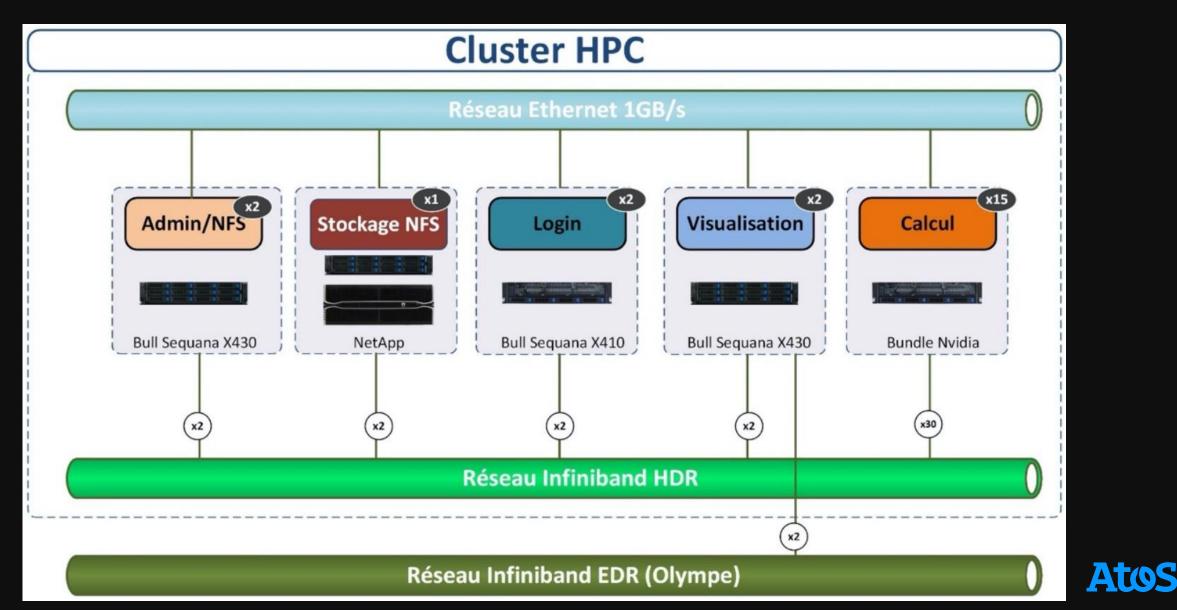
Turpan Architecture

Okba Hamitou





Turpan Architecture General



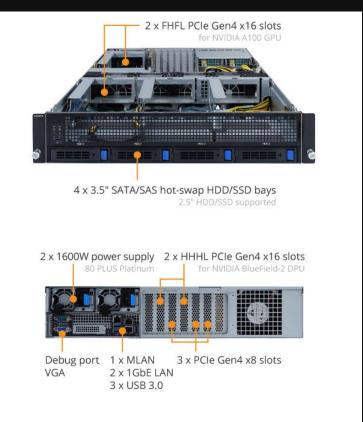
Turpan Architecture General

- Compute nodes
 - 15 Arm and Nvidia compute nodes, 1200 CPU cores, 30 GPU units
 - 1 Arm Ampere Q80-30 processor, 80 CPU cores, 3,0 GHz, RAM (8 x 64GB) 512GB
 - 2 NVIDIA A100-80GB GPU cards, 6912 CUDA cores, 80GB
- Login nodes
 - 2 Arm login nodes
 - 1 Arm Ampere Q80-30 processor, 80 CPU cores, 3,0GHz, RAM (8 x 32GB) 256GB
- Visualization nodes
 - 2 Intel x86 Visual Nodes
 - 2 Intel Icelake 6326 processors, 16 cores, 2.8GHz, RAM (16 x 32GB) 512GB
 - 2 NVIDIA A40-48GB GPU cards
- Storage
 - 1 NetApp E5760 + DE224C storage, 25TB with SSD, 350TB with HDD
 - 10 x 3.8 TB SSD, 3GB/s write, 8GB/s read
 - 60 x 8 TB HDD, 8GB/s write, 10GB/s read
- Network
 - Mellanox Infiniband HDR, 2 x 200 Gb/s



Turpan Architecture Processor : NVIDIA Arm HPC Developer kit

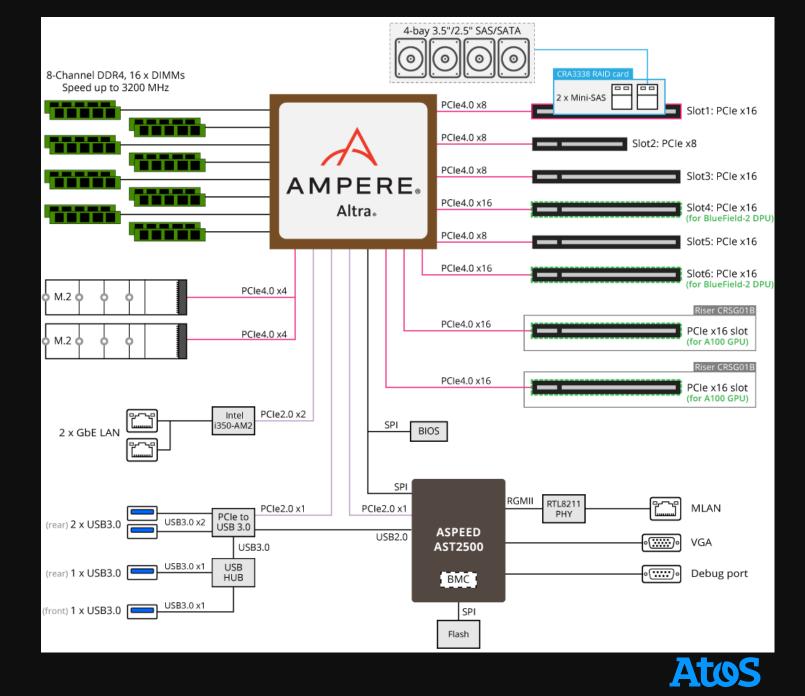
- Development platform for HPC and AI
- Applications porting from x86 to Arm with NVIDIA HPC and AI SDKs
- Enables experimentation and characterization of high-performance, NVIDIA-accelerated, Arm server-based system architectures





Turpan Architecture Processor design

- 1 Arm Ampere Q80-30 80c
- 8 channels DDR4 with 3200 MHz
 - 512 GB (8 x 64 GB)
- 2 Infiniband cards HDR
- 2 NVIDIA A100-80GB GPUs
- 1 local storage
 - HDD or SSD 6000 GB



Turpan Architecture Core description & features

- The Altra Processor Complex consists of 80 Processor Modules (PMDs)
- Each PMD contains a high-performance Altra core, each of which has
 - Neoverse N1
 - 3,0 GHz
 - Arm v8,2 architecture
 - Private 64 KB L1 I-cache,
 - Private 64 KB L1 D-cache,
 - Private 1 MB L2 cache.
 - Shared 32 MB System Level Cache (SLC) by all 80 PMDs,
- The Altra Processor Complex features include:
 - 128-bit double precision FPU
 - 2x full-width (128-bit wide) SIMD execution pipes
 - Coherent Mesh Interconnect (CMI)



Turpan Architecture NVIDIA GPU A100

- Since years ~2000, frequency scaling is over... We are now scaling cores !
- GPU is a massively multi-threaded many-cores architecture
- Thousands of threads executed in parallel
 - Kepler (K80) able to run 2048*13=26 624 threads
 - Pascal (P100) 2048*56=114 688 threads
 - Volta (V100) 2048*80=163 840 threads
 - Ampere (A100) 2048*108= 221 184 threads



GPU Features	NVIDIA Tesla P100	NVIDIA Tesla V100	NVIDIA A100
GPU Codename	GP100	GV100	GA100
GPU Architecture	NVIDIA Pascal	NVIDIA Volta	NVIDIA Ampere
GPU Board Form Factor	SXM	SXM2	SXM4
SMs	56	80	108
TPCs	28	40	54
FP32 Cores/SM	64	64	64
FP32 Cores/GPU	3584	5120	6912
FP64 Cores/SM (excl. Tensor)	32	32	32
FP64 Cores/GPU (excl. Tensor)	1792	2560	3456
INT32 Cores / SM	NA	64	64
INT32 Cores / GPU	NA	5120	6912
Tensor Cores / SM	NA	8	4 ²
Tensor Cores / GPU	NA	640	432
GPU Boost Clock	1480 MHz	1530 MHz	1410 MHz



Turpan Architecture Network

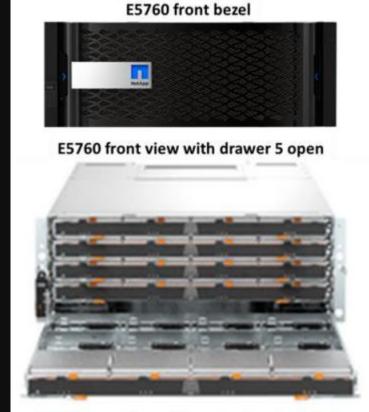
- Infiniband HDR based technology
- All equipments (login, visu, storage, service, etc...) are connected by one switch
- Compute nodes are connected to each other using two HDR links
- The topology is equivalent to Fat-Tree without blocking factor





Turpan Architecture Storage

- NFS type storage
 - 25 TB SSD type
 - 350 TB HDD type
- Hybrid storage type which enables fast response time with the SSD
 - SSD disks are used as cache to accelerate I/O operations



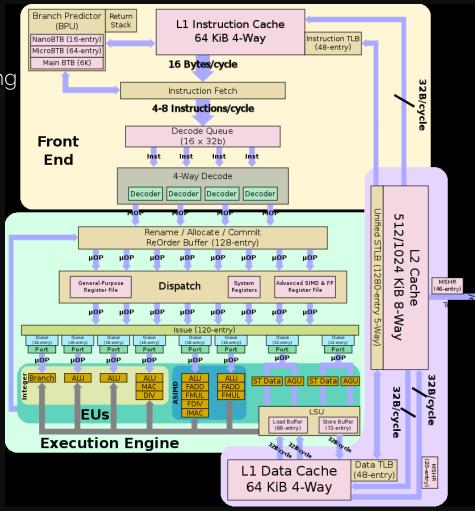
E5760 rear view with controllers installed





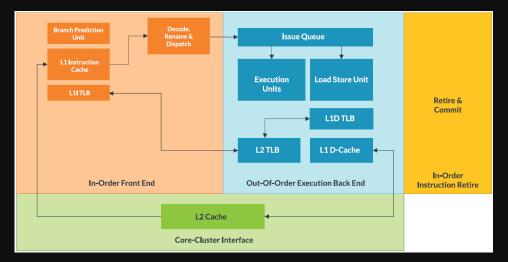
Turpan Architecture Core diagram

- The execution pipeline includes:
 - Integer execute unit that performs arithmetic and logical data processing operations.
 - Vector execute unit that performs Advanced SIMD and floating-point operations.



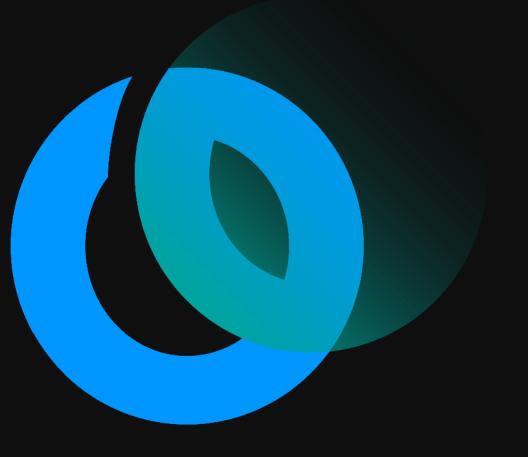
Turpan Architecture Core diagram

- The Back End of the CPU handles the execution of the micro-operations which are dispatched to the relevant execution units for processing.
- Neoverse N1 supports multiple execution units including the Branch unit, Load/Store unit and Arithmetic units including the advanced vector engines.
- The number of execution units and cycles taken for the execution of an instruction can vary per micro-architecture; therefore, instruction execution latency and throughput are implementation dependent.
- Once instruction execution is complete, the results are stored and committed in-order when dependencies are resolved.
- Neoverse N1 has
 - 4 integer execution units,
 - 2 Floating point/SIMD pipelines,
 - 2 load/store pipelines, which allows up to 8 micro-operations to be dispatched into the execution pipeline every cycle.



Turpan Supercomputer Software environment

Okba Hamitou





Access and data transfers

How to access, transfert, view data

- You must have a Mesonet account
 - Please refer to CALMIP Université de Toulouse for request
- Connect to Turpan
 - ssh your_login@turpanlogin[1,2].calmip.univ-toulouse.fr
- Data transfers (rsync [options] ORIGIN DESTINATION)
 - Always from outside the cluster
 - Get data from Turpan:

rsync -avP -e "ssh -p XXX" user@turpanlogin[1,2].calmip.univ-toulouse.fr:/path/to/data.tgz local_copy.tgz

• Get data to Turpan:

rsync -avP -e "ssh -p XXX" /path/to/data.tgz user@turpanlogin[1,2].calmip.univ-toulouse.fr:/path/to/directory/ local_copy.tgz

- Data Visualization
 - No need to transfer large data to your computer
 - Use the visualization node (refer to Turpan webpage for more information about it)



Disk spaces home/, work/, tmpdir/

- Home directory:
 - Dedicated to the installation of software and binaries,
 - Located in /users/\${GROUPE}/\${USER}" directory
 - Shortcut in environment variable \$HOME
- Work directory:
 - Dedicated to inputs and outputs,
 - Located in /work/\${PROJET}/\${USER}" directory
 - Shortcut in environment variable \$WORK

Temporary space

- Dedicated to temporary files
- Located in /tmpdir/\${USER}" directory
- Shortcut in environment variable \$SCRATCH}
- 200TB shared by all users and accelerated by an 8.5TB SSD cache.
- Files not accessed for more than 100 days are automatically deleted.

• Quotas on the different spaces

Quota	Groupe	User	File group	File user
home		10 Go		100 K
work	1 To		5 M	
tmpdir				5 M

Partitions Full, big, small, shared, visu

- small:
 - exclusive,
 - 2 jobs max,
 - no more than 6 nodes per job,
 - max walltime per job 4 hours
- big:
 - exclusive,
 - 1 job max,
 - no more than 13 nodes per job,
 - max walltime per job 2 hours
- full:
 - exclusive,
 - 1 jobs max,
 - at least 14 nodes per job,
 - max walltime per job 20 hours

• shared:

- non-exclusive,
- 2 jobs max,
- no more than 1 GPU, 40 cpu and 256G ram per job,
- max walltime per job 4 hours
- visu:
 - non-exclusive,
 - 1 job max,
 - max 50GB RAM
 - max 8 cpu per job,
 - max walltime per job 4 hours



Software environment Modules

- What is a module ?
 - a convenient way to use software/library/compiler which are available on the cluster
- Usage
 - display all available software installed on the cluster
 - load/unload a module
 - switch between 2 modules
 - unload all modules
 - list all loaded modules
 - Strong recommendation to use module show to have details

hamitouo@turpanlogin1:~> module avail

hamitouo@turpanlogin1:~> module load nvhpc/22.9
hamitouo@turpanlogin1:~> module unload nvhpc/22.9

hamitouo@turpanlogin1:~> module swap nvhpc/22.9 nvhpc/22.11

hamitouo@turpanlogin1:~> module purge

hamitouo@turpanlogin1:~> module list Currently Loaded Modulefiles: 1) binutils/11.2.0 2) gnu/11.2.0 3) openmpi/gnu/4.1.4-gpu



Software environment NVIDIA compiler collection

- Compilers
 - nvc pour C
 - nvc++ pour C++
 - nvfortran pour Fortran
- Without OpenMPI, with cuda

hamitouo@turpanlogin1:~> module load nvidia
hamitouo@turpanlogin1:~> module load nvhpc-nompi/22.9

• With OpenMPI, for CPU computing only

hamitouo@turpanlogin1:~> module load openmpi/nvidia/4.1.4-cpu

• With OpenMPI for GPU

hamitouo@turpanlogin1:~> module load openmpi/nvidia/4.1.4-gpu



Software environment Arm compiler collection

Compilers

- armclang pour C
- armclang++ pour C++
- armflang pour Fortran
- Without OpenMPI

hamitouo@turpanlogin1:~> module load arm
hamitouo@turpanlogin1:~> module load acf1/22.1

• With OpenMPI, for CPU computing only

hamitouo@turpanlogin1:~> module load openmpi/arm/4.1.4-cpu

• With OpenMPI for GPU

hamitouo@turpanlogin1:~> module load openmpi/arm/4.1.4-gpu



Software environment GNU compiler collection

- Compilers
 - gcc pour C
 - g++ pour C++
 - gfortran pour Fortran
- Without OpenMPI

hamitouo@turpanlogin1:~> module load gnu/11.2.0

• With OpenMPI, for CPU computing only

hamitouo@turpanlogin1:~> module load openmpi/gnu/4.1.4-cpu

• With OpenMPI for GPU

hamitouo@turpanlogin1:~> module load openmpi/gnu/4.1.4-gpu



Software environment Available software

- Communication libraries :
 - OpenMPI
 - HPC-X (can be found in nvhpc)
- Math librairies/application :
 - Julia
 - Blas, cuBlas, Lapack, Scalapack, cuSparse, AMGX,
 - FFT, CuFFT,
 - PetSC, AMGX,
- I/O libraries
 - HDF5
 - NetCDF
 - pNetCDF

- Scientific applications :
 - OpenFoam,
 - Magma,
 - CGAL
- Debug & profile :
 - Arm MAP (CPU / GPU),
 - NVIDIA Nsight (GPU)



Software environment Available software

/usr/local/nvidia/nvhpc/modulefiles						
			/usr/local/a	rm/modulefiles		
acfl/22.1 binutils/11.	2.0 gnu/11.2.0					
		/usr/l	ocal/modules/modulef	iles/compilers_and_libr	aries	
amgx/nvidia/2.3.0 amgx/nvidia/2.3.0-test amgx/nvidia/2.4.0 amgx/nvidia/2.4.0-test arm binutils/11.2.0	boost/arm/1.81.0 boost/gnu/1.81.0 boost/nvidia/1.81.0 cgal/arm/5.5.1 cgal/gnu/5.5.1 cgal/nvidia/5.5.1	fftw/arm/3.3.10 fftw/gnu/3.3.10	gnu/11.2.0 magma/gnu/2.7.0 magma/nvidia/2.7.0 mpc/arm/1.3.1 mpc/gnu/1.3.1 mpc/nvidia/1.3.1	mpfr/arm/4.1.1 mpfr/gnu/4.1.1 mpfr/nvidia/4.1.1 nvidia openmpi/arm/4.1.4-cpu openmpi/arm/4.1.4-gpu	openmpi/gnu/4.1.4-cpu openmpi/gnu/4.1.4-gpu openmpi/nvidia/4.1.4-cpu openmpi/nvidia/4.1.4-gpu petsc/arm/3.18.2 petsc/gnu/3.18.2	petsc/nvidia/3.18.2 scalapack/arm/2.2.0 scalapack/gnu/2.2.0 scalapack/nvidia/2.2.0
		/usr/l	ocal/modules/modulef	iles/scientific_applica	tions	
hdf5/arm/1.12.2-paralle hdf5/arm/1.12.2-seq hdf5/gnu/1.12.2-paralle	hdf5/nvidia/1.12.2	q julia/gnu -parallel netcdf/ar		ia/4.8.1 openfoam/gnu/ m/10 openfoam/gnu/	10 openfoam/nvidia/v22 v2212 pnetcdf/arm/1.12.3	12 pnetcdf/nvidia/1.12.3
arm-forge/22.1.2 cmake/3.2 <u>5</u> .1 dcgm/3.1.3-1						

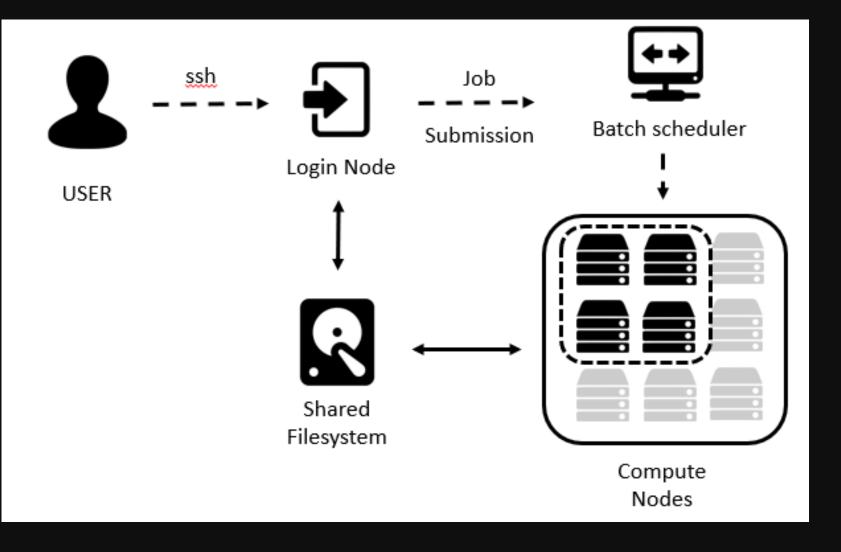
Turpan Supercomputer Fast Start

Okba Hamitou





Slurm Batch system



Atos

Slurm In a nutshell

- The Simple Linux Utility for Resource Management (SLURM) is used for submission, scheduling, execution, and monitoring of jobs
- Main Slurm commands :
 - *sinfo* show information about all partitions and nodes managed by SLURM as well as about general system state
 - *squeue* query the list of pending and running jobs
 - *sbatch* submit a batch script
 - *scancel* cancel a pending or running job or job step
 - *salloc* request interactive jobs/allocations
 - *srun* initiate parallel job steps within a job or start an interactive job
 - *scontrol* provides some functionality for the users to manage jobs or get some information about the system configuration such as nodes, partitions, jobs, and configurations
 - *sacct* retrieve accounting information about jobs and job steps. For completed jobs sacct queries the accounting database



Slurm Batch system

Advantages of a batch system are:

• It allows to run MANY jobs at the same time.

The system takes care that they are run efficiently on the available resources.

• Multiusers, queue system.

A batch system allows users to always submit jobs, even if a lot of people are using the system at the same time. In addition, take care of budgeting and fair resource usage.

• System load balance.

The system takes care of balancing the load across nodes and during time. In a batch system, most jobs may be submitted during office hours, but the scheduler will continue to start jobs at night as nodes become available.



Slurm Partitions

- There are 5 partitions :
 - Small (default)
 - Big
 - Full
 - Shared
 - Visu
- A partition request is done using the flag
 - -p
 - --partition=



Slurm Resource allocation

• Every job submission starts with a resource allocation (nodes, cores, memory).

• An allocation is valid for a specific amount of time, and can be created using the salloc, sbatch or srun commands.

• salloc and sbatch only create resource allocations, srun launches parallel tasks within such a resource allocation, or implicitly creates an allocation if not started within one.

• The usual procedure is to combine resource requests and task execution (job steps) in a single batch script (job script) and then submit the script using the sbatch command.





Syntax

• sbatch [options] script [args...]

Job Script

- Usually, a job script consists of two parts. The first part is optional but highly recommended:
 - Slurm-specific options used by the scheduler to manage the resources (e.g. memory) and configure the job environment
 - Job-specific shell commands

The job script acts as a wrapper for your actual job. Command-line options can still be used to overwrite embedded options.

I strongly recommend to get familiar with sbatch options on Slurm website or using the man command.



- Allocating Resources with SLURM : the *salloc* and *sbatch* commands make resource allocations only. The *srun/mpirun* command launches parallel tasks.
- The usual way to allocate resources and execute a job is to write a batch script and submit them to SLURM with the *sbatch* command.

#!/bin/bash
#SBATCH --job-name=test_mpi
#SBATCH --partition=compute
#SBATCH --ntasks=96
#SBATCH --time=01:30:00
#SBATCH --output=job_%x_%j.out
#SBATCH --err=job_%x_%j.err
#SBATCH --exclusive

setup environment
module load applications

#launch executable with or without inputs
srun ./mybinary input1 input2

Specify the name of the partition

Specify a reasonable time limit. It may allow your job to start quickly

Specify the names of your output files.
%x : environment variable referencing the job
name
%j : environment variable referencing the job ID

• Running serial, OpenMP, MPI jobs

Sequential job	OMP job	MPI job
<pre>#!/bin/bash #SBATCHjob-name=test_serial #SBATCHpartition=compute #SBATCHntasks=1 #SBATCHtime=00:30:00 #SBATCHoutput=job_%x_%j.out #SBATCHerr=job_%x_%j.err #SBATCHexclusive</pre>	<pre>#!/bin/bash #SBATCHjob-name=test_omp #SBATCHpartition=compute #SBATCHntasks=1 #SBATCHcpus-per-task=28 #SBATCHtime=00:30:00 #SBATCHoutput=job_%x_%j.out #SBATCHerr=job_%x_%j.err #SBATCHexclusive</pre>	<pre>#!/bin/bash #SBATCHjob-name=test_mpi #SBATCHpartition=compute #SBATCHntasks=240 # or # or #SBATCHnodes=3 #SBATCHtime=00:30:00 #SBATCHoutput=job_%x_%j.out #SBATCHerr=job_%x_%j.err #SBATCHexclusive</pre>
<pre># setup environment module load app1 app2appN</pre>	<pre># setup environment module load app1 app2appN export OMP_NUM_THREADS=\$SLURM_CPUS_PER_TASK</pre>	<pre># setup environment module load app1 app2appN</pre>
<pre>#launch executable with or without inputs ./mybinary input1 input2</pre>	<pre>#launch executable with or without inputs ./mybinary input1 input2</pre>	<pre>#launch executable with or without inputs srun ./mybinary input1 input2</pre>



• Running hybrid jobs (OpenMP + MPI)

Hybrid job

```
#!/bin/bash
#SBATCH --job-name=test_hybride
#SBATCH --partition=compute
#SBATCH --ntasks=4
#SBATCH --cpus-per-task=40
#SBATCH --tasks-per-node=2
#SBATCH --gres=gpu:2
#SBATCH --gres=gpu:2
#SBATCH --time=00:30:00
#SBATCH --output=job_%x_%j.out
#SBATCH --err=job_%x_%j.err
#SBATCH --exclusive
```

setup environment
module load app1 app2 ..appN
export OMP NUM THREADS=\$SLURM CPUS PER TASK

#launch executable with or without inputs
srun ./mybinary input1 input2



• Environment Variables

- Slurm sets various environment variables available in the context of the job script. Some are set based on the requested resources for the job.
- For the full list, see man sbatch

Environment variables	Correspondence
SLURM_JOB_ID	Job id
SLURM_NTASKS	#SBATCH -n
SLURM_JOB_NUM_NODES	#SBATCH -N
SLURM_CPUS_PER_TASK	#SBATCH -c
SLURM_ACCOUNT	#SBATCH -A
SLURM_JOB_NODLIST	Nodelist which is allocated

#!/bin/bash		
#SBATCH -A <account name=""></account>		
#SBATCH -J test		
#SBATCH -N 2		
#SBATCH -n 32		
#SBATCH -t 00:10:00		
#SBATCH -o test.%j.out		
#SBATCH -e test.%j.err		
NP=\$SLURM_NTASKS		
echo "jobid:\$SLURM_JOB_ID"		
echo "numnodes:\$SLURM_JOB_NUM_NODES"		
echo "nodelist:\$SLURM_JOB_NODLIST"		
mpirun -np \$NP ./a.out		



Slurm Monitoring jobs

- Different Slurm commands provide information about jobs/job steps on different levels.
- The command squeue provides high-level information about jobs in the Slurm scheduling queue (state information, allocated resources, runtime, ...).
- The command sstat provides detailed usage information about running jobs, and sacct provides accounting information about active and completed (past) jobs.
- The command scontrol provides even more detailed information about jobs and job steps.

Slurm Monitoring jobs

- squeue
 - Use the squeue command to get a high-level overview of all active (running and pending) jobs in the cluster.
- The default output format is as follows:
 - JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)
- Job States
 - During its lifetime, a job passes through several states.
 - The most common states are PENDING, RUNNING, SUSPENDED, COMPLETING, and COMPLETED.
 - PD Pending. Job is waiting for resource allocation
 - R Running. Job has an allocation and is running
 - S Suspended. Execution has been suspended and resources have been released for other jobs
 - CA Cancelled. Job was explicitly cancelled by the user or the system administrator
 - CG Completing. Job is in the process of completing. Some processes on some nodes may still be active
 - CD Completed. Job has terminated all processes on all nodes with an exit code of zero
 - F Failed. Job has terminated with non-zero exit code or other failure condition

Slurm Monitoring jobs

- List all currently running jobs of user foo:
 - squeue --user=foo --states=PD,R
- List all currently running jobs of user foo in partition bar:
 - squeue --user=foo --partition=bar --states=R
- scontrol
 - Use the scontrol command to show more detailed information about a job
 - Syntax : scontrol [options] [command]
- Examples
 - Show detailed information about job with ID 354684: scontrol show jobid 354684
 - Show even more detailed information about job with ID 35464 (including the jobscript): scontrol -dd show jobid 3546
- sacct
 - Use the sacct command to query information about past jobs
 - Syntax: sacct [options]
 - See man sacct

Slurm Deleting jobs

- scancel
 - Use the scancel command to delete active jobs
- Syntax : scancel [options] <jobid> ...
- scancel can be restricted to a subset of jobs, using the following options with the related value, e.g.
 - -u, --user \$USER jobs of current user
 - -A, --account jobs under this charge account
 - -n, --jobname jobs with this job name
 - -p, --partition jobs in this partition
 - -t, --state jobs in this state
- Delete specific job:
- Delete all running jobs:
- Delete all of your jobs:
- scancel 12345678 scancel --state=R
 - scancel --user \$USER



Turpan Supercomputer Fast Start

Okba Hamitou





Compiling on Arm Ampere Altra Compilers and Build Systems

- All popular build systems are supported and performant on Arm
- GCC, Arm, NVIDIA are excellent Arm compilers
 - Auto-vectorizing, auto-parallelizing, tested, in production
 - Arm & partners are the majority of GCC contributors
- All major build systems and tools work on Arm
 - CMake, Make, GNUMake, EasyBuild, Spack etc...

Compiling on Arm Ampere Altra Neon for Armv8-A

- Arm Neon technology implements SIMD
- Enabled through :
 - Arm Performance Libraries, FFTW
 - Auto-vectorization features of compilers
 - Neon intrinsic functions
 - Hand-coded Neon assembler (for experienced programmers)

Compiling on Arm Ampere Altra Neon for Armv8-A

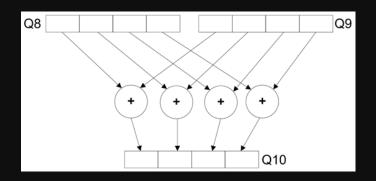
- Single Instruction Single Data (SISD)
 - Each instruction performs its specified operation on a single piece of data
 - Performing four addition operations requires four instructions to add values from four pairs of registers

ADD x0, x0, x5 ADD x1, x1, x6 ADD x2, x2, x7 ADD x3, x3, x8

• Single Instruction Multiple Data

- The same operation is executed simultaneously for multiple items
- The following instruction adds four pairs of singleprecision (32-bit) values together
- This operation adds two 128-bit (quadword) registers, Q8 and Q9, and stores the result in Q10. Each of the four 32-bit lanes in each register is added separately

ADD Q10.4S, Q8.4S, Q9.4S



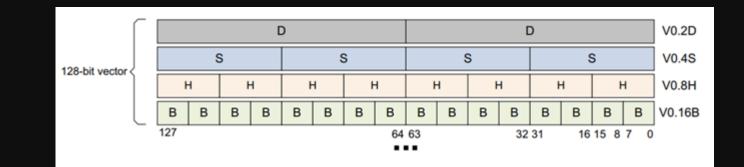


Compiling on Arm Ampere Altra Neon for Armv8-A

- A 128-bit Neon vector can contain the following element sizes:
 - Sixteen 8-bit elements
 - Eight 16-bit elements
 - Four 32-bit elements
 - Two 64-bit elements

(operand suffix .16B, where B indicates byte)

- (operand suffix .8H, where H indicates halfword)
- (operand suffix .4S, where S indicates word)
- (operand suffix .2D, where D indicates doubleword)





Compiling on Arm Ampere Altra

Arm compiler & Arm performance libraries Now free to use – No license required

• Free to use, no licence required

https://developer.arm.com/Tools%20and%20Software/Arm%20Compiler%20for%20Linux

arm Developer		IP Explorer	Documentation	Downloads	Community	Support	Q	Ŷ	Do
Developing on Arm \vee Architecture and Processors \vee Too	Is and Software $ imes $					<u>e</u>	0	۶	۲
Technical Specifications Resources Support and T	Training Supported Devices								
Specifications Arm Compiler for Linux is tailored to the development of High Performance Computing (HPC) applications.									
armclang armclang++(ArmC/C++Compiler)	 Built on modern LLVM and Clang technology Tailored for HPC and scientific codes, with support for C/C++ Implements specifications including ABI for the 64-bit Arm and the specifications including ABI for the 64-bit Arm and the specifications including ABI for the 64-bit Arm and the specifications including ABI for the 64-bit Arm and the specifications including ABI for the specifications					for SVE and S	SVE2.		
armflang (Arm Fortran Compiler)	 Built on modern LLVM and Flang technology Tailored for HPC and scientific codes, with support for moder 	n Fortran, Op	enMP standards, a	and SVE code					
Arm Performance Libraries	 Library routines with Fortran and C/C++ interfaces. BLAS, LAPACK, FFT, Sparse linear algebra, and certain libm f Built with OpenMP across many BLAS, LAPACK, FFT, and spa 								Feedback

Compiling on Arm Ampere Altra Arm compiler with Neon for Armv8-A

- Optimization options
 - -Ox with x in {0, 1, 2, 3, fast}
 - Auto-vectorization is enabled by default at optimization level -O2 and higher. The -fno-vectorize option lets you disable auto-vectorization.
 - At optimization level -O1, auto-vectorization is disabled by default. The -fvectorize option lets you enable auto-vectorization.
 - At optimization level -O0, auto-vectorization is always disabled. If you specify the -fvectorize option, the compiler ignores it.
 - Specifying the -Rpass=loop and -Rpass-analysis=loop compiler options displays useful diagnostic and analysis information.

- Specify Neon target
 - -mcpu=native option is a combination of -march and -mtune. It simultaneously specifies the target architecture and optimizes for a given microarchitecture.
- More information here Porting and Optimizing HPC Applications for Arm Documentation

Compiling on Arm Ampere Altra NVHPC compiler with Neon for Armv8-A

- Optimization options
 - -Ox with x in {0, 1, 2, 3, 4} and -fast
 - SIMD code generation is enabled by default at optimization level -O2 and higher.
 - At optimization level -O1, local optimizations are performed (register allocations)
 - At optimization level -Oo, no optimizations are performed.
 - Specifying the –Minfo compiler options displays useful diagnostic and analysis information.

Specify Neon target

• -tp=native|neoverse-n1 is used to specify a CPU target.

• More information here : <u>NVIDIA HPC SDK Version 22.11 Documentation</u>



Compiling on Arm Ampere Altra GNU compiler with Neon for Armv8-A

- Optimization options
 - -Ox with x in {0, 1, 2, 3, fast}
 - SIMD code generation is enabled by default at optimization level -O2 and higher.
 - At optimization level -O1, reduce code size and execution time.
 - At optimization level -O0, no optimizations are performed. Reduce compilation time and make debugging produce the expected results. This is the default.
 - -fopt-info-optimized -fopt-info-missed -fopt-info-all -fopt-info-vec-optimized -fopt-info-vec-missed to print information about performed or missed optimizations.

- Specify Neon target
 - -mcpu=native|neoverse-n1 to target Arm Ampere Altra.
- More information here Optimize Options (Using the GNU Compiler Collection (GCC))

Turpan Supercomputer Fast Start

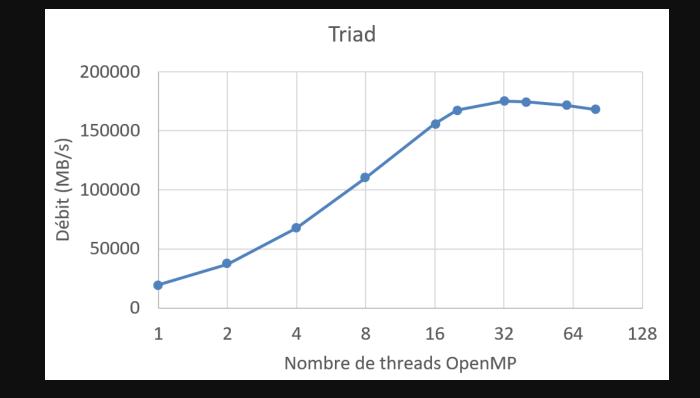
Okba Hamitou





Stream

- armclang -Ofast -mcpu=native -mcmodel=large -fopenmp -ffast-math -ffp-contract=on -DSTREAM_ARRAY_SIZE=100000000 -DNTIMES=20 stream.c -o stream.armclang
- Theoretical peak performance : 204 GB/s
- Measured peak performance : 175 GB/s





HPL & HPCG With Arm Performance Libraries

• HPL

- CCFLAGS = \$(HPL_DEFS) Ofast mcpu=neoverse-n1
- Theoretical peak performance : 1,92 TFlops
- Measured peak performance : 1,18 TFlops (61,4% efficiency)

• HPCG

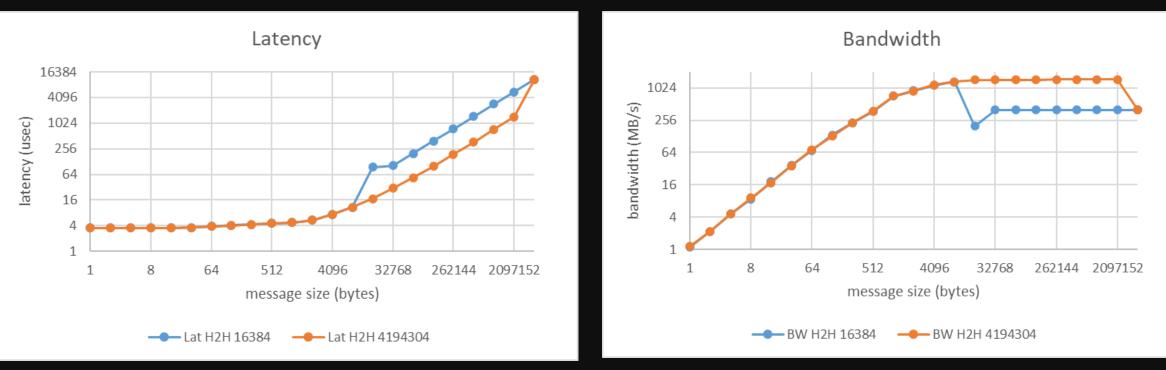
- CXXFLAGS = \$(HPCG_DEFS) -O3 -mcpu=native -ffp-contract=fast -fvectorize -funroll-loops -std=c++11 ffast-math
- Measured peak performance : 24,22 GFlops

- Compilation with GNU (CPU) and NVCC (GPU)
- Libraries : OpenMPI and UCX with CUDA and GDRCopy support

• Important environment variables :

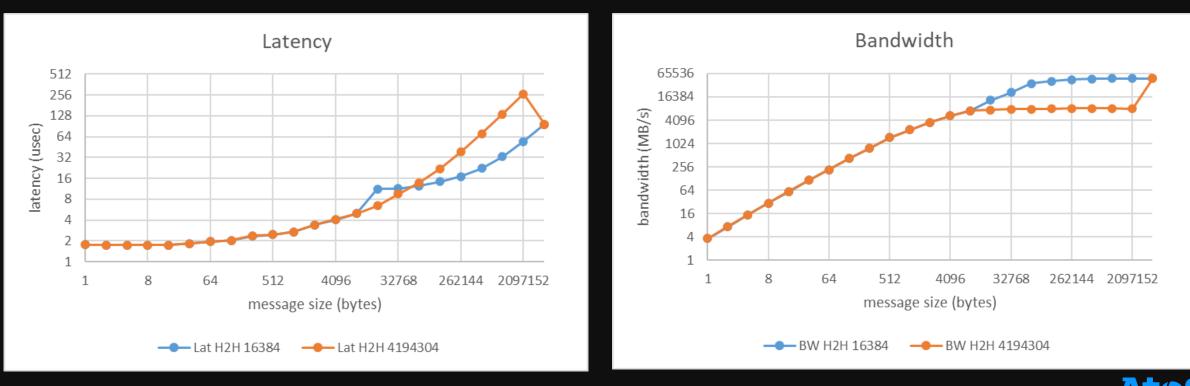
- export UCX_TLS=cma,rc,mm,cuda_copy,cuda_ipc,gdr_copy
- export UCX_RNDV_THRESH=16384
- export UCX_RNDV_SCHEME=put_zcopy
- export UCX_IB_GPU_DIRECT_RDMA=yes
- export UCX_NET_DEVICES=all
- Important environment variables :
 - export UCX_RNDV_THRESH=16384
 - This option set the message size rendezvous threshold (the UCX will switch from eager algorithm to rendezvous).

- Device to Device latency and bandwidth
- Influence of the UCX_RNDV_THRESH variable
 - UCX_RNDV_THRESH = 16 KB
 - UCX_RNDV_THRESH = 4 MB

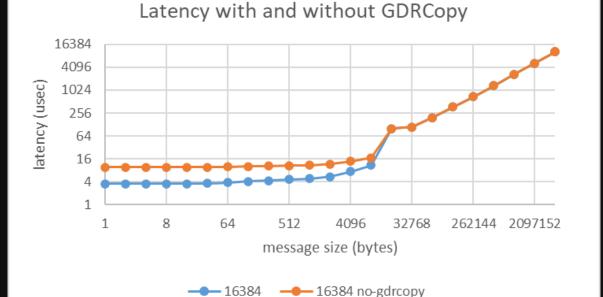




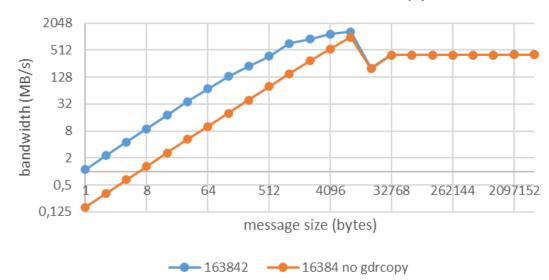
- Host to Host latency and bandwidth
- Influence of the UCX_RNDV_THRESH variable
 - UCX_RNDV_THRESH = 16 KB
 - UCX_RNDV_THRESH = 4 MB



- Device to Device latency and bandwidth
- Influence of GDRCopy
 - Bandwidth x7
 - Latency x3



BW with and without GDRCopy



Atos

Okba-nafie.hamitou@atos.net

Atos is a registered trademark of Atos SE. February 2022. © 2022 Atos. Confidential information owned by Atos, to be used by the recipient only. This document, or any part of it, may not be reproduced, copied, circulated and/or distributed nor quoted without prior written approval from Atos.



