Overview of the KAUST’s Cray X40 System – Shaheen II

Bilel Hadri, Samuel Kortas, Saber Feki, Rooh Khurram, Greg Newby

KAUST Supercomputing Laboratory
KAUST is located on the shores of the Red Sea, in Saudi Arabia
King Abdullah University of Science and Technology (KAUST) is an international, graduate research university in Saudi Arabia, dedicated to advancing science and technology through interdisciplinary research, education and innovation. KAUST has 3 main divisions:

- **Biological Science and Engineering (BESE)**
  - Bioscience
  - Environmental Science & Engineering
  - Marine Science
  - Plant Science

- **Computer, Electrical & Mathematical Science & Engineering (CEMSE)**
  - Applied Mathematics and Computational Science
  - Computer Science
  - Electrical Engineering

- **Physical Science & Engineering (PSE)**
  - Chemical and Biology Engineering
  - Chemical Science
  - Earth Science and Engineering
  - Material Science and Engineering
  - Mechanical Engineering
KAUST Research Centers

• The University has 11 Research Centers:
  ① Advanced Membranes and Porous Materials Center (AMPMC)
  ② Catalysis (KCC)
  ③ Clean Combustion (CCRC)
  ④ Computational Bioscience (CBRC)
  ⑤ Center for Desert Agriculture (CDA)
  ⑥ Extreme Computing Research Center (ECRC)
  ⑦ Red Sea Research Center (RSRC)
  ⑧ Solar and Photovoltaics Engineering Research Center (SPERC)
  ⑨ Upstream Petroleum Engineering Center (UPEC)
  ⑩ Visual Computing Center (VCC)
  ⑪ Water Desalination and Reuse (WDRC)

• The Academic Divisions and Research Centers support the University’s research mission by bringing together faculty members, researchers, and graduate students from across the disciplines. Together, they leverage the interconnectedness of science and engineering and develop interdisciplinary approaches to fundamental and goal-oriented research.
Core Labs

• The Core Labs and Major Facilities offer state-of-the art research equipment operated by more than one hundred expert staff scientists to support KAUST’s research community.

• The University has 8 Core Labs and Major Facilities:
  ① Advanced Nanofabrication and Thin Film Core Lab
  ② Analytical Core Lab
  ③ Biosciences Core Lab
  ④ Costal and Marine Resources Core Lab
  ⑤ Imaging and Characterization Core Lab
  ⑥ Supercomputing Core Lab (KSL)
  ⑦ Visualization Core Lab
  ⑧ Central Workshop
KAUST’s three-fold mission
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Advance science and technology through education and research
KAUST’s three-fold mission

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Catalyze diversification of Saudi economy through innovation and enterprise
KAUST’s three-fold mission

- Advance science and technology through education and research
- Catalyze diversification of Saudi economy through innovation and enterprise
- Connect globally to best practices in academia (70 nationalities)
KAUST is like a city (36 km2 - 14 sq mi):

• Campus
• K12 schools
• Daycare centers
• Restaurants, cafes, fine dining
• Cinemas, concert theatre
• Bank, post office, travel agent
• Beauty salon, dry cleaner
• Golf

• Supermarket
• Student Housing
• Faculty Villas and Staff Housing
• Recreational Facilities
• Stadium
• Beaches
• Hotels
• Security and Fire Protection
• Health Clinic and Heliport

More info on http://www.kaust.edu.sa/
## KAUST Applications

<table>
<thead>
<tr>
<th>Science Area</th>
<th>Codes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Atmospheric Modeling</td>
<td>WRF, WRF-Chem, HIRAM</td>
</tr>
<tr>
<td>Ocean Modeling</td>
<td>WRF, MITgcm</td>
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<tr>
<td>Combustion</td>
<td>NGA, S3D</td>
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<tr>
<td>CFD/Plasma</td>
<td>Plasmoid – in house code</td>
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<tr>
<td>Biology</td>
<td>In-house genomic motif identification code</td>
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<tr>
<td>Earthquake Seismology</td>
<td>SORD, SeisSol, SPECFEM_3D_GLOBE</td>
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<tr>
<td>Electromagnetism</td>
<td>In house explicit code</td>
</tr>
<tr>
<td>Big Data/</td>
<td>Mizan - in house code (Analysis of Large Graphs)</td>
</tr>
<tr>
<td>Chemistry</td>
<td>VASP, LAMMPS, Gaussian, WEIN2k, Quantum Espresso</td>
</tr>
<tr>
<td>Seismic imaging/Oil &amp; gas</td>
<td>In house 3D reverse time migration code</td>
</tr>
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More details http://www.hpc.kaust.edu.sa/sc14/presentations/

- Environment: 34%
- Combustion/CFD: 23%
- Chemistry: 21%
- Electromagnetics: 9%
- Biology: 5%
- Earth Sciences/Oil & Gas: 4%
- Others: 4%
Shaheen I Utilization

Core hours utilization by department at KAUST

Core hours utilization

Disk Utilization on Shaheen

Overview on KAUST Cray XC40 Shaheen II - CUG 2015
Shaheen II Overview

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<tr>
<th>COMPUTE</th>
<th>Node</th>
<th>Processor type: Intel Haswell</th>
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<td>2 CPU sockets per node, 16 processors cores per CPU, 2.3GHz</td>
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<td>6174 Nodes</td>
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<td><strong>ANALYZE</strong></td>
<td>Analyzing</td>
<td>Urika - GD 2TB of global shared-memory, 64 Threadstorm4 processors with 128 hardware threads per processor Over 75 TB of Lustre PFS</td>
<td></td>
</tr>
</tbody>
</table>
Shaheen II: Software ecosystem

• Shaheen II system is tightly integrated with compute, storage and data analytics solutions
  – Increases the difficulty to manage efficiently the hardware and software.

• KSL supports hundreds of third party packages.
  – Need to keep the installations consistent, up-to-date and providing reproducible performance and correctness of the results.

• Solution: Shaheen II software ecosystem:
  – monitoring,
  – software management,
  – regression tools
  – Efficient scheduling manager

• Strategy: not to re-invent the wheel.
Monitoring

- **Monitor SW usage:**
  - What are the most linked, compiled and executed applications your HPC system? How do we find who is using deprecated software or versions with bugs?....
  - **Solution: XALT:**
    - improves the functionalities of ALTD by tracking users, codes and environments. It collects job-level and link-time level data and subsequent analytics automatically and transparently.
    - Already in place on many centers, more than dozen in US and Europe (NICS, ORNL, CSCS, NERSC, NSCA,, TACC, KAUST ... )
    - Great Tutorial 2B by M. Fahey and R. Budiardja (easy instructions to install !)
    - At KAUST, ported ALTD on BG/P in 2013
      - Helped to extract most used libraries and applications with **real metrics**
      - Assisted in the design of benchmarks used for procurements benchmarking
      - Detected some bloopers (ref. blas/lapack, mpirun –np 4 ./config –prefix=...!!!)
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• Monitor I/O performance
  – Checking the performance of the PFS.
  – Solution: Darshan

• Monitor Power Usage
  – SLURM Native with on-the-fly dynamic steering of the frequencies of every running jobs.
SWTools

• To maintain infrastructure for software management of the third-party installation, SWTools has been put in place.

<table>
<thead>
<tr>
<th>/base</th>
<th>/machine</th>
<th>/appli</th>
<th>/version</th>
<th>/build</th>
</tr>
</thead>
<tbody>
<tr>
<td>/sw</td>
<td>/tds</td>
<td>/gsl</td>
<td>/1.15</td>
<td>cnl5.2_cce8.3.2</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>cnl5.2_intel15.2.2</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>cnl5.2_gnu4.9.1</td>
</tr>
</tbody>
</table>

• Standardize workflow for software installations in order to get:
  • a clear documentation on installations
  • an automated building, linking and testing of installations
  • an inventory of currently installed software
  • an easily maintainable installation
  • an automate generation of many user documents

• Each Software installation needs to have test case (small and big) used
  • Validating installation
  • User documentation
  • For regression
Along with the software management, KSL developed an early version of an automatic testing tool for the non-regression testing

Needed to detect errors and/or performance degradation, allowing the center to monitor issues such as reproducibility.

Used a python based tool, which compiles, launches, and checks the outputs of parallel jobs. The tool is managed through a continuous integration of Jenkins server.

Every application testing script or benchmark suite is made available as an elementary test unit. Regularly, through well-defined campaigns or random pick-up, a set of these tests will be initiated and run on Shaheen II via Jenkins.

The results (performance or accuracy) will be carefully archived by Jenkins along with the detailed system state on the service, login or computer nodes at that time.
Shaheen II Regression Workflow
Complete cycle

Overview on KAUST Cray XC40 Shaheen II - CUG 2015

SWTools
Test scripts

Workstation
Jenkins

Performance

Is Test OK?
Yes
No
Send Alert!

Linking traces
Run traces
I/O traces
Core-hour accounting

XALT
Darshan
SLURM accounting

TDS System
CDL nodes
TDS PFS

XC40-LC Computing System

Storage System

Tape Library

KAUST 40G Network
KAUST 1/10G Network

NFS GW nodes
CDL nodes
External LNET nodes
TAS

Send Alert!
Jenkins Script

Build History

Max # of builds to keep

This build is parameterized

Disable Build (No new builds will be executed until the project is re-enabled.)

Execute concurrent builds if necessary (beta)

Restrict where this project can be run

Label Expression

shaheen_2

Source Code Management

None

Build Triggers

Build after other projects are built

Trigger builds remotely (e.g., from scripts)

Build periodically

Schedule

*/* * * * *

Build SCM

Execute shell

Command

export WORK=$HOME/tmp/$USER/jenkins-$[JOB_NAME]-$[BUILD_NUMBER]
mkdir -p $WORK

cd $WORK
tar cvf zephyr.tar -C $HOME ZEPHYR > tar_fcv.out 2> tar_fcv.err

if [ $? -ne 0 ]; then
echo "FAILED : could not create the tar"
echo ----- out ----------------------
cat tar_fcv.out
echo ----- err ----------------------
cat tar_fcv.err
echo ----- end ----------------------

More...

RSS for all RSS for failures
## Jenkins GUI

### Build History

<table>
<thead>
<tr>
<th>Name</th>
<th>Last Success</th>
<th>Last Failure</th>
<th>Last Duration</th>
</tr>
</thead>
<tbody>
<tr>
<td>shaheen 2 filesystem</td>
<td>1 min 19 sec (#2950)</td>
<td>6 days 7 hr (#680)</td>
<td>20 sec</td>
</tr>
<tr>
<td>shaheen 2 get.powercap</td>
<td>33 min (#28)</td>
<td>N/A</td>
<td>0.21 sec</td>
</tr>
<tr>
<td>shaheen 2 slurm is alive</td>
<td>1 min 19 sec (#4704)</td>
<td>11 hr (#4362)</td>
<td>15 sec</td>
</tr>
<tr>
<td>shaheen 2 SPECFM</td>
<td>3 days 3 hr (#18)</td>
<td>3 days 5 hr (#9)</td>
<td>63 ms</td>
</tr>
<tr>
<td>shaheen 2 ssh</td>
<td>3 min 19 sec (#567)</td>
<td>1 day 17 hr (#75)</td>
<td>0.59 sec</td>
</tr>
<tr>
<td>shaheen 2 workload</td>
<td>19 sec (#2344)</td>
<td>7 hr 35 min (#2253)</td>
<td>7.1 sec</td>
</tr>
<tr>
<td>shaheen 2 xtnodestat</td>
<td>3 min 19 sec (#926)</td>
<td>N/A</td>
<td>2.1 sec</td>
</tr>
</tbody>
</table>
Workload monitor

3 last hours Shaheen 2 workload up to 16:34 (15/04/28)

percent of Busy nodes

Nodes running a job (%)

config: 6174
resv: 6144
use: 6144
avail: 17
down: 13
load: 99%

Load Peaks
99% 95%

Jobs OK
2015-04-28 16-29-21
2015-04-28 16-24-21
2015-04-28 16-19-21

Jobs Failed
None
Conclusions

• With acquisition of the new Cray XC40, Shaheen II, KAUST is once again the owner of a world-class supercomputer.

• Shaheen II will enable and grow collaboration with several in-Kingdom universities, industrial partners and other international leadership class supercomputers centers.

• XALT+DARSHAN+SLURM+SWTool (all open-source)
  → Real image of what is happening in the system
  → Preventive detection of performance issue

• Shaheen II software ecosystem: Jenkins will allow to detect any regression
Thanks!