Software Ecosystem for Arm-based HPC

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CUG 2018 - Stockholm Florent.Lebeau@arm.com

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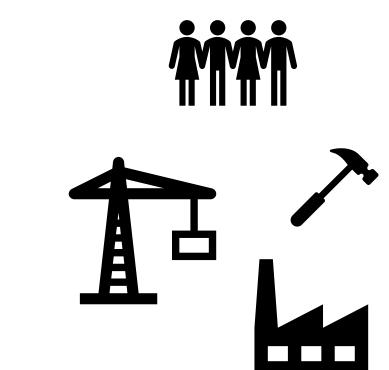
Ecosystem for HPC

List of components needed:

- Linux OS availability
- Compilers
- Libraries
- Job schedulers
- Debuggers
- Profilers

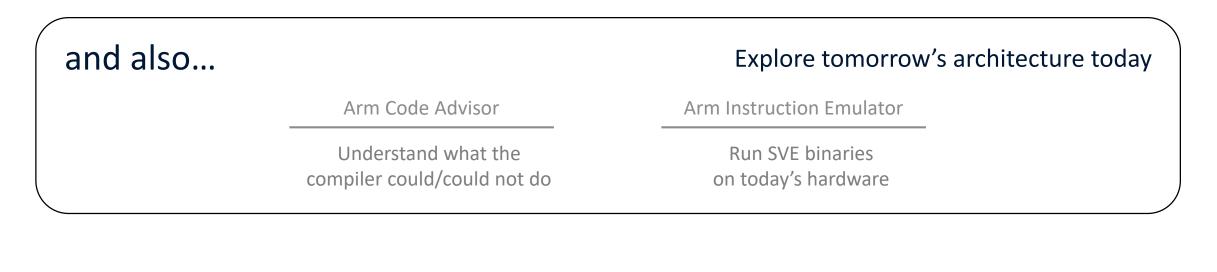
Mix of open source and commercial products and applications...

https://developer.arm.com/hpc/hpc-software

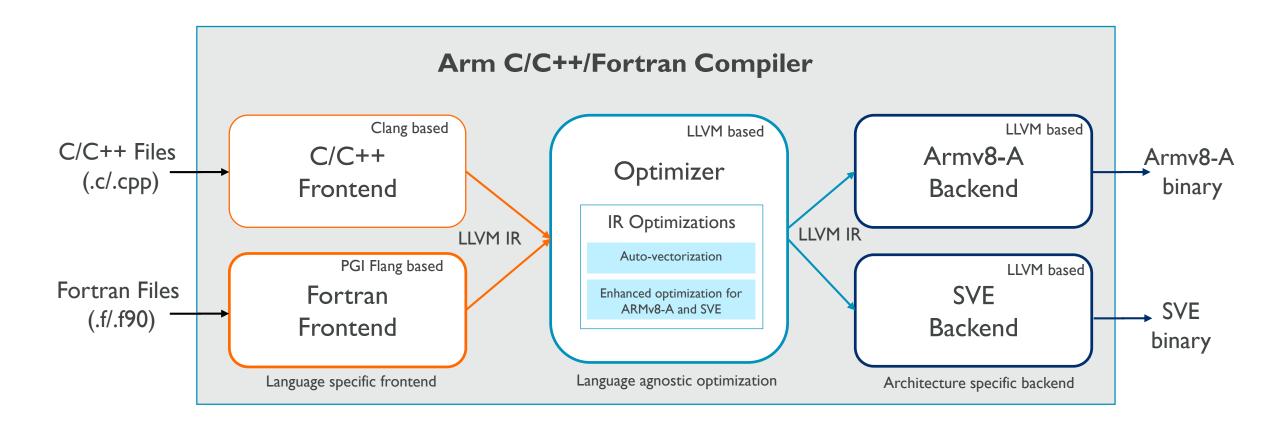


Arm development tools portfolio for HPC

Arm Allinea Studio		Develop and run on today's hardware			
Arm Compiler for HPC	Arm Performance Libraries	Arm Forge Professional	Arm Performance Reports		
Linux user space compiler for HPC applications	BLAS, LAPACK and FFT	Multi-node interoperable profiler and debugger	Interoperable application performance insight		



Arm Compiler – Building on LLVM, Clang and Flang projects





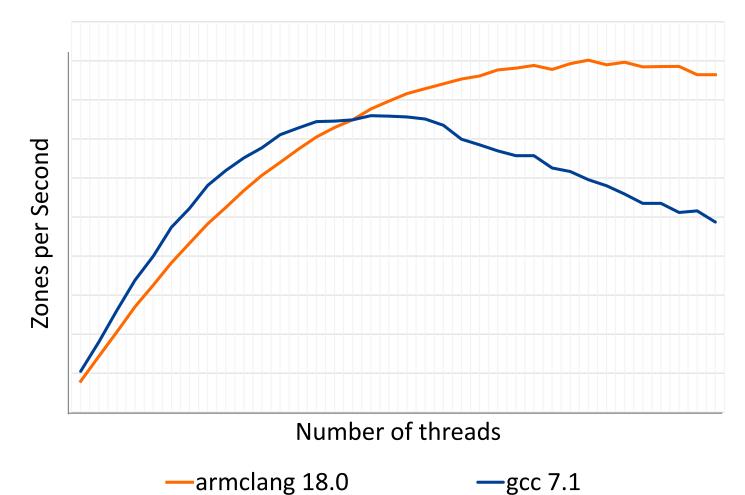
Arm Compiler – OpenMP scaling

Better scaling at higher thread count

Lulesh – size 40

Arm Compiler uses libomp based optimized OpenMP runtime

For Lulesh (Livermore Unstructured Lagrangian Explicit Shock Hydrodynamics), Arm Compiler shows better scaling than GCC for higher thread count



DGEMM performance on Cavium ThunderX2

Excellent serial and parallel performance

Achieving very high performance at the node level leveraging high core counts and large memory bandwidth

Single core performance at 95% of peak for DGEMM

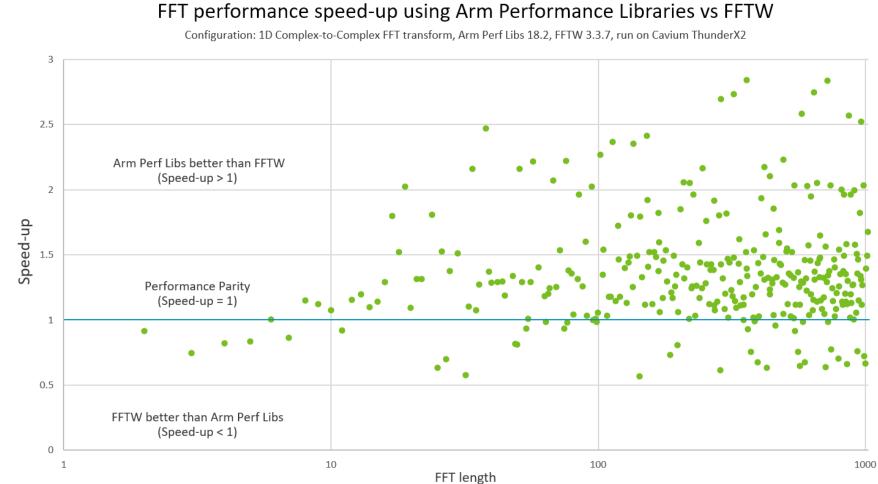
Parallel performance significantly higher than OpenBLAS

100% 90% 80% Percentage of peak 70% 60% 50% 40% 30% 20% 10% 0% 0 2000 4000 6000 8000 10000 Matrix dimension (M=N=K)

DGEMM – 56 threads on Cavium ThunderX2 CN99

ARM Performance Libraries — OpenBLAS

Arm Performance Libraries



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Arm HPC ecosystem

Porting to Arm

Arm is engaging directly with partners and HPC scientific code developers to support porting and optimisation of common HPC libraries, tools and applications

Initial focus on successfully building with both Arm and GCC compilers across a broad front

Often only modest changes to environment variables, build scripts and architecture files are needed

Degree of commonality between codes



Example: Particle in Cell codes

Two different approaches

VPIC

Explicit 2nd order push, charge conserving

FDTD fields

C & C++ with MPI & pthreads

Low particle order

Heavily optimised push, previously tuned for specific platforms

Vector kernel

https://github.com/lanl/vpic

EPOCH

Explicit 2nd order push, charge conserving
FDTD fields
Fortran with MPI
High order particles
Flexible, extensible, versatile
Linked list storage
Dependencies: SDF
http://www.ccpp.ac.uk

Example: Leveraging Arm intrinsics from C

VPIC

VPIC's v4 kernel pushes four particles at a time – optimised with SSE SIMD calls

Arm's NEON instructions offer similar functionality

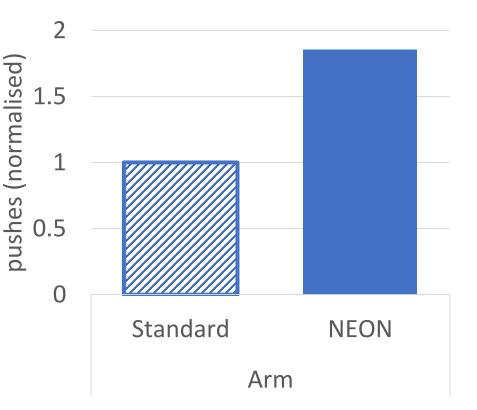
Datatypes and intrinsic calls from SSE can be mapped over to NEON in many cases

Projects like SIMD Everywhere:

https://github.com/nemequ/simde

may help generate portable code able to exploit Arm's vector calls

Could such vectorised kernels stand to benefit from Arm's SVE instructions?



Example: Leveraging Arm intrinsics from Fortran

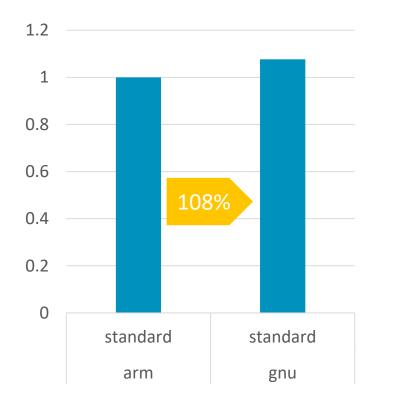
EPOCH

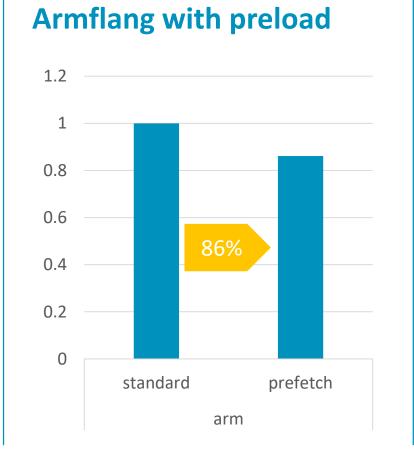
Particle prefetch Arm C compiler preload C wrapper src/housekeeping/arm intrinsics.c Uses intel's mm prefetch to improve Use pld in place of mm prefetch performance of linked-list Requires Fortran 2003's C-binding src/housekeeping/prefetch.f90 SUBROUTINE prefetch particle(p) INTERFACE #include<arm acle.h> TYPE (particle), INTENT (INOUT) :: p SUBROUTINE arm prefetch (p, x, w) BIND (C) void arm prefetch(void const* p) USE, INTRINSIC :: iso c binding #ifdef PREFETCH { CALL mm prefetch (p%part p(1)) REAL(c double),DIMENSION(3) :: p pld(p); CALL mm prefetch (p%weight) REAL(c double), DIMENSION(c ndims) :: x return; #endif REAL(c double) :: w END SUBROUTINE prefetch particle END SUBROUTINE arm prefetch END INTERFACE A similar approach can be used to call GCC's ____builtin_prefetch

Example: Performance improvement

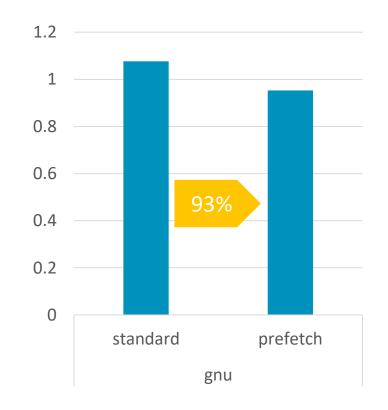
Speed-up memory-bound code

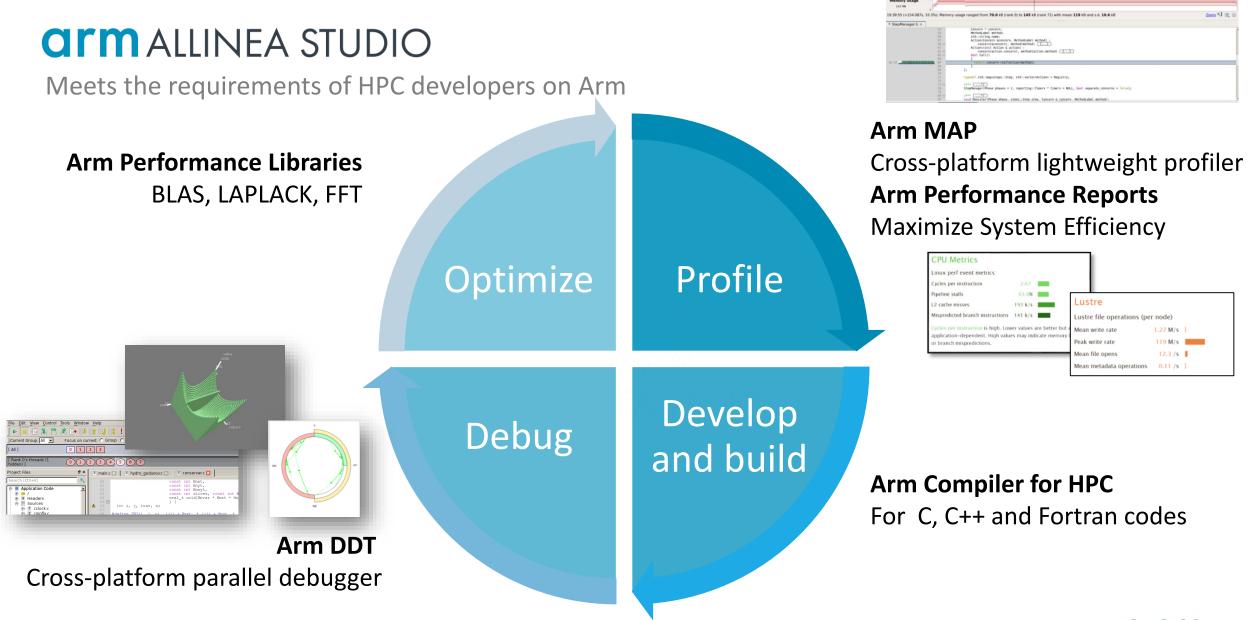
Armflang vs. GNU





GNU with prefetch





Community building

Outside the people we collaborate with, various complementary Arm HPC communities already exist:

Going - Arm HPC User Group (SC) and GoingArm (ISC/ArmRS)

Arm HPC Google Group

https://groups.google.com/forum/#!forum/arm-hpc

Arm HPC GitLab pages (<u>https://gitlab.com/arm-hpc/</u>)

Encouraging our partners to use GitLab is a priority

Our app work is **engaging with code owners and users** to get suitable test cases, to get Arm support built in, and including helping them make AArch64 testing part of their development processes

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Community site – gitlab.com/arm-hpc

https://gitlab.com/arm-hpc/packages/wikis/home

Dynamic list of common HPC applications

Provides focus for porting progress

Community driven.

Maintained by Arm, but anyone can join and contribute.

Allows developers to share recipes, and learn from progress on other applications

Provides a mechanism for tracking status of applications and package sets (e.g. OpenHPC packages, Mantevo, etc.)

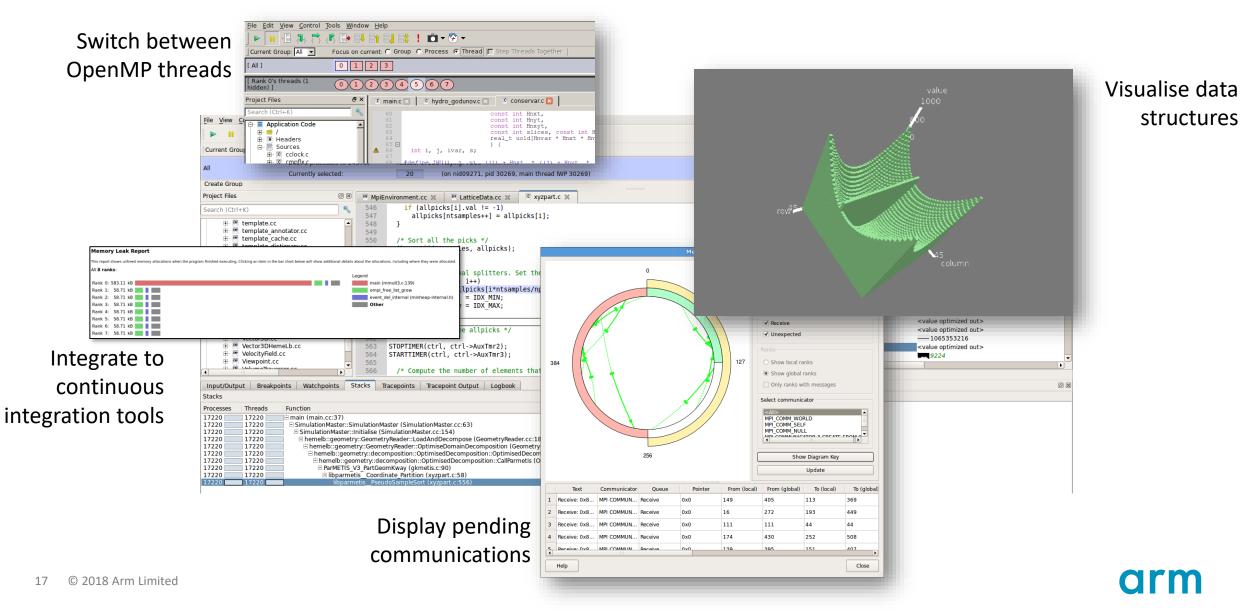
Up-to-date summary of package status

Package	External URL	Last Wiki Update	BuildMaturity	CompilesARMCompiler	CompilesGCC	NEONOptimized
EPOCH	http://www.ccpp.ac.uk	19/10/17 22:10:20	NeedsPatch	Yes	Yes	-
SDF	https://github.com/keithbennett/SDF	20/10/17 00:13:45	NeedsPatch	Yes	Yes	-
VPIC	https://github.com/lanl/vpic	19/10/17 22:10:20	-	Yes	Yes	-
adios	http://www.olcf.ornl.gov/center-projects/adios/	17/07/17 23:33:11	-	Yes	Yes	-
arpack	http://www.caam.rice.edu/software/ARPACK/	17/07/17 23:33:11	-	Yes	-	-
autoconf	http://www.gnu.org/software/autoconf/autoconf.html	01/08/17 21:48:30	-	Yes	Yes	-
automake	http://www.gnu.org/software/automake	18/07/17 13:41:43	-	Yes	Yes	-
bookleaf	https://uk-mac.github.io/BookLeaf/	17/07/17 23:33:11	-	Yes	Yes	-
boost	http://www.boost.org	18/07/17 11:29:00	-	Yes	Yes	-
ccs-qcd	https://github.com/fiber-miniapp/ccs-qcd	01/08/17 21:43:40	-	Yes		
cloverleaf	http://uk-mac.github.io/CloverLeaf/	19/10/17 22:10:20	Upstream	Yes	Yes	
cloverleaf3d	http://uk-mac.github.io/CloverLeaf3D/	24/07/17 21:41:31	Upstream	Yes	Yes	
<u>comd</u>	http://exmatex.github.io/CoMD	24/07/17 21:36:31	Upstream	Yes	Yes	-
dgemm	http://www.nersc.gov/research-and-development/apex/apex-bend	24/07/17 21:36:31	NeedsPatch	Yes	Yes	-
ffb	http://www.ciss.iis.u-tokyo.ac.jp/riss/english/project/fluid/	24/07/17 21:36:31	-		-	-
fftw	https://github.com/FFTW/fftw3	17/07/17 23:33:11	-	Yes	Yes	Yes
gnu-scientific-library	http://www.gnu.org/software/gsl/	18/07/17 07:08:24	-	Yes	Yes	-
gromacs	http://www.gromacs.org/	24/07/17 21:36:31	-	Yes	Yes	-
hdf5	http://www.hdfgroup.org	17/07/17 23:33:11	-	Yes	Yes	-
hpc-challenge	http://icl.cs.utk.edu/hpcc/index.html	24/07/17 21:36:31	Upstream	Yes	Yes	-
hpccg	http://mantevo.org/downloads/HPCCG-1.0.html	24/07/17 21:36:31	Upstream	Yes	Yes	-
hpcg	http://www.nersc.gov/research-and-development/apex/apex-bend	24/07/17 21:48:22	Upstream	Yes	Yes	-
hypre	https://computation.llnl.gov/project/linear_solvers/software.php	17/07/17 23:33:11	-	Yes	Yes	
imb		17/07/17 23:33:11	-	Yes	Yes	
lammps	http://lammps.sandia.gov/	19/10/17 22:10:20	-	Yes	Yes	
libtool		18/07/17 13:41:43	-	Yes	Yes	
lulesh	https://codesign.llnl.gov/lulesh.php	17/07/17 23:33:11	-	Yes		
metis		17/07/17 23:33:11	-	Yes	Yes	
<u>miniaero</u>	http://mantevo.org/downloads/miniAero 1.0.html	24/07/17 21:36:31	NeedsPatch	Yes	Yes	-
<u>miniamr</u>	http://mantevo.org/downloads/miniAMR_1.0.html	24/07/17 21:36:31	Upstream	Yes	Yes	-
minife	http://www.nersc.gov/users/computational-systems/cori/nersc-8-	24/07/17 21:36:31	Upstream	Yes	Yes	-
minighost	http://www.nersc.gov/users/computational-systems/cori/nersc-8-	24/07/17 21:36:31	Upstream	Yes	Yes	-
minimd	http://mantevo.org/downloads/miniMD_1.2.html	24/07/17 21:36:31	NeedsPatch	Yes	Yes	-
minixyce	http://mantevo.org/downloads/miniXyce_1.0.html	24/07/17 21:36:31	Upstream	Yes	Yes	-
mpich		19/10/17 22:10:20	NeedsPatch	Yes	Yes	-
mumps		17/07/17 23:33:11	-	Yes	Yes	
mvapich-2	http://mvapich.cse.ohio-state.edu	21/08/17 13:26:19	Upstream	Yes	Yes	
namd	http://www.ks.uiuc.edu/Research/namd/	24/07/17 21:36:31	NeedsPatch			-

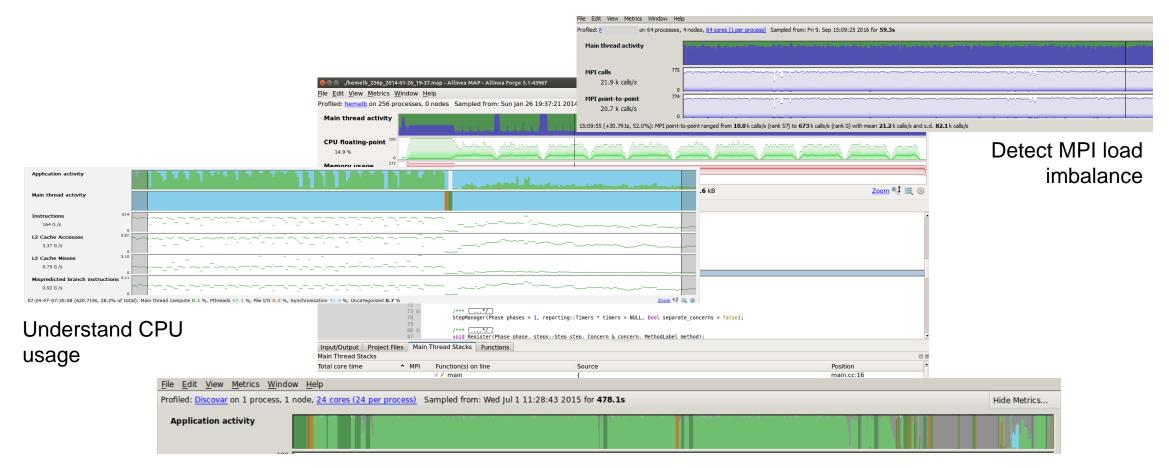
Tack! Thank You! Danke! Merci! 谢谢! ありがとう! **Gracias!** Kiitos! 감사합니다 धन्यवाद



Migrate and debug application to Arm



Optimise for Arm platforms



Identify regions of high OpenMP synchronisation

arm

Maximize System Efficiency

