

Issue 22

### **Uncertainty Quantification with Rappture**

Inputs to simulations often have some uncertainty in their values. It is essential to know how these uncertainties propagate to the output(s). Uncertainty Quantification (UQ) is a fundamental part of model verification and validation. With Rappture tools, it is used to do parameter sweeps for better understanding how output(s) respond to changing input(s). To learn more about UQ with Rappture visit <a href="https://nanohub.org/resources/25053/">https://nanohub.org/resources/25053/</a>

#### An Invitation from the nanoBIO Node

Dear nanoHUB User.

You and your research group members are invited to participate in a workshop on "Light/Matter Interactions at the nanoBIO interface" to be held Nov 28-29 at the University of Illinois at Urbana-Champaign. The workshop is being organized by the NSF-funded nanoBIO node at UIUC. The key details of the workshop are included at the end of this email and the application form is available through our webpage:

#### https://nanohub.org/groups/nanobio/nbnworkshop

In recent years, modeling and simulation-based design have become an integral part of the field of plasmonics and its applications to nanoBIO systems, an area where your group has been an active contributor. In order to aid the research community, the nanoBIO node at UIUC has developed a suite of modeling and design tools, most notably <u>nanoDDSCAT</u> for plasmonics design and modeling. While being free and easy to use, these are powerful, rigorous research-oriented tools. nanoDDSCAT has a worldwide user base of 600+ users and already 10 publications have resulted from use of this tool. But we would like to expand this community even further by offering training and education to practitioners in the field. The workshop is being conducted with this goal in mind. As a secondary objective, we would like to bring this community together and solicit feedback that will allow us to further enhance the capabilities of the nanoBIO node and nanoDDSCAT. One of the highlights of the workshop will be the integration of plasmonics and biomolecular dynamics for the design of complex nanoBIO nanostructures. I hope you and/or members of your group are able to participate. We look forward to welcoming you to our growing community.

Thank you.

Nahil A. Sobh (On behalf of the organizing committee and the nanoBIO node)

# 19th International Workshop on Computational Nanotechnology (IWCN)

### **Upcoming Events**

Applied Nanotechnology and Nanoscience International Conference – ANNIC 2016

When: November 9<sup>th</sup>, 2016
Where: Barcelona, Spain

2016 SNO CONFERENCE -Sustainable Nanotechnology Systems

When: November 10<sup>th</sup>, 2016
Where: Orlando, Florida

**Explore Events** 

#### **New Resources**

#### M-file/Mif Automatic GEnerator

#### **OpenKIM Explorer**

The Role of Dimensionality on Phonon-Limited Charge Transport: from CNTs to Graphene

Bringing Quantum Mechanics to Life: From Schrödinger's Cat to Schrödinger's Microbe

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research on the development and application of advanced simulations of nanostructures, nanomaterials and nanodevices.

Topics include electronic structure calculations; simulations of electronic, optical and mechanical properties of nanostructures; simulations of electronic, thermal, spin and molecular transport processes; multiscale and multiphysics simulations; computational design and evaluation of engineered nanomaterials and nanostructures; simulation of nanodevice processing and performance.

The IWCN is the 19th in the series of International Workshops previously titled "Computational Electronics". The new name, IWCN, reflects the longstanding aim of the Workshop to generate interdisciplinary research and collaboration in solid-state materials and device simulation, and the increasingly dominant presence of nanoscale structures and devices in high performance electronics and photonics.

The conference website (<a href="http://iwcn2017.iopconfs.org">http://iwcn2017.iopconfs.org</a>) contains more details including key personnel and the abstract deadline (15<sup>th</sup> January 2017).

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