First public disclosure of Isambard performance results

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Why explore Arm-based supercomputers?

- The architecture development is driven by the ***fast-growing mobile space***
- Multiple vendors of Arm-CPUs:
  - Greater **competition**
  - More **choice**
  - Rapid **innovations**, e.g. in vector instruction set
- MONT-BLANC proved the approach is feasible

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'Isambard', a new Tier 2 HPC service from GW4.

Named in honour of Isambard Kingdom Brunel

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UNIVERSITY OF BATH

UNIVERSITY OF EXETER

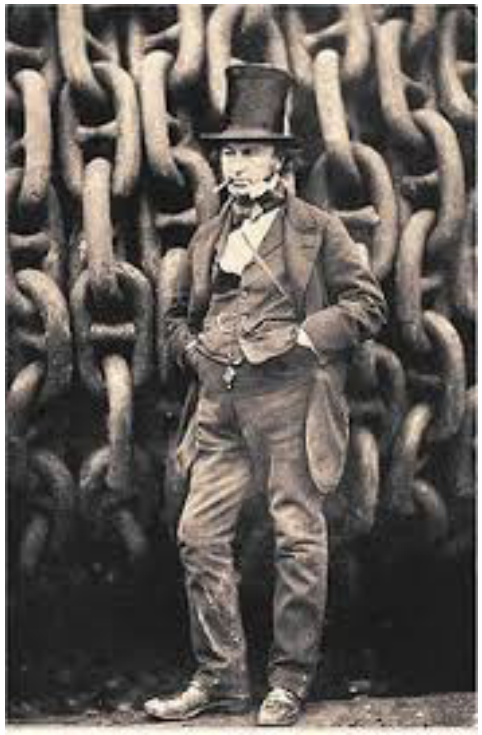
CARDIFF UNIVERSITY
PRIFYSGOL CAERDYDD

Met Office

EPSRC

CRAY
THE SUPERCOMPUTER COMPANY

ARM



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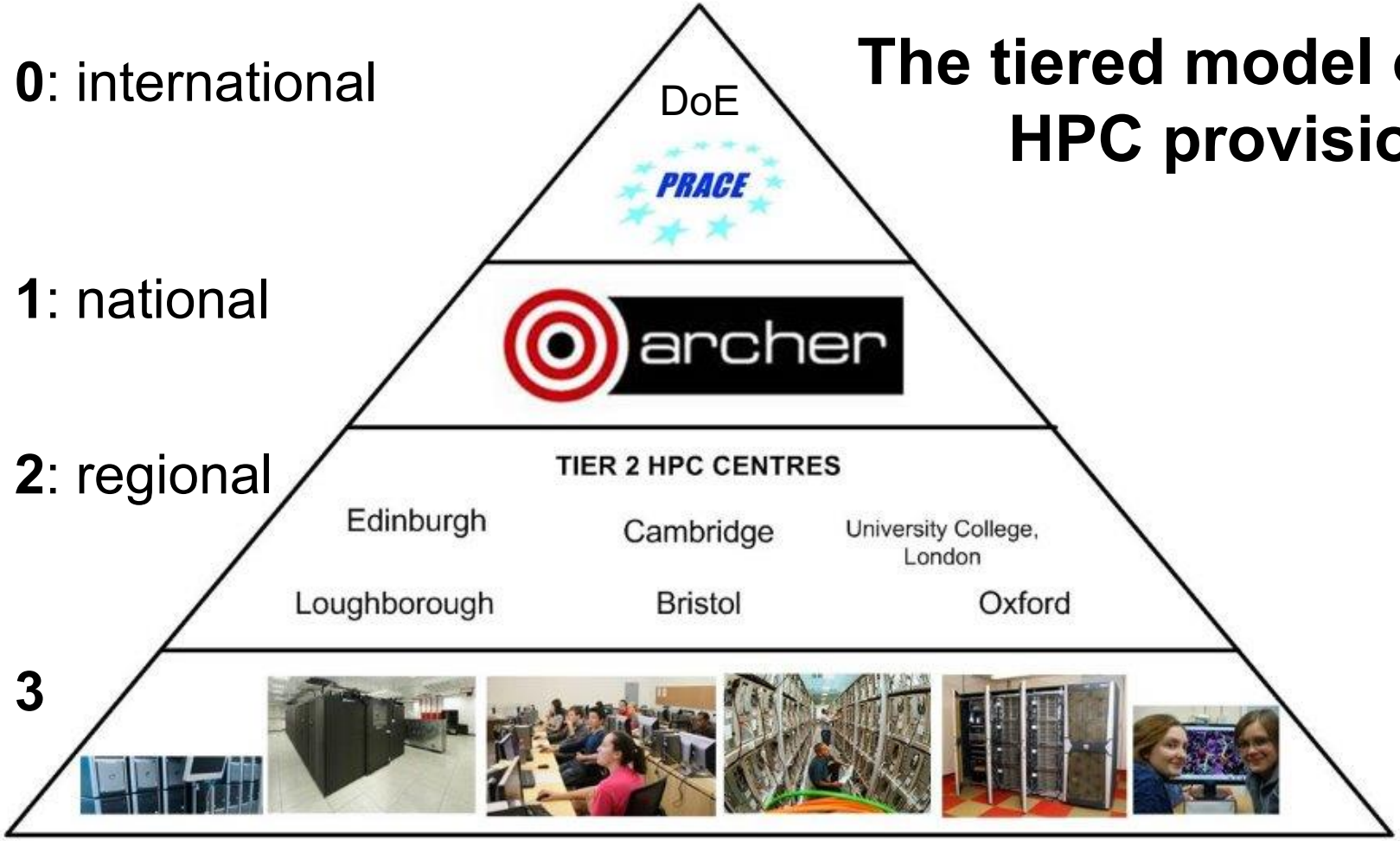
The tiered model of HPC provision

Tier 0: international

Tier 1: national

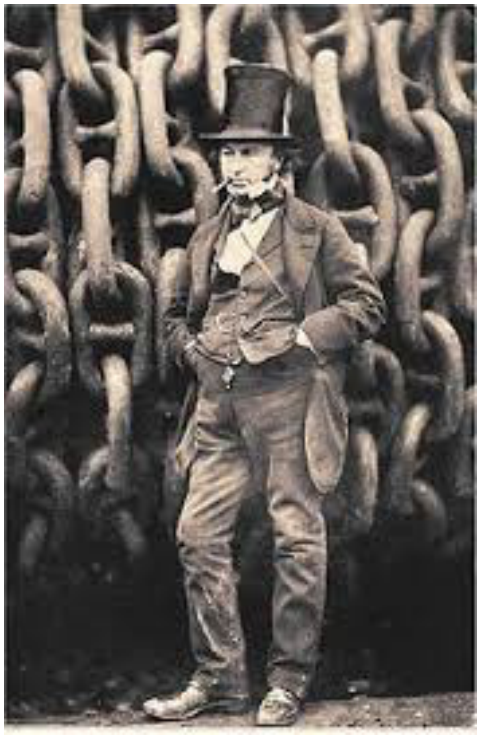
Tier 2: regional

Tier 3



Isambard system specification (red = new info):

- Cray "Scout" system – XC50 series
  - Aries interconnect
- **10,000+** Armv8 cores
  - Cavium ThunderX2 processors
  - 2x 32core @ >2GHz per node
- Cray software tools
- Technology comparison:
  - x86, Xeon Phi, Pascal GPUs
- Phase 1 installed March 2017
- The Arm part arrives early 2018



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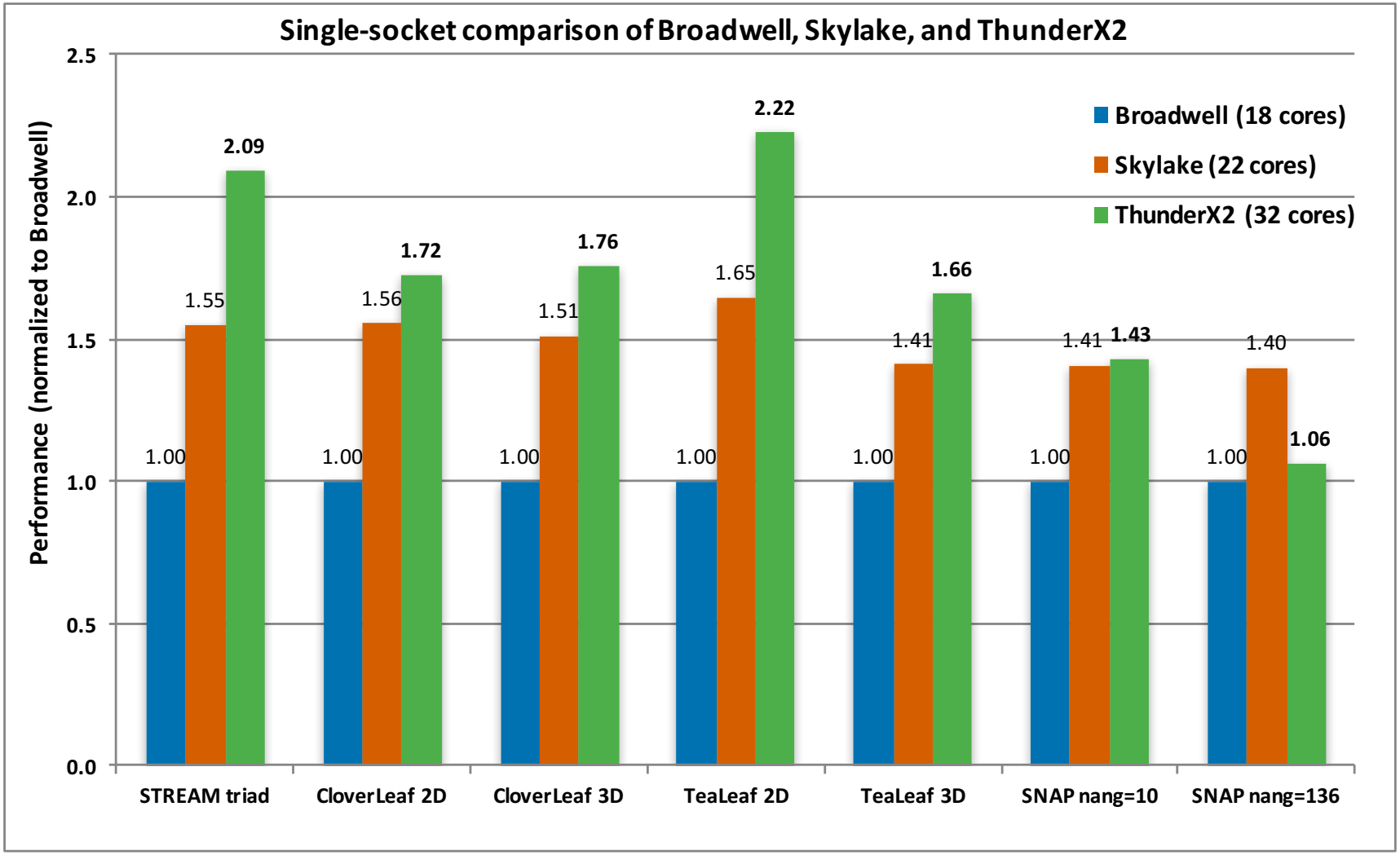
- The Isambard project's focus will be on the top 10 most heavily used codes on Archer in 2017:
  - VASP, CASTEP, GROMACS, CP2K, UM, HYDRA, NAMD, Oasis, SBLI, NEMO
  - Note: 8 of these 10 codes are written in **FORTRAN**
- Additional important codes for project partners:
  - OpenFOAM, OpenIFS, WRF, CASINO, LAMMPS, …
- We want to collaborate wherever possible!
  - Accelerate the adoption of Arm in HPC


Single-socket comparison of Broadwell, Skylake, and ThunderX2
Performance (normalized to Broadwell)
2.5
2.0
1.5
1.0
0.5
0.0
Broadwell (18 cores)
Skylake (22 cores)
ThunderX2 (32 cores)
1.00
1.55
2.09
1.00
1.56
1.72
1.00
1.51
1.76
1.00
1.65
2.22
1.00
1.41
1.66
1.00
1.41
1.43
1.00
1.40
1.06
STREAM triad
CloverLeaf 2D
CloverLeaf 3D
TeaLeaf 2D
TeaLeaf 3D
SNAP nang=10
SNAP nang=136

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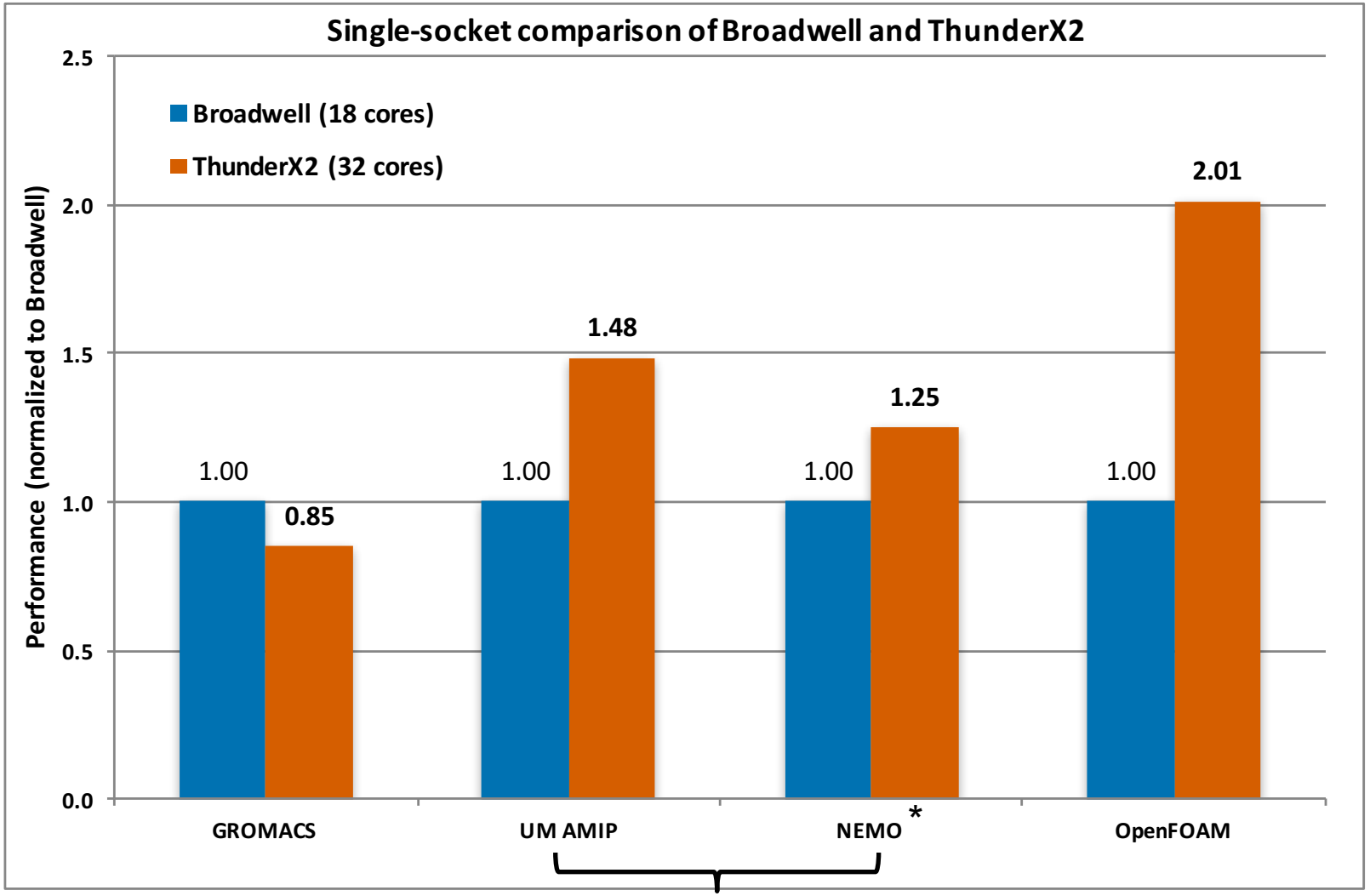

Benchmarked by the UK's Met Office

* = NEMO runs from a 28 core, 2.0GHz TX2

Details for benchmarks comparisons:

- ThunderX2 early access systems
  - 32c, 2.5GHz, 2667MHz DDR4, Ubuntu 16.04
  - 28c, 2.0GHz, 2400MHz DDR4, SLES 12 SP3
  - All alpha release (pre-production) hardware
- Broadwell system
  - 18c, 2.1GHz, 2400MHz DDR4, Xeon E5-2695 v4
- Skylake system
  - 22c, 2.1GHz, 2667MHz DDR4, Xeon Gold 6152

Software used for ThunderX2:

- UM, NEMO and TeaLeaf: Cray CCE 8.6.4
  - UM and NEMO results produced by the UK's Met Office
- GROMACS, OpenFOAM and STREAM: GCC 7.1
- CloverLeaf: 2D armflang 18.0, 3D armflang 1.4
- SNAP: nang=10 armflang 1.4, nang=136 CCE 8.6.3

Software used for Broadwell:

- UM and NEMO: Cray CCE 8.5.8, produced by the Met Office
- GROMACS: GCC 7.1
- Intel 2017 compiler for everything else

Software used for Skylake:

- Intel 2018 compiler

Benchmark test case parameters:

- **UM AMIP** (v10.8): 6day
- **NEMO**: GYRE_PISCES, idealised calculation, 720 timesteps
- **GROMACS**: rnase_cubic
- **OpenFOAM**: motorBike
- **STREAM**: test size of 2^{25} double precision elements per array with 100 iterations
- **CloverLeaf**: 2D bm_16, 3D bm1s_short
- **TeaLeaf**: 2D bm_5, 3D bm_3 0.04
- **SNAP**: 1024x16x(NC/2), ng=32

Other applications being ported to Isambard include:

VASP, CASTEP, CP2K, HYDRA, NAMD, Oasis, SBLI, OpenIFS, WRF, CASINO, LAMMPS…

Early results suggest that for compute-bound applications such as GROMACS, CP2K and VASP, performance between the different processors is closer than for memory bandwidth bound codes. This is because, while the codes benefit from the wider vector units of the x86 processors, ThunderX2 compensates with higher core counts and clock speeds

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For more information:

- http://gw4.ac.uk/isambard/
- http://investors.cray.com/phoenix.zhtml?c=98390&p=irol-newsArticle&ID=2316352
- https://github.com/UoB-HPC/GW4-Isambard
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