

**Prof Simon McIntosh-Smith**

@simonmcs

Isambard PI

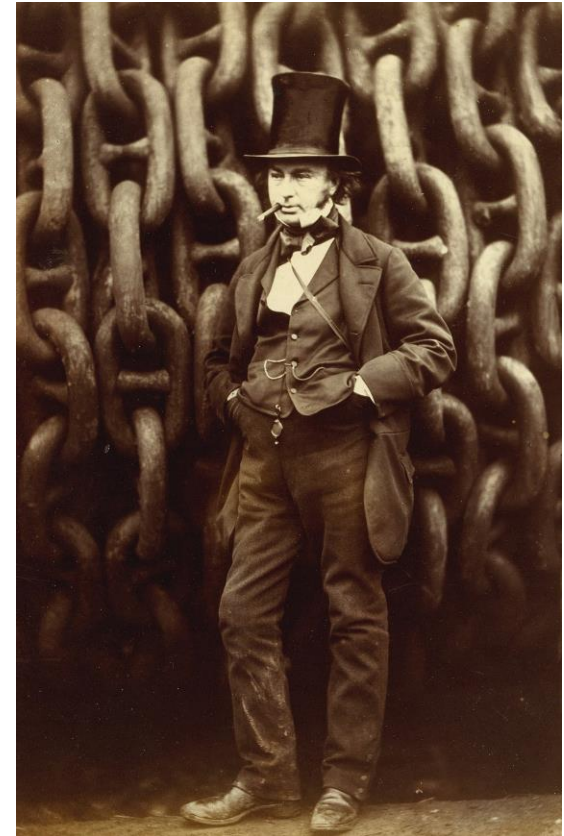
University of Bristol /

GW4 Alliance



# Arm in HPC: From Prototype to Production

# Isambard is a UK Tier 2 HPC service from GW4 and the world's first, Arm-based production supercomputer



Isambard Kingdom Brunel  
1804-1859





# Isambard system specification

- **10,752** Armv8 cores (168n x 2s x 32c)
  - **Marvell ThunderX2 32core 2.1→2.5GHz**
- Cray XC50 'Scout' form factor
- High-speed **Aries** interconnect
- Cray HPC optimised software stack
  - **Compiler, MPI, math libraries, tools, ...**
- **Phase 2 (the Arm part):**
  - **Accepted Nov 9<sup>th</sup> 2018**
  - **Upgrade to final B2 TX2 silicon, firmware, CPE completed March 15<sup>th</sup> 2019**
  - **Production service May 28<sup>th</sup> 2019**
- **>230 registered users**, ~80 of whom are from outside the consortium

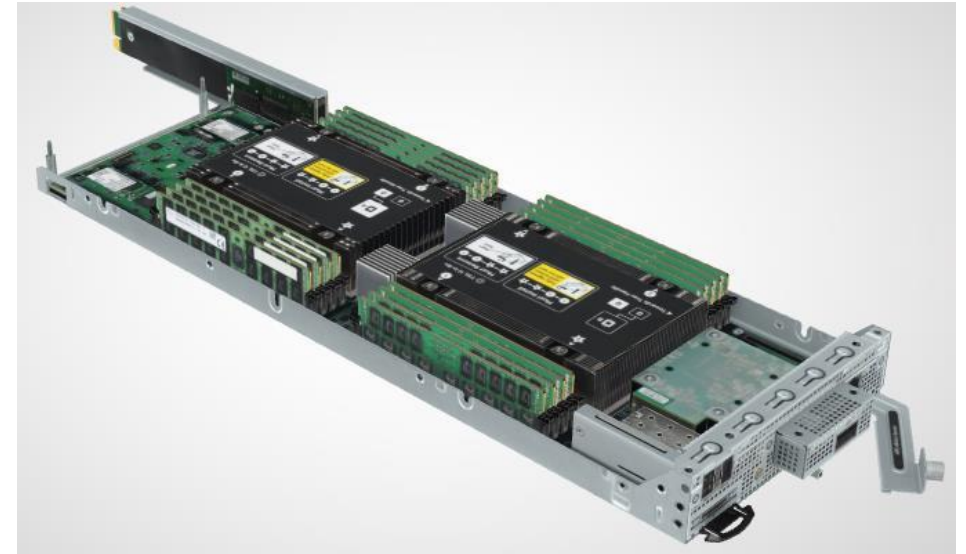


# HPE Catalyst system specification

- **4,096** Armv8 cores (64n x 2s x 32c)
  - **Marvell ThunderX2 32core 2.2GHz**
- HPE Apollo 70 form factor
- 100Gbps Infiniband interconnect
- Open Source software stack
  - **Compilers from Arm, GNU**
- Most users from Bristol today



Up to 4 servers in 2U



# Isambard's core mission: enabling Arm for production HPC

Initial focus on most heavily used codes on Archer, (#1 in UK)

- **VASP**, **CASTEP**, **GROMACS**, **CP2K**, **UM**,  
HYDRA, **NAMD**, **Oasis**, **SBLI**, **NEMO**
- Note: most of these codes are written in FORTRAN

Additional important codes for project partners:

- **OpenFOAM**, **OpenIFS**, WRF, CASINO, LAMMPS, ...

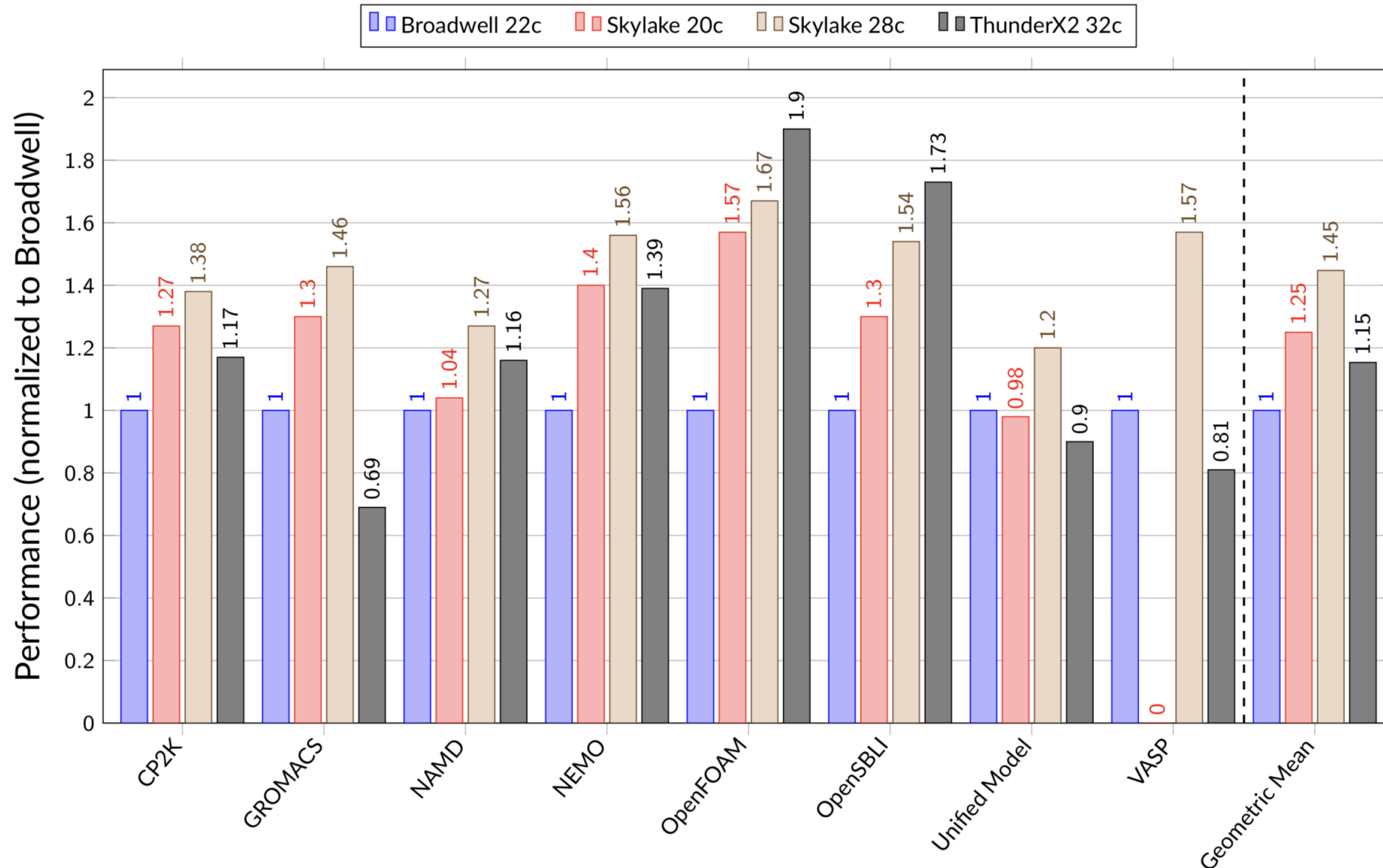
**RED** = codes optimised at the first Isambard hackathon

**BLUE** = codes optimised at the second hackathon

Processor	Cores	Clock speed GHz	TDP Watts	FP64 TFLOP/s	Bandwidth GB/s
Broadwell	2 × 22	2.2	145	1.55	154
Skylake Gold	2 × 20	2.4	150	3.07	256
Skylake Platinum	2 × 28	2.1	165	3.76	256
ThunderX2	2 × 32	2.1 (2.5)	175	1.28	320

- BDW 22c** Intel Broadwell E5-2699 v4, **\$4,115** each (near top-bin)
- SKL 20c** Intel Skylake Gold 6148, **\$3,078** each
- SKL 28c** Intel Skylake Platinum 8176, **\$8,719** each (near top-bin)
- TX2 32c** Cavium ThunderX2, **\$1,795 each** (near top-bin)

# Previously published Isambard single node performance

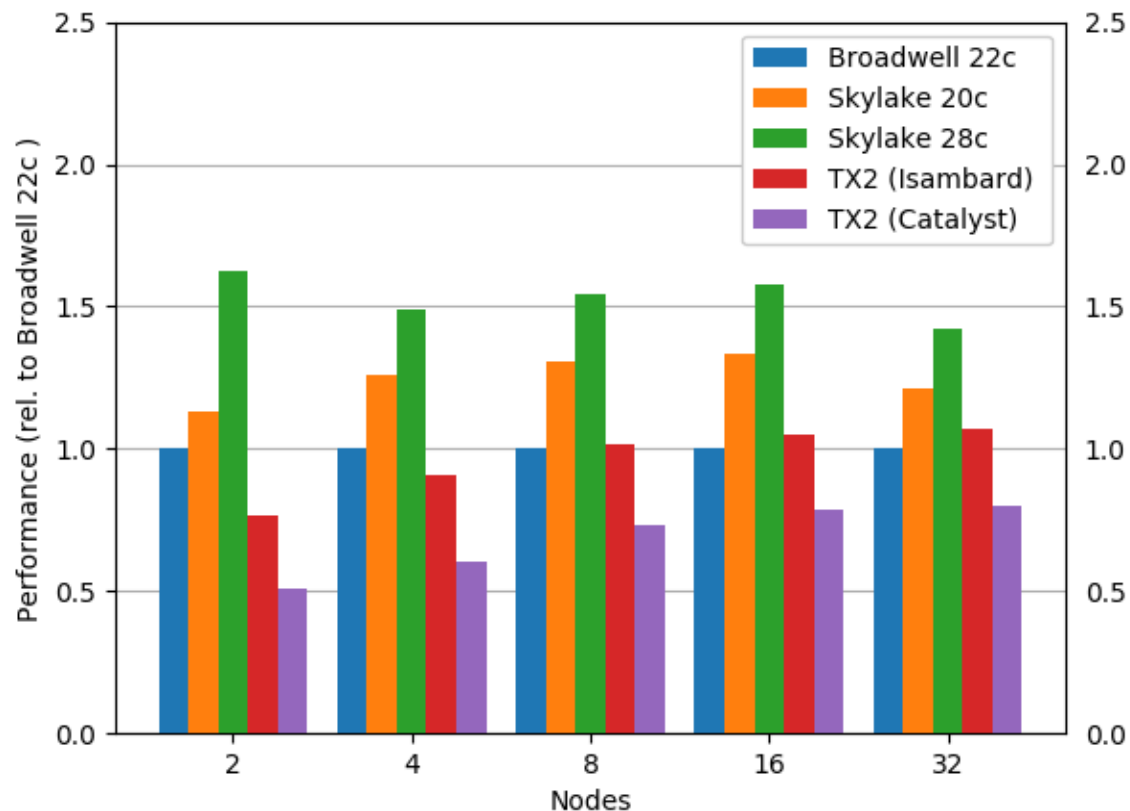


**Comparative Benchmarking of the First Generation of HPC-Optimised Arm Processors on Isambard**

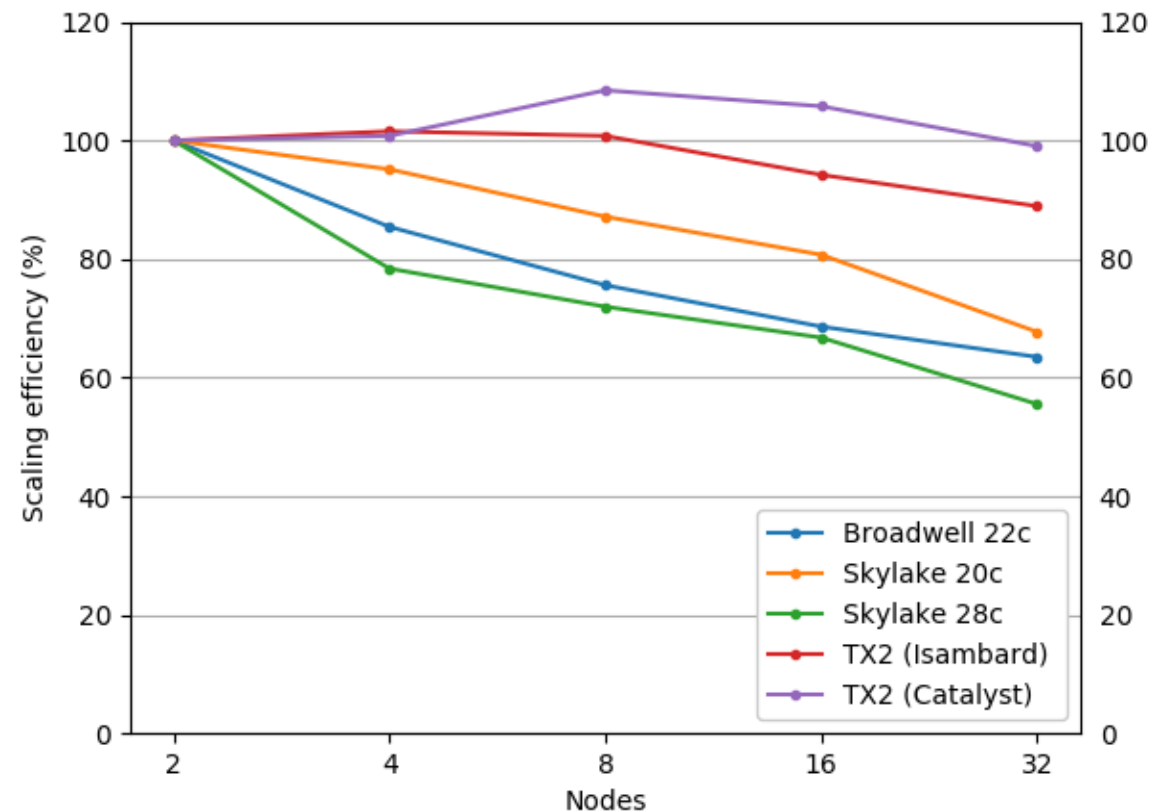
S. McIntosh-Smith, J. Price, T. Deakin and A. Poenaru, CUG 2018, Stockholm



# GROMACS (42 million atoms, ARCHER benchmark)



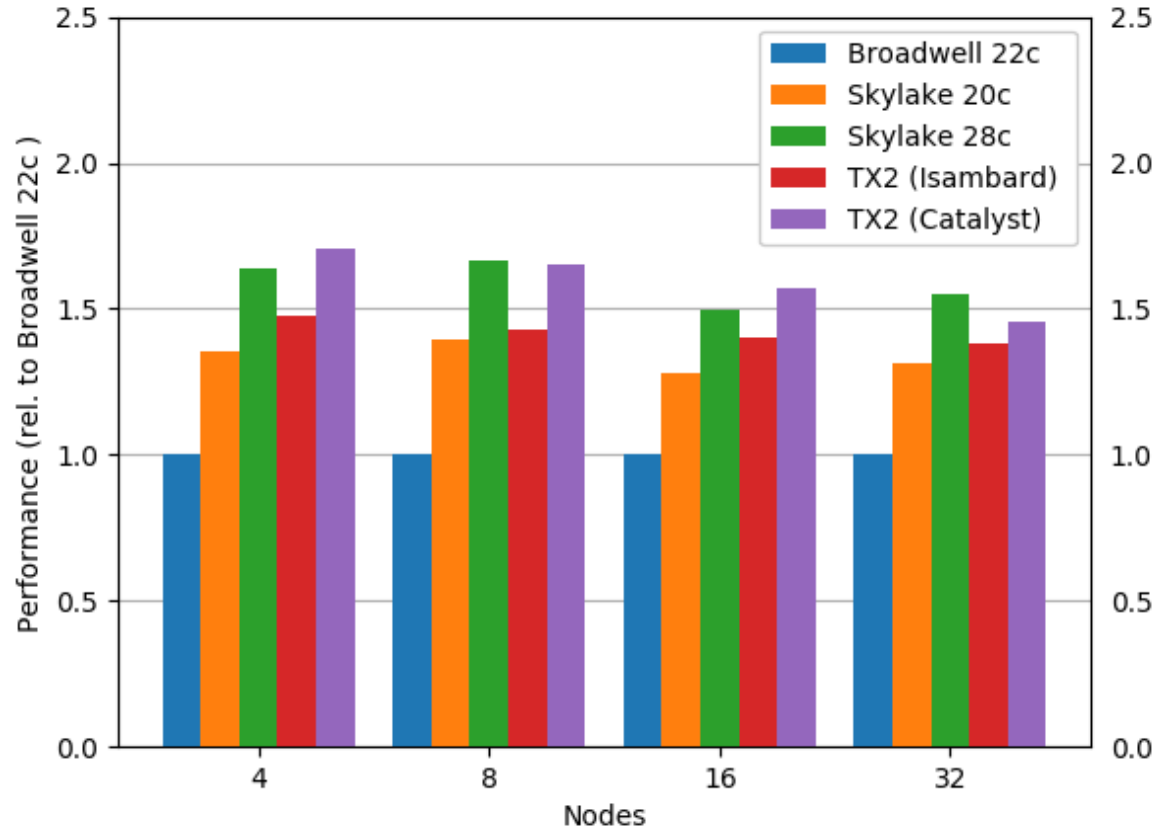
**Relative performance**



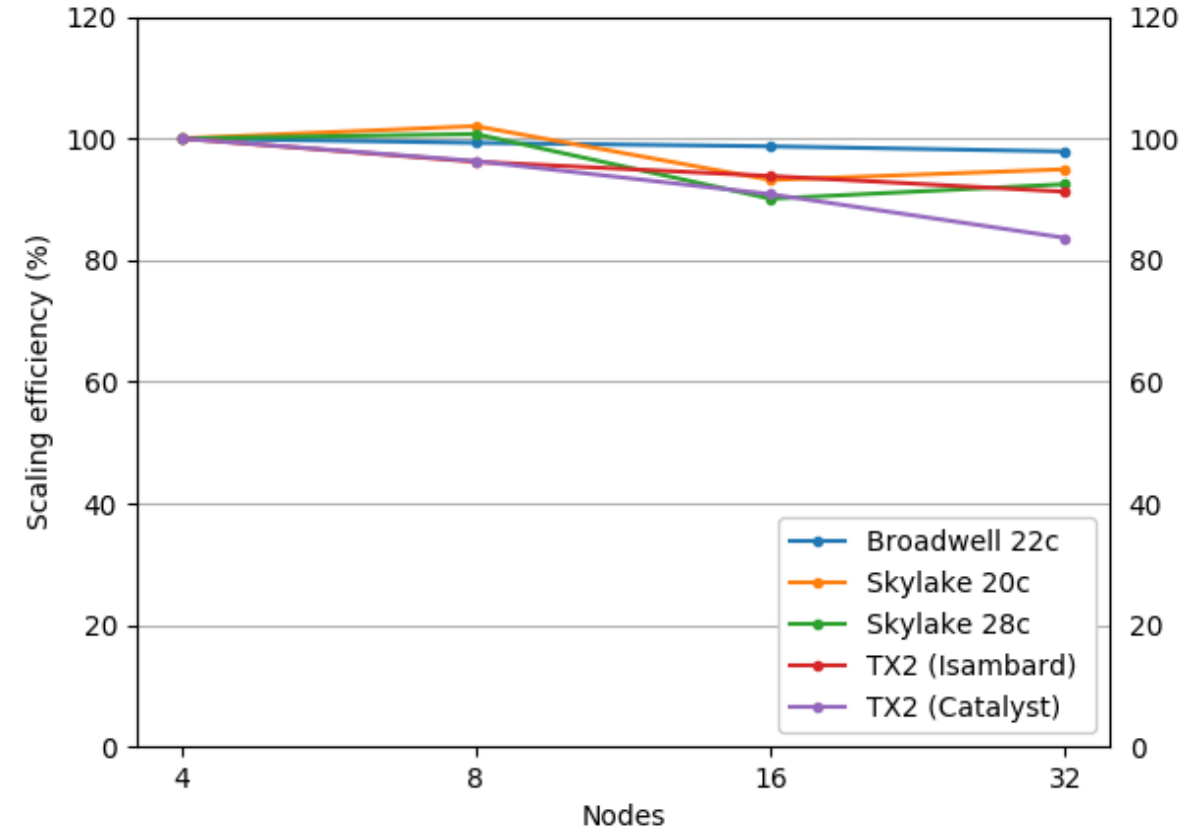
**Parallel efficiency**



# OpenSBLI (1024<sup>3</sup>, ARCHER benchmark)

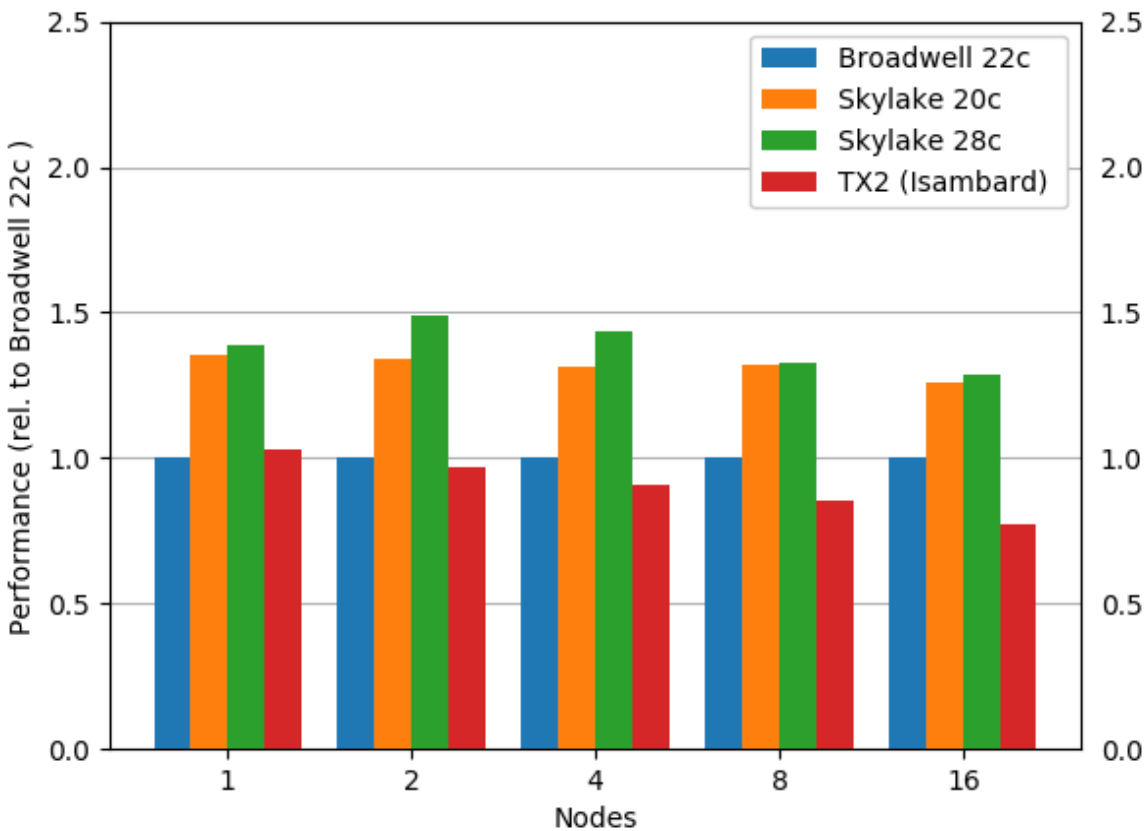


**Relative performance**

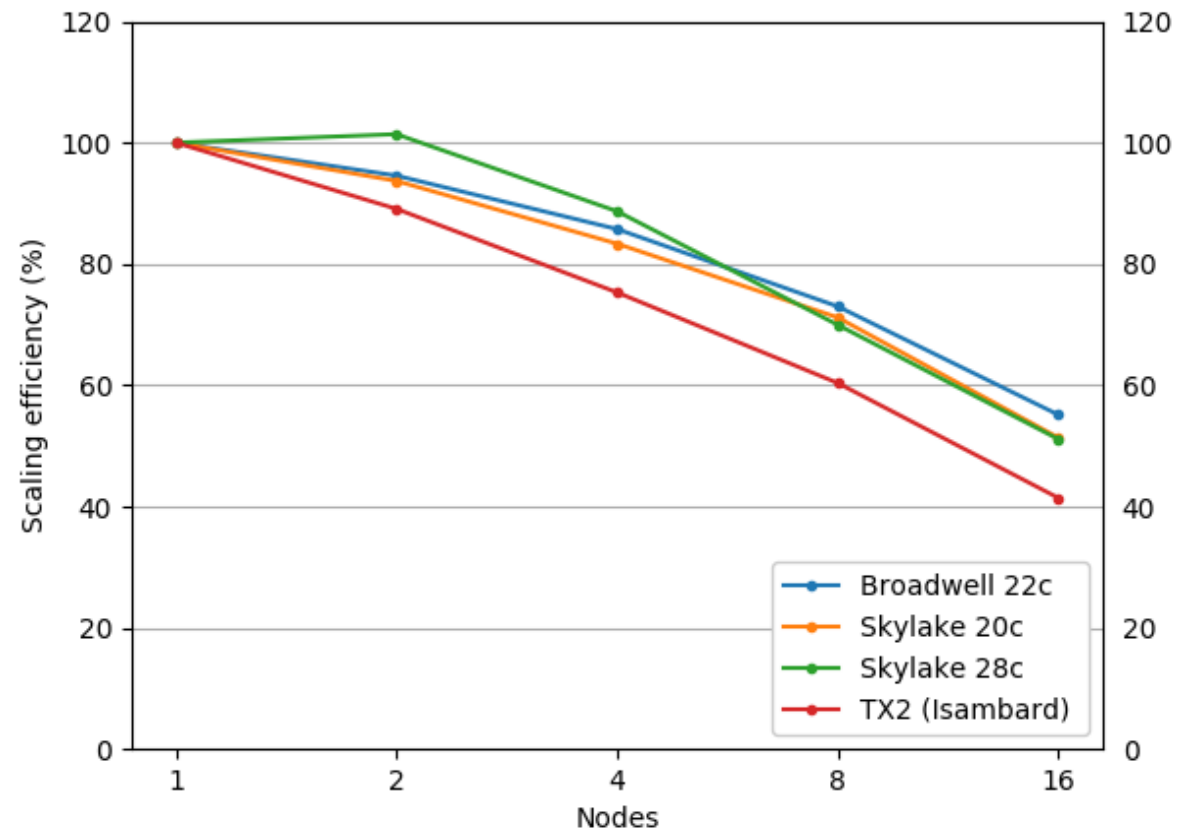


**Parallel efficiency**

# VASP (PdO, 1392 atoms)

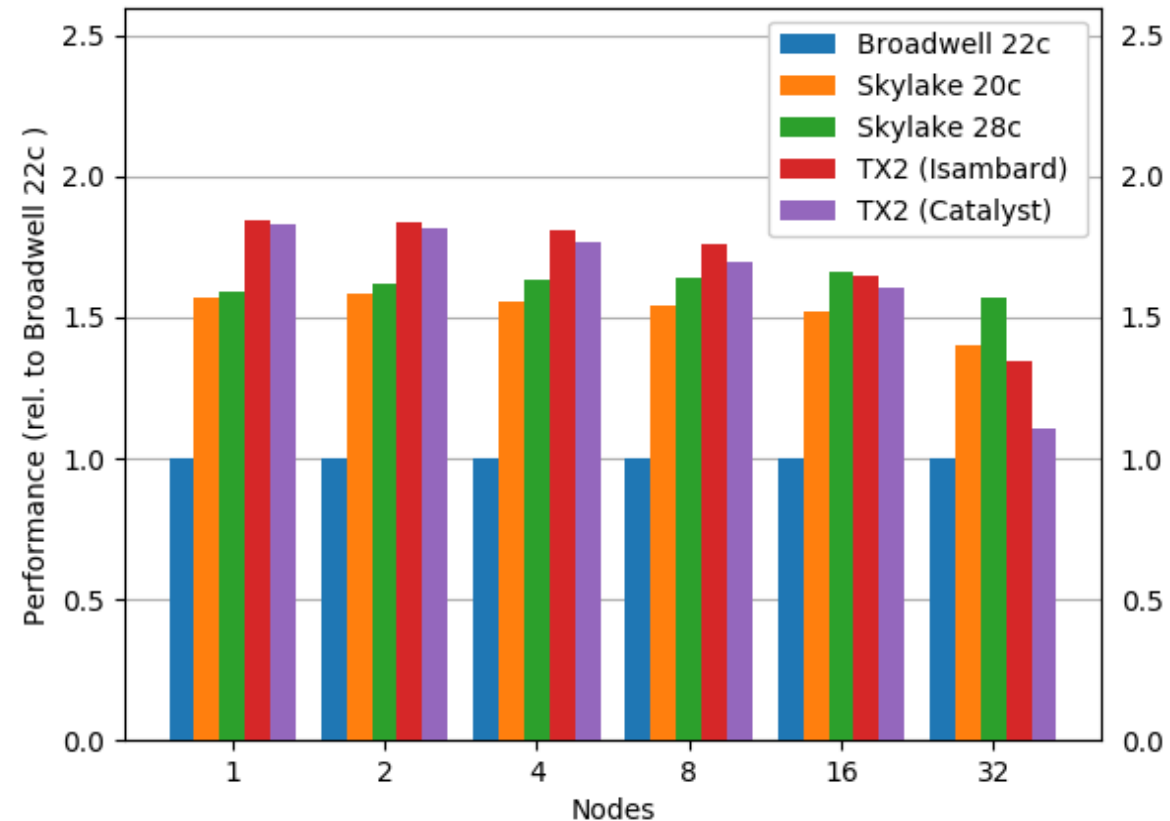


**Relative performance**

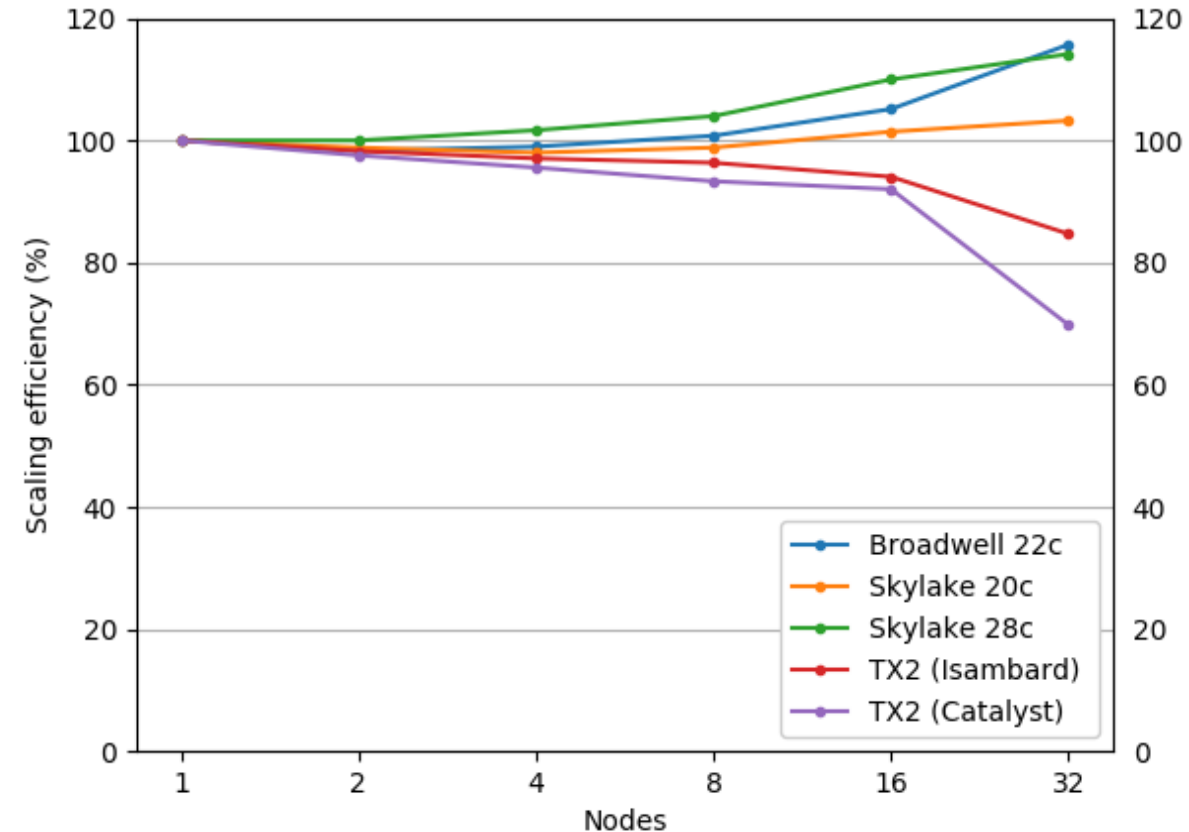


**Parallel efficiency**

# OpenFOAM (RANS DrivAer, ~64 million cells)



## Relative performance



## Parallel efficiency

**Which  
compiler  
was fastest\*  
on each  
code?**

Benchmark	Broadwell	Skylake	Isambard	Catalyst
CloverLeaf	Intel 2019	Intel 2019	CCE 9.0	Arm 19.0
TeaLeaf	Intel 2019	Intel 2019	GCC 8.3	Arm 19.0
SNAP	Intel 2019	Intel 2019	CCE 9.0	GCC 8.2
GROMACS	GCC 8.3	GCC 8.3	Arm 19.2	GCC 8.2
OpenFOAM	GCC 7.3	GCC 7.3	GCC 7.3	GCC 7.1
OpenSBLI	CCE 9.0	GCC 8.3	GCC 8.3	GCC 8.2
VASP	Intel 2019	Intel 2019	GCC 7.3	-

\* Fastest when running across 32 nodes using all cores.



Comparison of compilers on Isambard

CloverLeaf	88%	92%	100%
TeaLeaf	100%	91%	87%
SNAP	58%	CRASH	100%
GROMACS	96%	100%	88%
OpenFOAM	100%*	79%	BUILD
OpenSBLI	100%	91%	96%
VASP	100%*	BUILD	BUILD
	GCC 8.3	Arm 19.2	CCE 9.0

# Conclusions

- Arm-based supercomputers are now in production, doing real science
- Available from multiple vendors
- **Solid, robust software toolchains from multiple vendors**
  - Both open source and commercial
- Arm-based systems scale just as well as x86 ones
- **Arm-based systems are real alternatives for HPC**, reintroducing much needed competition to the market

# For more information

## Comparative Benchmarking of the First Generation of HPC-Optimised Arm Processors on Isambard

S. McIntosh-Smith, J. Price, T. Deakin and A. Poenaru, CUG 2018, Stockholm

<http://uob-hpc.github.io/2018/05/23/CUG18.html>

## Scaling Results From the First Generation of Arm-based Supercomputers

S. McIntosh-Smith, J. Price, A. Poenaru and T. Deakin, CUG 2019, Montreal (Best Paper)

<http://uob-hpc.github.io/2019/06/07/CUG19.html>

**Bristol HPC group:**

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

**Isambard:**

<http://gw4.ac.uk/isambard/>

**Build and run scripts:**

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