LEADING FUTURE ELECTRONICS INTO THE NANO REGIME USING QUANTUM ATOMISTIC SIMULATIONS IN NEMO5

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EXECUTIVE SUMMARY

With a revenue of $338.9 billion in 2016, and as an enabler for larger economy chains such as electronic systems, the semiconductor industry influences approximately 10% of the world GDP [1]. The transistor is at the heart of this enormous industry, and continuous improvements of transistors, in terms of speed and power consumption, are essential for the stability and growth of the semiconductor industry as well as its dependent product chains and economies. Needed improvements in the performance of transistors have driven the semiconductor industry to push for smaller transistors, reaching 14 nanometers (nm) in the latest technology mode, while development is ongoing for 10-nm technology and beyond. Such aggressive downscaling into a countable number of atoms in the critical dimensions makes atomistic simulations necessary pathfinders in the quantum regime. NEMO5 is designed to comprehend the critical multiscale, multiphysics phenomena for nanoscale technology through efficient computational approaches and enables quantitative study of new generations of nanoelectronic devices even beyond transistors [2,3].

RESEARCH CHALLENGE

The United States has always been a world leader in the semiconductor industry, with 40% of the worldwide semiconductor device-related patents originating here [4]. The industry is one of the nation's largest and most strategic, and the U.S. holds one-third of the global semiconductor device market, which is worth over $300 billion per year. Simultaneously, a relentless downscaling is occurring, with devices expected to be about 5-nm long in their critical active region within 10 years. Further improvements in shrinking dimensions will come only through the detailed study of device designs, materials, and of quantum effects such as tunneling, state quantization, and atomistic disorder. Fundamental questions remain about the downscaling of the CMOS (complementary metal–oxide–semiconductor) switch and its eventual replacement. What is the influence of atomistic local disorder from alloy, line-edge roughness, dopant placement, and fringe electric fields? How do lattice distortions due to strain affect carrier transport in nanometer-scale semiconductor devices such as nanowires, finFETs, quantum dots, and impurity arrays? What are the effects of interconnects' sidewall roughness, grain boundaries, electron–phonon scattering, and roughness of metal–dielectric interfaces? Can inserting new materials and devices reduce power consumption?

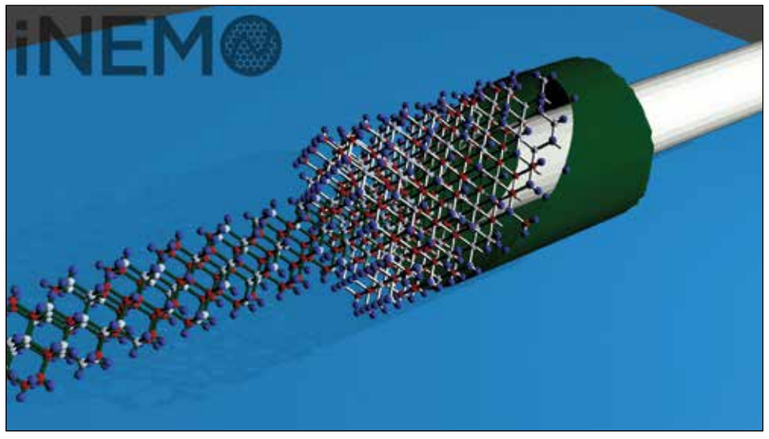

Figure 1: Cylindrical gallium arsenide nanowire transistor represented in a mixed atomistic and solid mechanics basis. The number of atoms in such a device is countable, and the local atom arrangements are critical. The source and drain of the nanowire transistor are conceptualized as thin. The wrap-around gate is indicated by the green solid.

NEMO5 was developed and used by the Institute for NanoElectronic Modeling (iNEMO) at Purdue University to address these fundamental questions on a variety of semiconductor devices. Besides enabling basic engineering, physics, and materials science research, NEMO5 is used by leading semiconductor firms to design future devices. The source code, binaries, and support for academic use are available through nanoHUB.org.

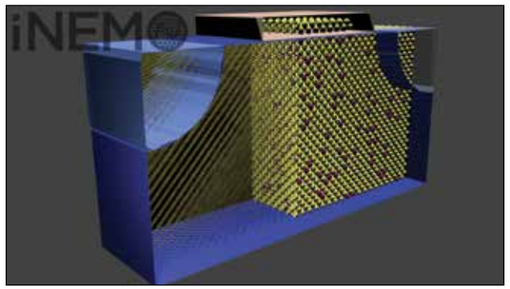

Figure 2: Atomistic representation of a silicon–germanium (SiGe) ultra-thin-body transistor. SiGe is a random alloy with atomistic local disorder. The source and drain are indicated by the rounded shapes. The top gate regulates the electron flow from source to drain.

METHODS & CODES

iNEMO's research on Blue Waters encompasses multiphysics atomistic quantum simulations implemented in NEMO5. The needed physics vary from one device to another, but all can be simulated inside NEMO5. For example, for transistors, quantum transport simulations are performed using the self-consistent Poisson with a nonequilibrium Green's function (NEGF) approach employing semiempirical tight-binding methods. The current mechanism of tunneling field effect transistors (TFETs) is through interband tunneling rather than thermionic emission in typical MOSFETs (metal–oxide semiconductor field-effect transistors). For realistic performance predictions, incoherent scattering effects are also included.

Several classes of devices demand a multiscale decomposition into regions of high- and low-electron densities. These different charge densities imply very different scattering mechanisms and thermalization processes. For example, for nitride-based light emitting diodes and alloy-engineered nitride TFETs, we use a multiscale quantum transport model, which treats high-density regions as local charge reservoirs where each reservoir serves as a carrier injector/receptor to the next/previous reservoir.

Atomistic basis sets are mapped from fundamental *ab initio* methods such as Density Functional Theory into reduced-order tight-binding or localized basis sets. With such reduced-order models, we can represent realistically extended devices.

RESULTS & IMPACT

Interconnect modeling: Orientation effects on the specific resistance of copper grain boundaries are studied systematically with two different atomistic tight-binding methods. A methodology is developed to model the specific resistance of grain boundaries at the ballistic limit using the embedded atom model, tight-binding methods, and nonequilibrium Green's functions. The methodology is validated against first-principles calculations for thin films with a single coincident grain boundary resulting in a 6.4% deviation in the specific resistance compared to DFT. A statistical ensemble of 600 large, random structures with grains is studied. For structures with three grains, we found that the distribution of specific resistances is close to normal. Finally, we constructed a compact model for grain-boundary-specific resistance based on a neural network.

Quantum device modeling: The discovery of integer (1980) and fractional (1982) quantum Hall effects revolutionized the field of condensed-matter physics by providing a platform for testing the effects of strong interactions among electrons, which are difficult to observe elsewhere. Strong interelectron interactions create a liquid-like state in which the current is carried by fractionally charged quasiparticles known as composite-Fermions (CFs). Further interactions among CFs could lead to the formation of quasiparticles that follow non-Abelian statistics, meaning they would hold a memory of the way in which their world lines are braided. These yet-unobserved non-Abelian quasiparticles could provide a platform for fault-tolerant topological quantum computing applications. In this work, we developed a computational model for devices that could be used to observe these quasiparticles and to propose better designs.

These devices consist of gallium arsenide-based nanostructures that are used for confining electrons in two dimensions. We applied a perpendicular magnetic field to limit electron/CF flow to the edges of the sample in one-dimensional channels. Such channels can be brought together from across the device and made to interfere with each other, like photons using gate-defined one-dimensional constrictions called quantum-point contacts. Observation of these interference oscillations can shed light on the properties of the non-Abelian quasiparticles. These quasiparticles must be traveling fast enough to maintain their phase while interfering and show a strong interference pattern.

We propose new designs for quantum-point contacts with high electron velocity along the edge channels using our modeling tool. Blue Waters has provided us with a unique and reliable computing environment to support these kinds of simulations.

WHY BLUE WATERS

Quantum transport simulations are very computationally expensive and demanding of memory due to the high degree of complexity of the equations used, especially if incoherent scattering of particles is needed. A toy quantum transport calculation of a

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MODELING MILLIONS OF ATOMS AND THEIR ELECTRONS: TIGHT-BINDING USING A SPECTRAL PROJECTION PURIFICATION METHOD

Allocation: Exploratory/50 Knh
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EXECUTIVE SUMMARY

In this project, we demonstrated a new method for accurately computing properties of material systems containing up to 10 million atoms and their electrons. The method is based on a linear scaling version of tight binding, which is a semiempirical approach for computing, from a model, the energy of a collection of atoms for the interactions among the electrons and the nuclei. We computed the density matrix—a fundamental property of such a system—using a spectral projection purification method. The method scaled well on Blue Waters to millions of atoms over thousands of processors. As an example, we computed the electronic properties of an SiO_2 crystal, which we reported in the form of the density of states. The results show the feasibility of the approach as a general-purpose total-energy electronic structure computational tool for materials science.

RESEARCH CHALLENGE

Our interest is in testing more efficient methods for computing the electronic structure of systems with millions and tens of millions of atoms. Properties of material domains of this size are important in many different technologies, from microelectronics to medical science to energy technologies. Our interest is in the properties of dielectric materials of plasma generation, which are important in combustion, materials processing, and catalysis. Traditional electronic structure calculations for these kinds of materials have cubic scaling in N—the number of atoms in the system—making the calculations prohibitively computationally expensive for systems larger than 10^4 atoms.

METHODS & CODES

We used the code we developed to compute the density matrix, a fundamental electronic structure quantity for a system of atoms and their electrons. Our computational method [1] combines the advantages of two existing linear scaling methods: the Kernel Polynomial Expansion (KPE) [2] and second-order spectral projection purification (SP2) [3]. The KPE method is computationally efficient and can be easily expressed in terms of sparse matrix–vector multiplications (SpMVs), but cannot satisfy one of the required constraints on its own. On the other hand, the SP2 method is highly accurate but can be prohibitively costly in terms of memory and communication when expressed in terms of sparse matrix–matrix multiplications (SpGEMM). When expressed in terms of SpMVs, the SP2 method scales exponentially with the number of iterations required to converge. An advantage of SP2, however, is that near the correct solution P, the method converges quadratically [3]. Thus, we have constructed a hybrid method that takes the inexpensive KPE solution and purifies P_{kpe} with a few SP2 iterations that are more expensive.

RESULTS & IMPACT

Our recent work has shown the feasibility of this method for computing properties of million-atom systems [1]. We will apply the method and have impact in the area of surface and dielectric properties for combustion, catalysis, and materials processing. The method can also have impact in other areas of physics and materials science. With the scaling observed during the outcome of the Blue Waters work, we have demonstrated that this method is fast, accurate, and efficient in 10-million-atom systems and beyond, which will increase its impact significantly.

WHY BLUE WATERS

Access to the Blue Waters system made this work possible by permitting our studies on a single platform that offered both large parallelism and resources for memory-intensive computations. Depending upon the tuning of the method, it is possible to carry out the entire computation on a single node in a very memory-intensive approach or, by distributing the computation over many processors, it is possible to perform the algorithm in a massively parallel way. The Blue Waters system allowed us to study the approach and plan for future studies with more optimized tuning.

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50-nm-long wire with a 3-nm diameter requires around 1 teraflop for a single energy point where more than 1,000 energy points are needed. And this calculation must be repeated perhaps a hundred times for a full current–voltage sweep. The treatment of a realistic device would require an atomistic resolution of a device with a cross-section of more than (20 × 20) nm^2, which includes the core semiconductor and the surrounding gate material. Such devices of larger sizes are especially an issue due to the $O(n^3)$ scaling of matrix operation time-to-solution and $O(n^2)$ scaling of memory. Blue Waters was used for running such simulations on up to 16,384 cores per simulation. In many cases, the work could not be accomplished in a reasonable amount of time without Blue Waters, and for the larger simulations the work could not be accomplished on other available systems. Blue Waters' staff provide exemplary support and user outreach to guide system usage, help with issues as they arise, and assist with code performance and scaling.

PUBLICATIONS & DATA SETS

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