EasyBuild Tech Talk: Yes! You Can Run Your Software on Arm

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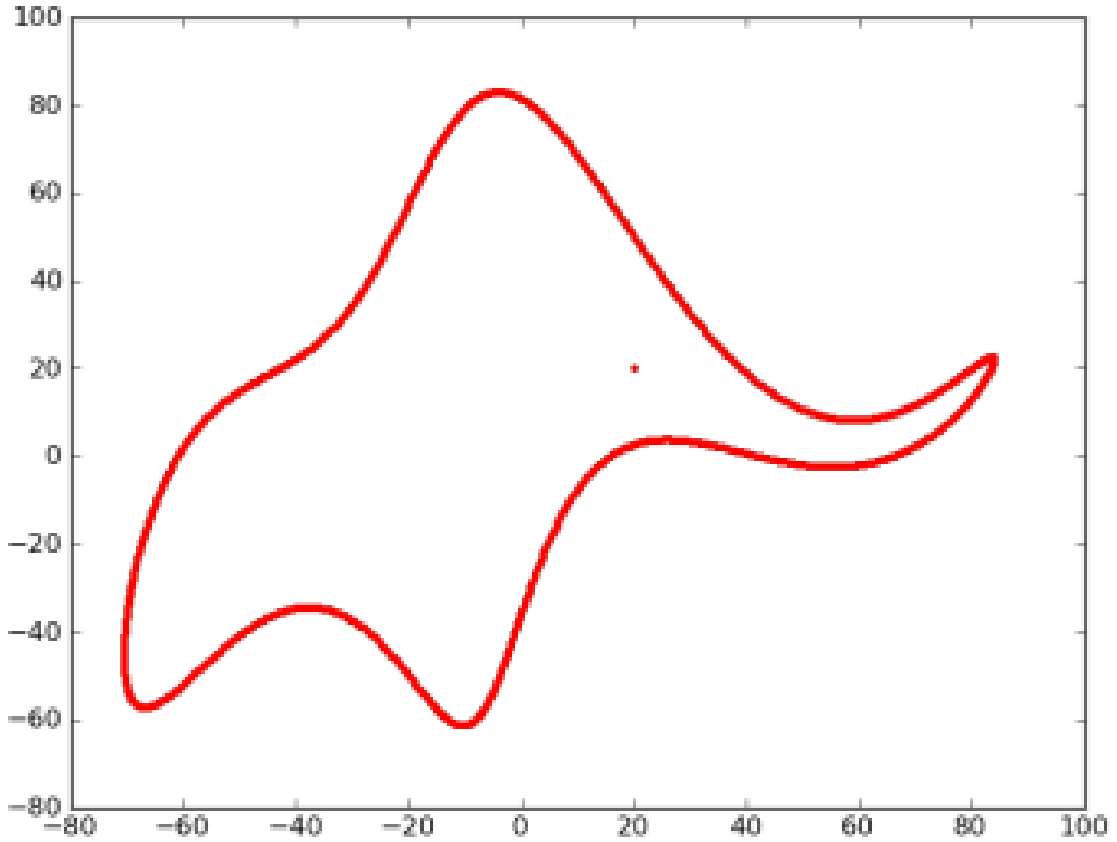
Outline

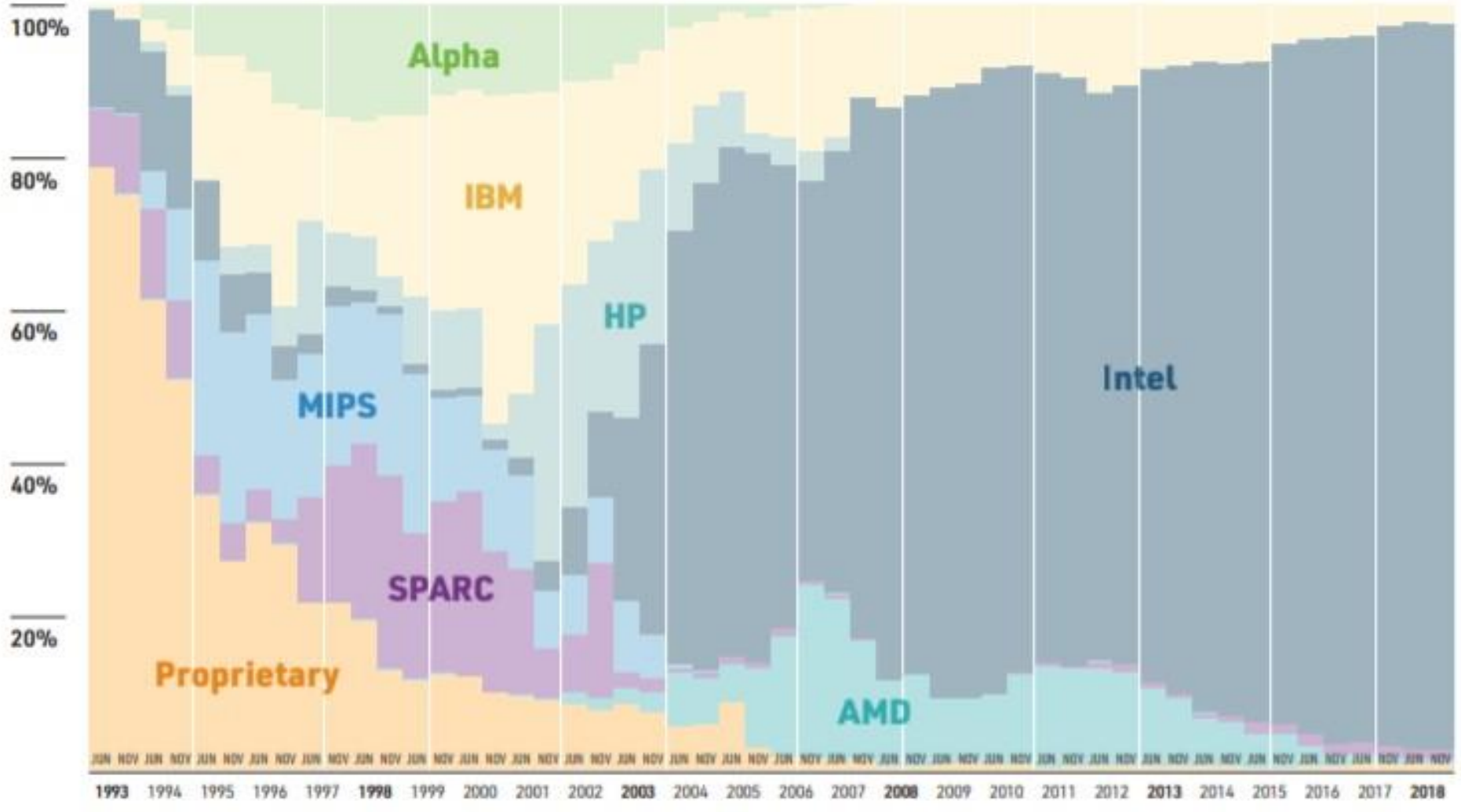
- Architectures
- ISAs
- Arm
- Arm CPU Implementations
- Systems with Arm CPUs
- Clouds with Arm
- Continuous Integration
- Software
- Vector Instructions
- SVE
- Compilers

The Elephant in the Room – NVIDIA Acquisition



https://www.johndcook.com/blog/2011/06/21/how-to-fit-an-elephant/

Top 500 Processor Architecture Over Time



Data: top500.org, Chart: The Next Platform

What is an Instruction Set Architecture (ISA)?

- x86_64

C++ source #1

```
1  int square(int num) {
2      return num * num;
3  }
```

- aarch64

x86-64 clang 10.0.0 (Editor #1, Compiler #1) C

x86-64 clang 10.0.0 | Compiler options... | Output... | Filter... | Libraries | Add new...

```
1  square:                                 # @square
2          push    rbp
3          mov     rbp, rsp
4          mov     dword ptr [rbp - 4], edi
5          mov     eax, dword ptr [rbp - 4]
6          imul    eax, dword ptr [rbp - 4]
7          pop     rbp
8          ret
```

armv8-a clang 10.0.0 (Editor #1, Compiler #1) C

armv8-a clang 10.0.0 | Compiler options... | Output... | Filter... | Libraries | Add new...

```
1  square:                                 // @square
2          sub     sp, sp, #16             // =16
3          str     w0, [sp, #12]
4          ldr     w8, [sp, #12]
5          ldr     w9, [sp, #12]
6          mul     w0, w8, w9
7          add     sp, sp, #16             // =16
8          ret
```

Credit: Compiler Explorer - https://godbolt.org/

Arm AArch64

- Different ISA to x86_64
- Defines the:
  - Instruction Set: A64
  - Encoding, Endianness, Registers …
- Variants, e.g.
  - Armv8.1-A - e.g. thunderx2
  - Armv8.3-A – has SVE, e.g. A64fx
- Business model:
  - Arm licenses the core designs (IP)
  - Small number of architecture licencees
  - The Licensees fabricate SoCs
    - Choose number of fp units, memory controllers, fab and packaging technologies

ARM Origin Story

- BBC Model B
- Acorn Archimedes
- Steve Furber, Sophie Wilson
- @bbcbasicbot

ARM HPC Processors

- Currently available
  - ThunderX2
  - A64fx
  - Ampere
  - Graviton2
- News from HotChips 2020
  - ThunderX3

European Processor Initiative

- Part of €8b EuroHPC Joint Undertaking
- SiPearl
- Codenames
  - Rhea – Zeus ARM Neoverse V1 cores, ETA 2021
  - Chronos, Titan

Astra – Sandia National Labs (top500: #244)

Photo: Regina Valenzuela

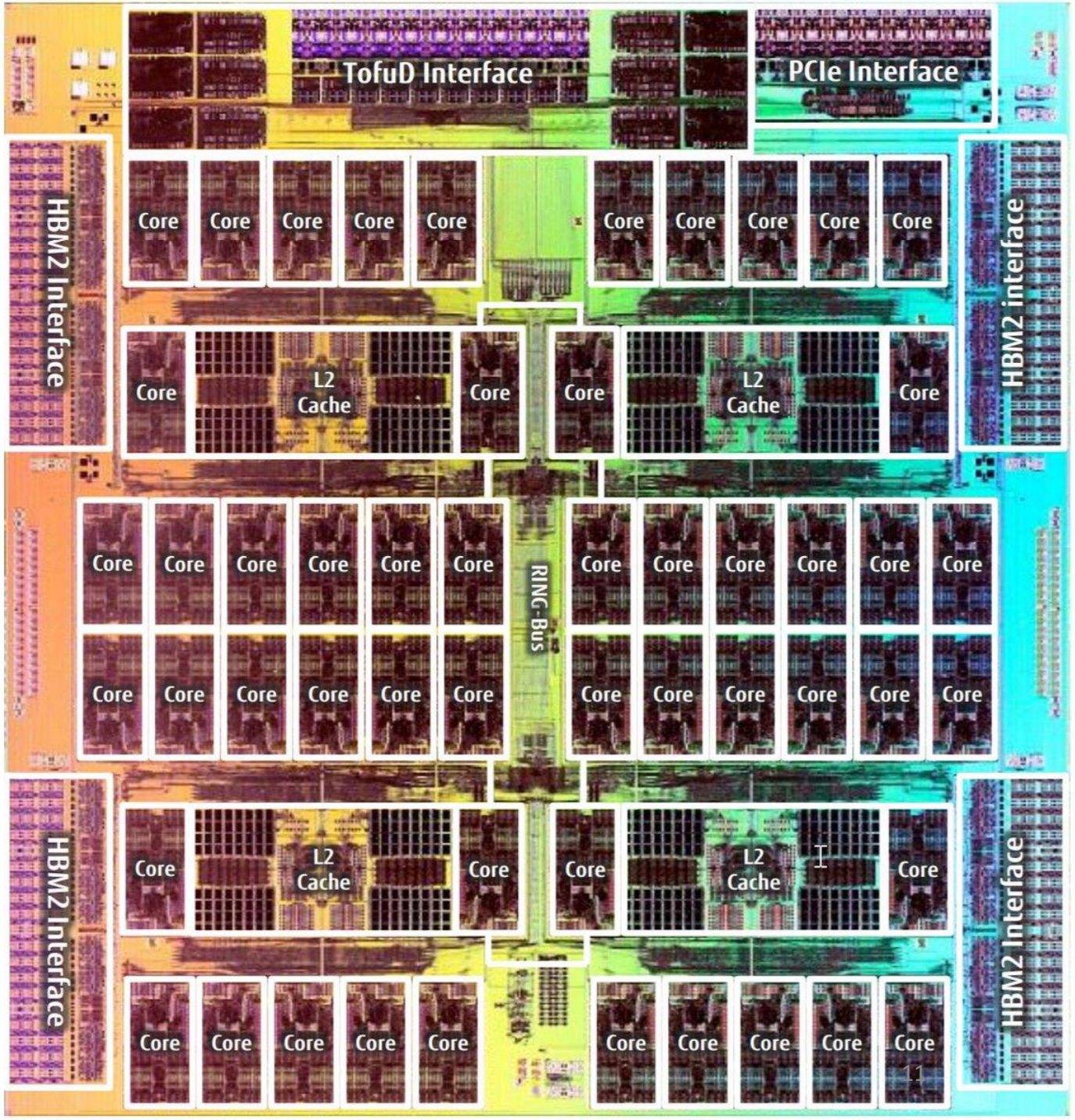
A64FX

Architecture Features
- Armv8.2-A(AArch64 only)
- SVE512-bit wide SIMD
- 48 computing cores + 4assistant cores
- HBM2 32GiB
- Tofu 6D Mesh/Torus28Gbps x 2 lanes x 10 ports
- PCIeGen3 16 lanes

Fabrication Process
- 7nm FinFET
- 8,786M transistors
- 594 package signal pins

Peak Performance (Efficiency)
- >2.7TFLOPS (>90%@DGEMM)
- Memory B/W 1024GB/s (>80%@Stream Triad)

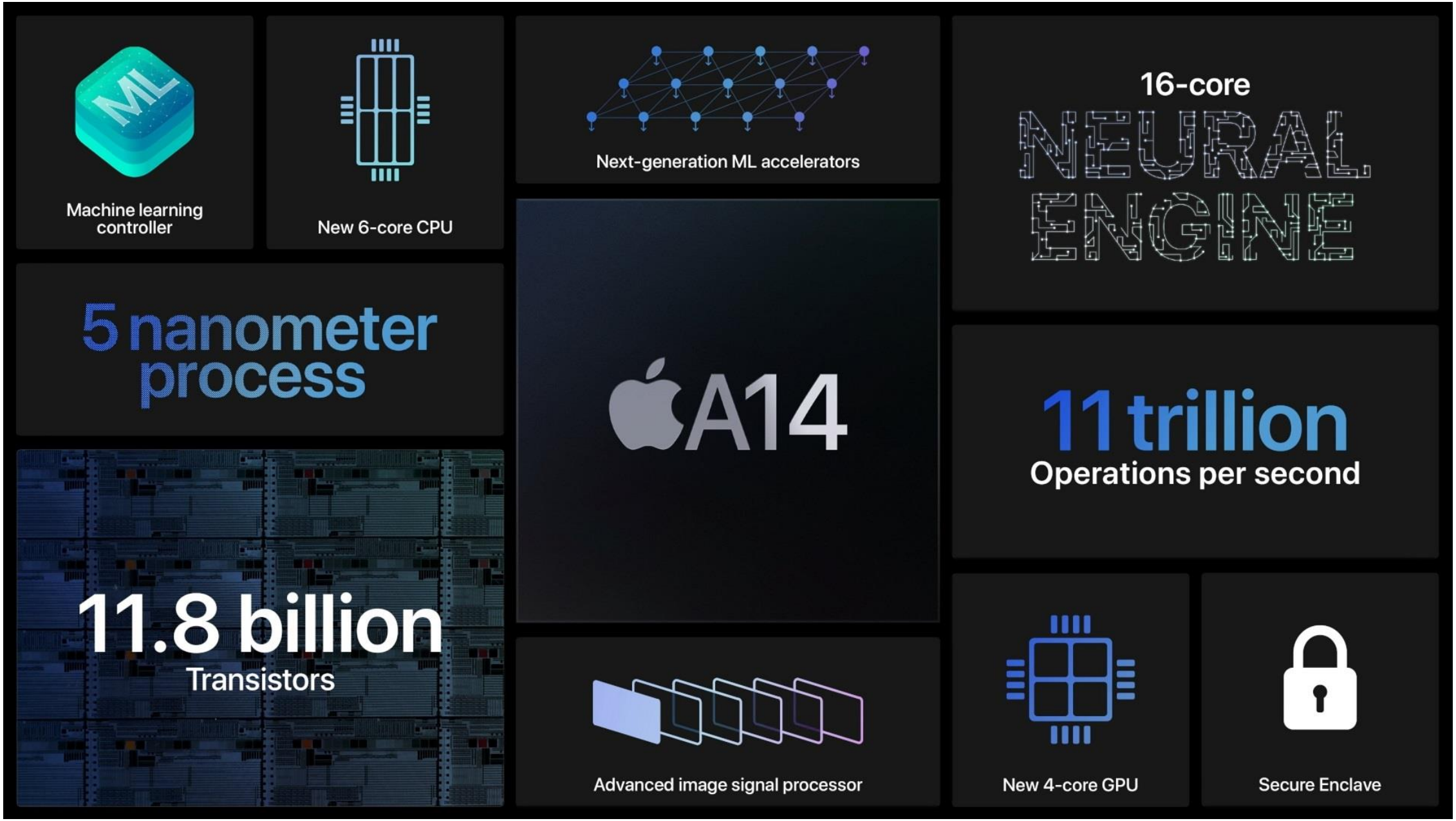
Credit: Fujitsu / RIKEN CCS



Fugaku – RIKEN (top 500 #1)

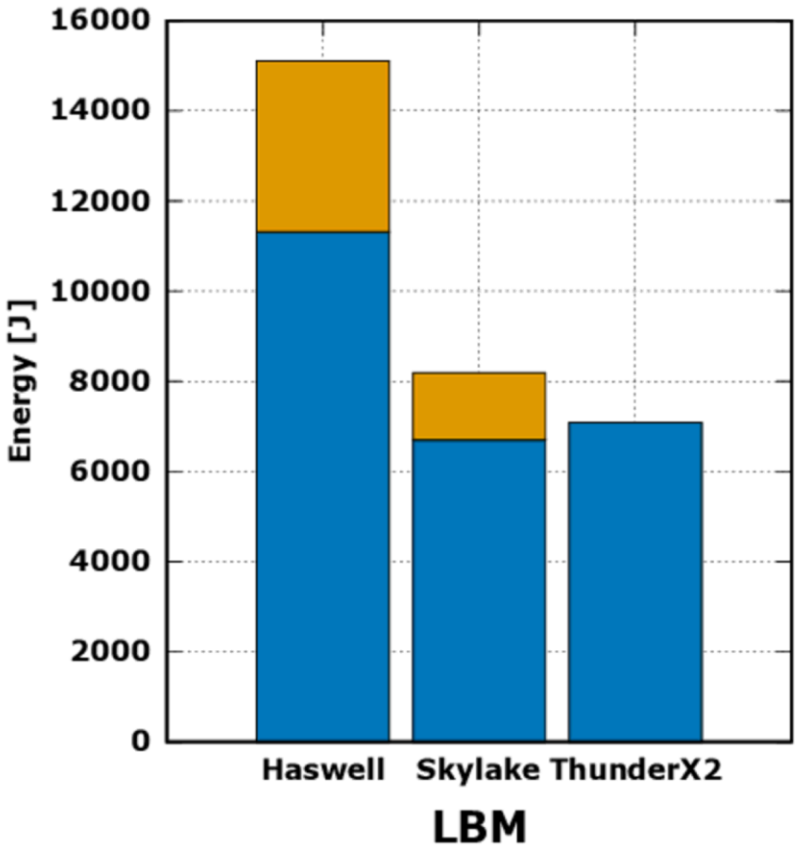
Apple's next Desktop CPU will be Arm

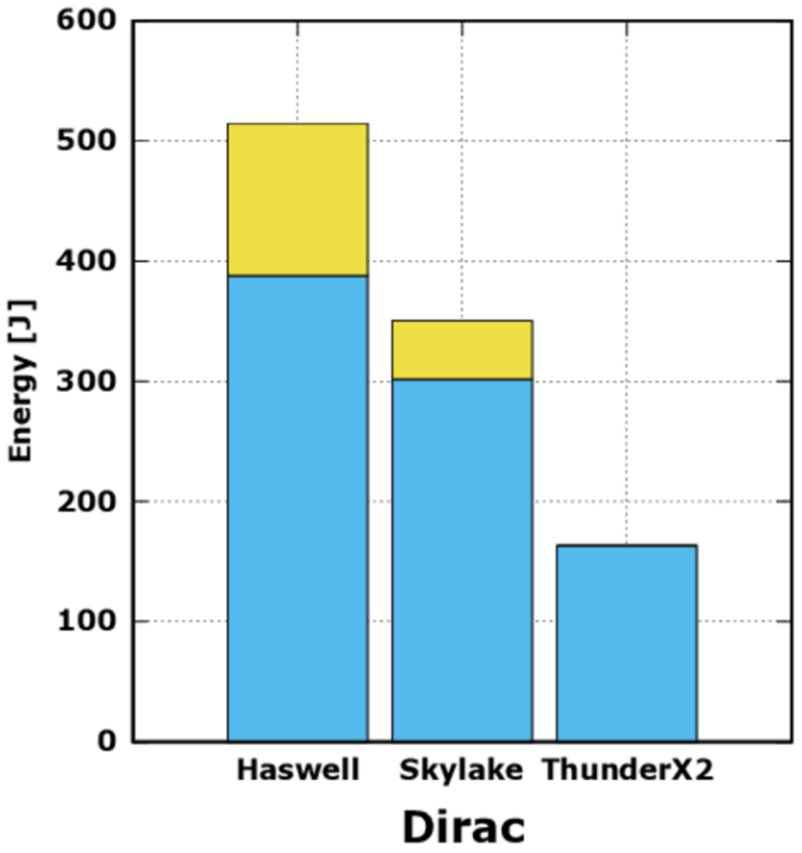
Credit: Apple.com


ML
Machine learning controller
New 6-core CPU
Next-generation ML accelerators
16-core
NEURAL ENGINE
5 nanometer process
A14
11 trillion
Operations per second
11.8 billion
Transistors
Advanced image signal processor
New 4-core GPU
Secure Enclave

Energy efficency

- ThunderX2 ~= Skylake





Computation **2020**, *8*(1), 20; https://doi.org/10.3390/computation8010020

Green500 Data

- Shaded entries in the table below mean the power data is derived and not meassured.

Rank	TOP500 Rank	System	Cores	Rmax (TFlop/s)	Power (kW)	Power Efficiency (GFlops/watts)
4	204	**A64FX prototype** - Fujitsu A64FX, Fujitsu A64FX 48C 2GHz, Tofu interconnect D, Fujitsu Fujitsu Numazu Plant Japan	36,864	1,999.5	118	16.876
9	1	**Supercomputer Fugaku** - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science Japan	7,299,072	415,530.0	28,335	14.665
172	244	**Astra** - Apollo 70, Marvell ThunderX2 ARM CN9975-2000 28C 2GHz, 4xEDR Infiniband, HPE Sandia National Laboratories United States	143,640	1,833.0	1,193	1.537

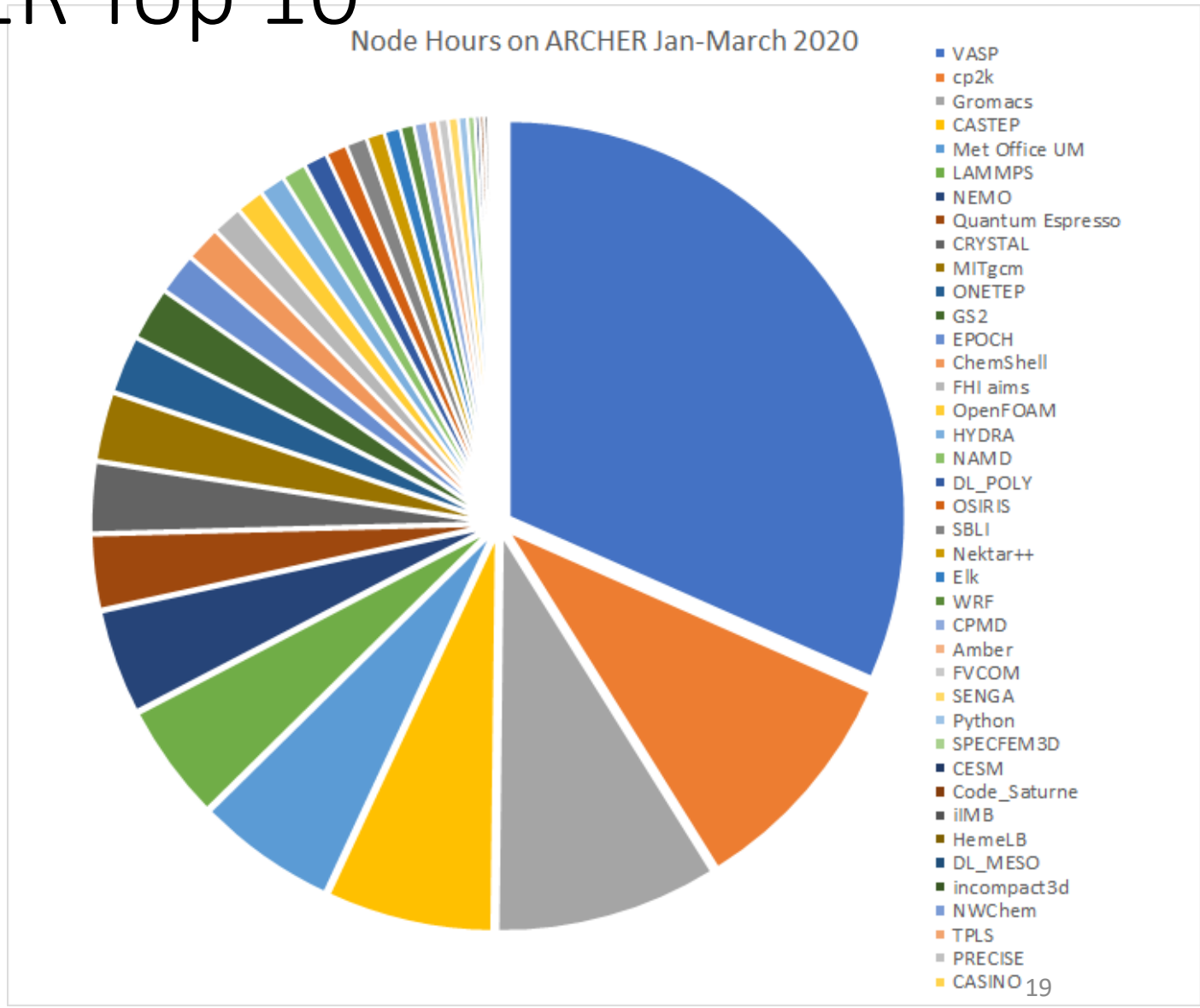
software

Software – It Just Works *

- Built from source
  - Beware intrinsics
- Interpreters
  - Python
  - R
  - Julia

Applications -ARCHER Top 10

- Periodic electronic structure:
  - VASP,
  - CASTEP,
  - CP2K
- N-body models:
  - GROMACS,
  - LAMMPS,
  - NAMD
- Grid-based climate modelling:
  - Met Office UM,
  - MITgcm
- Grid-based computational fluid dynamics:
  - SBLI,
  - OpenFOAM



The "Matlab Question" – ISV codes

- Ian Cutress quotes Fujitsu https://www.anandtech.com/show/15885/hpc-systems-special-offer-two-a64fx-nodes-in-a-2u-for-40k

" listed support for quantum chemical calculation software Gaussian16, molecular dynamics software AMBER, non-linear structure analysis software LS-DYNA."

SIMD instructions - NEON

- Compare with Intel SSE, AVX2, AVX512 etc.
- Porting codes with Intrinsics
  - GROMACS Isambard Hackathon
  - Phylobayes out of the box, needed compiler pragmas
  - IQ-Tree, 100s of intel intrinsics
  - sse2neon
  - SIMD everywhere

Scaleable Vector Extensions (SVE)

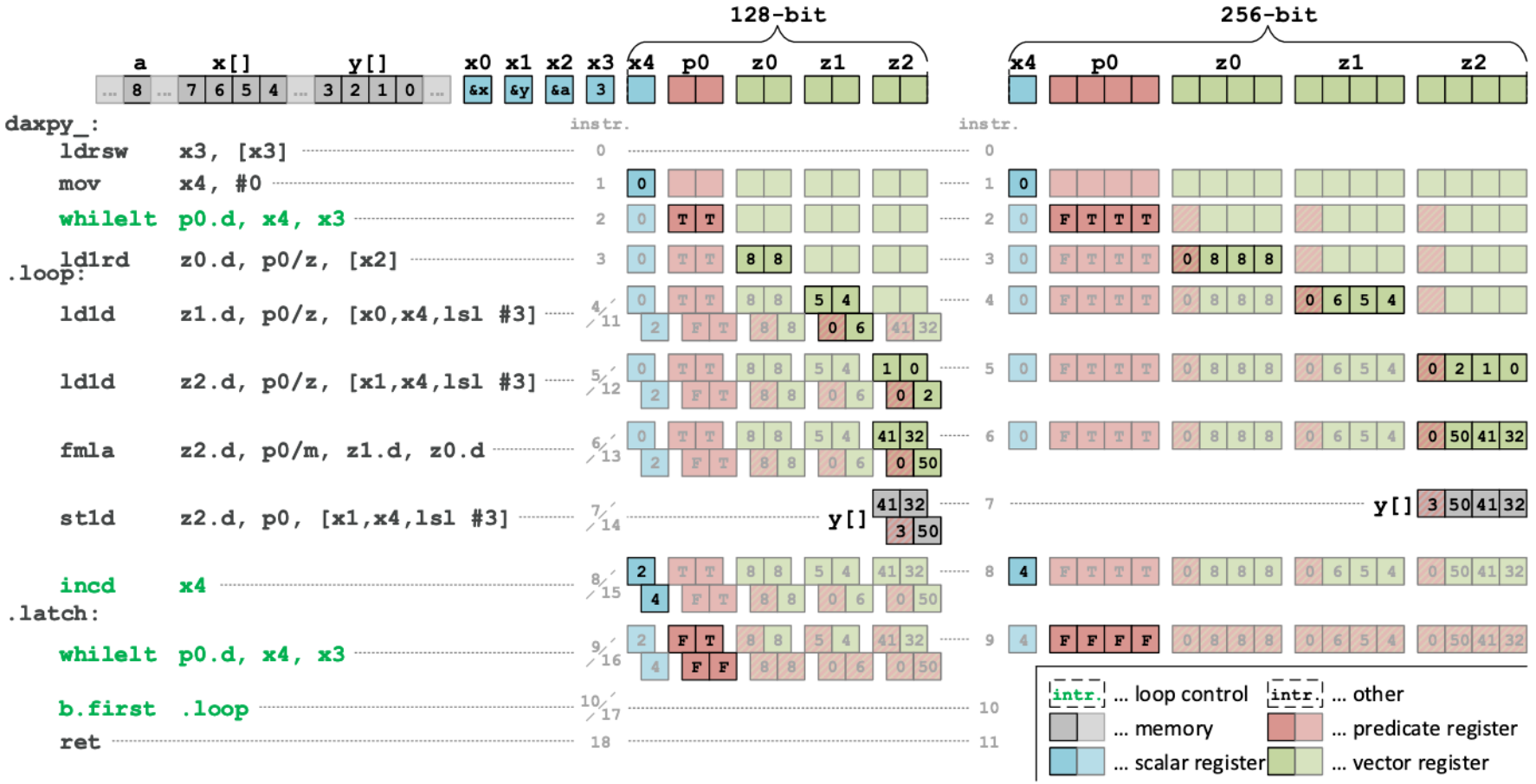


Fig. 3: Cycle by cycle example of daxpy with $n = 3$ and hardware vector lengths of 128- and 256-bit

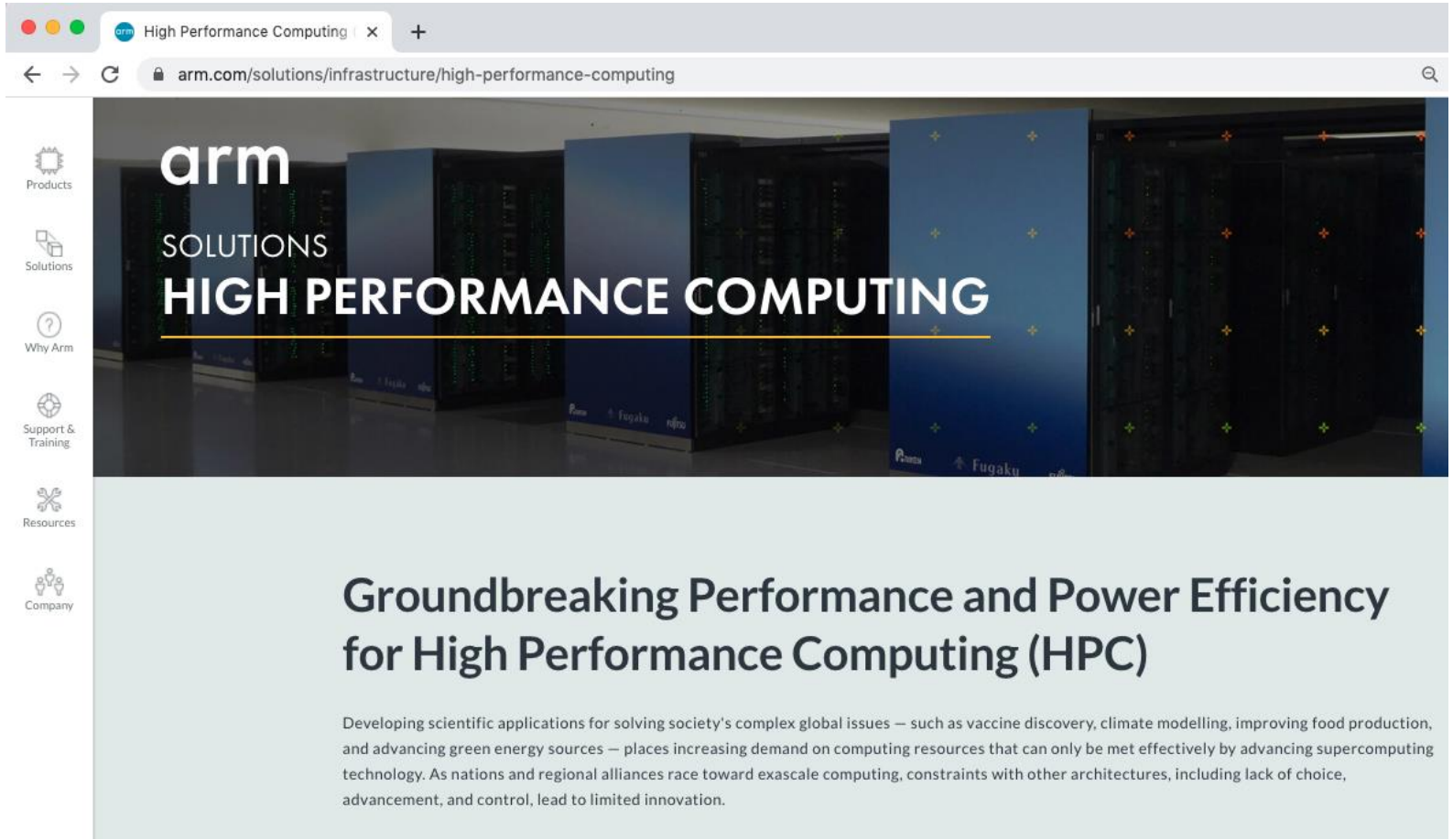
https://dl.acm.org/doi/abs/10.1109/MM.2017.35

Scalable Vector Extensions (SVE)

- Gem5
- ARMIE
- UoB writing our own simulator

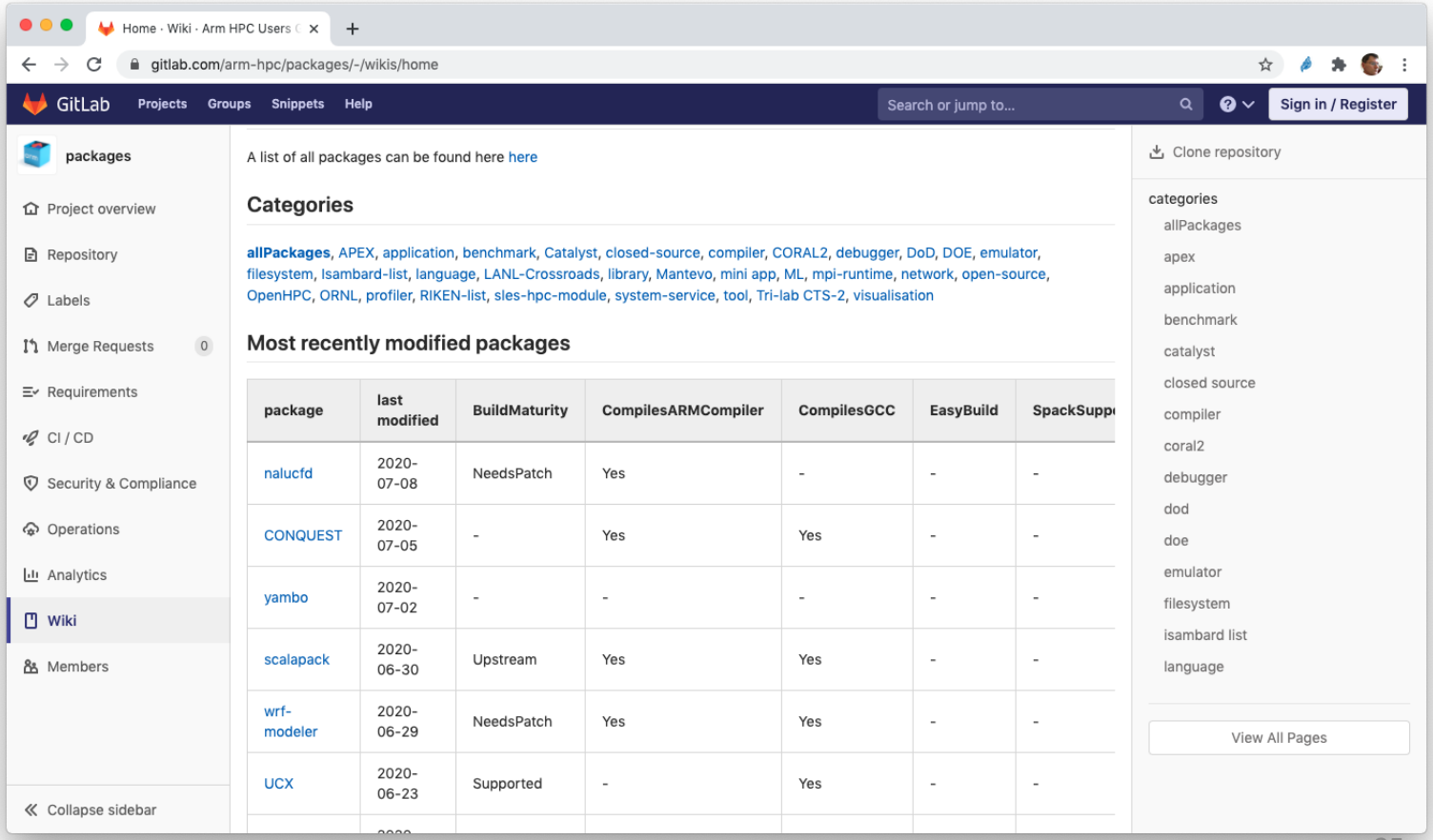
- Vector Length Agnostic code
  - Fujitsu compiler targets A64fx, assumes length 512
  - Cray generates fixed width, but can take the width as a compiler option
  - Arm Compiler only VLA
  - GCC, can do both, defaults to VLA

ARM HPC website



ARM HPC Wiki

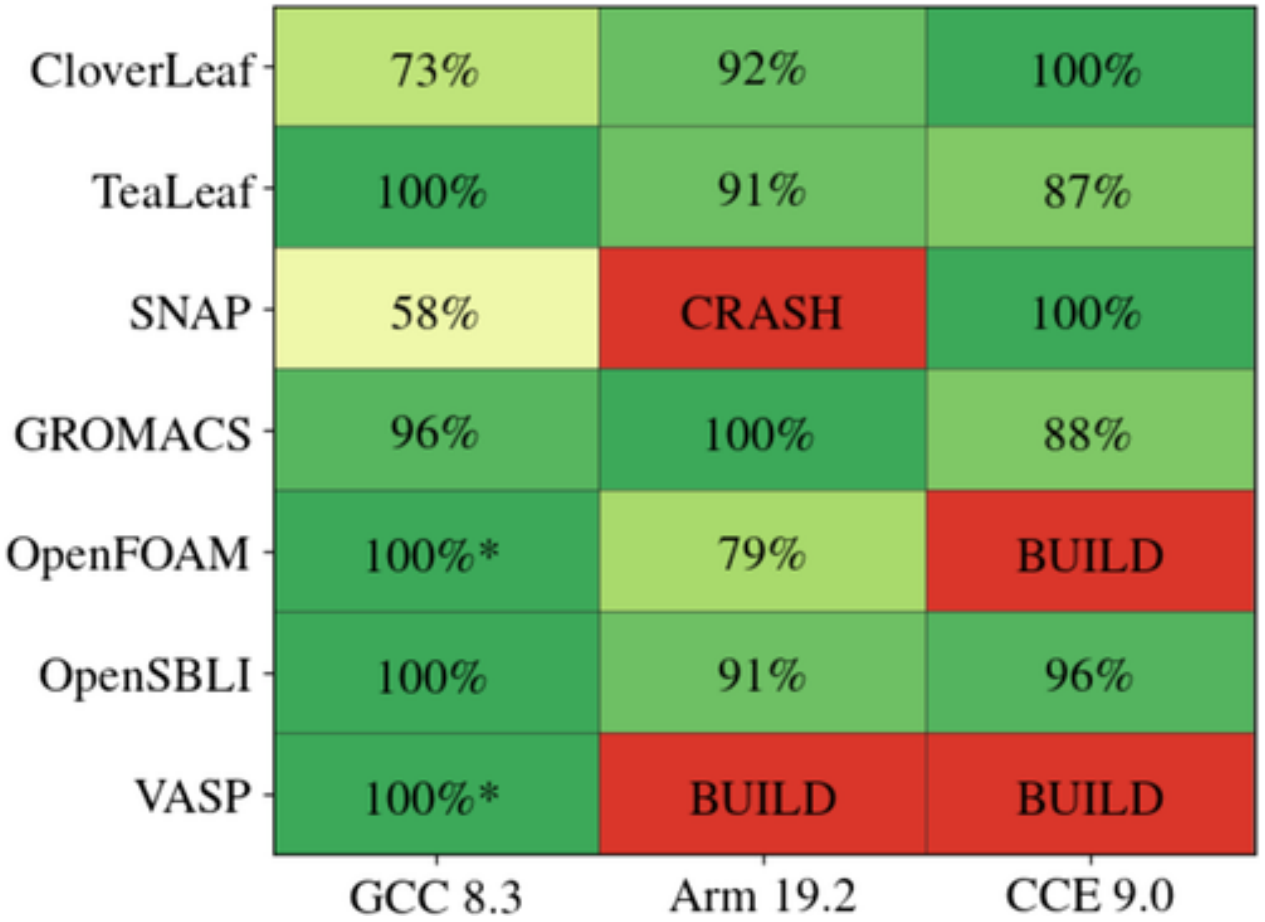
- List of apps known to work
- Build instructions



Compilers

- GCC
- Clang
- Arm (based on Clang)
- Cray (classic and Clang based)
- Fujitsu
- NVIDIA HPC SDK (formerly PGI)

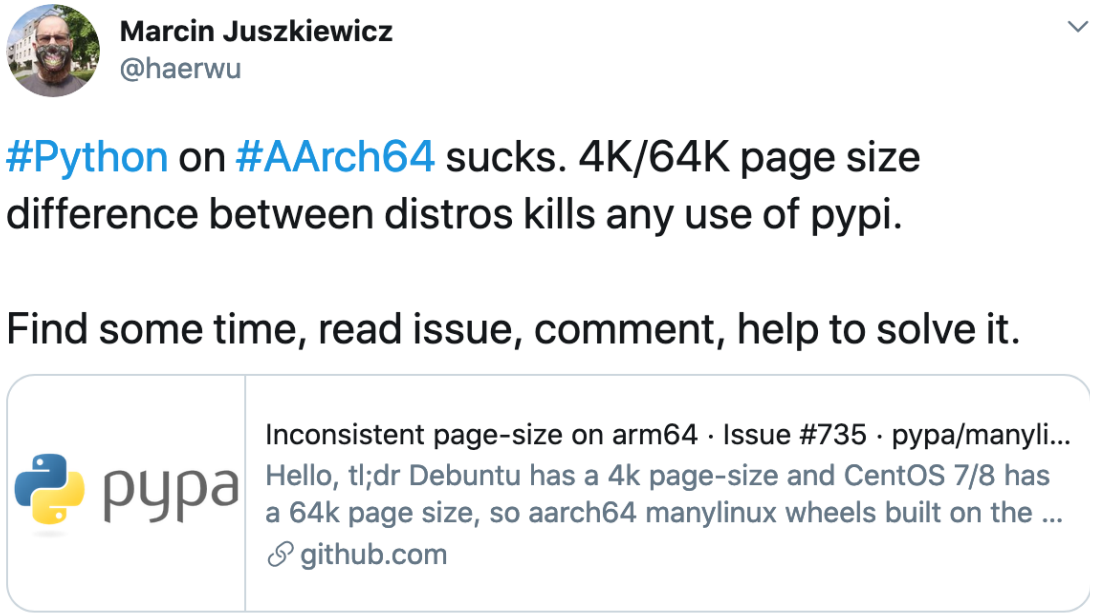
Perfromance of Different Compilers - YMMV

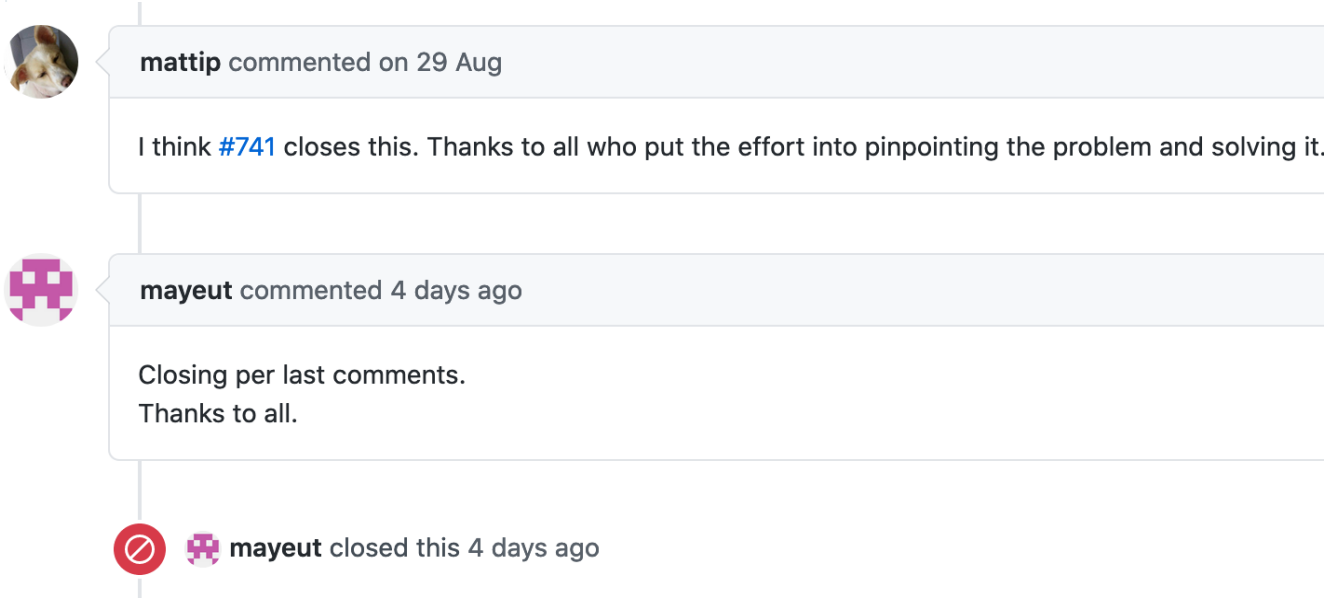


https://doi.org/10.1002/cpe.5569

Tracking down obscure bugs

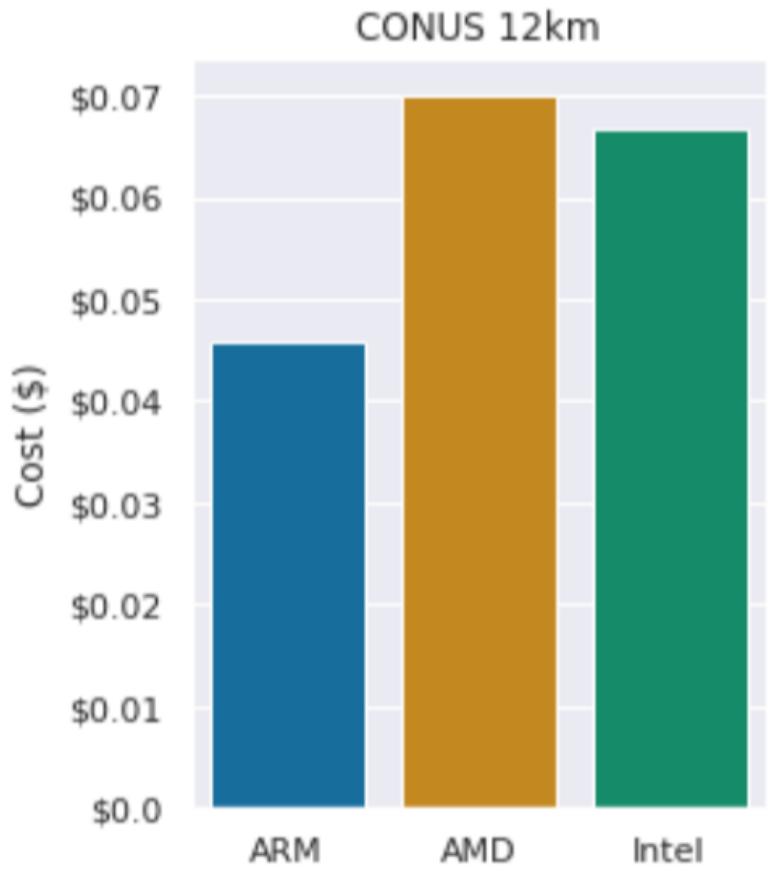
- https://github.com/pypa/manylinux/issues/735





Cloud Service Providers with Arm

Amazon Web Services - Graviton2



- Initial implementation Graviton
- Graviton2 generally available
- Very price/performance competitive

Cluster in the Cloud

- https://cluster-in-the-cloud.readthedocs.io
- Terraform + Ansible
- Multi-cloud (Currently AWS, Google, Oracle)
- Supports Graviton2

- HOWTO
  - Git clone
  - Edit creds
  - Terraform apply
  - Ssh to login node
  - Run EasyBuild

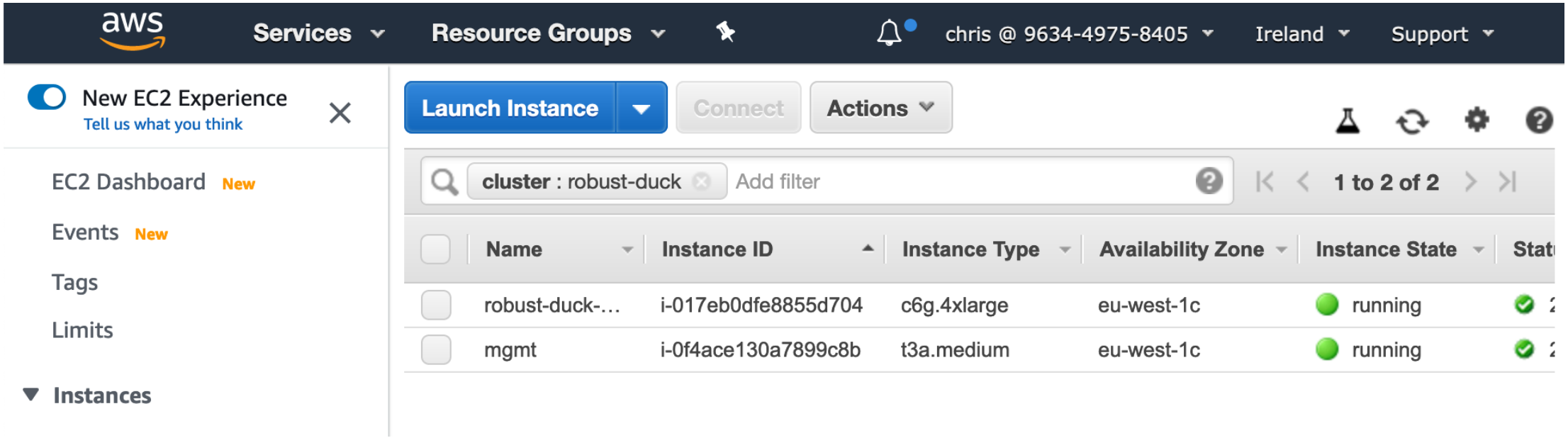
Installing software on your cluster

To make software available across your cluster, the best way is to install it onto the shared filesystem at `/mnt/shared`. Make sure that all the dependencies for it are available either on the shared filesystem or in the base image you're using. i.e. don't use `yum install` to provide dependencies.

Consider using a tool like EasyBuild or Spack to manage your software stack.

Monitoring

```
[chris@mgmt ~]$ srun -I --constraint="shape=c6g.4xlarge" -- /bin/bash
```



Ampere in Oracle Cloud Announcement

Announcing: First ARM Compute Offering
First Half of 2021

- First ARM offering in OCI powered by Ampere Altra Processors
- Easily develop and test ARM workloads in the cloud
- Best price/performance for many workloads
- Flexible VMs and BareMetal with up to 160 cores per instance, single threaded performance at 3.3GHz per core, 1TB of memory and 100Gb/s of bandwidth

AMPERE

Continuous Integration

- Travis (uses Graviton2)
- GitHub Actions (self hosted runner)
- Gitlab Runners
- Buildkite

HPC Clusters

HPE Catalyst Program

- Apollo 70 system
- Three systems in collaboration with the UK academic community
  - Bristol
  - Leicester
  - Edinburgh
- Hardware
  - Marvel ThunderX2
  - Infiniband EDR
  - Soon! 8x v100
- SW environment
  - Arm Compiler / GCC avail.
  - Arm Performance Libraries
  - MPI library: HPE HMPT, OpenMPI avail.

Isambard Project

- World's first production ARM based supercomputer
- GW4 + Met Office + Cray
- Purpose
  - Test limits
  - Platform for development
    - Open to UK academic researchers
    - Hackathons with international collaborators
  - Demonstrate production

Cray PrgEnv

- Modules for the programming environment
  - PrgEnv-cray, PrgEnv-allinea, PrgEnv-gnu
- Compiler wrappers
  - cc
  - CC
  - ftn

Packages already built (manually)

GW4-Isambard

Search docs

ISAMBARD USER GUIDE

- Request Account
- Connecting to Isambard
- Filesystem
- Running jobs
- Phase 1
- Phase 2 - XC50 ARM
- Debugging
- Profiling
- End of life procedures

Applications

- CASTEP
- CovidSim
- CP2K
- Dedalus
- DL_MONTE 2
- Firedrake
- GROMACS
- Hydro3D
- MolPro
- NAMD
- NEMO
- OpenFOAM
- OpenSBLI
- Unified Model
- VASP

```
    arch config     up   resv    use  avail   down rebootq
      XT    163    156    146    139     10      7       0

No pending applications are present

Total placed applications: 42
   Apid  ResId         User  PEs Nodes    Age State Command
1347394 547822  ca-nastases  192     3 22h03m   run chemsh.x
1347421 547833       ri-zwu 1312    21 19h57m   run mdrun_mpi
1347583 547870     ex-echan  384     6 17h36m   run vasp_std
1347643 547886  brx-hsenger   16     1 17h29m   run python3
1347761 547916  brx-hsenger   64     1 17h10m   run python3
1347817 547927  brx-hsenger    8     1 17h01m   run python3
1347841 547935   ba-rsharpe   64     1 16h01m   run vasp_std
1347847 547938   ba-rsharpe   64     1 15h56m   run vasp_std
1347853 547941   ba-rsharpe   64     1 15h55m   run vasp_std
1347869 547948 ba-tsmolders  256     4 15h11m   run vasp_gam
1347874 547950 ba-tsmolders  256     4 14h59m   run vasp_gam
1347876 547951 ba-tsmolders  256     4 14h58m   run vasp_gam
1347878 547952 ba-tsmolders  256     4 14h50m   run vasp_gam
1347885 547953     ex-echan 1024    16 13h42m   run vasp_std
1348020 547992  brx-hsenger    1     1  5h49m   run python3
1348024 547993  brx-hsenger    2     1  5h45m   run python3
1348092 547994  brx-hsenger    4     1  1h27m   run python3
1348093 547995  brx-hsenger    8     1  1h17m   run python3
1348037 547996  ba-oleyorla   15     1  4h33m   run python
1348039 547997  ba-oleyorla   15     1  4h33m   run python
1348038 547999  ba-oleyorla   15     1  4h33m   run python
1348059 548005  ba-oleyorla   15     1  3h05m   run python
1348060 548006  ba-oleyorla   15     1  3h05m   run python
1348061 548007  ba-oleyorla   15     1  3h05m   run python
1348065 548008  ba-oleyorla   15     1  3h05m   run python
1348064 548009  ba-oleyorla   15     1  3h05m   run python
1348068 548010     ex-echan  576     9  3h00m   run vasp_std
1348081 548015 ba-tsmolders   64     1  1h39m   run vasp_std
1348084 548017 ba-tsmolders   64     1  1h37m   run vasp_std
1348089 548018  brx-hsenger    1     1  1h30m   run python3
1348088 548019 ba-tsmolders   64     1  1h30m   run vasp_std
1348091 548020 ba-tsmolders   64     1  1h28m   run vasp_std
1348095 548021 ba-tsmolders   64     1  1h10m   run vasp_std
1348098 548022  brx-hsenger    2     1  1h03m   run python3
1348100 548023 ba-tsmolders   64     1  0h59m   run vasp_std
1348105 548024  ba-oleyorla   15     1  0h56m   run python
1348106 548025  ba-oleyorla   15     1  0h56m   run python
1348108 548026    ex-ebaker  512     8  0h56m   run vasp_std
1348113 548027  ca-rundlej2   64     1  0h27m   run cp2k.popt
1348119 548031  brx-hsenger    4     1  0h11m   run python3
1348121 548032    ex-ebaker  512     8  0h10m   run vasp_std
1348123 548033     ex-echan 1408    22  0h04m   run vasp_std
```

Isambard2

- Hackathons
- Isambard2 new hardware
  - Double the XC50 164 -> 328 nodes (10k -> 20k cores)
  - Add 72x A64fx (HPE Cray Apollo 80)
  - AMD Rome
  - Intel Cascade Lake
  - NVIDIA V100

How to Access Isambard

- Eligibility
- Process

Credits

- UoB HPC Research group
  - Simon McIntosh-Smith
  - James Price
  - Tom Deacon
  - Andrei Poenaru
- Joe Heaton
- GW4 and Isambard Partners
- Isambard RSE and Ops teams
- Cray
- ARM
- Amazon Web Services
- University of Bristol
  - ACRC – Simon Burbidge
  - RSE Group - @BristolRSE - Matt Williams - @milliams

Summary

- Things changing fast in the Arm world
- Performant and price preformant HPC implementations of Arm arch.
- Your software will almost certainly work
- Give it a go!

Questions?

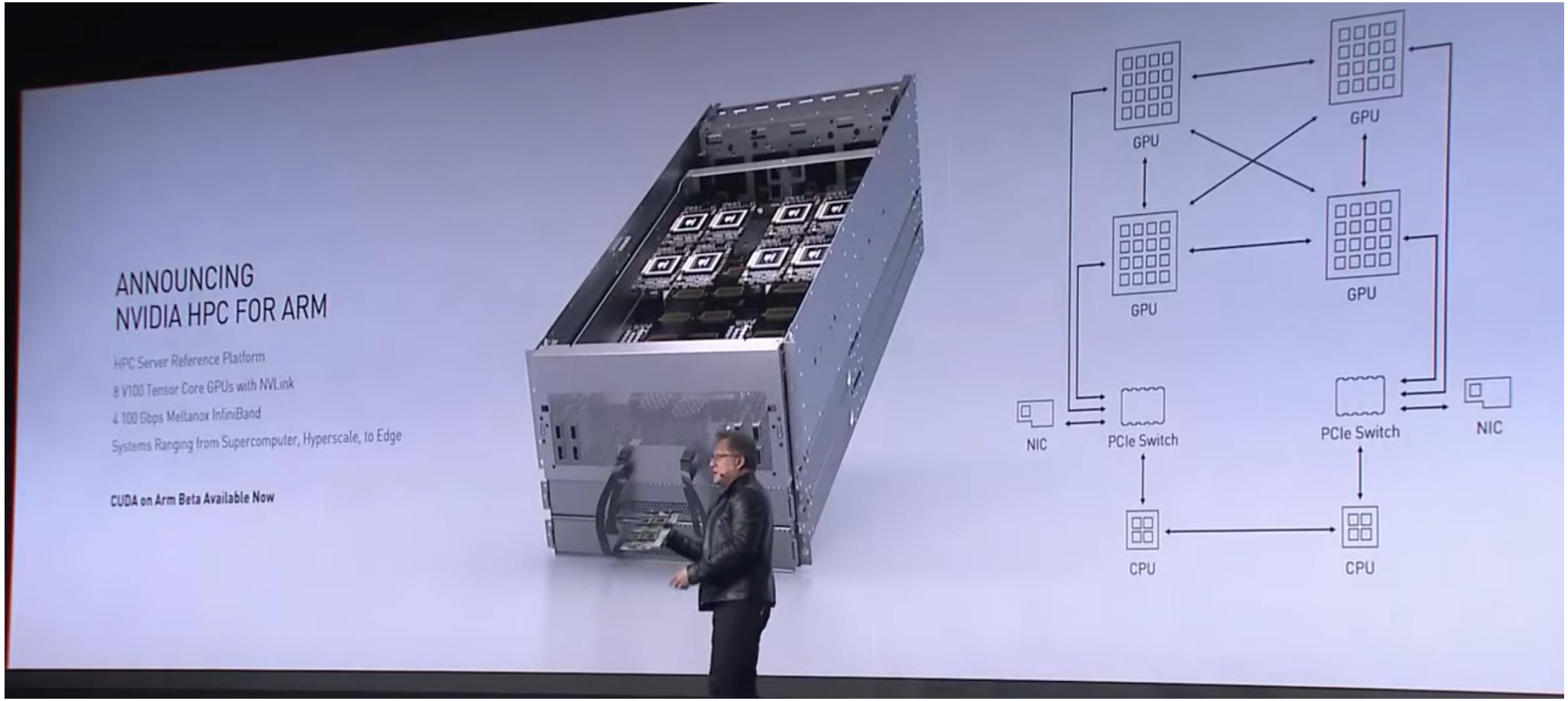
- Twitter: @hpcchris
- Email: chris.edsall@bristol.ac.uk
- Isambard: https://gw4-isambard.github.io/docs/
- CitC: https://cluster-in-the-cloud.readthedocs.io/

Backup Slides

Energy Efficiency

- https://chryswoods.github.io/howmuchisenough/

NVIDIA GPUs


ANNOUNCING
NVIDIA HPC FOR ARM
HPC Server Reference Platform
8 V100 Tensor Core GPUs with NVLink
4 100 Gbps Mellanox InfiniBand
Systems Ranging from Supercomputer, Hyperscale, to Edge
CUDA on Arm Beta Available Now
GPU
GPU
GPU
GPU
NIC
PCIe Switch
PCIe Switch
NIC
CPU
CPU