

Purdue 'nanoHUB' tops 100,000 annual users, popularity growing

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WEST LAFAYETTE, Ind. - An interactive Web site called [nanoHUB.org \(http://www.nanohub.org/\)](http://www.nanohub.org), which makes available scientific simulations, seminars, interactive courses and other specialized nanotech-related materials, has reached a milestone: 100,000 users in one year.

Researchers and educators from New York to London and Moscow to Madrid are logging onto nanoHUB.org because it offers a wide range of nanotech-related content.

Gerhard Klimeck



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"Attracting 100,000 users in a single year demonstrates the practical utility of nanoHUB," said Gerhard Klimeck, associate director of the [Network for Computational Nanotechnology \(http://www.ncn.purdue.edu/\)](http://www.ncn.purdue.edu/) and a professor of electrical and computer engineering at Purdue University. "Growing popularity has been directly tied to the dramatic improvement of user interfaces and content that cannot be found anywhere else."

The site now has more than 2,000 content items, most of them cutting-edge research seminars and complete courses on various aspects of nanotechnology.

"The popular items are getting the attention of literally thousands of users," Klimeck said. "They are delivered in several forms and formats, many of which do not require a large network bandwidth."

Intuitive graphical user interfaces are making it easier for researchers and educators to access and operate simulation tools.

"We're putting simulation tools into the hands of people who normally wouldn't touch them with a 10-foot pole," Klimeck said. "These are not computer geeks. They are experimentalists, educators and students whose work could benefit greatly through modeling and simulation but who are unable to install, run and maintain the software."

Chris Bowen, a researcher from Lockheed Martin in Cherry Hill, N.J., said nanoHUB has been an important component in patent applications.

"It has provided me with a means to quickly test the concept of a new gated resonant tunnel device for electronic applications," he said. "It allowed me to see if the concept was worth pursuing in more detail. I pushed a nanoHUB tool into a regime where it was never intended to operate and was able to get a concise answer to the question of viability. In the end it allowed me to get a patent through the initial approval

process."

Researchers from a six-university collaboration funded by the National Science Foundation began developing nanoHUB in 1998. Now based at the [Birck Nanotechnology Center \(http://www.purdue.edu/discoverypark/nanotechnology/\)](http://www.purdue.edu/discoverypark/nanotechnology/) in Purdue's [Discovery Park \(http://purdue.edu/discoverypark\)](http://purdue.edu/discoverypark), nanoHUB is an NSF science gateway and portal that enables the creators of specialized nanotechnology-related simulations to make them available to other researchers and educators.

The addition of user interfaces has dramatically increased traffic to various simulations on nanoHUB, Klimeck said.

"The key is usability," he said. "Researchers and educators will use a simulation because they can, even if it isn't really applicable to what they are doing. There could be a perfect piece of software out there that would solve their problem correctly, but they don't have access, they don't have the ability to use it."

Researchers in the Network for Computational Nanotechnology have solved this problem by creating programs that make it easier for simulation developers to also create user interfaces. The result has been a seven-fold increase in the annual number of simulation users over the past four years.

Mark Lundstrom



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"The growth in nanoHUB's user population from fewer than 1,000 in 2002 to more than 100,000 per year today is a clear indication of the success of nanoHUB's approach," said Mark Lundstrom, Purdue's Don and Carol Scifres Distinguished Professor of Electrical and Computer Engineering and chairman of the executive committee for the Network for Computational Nanotechnology.

Bruce Barker, president of the Chippewa Valley Technical College in Eau Claire, Wis., said nanoHUB has proved a valuable teaching tool.

"We can't afford to duplicate the facilities nanoHUB offers," he said. "Nanotechnology is the coming wave of the future. It will be integrated into every aspect of our lives, from building materials and clothing to medicine and agriculture. And nanoHUB allows our students access to resources that we can't duplicate, nor should we."

A selection of the educational nanoHUB content is now on iTunesU at <https://nanohub.org/itunes/> (<https://nanohub.org/itunes/>)

Using nanoHUB enables researchers to run simulations on three levels: generating an answer within seconds, hours or days.

"Users want to be able to ask the 'what if questions,'" Klimeck said. "'If I make the device this way, what will I see differently?' At first, they don't care if the answer is exact. All they want to see is trends. Then they can do another run that takes four hours to get more precise results, and then after that an overnight or two day-run that's even better."

The new user interfaces enable researchers to more easily conduct these "hierarchical" simulations.

"The user interface is like a more sophisticated version of what you see on your bank's site, but instead of

wanting to see certain records or make transactions you might want to run a simulation that shows quantum dots for future computers or artificial atoms for advanced sensors," Klimeck said. "I may want to rotate it, see how effective it is at absorbing light. It's real science or engineering code that can be used for training and research."

The appropriate computer resources for a given task are provided by nanoHUB. A cluster of 48 computers might be sufficient for simulations that take seconds, whereas the longest simulations might require 1,000 processors.

Future expansion may provide additional tools on nanoHUB, which is part of HUBzero, a platform that provides user-interface software for any technical field. About a dozen hubs now exist, while others are under development.

Klimeck said nanoHUB is powered by HUBzero software, which is a project of Information Technology at Purdue, or ITaP.

Other members of Network for Computational Nanotechnology include the University of California at Berkeley and the Department of Energy Molecular Foundry, University of Illinois, Massachusetts Institute of Technology, Norfolk State University, Northwestern University, and the University of Texas at El Paso.

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