**Docs:** <https://gw4-isambard.github.io/docs/index.html>

**A64fx:** <https://gw4-isambard.github.io/docs/user-guide/A64FX.html>

**Slack:**

[https://join.slack.com/t/isambard-hackathons/shared\\_invite/zt-nqmn6tmb-Tu5wLDnoLKgzbOcfkC2~bg](https://join.slack.com/t/isambard-hackathons/shared_invite/zt-nqmn6tmb-Tu5wLDnoLKgzbOcfkC2~bg)

**Tuesday Zoom:**

<https://bristol-ac-uk.zoom.us/j/98721814432?pwd=djFwQm0rTDVTNIRscVdmYmczMDRBQT09>

**Wednesday Zoom:**

<https://bristol-ac-uk.zoom.us/j/94919260730?pwd=WEJuenlEckpVSGpZMUICcDlkMIZXQT09>