NANO HIGHLIGHT
Multimillion-atom simulation and visualization of quantum dot systems

Network for Computational Nanotechnology Grant EEC-0228390
PIs: **Mark S. Lundstrom, Gerhard Klimeck**
Purdue University

Mullti-million atom simulations: The Nanoelectronic Modeling tool (NEMO 3-D) enables users to study long-range strain effects and quantum confined electronic structure effects. NEMO 3-D was originally developed at NASA/JPL from 1998-2003. NEMO 3-D had previously demonstrated strain calculations for up to 16 million atoms and eigen value computations for up to 9 million atoms. However, the eigen state calculation were limited to around 100,000 atoms due to algorithmic limitations. With NCN high performance computing team we were able to increase the simulation capability to 64 million atom strain systems and 21 million electron state systems. This corresponds to physical volumes of (110nm)3 and (77nm)3, respectively. This simulation capability was demonstrated in the NSF TeraGrid. We are now beginning to fully explore this capability to simulate the effect of long-range strain in the system [1] and the effects of coupled quantum dots.
Multi-millionatom visualization has been demonstrated [2] through a graphics hardware accelerated platform. The simulation data contains the probability density function values of multiple electron orbitals for up to tens of millions of atoms. The visualization component of the system utilizes hardware-accelerated direct volume rendering. To facilitate such interactive visualization, a number of novel techniques have been developed, including compact representation techniques for the FCC lattice within PC graphics hardware texture memory, hardware-accelerated trilinear and cubic reconstruction schemes, and multi-field rendering techniques utilizing logarithmic scale transfer functions. The system also enables the user to drill down through the simulation data and execute statistical queries using general-purpose computing on the GPU (GPGPU).

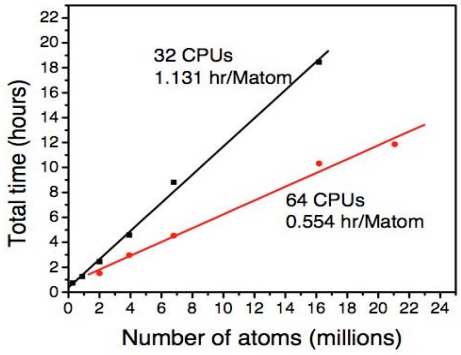

Figure 1: Required end-to-end time to obtain 4 eigenvectors as a function of system size for a 32 and 64 CPU configuration. Calculations were performed on NSF TeraGrid on Itanium2.

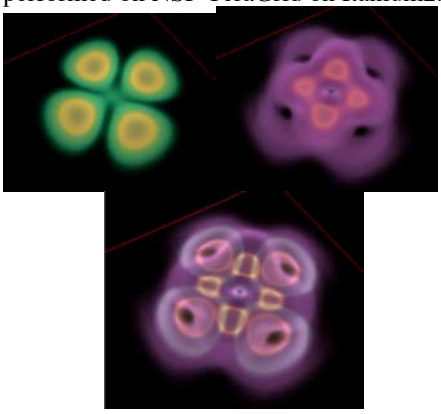

Figure 2: second excited state in an InAs quantum dot computed in an sp3d5s* tight binding model. Left: p,d orbital contributions. Right: s,s* orbital contributions. The two sets of contributions have different nodal symmetries. Bottom: combined wavefunction of all orbital contributions

References (10 point font)

[1] Marek Korkusinski, Gerhard Klimeck, Haiying Xu, Seungwon Lee, Sebastien Goasguen, Faisal Saied,
"Atomistic Simulations in Nanostructures Composed of Tens of Millions of Atoms:Importance of long-range Strain Effects in Quantum Dots", 2005 NSTI Nanotechnology Conference and Trade Show, Anaheim, CA, May 8-12, 2005.
[2] Wei Qiao, David S. Ebert ,Alireza Entezari, Marek Korkusinski, Gerhard Klimeck,
"VolQD: Direct Volume Rendering of Multi-million Atom Quantum Dot Simulations", IEEE Visualization 2005, October 23-28, Minneapolis, MN.