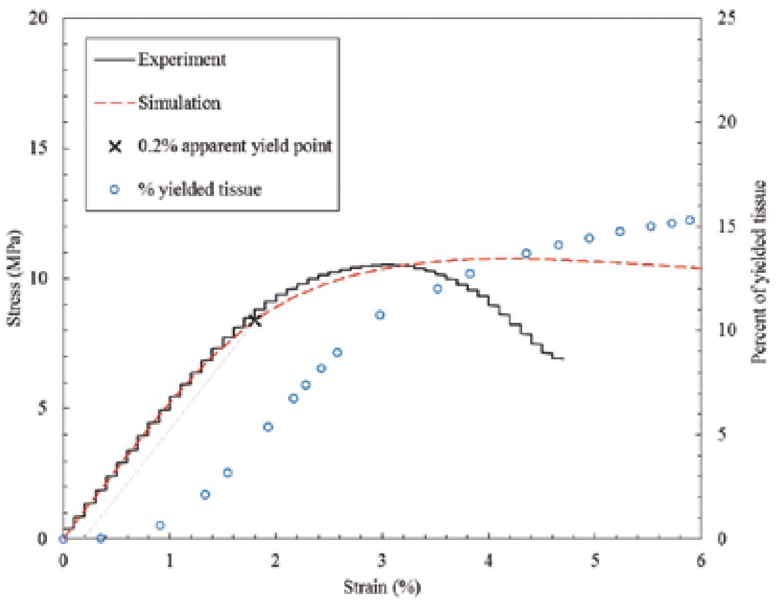

affected by diseases like osteoporosis, or diabetes and also aged bone will be modeled to better understand how the properties of bone are affected by various factors, assess effects of medications and to predict risk of bone fracture for patients.

PUBLICATIONS AND DATA SETS

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FIGURE 3: Prediction of stress-strain behavior of trabecular bone under compression along with percent of yielded tissue.

NANOSCALE ELECTRONIC DEVICES WITH NEMO5

Allocation: NSF PRAC/1.24 Mnh
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EXECUTIVE SUMMARY

Relentless downscaling of transistor size has continued according to Moore's Law for the past 50 years. According to the International Technology Roadmap for Semiconductors (ITRS), transistor size will continue to decrease in the next 10 years, but foundational issues with currently unknown technology approaches must be pursued. The number of atoms in critical dimensions is now countable. As the materials and designs become more dependent on atomic details, the overall geometry constitutes a new material that cannot be found as such in nature. NEMO5, the software package developed by the Institute for Nanoelectronic Modeling (iNEMO), is designed to comprehend the critical multi-scale, multi-physics phenomena through efficient computational approaches and to quantitatively model new generations of nanoelectronic devices including transistors and quantum dots, as well as to predict novel device architectures and phenomena [1,2].

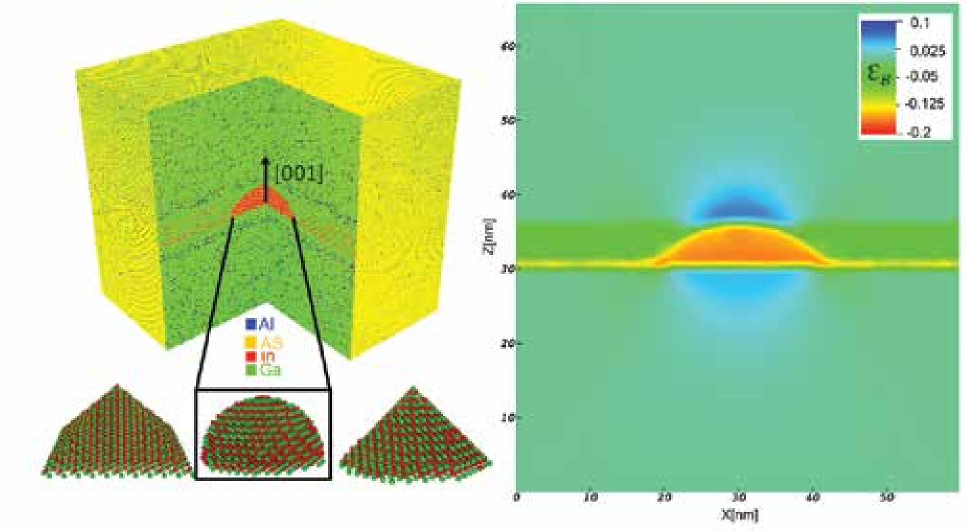

FIGURE 1: NEMO5 can simulate alloys such as this AlGaAs/InGaAs quantum dot system. On the left is the atomistic structure of a simulated 10 million atom system. The right shows the biaxial strain distribution dome-shaped quantum dot of size 20 nm by 5nm. Strain calculations are one of the first steps toward ensuring accurate treatment of the electronic qualities of devices.

INTRODUCTION

The U.S. is a market leader in the semiconductor industry, which produces many high-paying, high-technology jobs. The U.S. semiconductor industry is one of the nation's largest export industries, and the U.S. holds one-third of the global semiconductor device market worth over $300 billion. Simultaneously, the end of Moore's Law scaling as we know it will be reached in 10 years, with devices expected to be about 5 nm long and 1 nm in their critical active region width. 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? Can power consumption be reduced by inserting new materials and device concepts?

NEMO5 is developed and used by the Institute for NanoElectronic Modelling (iNEMO) at Purdue 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.

METHODS & RESULTS

iNEMO's research on Blue Waters encompasses simulations of incoherent scattering effects on tunnel FET devices, time-resolved quantum transport, a compact model for self-assembled quantum dot heterostructures, and a multiscale approach for nitride-based light emitting diodes.

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). Tunneling from the valence to conduction band has the potential to yield significantly improved subthreshold slopes to allow lower supply voltages and better efficiency than MOSFETs. Electron transport through the overall device, including the source and drain, entails significant amounts of computationally demanding scattering, which cannot be ignored in realistic device performance predictions, and these simulations agree well with experimental resistivity data. In an ultra-scaled silicon TFET, simulation also found that incoherent scattering has a significant impact on performance.

Time-resolved quantum transport data allow more accurate calculation of energy/delay device characteristics during turn-on for studying novel effects based on wave function phase manipulation, and as an alternative research path to simulating dissipation and nonlocal scattering. Time-resolved quantum transport simulations are performed with the semi-empirical tight binding method. Initial work shows that this approach is valid up to about 1 mV/ps, corresponding to a few GHz in realistic transistors.

Self-assembled quantum dots are highly strained heterostructures with optoelectronic applications, such as infrared photodetectors, intermediate band solar cells, optical amplifiers, and quantum dot lasers. A universal behavior in terms of strain magnitude and profile is observed in atomistic strain simulations of dots with different shapes and materials. Atomistic strain simulations are more accurate but more expensive than analytic continuum solutions. Simulations on Blue Waters showed that both techniques indicate that the strain depends on the aspect ratio of the dot, and not on the individual dimensions. This has allowed for the formulation of a compact model of strain effects on self-assembled quantum dots.

Multi-quantum well LEDs have carrier flow through complex quantum states and the NEGF (non-equilibrium Greens function) approach has been used to model nitride-based diodes that provide blue mid-to-high power light. Strong electron-electron/phonon scattering thermalizes carrier distribution in the wells. A multiscale approach models the barriers in non-equilibrium with the wells in equilibrium. Simulations of 120 nm long devices show IV characteristics matching experimental results when accounting for temperature differences and external resistance. This research has revealed how p-side wells provide higher radiative recombination, supporting experimental evidence, due to more deeply filled electronic states, leading to a stronger overlap in the electron-hole densities.

WHY BLUE WATERS

In many cases the work could not be accomplished in a reasonable amount of time without Blue Waters, and for 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. In particular, they have provided custom scripts and permissions to facilitate management of an allocation with a large research group.

NEXT GENERATION WORK

A next-generation Track-1 system will enable efficient reliability predictions of modern nanodevices—a crucial milestone in their design. Atomistic deviations due to statistical and fabrication fluctuations can have increasingly large effects on a device's operation as devices are scaled, and it is imperative to have a strong grasp on these phenomena in the coming years.

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COMPRESSIBLE LARGE EDDY SIMULATION OF A FILM-COOLED STAGE-ONE NOZZLE AT DIFFERENT FREESTREAM TURBULENCE LEVELS

Allocation: Innovation and Exploration/300 Knh

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Co-PI: Gustavo Ledezma[2]
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EXECUTIVE SUMMARY

Gas turbines are the backbone of aircraft propulsion. Therefore, technologies that improve the fuel efficiency of these turbines can have a significant impact on the U.S. economy and can substantially reduce polluting emissions. The quest for greater turbine efficiency has led to increased firing temperatures, subjecting turbine components to extremely high temperatures. One common technique for abating these temperatures is film cooling, which bleeds cool air from the compressor stage of the engine and discharges it through small holes in the turbine blade walls, providing an insulating layer of cool air. The focus of this project is to investigate the impact of freestream turbulence on film cooling, including mixing, turbulence decay, and boundary layer development.

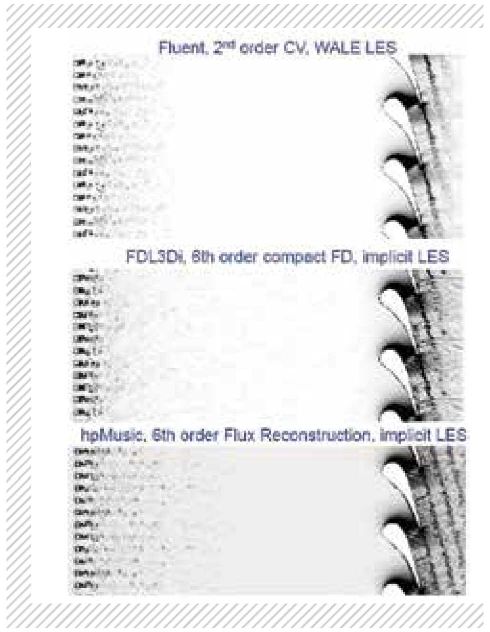

FIGURE 1: Numerical schlieren for an uncooled transonic vane and 6% turbulence intensity (a) unstructured 2nd order solver (b) structured 6th order solver (c) unstructured 6th order solver.

INTRODUCTION

Because of their power density and efficiency, gas turbines are, and will continue to be, the backbone of narrow- and wide-body aircraft propulsion. According to the Federal Aviation Administration, the United States alone consumed approximately 35.6 billion gallons of aviation fuel in 2012. Technologies that can further improve fuel efficiency can have a significant impact on the U.S. economy while reducing emissions.

The modern high-bypass turbofan engine is based on the Brayton cycle. Air is ingested in the engine and passes through the fan. A majority of the airflow bypasses the core of the engine to increase propulsive efficiency. The core flow is compressed, increasing total pressure (Pt) and total temperature (Tt). Fuel is added and burned in the combustor, increasing Tt and slightly reducing Pt, and the flow is expanded through the turbine, reducing Pt and Tt. Work extracted by the turbine drives the compressor. The turbine also drives a fan at the front of the engine in order to increase the mass flow through the engine, thus increasing the propulsive efficiency. In order to improve thermal efficiencies the turbine inlet temperature and compressor pressure ratio have historically increased with time.

The need for higher turbine efficiencies to reduce fuel consumption keeps pushing the firing temperature up. As a result, all components in the high-pressure turbine (HPT) are subject to extremely