HPC Challenges for NanoElectronic Modeling (NEMO)

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NEMO 1-D

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NEMO 3-D / Synthesis

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R. Chris Bowen, JPL

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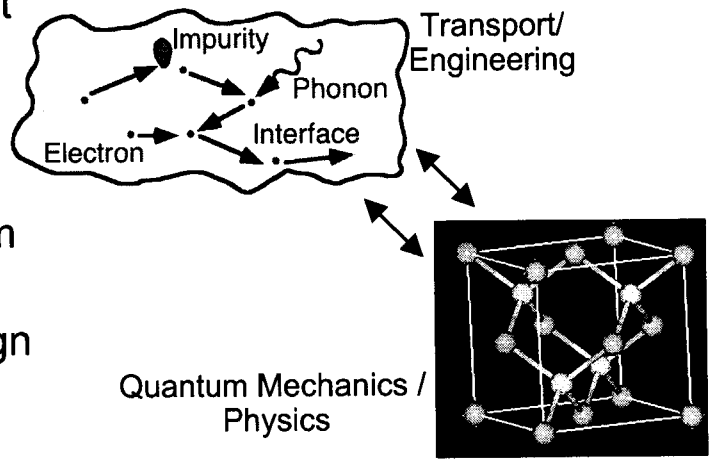
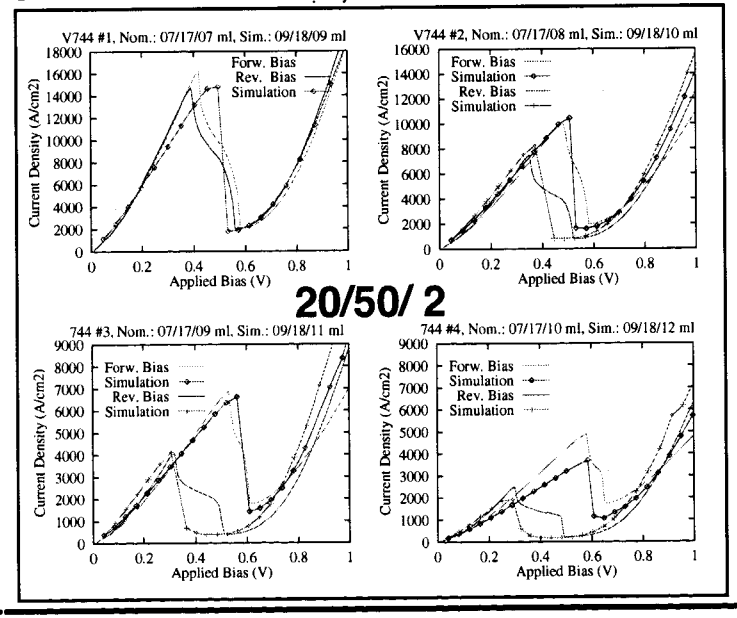
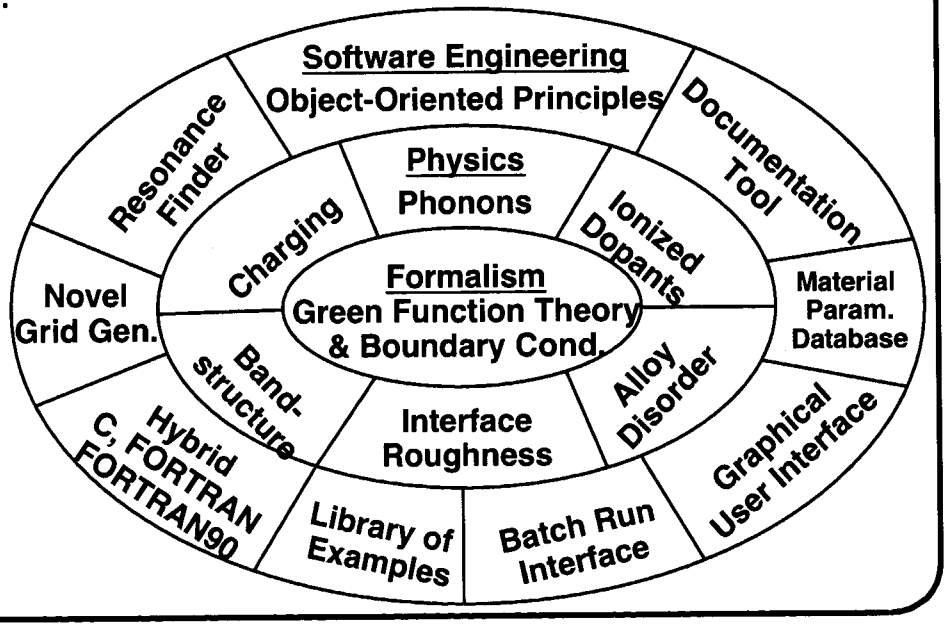
NEMO 1-D:
A User-friendly Quantum Device Design Tool

- 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.

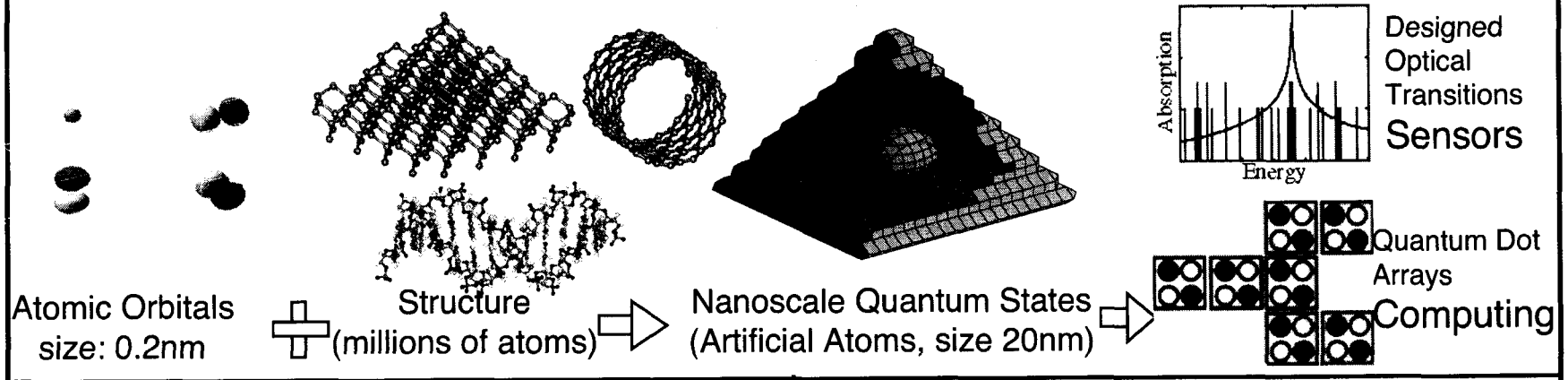


Testmatrix





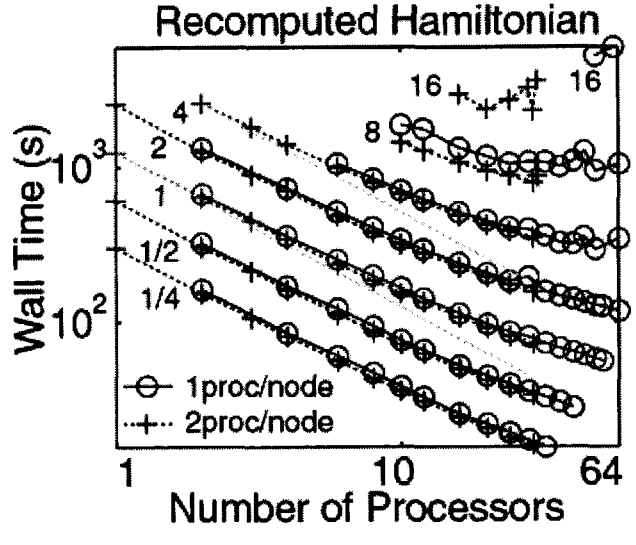
Development of NEMO 3-D



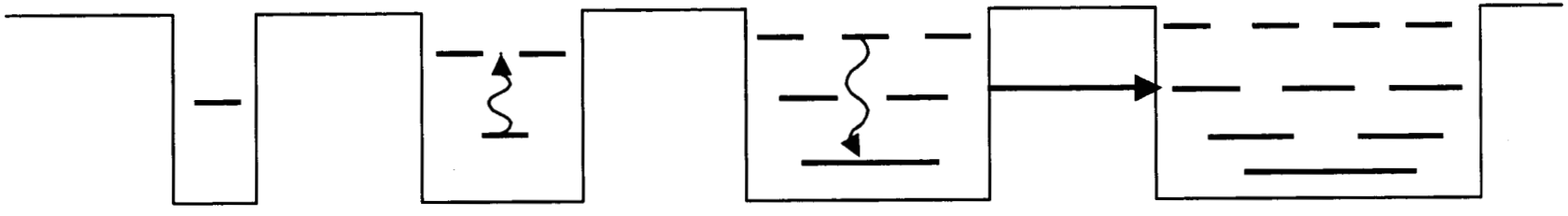
Approach:

- 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 ($N=3.2\times10^8$ 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



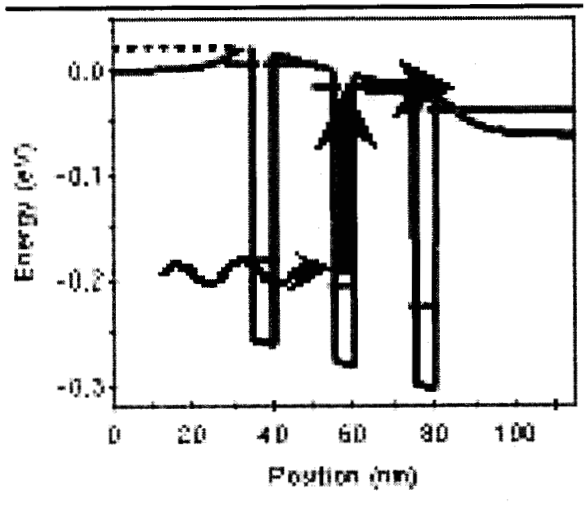
Heterostructure Applications:
Transitions & Functionality Controlled by Design



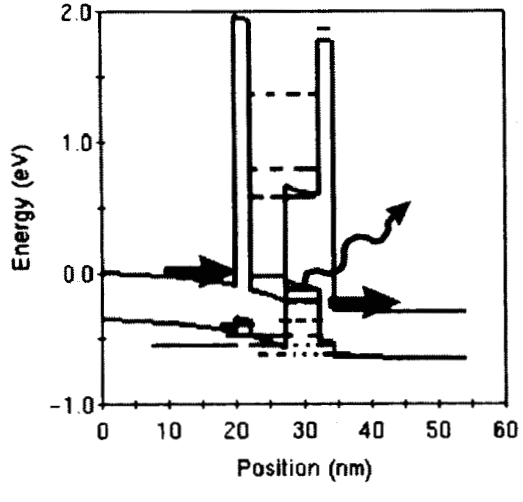
Photon Absorption → Detectors

Photon Emission → Lasers

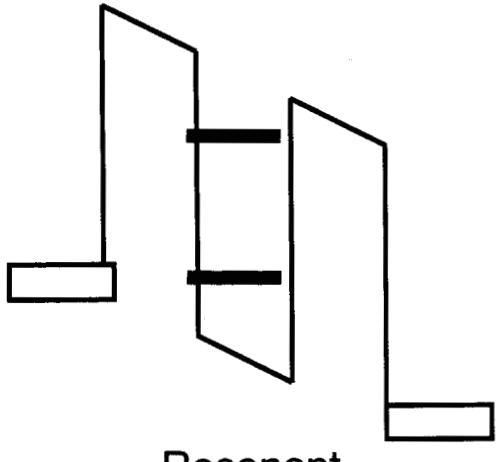
Tunneling → Logic / Memory



Quantum Well Infrared Detector



Quantum Cascade Laser



Resonant Tunneling Diode

Genetically Engineered Nanoelectronic Structures (GENES)

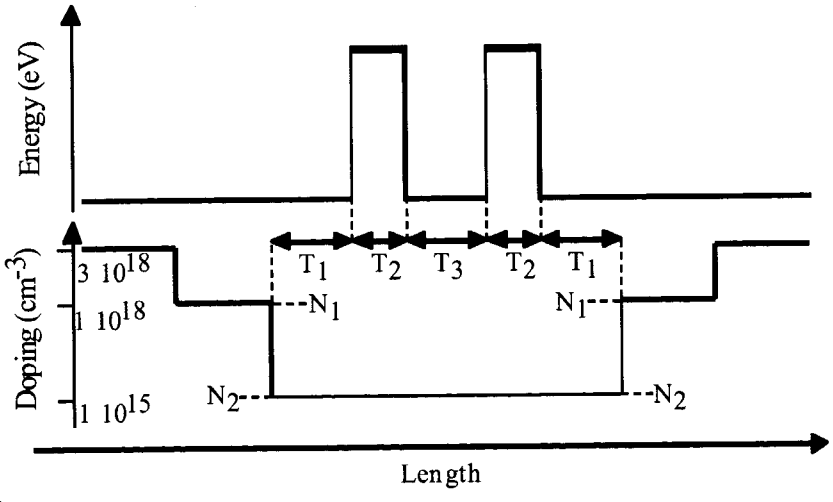
Objectives:

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

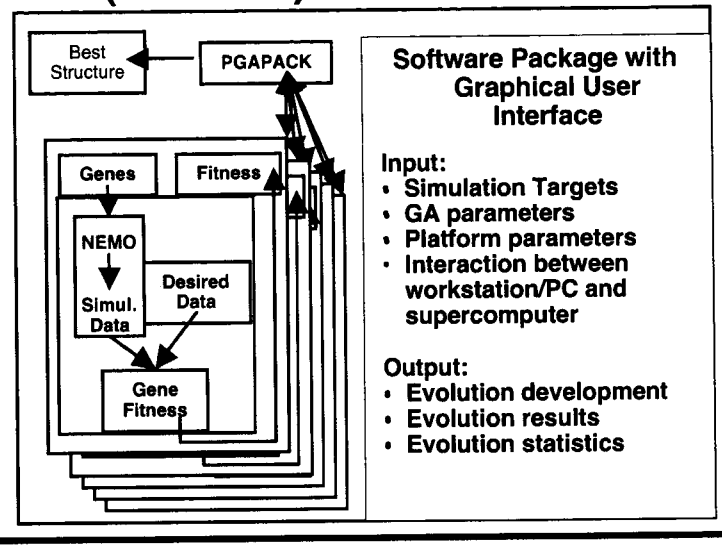
Approach:

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

How do you know what you have built?

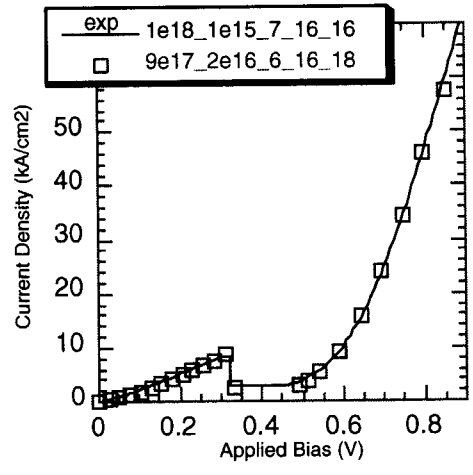


Architecture



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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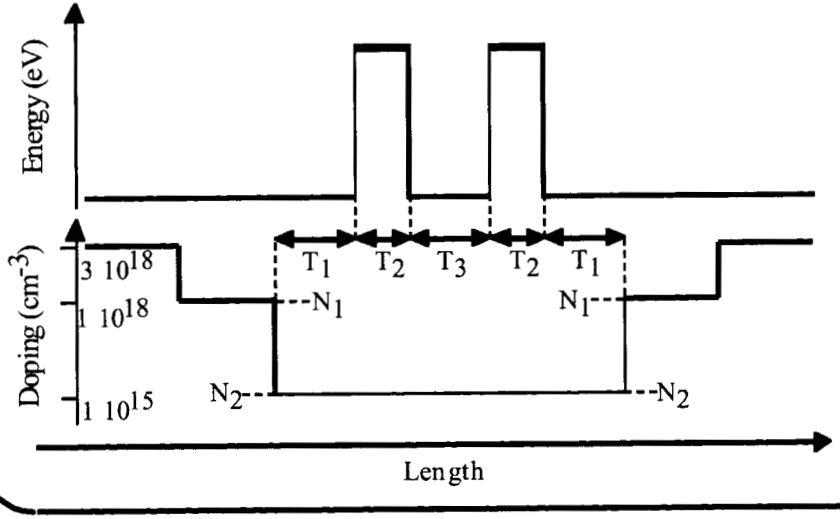
Applied Cluster Computing Technologies Group

Genetically Engineered Nanoelectronic Structures (GENES)

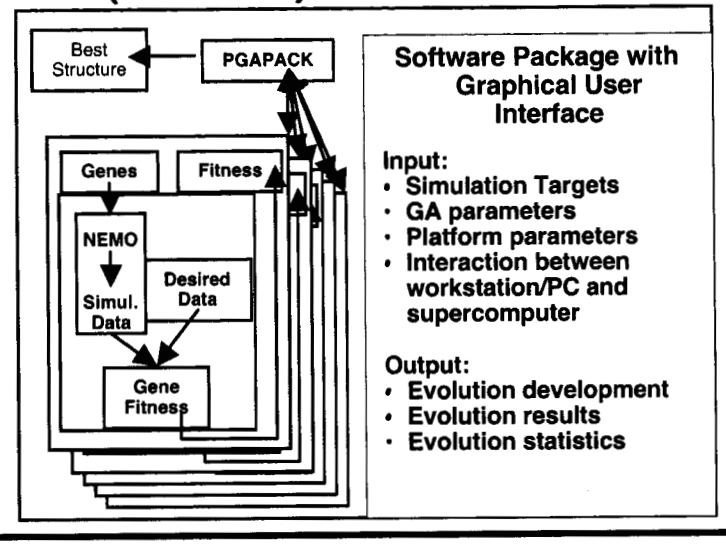
Computational cost:

- 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)



Architecture



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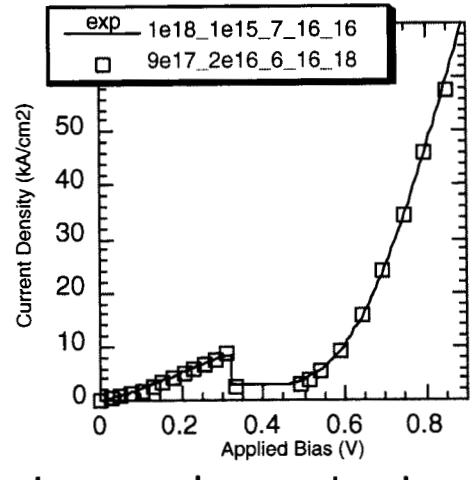

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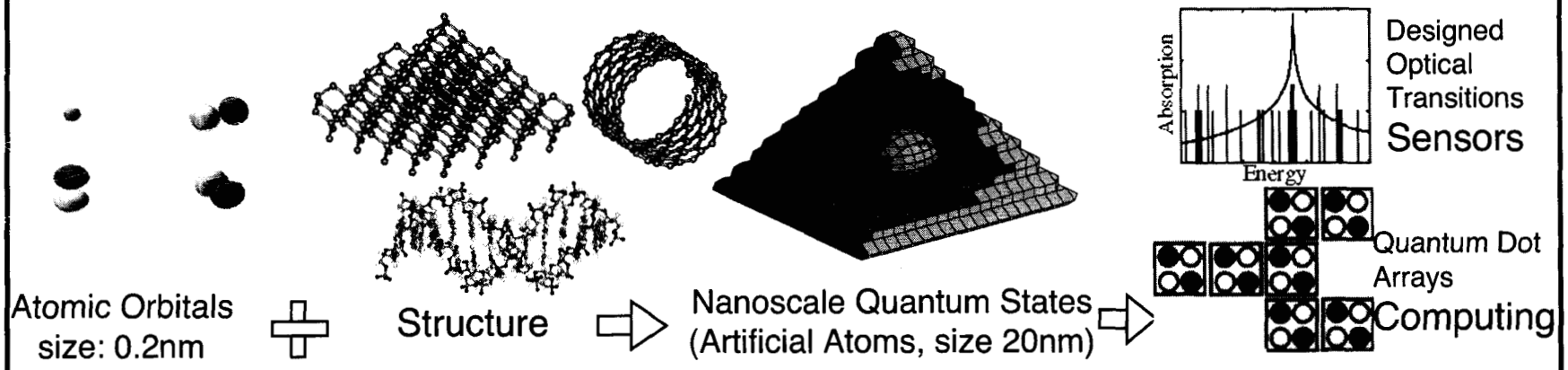
Bottom-up, Atomistic 3-D Quantum Dot Simulation for Revolutionary Computing and Sensing

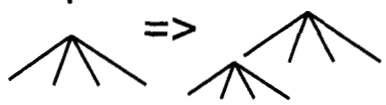


Computational Cost:

- **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**

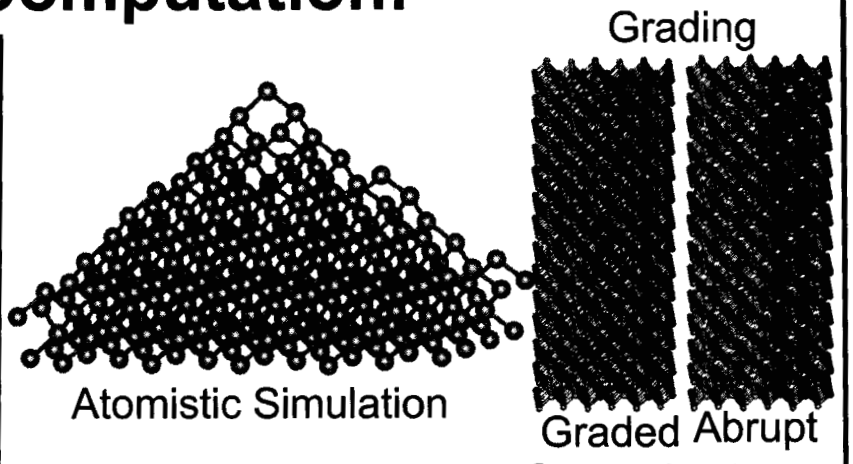
Need multiple parallelisms

=>

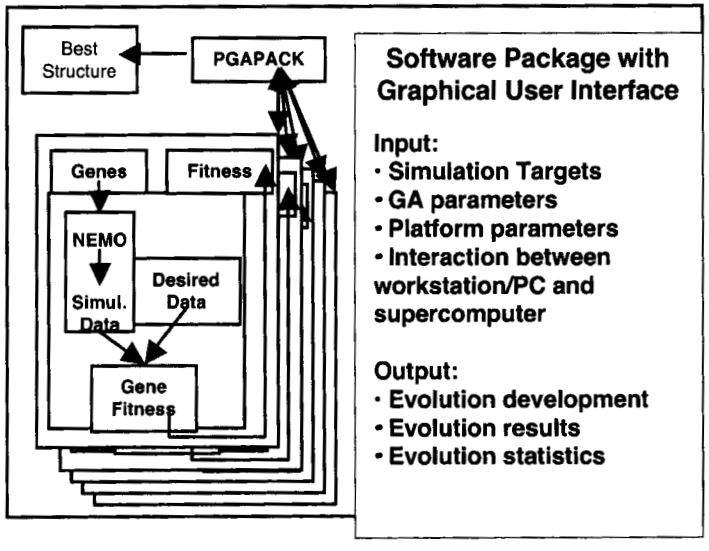


Exploration of the Design Space is Bound By Computation!

- 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



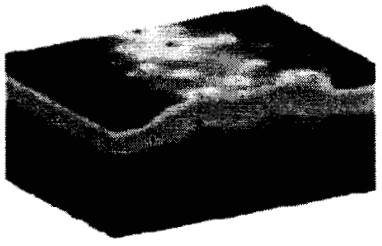
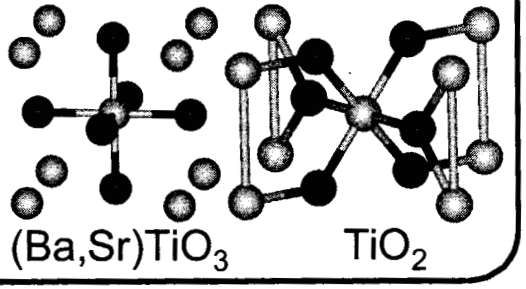
Software Package with Graphical User Interface

Input:
- **Simulation Targets**
- **GA parameters**
- **Platform parameters**
- **Interaction between workstation/PC and supercomputer**

Output:
- **Evolution development**
- **Evolution results**
- **Evolution statistics**

End of SIA Roadmap

Dopant Fluctuations in Ultra-scaled CMOS



Electron Transport in Exotic Dielectrics