CIM

Performance Engineering with MVAPICH2 and Arm's Scalable Vector Extension

> John Linford <john.linford@arm.com> 24 August 2020

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Schedule

https://gitlab.com/arm-hpc/training/mug20

- [5] Introduction to Arm in HPC
 - Training cluster coordinates
 - MVAPICH2 quick start
- [30] Arm Allinea Studio and Arm Forge
 - DDT Debugger
 - MAP Profiler
 - Forge Remote connect
 - Hands-on demo
- [20] SVE Introduction
 - Vector length agnostic (VLA) programming
 - Tools and approaches for programming SVE
- [2] Summary

Download slides and hands-on materials here!

Cluster access and hands-on materials

gitlab.arm-hpc.org/training/mug20

Accessing the Cluster

- ssh student@cluster.arm-hpc.org
- Password: Tr@ining!
- A private AWS Graviton 2 instance with all the necessary software installed and configured will be allocated for you.
- Introductory hands-on materials are in \$HOME.
- Instructions on how to connect to your AWS instance via Forge Remote Client are given when you log in.





arm

MVAPICH2 on AWS Graviton 2 Quick Start

module load Neoverse-N1/RHEL/7/gcc-9.3.0/mvapich2/2.3.4

or, to use MVAPICH2 with Arm Compiler

module load Neoverse-N1/RHEL/7/arm-linux-compiler-20.2/mvapich2/2.3.4

- module load Generic-AArch64/RHEL/7/forge/20.1
- module load Generic-AArch64/RHEL/7/arm-instruction-emulator/20.0
- See "Slides" folder or "README" files for instructions
- Hands-on code examples:
 - 01_Compiler
 - 02_Forge
 - 03_ArmIE
 - 04_ACLE

Install Arm Forge Remote Client

https://developer.arm.com/tools-and-software/server-and-hpc/downloads/arm-forge

- Go to the <u>Arm Forge download page</u>
- Linux:
 - Use the full Arm Forge installation package
 - For Ubuntu 19.04 and later, also install libncurses5 and libtinfo5
- Windows and macOS:
 - Navigate to the bottom of the page and use the appropriate link

Note: • For Centos, Fedora, and Sc	ientific Linux, use a Red Hat Enterprise Linux build
Intel Xeon Phi (Knight's Landing)	RHEL 7.0 (and later) 64-bit (AMD/Intel) SLES 12:0 (and later) 64-bit (AMD/Intel)
Cray X-series	SLES 15.0 (and later) 64-bit (AMD/Intel) SLES 12.0 (and later) 64-bit (AMD/Intel) SLES 15.0 (and later) 64-bit (Arm) SLES 12.3 (and later) 64-bit (Arm)
Ubuntu	13:04 (and later) 64-bit (AMD/Intel) 18:04 (and later) 64-bit (AMD/Intel) 16:04 (and later) 64-bit (Arm) 16:04 (and later) 64-bit (Arm) Note: For Ubuntu 19:04 (and later), you must install the libncurses5 and libtinfo5 packages on your system.
SuSE Linux Enterprise Server	15.0 (and later) 64-bit (AMD/Intel) 12.0 (and later) 64-bit (AMD/Intel) 15.0 (and later) 64-bit (Arm) 12.3 (and later) 64-bit (Arm) 18.04 (and later) 64-bit (Arm)
Red Hat Enterprise Linux	8.0 (and later) 64-bit (Arm) 7.6 (and later) 64-bit (Arm) 7.2 (and later) 64-bit (POWER little-endian)

Remote Client Downloads

 Windows and OS/X builds are remote clients only. They allow you to connect to a cluster and debug or profile on it but do not let you debug and profile programs running on Windows or OS/X. All Linux installs also function as remote clients.

 Platform
 Operating System/Distribution Version

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 Windows
 Vindows 7 (and later) 64-bit (AMD/Intel)

 Windows
 Note: For more information conclusion for the second client on Windows

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Arm in HPC

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Arm Neoverse Momentum in Servers & HPC



| + | | Applic
Open-source, owned, c | ommercial ISV codes, | Debuggers &
Profilers | | |
|---|--|---|--|--|---------------------------------|---------------------------------------|
| + | | Containers, In
Singularity, PodMar | Arm Forge (DDT, MAP),
Rogue Wave, HPC Toolkit,
Scalasca, Vampir, TAU, | SLURM, IBM | BT | |
| + | | Mellanox IB/OFED/HPC-X, | Middleware
OpenMPI, MPICH, MVAPICH2, OpenSH | IMEM, OpenUCX, HPE MPI | eduler
LSF, Altair PB | ISTER N
ight, HPE CM |
| + | OEM/ODM's
Cray-HPE, ATOS-Bull,
Fujitsu, Gigabyte, | Compilers
Arm, GNU, LLVM, Clang, Flang,
Cray, PGI/NVIDIA, Fujitsu, | + + +
Libraries
ArmPL, FFTW, OpenBLAS,
NumPy, SciPy, Trilinos, PETSc,
Hypre, SuperLU, ScaLAPACK, | Filesystems
BeeGFS, Lustre, ZFS,
HDF5, NetCDF, | S
S Pro, | lanageme
U, xCat, Warewulf, |
| | Silicon | OS
RHEL, SUSE, CentOS, Ubuntu, | | | | nt |
| F | Suppliers
Marvell, Fujitsu,
Mellanox, NVIDIA, | A | Arm Server Ready P
Standard firmware and RA | latform | | |

A Rich and Growing Application Ecosystem

| GROMACS | LAMMPS | CESM2 | MrBayes | Bowtie | DeepBench |
|-----------|---------------------|----------|---------------|----------|-----------|
| NAMD | TensorFlow | ParaView | SIESTA | UM | AMBER |
| WRF | Quantum
ESPRESSO | VASP | Torch | MILC | GEANT4 |
| OpenFOAM | GAMESS | Mahout | Vislt | DL-Poly | NEMO |
| Weka | BLAST | NWCHEM | Abinit | BWA | QMCPACK |
| + + | + + | + | + + | + | + + |
| Chem/Phys | Weather | CFD | Visualization | Genomics | AI/ML |
| | | | | | |

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Fujitsu's Fugaku: Fastest Supercomputer in the World



500 CERTIFICATE TOP The List.

Supercomputer Fugaku - A64FX 48C 2.2GHz, Tofu interconnect D

RIKEN Center for Computational Science, Japan

is ranked

No. 1

among the World's TOP500 Supercomputers

with 415.53 Pflop/s Linpack Performance

in the 55th TOP500 List published at the ISC 2020 Digital

Conference on June 22nd, 2020.

Congratulations from the TOP500 Editors

Erich Strohmaier NERSC/Berkeley Lab

Jack Dongarra University of Tennessee

Horst Simon

Martin Meuer NERSC/Berkeley Lab Prometeus

WHIL MAURE

March Maries



1. High-Performance Arm CPU A64FX in HPC and AI Areas FUITSU



Architecture features

| ISA | Armv8.2-A (AArch64 only) SVE (Scalable Vector Extension) | |
|--------------|--|--|
| SIMD width | 512-bit | |
| Precision | FP64/32/16, INT64/32/16/8 | |
| Cores | 48 computing cores + 4 assistant cores (4 CMGs) | |
| Memory | HBM2: Peak B/W 1,024 GB/s | |
| Interconnect | TofuD: 28 Gbps x 2 lanes x 10 ports | |

Peak performance (Chip level)



Vanguard Astra by HPE

- 2,592 HPE Apollo 70 compute nodes
 - 5,184 CPUs, 145,152 cores, 2.3 PFLOPs (peak)
- Marvell ThunderX2 ARM SoC, 28 core, 2.0 GHz
- Memory per node: 128 GB (16 x 8 GB DR DIMMs)
 - Aggregate capacity: 332 TB, 885 TB/s (peak)

- Mellanox IB EDR, ConnectX-5
 - 112 36-port edges, 3 648-port spine switches
- Red Hat RHEL for Arm
- HPE Apollo 4520 All-flash Lustre storage
 - Storage Capacity: 403 TB (usable)
 - Storage Bandwidth: 244 GB/s



AWS Graviton 2 - an Arm Server Processor



Graviton Processor



First Arm-based processor available in major cloud



Built on 64-bit Arm Neoverse cores with AWS-designed silicon using 16nm manufacturing technology



Up to 16 vCPUs, 10Gbps enhanced networking, 3.5Gbps EBS bandwidth

Graviton 2 Processor



7x performance, 4x compute cores, and 5x faster memory



Built with 64-bit Arm Neoverse cores with AWS-designed silicon using 7nm manufacturing technology



Up to 64 vCPUs, 25Gbps enhanced networking, 18Gbps EBS bandwidth

AWS Graviton 2 for HPC workloads

The c6g instances have outstanding price/performance as compared to similar x86 instances

- The AWS Graviton 2 implements the Arm Neoverse N1
- Up to 40% improved price/performance over x86 instances









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Performance

Engineering

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Identifying and resolving performance issues



Arm Performance Engineering Tools Ecosystem

See the http://www.vi-hps.org/tools/ for an excellent view of the tools ecosystem.



Arm Allinea Studio: HPC Development Solutions from Arm

Commercially supported tools for HPC developers



• Profiler



Arm Forge = DDT + MAP + Performance Reports

An interoperable toolkit for debugging and profiling



Commercially supported by Arm





The de-facto standard for HPC development

- Available on the vast majority of the Top500 machines in the world
- Fully supported by Arm on x86, IBM Power, Nvidia GPUs, etc.

State-of-the art debugging and profiling capabilities

- Powerful and in-depth error detection mechanisms (including memory debugging)
- Sampling-based profiler to identify and understand bottlenecks
- Available at any scale (from serial to petaflopic applications)

Easy to use by everyone

- Unique capabilities to simplify remote interactive sessions
- Innovative approach to present quintessential information to users

Arm Forge – DDT Parallel Debugger



Arm DDT Feature Details

- Scalable debugging of threaded codes (with OpenMP or pthreads)
 - Support for asynchronous thread control
- GPU debugging
- Memory debugging: error detection, OOB detection (guard pages), leak detection
- Single or multiple Linux corefiles.
 - Core files are well supported on aarch64,
 - Can selectively dump core memory from specified processes or threads.
 - Standard core files as generated by all major Linux distributions. Lightweight core files not supported.
- Scalable launch via many vendor specific launch infrastructures, e.g. PMIx or MPIR

DDT: Production-scale debugging

Isolate and investigate faults at scale

- Which MPI rank misbehaved?
 - Merge stacks from processes and threads
 - Sparklines comparing data across processes
- What source locations are related to the problem?
 - Integrated source code editor
 - Dynamic data structure visualization
- How did it happen?
 - Parse diagnostic messages
 - Trace variables through execution
- Why did it happen?
 - Unique "Smart Highlighting"
 - Experiment with variable values

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Process Groups
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Update
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MPI COMMUN | 256
Queue
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149 | From (global)
405 | w Diagram Key
Update
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MPI COMMUN
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Memory Debugging Menu in Arm DDT

| Run | |
|---|------------------|
| Run: mpirun -n 8 ./mmult2_c.exe | Details |
| Command: mpirun -n 8 ./mmult2_c.exe | |
| □ OpenMP | Details |
| CUDA: Track allocations: enabled, Detect invalid accesses: disabled | Details |
| ☑ Track GPU allocations (also enables CPU memory debugging) | |
| Detect invalid accesses (memcheck) | |
| ☑ Memory Debugging: Fast, 1 guard page after, Backtraces, Preload | Details |
| Plugins: none | Details |
| Help Options | <u>R</u> un Quit |

MVAPICH2 Compatibility Hint

Set the environment variable **MV2_ON_DEMAND_THRESHOLD** to the maximum job size you expect. This setting should *not* be a system wide default; it should be set as needed.

When manual linking is used, untick "Preload" box

| <u> P</u> reload the memory debugging library <u>L</u> anguage: C++, threads ↓ | | | | | |
|---|-----------|------------|-----------------|--|--|
| Note: Preloading only works for programs linked against shared libraries. If your program is statically linked, you must relink it against the dmalloc library manually.
Heap Debugging | | | | | |
| Fast | Balanced | Thoroug | gh Custom | | |
| Enabled Checks: | basic | <u>M</u> | ore Information | | |
| Heap O <u>v</u> erflow/Underflow Detection | | | | | |
| $\blacksquare \underline{A}$ dd guard pages to detect out of bounds heap access | | | | | |
| <u>G</u> uard pages: $1 \xrightarrow{\bullet} A\underline{d}d$ guard pages: After \diamond | | | | | |
| Ad <u>v</u> anced | | | | | |
| \Box <u>Check heap consistency every</u> 100 $\frac{1}{\sqrt{2}}$ heap operations | | | | | |
| Store stack <u>b</u> acktraces for memory allocations | | | | | |
| □ <u>O</u> nly enable for these processes: | | | | | |
| 0 | 100% Sele | ect All x2 | x0.5 1% | | |
| Help | | | OK Cancel | | |



Run DDT in offline mode

Run the application under DDT and halt or report when a failure occurs.

- You can run the debugger in non-interactive mode
 - For long-running jobs
 - For automated testing, continuous integration...
- To do so, use the following arguments:
 - \$ ddt --offline --output=report.html mpirun ./jacobi_omp_mpi_gnu.exe
 - --offline enable non-interactive debugging
 - --output specifies the name and output of the non-interactive debugging session
 - Html
 - Txt
 - Add --mem-debug to enable memory debugging and memory leak detection

```
ddt --offline -o jacobi_omp_mpi_gnu_debug.txt \
    --trace-at _jacobi.F90:83,residual \
    srun ./jacobi_omp_mpi_gnu.exe
```

The Arm Forge GUI and where to run it

Forge includes a provide powerful GUI that can be run in a variety of configurations.



DDT somewhere over the Pacific at 41,000ft and 550MPH



arm

Install Arm Forge Remote Client

https://developer.arm.com/tools-and-software/server-and-hpc/downloads/arm-forge

- Go to the <u>Arm Forge download page</u>
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| Red Hat Enterprise Linux | 8.0 (and later) 64-bit (Arm)
7.6 (and later) 64-bit (Arm) |
|-----------------------------------|---|
| | 7.2 (and later) 64-bit (POWER little-endian) |
| | 15.0 (and later) 64-bit (AMD/Intel)
12.0 (and later) 64-bit (AMD/Intel) |
| SuSE Linux Enterprise Server | 15.0 (and later) 64-bit (Arm)
12.3 (and later) 64-bit (Arm) |
| | 18.04 (and later) 64-bit (AMD/Intel)
16.04 (and later) 64-bit (AMD/Intel) |
| Ubuntu | 18.04 (and later) 64-bit (Arm)
16.04 (and later) 64-bit (Arm) |
| | Note: For Ubuntu 19.04 (and later), you must install the libncurses5 and libtinfo5 packages on your system. |
| | SLES 15.0 (and later) 64-bit (AMD/Intel)
SLES 12.0 (and later) 64-bit (AMD/Intel) |
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Remote Client Downloads

 Windows and OS/X builds are remote clients only. They allow you to connect to a cluster and debug or profile on it but do not let you debug and profile programs running on Windows or OS/X. All Linux installs also function as remote clients.

 Platform
 Operating System/Distribution Version

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 Windows
 Vindows 7 (and later) 64-bit (AMD/Intel)

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Launching the Forge Remote Client

The remote client is a stand-alone application that runs on your local system

- Open Forge Remote Client
- Create a new connection: Remote Launch → Configure → Add
 - Hostname: <username>@<hostname>
 - -student0XX@cluster.arm-hpc.org
 - Remote installation directory: </path/to/arm-forge/X.Y/>
 _/opt/arm/forge/20.1
- Connect!

Remote connect

arm FORGE

arm DDT

arm MAP <u>R</u>UN Run and debug a program.

ATTACH Attach to an already running program.

OPEN CORE Open a core file from a previous run.

MANUAL LAUNCH (ADVANCED) Manually launch the backend yourself.

OPTIONS

Remote Launch: Configure...

<u>Q</u>UIT

| Configure Remote Connections Imars-rhel7 Immediate Statistics Connection Name: oxp09-nnm08@login.ace.hartree.stfc.ac.uk oxp09-nnm08@ace-login Host Name: oxp09-nnm08@login.ace.hartree.stfc.ac.uk oxp09-nnm08@ace-login How do I connect via a gateway (multi-hop)? Remote Installation Directory: /opt/ohpc/pub/utils/arm-forge/18.1.2/ Remote Script Optional Always look for source files locally Test Remote Launce | |
|---|----|
| Mars-rhel7 Add Immediate And Connects (allineas forme - 7.0. Redhat - 7.0.x86) Add Remote Launch Settings Add Connection Name: oxp09-nnm08@login.ace.hartree.stfc.ac.uk oxp09-nnm08@ace-login Host Name: oxp09-nnm08@login.ace.hartree.stfc.ac.uk oxp09-nnm08@ace-login How do I connect via a gateway (multi-hop)? Remote Installation Directory: /opt/ohpc/pub/utils/arm-forge/18.1.2/ Remote Script Optional Add | |
| Remote Launch Settings Connection Name: oxp09-nnm08@login.ace.hartree.stfc.ac.uk oxp09-nnm08@ace-login Host Name: oxp09-nnm08@login.ace.hartree.stfc.ac.uk oxp09-nnm08@ace-login How do I connect via a gateway (multi-hop)? Remote Installation Directory: /opt/ohpc/pub/utils/arm-forge/18.1.2/ Remote Script Optional Image: Always look for source files locally Test Remote Launce | |
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| Remote Installation Directory: /opt/ohpc/pub/utils/arm-forge/18.1.2/ Remote Script Optional Image: Always look for source files locally Image: Test Remote Launce Test Remote Launce Image: Test Remote Launce | |
| Remote <u>S</u> cript Optional Always look for source files locally Test Remote Launce | |
| Always look for source files locally | |
| Test Remote Launc | |
| | :h |
| | |
| Help OK Cancel | |
| | |
| 😣 💷 Test Remote Launch | |
| Remote Launch test completed successfully. | |
| Hostname: ace-login
OS: CentOS Linux release 7.4.1708 (AltArch)
Version: 18.1.2 | |
| Show Terminal >> | |
| ОК | |

arm

Arm MAP: Production-scale application profiling

Identify bottlenecks and rewrite code for better performance

- Run with the representative workload you started with
- Measure all performance aspects with Arm Forge Professional

Examples:

\$> map -profile mpirun -n 48 ./example

| Profiled: clover_leaf on 32 processes, 4 nodes, 32 cores (1 per process) Sampled from: Wed Nov 9 2016 15:28:37 (UTC) for 309.1s | Hide Metrics |
|---|--|
| Application activity | |
| Iterations / s ^{NO}
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Mana dan kanakan kanakan kanakan kanakan dan dan kanakan kanakan kanakan kanakan kanakan kanakan kanakan kanaka |
| Grind time | |
| Step time 1300 | In the dependence for |
| 15:28:37-15:33:46 (309.138s): Main thread compute 0.2 %, OpenMP 80.0 %, MPI 19.7 %, OpenMP overhead 0.1 %, Sleeping 0.1 % | Zoom 📲 🗮 💿 |
| ™ hydro.190 x | Time spent on line 75 |
| 3.2% 73 CALL flux_calc() | Breakdown of the 51.2% time spent on this line: Eventing instructions 0.0% |
| 51.2% T5 CALL advection() | Calling other functions 100.0% |
| 3.3% 77 CALL reset_field() | - |
| Input/Output Project Files OpenMP Stacks OpenMP Regions Functions
OpenMP Stacks | 0.9 |
| Total core time A MPI Overhead Function(s) on line | • |
| ie / clover_leat
i∈hydro | 2 |
| 01.2% 02% 01% -dovector_module_tadvector
22.2% 0.2% -0.1% istimation_module_timaten | |

| Profiled: My_code.exe on 64 proce | ises Started: Fri Sep 20 14:59:09 2013 Runtime: 35s Time in MPI: 45% | Hide Metrics |
|--|--|----------------|
| Memory usage (M)
9.4 - 777.9 (454.6 avg | | |
| MPI call duration (ms)
0 - 5,575.1 (341.0 avg | | |
| CPU floating-point (%)
0 - 90 (8.2 avg) | | |
| 14:59:09-14:59:44 (range 34.77 | 3s): Mean Memory usage 454.6 M; Mean MPI call duration 341.0 ms; Mean CPU floating-point 8.2 %; | Metrics, Reset |
| My_code.f90 | | |
| | 87 module wall_excitationn | Ê |
| | 100 MODULE EXCITATION | |
| | 102
103 ⊞ module derivativee | |
| | 140 !
141 ! MAIN CODE | |
| | | |
| | 143 D program Vel Vort 30 FP | |
| | 145 use wall excitation | |
| | 146 implicit none | |
| | 147 include 'mpif.h' | |
| | 18 double precision :: max_omx_dt,max_omy_dt,max_omz_dt,t,time_cal | |
| | 149 integer :: option, J, J, K, nn, Twent, Count_max, Counter, 105, next_file_at, w_cnt(1:4)
character#30 str file type str t num 2 str | |
| | 151
151 | |
| <0.1% | 152 call MPI_INIT(ierr) | |
| | 153 call MPI_COMM_SIZE(MPI_COMM_WORLD,npro,ierr) | |
| <u>ا ا</u> | | <u>۱</u> |
| Input/Output Project Files Pa | rallel Stark View | |
| Parallel Stack View | und start from | đ× |
| Total Time | MPI Function(s) on line Source Posi- | tion |
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| 63.0% | 31.4% Time_integration call time_integration My_ | ode.f90:330 |
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Arm MAP Overview

A lightweight sampling-based profiler for large scale jobs

Core Features

- MAP is a sampling based scalable profiler
 - Built on same framework as DDT
 - Parallel support for MPI, OpenMP
 - Designed for C/C++/Fortran
- Designed for simple 'hot-spot' analysis
 - Stack traces
 - Augmented with performance metrics
- Lossy sampler
 - Throws data away 1,000 samples / process
 - Low overhead, scalable and small file size

Performance Metrics

- Time classification
 - Based on call stacks
 - MPI, OpenMP, I/O, Synchronization
- Feature-specific metrics
 - MPI call and message rates
 - (P2P and collective bandwidth)
 - I/O data rates (POSIX or Lustre)
 - Energy data (IPMI or RAPL for Intel)
- Instruction information (hardware counters)
 - x86 instruction breakdown + PAPI
 - aarch64 perf metric for hardware counters

Hardware Performance Metrics on Arm

MAP uses perf or PAPI to gather data.

- On x86 MAP reports on instruction mix
 - CPU, vectorization, memory, etc
 - Arm are researching ways to provide the same
- Instruction activity via perf
 - Harder to read / action
 - Raw rates presented not interpolated



Python Profiling

From 19.1

New support for Python applications

- Native Python
- Cython Interpreter
- Called C/C++ code



Custom metrics interface

- MAP supports the development of user metrics
- We provide a custom metric interface
 - API for safe calls to common functions
- Let's you develop your own metrics of interest
 - Link to application metrics (units / s, error values)
 - Link to libraries (specialist communication or I/O)
 - System metrics (custom energy monitors)
- Integrates directly into MAP and Performance Reports
 - XML files for aggregation methods
- Need to consider overheads and thread safety

Arm Performance Reports

A high-level view of application performance with "plain English" insights

| Command:
PERFORMANCE
REPORTS
Resources:
Memory:
Tasks:
Machine:
Start time:
Total time:
Full path: | mpiexec.hydra -host node-1,node-2 -map-by
socket -n 16 -ppn 8 ./Bin/low_freq///Src//hydro
-i
./Bin/low_freq////Input/input_250x125_corner.nml
2 nodes (8 physical, 8 logical cores per node)
15 GiB per node
16 processes, OMP_NUM_THREADS was 1
node-1
Thu Jul 9 2015 10:32:13
165 seconds (about 3 minutes)
Bin//Src | I/O
A breakdown of the 16.2% I/O time:
Time in reads 0.0%
Time in writes 100.0%
Effective process read rate 0.00 bytes/s
Effective process write rate 1.38 MB/s |
|---|--|--|
| Summary: hydro | is MPI-bound in this configuration | Most of the time is spent in write operations with a very low
effective transfer rate. This may be caused by contention for the
filesystem or inefficient access patterns. Use an I/O profiler to
investigate which write calls are affected. |



This is **very low**; focus on improving MPI or I/O performance first Time spent in MPI calls. High values are usually bad. This is **high**; check the MPI breakdown for advice on reducing it

Time spent in filesystem I/O. High values are usually bad. This is **average**; check the I/O breakdown section for optimization advice

Arm Performance Reports Metrics

Lowers expertise requirements by explaining everything in detail right in the report.


Arm Forge and MVAPICH2

- To use DDT's memory debugging features, set the environment variable MV2_ON_DEMAND_THRESHOLD to the maximum job size you expect. This setting should not be a system wide default; it should be set as needed.
- To use mpirun_rsh with DDT, from File → Options go to the System page, check Override default mpirun path and enter mpirun_rsh. You should also add – hostfile <hosts>, where <hosts> is the name of your hosts file, within the mpirun_rsh arguments field in the Run window.
- To enable message Queue Support MVAPICH2 must be compiled with the flags --enable-debug --enable-sharedlib. These are not set by default.
- MVAPICH2 MPI programs cannot be started using Express Launch syntax.
 - Do use: "ddt ./a.out" and configure MPI launch parameters in the GUI.
 - Don't use: "ddt mpirun <mpi_args> ./a.out"

Hands-on demo

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Orm SVE: The Scalable Vector Extension

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What makes it a <u>Scalable</u> Vector Extension?

• There is no preferred vector length

- The vector length (VL) is a hardware choice, 128-2048b, in increments of 128b
- A Vector Length Agnostic (VLA) programming adjusts dynamically to the available VL

• SVE addresses traditional barriers to auto-vectorization

- Software-managed speculative vectorization of uncounted loops
- Extract more data-level parallelism (DLP) from existing C/C++/Fortran source code

• SVE is a new approach to vectorization, not an iteration on existing ISAs (e.g. NEON)

- SVE is a separate, optional extension with a new set of instruction encodings
- Initial focus is <u>HPC</u> and general-purpose server, not media/image processing







SVE ISA does not mandate a single, fixed vector length

The vector length is **LEN x 128-bit** up to 2048

- There is no preferred vector length
- No need to recompile
- No need to rewrite hand-coded SVE assembler or C intrinsics
- The programmer's intent is expressed in the binary → easier to optimize
- **Predicate Registers** indicate active vector lanes



SVE vs Traditional ISA

How do we compute data which has ten chunks of 8-bytes?

Aarch64 (scalar)

Ten iterations over an 8-byte register

NEON (128-bit vector engine)

Four iterations over a 16-byte register + two iterations of a drain loop over a 8-byte register

SVE (VLA vector engine)

Three iterations over a 32-byte VLA register with an adjustable predicate



How can you program when the vector length is unknown?

SVE provides features to enable VLA programming from the assembly level and up



Per-lane predication

Operations work on individual lanes under control of a predicate register.

| for (i | = 0; | i < | n; | ++i) |
|---------|------|-----|----|------|
| INDEX i | n-2 | n-1 | n | n+1 |
| CMPLT n | 1 | 1 | 0 | 0 |

Predicate-driven loop control and management Eliminate scalar loop heads and tails by processing partial vectors.



Vector partitioning & software-managed speculation

First Faulting Load instructions allow memory accesses to cross into invalid pages.

How do you count by vector width?

No need for multi-versioning: one increment to rule all vector sizes

ld1w z1.s, p0/z, [x0,x4,ls1 2] // p0:z1=x[i] ld1w z2.s, p0/z, [x1,x4,ls1 2] // p0:z2=y[i] fmla z2.s, p0/m, z1.s, z0.s stlw z2.s, p0, [x1,x4,ls1 2]

// p0?z2+=x[i]*a // p0?y[i]=z2

incw x4

// i+=(VL/32)

"Increment x4 by the number of 32-bit lanes (w) that fit in a VL."

Initialization when vector length is unknown

- Vectors cannot be initialized from compile-time constant, so...
 - INDEX Zd.S,#1,#4 : Zd = [1, 5, 9, 13, 17, 21, 25, 29]
- Predicates cannot be initialized from memory, so...
 - PTRUE Pd.S, MUL3 : Pd = [T, T, T, T, T, T, F, F]
- Vector loop increment and trip count are unknown at compile-time, so...
 - INCD Xi : increment scalar Xi by # of 64b dwords in vector
 - WHILELT Pd.D,Xi,Xe
- : next iteration predicate Pd = [while i++ < e]
- Vectors stores to stack must be dynamically allocated and indexed, so...
 - ADDVL SP,SP,#-4
- : decrement stack pointer by (4*VL)
- STR Zi, [SP,#3,MUL VL] : store vector Z1 to address (SP+3*VL)

SVE Registers

Layout

Scalable vector registers

- Z0-Z31 extending NEON's 128-bit v0-v31.
- Packed DP, SP & HP floating-point elements.
- Packed 64, 32, 16 & 8-bit integer elements.

Scalable predicate registers

- P0-P15 predicates for loop / arithmetic control.
- 1/8th size of SVE registers (1 bit / byte).
- FFR first fault register for software speculation.



Predicates: Active Lanes vs Inactive Lanes

Predicate registers track lane activity

- 16 predicate registers (PO-P15)
- 1 predicate bit per 8 vector bits (lowest predicate bit per lane is significant)
- On load, active elements update the destination
- On store, inactive lanes leave destination unchanged (p0/m) or set to 0's (p0/z)



SVE supports vectorization in complex code

Right from the start, SVE was engineered to handle codes that usually won't vectorize



Gather-load and scatter-store

Loads a single register from several non-contiguous memory locations.



Extended floating-point horizontal reductions

In-order and tree-based reductions trade-off performance and repeatability.

A64FX: Spec Summary

- Arm SVE, high performance and high efficiency
 - DP performance 2.7+ TFLOPS, >90%@DGEMM
 - Memory BW 1024 GB/s, >80%@STREAM Triad



CMG: Core Memory Group NOC: Network on Chip

| | A64FX |
|-------------------------|------------------|
| ISA (Base, extension) | Armv8.2-A, SVE |
| Process technology | 7 nm |
| Peak DP performance | > 2.7+ TFLOPS |
| SIMD width | SVE 512-bit |
| # of cores | 48 + 4 |
| Memory capacity | 32 GiB (HBM2 x4) |
| Memory peak bandwidth | 1024 GB/s |
| PCIe | Gen3 16 lanes |
| High speed interconnect | TofuD integrated |



Post-K performance evaluation

• Himeno Benchmark (Fortran90)



SC18, https://dl.acm.org/citation.cfm?id=3291728

CIM Programming Tools for SVE

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SVE Programming Approaches

Libraries > Autovectorization > compilers directives > intrinsics > assembly

- Libraries:
 - ArmPL supports SVE!
- Compilers:
 - Auto-vectorization: GCC, Arm Compiler for HPC, Cray, Fujitsu
 - Compiler directives, e.g. OpenMP
 - #pragma omp parallel for simd
 - #pragma vector always
- Intrinsics:
 - <u>Arm C Language Extensions for SVE</u>
 - Arm Scalable Vector Extensions and Application to Machine Learning
- Assembly:
 - Full ISA Specification: <u>The Scalable Vector Extension for Armv8-A</u>
 - Lots of worked examples: <u>A Sneak Peek Into SVE and VLA Programming</u>

SVE Support in OSS

Over four years of active, ongoing development

Arm actively posting SVE open source patches upstream
Beginning with first public announcement of SVE at HotChips 2016



- Available upstream
- Since GNU Binutils-2.28
- Since GCC 8:
- Since LLVM 7:
- Since QEMU 3:
- Since GDB 8.2

- Released Feb 2017, includes SVE assembler & disassembler Full assembly, disassembly and basic auto-vectorization Full assembly, disassembly User space SVE emulation HPC use cases fully included
- Constant upstream review
 - <u>LLVM</u>:
 - <u>Linux kernel</u>:

Since Nov 2016, as presented at LLVM conference Since Mar 2017, LWN article on SVE support

Automatic Arm support in latest version of all tools – peer to x86

Targeting SVE with Arm Compiler or GNU 8+

- Compilation targets a specific architecture based on an architecture revision
 - -mcpu=native -march=armv8.1-a+lse+sve
 - Learn more: <u>https://community.arm.com/.../compiler-flags-across-architectures-march-mtune-and-mcpu</u>
- -march=armv8-a
 - Target V8-a
 - Will generate NEON instructions
 - No SVE
- -march=armv8-a+sve
 - Will add SVE instruction generations
- Check the assembly (-S)
 - armclang++ -S -o code.s -Ofast -g -march=armv8-a+sve code.cpp
 - g++ -S -o code.s -Ofast -g -march=armv8-a+sve code.cpp

Arm Compiler Vectorization Control

OpenMP and clang directives are supported by the Arm Compiler for HPC

| C/C++ | Fortran | Description |
|--|----------------|--|
| <pre>#pragma ivdep</pre> | !DIR\$ IVDEP | Ignore potential memory dependencies and vectorize the loop. |
| <pre>#pragma vector always</pre> | !DIR\$ VECTOR | ALWAYS Forces the compiler to vectorize a loop irrespective of any potential performance implications. |
| <pre>#pragma novector</pre> | !DIR\$ NO VECT | TOR Disables vectorization of the loop. |
| | | |
| Clang compiler directives for C/C++ | | Description |
| <pre>#pragma clang loop vectorize(as</pre> | sume safetv) | Assume there are no aliasing issues in a loop. |

| 1 5 | 5 | • | | - | — | | 5 1 |
|---------|-------|------|---------|----------|-----------|------|---|
| #pragma | clang | loop | unroll_ | _count(_ | _value_) | | Force a scalar loop to unroll by a given factor. |
| #pragma | clang | loop | interle | ave_cou | unt(_valu | le_) | Force a vectorized loop to interleave by a factor |

Arm C Language Extensions (ACLE)

Intrinsics and other features for supporting Arm features in C and C++

- ACLE extends C/C++ with Arm-specific features
 - Predefined macros: ____ARM_ARCH_ISA_A64, ___ARM_BIG_ENDIAN, etc.
 - Intrinsic functions: __clz(uint32_t x), __cls(uint32_t x), etc.
 - Data types: SVE, NEON and FP16 data types

• ACLE for SVE enables VLA programming with ACLE

- Nearly one intrinsic per SVE instruction
- Data types to represent the size-less vectors used for SVE intrinsics
- Intended for users that...
 - Want to hand-tune SVE code
 - Want to adapt or hand-optimize applications and libraries
 - Need low-level access to Arm targets

SVE Intrinsics

When you don't know the vector length (VLA)

NEON: Fixed Width 128-bit (arm_neon.h)

Data types are encoded for 128-bit vectors:

float32x4_t va =
vld1q_f32(&a[i]);

• Load 4x32-bit floating point values

SVE: VLA (arm_sve.h)

Intrinsics are same for 128-bit -> 2048-bit vectors

svfloat32_t va = svld1(Pg, &a[i]);

- Load a vector of 32-bit floating point values
- Don't know how many variables are in there

SVE data types are defined as 'sizeless' (more restrictive)

Don't get confused:

svfloat32x4_t va4 = svld4(Pg, &a[i]);

A tuple of 4 svfloat32_t vectors



Vectorizing A Scalar Loop With ACLE a[:] = 2.0 * a[:]

Original Code

}

for (int i=0; i < N; ++i) {</pre>

```
a[i] = 2.0 * a[i];
```

128-bit NEON vectorization

int i;

```
// vector loop
for (i=0; (i<N-3) && (N&~3); i+=4) {
  float32x4_t va = vldlq_f32(&a[i]);
  va = vmulq_n_f32(va, 2.0);
  vstlq_f32(&a[i], va)</pre>
```

```
}
// drain loop
for (; i < N; ++i)
    a[i] = 2.0 * a[i];</pre>
```

This is NEON, <u>not</u> SVE!



Vectorizing A Scalar Loop With ACLE a[:] = 2.0 * a[:]

```
for (int i=0; i < N; ++i) {
    a[i] = 2.0 * a[i];
}</pre>
```

128-bit NEON vectorization

int i;

```
// vector loop
for (i=0; (i<N-3) && (N&~3); i+=4) {
  float32x4_t va = vldlq_f32(&a[i]);
  va = vmulq_n_f32(va, 2.0);
  vstlq_f32(&a[i], va)
}
// drain loop
for (; i < N; ++i)
  a[i] = 2.0 * a[i];</pre>
```

SVE vectorization

```
for (int i = 0 ; i < N; i += svcntw() )
{
    svbool_t Pg = svwhilelt_b32(i, N);
    svfloat32_t va = svld1(Pg, &a[i]);
    va = svmul_x(Pg, va, 2.0);
    svst1(Pg, &a[i], va);
}</pre>
```

Vectorizing A Scalar Loop With ACLE a[:] = 2.0 * a[:]

```
for (int i=0; i < N; ++i) {
    a[i] = 2.0 * a[i];
}</pre>
```

armclang -march=armv8.2-a+sve -O3 -S sve2.c

```
SVE vectorization
for (int i = 0; i < N; i += svcntw())
{
  svbool t Pg = svwhilelt b32(i, N);
  svfloat32 t va = svld1(Pg, &a[i]);
  va = svmul x(Pg, va, 2.0);
  svst1(Pg, &a[i], va);
}
```

Assembly

| | cmp | w0, #1 |
|----------|---------|---|
| | b.lt | .LBB0_3 |
| | mov | w8, wzr |
| .LBB0_2: | | |
| | whilelt | p0.s, w8, w0 |
| | sxtw | ×9, w8 |
| | ld1w | <pre>{ z0.s }, p0/z, [x1, x9, lsl #2]</pre> |
| | incw | x8 |
| | cmp | w8, w0 |
| | fmul | z0.s, p0/m, z0.s, #2.0 |
| | st1w | { z0.s }, p0, [x1, x9, lsl #2] |
| | b.lt | .LBB0_2 |
| | | |

.LBB0_3:

ret

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Cluster access and hands-on materials

gitlab.arm-hpc.org/training/mug20

Accessing the Cluster

- ssh student@cluster.arm-hpc.org
- Password: Tr@ining!
- A private AWS Graviton 2 instance with all the necessary software installed and configured will be allocated for you.
- Introductory hands-on materials are in \$HOME.
- Instructions on how to connect to your AWS instance via Forge Remote Client are given when you log in.



👔 johlin02 — student002@ip-172-31-27-255:~ — ssh student@cluster.arm-hpc Last login: Sat Nov 16 14:33:20 on ttys001 \$ ssh student@cluster.arm-hpc.org student@cluster.arm-hpc.org's password: Warning: No xauth data; using fake authentication data for X11 forwarding. Last login: Sat Nov 16 21:24:40 2019 from 38.109.203.254 http://www.arm-hpc.org Download materials at https://gitlab.com/arm-hpc/training/arm-sve-tools/-/archiv e/master/arm-sve-tools-master.tar.gz sinfo: error: If using PrologFlags=Contain for pam_slurm_adopt, either proctrack /cgroup or proctrack/cray_aries is required. If not using pam_slurm_adopt, plea se ignore error. Welcome! Your student ID is 002. Please Install Arm Forge Remote Client: https://developer.arm.com/tools-and-software/server-and-hpc/arm-architecture-too ls/downloads/download-arm-forge lost Name: student002@cluster.arm-hpc.org Remote Installation Directory: /opt/arm/forge/19.1.3 Password: Tr@ining!002 srun: error: If using PrologFlags=Contain for pam_slurm_adopt, either proctrack/ cgroup or proctrack/cray_aries is required. If not using pam_slurm_adopt, pleas e ignore error. [student002@ip-172-31-17-83 ~]\$

MVAPICH2 on AWS Graviton 2 Quick Start

module load Neoverse-N1/RHEL/7/gcc-9.3.0/mvapich2/2.3.4

or, to use MVAPICH2 with Arm Compiler

module load Neoverse-N1/RHEL/7/arm-linux-compiler-20.2/mvapich2/2.3.4

- module load Generic-AArch64/RHEL/7/forge/20.1
- module load Generic-AArch64/RHEL/7/arm-instruction-emulator/20.0
- See "Slides" folder or "README" files for instructions
- Hands-on code examples:
 - 01_Compiler
 - 02_Forge
 - 03_ArmIE
 - 04_ACLE

Install Arm Forge Remote Client

https://developer.arm.com/tools-and-software/server-and-hpc/downloads/arm-forge

- Go to the <u>Arm Forge download page</u>
- Linux:
 - Use the full Arm Forge installation package
 - For Ubuntu 19.04 and later, also install libncurses5 and libtinfo5
- Windows and macOS:
 - Navigate to the bottom of the page and use the appropriate link

| Note:
• For Centos, Fedora, and Sc | ientific Linux, use a Red Hat Enterprise Linux build |
|---------------------------------------|---|
| Intel Xeon Phi (Knight's Landing) | RHEL 7.0 (and later) 64-bit (AMD/Intel)
SLES 12:0 (and later) 64-bit (AMD/Intel) |
| Cray X-series | SLES 15.0 (and later) 64-bit (AMD/Intel)
SLES 12.0 (and later) 64-bit (AMD/Intel)
SLES 15.0 (and later) 64-bit (Arm)
SLES 12.3 (and later) 64-bit (Arm) |
| Ubuntu | 13:04 (and later) 64-bit (AMD/Intel) 18:04 (and later) 64-bit (AMD/Intel) 16:04 (and later) 64-bit (Arm) 16:04 (and later) 64-bit (Arm) Note: For Ubuntu 19:04 (and later), you must install the libncurses5 and libtinfo5 packages on your system. |
| SuSE Linux Enterprise Server | 15.0 (and later) 64-bit (AMD/Intel) 12.0 (and later) 64-bit (AMD/Intel) 15.0 (and later) 64-bit (Arm) 12.3 (and later) 64-bit (Arm) 18.04 (and later) 64-bit (Arm) |
| Red Hat Enterprise Linux | 8.0 (and later) 64-bit (Arm)
7.6 (and later) 64-bit (Arm)
7.2 (and later) 64-bit (POWER little-endian) |

Remote Client Downloads

 Windows and OS/X builds are remote clients only. They allow you to connect to a cluster and debug or profile on it but do not let you debug and profile programs running on Windows or OS/X. All Linux installs also function as remote clients.

 Platform
 Operating System/Distribution Version

 Mac OS/X
 High Sierra (10.13 and later) 64-bit (AMD/Intel)

 Windows
 Vindows 7 (and later) 64-bit (AMD/Intel)

 Windows
 Note: For more information conclusion for the second client on Windows

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Arm DDT cheat sheet

Start DDT interactively, remotely, or from a batch script.

- Load the environment module:
 - \$ module load forge
- Prepare the code:
 - \$ mpicc -OO -g myapp.c -o myapp.exe
 - \$ mpfort -**OO** -g myapp.f -o myapp.exe
- Start DDT in interactive mode:
 - \$ ddt mpirun -n 8 ./myapp.exe arg1 arg2 ...
- Or use reverse connect:
 - On the login node:
 - \$ ddt &
 - (or use the remote client)
 - Then, edit the job script to run the following command and submit:
 - **ddt --connect** mpirun -n 8 ./myapp.exe arg1 arg2 ...

DDT command line options

\$ ddt --help

```
Arm Forge 18.2.1 - Arm DDT
```

```
Usage: ddt [OPTION...] [PROGRAM [PROGRAM_ARGS]]
ddt [OPTION...] (mpirun|mpiexec|aprun|...) [MPI_ARGS] PROGRAM [PROGRAM_ARGS]
```

```
--connect
```

```
--attach=[host1:]pid1,[host2:]pid2... [PROGRAM]
--attach-mpi=MPI_PID [--subset=rank1,rank2,rank3,...] [PROGRAM]
--break-at=LOCATION[,START:EVERY:STOP] [if CONDITION]
--trace-at=LOCATION[,START:EVERY:STOP],VAR1,VAR2,...
--cuda
--mem-debug[=(fast|balanced|thorough|off)]
--mpiargs=ARGUMENTS
-n, --np, --processes=NUMPROCS
--nodes=NUMNODES
--procs-per-node=PROCS
--offline
```

-s, --silent

Reverse Connect (launch as a server and wait) attach to PROGRAM being run by list of host:pid attach to processes in an MPI program. set a breakpoint at LOCATION set a tracepoint at LOCATION enable CUDA configure memory debugging (defaults to fast) command line arguments to pass to mpirun specify the number of MPI processes configure the number of nodes for MPI jobs configure the number of processes per node run through program without user interaction don't write unnecessary output to the command line

Arm MAP cheat sheet

Generate profiles and view offline

- Load the environment module
 - \$ module load forge
- Prepare the code
 - \$ mpicc -O -g myapp.c -o myapp.exe
 - \$ mpfort -O -g myapp.f -o myapp.exe
- Offline: edit the job script to run Arm MAP in "profile" mode
 - \$ map --profile mpirun ./myapp.exe arg1 arg2
- View profile in MAP:
 - On the login node:
 - \$ map myapp_Xp_Yn_YYY-MM-DD_HH-MM.map
 - (or load the corresponding file using the remote client connected to the remote system or locally)

MAP command line options

\$ map --help
Arm Forge 18.2.1 - Arm MAP

Usage: map [OPTION...] [PROGRAM [PROGRAM_ARGS]]
map [OPTION...] (mpirun|mpiexec|aprun|...) [MPI_ARGS] PROGRAM [PROGRAM_ARGS]
map [OPTION...] [MAP_FILE]

--connect

Analysis of the CUDA kernel source code lines --cuda-kernel-analysis --list-metrics Display metrics IDs which can be explicitly enabled or disabled. --disable-metrics=METRICS Explicitly disable metrics specified by their metric IDs. --enable-metrics=METRICS Explicitly enable metrics specified by their metric IDs. --export=FILE.json Exports a specified .map file as JSON --export-functions=FILE Export all the available columns in the functions view to a CSV file (use --profile) --select-ranks=RANKS Select ranks to profile. --mpiargs=ARGUMENTS command line arguments to pass to mpirun -n, --np, --processes=NUMPROCS specify the number of MPI processes --nodes=NUMNODES configure the number of nodes for MPI jobs --procs-per-node=PROCS configure the number of processes per node run through program without user interaction --profile

Reverse Connect (launch as a server and wait for the GUI to connect)

Arm Performance Reports cheat sheet

Generate text and HTML reports from application runs or MAP files

- Load the environment module:
 - \$ module load reports
- Run the application:
 - **perf-report** mpirun -n 8 ./myapp.exe
- ... or, if you already have a MAP file:
 - **perf-report** myapp_8p_1n_YYYY-MM-DD_HH:MM.txt
- Analyze the results
 - \$ cat myapp_8p_1n_YYYY-MM-DD_HH:MM.txt
 - \$ firefox myapp_8p_1n_YYYY-MM-DD_HH:MM.html

Performance Reports command line options

\$ perf-report --help
Arm Performance Reports 18.2.1 - Arm Performance Reports

```
Usage: perf-report [OPTION...] PROGRAM [PROGRAM_ARGS]
perf-report [OPTION...] (mpirun|mpiexec|aprun|...) [MPI_ARGS] PROGRAM [PROGRAM_ARGS]
perf-report [OPTION...] MAP_FILE
```

| list-metrics | Display metrics IDs which can be explicitly enabled or disabled. |
|------------------------------------|--|
| <pre>disable-metrics=METRICS</pre> | Explicitly disable metrics specified by their metric IDs. |
| <pre>enable-metrics=METRICS</pre> | Explicitly enable metrics specified by their metric IDs. |
| mpiargs=ARGUMENTS | command line arguments to pass to mpirun |
| nodes=NUMNODES | configure the number of nodes for MPI jobs |
| -o,output=FILE | writes the Performance Report to FILE instead of an auto-generated name. |
| -n,np,processes=NUMPROCS | specify the number of MPI processes |
| procs-per-node=PROCS | configure the number of processes per node for MPI jobs |
| <pre>select-ranks=RANKS</pre> | Select ranks to profile. |
SVE Resources

http://developer.arm.com/hpc

- Porting and Optimizing Guides
 - For SVE: <u>https://developer.arm.com/docs/101726/0110</u>
 - For Arm in general: <u>https://developer.arm.com/docs/101725/0110</u>

• The SVE Specification

<u>Arm Architecture Reference Manual Supplement, SVE for ARMv8-A</u>

ACLE References and Examples

- ACLE: https://developer.arm.com/docs/101028/latest
- ACLE for SVE: https://developer.arm.com/docs/100987/latest
- Worked examples: <u>A Sneak Peek Into SVE and VLA Programming</u>
- Optimized machine learning: <u>Arm SVE and Applications to Machine Learning</u>