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Reinforcing the Kingdom's Engineering Simulation Capability Through Training and Consulting

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The KAUST Supercomputing Laboratory has been serving the engineering community of Saudi Arabia for many years. This paper aims to highlight the KAUST Supercomputing Laboratory's educational, training, and consulting services that form their outreach program composed of two streams: modelling & simulation and deep learning for engineers. Since 2017, the KAUST Supercomputing Laboratory has conducted ten training workshops in collaboration with Ansys. The workshops were attended by researchers and students from KAUST and Saudi universities and industry, totaling 703 attendees. Based on the feedback from the participants, the training themes evolved with time from basic Computational Fluid Dynamics (CFD) and Computational Structural Mechanics (CSM) to multiphase flows, electromagnetism and multiphysics simulations. Hands-on sessions on workstations and Shaheen II are the key components of the workshops. In 2019, the KAUST Supercomputing Laboratory started a certification program that quickly gained popularity among Saudi students, certifying 353 students in CFD and CSM thus far. These engineering services of the KAUST Supercomputing Laboratory have a high potential to cater to the upcoming nuclear human capacity building within the Kingdom. In this paper, we describe the engineering services offered to the Kingdom, discuss the lessons we learned along the way, and outline the future direction these services can take to better prepare emerging Saudi engineers for meeting the needs of today's job market.

Keywords: Computational Fluid Dynamics (CFD), High Performance Computing (HPC), Supercomputing, Modeling and Simulation (M&S).

I. Introduction

Whether we – the older generation, like it or not, today's teenagers interact, enjoy, and even rely on technology in their day-to-day routine. For instance, it is common for middle school students to use ChatGPT [1] when completing their assignments. Consequently, it is imperative for parents and teachers to explain the concept of academic honesty to the students, and educate them on the consequences of breaching such policies. On the other hand, it is also critical for educators to first learn and integrate the latest technology into their syllabus to ensure their students gain proficiency in using various software, tools, and platforms, equipping them with the skillset to succeed in the evolving job market. Familiarity with technology-enhanced learning also nurtures a sense of adaptability and lifelong learning.

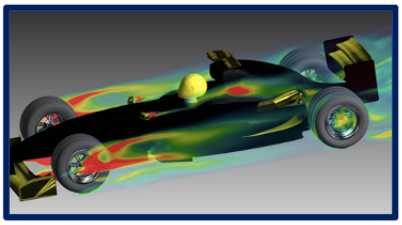
Theory and experimentation have been a cornerstone of our educational system for centuries. Computer based modeling & simulation (M&S) and data driven science are relatively recent paradigms for scientific discoveries [2]. It is imperative to introduce young students to M&S and data driven science at an early stage. The KAUST Supercomputing Laboratory has been serving the engineering community of Saudi Arabia for several years. This outreach program has two streams: M&S and deep learning for engineers. This paper describes various services that are being offered to the students, faculty and researchers. Figure 1 displays the various components of the KAUST

Supercomputing Laboratory's outreach program, and these are described in greater detail in the subsequent sections. The target audience range from undergraduate engineering students to experienced engineering professionals. Therefore, the language and technical details are simplified so that the larger audience can benefit from the contents. It is assumed that the readers have little to no background in computer science or High Performance Computing (HPC).

Fig. 1. Various components of the engineering services outreach program at the KAUST Supercomputing Laboratory

II. The Role of HPC in Modeling and Simulation

Most of the physical phenomena around us are modelled by partial differential equations (PDEs). PDEs are discretized by employing numerical methods such as finite difference, finite volume or finite element [3-6]. The discretization process converts PDEs into algebraic equations. Computers are very efficient in solving dense or sparse matrices. In order to minimize the discretization error, the computational domain must be modeled by extremely fine meshes which, in turn, results in large matrices that often exceed the memory of an average desktop computer.



F1 racecar; 140m; 100 iterations			
Cores	Time (sec)	Speedup	Ideal
1024	676.034	1	1
2048	380.671	1.8	2
4096	200.926	3.4	4

Fig. 2. Strong scalability of a CFD simulation of a F1 racecar on Shaheen II using Ansys-fluent [7]

To solve real world problems, HPC platforms enable the users to distribute a single large-scaled model on many processors, a strategy that reduces the time it takes to reach a solution as the number of processors increases. Figure 2 showcases the strong scalability of a F1 car simulation on KAUST's supercomputer – Shaheen II [8]. As the numbers of cores increased from 1024 to 4096, the time to reach a solution reduces by a factor of almost three and a half – which is given the term *speedup*. It must be noted that the speedup numbers depend on various factors (e.g., problem size, programing style of the software, interconnect type and topology used in the cluster etc.) and are problem-specific [9]. However, the intent here is that if the right software and infrastructure are utilized, engineers can significantly increase their productivity.

III. Infrastructure

KAUST has demonstrated its commitment to providing HPC infrastructure for not only KAUST researchers but for the Kingdom's academic and industrial users as well. Figure 3 shows three generations of Shaheen supercomputers, which were all highly globally ranked.

Fig. 3. Family of Shaheen supercomputers at the KAUST Supercomputing Laboratory [8, 10]

Shaheen's access is provided by following a rigorous allocation process. However, under this program, new users from all over the Kingdom are provided a chance to use Shaheen for hands-on training sessions by creating temporary accounts. Moreover, users of the KAUST Supercomputing Laboratory's consulting services are given the option to use Shaheen for speeding up their calculations.

In addition to Shaheen, cloud-based services are also offered to the participants via an easy-to-use interface. This solution is preferred by users lacking HPC expertise and would opt for a more workstation-like experience on the HPC infrastructure. Notably, first-time cloud users often require our guidance in properly sizing and pricing the cloud instances.

IV. Software Installation

The users transitioning from a workstation to a supercomputer must alter their workflow. In order to ease their transitioning experience. The majority of the continuum mechanics software are pre-installed on our HPC infrastructure. The users can simply load the environment and start using the software of their choice on Shaheen. Furthermore, there are sample tests available for the users to run a typical job on Shaheen. Users are also provided assistance with installing certain software on their workstations. For example, a user may require an Ansys workbench and Tecplot installations on their workstation for pre- and post-processing, respectively, as well as Fluent on the supercomputer. Figure 4 lists the supported software. Additional software can also be installed upon request.

Fig. 4. List of supported software for KAUST Supercomputing Laboratory users

V. Software Licenses

The software typically used for engineering simulations are either open source or licensed. Open-source software (e.g., OpenFOAM) are available for all users. Access to a licensed software like Tecplot requires individuals to purchase the license and share the license file to make the software available in a secure manner. To democratize the use of easy-to-use commercial engineering software, KAUST purchased 11,000 licenses of one of the most popular engineering software – Ansys, for KAUST researchers as well as researchers and students from any Saudi University with an Ansys license. The Ansys license provided by KAUST are also available to users from the Saudi industry for open research purposes. Ansys suite consists of fluent, mechanical, aedt, CFD post, SpaceClaim, chemkin and discovery live, for performing fluid mechanics, solid mechanics, electromagnetics, visualization, geometric modeling, chemistry, and real-time simulation, respectively. The licenses are shared by all users at a given time. If only a single user is accessing an Ansys license at a given time, he/she can potentially scale the simulation on Shaheen and reduce the time to reach the solution by a factor of 11,000 – thus tremendously increasing his/her productivity.

VI. Helpline

KAUST Supercomputing Laboratory provides a helpline, where a user or any member of the general public can send a question via email (i.e., CFD-Helpline@hpc.kaust.edu.sa) and get a response within 24 hours. In the last two years, since the launch of this service, over 250 tickets have been logged and closed. The requests generally fall into the following categories:

- Installation, automation and scripting
- Speeding up of simulations
- Numerical analysis based academic questions
- Student mentoring
- Laboratory experiment scientist (e.g., wind tunnel engineer) seeking simulation assistance for verification
- Developers seeking validation of their code's results with a third-party code

VII. Training

Since 2017, the KAUST Supercomputing Laboratory has conducted ten training workshops in collaboration with Ansys and Fluid Codes (Ansys channel partner [11]). The workshops were attended by researchers and students from KAUST and by Saudi universities and industry, totaling 703 attendees. Participant's feedback helped shape the design of future workshops, where the training themes evolved from basic CFD and CSM to multiphase flows, electromagnetism and multiphysics simulations. Hands-on sessions on workstations and Shaheen II are the key components of the workshops, as shown in Figure 5.

Fig. 5. Students performing hands-on training sessions on their computers

Numerous step-by-step trainings are provided online for data science, machine learning and deep learning. However, emerging engineers usually come to the consensus that Python tools are challenging to apply and maintain. These students attend conferences, watch tutorials and learn a particular example crafted conveniently for the platform provided by the trainer. When these students try to run the acquired example on their personal workstation, they learn about the various dependencies they are missing. While computer science students usually independently manage such situations, engineering students may need additional support and guidance to proceed to the next step. To tackle this problem, the KAUST Supercomputing Laboratory teamed up with MathWorks [12] and CES (the exclusive partner of MathWorks in the Middle East [13]) to offer MATLAB-based deep learning trainings for engineers – a platform that provides robust and easy-to-learn tools for beginners. In the last three years, over 350 people from all over the Kingdom were trained on MATLAB's machine learning and deep learning toolkit in the area of computer vision, classification, transfer learning, time series, analyzing sensor data, LSTM, and seismic facies classification.

VIII. Consulting

In 2022, the KAUST Supercomputing Laboratory launched a pilot consulting program for engineering simulations. The consulting service is available for all researchers and students in the Kingdom. To get paired with an expert consultant, an individual must submit a simple project proposal which then gets reviewed by a recently formed national review and steering committee. Upon successful review, an expert is assigned to the approved project. To submit a project for review, one can scan the QR code featured in Figure 6.

Fig. 6. QR code for consulting project proposal

During the pilot program, a CFD expert is hired by the KAUST Supercomputing Laboratory for 6-months for providing consulting support. Data obtained during the pilot phase will clarify ways to improve and scale-up the program, eventually charging the users for the consulting services. The pilot phase, however, is free of cost at this time.

IX. Education

In 2019, the KAUST Supercomputing Laboratory started a certification program that rapidly gained popularity among Saudi students. Thus far, 353 students successfully passed the certificate exam, certifying them in CFD and CSM.

As discussed earlier, the younger generation uses technology much more proficiently than the older one. In the KAUST School (TKS), grade 9 and 10 International Baccalaureate (IB) Design Technology students are developing 3D models of F1 racecars using Fusion360. With some extra support and a few training sessions, these students have learned to import their models in Fluent, place a box around it, mesh the computational domain, apply boundary conditions and run the simulation. In partnership with TKS teachers, the middle school students were introduced to an easy-to-use simulation tool – Ansys Discovery Live. The students were given a demonstration on how they can perform a basic CFD simulation within minutes, as shown in Figure 7. This real-time CFD tool became rather popular among the grade 9 & 10 students and is now being used by several departments at TKS.

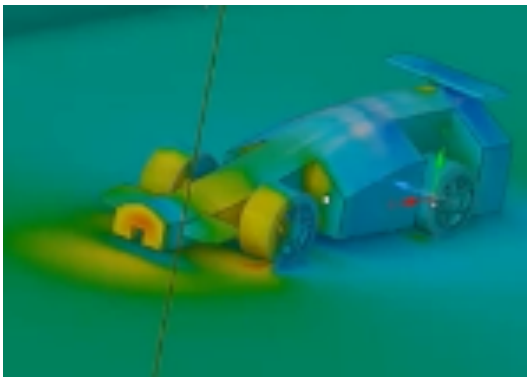


Fig. 7. High school students perform CFD analysis on F1 car model using Ansys Discovery Live

X. Community Building

Scientific education community building involves the creation of a collaborative ecosystem where individuals with a shared passion for science can connect, learn, and grow together. This process encompasses a variety of activities, such as organizing or participating in workshops, seminars, and conferences that facilitate the exchange of knowledge and ideas. In order to outreach to the Kingdom's engineering community, various KAUST-based workshops were organized, helpline is established, talks were delivered in national conferences (e.g., HPC Saudi), a national review and steering committee was created, and booths were setup in Saudi universities (see Figure 8) throughout the Kingdom [14, 15]. It is envisioned that these steps will contribute to the Saudi Vision2030 [16] movement by preparing a workforce ready to tackle today's growing digital job market.

Fig. 8. Discussion with the faculty at Imam Abdulrahman bin Faisal University (IAU)

XI. Proposed Services for the Kingdom's Nuclear Industry

Due to the rapid increase in energy demand and to use petroleum for higher value purposes and export, the Kingdom is planning a sustainable energy mix that includes atomic energy to meet the energy needs of the Kingdom to produce electricity, desalinated water and thermal energy [17]. Numerical simulations, such as thermal hydraulic analysis, is a critical component of designing and analyzing nuclear reactors. A new training module about thermal hydraulics application in nuclear industry will be added to the ongoing KAUST Supercomputing Laboratory's training program. Equipping Saudi students with skills relevant to the nuclear industry enhances their career readiness. They are better prepared to enter industries that rely heavily on technology, as they already have experience with advanced tools commonly used in thermal hydraulics simulations.

Starting in 2025, the International Thermonuclear Experimental Reactor (ITER) is set to initiate a 15-year phase dedicated to showcasing the scientific and technological viability of fusion energy [18, 19]. Engineers from various corners of the world have joined forces for many years to create this cutting-edge achievement, crafted to achieve unprecedented levels of fusion power gain. The scope of consulting projects will be broadened to include projects from the Saudi faculty to overcome the challenges of designing and sustaining self-sufficient fusion reaction that needs to be maintained at 150 million °C. The research could entail cooling design of various components and structural design of materials under extremely high temperature and severe cyclic loading.

XII. Summary

The paper introduces the KAUST Supercomputing Laboratory's outreach program, with streams in modeling and simulation and deep learning. The program serves a broad audience from undergraduates to experienced professionals. It emphasizes simplifying technical language for a wider audience. The role of high-performance computing (HPC) in M&S is discussed, focusing on solving complex problems by distributing them across processors. The scalability of simulations on KAUST's supercomputer, Shaheen II, is exemplified.

The software suite supported by the KAUST Supercomputing Laboratory, including both open-source and licensed software, is detailed. A helpline assists users in various categories, while training workshops and online resources educate users on data science, machine learning, and deep learning. A consulting program for engineering simulations is described, and an education initiative certifies students in computational fluid dynamics (CFD) and computational solid mechanics (CSM).

The paper highlights community building efforts, including workshops, seminars, and national conferences, to foster knowledge sharing. The broader aim is aligning with Saudi Vision 2030 by preparing a digitally adept workforce. The example of high school students using Ansys Discovery Live for CFD analysis underscores the success of these efforts in equipping students with essential skills for a technology-driven future.

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