

**HPC User Forum, May 2021**



# Building HPC/AI Ecosystem in the Kingdom of Saudi Arabia

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King Abdullah University of Science and Technology





# Shaheen II Supercomputer



جامعة الملك عبد الله  
للعلوم والتقنية  
King Abdullah University of  
Science and Technology

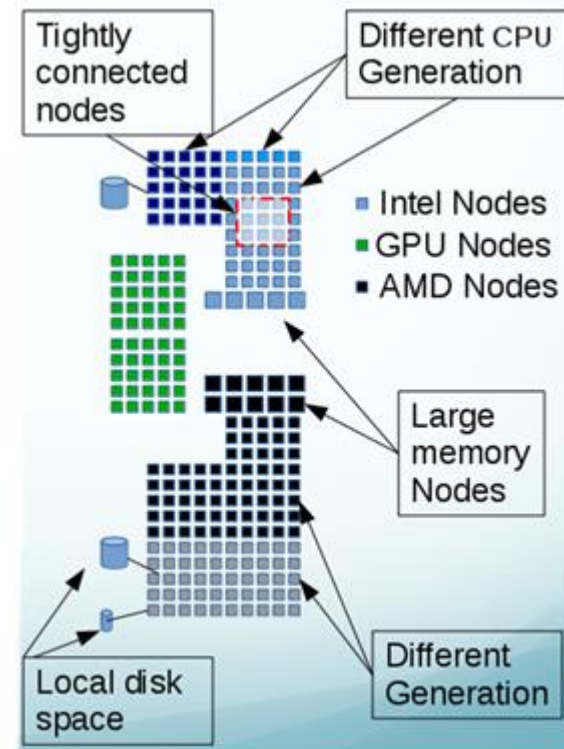
<b>Compute</b>	Node	Processor type: Intel Haswell	2 CPU sockets per node @2.3GHz 16 processor cores per CPU
		6174 nodes	197,568 cores
		128 GB of memory per node	Over 790 TB total memory
	Power	Up to 3.5MW	Water cooled
	Weight/Size	More than 100 metrics tons	36 XC40 Compute cabinets, disk, blowers, management nodes
	Speed	7.2 Peta FLOPS peak performance	5.53 Peta FLOPS sustained LINPACK and ranked 52 <sup>th</sup> in the latest Top500 list
	Network	Cray Aries interconnect with Dragonfly topology	57% of the maximum global bandwidth between the 18 groups of two cabinets
<b>Storage</b>	Storage	Sonexion 2000 Lustre appliance	17.6 Peta Bytes of usable storage Over 500 GB/s bandwidth
	Burst Buffer	DataWarp	Intel Solid State Devices (SSD) fast data cache Over 1.5 TB/s bandwidth
	Archive	Tiered Adaptive Storage (TAS)	Hierarchical storage with 200 TB disk cache and 20 PB of tape storage, using a spectra logic tape library (Upgradable to 100 PB)



# Ibex Cluster

## Total of 408 Computing Nodes

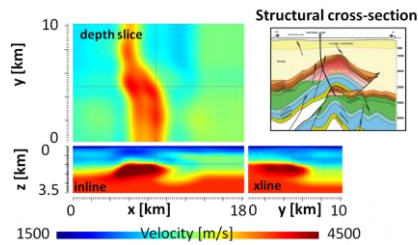
- **Intel Nodes (216)**  
Skylake (108), Cascade Lake (108)
- **AMD Nodes (108)**  
Rome (108)
- **GPU Nodes (62), GPU Cards (394)**  
V100 (30x8, 8x4, 1x2),  
1080Ti (4x8, 8x4), 2080Ti (4x8),  
P100 (5x4), P6000 (2x2)
- **Large Memory Nodes (22)**  
Skylake (4, 3TB), Cascade Lake (18, 3TB)
- **Storage (11.2PB)**  
Scratch (4.1PB + 1.2PB + 1.0PB),  
Fast Scratch (90TB),  
Encrypted (4PB + 330TB),  
NetApp (500TB)



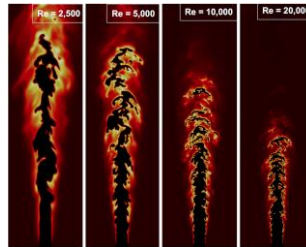
# Applications on Shaheen



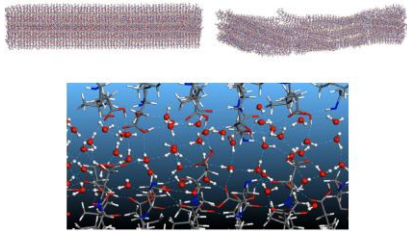
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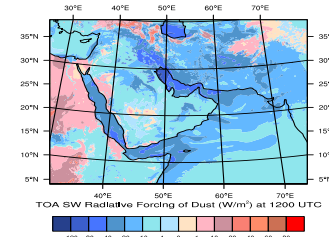
Geoscience



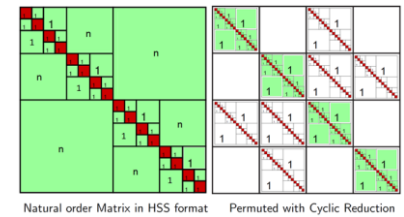
Computational Fluid  
Dynamics and  
Computational Solid  
Mechanics



Bioscience, Chemistry,  
and Material Science



Atmospheric  
Science

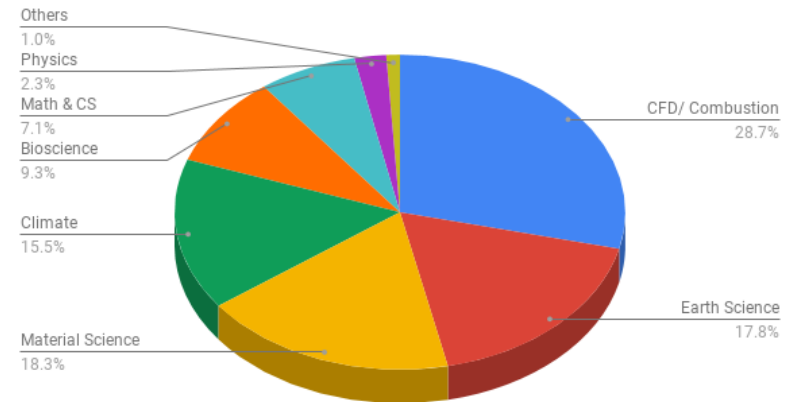


Computer Science and  
Applied Mathematics

# Shaheen Utilization

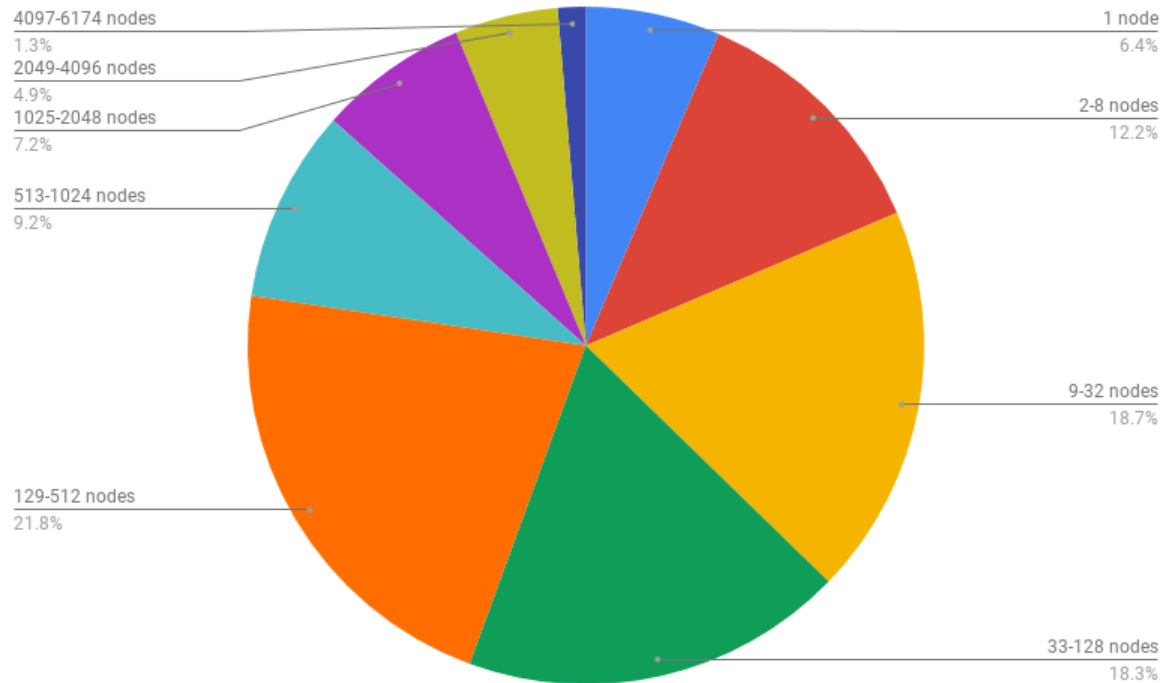
- Provided 5.62 Billion Core Hours
- Supported 540 Projects from 180 PIs

Field of Science	Core hours used	% of core used
CFD/ Combustion	1,615,447,801	28.73%
Earth Science	1,003,447,004	17.85%
Material Science	1,028,356,558	18.29%
Atmospheric Science	873,688,560	15.54%
Bioscience	521,047,178	9.27%
Math & CS	396,834,705	7.06%
Physics	128,530,748	2.29%
Others	54,640,798	0.97%



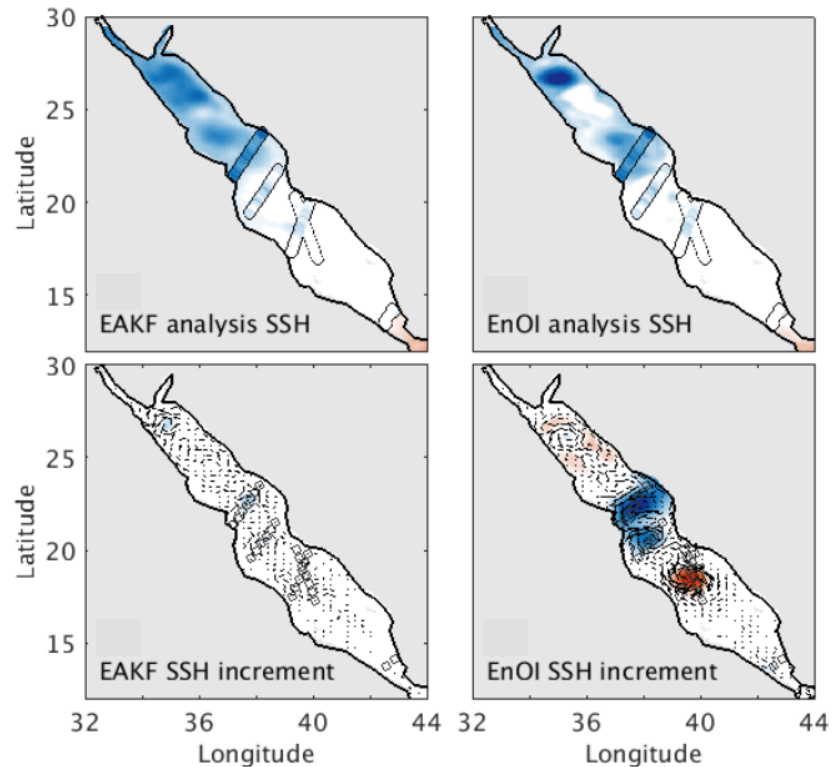
# Shaheen Workloads

- 62.7% hours for > 1024 Cores
- 25% hours for > 16K Cores



# Modeling and Forecasting the Red Sea with Data Assimilation

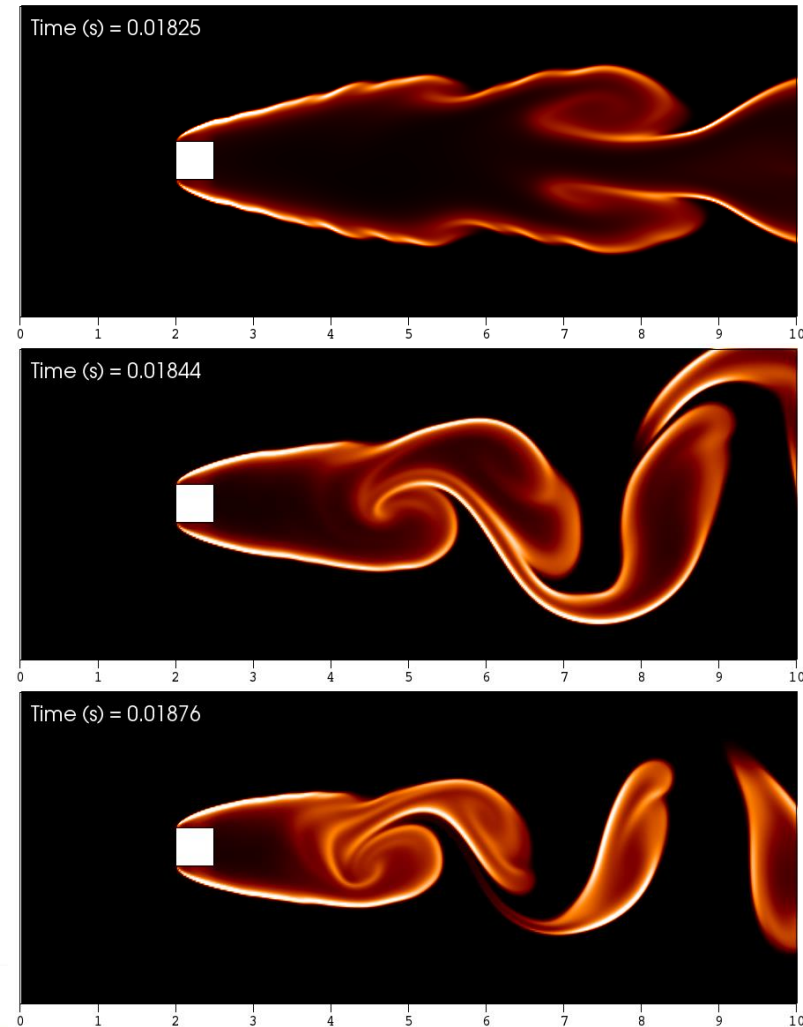
- PI: Ibrahim Hoteit
- A fully parallel ensemble-based ocean data assimilation and forecasting system has been implemented for the Red Sea
- We have investigated the best ensemble approach for forecasting and reconstructing the history of the Red Sea circulations
- A one-year ensemble assimilation experiment with 250 members cost about 250K core-hours on KAUST Shaheen supercomputer. We have conducted dozens of these.



Toye et al. "Ensemble Data Assimilation in the Red Sea: Sensitivity to Ensemble Selection and Atmospheric Forcing." *Ocean Dynamics*, 2016

# Direct Numerical Simulation on Dynamics of Bluff-Body Stabilized Flames

- PI: Hong G. Im, PSE/CCRC
- Direct numerical simulations of the dynamics of bluff-body-stabilized flames
- High fidelity simulations with full temporal and spatial resolution and description of detailed hydrogen and syngas chemistry provide fundamental insights into the mechanism of flame blow-off, which is a critical practical issue in gas turbine combustors.
- The simulations consumed about 6 million CPU-hours on KAUST's Shaheen supercomputer utilizing 3,200 cores

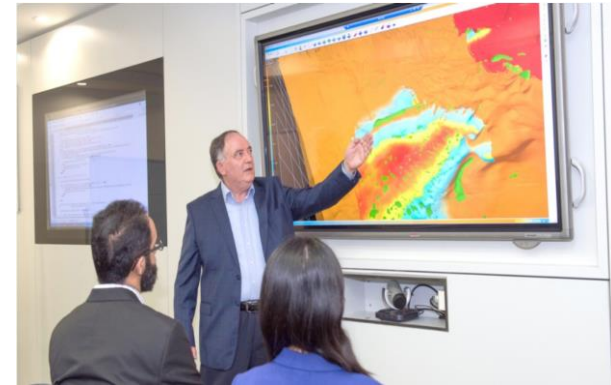


# Providing HPC Services to the Kingdom

- **Industry (3)**
  - Aramco, SABIC, UnitX
- **Government (4)**
  - GAMEP, KACST, KACARE, LBS
- **Academia (11)**
  - Alfaisal University
  - Imam Abdulrahman Bin Faisal University
  - Jouf University
  - Jubail University
  - King Abdulaziz University
  - King Fahd University of Petroleum & Minerals
  - King Faisal University
  - King Faisal Specialist Hospital & Research Centre
  - King Khaled University
  - King Saud University
  - Taif University

# Aramco 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*

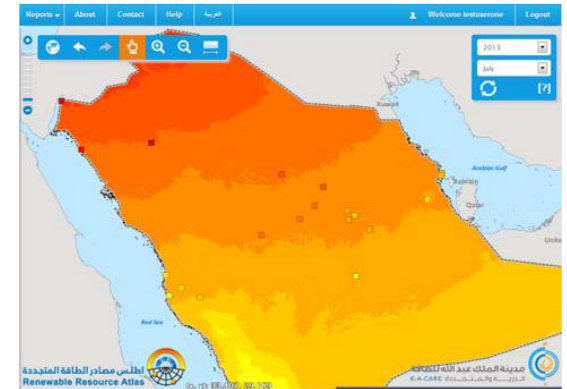


The EXPEC Advanced Research Center (EXPEC ARC) TeraPOWERS Technology Team, under the leadership of Saudi Aramco fellow Ali Dogru, achieved a major breakthrough with the industry's first trillion cell reservoir simulation run on October 28, 2016

**Aramco news, Dhahran, November 23, 2016**

# Enhanced Forecasting of Solar Radiation in the Kingdom

- KAUST has been working with KACARE (King Abdullah City for Atomic and Renewable Energy) to understand the Kingdom's solar irradiation and atmospheric weather conditions
- Completed simulating and archiving weather and atmospheric conditions from 2005 to 2018
- Currently working to provide daily forecast of weather and atmospheric conditions (dust and air pollutants) over the Arabian Peninsula





# Reduce Non-Technical Losses in KSA Residential Power Sector

- KAUST has been working with SEC (Saudi Electricity Company) to apply visualization and machine learning tools to reduce non-technical losses in residential power sector
- KAUST scientist helped SEC to build BI (Business intelligence) dashboard for easy display and analysis of customer data
- KAUST scientist applied machine learning tools to detect anomalous billing transactions. This method predict anomalous power consumption with 75% accuracy (compared to 3% by random survey of customers) with potential savings of \$20M annually

# Training on Engineering Simulation

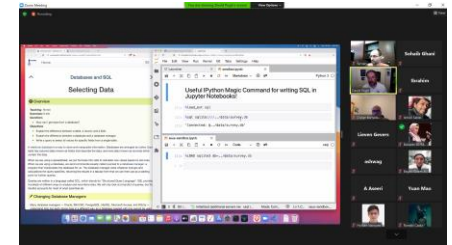
- Educate the next generation of leaders in the field of engineering simulation for the era of digital economy
- Providing training on tools from Altair, ANSYS COMSOL, Convergent Science, MathWorks, Tecplot
- ANSYS
  - Held 7 workshops since: total attendee of 408
  - Held 4 certification programs: total certified of 188
  - Associate License: Paving the way for industrial use of ANSYS on Shaheen
- MATLAB
  - Provide easy way to apply deep-learning to engineering problems
  - Online event with 192 attendees





# Introduction to Data Science Workshops

- Help research community to get started with core data science tools, and to enable future data science applications
- Consists of seven individual workshops; given at each semester
  - Introduction to Shell for (Data) Scientists
  - Introduction to Conda for (Data) Scientists
  - Introduction to Python for Data Science
  - Introduction to Git for (Data) Scientists
  - Introduction to SQL for Data Science
  - Introduction to Machine Learning with Scikit-Learn
  - Introduction to Deep Learning Image Classification with Keras



415 Attendees in 2020 Fall Workshop

# HPC

## SAUDI ARABIA

Building the HPC Community in the Kingdom

Conference  
Plenary Sessions  
Tutorials  
✉ email  
Social

March 13th - 15th, 2017

March 13th - 14th, 2017

March 15th, 2017

[contact@hpcSaudi.org](mailto:contact@hpcSaudi.org)

[f](#) | [t](#) | [in](#)

[REGISTRATION »](#)

High Performance Computing Saudi Arabia (HPC Saudi) is the premier regional event in the field, where participants can meet each other, share ideas and experiences, and discuss cooperation and collaboration. This is the seventh HPC Saudi event and this year it will focus on coordinated efforts for the advancement of the HPC ecosystem in the Kingdom.

Hosted by

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[About KAUST »](#)

## Keynote Speakers



Dr. Steven E. Koonin

Director, NYU Center for  
Urban Science and  
Progress



Dr. Thomas Schulthess

Director, Swiss National  
Supercomputing Centre  
(CSCS) at Lugano



Dr. Robert G. Voigt

Senior Member of  
Technical Staff, Krell  
Institute, US DOE

## Important Dates

**January 7th, 2017**

Tutorial Proposal Submissions

[Poster Submission](#)

**February 1st, 2017**

KAUST Inn [Hotel Reservations](#)

Application for [Student Travel Awards](#)

**March 1st, 2017**

[Registration Deadline](#)

**Are there special challenges  
associated with operating  
an HPC center in Saudi Arabia?**

# Thank You!

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