HPC Challenges for NanoElectronic Modeling (NEMO)

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NEMO 1-D
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NEMO 1-D:
A User-friendly Quantum Device Design Tool

- NEMO was developed under a government contract to Texas Instruments and Raytheon from 1993-97
  - >50,000 person hours of R&D
  - 250,000 lines of code in C, FORTRAN and F90
- Based on Non-Equilibrium Green function formalism (Datta, Lake, Klimeck).
- NEMO in THE state-of-the-art heterostructure design tool.
- Used at Motorola, HP, Texas Instruments, US Government Labs, and >10 Universities.
Development of NEMO 3-D

**Approach:**
- Leverage NEMO 1-D:
  - 25 person years at TI / Raytheon
  - 250,000 lines of code.
- Use local orbital description for individual atoms in arbitrary crystal / bonding conf.
  - Use s, p, and d orbitals
  - Use genetic algorithm for fitting
- Compute mechanical strain in the system.
- Develop parallel algorithms to generate eigenvalues/vectors of very large matrices (N=3.2x10^8 for a 16 million atom system).
- Develop prototype GUI for (NEMO-3D)

**Electronic Structure for Systems of up to 30 Million Atoms on Beowulf Cluster**

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Heterostructure Applications:
Transitions & Functionality Controlled by Design

Photon Absorption

Photon Emission

Tunneling

Detectors

Lasers

Logic / Memory

Quantum Well
Infrared Detector

Quantum Cascade
Laser

Resonant
Tunneling
Diode

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Genetically Engineered NanoElectronic Structures (GENES)

Objectives:
- Automate nanoelectronic device synthesis, analysis, and optimization using genetic algorithms (GA).

Approach:
- Augment parallel genetic algorithm (PGApack).
- Combine PGApack with NEMO.
- Develop graphical user interface for GA.

How do you know what you have built?

Results:
- Nanoelectronic Device Structural analysis

GA analyzed atomic monolayer structure and doping profile of RTD device
Black: structure specs, Blue: Best fit

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Computational cost:
- 30 minutes compute time / individual
- 2000 individuals evaluated
- 1000 serial compute hours
- 31 hours compute time on 32 CPUs
  (in 1998 on neptune.cacr.caltech.edu)

Results:
- Nanoelectronic Device
- Structural analysis

GA analyzed atomic monolayer structure and doping profile of RTD device
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Bottom-up, Atomistic 3-D Quantum Dot Simulation for Revolutionary Computing and Sensing

Atomic Orbitals size: 0.2nm \( \rightarrow \) Structure \( \rightarrow \) Nanoscale Quantum States (Artificial Atoms, size 20nm) \( \rightarrow \) Designed Optical Transitions Sensors

Computational Cost:
- One structure / individual: 1-10 hours on 20-40 CPUs running in parallel
- Cannot even think about running GA based evolution right now!!!!
- Have no implemented architecture
  - Need a parallel GA running parallel applications underneath

Need multiple parallelisms

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Exploration of the Design Space is Bound By Computation!

- Fundamental nanoelectronic tools exist already and are being improved!
  - 1-D Quantum Transport is Solved!
  - 2-D / 3-D Quantum Transport bound by Computation
- GENES - Design Synthesis needs compute power!

Advanced Device Simulation

End of SIA Roadmap

Dopant Fluctuations in Ultra-scaled CMOS

Electron Transport in Exotic Dielectrics

(Ba,Sr)TiO₃  TiO₂

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