Arm Supported HPC Tools

Geraint North
Distinguished Engineer, Arm HPC Tools

Arm Research Summit
12 September 2017

Continuity

across Arm-compatible cores, and beyond.

Community

through our partnership and open-source.

Consumability

through integrated, tested, supported products.

Serious Arm HPC deployments starting in 2017

Two big announcements about Arm in HPC in Europe

insideHPC

Bull Atos to Build HPC Prototype for Mont-Blanc Project using Cavium ThunderX2 Processor

January 16, 2017 by staff

Today the Mont-Blanc European project announced it has selected Cavium's ThunderX2 ARM server processor to power its new HPC prototype.

The new Mont-Blanc prototype will be built by Atos, the coordinator of phase 3 of Mont-Blanc, using its Bull expertise and products. The platform will leverage the infrastructure of the Bull sequana pre-exascale supercomputer range for network, management, cooling, and power. Atos and Cavium signed an agreement to collaborate to develop this new platform, thus making Mont-Blanc an Alpha-site for ThunderX2.

Bull atos technologies

University of BRISTOL GW4

January 17th 2017

Announcing the **GW4 Tier 2 HPC service, 'Isambard':** named after Isambard Kingdom Brunel

System specs:

- Cray CS-400 system
- **10,000+** ARMv8 cores
- HPC optimised software stack
- Technology comparison:
  - x86, KNL, Pascal
- To be installed March-Dec 2017
- £4.7m total project cost over 3 years

I.K.Brunel 1804-1859

Simon McIntosh Smith, simonm@cs.bris.ac.uk, @simonmcs

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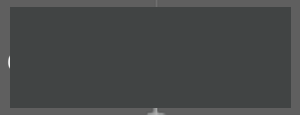
bristol.ac.uk

arm

Open-source Arm HPC

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openHPC – Now on Arm

OpenHPC is a community effort to provide a common, verified set of open source packages for HPC deployments

Arm's participation:

- Silver member of OpenHPC
- Arm is on the OpenHPC Technical Steering Committee in order to drive Arm build support

Status: 1.3.2 release out now

- All packages built on ARMv8 for CentOS and SUSE
- Arm machines are being used for building and also in the OpenHPC build infrastructure.
- Great work from Linaro for testing the release and addition of new packages (plasma, pnetcdf, scotch, slepc)

Functional Areas	Components include
Base OS	RHEL/CentOS 7.1, SLES 12
Administrative Tools	Conman, Ganglia, Lmod, LosF, ORCM, Nagios, pdsh, prun
Provisioning	Warewulf
Resource Mgmt.	SLURM, Munge. Altair PBS Pro*
I/O Services	Lustre client (community version)
Numerical/Scientific Libraries	Boost, GSL, FFTW, Metis, PETSc, Trilinos, Hypre, SuperLU, Mumps
I/O Libraries	HDF5 (pHDF5), NetCDF (including C++ and Fortran interfaces), Adios
Compiler Families	GNU (gcc, g++, gfortran)
MPI Families	OpenMPI, MVAPICH2
Development Tools	Autotools (autoconf, automake, libtool), Valgrind,R, SciPy/NumPy
Performance Tools	PAPI, Intel IMB, mpiP, pdtoolkit TAU

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Arm HPC Users Group

Community Resources

- Mailing List
- Community Gitlab Group (Source Code, Wiki, Issue Tracking, etc.)
- Slack Channel- request invitation on the mailing list
- Arm HPC Package List

Events

- Going ARM Workshop (ISC 2017)
- Designing, Porting & Optimizing HPC Workloads for ARM Based Systems
- Arm Research Summit (Cambridge, UK) - Sept 2017

Arm Resources

- Arm HPC Developers Site
- Arm Research Github Site

https://arm-hpc.gitlab.io

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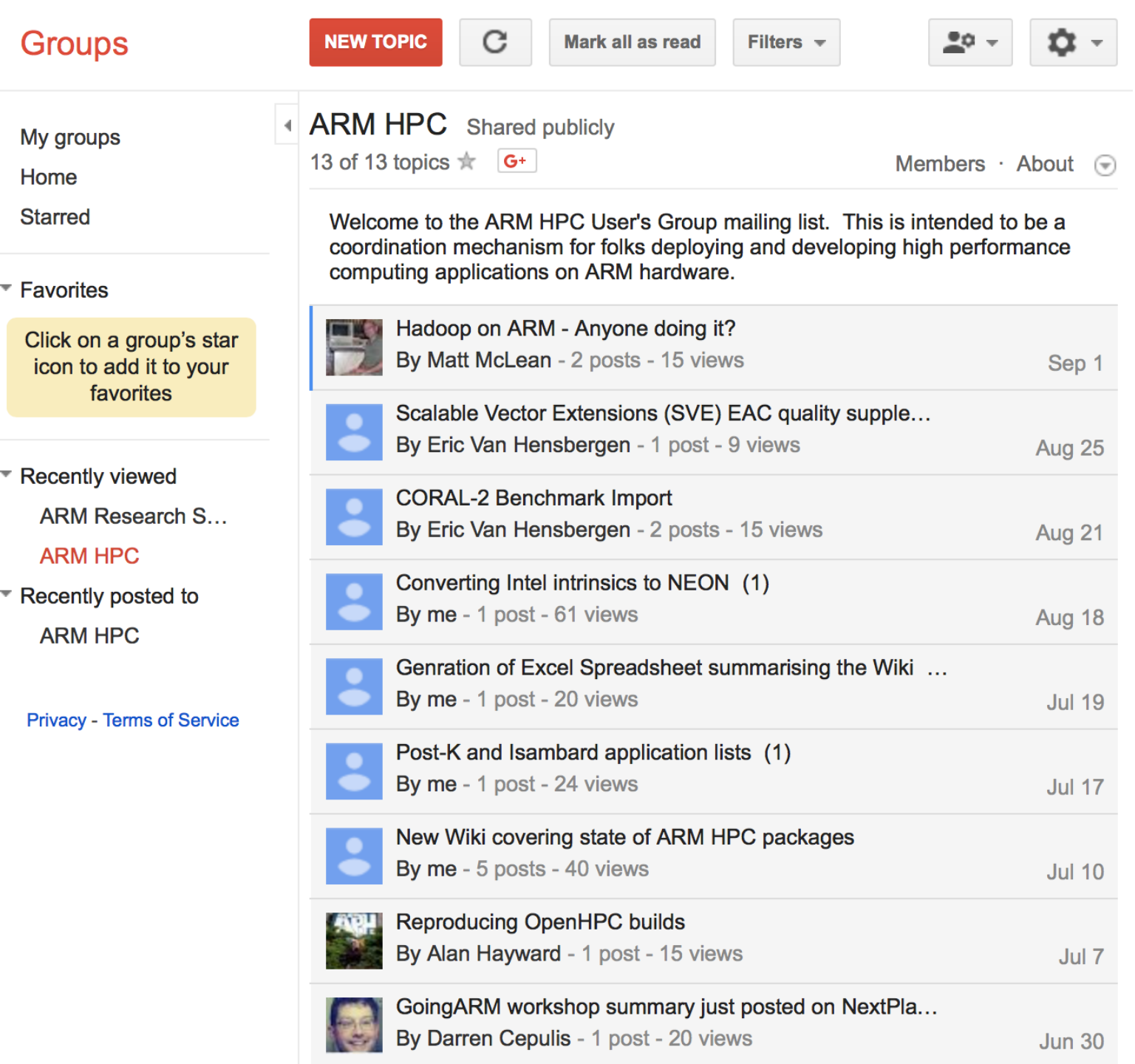

- 50 members joined since ISC.
- Mostly used by Arm to draw attention to new resources and announcements.
- Some involvement from others in the community.

https://arm-hpc.gitlab.io

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Arm HPC Users Group / packages

Project | Repository | Merge Requests 0 | Pipelines | **Wiki** | Snippets | Members | Settings

Home

Home

New page | Page history | Edit

Last edited by **arm-hpc packages pipeline** 2 days ago

This Wiki exists to capture and link to information regarding the packages considered critical for HPC.

Download the summary Excel Spreadsheet

Please make any modifications you like to the individual package pages. Especially desirable contributions are:

- Elaborating on details of what the package is, where they are sparse.
- Mentioning yourself if you are actively working on it or have some expertise that you'd like to share.
- Adding labels to the relevant pages if you (for example) know that something includes NEON optimisations or is known to compile on Arm (with either GCC or the Arm Compiler suite).
- Sharing instructions, gotchas, recipes, results and anything else that you think could help those who want to evaluate a particular package on Arm.

The Arm HPC Packages Wiki is a community site to share knowledge about:

- What builds (GCC and ARM Compiler)
- What is important
- What has been tuned
- What flags/patches are needed for good performance.

https://arm-hpc.gitlab.io

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This is a list of packages of interest to the GW4 group of universities for their "Isambard" ARM-based supercomputer, as presented by Simon McIntosh-Smith in his presentation at the GoingARM workshop at ISC2017.

Packages in the 'isambard-list' category

Package	Last Modified	BuildMaturity	CompilesARMCompiler	CompilesGCC	NEONOptimized
bookleaf	2017-07-17		Yes	Yes	
castep	2017-07-24				
cloverleaf	2017-07-24	Upstream	Yes	Yes	
cp2k	2017-07-24			Yes	
gromacs	2017-07-24		Yes	Yes	
hipstar	2017-07-17				
lammps	2017-07-24				
oasis	2017-07-24				
onetep	2017-07-24				
openfoam	2017-07-24	NeedsPatch	Yes	Yes	
openfoamplus	2017-07-26	NeedsPatch	Yes	Yes	
snap	2017-07-24	Upstream	Yes	Yes	

Categories group pages together into lists, e.g.:

- Benchmarks, debuggers, compilers, etc.
- Applications interesting to specific end-users.
- Open/Closed source
- Included in OpenHPC etc.

https://arm-hpc.gitlab.io

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Openfoamplus

Page history

Last edited by **Alan Hayward** about 21 hours ago

URL: http://openfoam.com/download/install-source.php

Categories: application, open-source, isambard-list

Free open-source CFD package, built on top of OpenFOAM

Label: BuildMaturity=NeedsPatch, see script below.

Build Instructions

Install system requirements

Install system requirements, using http://www.openfoam.com/documentation/system-requirements.php

If using ARM compiler, module load it.

Label: CompilesARMCompiler=Yes (Tested at 1.3)

Set user options

Run the following, editing as required

```
# Where to put everything.
BENCH_ROOT=~/OpenFOAM+
BENCH_ARCHIVE=$BENCH_ROOT/Archive

# Parallel builds.
```

The Wiki pages themselves mark up Categories and Labels, which cause the summaries and spreadsheets to be automatically updated.

https://arm-hpc.gitlab.io

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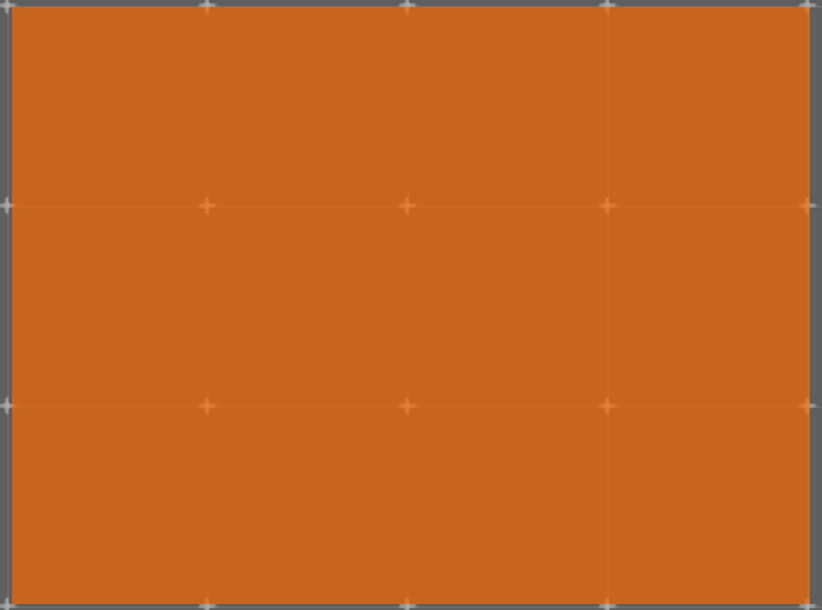
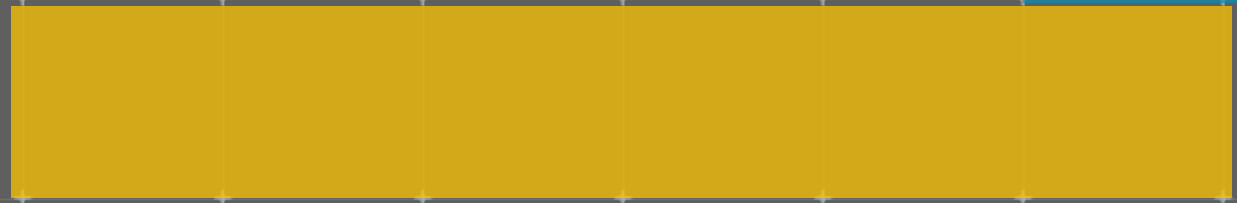
Package	External URL	Last Wiki Update	BuildMaturity	CompilesARMCompiler	CompilesGCC	NEONOptimized	Categories		
abinit	http://www.abinit.org/	19/07/17 16:26:26					application	open-source	
adios	http://www.olcf.ornl.gov/center-projects/adios/	17/07/17 23:33:11		Yes	Yes		open-source	openhpc	
adventure	http://adventure.sys.t.u-tokyo.ac.jp/	17/07/17 14:43:13					application	closed-source	riken-list
allinea-ddt	https://www.allinea.com/products/ddt	24/07/17 21:50:22	Supported				closed-source	debugger	
allinea-map	https://www.allinea.com/products/map	24/07/17 21:50:43	Supported				closed-source	profiling	
alya	https://www.bsc.es/es/computer-applications/alya-system	17/07/17 13:52:45			Yes		application	closed-source	
arpack	http://www.caam.rice.edu/software/ARPACK/	17/07/17 23:33:11		Yes			library	open-source	
asearch-blas	https://ccpforge.cse.rl.ac.uk/gf/project/asearchralna/	10/07/17 19:52:09					application	open-source	
atlas	http://sourceforge.net/projects/math-atlas/	18/07/17 18:53:49			Yes	Yes	library	open-source	
autoconf		18/07/17 13:41:43		Yes	Yes		open-source	openhpc	tool
automake	http://www.gnu.org/software/automake	18/07/17 13:41:43		Yes	Yes		open-source	openhpc	tool
beegfs	http://www.beegfs.com/content/	10/07/17 19:52:09					filesystem	open-source	
bioconductor	https://www.bioconductor.org	10/07/17 19:52:09					application	open-source	
blis	https://github.com/flame/blis/	10/07/17 19:52:09					library	open-source	
bookleaf	https://uk-mac.github.io/BookLeaf/	17/07/17 23:33:11		Yes	Yes		benchmark	isambard-list	open-source
boost	http://www.boost.org	18/07/17 11:29:00		Yes	Yes		library	open-source	openhpc
bowtie	http://bowtie-bio.sourceforge.net/index.shtml	10/07/17 19:52:09					application	open-source	
bqcd	https://www.rrz.uni-hamburg.de/services/hpc/bqcd	10/07/17 19:52:09					application	open-source	
bwa	https://github.com/lh3/bwa	18/07/17 18:57:29			Yes		application	open-source	
castep	http://www.castep.org	24/07/17 21:36:31					application	isambard-list	open-source
ccs-qcd		17/07/17 23:33:11		Yes			application	closed-source	riken-list
ceph	http://ceph.com	17/07/17 16:13:35					filesystem	open-source	
cloverleaf	http://uk-mac.github.io/CloverLeaf/	24/07/17 21:42:47	Upstream	Yes	Yes		benchmark	isambard-list	mantevo
cloverleaf3d	http://uk-mac.github.io/CloverLeaf3D/	24/07/17 21:41:31	Upstream	Yes	Yes		benchmark	mantevo	open-source
clustershell	http://clustershell.sourceforge.net/	10/07/17 19:52:09			Yes		open-source	openhpc	tool
code-aster	http://www.code-aster.org	19/07/17 12:21:38					application	open-source	
code-saturne	http://code-saturne.org/cms/	10/07/17 19:52:09					application	open-source	
comd	http://exmatex.github.io/CoMD	24/07/17 21:36:31	Upstream	Yes	Yes		benchmark	mantevo	open-source
confuse	https://github.com/martinh/libconfuse	10/07/17 19:52:09			Yes		library	open-source	openhpc
conman	https://github.com/dun/conman	10/07/17 19:52:09			Yes		open-source	openhpc	sles-hpc-module
cp2k	http://www.cp2k.org/	24/07/17 21:36:31			Yes		application	isambard-list	open-source
crass-crispr	https://github.com/ctSkennerton/crass	10/07/17 19:52:09					application	open-source	
cube	http://www.scalasca.org/software/cube-4.x/download.html	10/07/17 19:52:09					open-source	profiler	
cython	http://cython.org	10/07/17 19:52:09			Yes		compiler	open-source	openhpc
dgemm	http://www.nersc.gov/research-and-development/apex/apex-benc	24/07/17 21:36:31	NeedsPatch	Yes	Yes		apex	benchmark	open-source
dl-meso	http://www.scd.stfc.ac.uk/SCD/research/app/cse/software/DL_MF	10/07/17 19:52:09					application	open-source	

arm

Commercial HPC Tools





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Commercial HPC products simplify the ecosystem

Comprehensive

- Comprehensive suite of tools – compiler, libraries, debuggers and profilers

Performant

- Best in class performance with latest features
- Tuned for a wide range of 64-bit ARMv8-A-based platforms

Supported

- Commercially supported by Arm

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Arm commercial HPC software portfolio

Arm HPC Compilers

COMMERCIALLY SUPPORTED
FORTRAN, C AND C++

Arm Performance Libraries

BLAS, LAPACK and FFT
MICRO-ARCHITECTURALLY TUNED

+

Allinea Forge (DDT+MAP)

PARALLEL DEBUGGING and PROFILING

Allinea Performance Reports

PERFORMANCE SUMMARY

arm

Arm C/C++/Fortran Compiler

Commercially supported by ARM

Linux user-space compiler tailored for HPC on Arm

- Maintained and supported by Arm for a wide range of Arm-based SoCs running leading Linux distributions
- Based on Clang/LLVM, the leading compiler framework with Flang for Fortran support.

Latest features and performance optimizations

Latest features go into the commercial releases first

- Ahead of upstream LLVM by up to an year with latest performance improvement patches
- SVE support in the assembler, disassembler, intrinsics and autovectorizer

Optimized OpenMP

OpenMP

- Uses latest open source (now Arm) LLVM OpenMP runtime
- Changes pushed back to the community

arm

Arm Performance Libraries

Optimized BLAS, LAPACK and FFT

Commercial 64-bit ARMv8 math libraries

- Commonly used low-level math routines - BLAS, LAPACK and FFT
- Validated with NAG's test suite, a de-facto standard

Performance on par
with best-in-class math libraries

Best-in-class performance with commercial support

- Tuned by Arm for Cortex-A72, Cortex-A57 and Cortex-A53
- Maintained and supported by Arm for a wide range of Arm-based SoCs
  - Including Cavium ThunderX and ThunderX2 CN99 cores

Commercially Supported
by ARM

Silicon partners can provide tuned micro-kernels for their SoCs

- Partners can contribute directly through open source route
- Parallel tuning within our library increases overall application performance

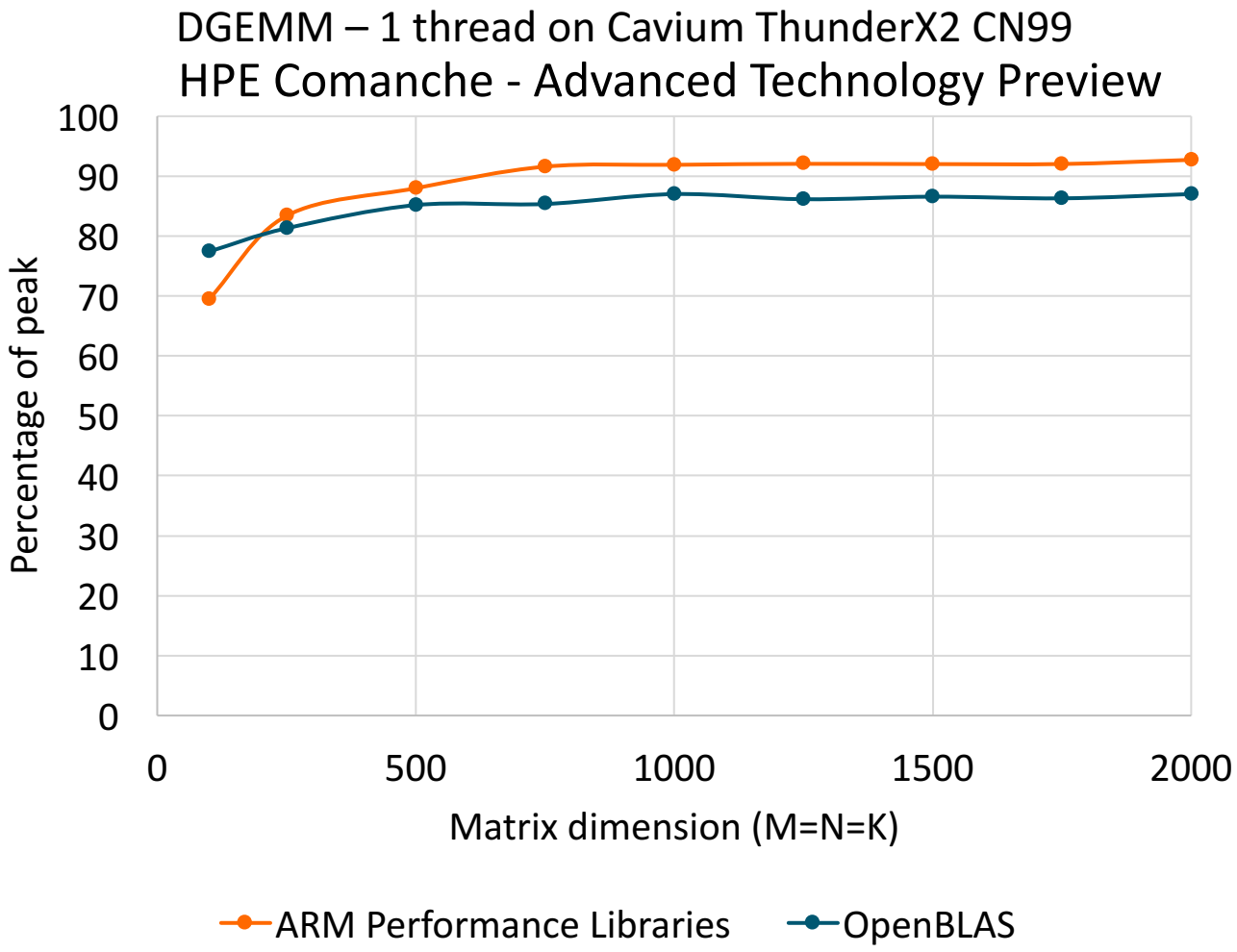
Validated with
NAG test suite

arm

Arm Performance Libraries

Micro-architectural tuning

- Arm cores have a variety of designs, created by both ARM and our partners
- Arm Performance Libraries are creating tailored versions of routines to target these different *micro-architectures*
- It is important to ensure that the correct version is installed on your system



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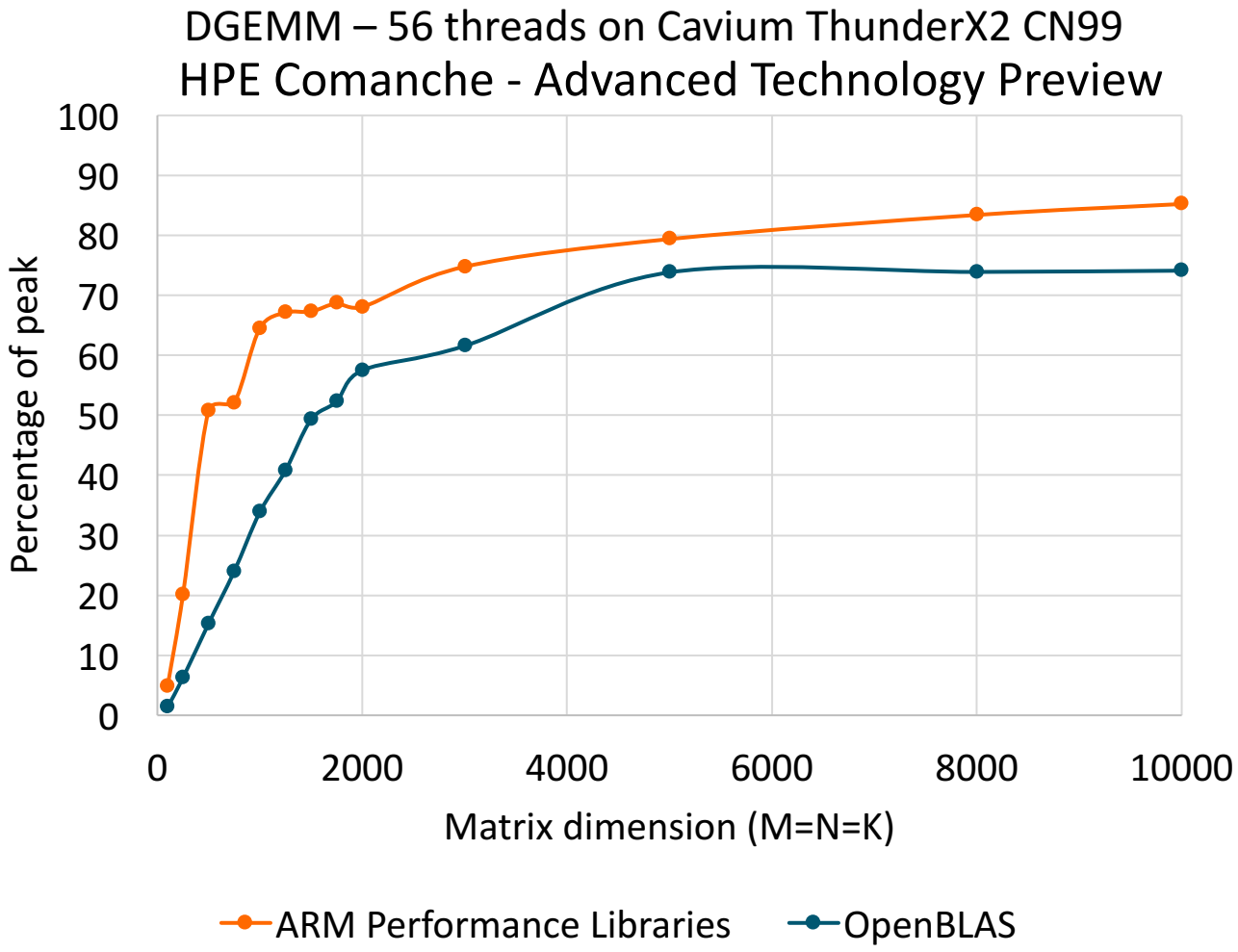

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New in Arm Compiler for HPC 1.4

Arm Performance Libraries 2.3.0

- Supports GCC 7.1.0 and Arm Compiler 1.4

Arm Compiler 1.4

- Support for some gfortran flags in armflang for compatibility:
  `-ffree-form -ffixed-form -ffixed-line-length-0 -ffixed-line-length-132 -ffixed-line-length-none`
  `-ffree-line-length-0 -ffree-line-length-132 -ffree-line-length-none`
  `-fconvert={native|swap|little-endian|big-endian}`
- Support for `-mcpu=native` flag.
- Support for vectorized math routines (from SLEEF) – undocumented feature.

Packaging

- Module files are now compatible with lmod

arm

Experimental tools to support SVE

With Arm Compiler, Instruction Emulator and Code Advisor

Compile → Emulate → Analyse

ARM HPC Compiler

C/C++/Fortran

SVE via auto-vectorization, intrinsics and assembly.

Compiler Insight: Compiler places results of compile-time decisions and analysis in the resulting binary.

Instruction Emulator

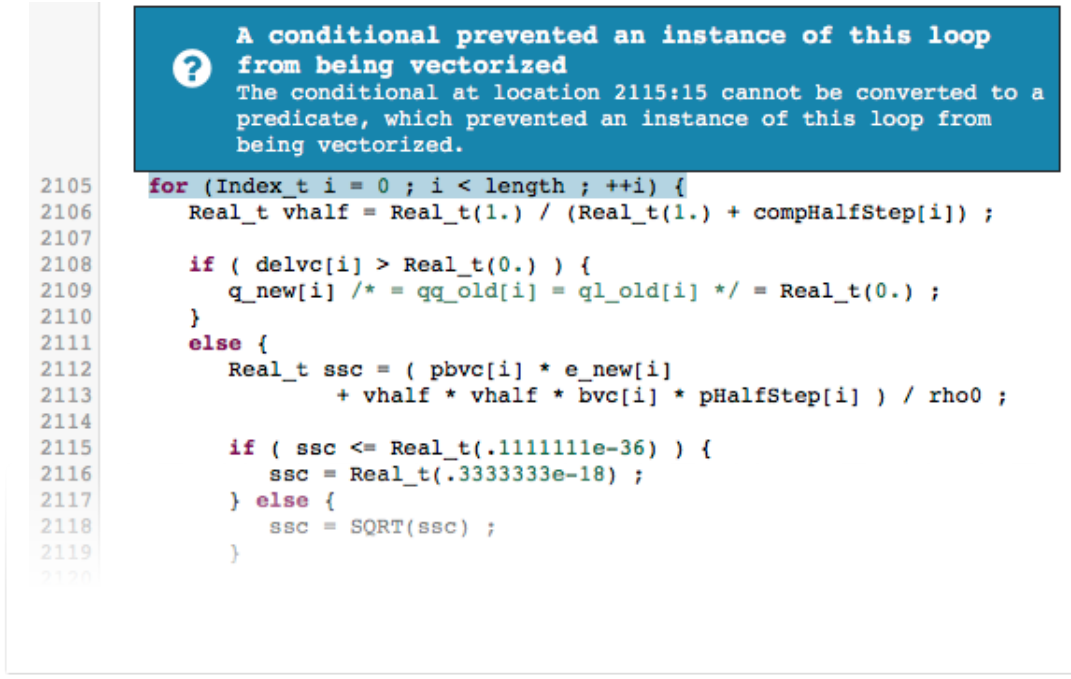
Runs **userspace** binaries for future ARM architectures on today's systems.

Supported instructions run **unmodified**.

Unsupported instructions are **trapped and emulated**.

Code Advisor

Console or web-based output shows prioritized advice in-line with original source code.



New in Arm Instruction Emulator 1.2.1

Experimental feature to integrate with DynamoRIO to generate memory access traces.
Thanks to Chris Adeniyi-Jones and Miguel Tairum-Cruz for their design input!

Output file format:

```
sequence, tid, bundle, isWrite, size, addr, pc
```

Where:

sequence	sequence number which orders the load/stores across multiple trace files
tid	thread id
bundle	support bundling of multiple mem_refs for gather/scatter/strided accesses
isWrite	true if store, false if load
size	number of bytes stored or loaded
addr	load/store address
pc	instruction address

Introducing the *Compute Library*

Optimized low-level functions for CPU and GPU

- Most popular Computer Vision (CV) and Machine Learning (ML) functions
- Supports common ML frameworks

Enable faster deployment of CV and ML

- Targeting CPU (NEON) and GPU (OpenCL)
- Significant performance uplift compared to OSS alternatives

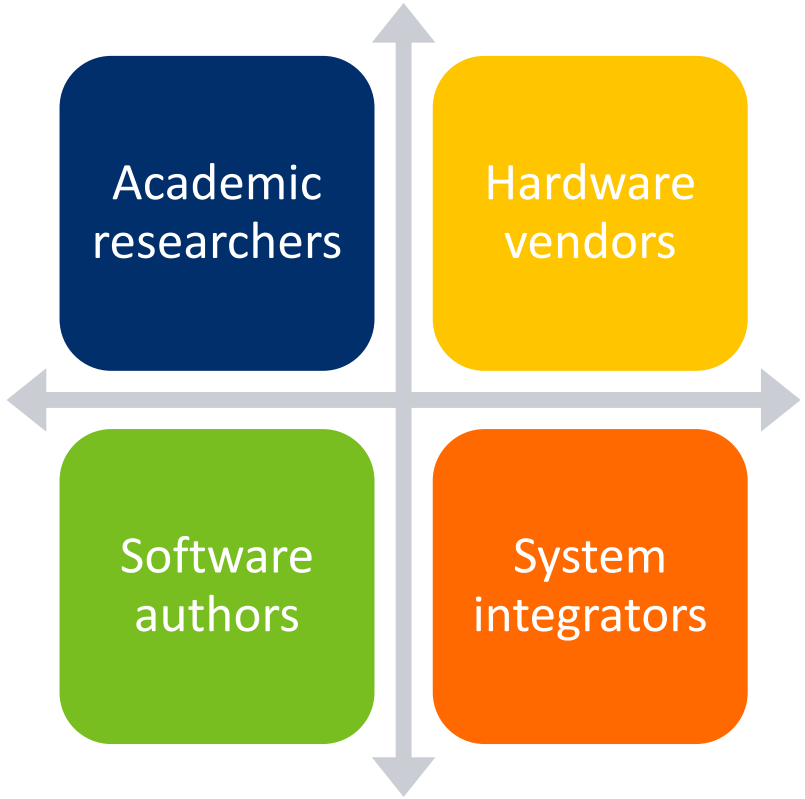
Publicly available now (no fee, MIT license)

Key Functions categories
Basic arithmetic
Convolutions
Colour manipulation
Feature detection
Neural network
GEMM
Pyramids
Filters
Image reshaping
Mathematical functions

Software Grants Overview

We will provide free access to HPC tools (ARM compiler, libraries, Emulator, Forge and Reports) for:

- Researchers experimenting with and porting codes to ARM hardware
- Partners porting applications and developing systems for the ARM ecosystem



We will assess eligibility on a case-by-case basis for each grant application with the sales manager for the relevant region.

Guidelines for acceptance

- Single nodes and small systems intended to explore ARM technology
- Research projects with limited scope and duration
- Contribution to the ARM ecosystem

Unlikely to be eligible

- Production systems
- Long-term use for large teams
- Prevents a sale in progress

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Summary

Arm's ecosystem is built on partnership and choice

- We work with many organizations to drive hardware design and deliver better software
- This method enables partners to design different products for different markets

We license IP at all levels of the stack to help customers be successful

Our 64-bit server platforms are beginning to see large, main-stream deployments

Building the software ecosystem and tools is an important part of this story

- We enhance open source software as well as developing commercially supported options