



Issue 54

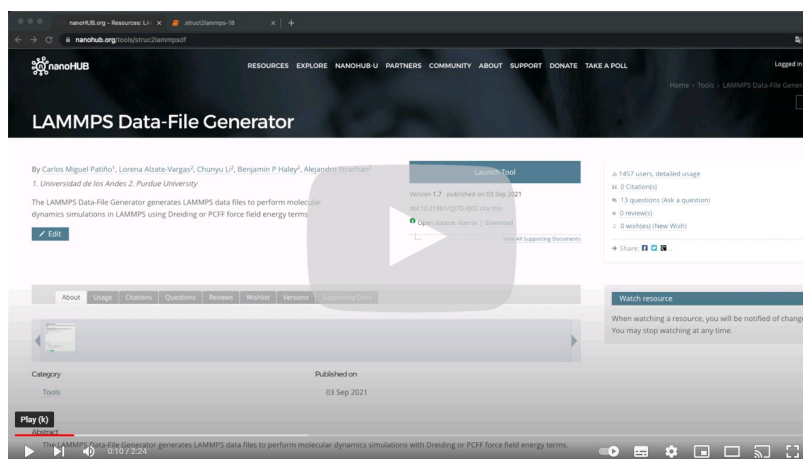
Stay informed about what's happening on nanoHUB! Check out new resources, upcoming online workshops, and more below.

nanoHUB App Spotlight

LAMMPS Data-File Generator Tool

The [LAMMPS Data-File Generator](#) takes input from a number of different types of structure files, such as xyz or pdb, and generates a LAMMPS data file that can be used to run molecular dynamics simulations.

Check out [this video by Carlos Patino](#), one of the tool authors, to learn more about this handy Jupyter notebook app that can make it easier to create the input files you need to run LAMMPS!



Featured Resources on nanoHUB

EngrTEAMS Curricular Units

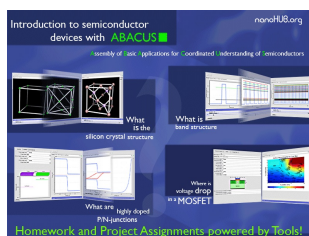
[This series](#) is designed to increase the learning of science concepts for 4th through 8th grade students, as well as mathematical concepts related to data analysis and measurement, by using an engineering design-based approach to teacher professional development and curriculum development.



Each resource is an engineering design-based STEM curricular unit that includes teacher guides, class activities with solutions, and assessment guidelines. The units aim to facilitate the learning of major science and mathematical concepts and skills within the Next Generation Science Standards (NGSS) and Common Core State Standards (CCSS).

These resources were provided by [EngrTeams](#), a five-year, \$8 million National Science Foundation award made to a partnership involving the University of Minnesota and Purdue University.

Recitation Series for Semiconductor Education

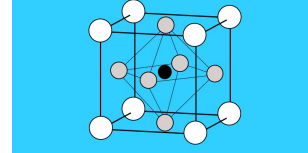


This [seven-part series](#) covers the [ABACUS Tool Suite](#) in nanoHUB. In each session, Dr. Gerhard Klimeck gives a brief overview of the featured tool, shows several sample simulations, and shares resources for the tool that can be found on nanoHUB (including the tools and materials needed to easily integrate these resources into new and existing coursework).

This series was presented twice, in the winter of 2021 and spring of 2022. All recordings from both sessions can now be found on the [Recitation Series for Semiconductor Education page](#).

Materials Science Resources

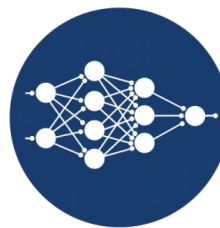
The [Materials Science Page](#) provides nanoHUB resources for materials science. These include complete courses, seminars and tutorials on specialized topics, simulation tools that run in the cloud using nanoHUB's computing resources, and learning activities that use simulations.



There are also activities for Materials Science outreach that you can use to teach high school and middle school students about the wonders of materials science.

Gaussian Process Regression for Surface Interpolation

Want to learn more about the fundamentals of Gaussian Process Regression and its application to surface interpolation? Attend nanoHUB's free summer workshop, Gaussian Process Regression for Surface Interpolation. This session is part of our [Hands-on Data Science and Machine Learning Training Series](#).



Presenters:

Zhiqiao Dong, Ph.D. candidate, University of Illinois Urbana-Champaign and Manan Mehta, Ph.D. candidate, University of Illinois Urbana-Champaign

Date/Time:

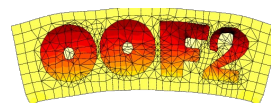
Wednesday, July 6, 2022 from 1:30 PM – 2:30 PM EDT

Abstract:

Gaussian process regression (GPR) is a nonparametric regression method with widespread applications in various scientific and engineering fields. In manufacturing, it has been used for surface interpolation that generates high-resolution surface estimations from coarser measurement data. This tutorial will introduce the fundamentals of GPR and its application to surface interpolation. We will also introduce a new technique called filtered kriging (FK), which uses a pre-filter to improve interpolation performance. The FK method will be illustrated using periodic surfaces manufactured by two photon lithography.

Microstructure Modeling with OOF2 and OOF3D

Join us for a free, online tutorial on Microstructure Modeling with [OOF2](#) and [OOF3D](#).



Presenters:

Dr. Andrew Reid, NIST and Dr. Steve Langer, NIST

Date/Time:

Wednesday, July 27, 2022 from 3:00 - 4:00 p.m. EDT



Abstract:

The OOF object-oriented finite element software, developed at the National Institute of Standards and Technology, provides an interactive FEM tool which packages sophisticated mathematical capabilities with a user-interface that speaks the language of materials science.

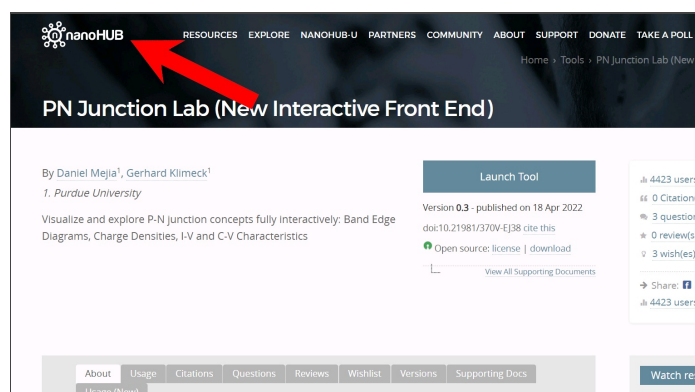
Users can assign material properties to the constituent phases of a microstructural image, and then construct finite-element meshes from these images, in either 2D or 3D. The tool then allows users to perform virtual experiments using a variety of boundary conditions to explore structure-property relationships within the system, including effective properties.

[Register Here](#)

nanoHUB Tips and Tricks

Return to the nanoHUB homepage instantly

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