

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

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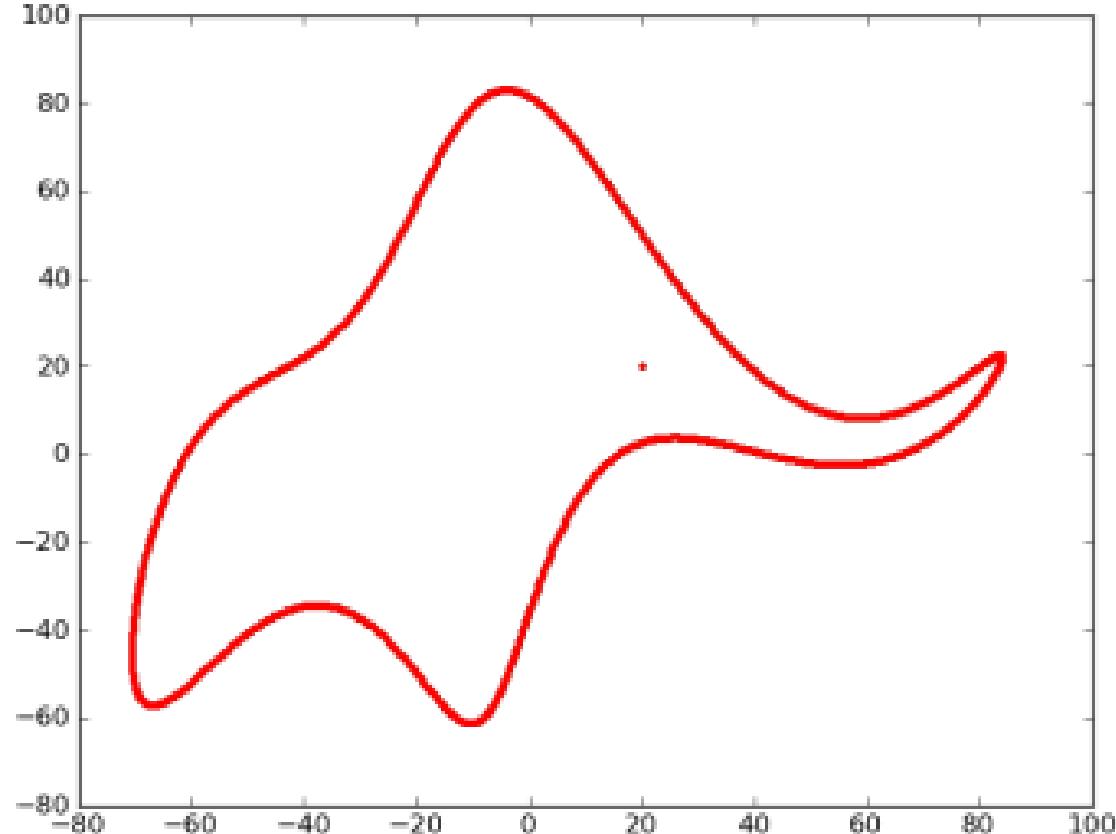
arm



Outline

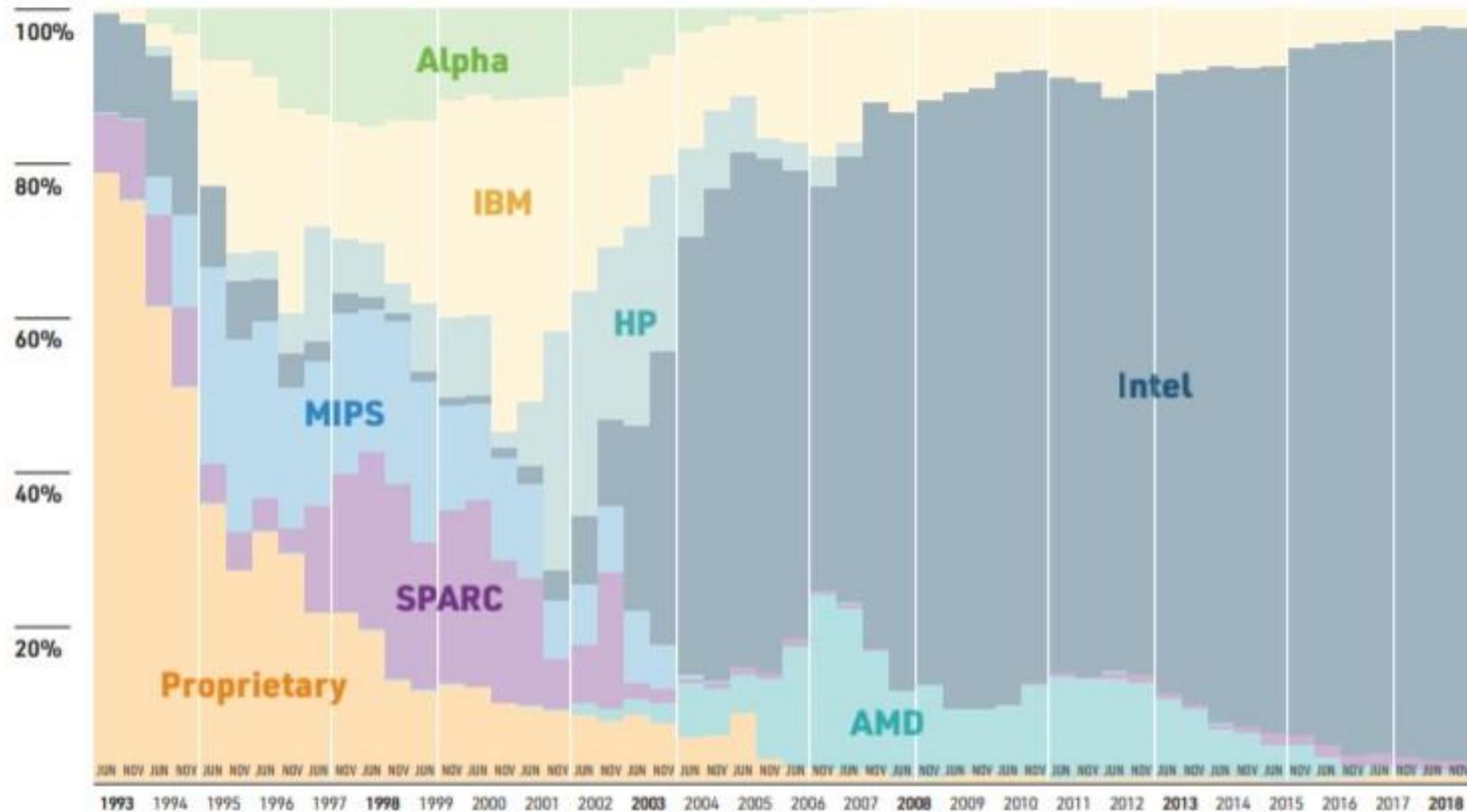
- Architectures
- ISAs
- Arm
- Arm CPU Implementations
- Systems with Arm CPUs
- Clouds with Arm
- Continuous Integration
- Software
- Vector Instructions
- SVE
- Compilers

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



What is an Instruction Set Architecture (ISA)?

- x86_64

C++ source #1 ×

A ▾ Save/Load + Add new... ▾

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

- aarch64

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

x86-64 clang 10.0.0 ✓ Compiler options...

A ▾ Output... ▾ Filter... ▾ Libraries ▾ + Add new... ▾ Add toc

```
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 X

armv8-a clang 10.0.0 ✓ Compiler options...

A ▾ Output... ▾ Filter... ▾ Libraries ▾ + Add new... ▾ Add toc

```
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



Kieran HJ Connell
@khconnell

Replying to @bbcbasicbot

```
OMO.13:DIM P% 256:[.s equd148:equd-1
1.t adr 0,s:mov 1,0:swi &31:mov 0,#0
2.m ldr 7,s:mov 2, #255
3.y mov 1,#320
4.x add 3,1,0:add 5,2,1:eor 4,1,5:eor 3,3,4:str 3,
[7],#4:subs 1,1,#4:bne x:subs 2,2,#1:bge y:add 0,0,#4:b
m
5]:CALL t
```

[Translate Tweet](#)

7:37 pm · 14 Aug 2020 · Twitter Web App

1 Retweet 15 Likes

Replying to @khconnell

A screenshot of a tweet from the account "Acorn Arc (1987) - BETA BOT" (@bbcbasicbot). The tweet shows a colorful, abstract graphical output, likely a test pattern or a simple game, displayed on a screen.

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)



A64FX

Architecture Features

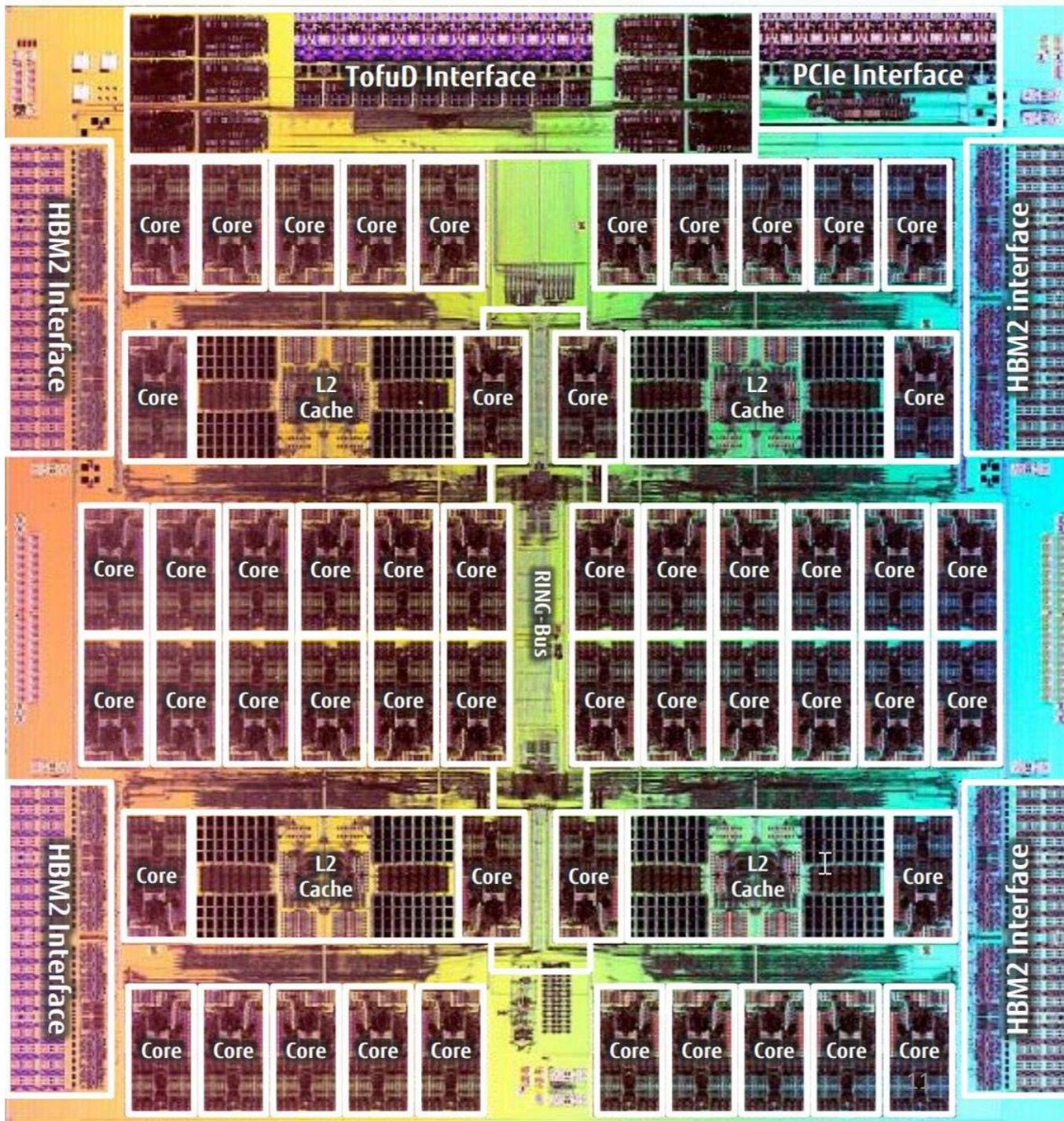
- Armv8.2-A(AArch64 only)
- SVE512-bit wide SIMD
- 48 computing cores + 4assistant cores
- HBM2 32GiB
- Tofu 6D Mesh/Torus28Gbps x 2 lanes x 10 ports
- PCIeGen3 16 lanes

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)

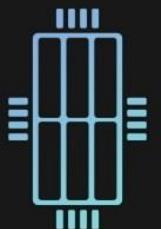


Apple's next Desktop CPU will be Arm





Machine learning controller



New 6-core CPU



Next-generation ML accelerators

5 nanometer process



11.8 billion
Transistors

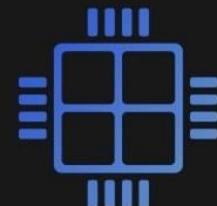
A14



Advanced image signal processor

16-core
**NEURAL
ENGINE**

11 trillion
Operations per second



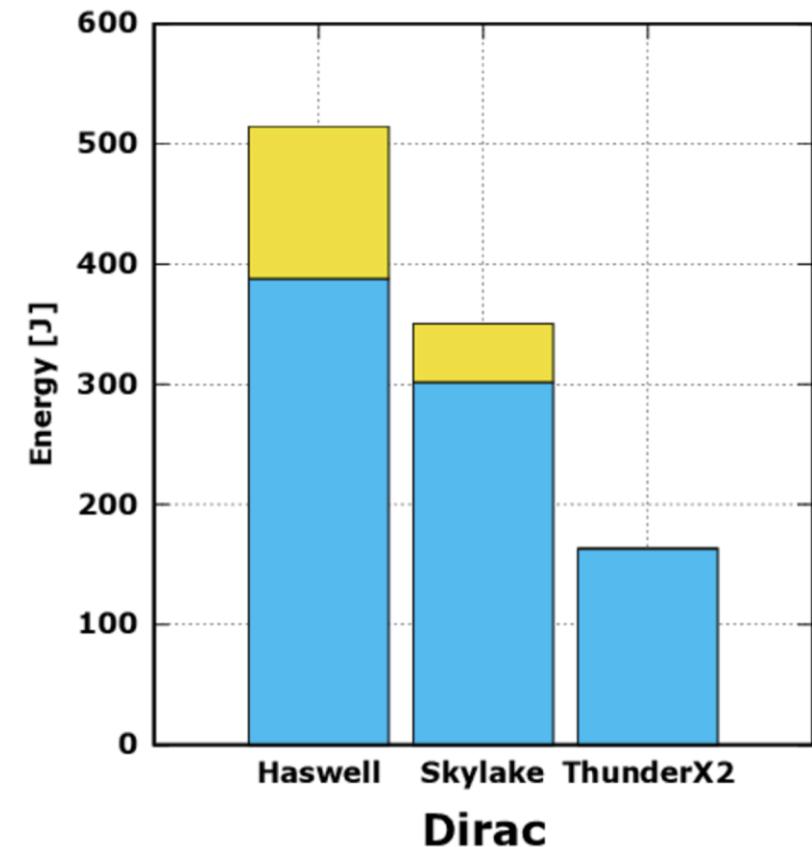
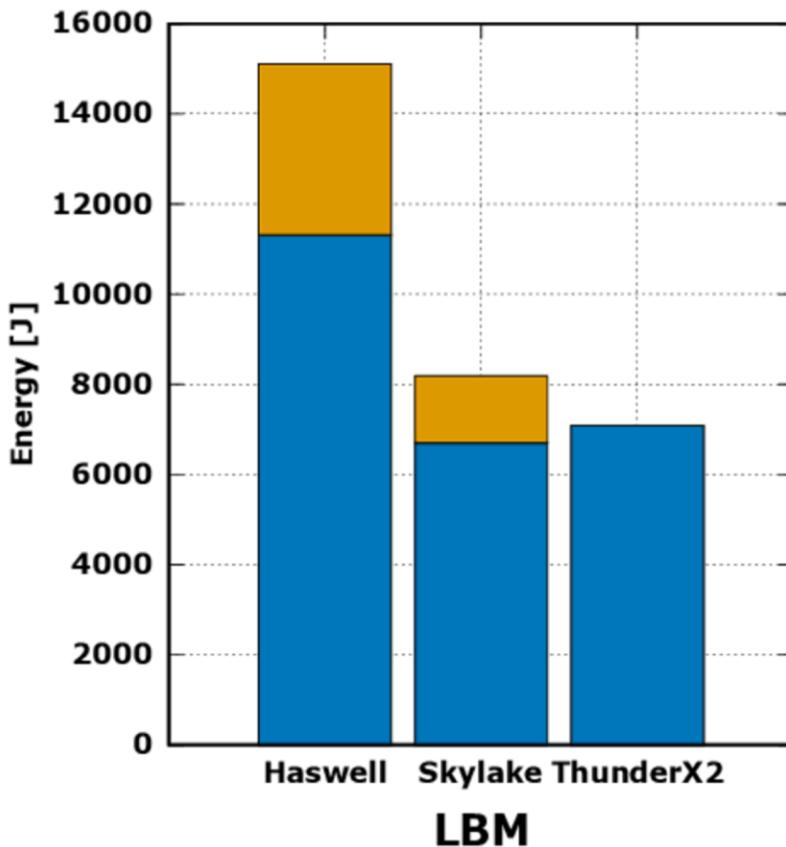
New 4-core GPU



Secure Enclave

Energy efficiency

- ThunderX2 ≈ Skylake



Green500 Data

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

TOP500			Cores	Rmax (TFlop/s)	Power (kW)	Power Efficiency (GFlops/watts)
Rank	Rank	System				
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

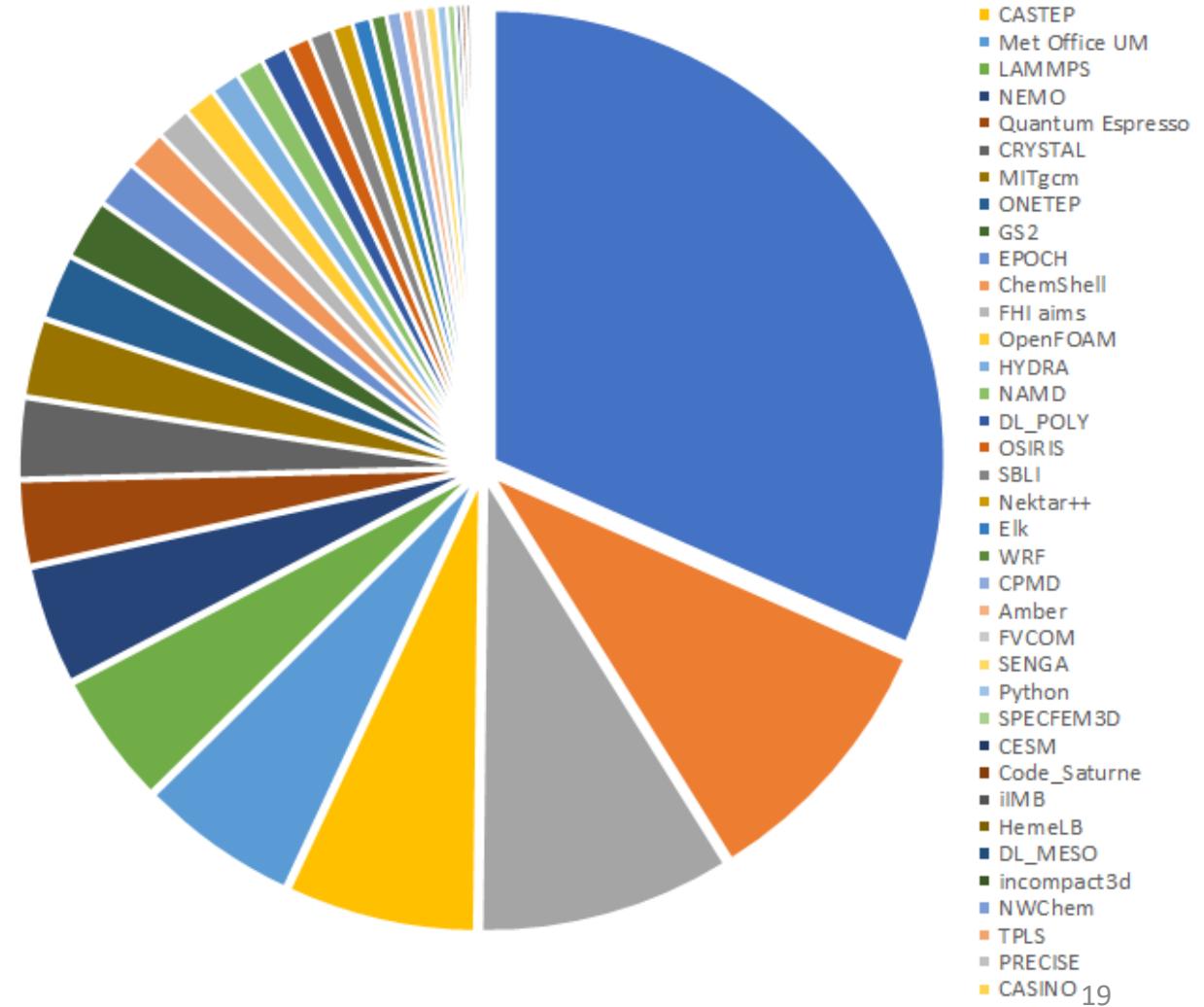
Software – It Just Works *

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

Applications -ARCHER Top 10

Node Hours on ARCHER Jan-March 2020

- 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)

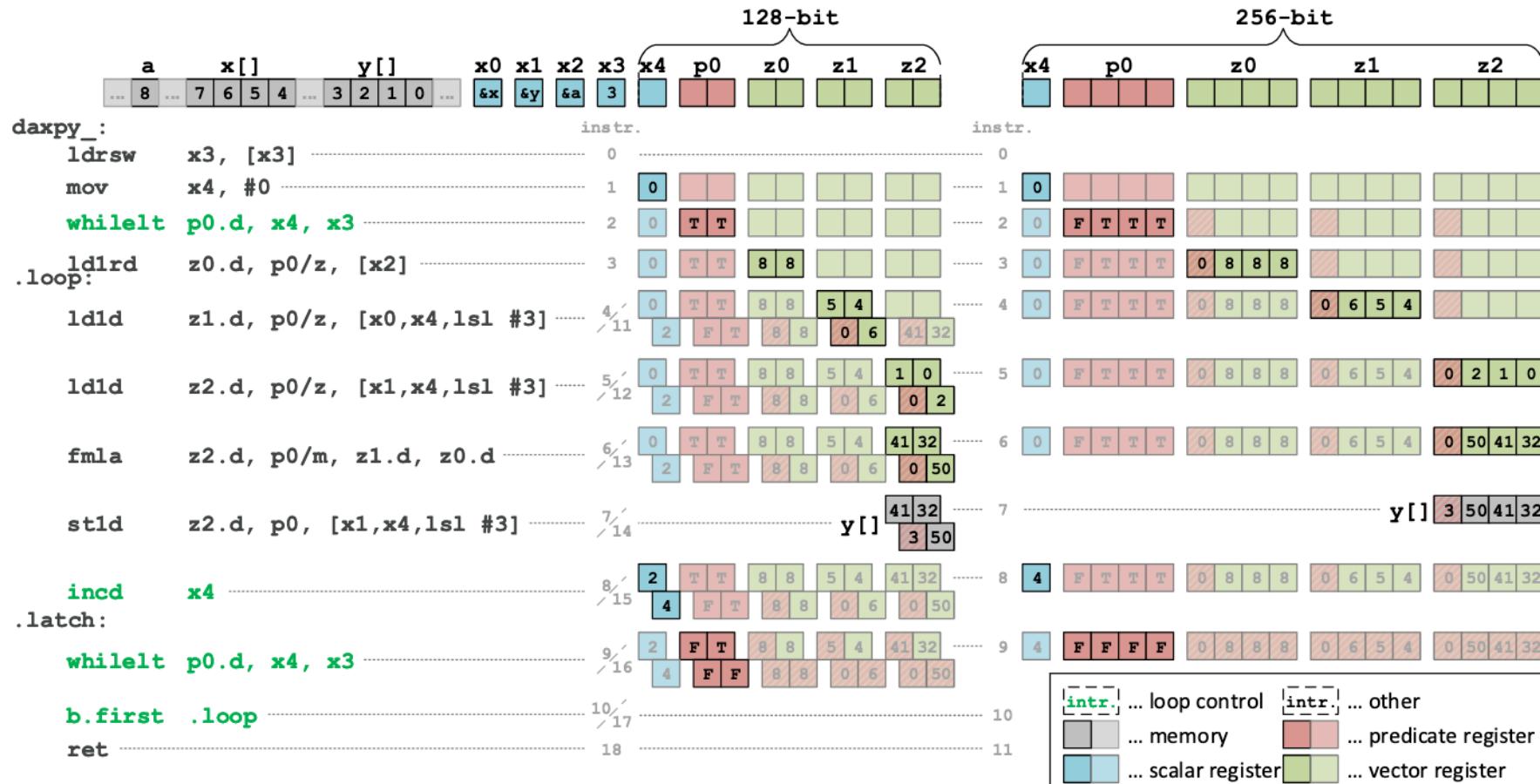
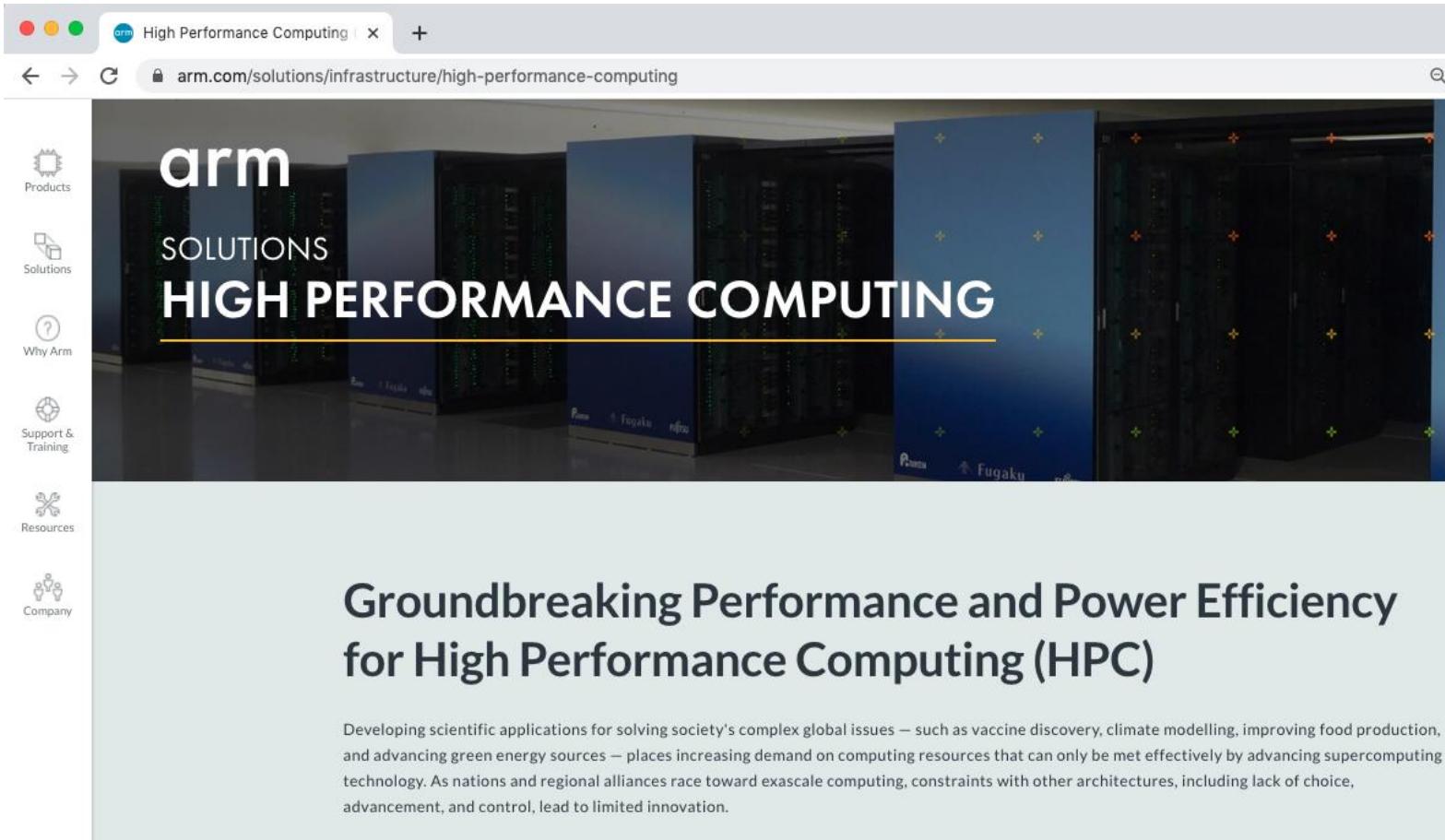


Fig. 3: Cycle by cycle example of `daxpy` with $n = 3$ and hardware vector lengths of 128- and 256-bit

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



The screenshot shows a web browser window for the ARM High Performance Computing page at arm.com/solutions/infrastructure/high-performance-computing. The page features a dark background image of server racks with glowing blue lights. Overlaid on the image is the ARM logo, the word "SOLUTIONS", and the large, bold text "HIGH PERFORMANCE COMPUTING". To the left of the main content area is a vertical sidebar with navigation icons and labels: Products (chip icon), Solutions (cube icon), Why Arm (question mark icon), Support & Training (globe icon), Resources (cross icon), and Company (people icon).

Groundbreaking Performance and Power Efficiency for High Performance Computing (HPC)

Developing scientific applications for solving society's complex global issues — such as vaccine discovery, climate modelling, improving food production, and advancing green energy sources — places increasing demand on computing resources that can only be met effectively by advancing supercomputing technology. As nations and regional alliances race toward exascale computing, constraints with other architectures, including lack of choice, advancement, and control, lead to limited innovation.

ARM HPC Wiki

- List of apps known to work
- Build instructions

The screenshot shows a GitLab project page for 'packages'. The sidebar on the left includes links for Project overview, Repository, Labels, Merge Requests (0), Requirements, CI / CD, Security & Compliance, Operations, Analytics, and Wiki (which is selected). The main content area displays a table of recently modified packages:

package	last modified	BuildMaturity	CompilesARMCompiler	CompilesGCC	EasyBuild	SpackSupport
nalucfd	2020-07-08	NeedsPatch	Yes	-	-	-
CONQUEST	2020-07-05	-	Yes	Yes	-	-
yambo	2020-07-02	-	-	-	-	-
scalapack	2020-06-30	Upstream	Yes	Yes	-	-
wrf-modeler	2020-06-29	NeedsPatch	Yes	Yes	-	-
UCX	2020-06-23	Supported	-	Yes	-	-

On the right side, there is a sidebar with categories and a 'View All Pages' button.

allPackages	APEX	application	benchmark	Catalyst	closed-source	compiler	CORAL2	debugger	DoD	DOE	emulator	filesystem	Isambard-list	language	LANL-Crossroads	library	Mantevo	mini app	ML	mpi-runtime	network	open-source	OpenHPC	ORNL	profiler	RIKEN-list	sles-hpc-module	system-service	tool	Tri-lab CTS-2	visualisation
-------------	------	-------------	-----------	----------	---------------	----------	--------	----------	-----	-----	----------	------------	---------------	----------	-----------------	---------	---------	----------	----	-------------	---------	-------------	---------	------	----------	------------	-----------------	----------------	------	---------------	---------------

Categories

Most recently modified packages

View All Pages

Compilers

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

Perfromance of Different Compilers - YMMV

	GCC 8.3	Arm 19.2	CCE 9.0
CloverLeaf	73%	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

Tracking down obscure bugs

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



Marcin Juszkiewicz
@haerwu

#Python on #AArch64 sucks. 4K/64K page size difference between distros kills any use of pypi.

Find some time, read issue, comment, help to solve it.



Inconsistent page-size on arm64 · Issue #735 · pypa/manyli...
Hello, tl;dr Debuntu has a 4k page-size and CentOS 7/8 has a 64k page size, so aarch64 manylinux wheels built on the ...
[🔗](#) [github.com](#)



mattip commented on 29 Aug

I think #741 closes this. Thanks to all who put the effort into pinpointing the problem and solving it.



mayeut commented 4 days ago

Closing per last comments.
Thanks to all.



mayeut closed this 4 days ago

Cloud Service Providers with Arm

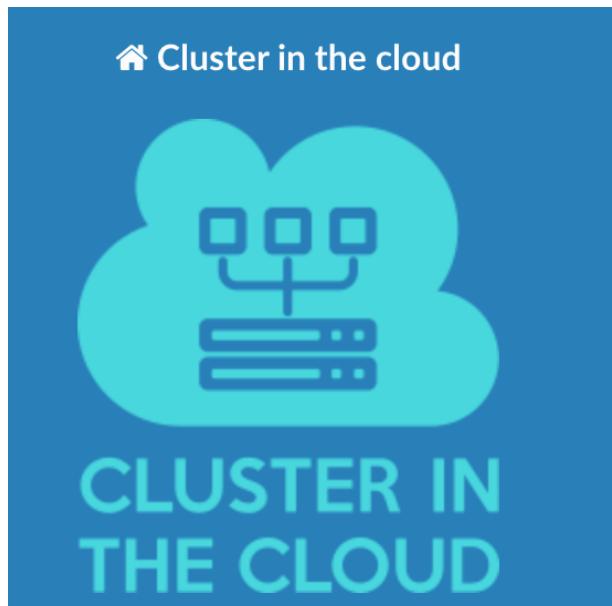
Amazon Web Services - Graviton2



- 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
```

AWS Services Resource Groups chris @ 9634-4975-8405 Ireland Support

New EC2 Experience Tell us what you think

EC2 Dashboard New

Events New

Tags

Limits

Instances

Launch Instance Connect Actions

cluster : robust-duck Add filter 1 to 2 of 2

<input type="checkbox"/>	Name	Instance ID	Instance Type	Availability Zone	Instance State	Status
<input type="checkbox"/>	robust-duck-...	i-017eb0dfe8855d704	c6g.4xlarge	eu-west-1c	running	✓ 2
<input type="checkbox"/>	mgmt	i-0f4ace130a7899c8b	t3a.medium	eu-west-1c	running	✓ 2

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



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-rsharp	64	1	16h01m	run	vasp_std
1347847	547938	ba-rsharp	64	1	15h56m	run	vasp_std
1347853	547941	ba-rsharp	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/howmuchisenoough/>

NVIDIA GPUs

