LDRD@SNL

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A Universal Quantum Transport Computational Capability for Cross-Technology Comparisons of Beyond-CMOS Nano-electronic Devices

Denis Mamuluy (PI) and Xujiao Gao

Sandia researchers have discovered the fundamental downscaling limit of existing transistor technology through developing and testing a tool to aid in identifying and characterizing new technologies for post-Moore's law computing.

How small can transistors get? Transistors are the basic building blocks of modern electronics that currently drive the $250-billion semiconductor industry. Are there any fundamental limits for Moore's law besides the obvious atomic size limit? If so, are there any ways to overcome such limits? Quantifying these limits, and when they might be reached, is an active subject of research and debate, with implications for both commercial and scientific computing.

Existing modeling tools work only with conventional complementary metal-oxide semiconductor (CMOS) devices and are unable to account for quantum effects. This makes them impractical for characterizing new and novel nanodevice behavior at sub-10 nanometer (nm) gate lengths, where such effects dominate the governing physics of conventional technology. To address this problem, Sandia researchers have created a universal 3D quantum transport simulator that allows—for the first time—the accurate simulation and optimization of a large number of realistic "beyond-CMOS" devices. The tool can predict the performance of both existing and unstudied nanodevices in order to select the best design options. Using this new tool to simulate behaviors of various field effect transistors (FETs) at sub-10 nm gate lengths, the team discovered the fundamental downscaling limit for CMOS/FETs.

The LDRD-developed simulator, CBR3D, is based on contact block reduction (CBR), a numerical method developed by the team. It provides a highly efficient and scalable technique of implementing the mathematics that provide a quantum mechanical description of energy transport—the nonequilibrium Green's function formalism for quantum transport simulation. The CBR method is significantly faster that existing methods and scales linearly with problem size and number of CPUs.

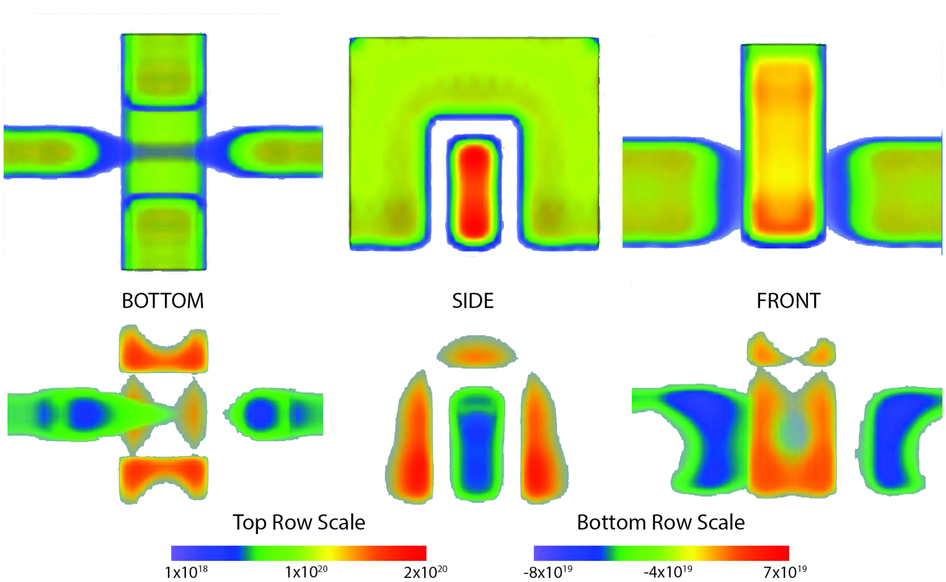

Figure 1. Projected views of on-state (Vg=0.5 Volts) electron density (top row) and corresponding induced charge distribution (bottom row) for an optimized 6 nm MuGFET device. The electronic channel is located in the center of the intrinsic silicon region. Electron densities in the source, channel, drain, and gate regions are all set back from the surfaces due to quantum confinement.

CBR3D was used to simulate and optimize the electrical performance of numerous multi-gate FETs (MuGFETs) at gate lengths of 6-, 5-, and 4-nm using various geometries, channel materials, and wafer/channel orientations (e.g., Figure 1). The team was able to show that at room temperatures, all FETs will begin to experience levels of thermally induced errors at gate lengths around 5 nm. The International Technology Roadmap for Semiconductors gate length projections indicate that a 5 nm limit would be reached within the next 15 years. This important result, published in Applied Physics Letters, helps constrain current technology longevity. The tool developed through the research will significantly aid in identifying, characterizing, and comparing new technologies for post-Moore's law computing.

READ MORE:

D. Mamuluy and X. Gao, The fundamental downscaling limit of field effect transistors, *Applied Physics Letters, 106, 193503, 2015.*

Sandia National Laboratories
Laboratory Directed Research and Development

We welcome your questions, comments, and ideas for future LDRD projects to feature!
Email your feedback to Marie Arrowsmith, mdarrow@sandia.gov

Digital Holography for Quantification of Fragment Size and Velocity from High Weber Number Impacts

Dan Guildenbecher (PI), Phillip Reu, Jun Chen (Purdue), Jian Gao (Purdue)

An LDRD-developed technology based on digital in-line holography provides a rapid and robust method for predicting the behavior of burning droplets of fuel.

Large transportation accidents can create catastrophic fires, as tanks containing flammable or hazardous liquids impact surfaces at high velocity. Understanding how burning droplets of fuel are generated and behave in these types of events is critical to hazard prediction and mitigation and applicable to many governmental agency missions. Historical techniques used to characterize droplet dispersion, based on phase-Doppler anemometry, were spatially limited and provided information only in a two-dimensional plane. Sandia researchers have developed three-dimensional (3D) measurement techniques based on digital in-line holography (DIH) that automatically extract 3D particle position and morphology.

DIH is a laser-based optical technique used to measure particle sizes and three-dimensional positions and velocities. The team significantly advanced the technique, particularly for diagnostics of high-velocity droplet fields by (1) using nano--second laser pulses to improve temporal resolution, (2) developing advanced algorithms to detect individual droplets and track them through multiple exposures, and (3) applying tomographic methods to improve the out-of-plane resolution of large-scale flow fields. Results show that the accuracy of the particle positions measured using the newly developed algorithms was improved by an order of magnitude compared to previous literature results.

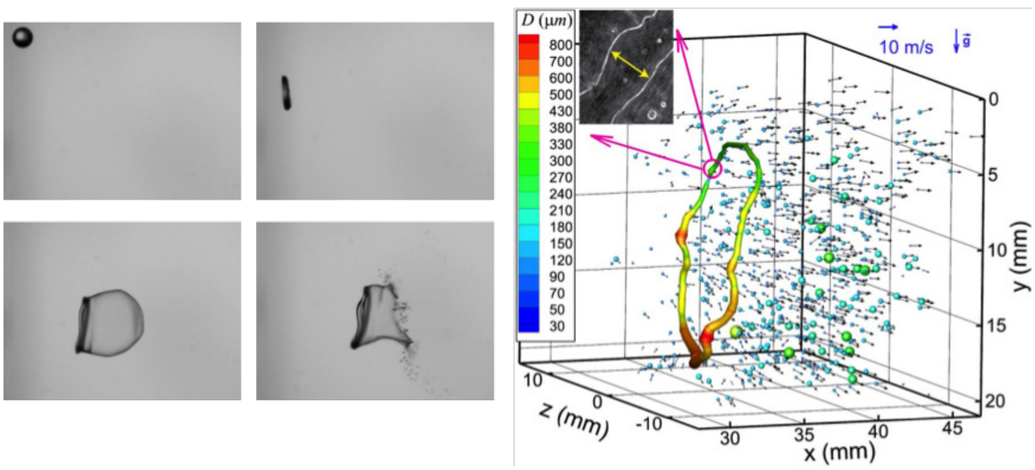

Figure 1. Typical white light recording of the breakup of an ethanol drop in an air stream (left) along with the 3D DIH results (right); from Gao et al. (2013).

In addition to measuring fuel breakup at high velocities (Figure 1), this LDRD-developed technology has been applied to other challenging 3D phenomena, such as particles in environments containing shock waves and aluminum drops from propellant fires. An ongoing LDRD project will extend the technique to quantify the breakup of molten components in shock-induced flows.

READ MORE:

Gao, J., Guildenbecher, D. R., Reu, P. L., Kulkarni, V., Sojka, P. E., and Chen, J., 2013, *Quantitative, 3D diagnostics of multiphase drop fragmentation via digital in-line holography*, Opt. Lett., 38(11), pp. 1893-1895.

UPCOMING LDRD EVENTS

MAY 26 – JUNE 16
Technical and Programmatic Proposal Reviews

JUNE 17 – JUNE 30
Proposal Reviews by Investment Area Representatives

LDRD PROJECTED BUDGET AND STATUS

FY15 Q3 $146 MILLION 373 PROJECTS FUNDED AT $140.5 MILLION

AWARDS & RECOGNITION for LDRD Participants

Mark Taylor received the highest non-monetary award from the U.S. Department of Energy—the 2014 Secretary's Honor Award—for his work as chief computational scientist for DOE's Accelerated Climate Modeling for Energy executive council team.

Aleksandra Faust was awarded the 2015 Tome L. Popejoy Dissertation Prize by the University of New Mexico for her work in robotics. This award recognizes the highlest levels of excellence among doctoral students.