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NANOHUB AS A PLATFORM FOR IMPLEMENTING ICME SIMULATIONS IN RESEARCH AND EDUCATION

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Abstract

nanoHUB.org is an open-access cyberinfrastructure supported by the US National Science Foundation. It provides a powerful and versatile platform for delivering computational resources to support the implementation of Integrated Computational Materials Engineering (ICME) solutions and associated educational efforts. nanoHUB provides free cloud scientific computing, where users can access simulation tools for research and education using a web-browser or iPad, without the need to install software or have access to local computing resources. The tools have friendly, fully-interactive graphical user interfaces, meaningful default values, output of both numerical data and visualizations, and extensive support material that provides an accessible pathway towards advanced materials simulations. On the back end, nanoHUB computational resources include high performance computing clusters that enable research-quality simulation.

The nanoHUB platform can empower ICME researchers and educators in two distinct ways: by using existing tools or by creating and publishing new, customized nanoHUB tools. Existing nanoHUB tools are currently used to introduce ICME simulations in courses in a variety of areas such as electronic structures, diffusion kinetics, and mechanics of materials. These tools were created by installing the available open source code into nanoHUB, then building custom graphical user interfaces (GUIs) using the Rappture toolkit (*R*apid *App*lication Infrastruc*ture*; http://rappture.org), which is integrated into the nanoHUB workspace. In a similar manner, instructors can install other simulation tools into nanoHUB using Rappture to easily customize their tools to meet their learning objectives. This paper introduces existing nanoHUB ICME tools, additional resources for materials science education, and the procedure for customizing and publishing new simulation tools on nanoHUB.

Introduction

Motivated by the report Committee on Integrated Computational Materials Engineering of the National Materials Advisory Board [1] and following ICME documents, see for example Ref. [2] there has been growing interest in making computational materials simulations tools widely accessible to engineers, researchers, educators and students [3]. The announcement of the Materials Genome Initiative in 2011 [4], with the goal of accelerating the pace of materials development from discovery to production by integrating simulation into the various parts of the materials development process provides increased motivation to make robust simulations widely available. There are, however, a few barriers to be overcome when attaining these simulation tools. Many of the popular software packages have academic licensing fees that must be borne by the department, university or company. The software is often restricted to use on specific lab computers, or available to students on a limited basis if floating licenses are available. Alternatively, free software can be downloaded from various repositories and installed on local

computers, but this process can be a little daunting, especially to the uninitiated. An alternative to purchasing, downloading and installing software is to use the open-access, cloud-based simulations available on nanoHUB.org. No installation or local computing power is required: many of these simulations are run on servers at Purdue University while more computationally intensive simulations are sent to grid computing resources such as NSF's XSEDE or the Open Science Grid [5]. The simulations are available to run via most web browsers, and can even be accessed on an iPad tablet computer. Several advantages to using simulations on nanoHUB for educational purposes were noted [5] as follows. No installation of software on classroom computers means that administrator privileges are not required, the tools are available on all platforms (Windows, MacOS, and Linux), the tools are easy to use and efficient, they have integrated visualization capabilities, and they come with supporting materials to help learners get to the underlying concepts. Additionally, the nanoHUB support team is available through the built-in help feature. The web-based simulation tools on nanoHUB provide access to research-grade simulations to users at institutions world-wide, including those whose computing infrastructure may not be set up to support computational modeling and simulation of materials.

The advantages of using the nanoHUB infrastructure continue into the classroom environment, where instructors can share live simulation tool sessions with their students, both face-to-face or remote, via the web. They can also prepare and save a set of simulation runs ahead of time, as tool sessions remain active for several days unless terminated.

The next sections will present several materials science simulation tools that are already available for use on nanoHUB, nanoHUB features that instructors may find useful for classroom use, and information that researchers who are developing their own materials simulation tools can use to publish their tools in nanoHUB using the self-serve publication process and the Rappture Toolkit.

Materials Science Simulations Available on nanoHUB

nanoHUB simulation tools have been used for various educational purposes in hundreds of classes [6]. In particular, three out of the four simulation tools featured in the 3rd Summer School for Integrated Computational Materials Education (http://icmed.engin.umich.edu/) in July 2014, were nanoHUB simulations. This international workshop was organized by professors at the University of Michigan and UC Berkeley with the goal of training instructors to be able to incorporate ICME simulations in their courses. The nanoHUB simulations used in the course were DFT Calculations with Quantum Espresso [7] to teach how to use Density Functional Theory (DFT) to calculate equilibrium lattice parameters, bulk modulus and elastic constants for a single crystal; Virtual Kinetics of Materials Laboratory [8] to explore numerical aspects of the computational technique for studying diffusion; and OOF2 [9] to work with different skeleton meshes and boundary conditions in order to calculate materials properties of polycrystalline materials, starting from a material micrograph and a set of known properties.

These and other resources for materials science, including full courses and additional computational simulation tools, have been collected in the Materials Science group within nanoHUB (https://nanohub.org/groups/materials) and are freely available to use by instructors and students. The simulation tools in this group are distributed into general categories: *Ab initio* electronic structure simulations tools, Molecular Dynamics (MD) Simulation Tools, Finite Element Analysis of Microstructures, Virtual Kinetics of Materials, Structure of Materials, and Phase Field Simulations of Plastic Deformation. A large number of computational materials

simulation tools are currently available and new simulation tools continue to be added by members of the nanoHUB community. These additional materials simulation tools on nanoHUB can be found using the search bar, and are added to the Materials Science group as they are identified.

The *ab initio* tools include: ABINIT [10], SIESTA [11], nanoMATERIALS SeqQuest DFT [12], QC Lab [13], Strain Bands [14], DFT Calculations with Quantum ESPRESSO [7], and QWalk Quantum Monte Carlo Tutorial [15].

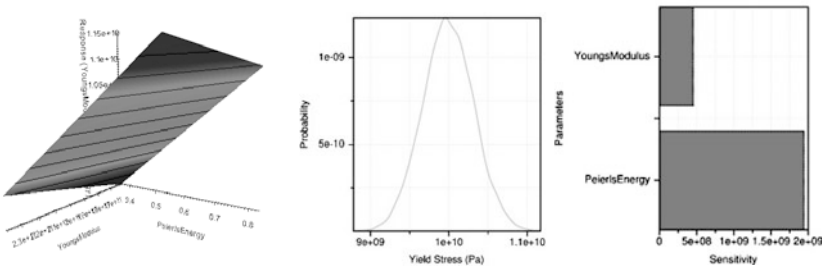
The MD simulation tools include minimol [16], nano-Materials Simulation Toolkit [17], LAMMPS for Carbon Nanostructures and the Lennard-Jones Potential for LAMMPS, both in the MIT Atomic Scale Modeling Toolkit [18].

The finite element analysis tool is OOF2 [9], which is a public domain tool created at the National Institute of Standards and Technology (NIST) to investigate the properties of microstructures. OOF2 can be downloaded, installed and run on a local machine, or run on nanoHUB with no installation.

The Virtual Kinetics of Materials Laboratory [8] is a web environment to develop microstructural evolution models using FiPy, which is a powerful set of libraries for solving partial differential equations. Several example modules are provided as example for users—Dendritic Growth, Polycrystalline Growth and Coarsening, Spinodal Decomposition and Spinodal Decomposition 3D. Additionally, Gibbs [19] is a Python-based set of libraries for calculation of phase diagrams and thermodynamic properties.

Crystal structures can be probed with Crystal Viewer Tool [20, 21], which allows 3D rotation of the structures and enables Miller planes to cut through the lattice, showing dangling bonds. Polymer Modeler [22] enables users to build polymer chains by specifying the monomers, monomer arrangements, torsion angles between monomers, and other system parameters such as density and temperature. The resulting structure file can be used in LAMMPS.

Finally, the newest feature of nanoHUB simulation tools, uncertainty quantification, is now available in the NanoPlasticity Lab [23], which is a phase field approach to simulate plastic deformation in nanocrystalline materials. The integration of uncertainty quantification in this tool allows users to quantify how uncertainties in the input parameters affect the yield stress calculation, and provides a sensitivity analysis to quantify the relative importance of each of the input variables. The PRISM Uncertainty Quantification (PUQ) framework [24] enables users to select from various state-of-the-art methods for uncertainty propagation. Figure 1a shows the calculated yield strength output when the inputs for the Peierl's Energy Barrier and elastic modulus are Gaussian distributions instead of single-valued quantities. Figure 1b shows the Gaussian probability distribution of the calculated yield stress and figure 1c shows the sensitivity of the output to the input Young's modulus and Peierl's Energy.



1a 1b 1c

Figure 1: NanoPlasticity Lab output incorporating uncertainty quantification. Figure 1a) shows the Response curve for the yield stress, given a single value for the Poisson's ratio and grain boundary sliding energy barrier, and Gaussian distributions for the elastic constants and Pierel's energy barrier using a first degree polynomial expansion with the Smolyak and Polynomial Chaos with Legendre basis functions method.

nanoHUB Educational Resources and Features for Instructors

Thousands of resources on nanoHUB provide additional information on nanotechnology- and simulation-related topics, and can support the use of simulations in the classroom. nanoHUB's signature lecture effort, nanoHUB-U (https://nanohub.org/groups/u), provides free, self-paced short courses on a number of cutting-edge topics of interest to materials scientists and engineers, including Fundamentals of Atomic Force Microscopy, Thermal Energy at the Nanoscale, Thermoelectricity: from Atoms to Systems, Principles of Electronic Nanobiosensors and Quantum Transport. The nanoHUB-U course packages contain online lectures with a student-friendly format that allows for one-click access to any lecture slide within a presentation, an adjustable play-back rate, the ability to append time-stamped notes to the lectures, and homework problems and quizzes with instant feedback. Many of the courses incorporate simulations and include instruction and tutorials on how to use the simulations, and practice problems that use simulations are included in the homework.

One nanoHUB-U course in particular should be of interest to the ICME community: From Atoms to Materials: Predictive Theory and Simulations (https://nanohub.org/courses/FATM) develops a unified framework for understanding essential physics that governs material behavior at atomic scales and relates these processes to the macroscopic world. Background instruction is provided on quantum mechanics, *ab initio* calculations, the methods of density functional theory, statistical mechanics and molecular dynamics theory. Several simulation tools are used in the course, with instruction provided in the lecture videos and tutorials. These simulation tools are nanoMATERIALS SeqQuest DFT [12], DFT calculations with Quantum ESPRESSO [7], nano-Materials Simulation Toolkit [17], and nano-Material nanoscale Thermal Transport Tool [25].

In addition to providing content that supports learning, the nanoHUB platform has features such as groups, collections, databases and projects that instructors may find useful in a course. These features are summarized on nanoHUB [26] and can be easily explored. Groups provide a means for assembling material for a given class. Access the material can be open to any nanoHUB user or restricted to group members only. Additionally, threaded discussion forums can be created within groups, where students can comment on assigned topics or ask questions, and group collections offers a way for group members to collect and share material found within nanoHUB,

elsewhere on the web, or uploaded from an individual's computer. Collections can be a useful way to have class members assemble content in a specific area, and vote up those resources that they find most useful.

nanoHUB Simulation Tools in Research

The same simulation tools used for educational purposes can also be used for research, and several of the materials science simulation tools have been cited in research publications. The citations for each tool are collected and presented in the "citations" tab on the tool home page. For example, nanoMATERIALS Sequest DFT has been cited in 3 research papers to date (https://nanohub.org/resources/nmst_dft/citations), in the journals *Phys. Rev. B*, *Applied Physics Letters*, and IEEE's *Journal of Microelectromechanical Systems.* This particular tool is suitable to study a wide range of topics, and those published are dielectric charging, the effects of surface orientation on interface structure and Fermi level pinning at an oxide/ semiconductor interface, and estimating the elastic modulus in a MEMs structure. Six other materials science simulation tools cited in this paper have been cited in research publications. It should be noted that each simulation tool contributed to nanoHUB is an official publication, and receives a Digital Object Identifier (DOI). Information is provided with each tool on how to properly cite the simulation tool in publications, and such publications go towards increasing the author's impact. In all nanoHUB has been cited in the scientific literature over 1,200 times to date and these papers have over 16,000 secondary citations resulting in a nanoHUB h-index of 59.

Publishing Simulations on nanoHUB

The simulation tools on nanoHUB are contributed from members of the community, in a process that is self-serve and streamlined [27]. The starting page for contributing a new simulation tool on nanoHUB is https://nanohub.org/tools/create, and once the tool contribution process has been initiated, *Workspace* [28] access can be requested. *Workspace* is a virtual full-fledged Linux workstation that exists in a browser and provides access to the complete nanoHUB software stack including the Rappture toolkit and grid computing access. As such *Workspace* serves as a development and staging area for new tools. Code can be uploaded, compiled, tested and debugged in *Workspace*, and once it is ready, it can be deployed on nanoHUB from *Workspace*. A course on nanoHUB (https://nanohub.org/courses/tools) provides exercises to guide you in creating and deploying your scientific tools on nanoHUB and additional video tutorials stemming from a Rappture summer training [29] give instruction as well as solutions to the exercises.

The Rappture toolkit is a GUI builder and data management tool for simulation tools, allowing guided input and graphical output in many formats. The GUIs can be built on top of simulation tools in many languages, without modification of the simulation code itself. The GUI can also be wrapped around a complex scientific workflow. These GUIs provide a consistent and user-friendly means for learners to interact with simulation tools, and can be designed to be more user-centered and intuitive than the text-based input decks that are commonly used for simulations. These GUIs make the nanoHUB versions of open source simulation tools more accessible to novices. Many advanced simulation users often prefer the flexibility of text-based entry, and the tool contributor has the option to create a dual interface, allowing either graphical or text-based entry. As such nanoHUB enables the tool developers as well as the users to trade off usability versus capability.

Conclusions

nanoHUB.org provides access to a number of computational materials science simulation tools that require no installation or local compute power. These simulations are run in an environment that is easily used in classrooms and that makes ICME simulations accessible to a wide range of learners, worldwide. Educators who have developed their own simulation tools can publish them on nanoHUB, using nanoHUB's *Workspace* and the Rappture toolkit to build user-friendly GUIs that can be customized to suit their desired learning objectives. In addition to simulation tools, nanoHUB hosts thousands of other resources for education, in nanotechnology, materials science, computation and simulation and related areas.

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