



Issue 55

Stay informed about what's happening on nanoHUB! Check out our featured resources, upcoming hands-on workshops, and more below.

nanoHUB App Spotlight

MIT Atomic-Scale Modeling Toolkit

The [toolkit](#) was developed for use with a [course on computational nanoscience](#), originally developed at UC Berkeley and taught by Jeffrey Grossman and Elif Ertekin. Together, the course and toolkit are a great package for learning about simulations for:

- Statistical analysis
- Molecular Dynamics (LAMMPS)
- Monte Carlo methods (Metropolis method and Ising model)
- Crystalline and molecular structure visualization (XCrysDen)
- Quantum Chemistry (GAMESS)
- Density-Functional Theory (Quantum Espresso and SIESTA)
- Quantum Monte Carlo (QWalk)

Atomic Scale Modeling Toolkit
Massachusetts Institute of Technology

Application:

About this Toolkit

MIT Atomic Scale Modeling Toolkit

These simulation tools have been developed for educational purpose, to complement the MIT Introduction to Modeling and Simulation course taught by Jeffrey Grossman and Markus Buehler.

Lectures, homeworks, and example simulations are available on the NanoHUB.

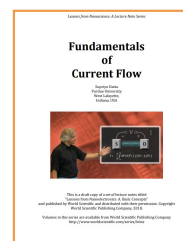
Select a tool from the "application" menu above to get started!

Toolkit Developers: David Strubbe, Daniel Richards, Lucas Wagner, Elif Ertekin, Jeffrey C. Grossman, Justin Riley

Featured Resources on nanoHUB

Semiconductor Education Textbooks on nanoHUB

Through an agreement with World-Scientific Publishing, nanoHUB offers several [free textbooks](#) that correspond to our [online semiconductor education courses](#). Browse our textbook offerings and find corresponding online courses for each on our [Semiconductor Workforce Development page](#).



MNT-CURN Seminar Series



Check out the latest [Seminar Series](#) from the MNT-CURN Research Program.

This series was recently added to nanoHUB and covers multiple topics including Ultrafast Spectroscopy of Nanomaterials, Colorful and Smart Nanoscale Materials, Blockchain & Proof of Useful Work, and more.

The [Micro Nano Technology Collaborative Undergraduate Research Network \(MNT-CURN\)](#) is an undergraduate research program for community college students.

New NACK Webinar Archive

The [Nanotechnology Applications and Career Knowledge \(NACK\) Resource Center](#) has a new [Webinar Archive](#) to go along with their other instructional modules and laboratory exercises published in nanoHUB. The archive spans a variety of topics including Shape-Changing Micromachines, Novel Two-dimensional Materials and Devices for Biomimetic Sensing and Computing, and more!



Upcoming Events

Visit nanoHUB at BCCE!

nanoHUB will be at the [Biennial Conference on Chemical Education \(BCCE\)](#) at Purdue University next week in **Booth #11**. Stop by and say hello!



Machine Learning Predicts Additive Manufacturing Part Quality: Tutorial on Support Vector Regression

This hands-on workshop will demonstrate the use of machine learning to accurately predict defects in additive manufacturing (3D printing). The session is part of our [Hands-on Data Science and Machine Learning Training Series](#).



Presenter

Davis McGregor, Ph.D., Senior Manufacturing Scientist at Fast Radius Inc.

Date/Time

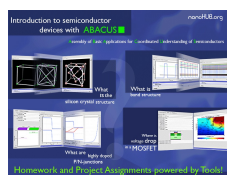
Wednesday, August 10, 2022 from 1:30 PM – 2:30 PM EDT

[Register Here](#)

Abstract

In additive manufacturing (AM, or 3D printing), part geometry can differ from the designed dimensions depending on the part size and shape, as well as manufacturing parameters such as the machine used or location of the part within the printer. The relationships between part design, manufacturing parameters, and geometric accuracy are not well understood for AM, and there is a need to develop methods that effectively predict these defects. This tutorial introduces and demonstrates the use of machine learning (ML) to address this need. Using data collected from an AM factory, you will train a support vector regression (SVR) model to predict the dimensions of AM parts based on the design geometry and manufacturing parameters. You will learn to combat ML bias using grid search hyperparameter tuning and nested cross validation, such as k-fold and Monte Carlo subsampling. Finally, you will compare SVR to other ML algorithms, such as k-nearest neighbors (KNN), and evaluate their computational cost and predictive accuracy.

Q&A Series on Semiconductor Education and Workforce Development using nanoHUB Simulation Tools



If you attended our [nanoHUB Recitation Series on nanoHUB tools for Semiconductor Education](#), or if you are interested in semiconductor education and workforce development using nanoHUB simulation apps, keep an eye out for an upcoming Q&A series. You will have the chance to meet with experts to have your questions answered. Specific topics and session dates will be announced in the upcoming weeks.

Semiconductor Industry News

SkyWater Technology chooses Discovery Park District at Purdue for \$1.8B semiconductor fabrication facility, to create 750 jobs in 5 years

SkyWater Technology recently announced that it plans to open a \$1.8 billion state-of-the-art semiconductor manufacturing facility in Discovery Park District at Purdue University. The company expects to create 750 new direct jobs within five years after it opens the new facility.

[Read the full article here.](#)

South Korean giant SK Group is pouring \$22 billion into the United States

SK Group's investments will include \$15 billion in the semiconductor industry through research and development programs, materials, and the creation of an advanced packaging and testing facility.

While the exact timeline for the investments was not disclosed, the Seoul-based corporation plans to grow its US workforce from 4,000 to 20,000 people by 2025

[Read the full article here.](#)

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