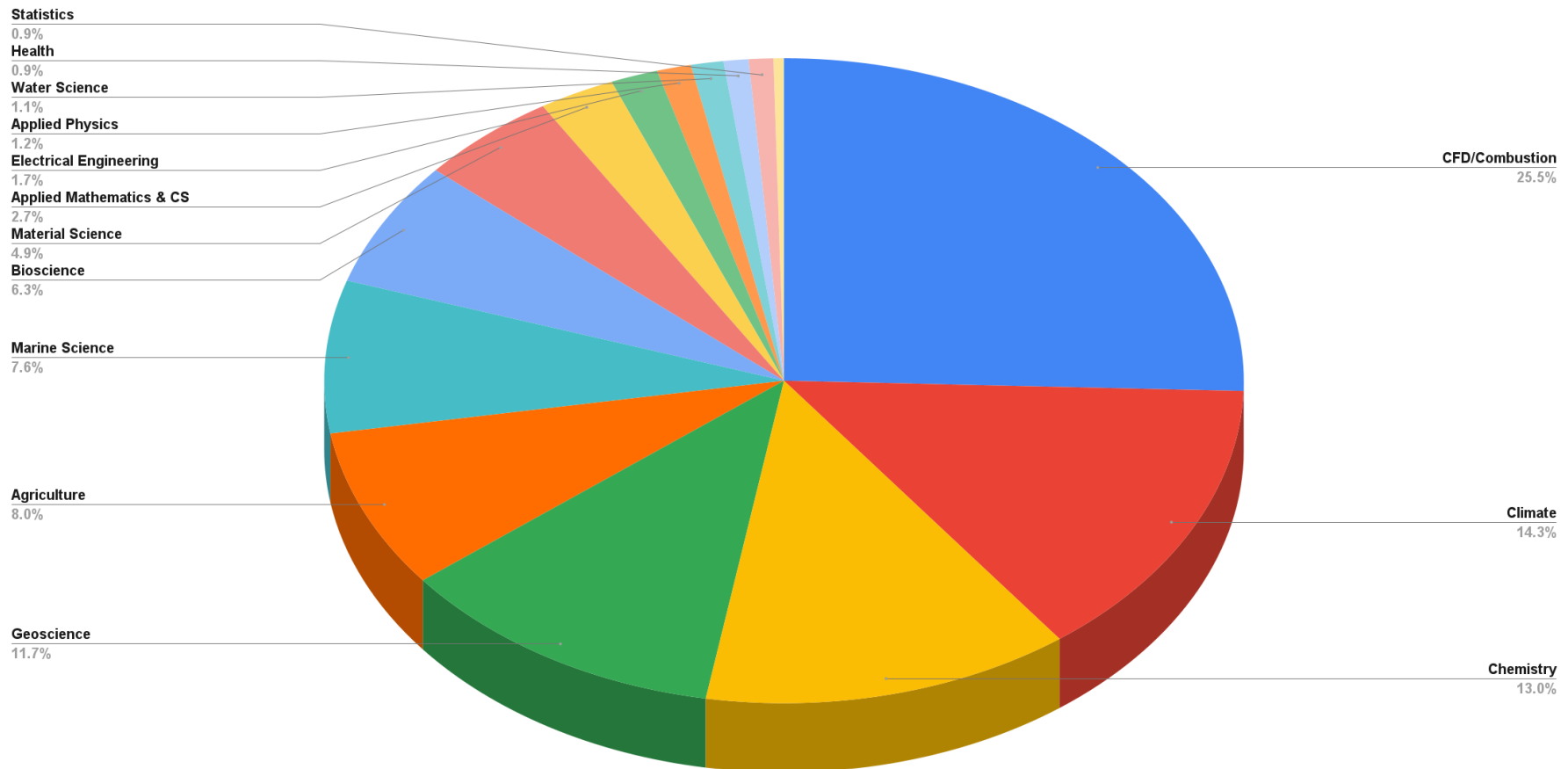


Shaheen III Access

Bilel Hadri, KAUST Supercomputing Lab

February 4th, 2025

Why access on Shaheen ?



Example of some early success !

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



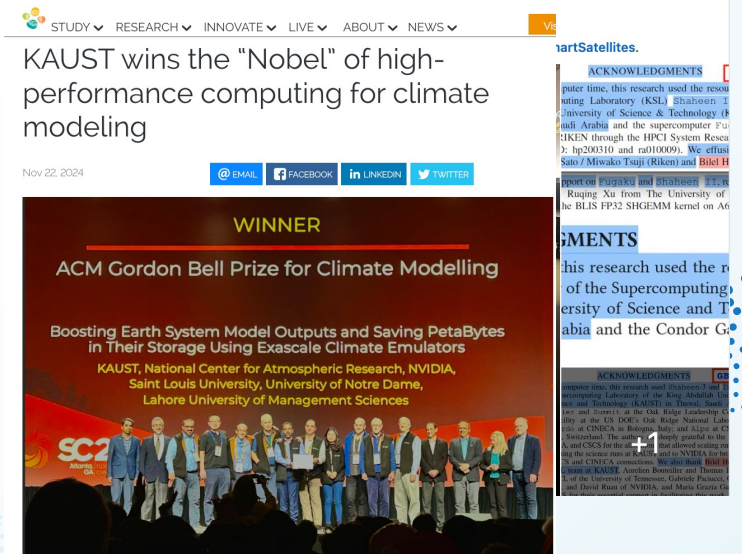
Hatem Ltaief · 1st
Principal Research Scientist at ECRC@KAUST
2mo · Edited · 🌐

These are the acknowledgment sections of our four #GordonBell campaigns in 2022, 2023, and 2024 (x2), including the winning paper on Climate Modeling this year. We would certainly not be able to reach the last stage without the support of our HPC leadership facility partners which granted us remote access to their supercomputers: #Fugaku at RIKEN, #CondorGalaxy at G42, #Leonardo at CINECA, #Frontier / #Summit at Computing at ORNL, and #Alps at CSCS.

One common HPC facility for these campaigns is obviously our own KAUST (King Abdullah University of Science and Technology) Supercomputing Lab from the KAUST Core Labs Admin, host to #Shaheen-2/3 and #Ibex.

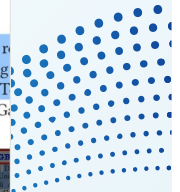
But one common person needs a particular attention: Bilel Hadri from the #KAUST Supercomputing Lab. With his 24/7 support and always on the phone line to deliver critical advices, we were like his pampered children! 😊

Thank you Bilel, you certainly deserve this award for being on the frontline with



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. Stenichkov, 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.



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.



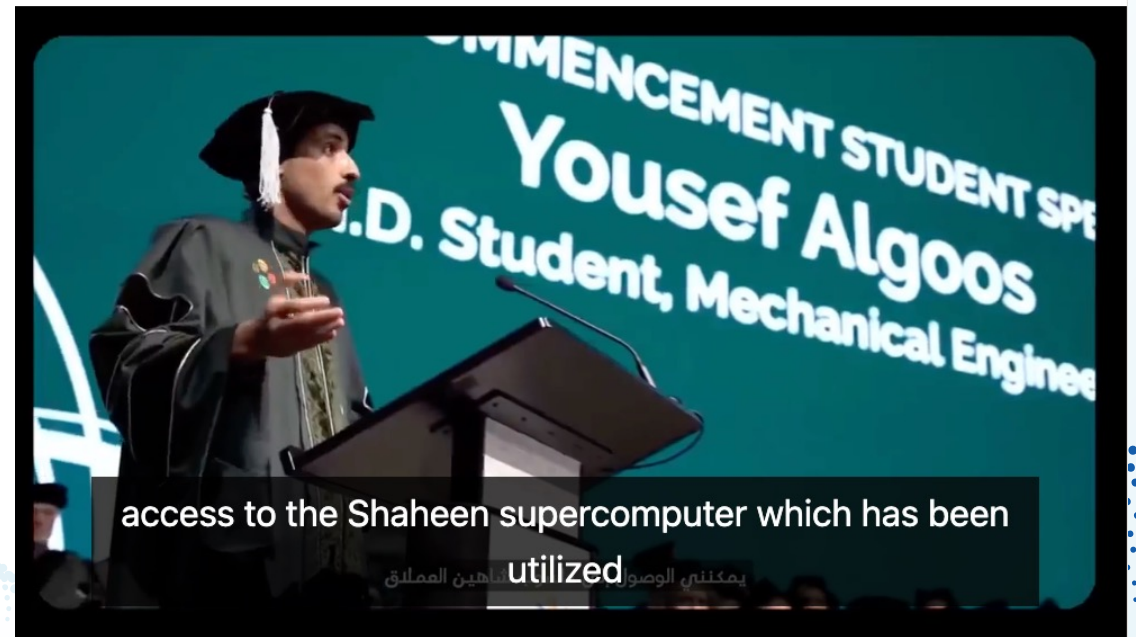
Shaheen mentioned during the graduation ceremony

Record number of Saudi students graduate from KAUST in 2024

Dec 13, 2024 Press Release



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

Many faculty are using Shaheen !

14

KAUST faculty among
Clarivate Highly Cited
Researchers 2024



Omar F. Mohammed
Cross-Field



Hylke Beck
Cross-Field



Osman M. Bakr
Chemistry



Carlos M. Duarte
Environment and
Ecology



Yoshihide Wada
Environment and
Ecology



Matthew F. McCabe
Cross-Field



Heribert Hirt
Cross-Field



Mohamed Eddaoudi
Chemistry



Luigi Cavallo
Cross-Field



Stefaan De Wolf
Cross-Field



Huabin Zhang
Cross-Field



Fernando T. Maestre
Environment and
Ecology



Yu Han
Materials Science



Salim Al-Babili
Plant and Animal
Science

Who are the KAUST PI on Shaheen III ?

- Aamir Farooq
- Andrea Fratalocchi
- Bernard Ghanem
- Cafer Yazuz
- Cristian Picioreanu
- David Keys
- 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
- Kuo-Wei Huang
- Luigi Cavallo
- Magdy Mahfouz
- Magnus Rueping
- Mani Sarathy
- Marc Genton
- Mark Tester
- Martin Heeney
- Martin Mai
- Matteo Parsani
- Min Suk Cha
- Mohamed Eddaoudi
- Mohamed Elhoseiny
- Nikos Hadjichristidis
- Noredine Ghaffour
- Omar Knio
- Omar Mohammed
- Panos Kalnis
- Pedro Castano
- Peter Richtarik
- Peter Schmid
- Robert Hoehndorf
- Rod Wing
- Rolf Krause
- Shadi Fatayer
- Shehab Elsayed
- Tariq AlKhalifa
- Udo Schwingschloegl
- Valerio Orlando
- Volker Vahrenkamp
- William Roberts
- Xin Gao
- Xixiang Zhang
- Ying Sun
- Yoji Kobayashi
- Yoshihide Wada

How to apply?

<https://hpc.kaust.edu.sa/>



Apply for Access

Home / Apply for Access

Getting an account on Shaheen is a three-step process. The KAUST Supercomputing Laboratory manages three user account entities - organisations, projects, and users. Every Shaheen user must be an official member of at least one project and every project must originate from an approved organisation.

1. For non-KAUST users, your organisation or department must submit the [Organisational Access Application \(OAA\)](#), establishing a relationship between your home organisation and the KAUST Supercomputing Laboratory (KSL). The form should be completed, printed, signed, scanned and emailed to help@hpc.kaust.edu.sa. Each external organisation must have submitted a completed Organisation Access Application before its account requests or project proposals can be considered.
2. The Principal Investigator (PI) must download and submit a Project Proposal Form. There are two distinct types of projects:
 - **Development project**: provides access for system familiarisation, code porting, performance assessment, and other pre-production work. **This form can be used only by KAUST PIs for assessing software not installed on Shaheen.** Development projects will **not** be allocated significant computing resources.
 - **Production project proposal**: can be allocated significant computing resources. The RCAC reviews each project based on not only the computational readiness reviews but also on scientific readiness reviews by faculty experts in the scientific field of the proposed project.
3. Each user must submit an [Individual Account Application \(IAA\)](#), supplying identification information from which we can generate login credentials.

Once the account is created, user will be notified by email and should follow [these](#) instructions to login.

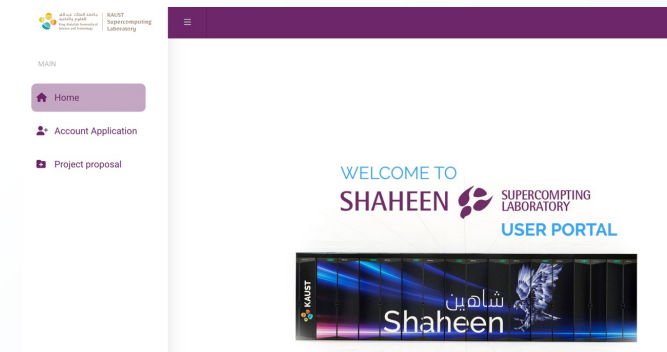
Steps 2 and 3 should be submitted through the [KSL Apply website](#) using KAUST portal (Active Directory) credentials. If you are an external user who has used Shaheen II and still have an **active** portal account, you may use these credentials to access the website. Otherwise, you should email help@hpc.kaust.edu.sa attaching a scan of your passport photo page in order to obtain your credentials.

Shaheen CPU usage is free of charge for KAUST PIs and their team members at KAUST. PIs and users should consult the [Terms and Conditions of Usage](#).

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

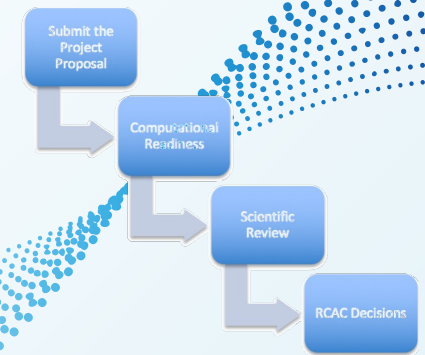
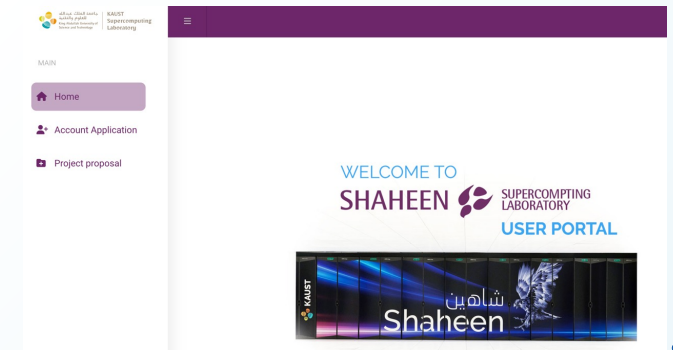
Any issue, send an email to help@hpc.kaust.edu.sa



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 عبد الله
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."

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):

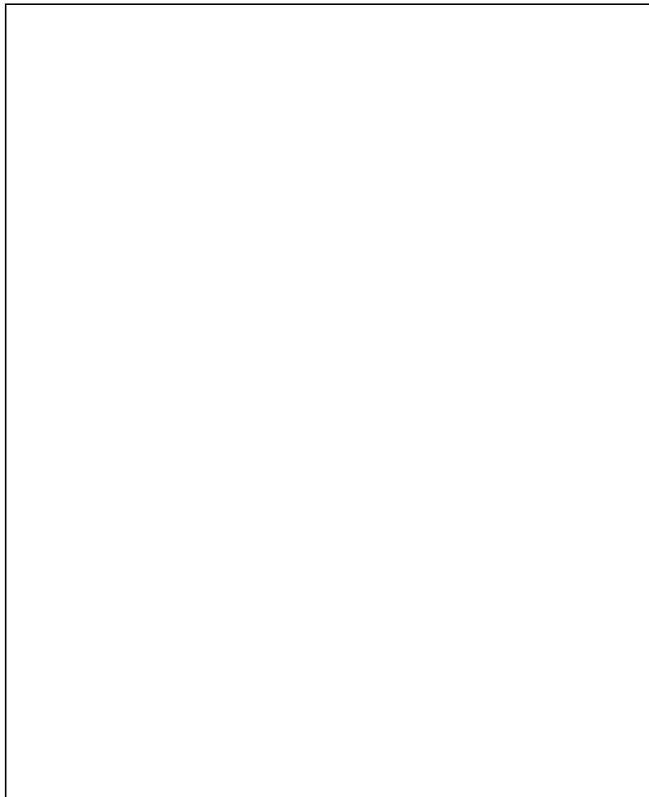
1	Name:	
	Email:	
	Tel:	
	Organisation:	
	Position:	
	Org Address:	

Project Description:

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

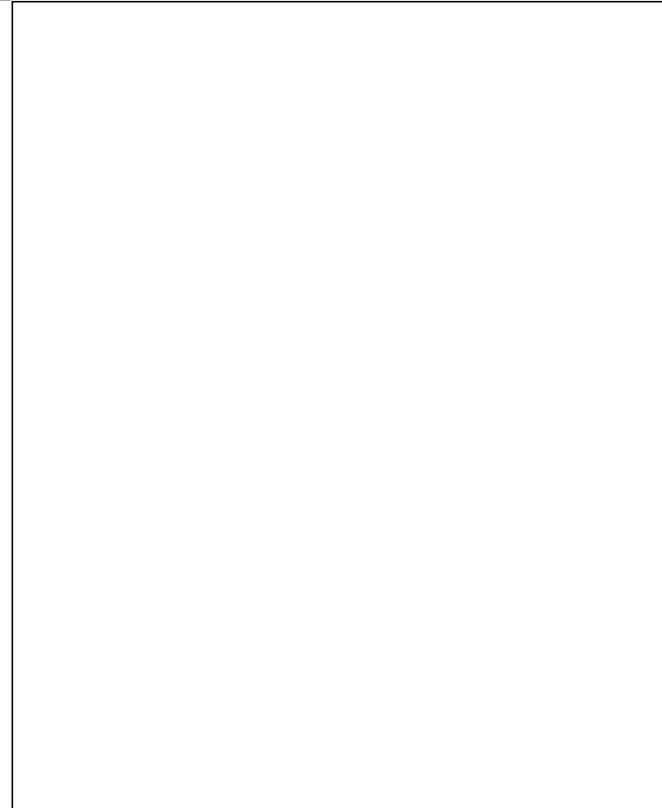
Please describe the activities proposed, including current state of art, research work proposed, expected milestones, and deliverables, as well as a summary description in the box below, and include the scientific field of the investigation as part of the description.

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.



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 (vii) If you have other major HPC projects on Shaheen 2 or elsewhere, please make a summary of its results, including publications and other deliverables



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:	

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 (<u>CPUs</u> nodes)	
Maximum size of runs (<u>CPUs</u> nodes)	

Typical problem description:

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

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 support.
- **Core Hour and Time Extension**
 - Specify the **additional Core Hours** and **Storage** required.
 - Complete the proposal document using the [designated form](#).
 - Send 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 form.

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.

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 Hardware 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

