CSCS
Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Using the Cray XK7 Todi at CSCS

CSCS-USI Summer School 2014

System Specifications: Todi

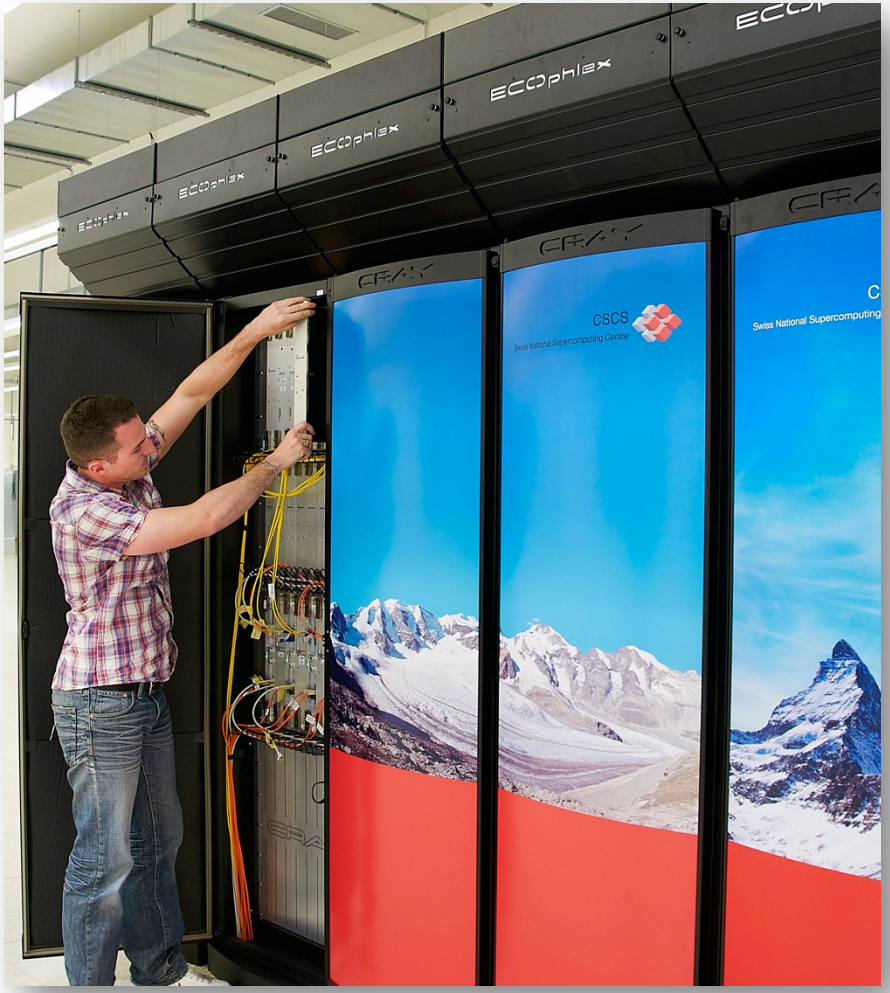
- **1st hybrid CPU/GPU system at CSCS**
- **272 nodes each with:**

➢ one 16-core AMD Opteron CPU (32 GB DDR3 memory)

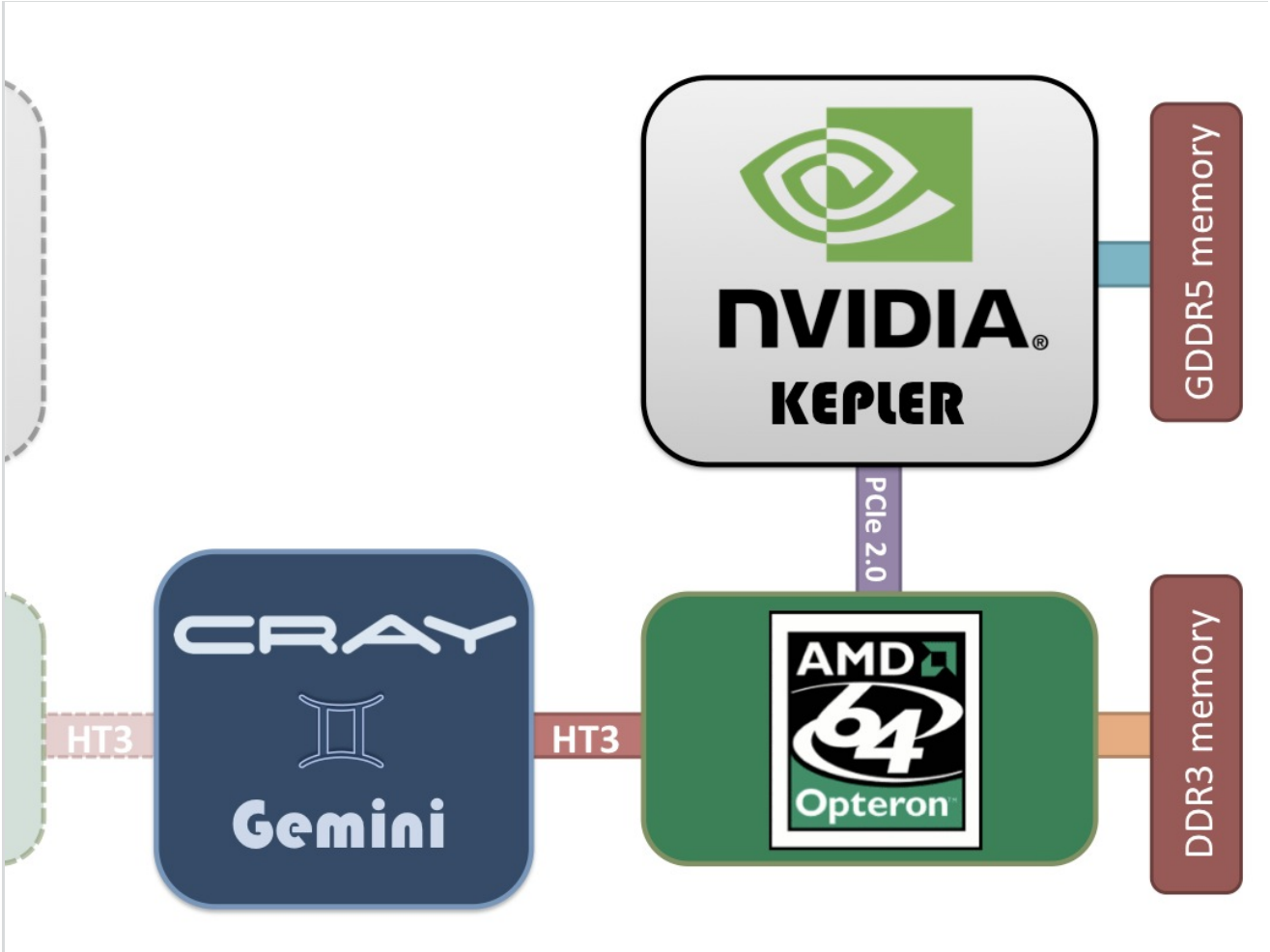
➢ one NVIDIA Tesla K20X GPU (6 GB of GDDR5)

- **Gemini interconnect** (5 GBytes/s injection bandwidth)

Grand total: 4352 cores
272 GPUs



Zoom-in of the Node



Getting started: Accessing the system

ssh -Y *username*@ela.cscs.ch

ssh -Y *username*@todi.cscs.ch

CSCS resources can be accessed through the frontend system Ela. Once logged in, proceed to Todi for compiling and running jobs.

Programming environment

CSCS systems use the modules framework:

- module avail (list of all available modules)
- module list (list of currently loaded modules)
- module show *modulename* (useful information)
- module load/unload *modulename*
- module swap *modulename/ver1 modulename/ver2*

Compilers are loaded when you load the appropriate programming environment

CRAY	INTEL	PGI	GNU
PrgEnv-cray	PrgEnv-intel	PrgEnv-pgi	PrgEnv-gnu

GPU-specific modules

CUDA

- module load cudatoolkit

OpenACC

- module load craype-accel-nvidia35

Compiler wrappers (mpi by default)

	Fortran	C	C++	w/OpenMP	w/OpenACC
CRAY	ftn	cc	CC	by default	-h acc
PGI	ftn	cc	CC	-mp=nonuma	-acc -ta=kepler
INTEL	ftn	cc	CC	-openmp	N/A
GNU	ftn	cc	CC	-fopenmp	announced

Compile CUDA kernels with nvcc !!

Running jobs on Todi

Interactively:

- salloc –N *<number of nodes>*
- aprun *<options>* *<myexecutable>*

Through a SLURM job script:

- sbatch *<jobscript>*

Sample SLURM jobscripts

```
#!/bin/bash -l
#SBATCH --nodes=8
#SBATCH --ntasks=128
#SBATCH --time=00:30:00
aprun -B ./test.exe
```

Fancier job script

```
#!/bin/bash -l
#SBATCH --job-name="test"
#SBATCH --nodes=2
#SBATCH --ntasks=2
#SBATCH --cpus-per-task=1
#SBATCH --ntasks-per-node=1
#SBATCH --time=00:05:00
#======START=====================================
echo "On which nodes it executes"
echo $SLURM_JOB_NODELIST
echo "Now run the MPI tasks..."
aprun -B ./mpicuda.x
#======END=======================================
```

Where do I compile/run?

Home filesystem $HOME=/users/$USER

- quota of 10 Gbytes per user and backed up
- not to be be used for simulation I/O, usually for keeping source code/binaries.

Scratch filesystem $SCRATCH=/scratch/<machine>/$USER

- to be used for I/O during a simulation
- no quota but no backup as well: temporary storage only!
- data subject to a cleaning policy: see details on CSCS User Portal

Checking/changing job status

- **squeue** [current job status]
- **scontrol show job <JOBID>**[detailed info about your job]
- **sacct** [status of recently completed jobs]
- **scancel <JOBID>** [cancels your running job]

JobID	JobName	Partition	Account	AllocCPUS	State	ExitCode
267073	N300	normal	s384	3072	COMPLETED	0:0
267073.batch	batch		s384	1	COMPLETED	0:0
267074	N300	normal	s384	3072	RUNNING	0:0
267075	N300	normal	s384	3072	PENDING	0:0
267076	N300	normal	s384	3072	PENDING	0:0
267077	N300	normal	s384	3072	PENDING	0:0
267078	N300	normal	s384	3072	PENDING	0:0
267079	N300	normal	s384	3072	PENDING	0:0
267080	N300	normal	s384	3072	PENDING	0:0
267081	N300	normal	s384	3072	PENDING	0:0
267082	N300	normal	s384	3072	PENDING	0:0
267083	N300	normal	s384	3072	PENDING	0:0
267084	N300	normal	s384	3072	PENDING	0:0
267837	H105	normal	s384	1536	COMPLETED	0:0
267837.batch	batch		s384	1	COMPLETED	0:0
267838	H105	normal	s384	1536	RUNNING	0:0
267839	H105	normal	s384	1536	PENDING	0:0
267840	H105	normal	s384	1536	PENDING	0:0
267841	H105	normal	s384	1536	PENDING	0:0
267842	H105	normal	s384	1536	PENDING	0:0
267843	H105	normal	s384	1536	PENDING	0:0
267844	H105	normal	s384	1536	PENDING	0:0
267845	H105	normal	s384	1536	PENDING	0:0
269690	N300	normal	s384	3456	COMPLETED	0:0
269690.batch	batch		s384	1	COMPLETED	0:0
269691	N300	normal	s384	3072	COMPLETED	0:0
269691.batch	batch		s384	1	COMPLETED	0:0
269693	H105	normal	s384	1536	COMPLETED	0:0
269693.batch	batch		s384	1	COMPLETED	0:0
269694	H105meas	normal	s384	768	FAILED	137:0
269694.batch	batch		s384	1	FAILED	137:0

Where do I find course material?

- **Git clone <URL>:**

https://github.com/fomics/SummerSchool2014

Thank you for your attention.