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nanoHUB.org - Towards On-Line Simulation for Materials and Nanodevices by Design[1]

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Challenges in nanoelectronics are the merging notions of material and device. Device lengths have reached the nanometer scale, where material properties are defined. Detailed atomic composition such as strain, interface, doping, and size fluctuations need to be treated. Here the material science and device engineering communities meet on the common ground of quantum mechanics. Success will depend on bridging language and approach barriers between communities. The development of accepted community software will be a significant step.

One element of such codes is the NanoElectronic MOdeling Tool. NEMO 3-D enables the computation of strain and electronic structure in an atomistic basis for over 60 and 23 million atoms, corresponding to volumes of $(107nm)^3$ and $(77nm)^3$, respectively. NEMO 3-D runs on a serial and parallel platforms, local cluster computers as well as the NSF Teragrid. About 400,000 atoms are treated efficiently on a single 32bit CPU. NEMO uses an atomistic valence force field method (strain) and the empirical tight binding method (electronic structure). Quantitative simulations for quantum dots in the InAs/GaAs and Si/SiGe material systems have been performed.

The Network for Computational Nanotechnology (NCN) is in the process of developing new community and research codes for the analysis of nano-(electronic/mechanical/bio) devices. These tools are hosted on http://nanohub.org for on-line simulation use free-of-charge. Last year over 1,000 people performed about 64,000 simulations. 2,200 others viewed seminars and nanotechnology curriculum items. nanoHUB is being developed as a community resource that encourages on-line simulation, collaborations and nanotechnology education.

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[1]This work has been performed in close collaboration with M Korkusinski, H Xu, F Saied, S Goasguen (all at Purdue), TB Boykin (at U of Alabama Huntsville), and FA Oyafuso, S Lee, H Hua, O Lazarankova, RC Bowen, and P von Allmen (at JPL)