



## 2<sup>nd</sup> International Computational Science and Engineering Conference

23 – 24 October 2017

Doha, Qatar

<http://icsec.qatar.tamu.edu/>

The 2<sup>nd</sup> International Computational Science and Engineering Conference will be held in Doha, Qatar on 23 and 24 October 2017. 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 and oral presentations.

The main themes of the conference are:

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

A list of representative topics includes:

A. Computational Materials Science and Engineering:

1. Different computational techniques at various time and length scales (quantum mechanics, Molecular Dynamics, Metropolis Monte Carlo simulations, etc.),
2. Different types of materials (soft materials, electronic materials, hybrid materials, etc.),
3. Energy capture and storage,
4. Reservoir modeling and simulation.
5. Electronic transport calculations
6. Dynamical phenomena applied to energy applications
7. Photovoltaic materials simulations

B. Computational Biology:

1. Genome analysis / annotation, Comparative genomics and Genome variations
2. Sequence analysis,
3. Epigenomics and transcriptomics data analysis
4. Genome-wide association study,
5. Computational methods in personalized medicine,
6. Structural Bioinformatics,
7. Modeling and simulation of biological networks,
8. High-throughput bimolecular analysis

C. High Performance Computing & Data Science

1. Large Scale Computing, parallel and distributed computing, cloud computing,
2. Hardware and software HPC architecture,
3. Uncertainty quantification and data assimilation (stochastic identification and uncertainty propagation),



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.

**Invited speakers:**

- ✓ Prof. David Bader, Georgia Institute of Technology
- ✓ Prof. Dimitris Maroudas, University of Massachusetts, Amherst
- ✓ Prof. Kenneth Merz, Michigan State University
- ✓ Prof. Udo Schwingschloegl, King Abdulla University of Science and Technology, KSA
- ✓ Prof. Perla Balbuena, Texas A&M University, USA
- ✓ Prof. Jorge Seminario, Texas A&M University, USA
- ✓

**Abstract submission deadline: 1 April 2017**

You are kindly invited to submit your abstract electronically through the conference website, at <http://icsec.qatar.tamu.edu/>. 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:**

- ✓ 15 December 2016: Abstract submission opens,
- ✓ 1 April 2017: Abstract submission ends,
- ✓ 15 May 2017: Abstract acceptance notification,
- ✓ 15 August 2017: Full paper submission to the Journal of Computational Science.

**Conference contact points:** [icsec@qatar.tamu.edu](mailto:icsec@qatar.tamu.edu)

- ✓ 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:**

- ✓ Ashraf Aboulnaga, Qatar Computing Research Institute, Hamad Bin Khalifa University
- ✓ Abdelkader Baggag, Qatar Computing Research Institute, Hamad Bin Khalifa University
- ✓ Halima Bensmail, Qatar Computing Research Institute, Hamad Bin Khalifa University
- ✓ Amine Bermak, Hamad Bin Khalifa University

- ✓ Othmane Bouhali, Texas A&M University at Qatar
- ✓ Ioannis G. Economou, Texas A&M University at Qatar
- ✓ Sami El Borgi, Texas A&M University at Qatar
- ✓ Fadwa El-Mellouhi, Qatar Environment & Energy Research Institute, HBKU
- ✓ Sebti Foufou, Qatar University
- ✓ Mohammad Karimi, Qatar Biomedical Research Institute, HBKU
- ✓ Valentin Ilyin, Carnegie Mellon University at Qatar.
- ✓ Hazem Nounou, Texas A&M University at Qatar
- ✓ Mohamed Nounou, Texas A&M University at Qatar
- ✓ Ting Huang, Texas A&M University at Qatar
- ✓ Munir Tag, Qatar National Research Fund

**Venue:** The conference venue will be announced later.

**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 2017!