

ENGINEERING

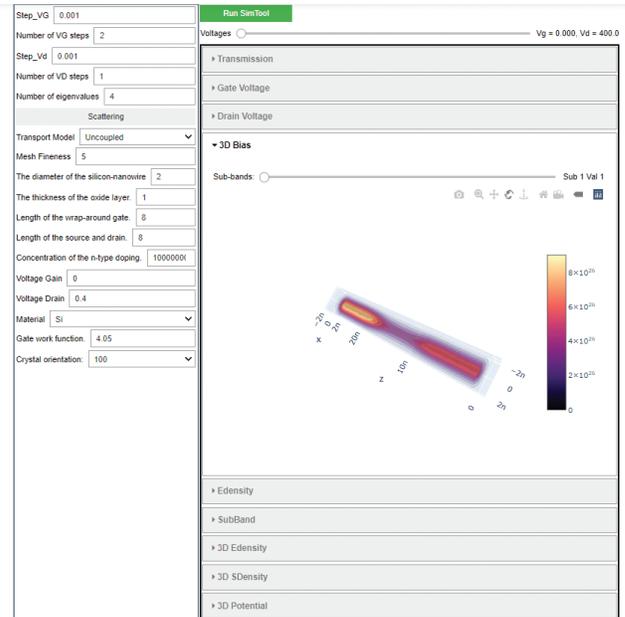
Redefining Research in Nanotechnology Simulations: A New Approach to Data Caching and Analysis

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As the world shifts deeper into the virtual workspace, previous models and systematic designs become obsolete or inconvenient. To keep up with the ever-growing field of nanotechnology simulations, nanoHUB, a public platform for computation research in nanotechnology and related fields, has recently created a code library called Sim2ls. Sim2ls is a revolutionary tool allowing data processed by a simulation to be saved into a globally accessible storage area. Implementation of Sim2ls instantly allows retrieval of output data that has been run before if the same inputs were to be used, skipping the entire calculation process that could take up to several hours of runtime.

In our study, outdated simulation code was optimized and separated into the “workflow,” which works with the user interface, and the “simtool” file that works to send and retrieve data to process. This infrastructure can be seen with the “workflow” acting like a display case with the “simtool” file acting as the inner machinery. With the “workflow” any user can comfortably make any visual representations of their research project.

Lack of documentation stifles progress, thus, throughout the study, the process of implementing Sim2ls has been documented along with retaining legibility and ease of comprehension for all end users. This provides a comprehensible foundation for multidisciplinary researchers to create their own workflows or modifications to existing simulations to suit their own research or educational endeavors.



One of many Sim2l implemented simulations, showing a configurable and interactable silicon nanowire with the 3D bias display, with additional options to analyze potential profile, electron density, and more.

This goal of this study is to drive the growth of simulation development. Through this implementation, a standard in information distribution and analysis can be set.

Research advisor Daniel Mejia writes “Darin, Alan, and Aloysius have been working as a cohesive team. They created sim2ls based on deprecated research codes following modern programming paradigms. Their work includes high-impact scientific visualizations, and their contributions are crucial in moving nanoHUB forward to deliver nanoelectronics simulations in the era of abundant data.”