Society of Engineering Science 51st Annual Technical Meeting

1–3 October 2014

Purdue University, West Lafayette, Indiana, USA

Cloud computing in nanoHUB powering education and research

Ale Strachan, strachan@purdue.edu

ABSTRACT

The synergistic integration of data from physics-based simulations and experiments within a decision-making framework has the potential to revolutionize the discovery, optimization, and certification of materials and devices. Transforming this vision into a reality requires the rapid transition of cutting-edge research codes from developers to researchers who can use them in design and optimization and to instructors who are training next generations of engineers and scientists. NSF's nanoHUB empowers simulation tool developers to make their codes universally accessible and useful via cloud computing, and users who can run these tools directly from their web browsers or iPads neither without the need to download or install any software nor to provide compute cycles. In this discussion, I will illustrate the use of nanoHUB tools in materials education and research focusing on ab initio electronic structure and molecular dynamics simulations. In the area of education, I will discuss learning modules for undergraduates designed to help students develop a more intuitive and deeper understanding of how materials look and work at atomic scales. Our research shows improved learning via hands-on simulations and powerful visualization tools. In the area of research I will demonstrate nanoHUB tools for electronic structure and thermal transport calculations with examples from the recent scientific literature.