





3rd International Computational Science and Engineering Conference 21 – 22 October 2019 Doha, Qatar http://icsec.qatar.tamu.edu/

The 3rd International Computational Science and Engineering Conference will be held in Doha, Qatar on 21 and 22 October 2019. The conference aims to bring together researchers from academia and industry from Qatar and abroad to discuss recent research advances and plan future collaborations. The conference consists of keynote lectures, oral presentations and posters.

The main themes of the conference are:

- A. Computational Materials Science and Engineering,
- B. Computational Biology,
- C. Artificial Intelligence, Data Science and High Performance Computing.

A list of representative topics includes:

- A. Computational Materials Science and Engineering:
 - 1. Advances in applying different computational techniques at various time and length scales (Quantum Mechanics, Molecular Dynamics, Monte Carlo simulations, Continuum Modelling, Statistical Machine learning, etc.),
 - 2. Novel materials discovery and design (soft materials, polymers, electronic materials, hybrid materials, etc.),
 - 3. Advances in Materials degradation and aging simulations,
 - 4. Materials for Energy conversion, capture and storage,
 - 5. Reservoir modeling and simulation.
- B. Computational Biology:
 - 1. Genome analysis / annotation, Comparative genomics and Genome variations,
 - 2. Sequence analysis, and Genome-wide association study,
 - 3. Epigenomics and transcriptomics data analysis
 - 4. Computational methods in personalized medicine,
 - 5. Structural Bioinformatics,
 - 6. Modeling and simulation of biological networks.
- C. AI, Data Science and High Performance Computing
 - 1. Artificial intelligence and its applications in engineering and science,
 - 2. Large Scale Computing, parallel and distributed computing, cloud computing,
 - 3. Hardware and software HPC architecture,
 - 4. State-of the art data management and data mining techniques,
 - 5. Big Data Science, data-driven techniques and systems-related,













6. 3D scientific visualization techniques.

Young Investigator awards:

3 prizes will be awarded to the best presentation/poster delivered by young investigators and researchers (below the age of 35 years). These awards are sponsored by the **Computational Materials and Processes Center of the Qatar Environment and Energy Research Institute at Hamad Bin Khalifa University:**

- 1st prize 1000 USD/team
- 2nd prize 500 USD/team
- 3rd prize 300 USD/team

Keynote and Invited Speakers:

- ✓ Prof. Ilja Siepmann, University of Minnesotta, USA.
- ✓ Prof. Stefano Sanvito, Trinity college Dublin, Ireland.
- ✓ Prof. Taylor Sparks, University of Utah, USA.
- ✓ Prof. Sanjay Chawla, Qatar Computing Research Institute, Hamad Bin Khalifa University, Qatar.
- ✓ Dr. Ligang Lu, Shell International Exploration and Production Inc, USA.
- ✓ Prof. Normand Mousseau, University of Montreal, Canada
- ✓ Prof. Charlotte Becquart, ENSCL, France.

Abstract submission deadline: 15 May 2019

You are kindly invited to submit your abstract electronically through the conference website, at <u>http://icsec.qatar.tamu.edu/</u>. Please use the template provided in the conference website for your abstract. Oral presentations at the conference will be based on a peer-reviewed selection of abstracts.

Moreover, full papers from the conference will be published in a special issue of the **Journal of Computational Science**, based on a standard peer-review process.

Important deadlines:

- ✓ 27 January 2019: Abstract submission opens,
- ✓ 15 May 2019: Abstract submission ends,
- ✓ 10 june 2019: Abstract acceptance notification,
- ✓ Post-conference: TBA

Conference contact points: <u>icsec@qatar.tamu.edu</u>

✓ Othmane Bouhali, Texas A&M University at Qatar, Qatar Computing Research Institute, Hamad Bin Khalifa University, Conference Chairman,













- ✓ Ioannis G. Economou, Texas A&M University at Qatar, Conference Program Chair,
- ✓ Fadwa El-Mellouhi, Qatar Environment & Energy Research Institute, Hamad Bin Khalifa University.

Conference organizing committee:

- ✓ Ahmad Abushaikha, Hamad Bin Khalifa University.
- ✓ Omar Albagha, Qatar Biomedical research Institute, Hamad Bin Khalifa University
- ✓ Abbes Amira, Qatar University
- ✓ Dhruv Arora, Qatar Shell Research & Technology Center
- ✓ Halima Bensmail, Qatar Computing Research Institute, Hamad Bin Khalifa University
- ✓ Faycal Bensaali, Qatar University
- ✓ Joseph Boutros, Texas A&M University at Qatar
- ✓ Abdesselam Bouzerdoum, Hamad Bin Khalifa University
- ✓ Othmane Bouhali, Texas A&M University at Qatar, Qatar Computing Research Institute, Hamad Bin Khalifa University
- ✓ Ioannis G. Economou, Texas A&M University at Qatar
- ✓ Fadwa El-Mellouhi, Qatar Environment & Energy Research Institute, HBKU
- ✓ Tamer Elsayed, Qatar University
- ✓ Mohamed Nounou, Texas A&M University at Qatar
- ✓ Mourad Ouazani, Qatar Computing Research Institute, Hamad Bin Khalifa University
- ✓ Munir Tag, Qatar National Research Fund

Venue: The conference will be held in the Marriott-Marquis City Center Hotel, Doha.

Accommodation, Visa, etc.: Additional details about accommodation, transportation, visa and other practical matters for participants from outside Doha can be found at the conference website.

We hope to see you all in Doha in October 2019!





