جامعة الملك عبدالله للعلوم والتقنية
King Abdullah University of Science and Technology

Core Labs and
Research Infrastructure

Shaheen III HPC 101

Agenda

- 8:30am Welcome
- **8:35am Shaheen III Overview**
- **8:55am How to apply on Shaheen III**
- 9:05am Getting Started on Shaheen III
- 9:15am Software Environment
- 9:35am Job Scheduling
- 10:00am Coffee Break
- 10:15am Storage overview & Best practices
- 10:30am Applications software example: VASP workflow
- 10:50 am Applications software example: CFD applications
- 11:10 am Applications software example: Bio informatics workflow
- 11:20-11.30am Q&A and Open Discussion

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King Abdullah University of Science and Technology
Core Labs and Research Infrastructure

KAUST SUPERCOMPUTING CORE LAB

KAUST Supercomputing Lab (KSL) & KAUST Visualization Lab

KAUST Supercomputing core Lab (KSL)

SABER FEKI,
DIRECTOR OF RESEARCH
COMPUTING CORE LAB (KSL + KVL)

BILEL HADRI

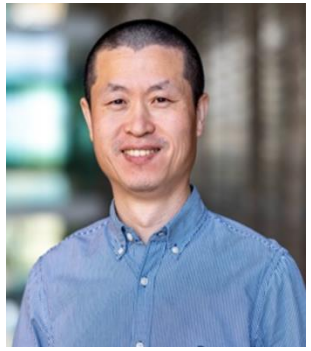
HPC SW ENV.
AND TOOLS

KADIR AKBUDAK

WEATHER
AND CLIMATE
SUPPORT

ROOH KHURRAM

CFD SERVICES



ZHIYONG ZHU

MATERIAL SCIENCE/
CHEMISTRY

MOHSIN A. SHAIKH

AI/ML

NAGARAJAN KATHIRESAN

BIO-SCIENCE

KAUST Supercomputing Core Lab

IaaS: (Infrastructure as-a Service)

SaaS: (Software as a Service)

PaaS:(Platform as-a Service)

CaaS: (Collaboration/Consultancy as-a Service)

Shaheen (s) global ranks over time

- Supercomputing is the cornerstone of KAUST from the beginning.
- KAUST has been maintaining world-class supercomputing facility for open research,
- Similar to US NSF Supercomputing Centers and EU PRACE Research Infrastructure

#20 November 2023

Shaheen3 HPE Cray EX CPU
884,736 cores
39.5PF/s; 5.5MW
7.2GF/W
Since Feb. 2024; 200 projects, 3Billion core hours

~5.5x Performance
3.1x Energy efficeincy

Ranked #7 TOP500 July 2015

Shaheen2 Cray XC40
197,568 cores
7.2 PF/s; 3.1MW
2.32GF/W

8Billion core hours; 700 projects; 1200 publications;
(66% of KAUST faculty using Shaheen)

~36x Performance
5.3x Energy efficeincy

Ranked #14 TOP500 June 2009

Shaheen 1 IBM Blue Gene
65,000 cores
0.2 PF/s; 500KW
0.44 GF/W

400Million Core hours, 200 projects

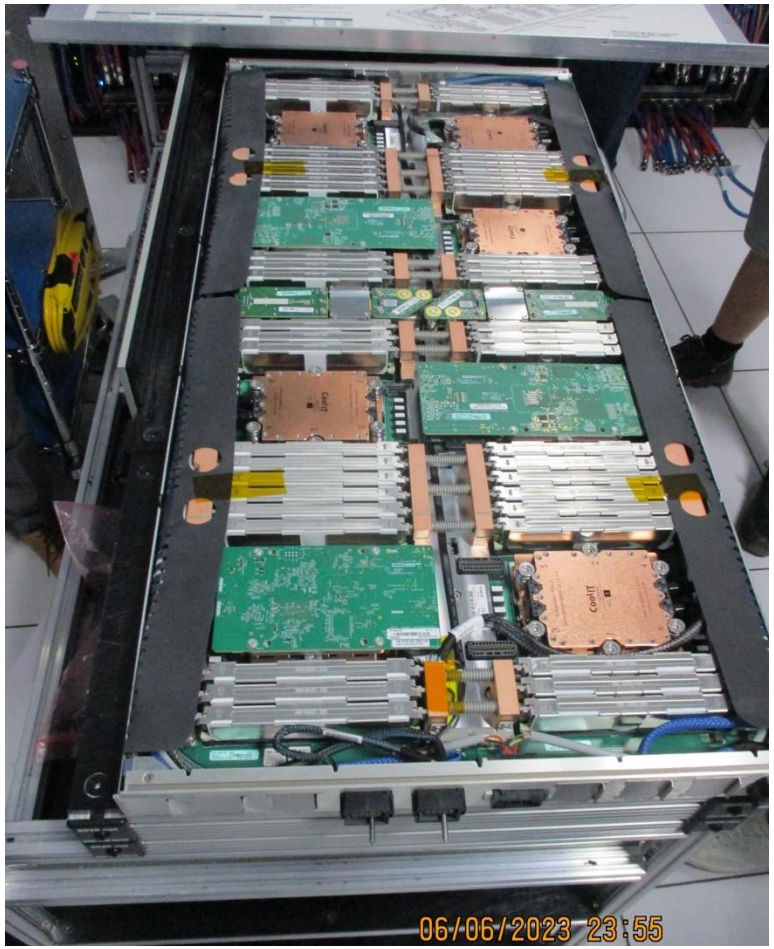
Shaheen III Hardware Overview

Shaheen III – CPU: #1 fastest supercomputer in the Middle East and #20 in the world in 2023

Shaheen III Hardware Specifications: Compute

Characteristics	Shaheen III CPU
Cabinets	18 x Cray EX4000
CPU Type	AMD Genoa 9654
#Socket X #Cores	2 x 96 = **192 cores**
HPL Performance (TFlops/s)	6.87 TF/s per node
Memory	2X12X16GB DDR5@4800Mhz **384GB**
Memory STREAM Bandwidth	800 GB/s per node
Total Number of Nodes	4608
Total Number of Cores	884,736
Theoretical/Sustained Peak (PFlops/s)	**35.66/39.61 (90%)**
Aggregated Theoretical Bandwidth	4.6 PB/s
Power (at highest load)	5.3 MW
Cooling	Direct Liquid Cooling

Shaheen III Hardware Specifications: Compute

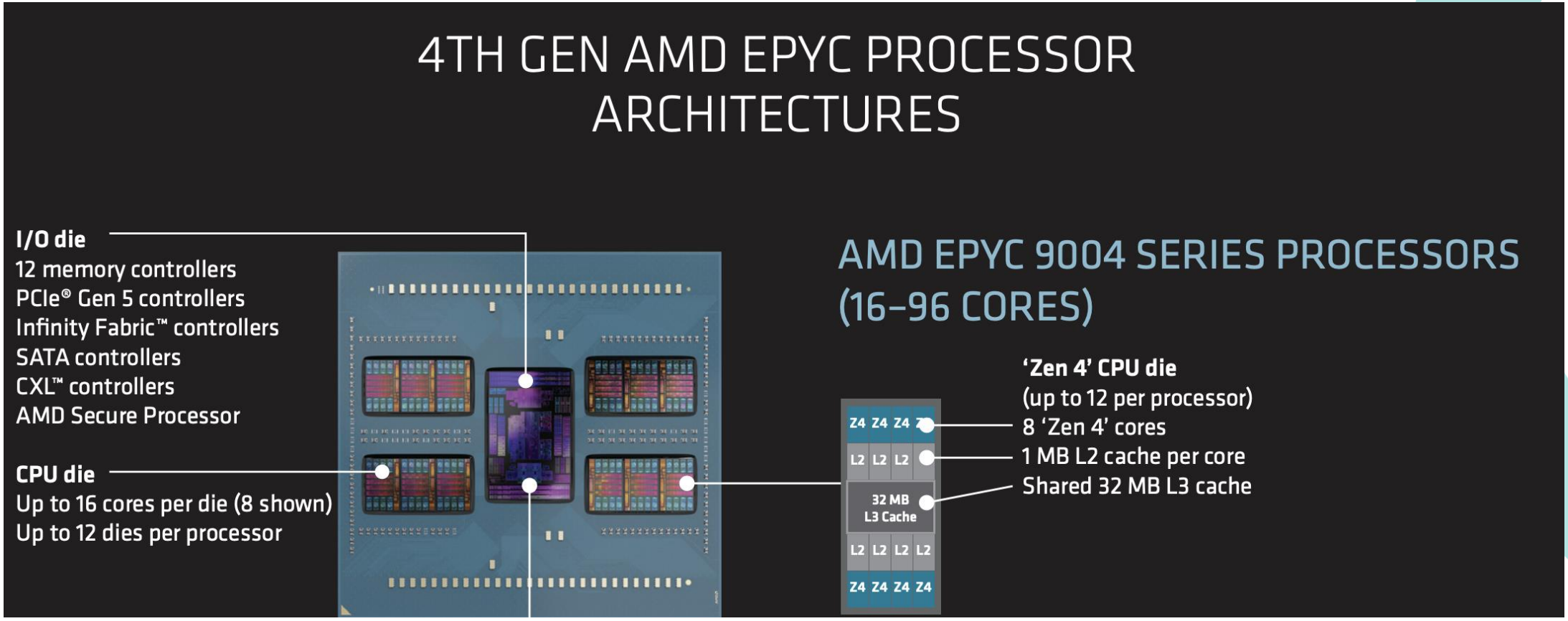


A Cray EX 4000 CPU Blade with 4 Dual Socket AMD EPYC compute nodes

AMD EPYC 9654 Socket

Shaheen III Hardware Specifications: Compute

AMD Genoa CPU Microarchitecture



Shaheen III GPUs Specifications : Early 2026

Characteristics	Shaheen III GPUs
Cabinets	7 x Cray EX4000
#Nodes	700 x 4 X GH Superchip
GPUs	H100 SXM 96GB HBM3 @ ~3TB/s
Host CPU Type	4 x NARM Grace - 72 ARM Cores each
Host Memory	4X 128GB = 512GB (LPDDR5)
CPU-GPU Interconnect	Memory Coherency
NICS	4 x Cassini 200 Gbps, 1 per superchip
GPU Perf **Peak FP64 Tensor**	54.5 TF/s @600W
Total Perf **/Peak FP64/ efficiency)**	152.6 PF/s / 100PF/s

Shaheen III Hardware Specifications: Interconnect

Characteristics	Shaheen III High Speed Network
Type	Slingshot-11
Topology	Dragonfly, multi-level all-to-all
Bandwidth	200 Gbps per link
Latency	Up to 2.6 µs for max 3 hops
Injections per node	CPU Nodes: 1 injection GPU Nodes: 4 injections
Features	Adaptive routing, RDMA, Decongestion, Ethernet compatible

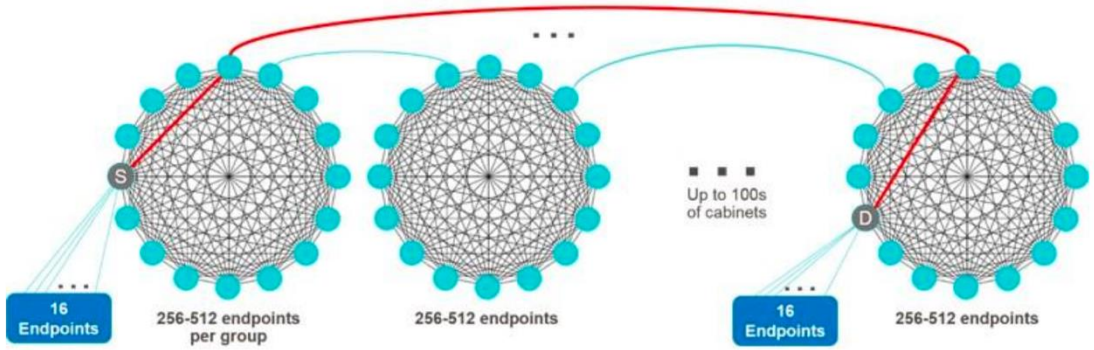
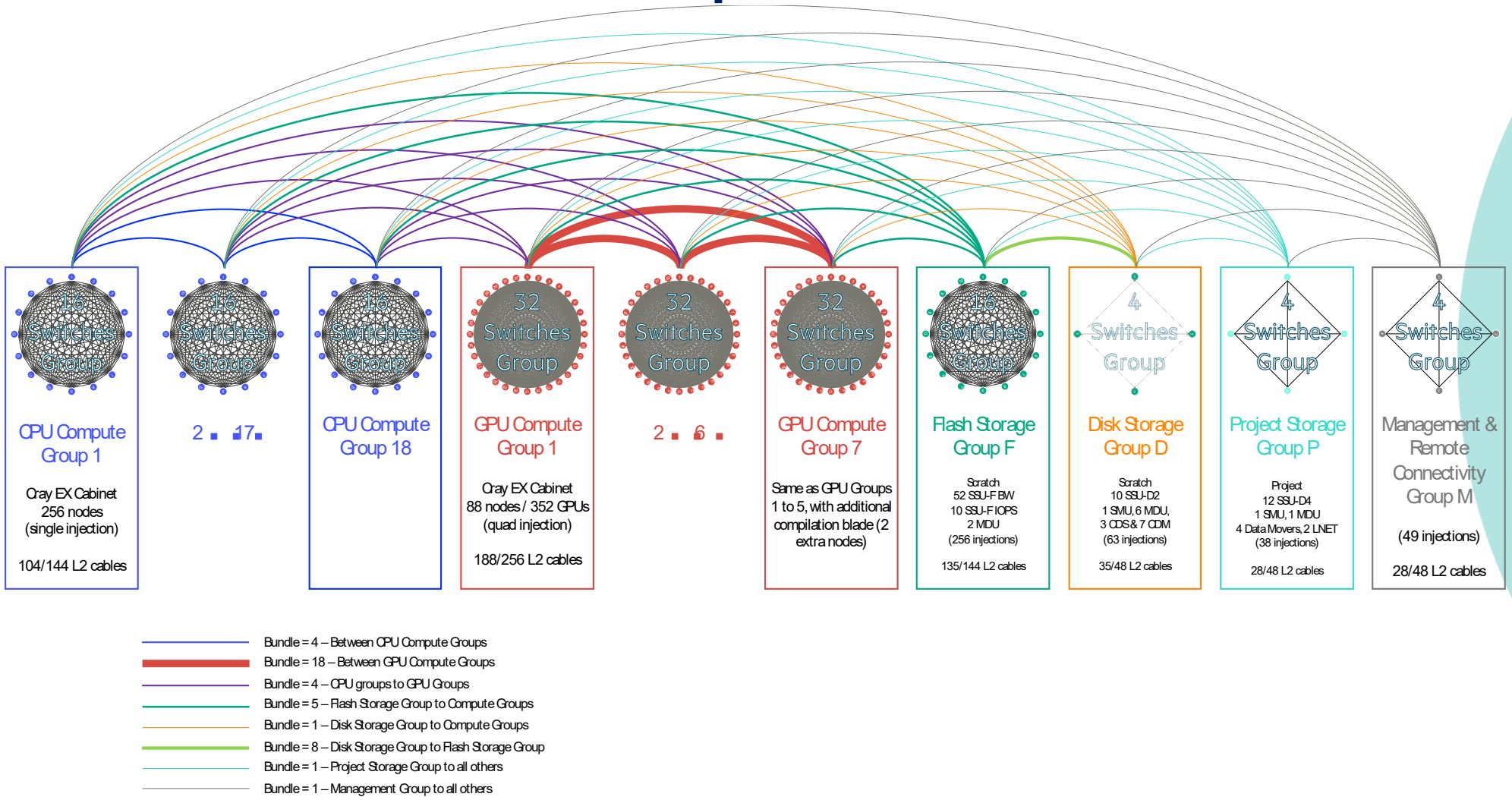


Figure 26: Slingshot Extreme Scale and Performance with Dragonfly Topology

Shaheen III Hardware Specifications: Interconnect



Shaheen III Hardware Specifications: Storage

Characteristics	Shaheen III /scratch storage
Total Capacity (usable)	32 PB
Capacity tier (HDD)	25 PB
Capacity tier perf Read/Write	330/260 GB/s
BW tier capacity	6.8PB (20.9%)
BW Perf. tier Read/Write	3750/2500 GB/s
IOPS tier capacity	338 TB
IOPS tier IOPS (Read/Write)	10+M IOPS

- I/O500: #3 in Overall Production, #7 in Bandwidth, The fastest Lustre on the list
- /project storage will be disconnected from Shaheen II
- Coming Soon on Shaheen III with upgraded capacity and performance !

Shaheen III Hardware Specifications

COMPUTE	CPU Nodes	Processor type: AMD EPYC Genoa	2 CPU sockets per node, 96 processors cores per CPU
		4608 Nodes	884,736 cores
		384 GB of memory per node	Over 1.770 PB total memory
	GPU Nodes	Host: Grace Hopper Superchip	4 X 72 ARM Cores directly attached to NVIDIA H100 GPUs
		700 Nodes	2800 H100 GPUs
	Weight/Size	More than 100 metrics tons	18+7 Cray EX Compute cabinets
	Speed	HPL: 35Pflops/s #20 HPCG: 651.5 TF #16	GPUs with more than 100 Pflops/s sustained HPL performance
	Network	Cray Slingshot interconnect	Dragonfly topology with a max of 3 hops
STORE	Scratch	E1000 Lustre appliance	32 Petabytes of usable storage including a performance and IOPS optimized tiers
	Project	E1000 Lustre appliance	57 PB of HDD
	Archiving	HPE Data Management Framework (DMF) for data backup	120 PB of tape storage, using a spectra logic tape library.

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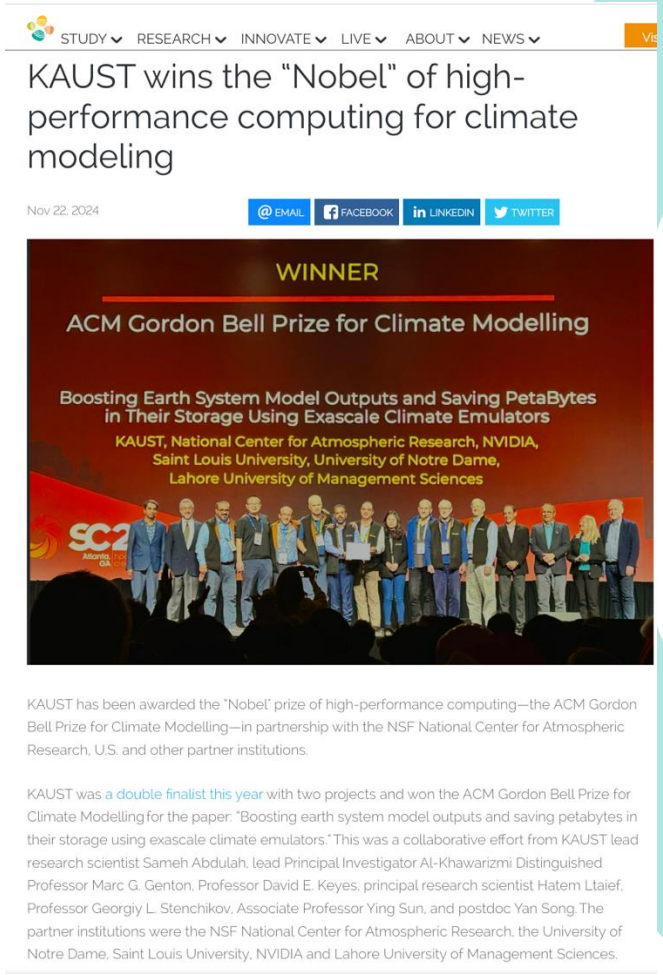
Thank you!

https://www.instagram.com/reel/CzoM8pxtnic/?igsh=MTNuM2lpaTFubHA0aA%3D%3D

Why and How to apply on Shaheen III?

Example of some early success !



STUDY RESEARCH INNOVATE LIVE ABOUT NEWS

KAUST wins the "Nobel" of high-performance computing for climate modeling

Nov 22, 2024

EMAIL FACEBOOK LINKEDIN TWITTER

KAUST has been awarded the "Nobel" prize of high-performance computing—the ACM Gordon Bell Prize for Climate Modelling—in partnership with the NSF National Center for Atmospheric Research, U.S. and other partner institutions.

KAUST was a double finalist this year with two projects and won the ACM Gordon Bell Prize for Climate Modelling for the paper: "Boosting earth system model outputs and saving petabytes in their storage using exascale climate emulators." This was a collaborative effort from KAUST lead research scientist Sameh Abdulah, lead Principal Investigator Al-Khawarizmi Distinguished Professor Marc G. Genton, Professor David E. Keyes, principal research scientist Hatem Ltaief, Professor Georgiy L. Stenchikov, Associate Professor Ying Sun, and postdoc Yan Song. The partner institutions were the NSF National Center for Atmospheric Research, the University of Notre Dame, Saint Louis University, NVIDIA and Lahore University of Management Sciences.

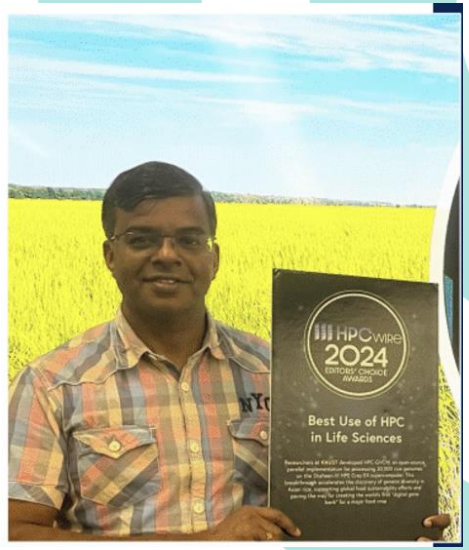
https://www.kaust.edu.sa/en/news/kaust-wins-prestigious-gordon-bell-prize-for-innovation-in-climate-modelling

Example of some early success !

Outstanding Leadership in HPC

•**Editors' Choice**

Since 2022, **David Keyes** has been a finalist for the ACM Gordon Bell Prize utilizing leadership-scale supercomputers such as Fugaku, Frontier, and Shaheen, and partnering with industry leaders like Cerebras, Nvidia, and HPE. These achievements, assisted by Hatem Ltaief, were demonstrated across various real scientific applications, including geostatistics, seismic analysis, climate modeling, and genomics.



Best Use of HPC in Life Sciences

Editors' Choice

Researchers at **KAUST** developed HPC-GVCW, an open-source parallel implementation for processing 20,000 rice genomes on the **Shaheen-III HPE Cray EX** supercomputer. This breakthrough accelerates the discovery of genetic diversity in Asian rice, supporting global food sustainability efforts and paving the way for creating the world's first "digital gene bank" for a major food crop.

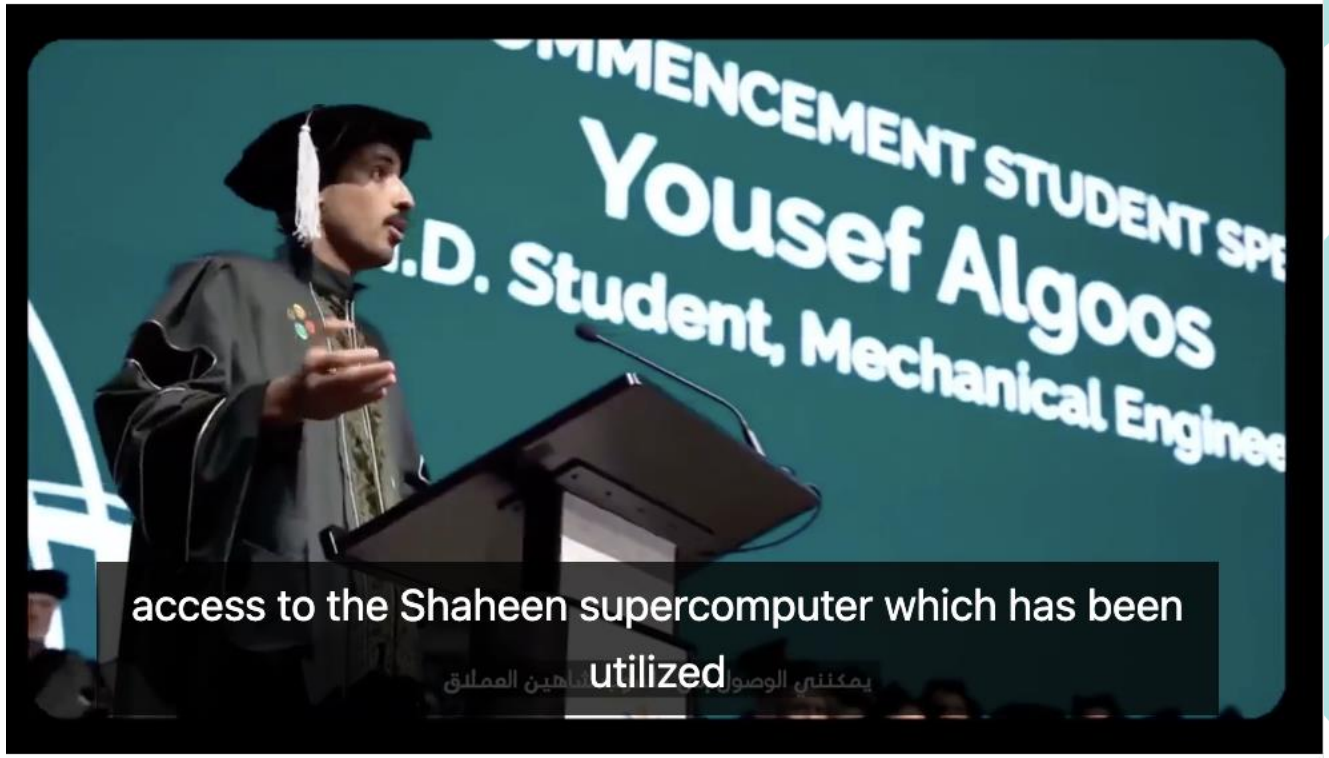
Shaheen mentioned during the graduation ceromony

Record number of Saudi students graduate from KAUST in 2024

Dec 13, 2024 Press Release

@ EMAIL FACEBOOK LINKEDIN TWITTER

As KAUST celebrated its 15th commencement ceremony in 2024, it also celebrated a significant milestone: the highest number of Saudi graduates in the University's history. Saudi students comprised a record-breaking 203, or nearly 44%, of the total 465 graduates. This milestone comes just a week after KAUST was named the top Arab university for the second consecutive year by Times Higher Education.



https://www.linkedin.com/posts/salman-aljabri-791257123_%D9%82%D8%B5%D8%A9-%D9%8A%D9%88%D8%B3%D9%81-%D9%82%D8%B5%D8%A9-%D9%88%D8%B7%D9%86%D8%A3%D8%B3%D8%B3-%D8%B9%D9%84%D9%89-%D8%A7%D9%84%D9%85%D8%B7%D8%A7%D9%8A%D8%A7-ugcPost-7274513644434968576-MhZN/?utm

Recent Alumna winnning IEE CS TCHPC Award

Collaboration and computation

Alomairy's research explores the intersection of algorithms and hardware, focusing on scalable, portable and energy-efficient solutions for scientific computing and artificial intelligence (AI). At MIT's JuliaLab, part of the university's Computer Science and Artificial Intelligence Laboratory (CSAIL), she develops advanced algorithms that account for hardware characteristics such as memory structures, low-precision processing units and parallel task execution—particularly on heterogeneous supercomputers.

She also co-develops matrix-aware methods that accelerate applications on supercomputers like Frontier, Summit, ALPS, and Shaheen-III. Her methods aim to bridge HPC with domain science, delivering insights faster in materials design, genomics, and climate science.

KAUST alumna Dr. Rabab Alomairy wins prestigious IEEE CS TCHPC Early Career Researchers Award

3 min read · Wed, Oct 22 2025
By David Murphy
Awards News
HPC

KAUST alumna and Ibn Rushd Postdoctoral Fellow Dr. Rabab Alomairy received the IEEE CS Early Career Researchers Award in HPC, becoming the first Middle Eastern and one of the youngest recipients professionally to earn this distinction in the award's decade-long history.

https://cemse.kaust.edu.sa/articles/2025/10/22/kaust-alumna-dr-rabab-alomairy-wins-prestigious-ieee-cs-tchpc-early-career

Who are the KAUST PI on Shaheen III ?

- Aamir Farooq
- Andrea Fratalocchi
- Bernard Ghanem
- Boon Ooi
- Cafer Yavuz
- Cristian Picioreanu
- David Keyes
- Deanna Lacoste
- Frederic Laquai
- Gabriel Wittum
- Geert Jan Witkamp
- Gyorgy Szekely
- Hakan Bagci
- Himanshu Mishra
- Hong Im
- Huabin Zhang
- Hylke Beck
- Ibrahim Hoteit
- Iman Roqan
- Ingo Pinnau
- James Turner
- Jesse Poland
- Jian Weng
- Jinchao Xu
- Jorge Gascon
- Juergen Schmidhuber
- Kangming Li
- Kuo-Wei Huang
- Luigi Cavallo
- Magdy Mahfouz
- Magnus Rueping
- Mani Sarathy
- Marc Genton
- Mark Tester
- Markus Hadwiger
- Martin Heeney
- Martin Mai
- Matteo Parsani
- Min Suk Cha
- Mohamed Eddaoudi
- Mohamed Elhoseiny
- Nazek Elatab
- Nikos Hadjichristidis
- Noredine Ghaffour
- Omar Knio
- Omar Mohammed
- Panos Kalnis
- Pedro Castano
- Peter Richtarik
- Peter Schmid
- Robert Hoehndorf
- Rolf Krause
- Sami Al-Ghamdi
- Shadi Fatayer
- Shehab Elsayed
- Sigurdur Thoroddsen
- Sigurjon Jonsson
- Tariq AlKhalifa
- Thomas Finkbeiner
- Udo Schwingenschloegl
- Valerio Orlando
- Volker Vahrenkamp
- William Roberts
- Xin Gao
- Xixiang Zhang
- Ying Sun
- Yoji Kobayashi
- Yoshihide Wada

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Shaheen External PI

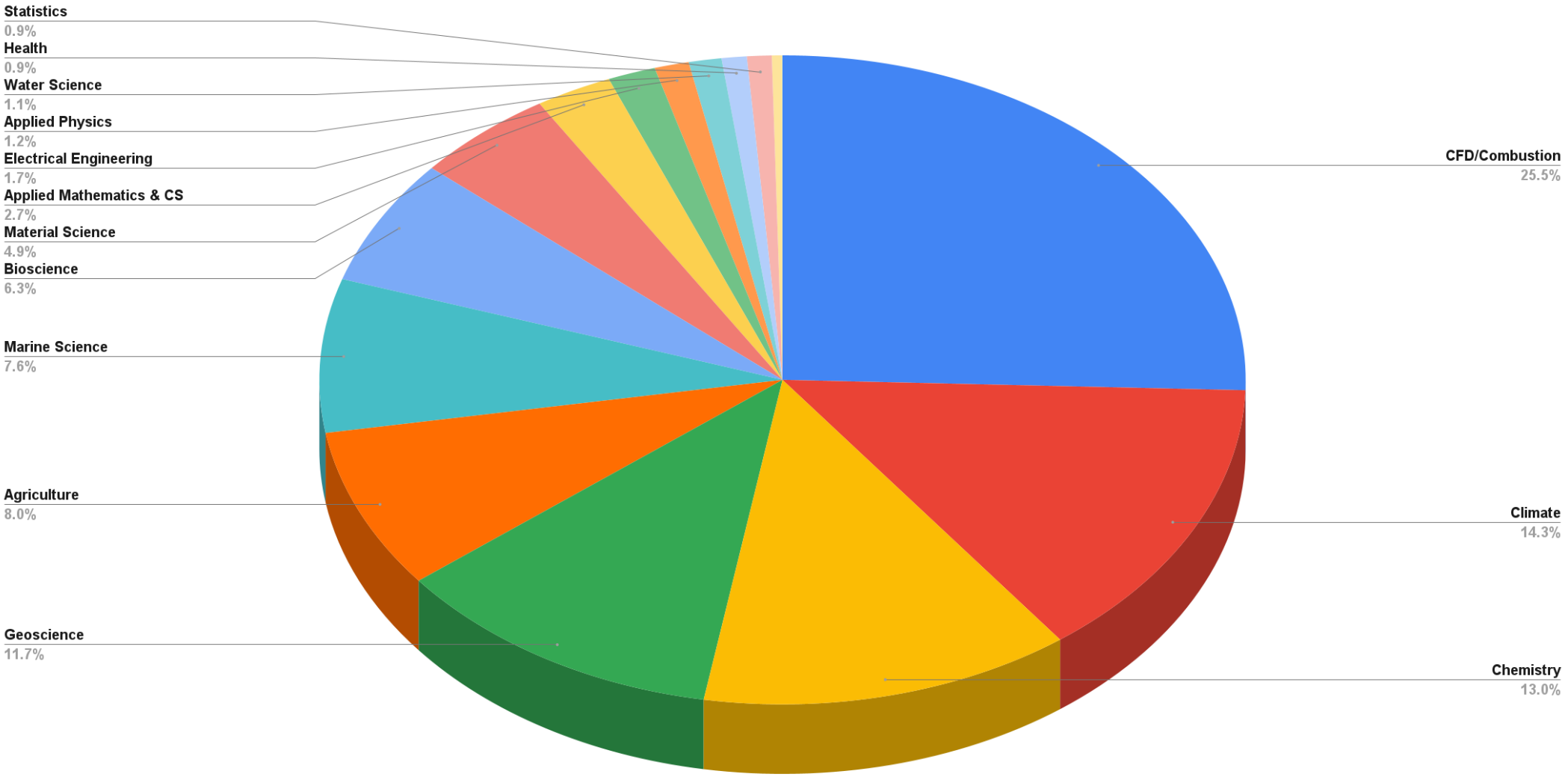
19 Saudi universities

جامعة أم القرى UMM AL-QURA UNIVERSITY
جامعة الجوف Jouf University
جامعة حفر الباطن University of Hafr Al Batin
Princess Nourah Bint Abdulrahman University
KFU جامعة الملك فيصل KING FAISAL UNIVERSITY
عهـة الأمـيـر سطام بن عبدالله INCE SATTAM BIN ABDULAZIZ UNIVERS
جامعة تبوك University of Tabuk
جامعة الفيصل Alfaisal University
KING KHALID UNIVERSITY
جامعـة الحـدود الشماليـة NORTHERN BORDER UNIVERSITY
كليات الأصالة ALASALA COLLEGES
جامعة الملك سعود King Saud University
كليـة الجبيـل الجامعيـة JUBAIL UNIVERSITY COLLEGE
جامعة الطائف TAIF UNIVERSITY TU
جامعة الإمام عبدالرحمن بن فيصل IMAM ABDULRAHMAN BIN FAISAL UNIVERSITY

سابك sabic
الهيئة الوطنية للأمن السيبراني National Cybersecurity Authority
مدينة الملك عبدالعزيز للعلوم والتقنية KACST
أرامكو السعودية saudi aramco
لين Lean
المركز الوطني للأرصاد National Center for Meteorology
UNITX
مدينة الملك عبد الله للطاقة الذرية والمتجددة K·A·CARE
مستشفى الملك فيصل التخصصي ومركز الأبحاث King Faisal Specialist Hospital & Research Centre
الشركة الكويتية لنفط الخليج KUWAIT GULF OIL COMPANY
KJO
أرامكو لاعمال الخليج Aramco Gulf Operations

10 Saudi industries & agencies

Which field of Science is being done on



Core Labs and Research Infrastructure

KAUST SUPERCOMPUTING CORE LAB

Collaboration with Prof. Matteo Parsani: Full Simulation of Flows Around Racing Cars

Performance Study of Sustained Petascale Direct Numerical Simulation on Cray XC40 Systems

Bilel Hadri*[1] | Matteo Parsani[2] | Maxwell Hutchinson[3] | Alexander Heinecke[4] | Lisandro Dalcin[2] | David Keyes[2]

[1]KAUST Supercomputing Lab, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia
[2]Extreme Computing Research Center, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia
[3]Citrine Informatics, Redwood City, California, USA
[4]Intel Corporation, Santa Clara, California, USA

Correspondence
*Bilel Hadri, KAUST Supercomputing Lab, Al Khawarizmi Bldg. (1) Office 126, 4700 King Abdullah University of Science and Technology, Thuwal 23955-6900 . Email: bilel.hadri@kaust.edu.sa

Abstract

We present in this paper a comprehensive performance study of highly efficient extreme scale direct numerical simulations of secondary flows, using an optimized version of Nek5000. Our investigations are conducted on various Cray XC40 systems, using a very high-order spectral element method. Single-node efficiency is achieved by auto-generated assembly implementations of small matrix multiplies and key vector-vector operations, streaming lossless I/O compression, aggressive loop merging and selective single precision evaluations. Comparative studies across different Cray XC40 systems at scale, Trinity (LANL), Cori (NERSC) and ShaheenII (KAUST), show that a Cray programming environment, network configuration, parallel file system and burst buffer all have a major impact on the performance. All three systems possess a similar hardware with similar CPU nodes and parallel file system, but they have different theoretical peak network bandwidths, different OSs and different versions of the programming environment. Our study reveals how these slight configuration differences can be critical in terms of performance of the application. We also find that with 9216 nodes (294,912 cores) on Trinity XC40 the applications sustains petascale performance, as well as 50% of peak memory bandwidth over the entire solver (500 TB/s in aggregate). On 3072 Xeon Phi™ nodes of Cori, we reach 378 TFLOP/s with an aggregated bandwidth of 310 TB/s, corresponding to time-to-solution 2.11× faster than obtained with the same number of (dual-socket) Xeon® nodes.

KEYWORDS:
Cray XC40, Haswell, KNL, Nek5000, Performance Analysis, Regression, Energy Efficiency

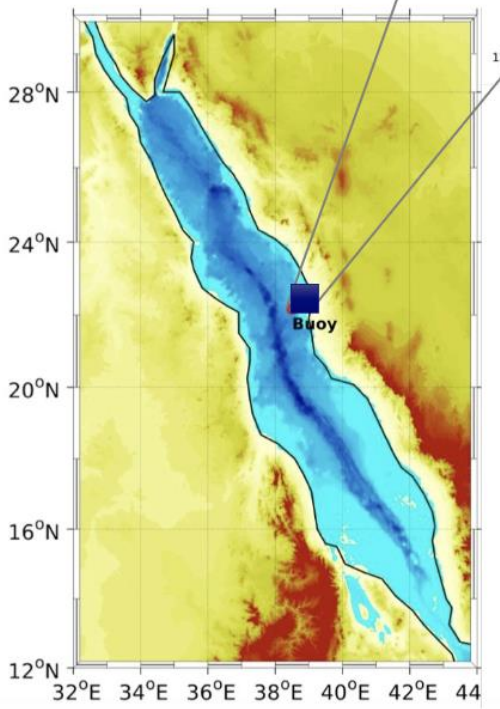
Significantly enhance simulation accuracy at the full vehicle scale

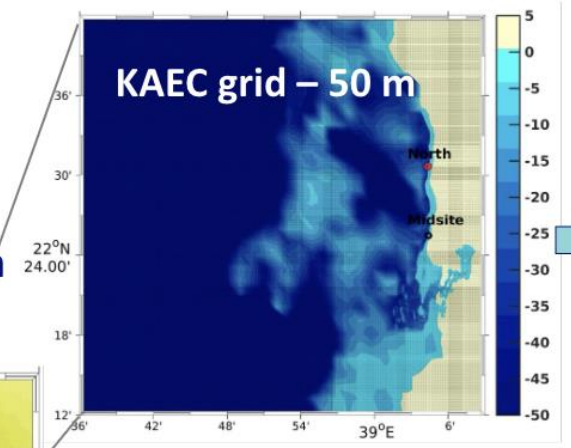
- Detect and improve performance bottleneck
- Scaling the code up to full Shaheen II

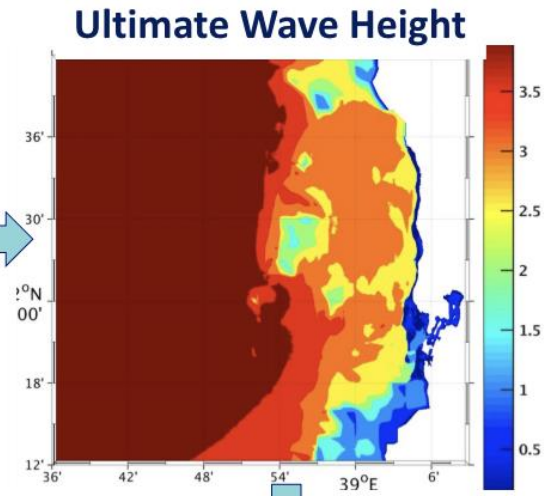
~5 Collaboration projects / year

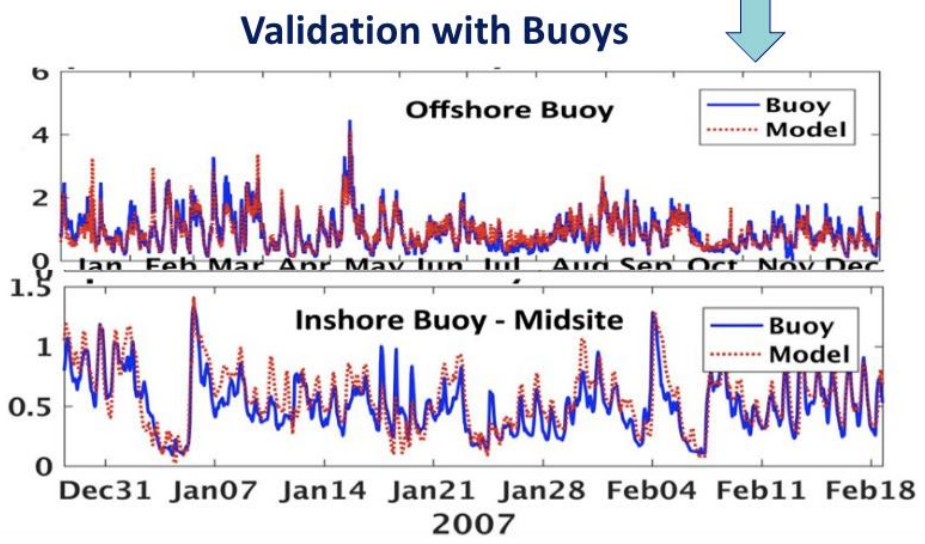
KAEC ULTIMATE WAVE HEIGHT PROJECT

- Nested wave models, at higher resolution 50m
- WRF at 1km
- Boundaries from a 38yr simulation









Donald Francis Jun 8 (5 days ago)

to Omar, me

Gents,

I want to thank you for the excellent effort provided by your team in preparing the Wave Study for the waterfront area adjacent to our property. This has become a key component of further review for setting the minimum safe floor elevation for structures and roadway design. We had previously used incomplete information from which we determined the safe elevation to be approx. 4.0 MSL and have been constructing accordingly. However, when using your data we have been able to lower that elevation to 2.23 MSL. This may not sound like a big change however this equates to a savings of some 90 million cubic meters of fill material or SR 1.8 billion across the City. As you can imagine this is a huge savings to our project.

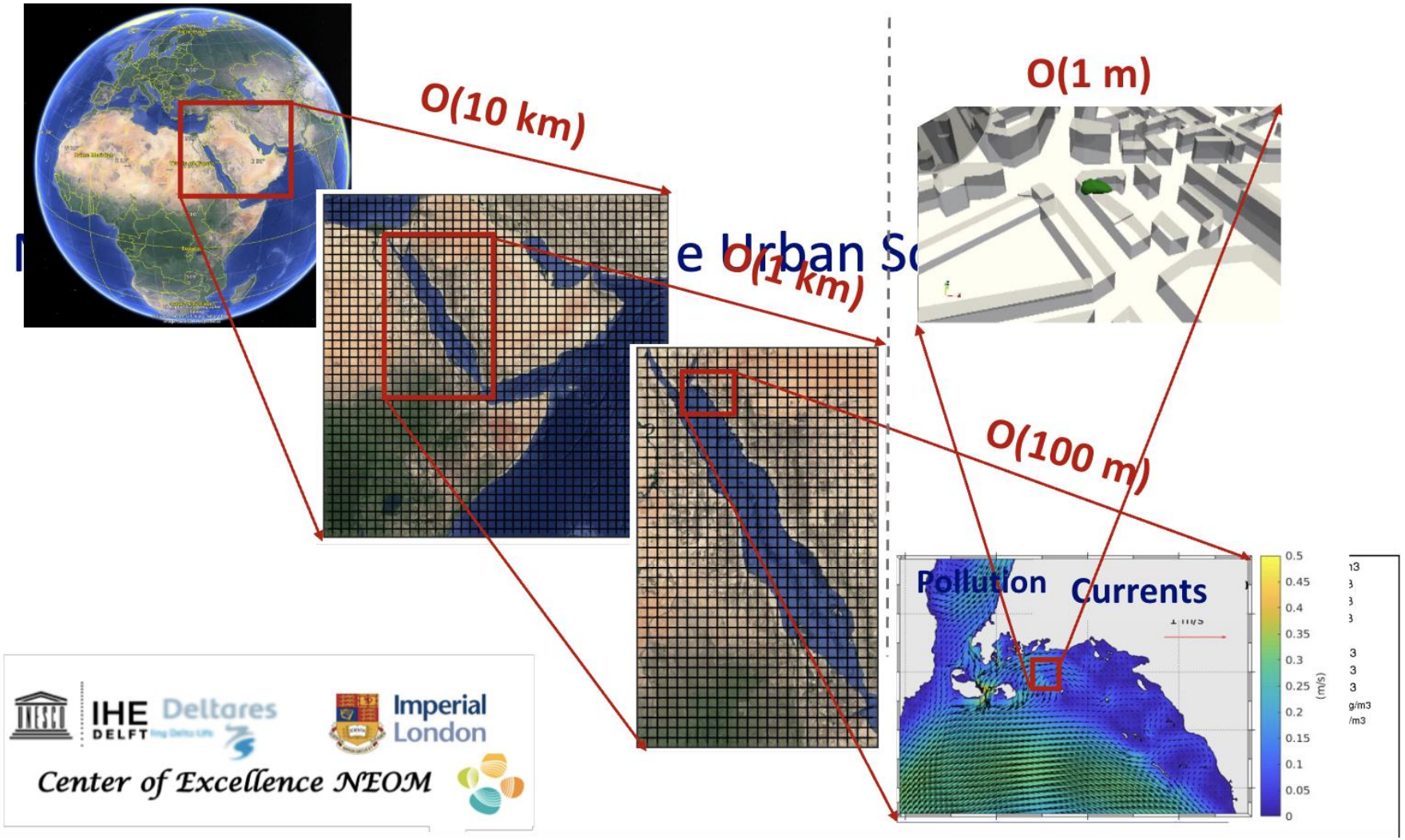
I look forward to your proposal to expand the work to study the tidal surge impact on these numbers as we are hoping to reduce our fill requirements further by some 10 million cubic meters or SR 200 million. As the previous tidal surge was a significant factor in the buildup of our elevation hopefully this can be reduced also. If this can be achieved we would then realize a balanced dirt work across the City and eliminate the need for further import of material.

Thanks again for your efforts.

Don Francis, PE
Head, Corporate Construction

KING ABDULLAH ECONOMIC CITY

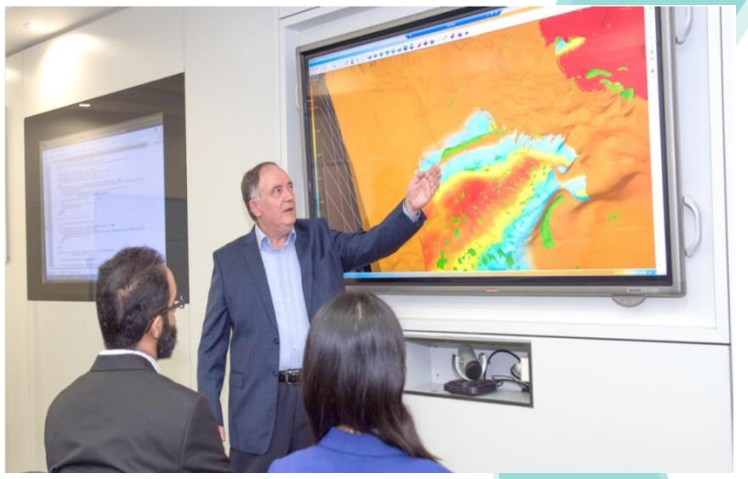
MODELING & PREDICTING NEOM AT ALL SCALES



IHE DELFT Deltares
Imperial London
Center of Excellence NEOM

Advanced Support for Saudi Aramco: Trillion Node Reservoir Simulation

- TeraPOWERS – new trillion node reservoir simulation to model oil migration problems in the Kingdom in a fraction of the time of previous run
- Shaheen II serves as the ONLY platform in the Kingdom for TeraPOWERS for developing capability and performing large scale production runs
- "*We simulated an oil migration problem in the Kingdom from the source rock to the trap with millions of years of history in 10 hours using 1 trillion active computational cells*", Ali Dogru
- "*We could not have achieved this incredible milestone without the expertise and resources from KAUST, which provided superb support*," Larry Fung



The EXPEC Advanced Research Center (EXPEC ARC) TeraPOWERS Technology Team, under the leadership of Saudi Aramco fellow Ali Dogru, achieved a major breakthrough with the industry's first trillion cell reservoir simulation run on October 28, 2016

Aramco news, Dhahran, November 23, 2016

http://www.saudiaramco.com/en/home/news-media/news/saudi-aramco-scientists-achieve-new-world-record.html

Training on Engineering Simulation

- Educate the next generation of leaders in the field of engineering simulation for the era of digital economy
- Providing training on tools from Altair, ANSYS, COMSOL, Convergent Science, MathWorks, Tecplot
- ANSYS
  - Held 9 workshops since: total attendee of ~500
  - Held 6 certification programs: total certified of ~250
- MATLAB
  - Provide easy way to apply deep-learning to engineering problems
  - Two online event with ~300 attendees

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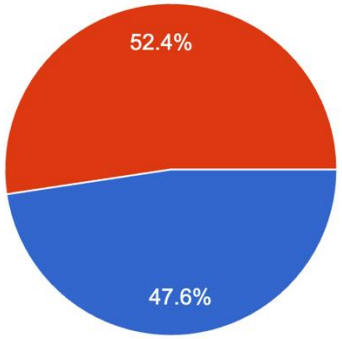
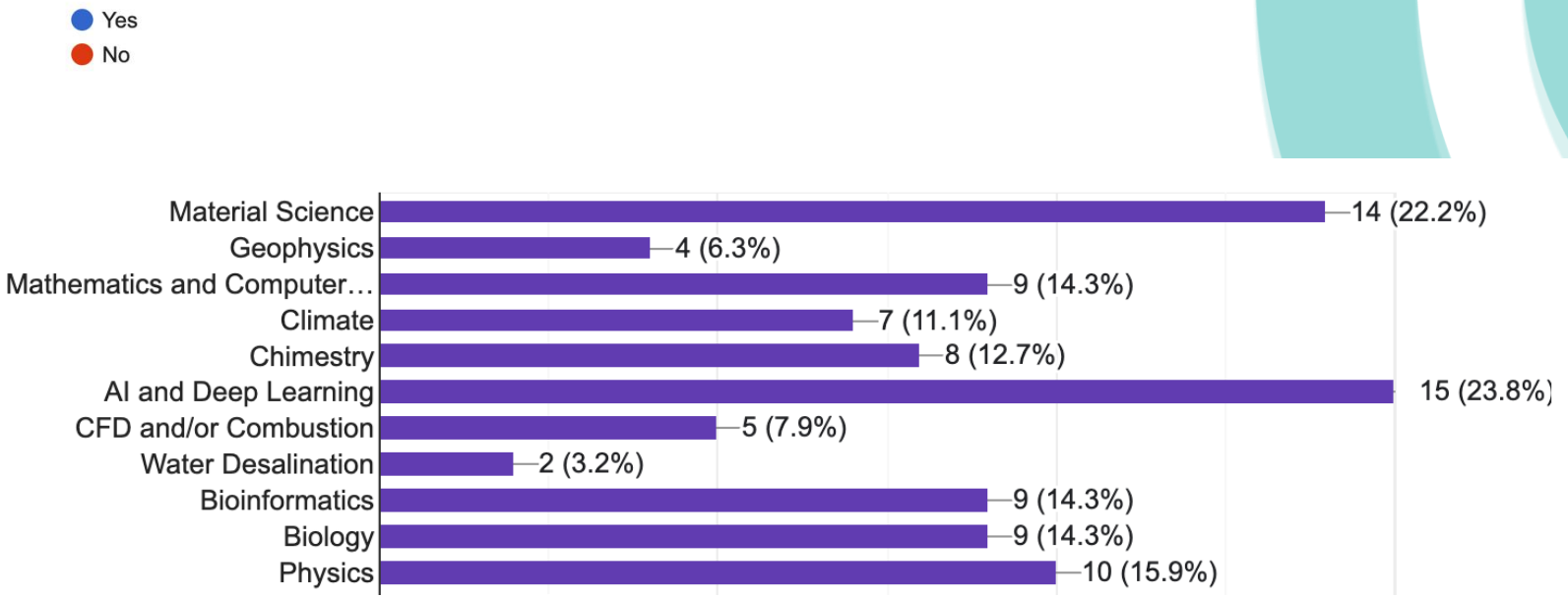
How to apply on Shaheen III?

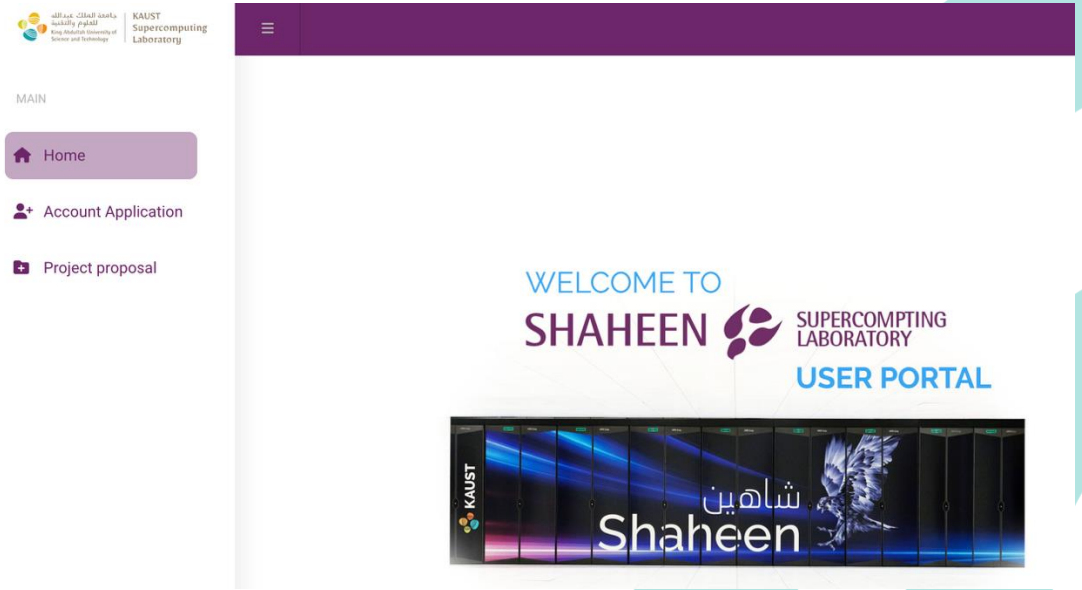
Do you have an account on Shaheen III?

63 responses



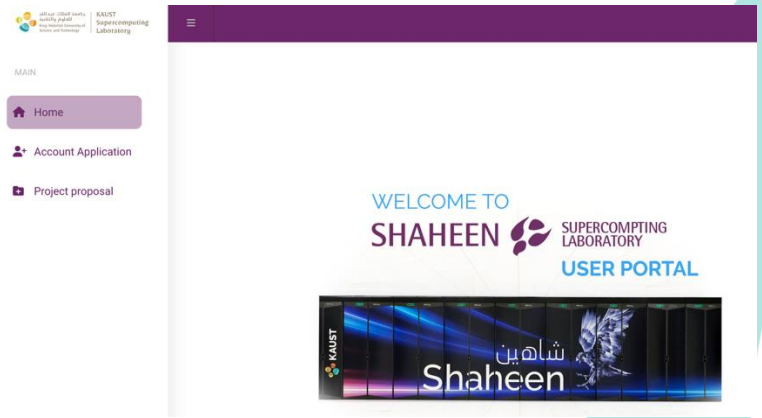


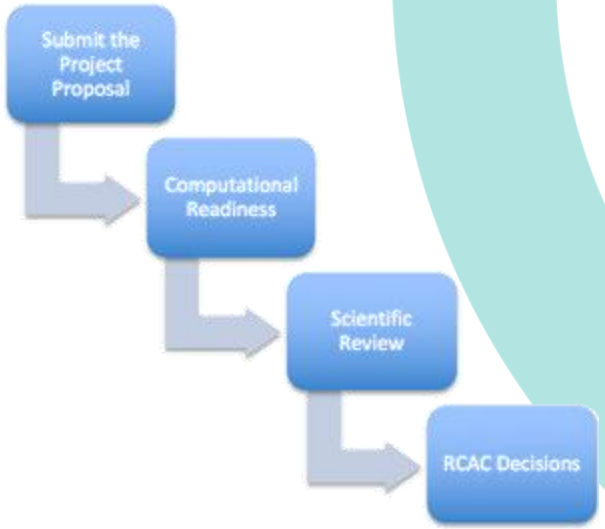
Development proposal



- The PI (faculty) completes the form and submit online
  - https://apply.hpc.kaust.edu.sa/
  - Dedicated only to KAUST faculty
    - First time PI's project or new developed code
    - Small amount of core hours (2M core hours)
      - Computational readiness review by KSL scientist team
      - KSL will send instructions for setting the account
- Any issue, send an email to help@hpc.kaust.edu.sa

Production Project proposal





- The PI (faculty) completes the form and submit online
  - https://apply.hpc.kaust.edu.sa/
  - Production project proposal
    - Needs RCAC approval (monthly reviewed)
    - Computational readiness review by KSL scientist team
    - Scientific review
    - RCAC final review and recommendation
    - KSL will send instructions for setting the account
- Any issue, send an email to projects@hpc.kaust.edu.sa

جامعة الملك عبدالله للعلوم والتقنية
King Abdullah University of Science and Technology

SHAHEEN SUPERCOMPUTING LABORATORY

KAUST Supercomputing Laboratory (KSL)

Production Project Proposal Shaheen III CPU

Project Title	
Principal Investigator (PI)	By submitting this proposal, I approve the entire content of this document and associated supporting documents.
Date of Proposal	
Details of competitive grant related to the project(name of award details with funds and duration)	

Core Hours Requested Shaheen III CPU	_____
Storage TB Requested	_____

Available System: Shaheen III Supercomputer : 18-cabinets Cray EX system, **comprising 4608 nodes, each with 192 AMD Genoa cores and 384GB of memory, with 30 Petabytes of usable storage including a performance and IOPS optimized tiers**.

Submission

Please submit your project proposal to https://apply.hpc.kaust.edu.sa/new_project/.

For any inquiries, please contact projects@hpc.kaust.edu.sa

Terms and Conditions regarding Research Publications

Whenever the results of research conducted on the HPC systems at KAUST are published, or the research involved personnel from KAUST Supercomputing Laboratory (KSL), Principal Investigators (PIs) are required to acknowledge the usage of the HPC systems at KAUST and/or the involvement of KSL personnel in their research in their publications. For example, the following statement could be used: **"For computer time, this research used Shaheen III managed by the Supercomputing Core Laboratory at King Abdullah University of Science & Technology (KAUST) in Thuwal, Saudi Arabia**.

KAUST Confidential (when completed)

KAUST Confidential (when completed)

Principal Investigator (PI):

Name:	
Email:	
Tel:	
Organisation:	
Position:	
Department:	
Organisation Address:	

Additional Investigators

1	**Name:**	
	Email:	
	Tel:	
	Organisation:	
	Position:	
	Org Address:	
2	**Name:**	
	Email:	
	Tel:	
	Organisation:	
	Org Address:	

Collaborators (External):

1	**Name:**	
	Email:	
	Tel:	
	Organisation:	
	Position:	
	Org Address:	

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Project Description:

Describe the project concretely and clearly define the unsolved research problem or question that the project is supposed to solve

Please describe the activities proposed, including current state of art, research work proposed, *expected milestones, and deliverables, as well as a summary description in the box below, and include the scientific field of the investigation as part of the description.*

***Note**: Citations of the scientific literature are encouraged in order to show where the proposed simulations stand with respect to the 'state of the practice' in terms of such factors as model generality, resolution, and advantages of simulation versus experiment and theory.*

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Project Background:

Please describe the background to this project, including (i) what is the existing work in this area; (ii) what is the novelty of the proposed project; (iii) why is the proposed work significant; (iv) what is the common methodology to tackle similar problems; (v) does the proposed project follow a similar/different methodology; (vi) what are the expected outcomes of this project (vi) If you have other major HPC projects on Shaheen 2 or elsewhere, please make a summary of its results, including publications and other deliverables

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Scientific Impact:

Please detail the expected scientific impact of the proposed research.

In-Kingdom impact:

Please detail how will the proposed computational research impacts the Kingdom, and what specific benefits and contributions can it bring to the in-Kingdom's aspirations and priorities in Research, Development and Innovation (RDI), in Health and Wellness; Sustainable Environment and Supply of Essential Needs; Energy and Industrial Leadership; and Economies of the Future.

Codes & Libraries:

- *Please provide the following information for each code or library that will be used.*
- *If needed, please include the same information for any other codes or libraries to be used in 'Additional Information' at the end of this proposal, or attached on a separate sheet.*

1	**Name of Code/Library:**	
	Ownership / Licensing:	
	URL (*for Open Source codes*)	
	Function:	
2	**Name of Code/Library:**	
	Ownership / Licensing:	
	URL (*for Open Source codes*)	
	Function:	

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Code Readiness:

- *Please provide details of code performance and scalability achieved, and note any known issues that might impact production execution.*
- *For code beyond 5 nodes (beyond 1000 cores), please share the scalability table below for each code/application.*

1	**Name of Code/Library:**	
	Scalability on CPUs:	
	Known Issues:	
2	**Name of Code/Library:**	
	Scalability on CPUs	
	Known Issues:	

Resource Requirements:

Compute Resource	Requirement (core hours)	Duration (in Days)
Shaheen III		

Resource Requirement Justification:

Please detail how the above requirements were calculated. The nodes are exclusive.
Example: 4 simulations x 512 nodes x 192 cores x 20hours = 7,864,320core hours

Minimum size of runs (CPUs nodes)	
Maximum size of runs (CPUs nodes)	

Typical problem description:

Please describe typical problem size and duration e.g. typical job will use 100 nodes for 2 hours.

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Shaheen III extensions of projects

- **Time Extension Only**
  - Enter 0 in the **Core Hours** and **Storage** fields.
  - Include a proposal document containing:
    - A brief progress report.
    - A list of any publications that acknowledge Shaheen s

d Time Extension

cify the **additional Core Hours** and **Storage** required.

nplete the proposal document using the designated form

d a list of any publications that acknowledge Shaheen.

Extending a Project on Shaheen

Overview

Principal Investigators (PIs) can request project extensions on Shaheen by submitting an application using the f

Please note that only PIs can access the form and only their own projects will be displayed.

Shaheen project extension proposal

Project:

Extension proposal No file chosen

Core hours requested

Total storage requested (please enter 0 for the default 80TB)

Please enter a number.

Submit

Shaheen III Individual Access

- Submit IAA (https://apply.hpc.kaust.edu.sa/)
- Every user must be a member of at least one Shaheen III project
- Once the account is created, user will be notified by email with instructions to login
- Setup and Scan your OTP QR for Shaheen III
    1. Login with your KAUST credentials to https://hpc.kaust.edu.sa/user/login
    2. Answer your security question
    3. Scan your OTP QR Code from (My KSL > View My OTP Seed)

- Any issue, send an email to help@hpc.kaust.edu.sa

Shaheen III Individual Access

- Justify the resource requirements
- Review your project with your PI
- Feel free to contact us before submitting it.
- Don’t forget to acknowledge KAUST Supercomputing in your future publications.
    - **“For computer time, this research used Shaheen III managed by the Supercomputing Core Laboratory at King Abdullah University of Science & Technology (KAUST) in Thuwal, Saudi Arabia. “**

Agenda

- 8:30am Welcome
- 8:35am Shaheen III Overview
- 8:55am How to apply on Shaheen III
- **9:05am Getting Started on Shaheen III**
- 9:15am Software Environment
- 9:35am Job Scheduling
- 10:00am Coffee Break
- 10:15am Storage overview & Best practices
- 10:30am Applications software example: VASP workflow
- 10:50 am Applications software example: CFD applications
- 11:10 am Applications software example: Bio informatics workflow
- 11:20-11.30am Q&A and Open Discussion

Shaheen III Survey