Using nanoHUB.org in Research and Education – A Hands-on Tutorial

G. Klimeck, A. Strachan, T. Faltens,
B. Hallberg, L. K. Zentner, M. G. Zentner, M. Hunt
Network for Computational Nanotechnology, Purdue University, West Lafayette, IN 47906
gekco@purdue.edu

If you had access to interactive modeling and simulation tools that run in any browser, could you introduce interactive learning into your classes? If you had easy access tools, which need no installation, could you use them to help guide your experiments? If you did not have to worry about compute cycles, would you benchmark your own tools against other state-of-the-art approaches? If you had your own tools and could easily share them with the community, would you do it? This tutorial will provide an overview of these processes and their impact as they are supported on nanoHUB.org today.

Recently we have begun to deploy Jupyter notebooks within nanoHUB. nanoHUB provides its users with a secure Jupyter installation with a large number of installed mathematical and graphical packages. Users can develop their own scripts in python or octave and deploy their own codes. More complex codes can also be installed in nanoHUB and called as a service. All the Rappture-based tools in nanoHUB can be called as a service in the Jupyter notebooks as well.

Annually, nanoHUB provides a library of 5,500+ learning resources to over 1.4 million users worldwide. Its 500+ simulation tools, free from the limitations of running software locally, are used in the cloud by over 16,000 annually. Its impact is demonstrated by 2,180+ citations to nanoHUB in the scientific literature with over 30,900 secondary citations, yielding an h-index of 82 and by a median time from publication of a research simulation program to classroom use of less than 6 months [1]. Cumulatively, over 35,600 students in over 1,500 formal classes in over 185 institutions have used 210 nanoHUB simulation tools. *The **Web of Science and Google Scholar** now both **list nanoHUB simulation tools** as proper publications giving credit to the tool authors.*

nanoHUB.org is a virtual nanotechnology user facility funded by the National Science Foundation and supports the National Nanotechnology Initiative with a highly successful cyber-infrastructure. nanoHUB.org has been supported by the U.S. National Science Foundation since 2002 to serve the nanotechnology community.

[1] Krishna Madhavan, Michael Zentner, Gerhard Klimeck, "Learning and research in the cloud", *Nature Nanotechnology* 8, 786–789 (2013); doi:10.1038/nnano.2013.231

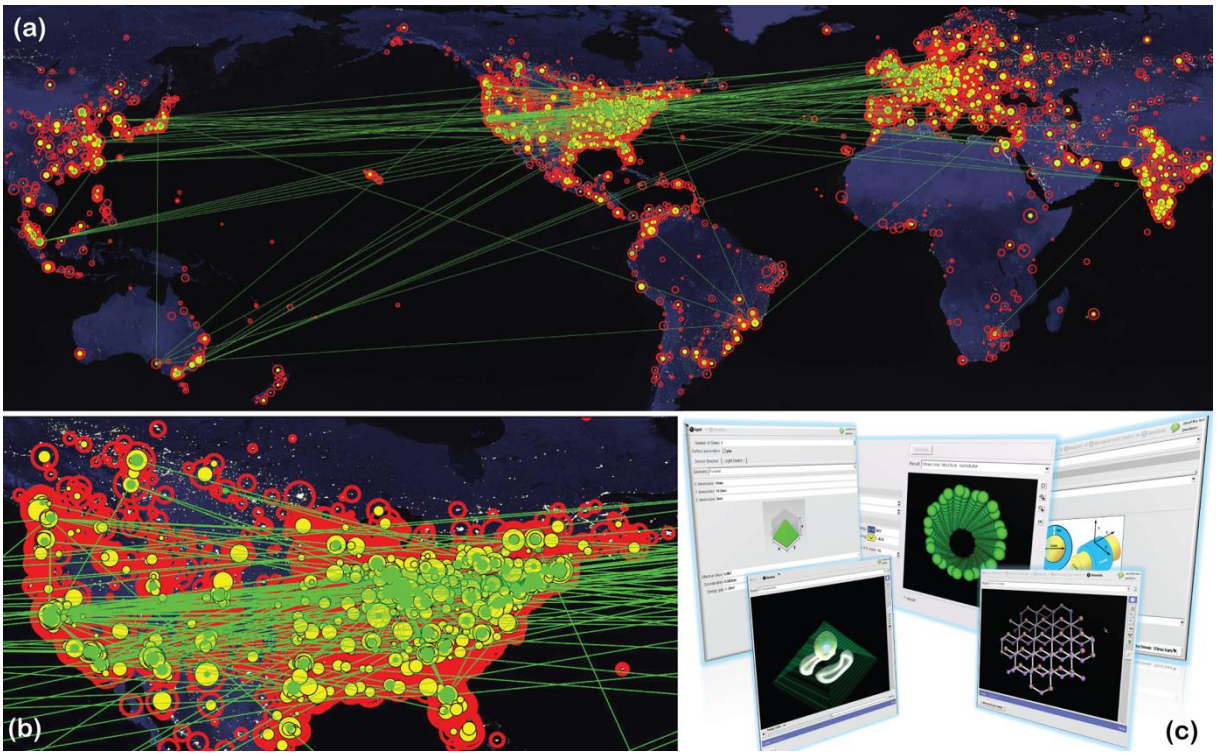

Fig.1: (a) annual nanoHUB user map superposed on NASA's world at night. Red circles designate users viewing lectures, tutorials, or homework assignments. Yellow dots are users of simulation. Green dots indicate authors of over 2,180 scientific publications citing nanoHUB. Dot size corresponds to the number of users, and lines show author-to-author connections proving intense research collaboration networks. (b) U.S. enlarged. (c) a collage of typical nanoHUB interactive tool sessions and 3D-rendered interactively explorable results (quantum dots, carbon nanotubes, nanowires).

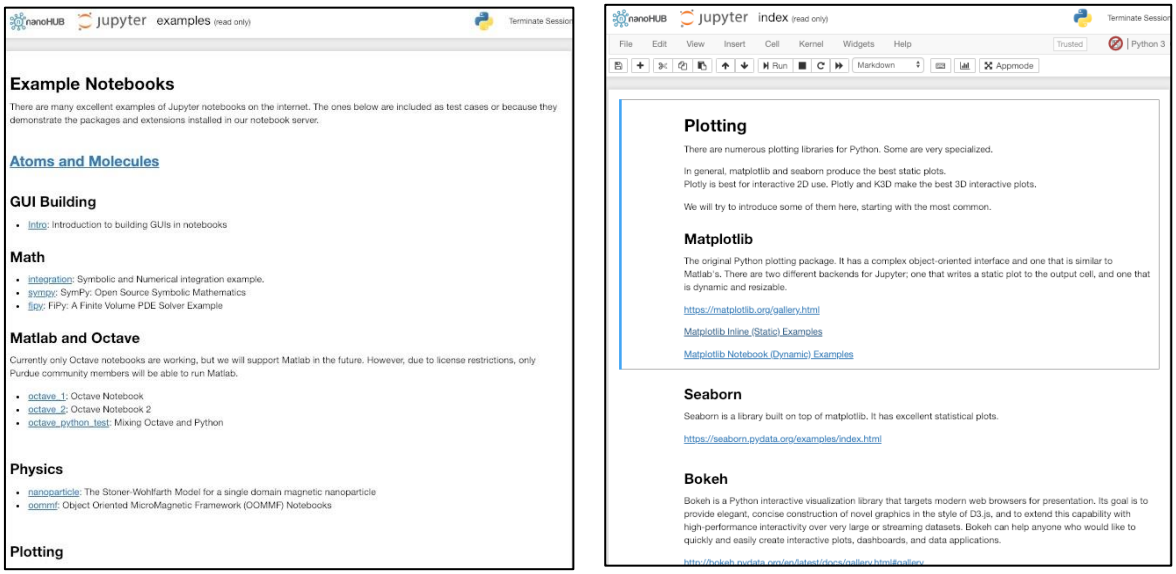

Fig.2: nanoHUB provides its users with a secure Jupyter installation with a large number of installed mathematical and graphical packages. Users can develop their own scripts in python or octave and deploy their own codes. More complex codes can also be installed in nanoHUB and called as a service. All the Rappture-based tools in nanoHUB can be called as a service in the Jupyter notebooks as well. Computational cycles and 24/7 operation as a service to these Jupyter notebooks is provided for nanoHUB users. (left) Example notebooks. (right) Tutorials for plotting libraries in Jupyter.