Genetically Engineered NanoElectronic Structures (GENES)

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Outline:

- NEMO genealogy and general features
- Structural device optimization:
    - Massively parallel genetic algorithm package
- Conclusion

NEMO Genealogy

- NEMO was developed under a government contract at Texas Instruments and Raytheon from 1993-1997
  - Theory
    - Roger Lake, Chris Bowen, Tim Boykin (UAH), GK
  - Graphical User Interface
    - Dan Blanks, GK
  - Programming Approach, Philosophy, and Prototypes
    - Bill Frensley (UTD), GK
  - Coding
    - Manhua Leng (UTD), Chenjing Fernando, Paul Sotirelis, Dejan Jovanovic, Mukund Swaminathan (UTA), GK
  - Experiments for verification
    - Ted Moise, Alan Seabaugh, Tom Broekaert, Berinder Brar, Yung-Chung Kao

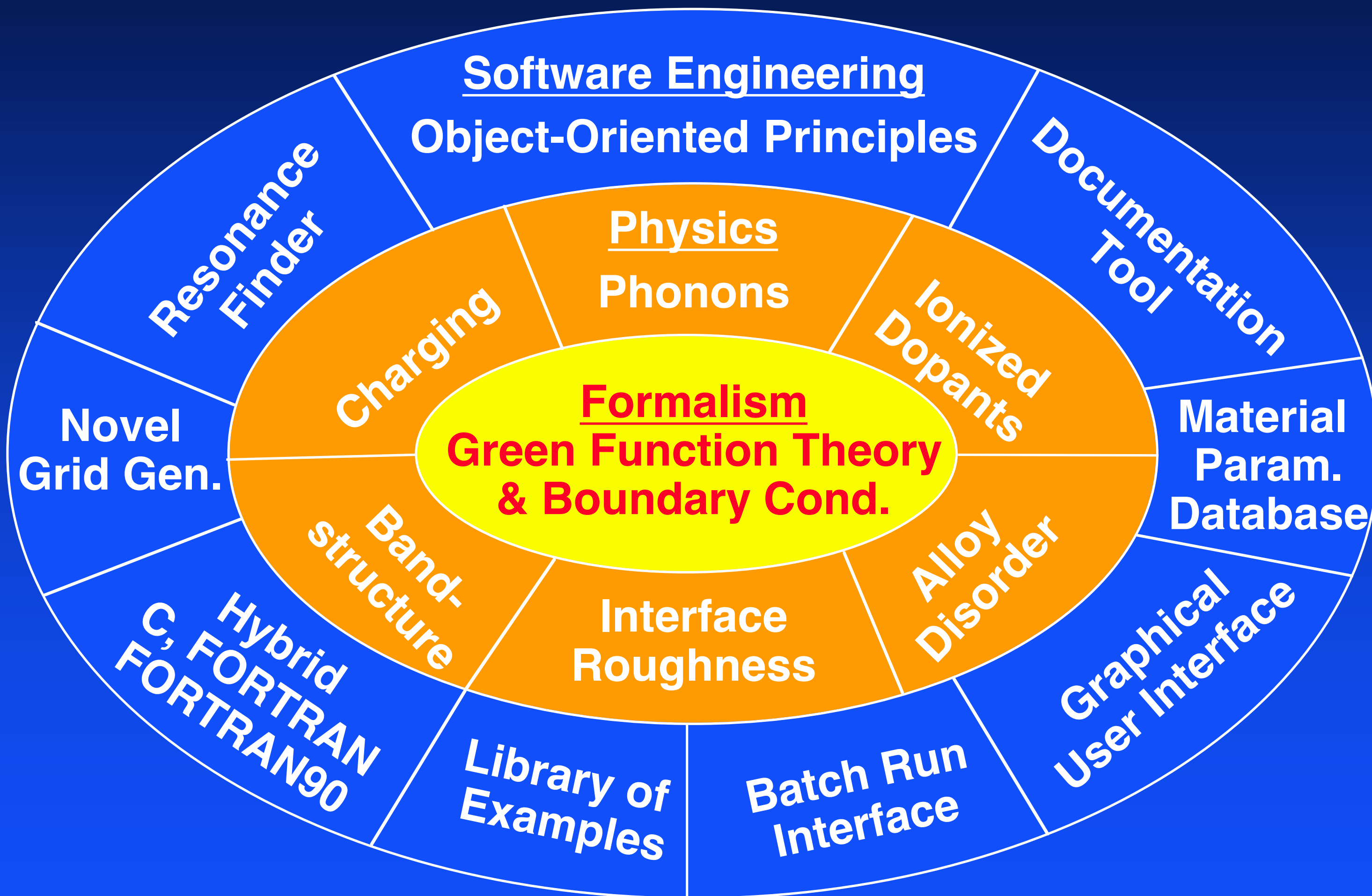
- NEMO is based on non-equilibrium Green functions, in an implementation that is novel. The development of NEMO has benefited from the vast research on resonant tunneling diodes that had been done before the project.

Summary of NEMO Capabilities

- **Interface / Users:**
  - FAST and dirty design. — interactive
  - Comprehensive analysis (SLOW). — batch
- **Physics**
  - Charging
    - Semi-classical self-consistency, quantum self-consistency
  - Scattering
    - Phonons, alloy disorder and interface roughness (1band)
  - Bandstructure
    - 1, 2, 10 tight binding band models nearest and next nearest neighbor coupling.
  - Realistically long devices
    - Novel boundary conditions

NEMO can trade off CPU time and memory against a variety of models.

All of NEMO's Facets: Formalism, Physics, and Technology



Approximately 250,000 lines of code at time of delivery

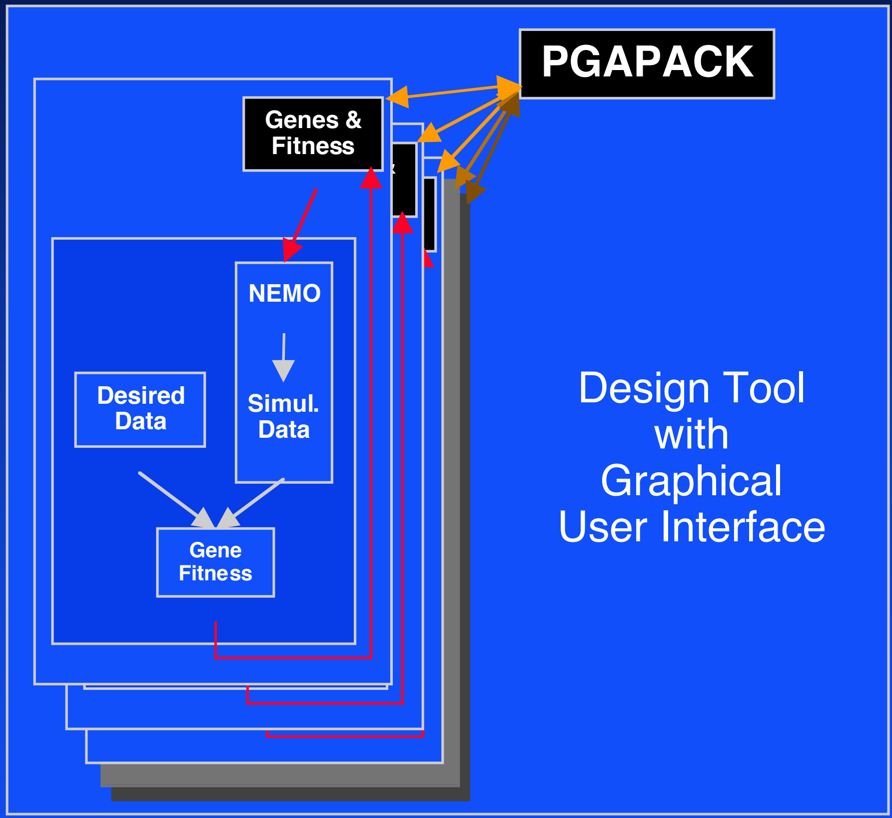
"Genetically Engineered" Nanostructure Devices

Objective:
- Automated device synthesis and analysis using genetic algorithms.
- Material spectroscopy through genetic algorithm analysis.

Justification:
- Empirical Design (usual process) is sub-optimal. Complete design space search is unfeasible.
  => Develop automated design tools.

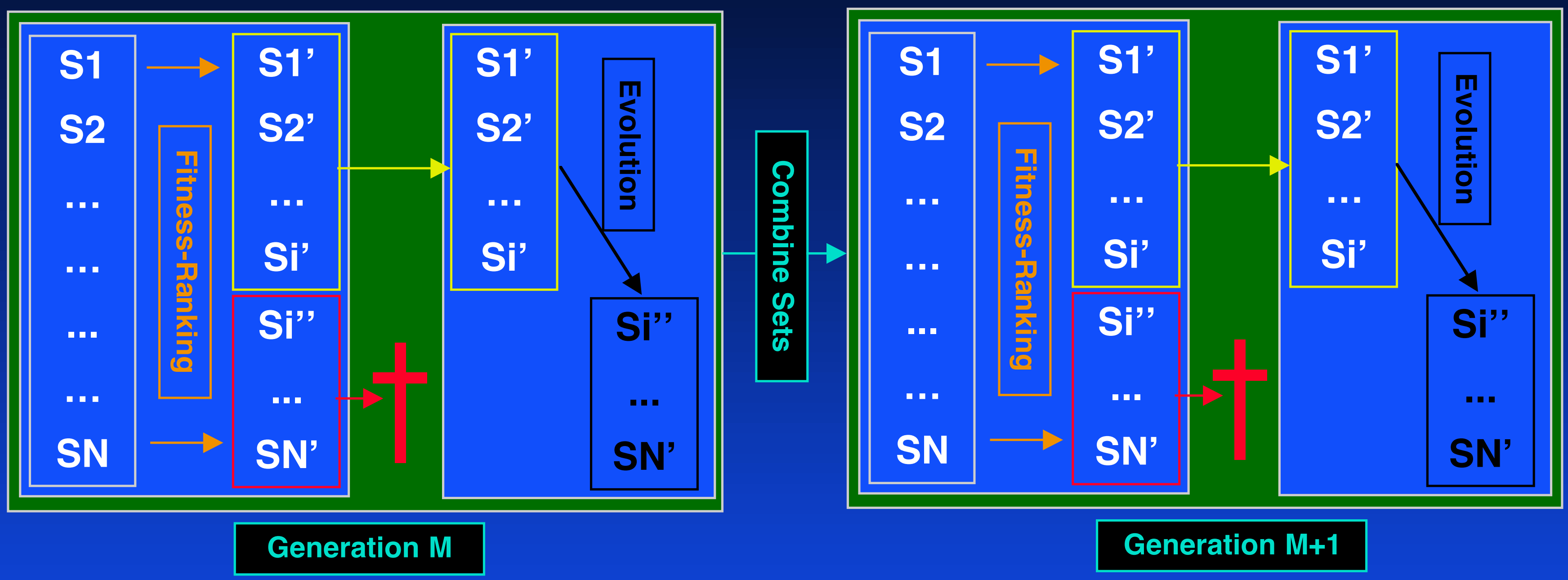
Impact:
- Rapid nanotechnology device synthesis and development.
- Generation of novel devices.

Approach:
- Augment NEMO to analyze individual structures in parallel.
- Augment parallel genetic algorithm package (PGApack) to optimize and select desired structures in NEMO.



Proposed system architecture.
Prototype is operable in batch mode.

Basic Genetic Algorithm Development

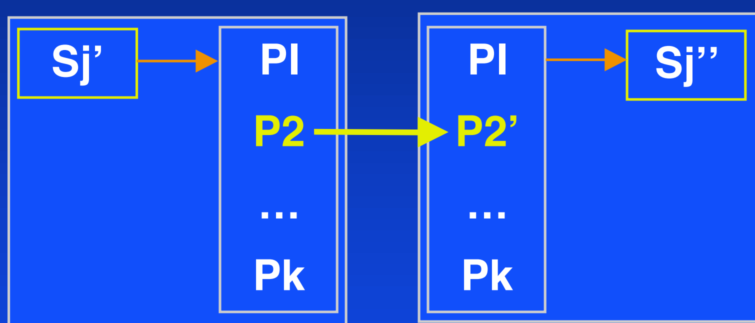


- Genetic algorithm parameter optimization is based on:
  - Survival of good parameter sets
  - Evolution of new parameter sets
  - Survival of a diverse population
- Optimization can be performed globally, rather than locally.

Basic Evolution Operations

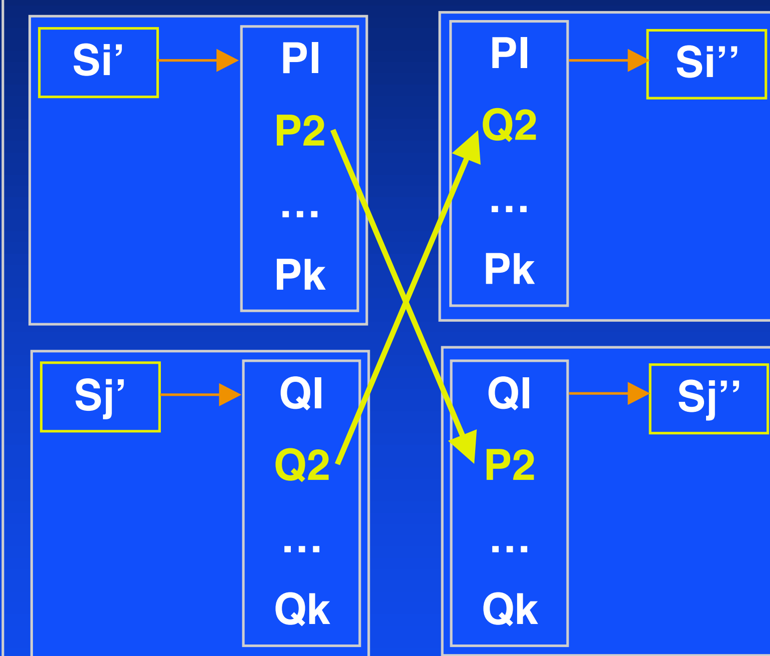
- Each set (Si) consists of several parameters (Pj)
- The parameters Pj can be of different kinds: real, integers, symbols, ….

Mutation operation



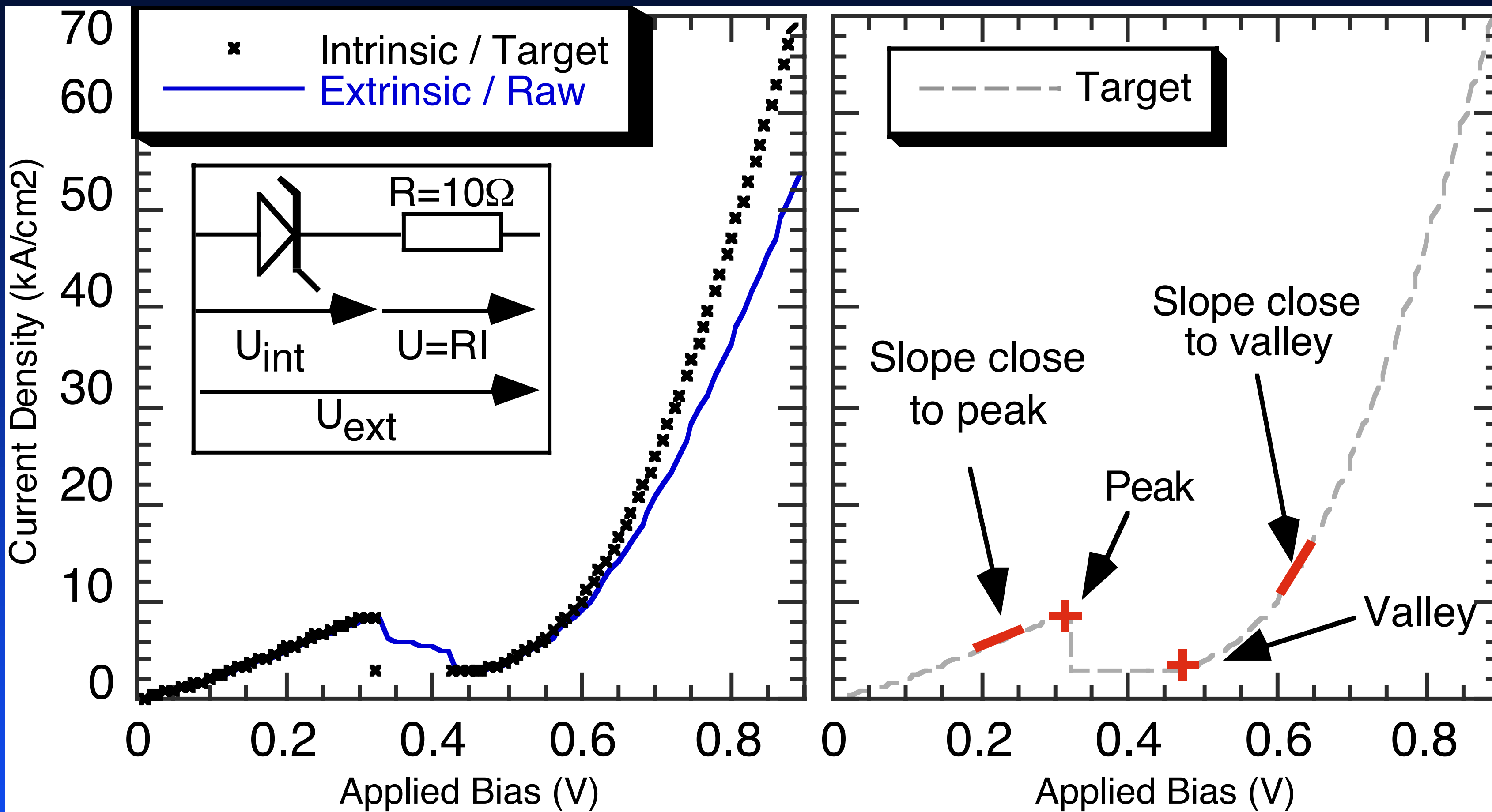
- Mutation may move parameters out of their original parameter range
  - E.g: original range [5,6,7,…100] 5 could be mutated to 4, or 3 …
- Mutation size may be random.
- Multiple parameters may be mutated at the same step.

Crossover operation



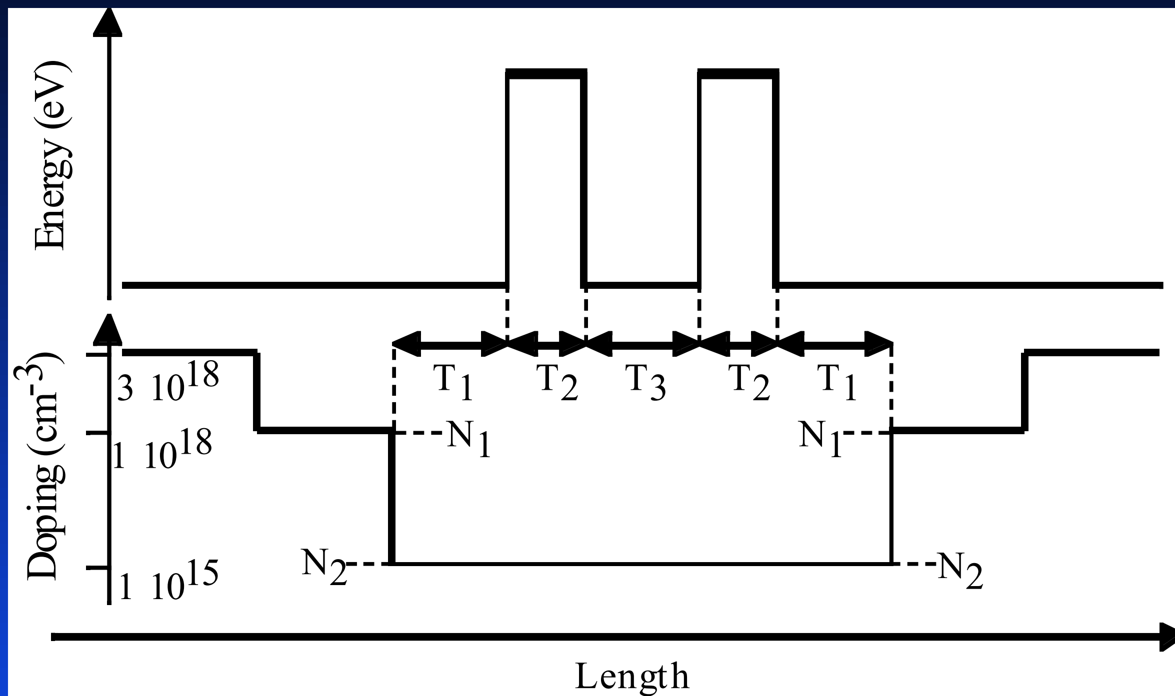
- Crossover maintains the original parameters range.
- Crossover explores different combinations of existing genes.

Development of a Fitness Function



- **Eliminate series resistance effects**
- **Eliminate NDR oscillations (step-like feature)**
- **Fitness from of 6 error contributions:**
  - **Peak and valley**
  - **Slope at peak and valley**
  - **Overall absolute and relative error**

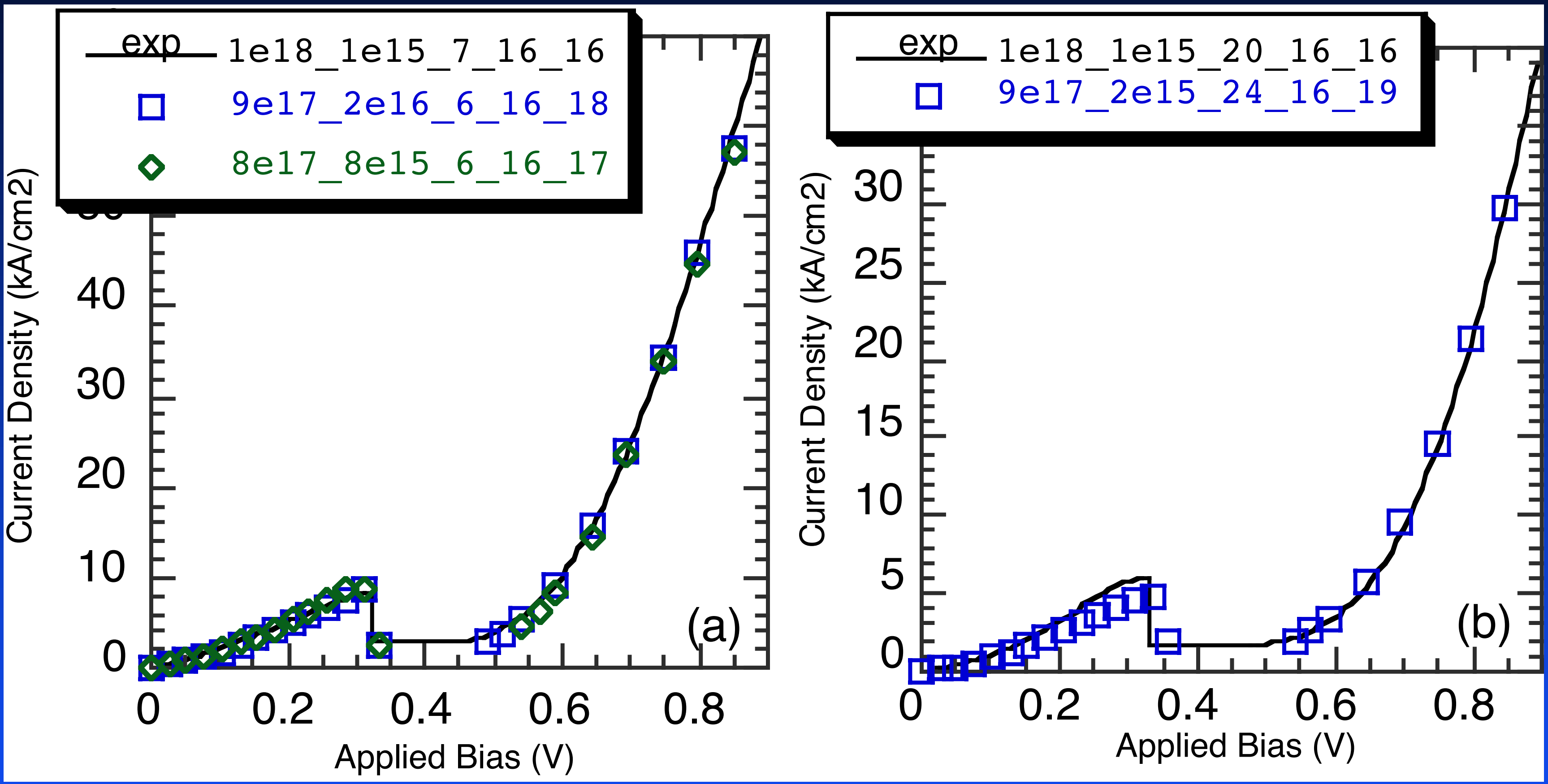
First Simulation Results: Structural Analysis



- Allow genetic algorithm to vary 5 different structural parameters:
  - 3 Thicknesses: well, barrier, spacer
  - 2 Dopings: low doped spacer, unintentional doping in center
- Employ parameterized non-parabolic single band model with full quantum charge self-consistency and transverse momentum integration.
- Developed fitness function for typical RTD I-V curves. Need to shoot for peak position and amplitude, slope at peak and relative and absolute errors.

JPL

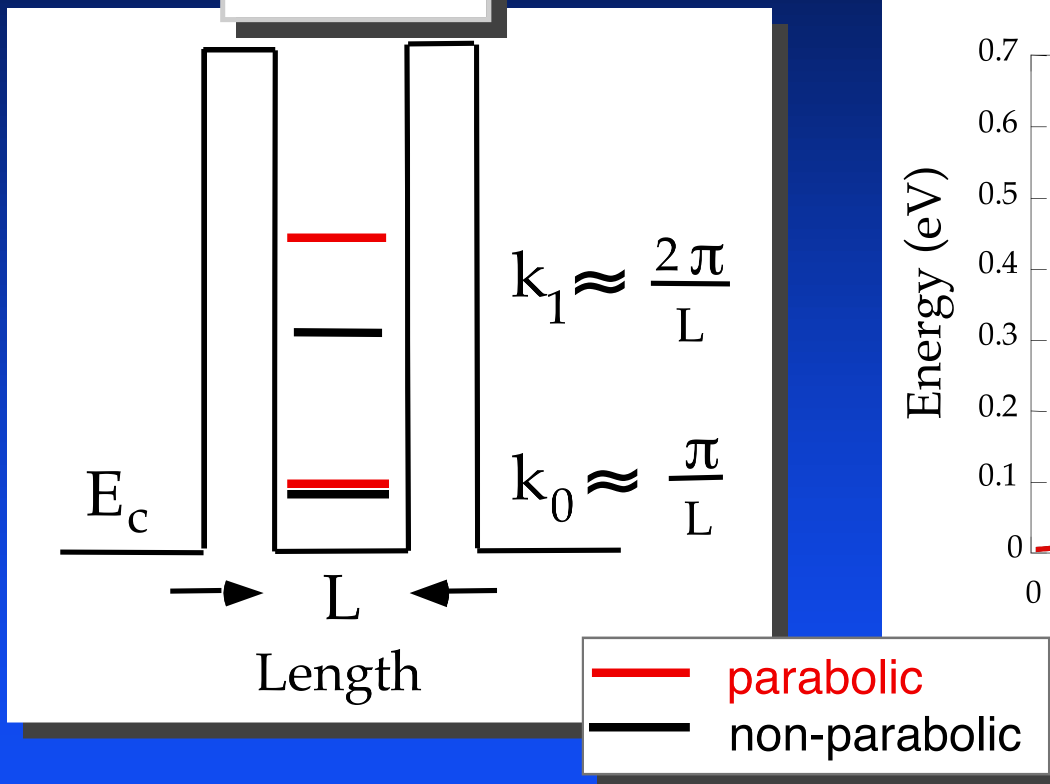
First Simulation Results: Structural Analysis



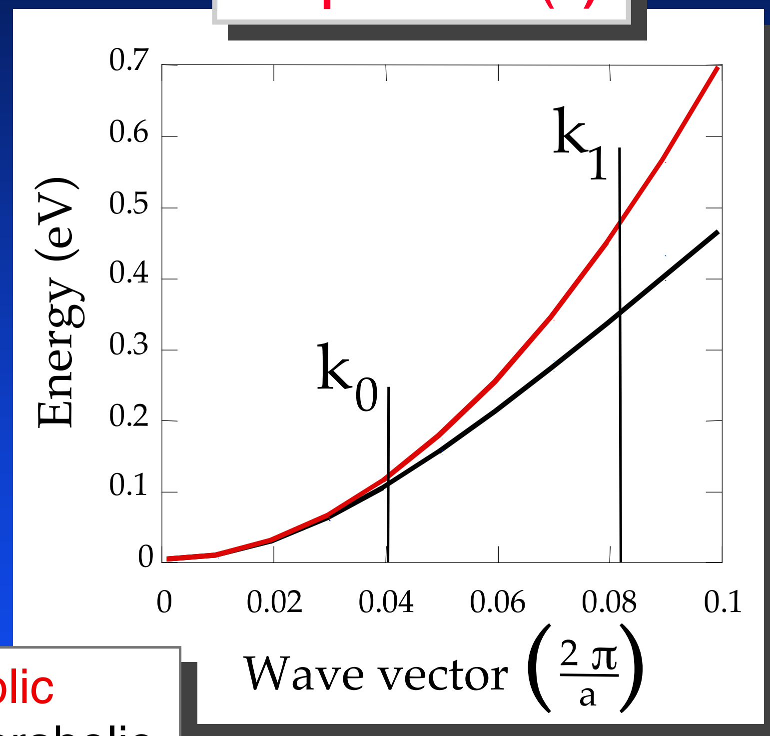
- **Analyzed two similar InGaAs/InAlAs structures :**
  - **RTD 1: N1=1e18/cm^3, D2=1e15/cm^3, T1=7ml, T2=16ml, T3=16ml**
  - **RTD 2: N1=1e18/cm^3, D2=1e15/cm^3, T1=20ml, T2=16ml, T3=16ml**

Resonance State Lowering due to Band Non-Parabolicity

Resonator

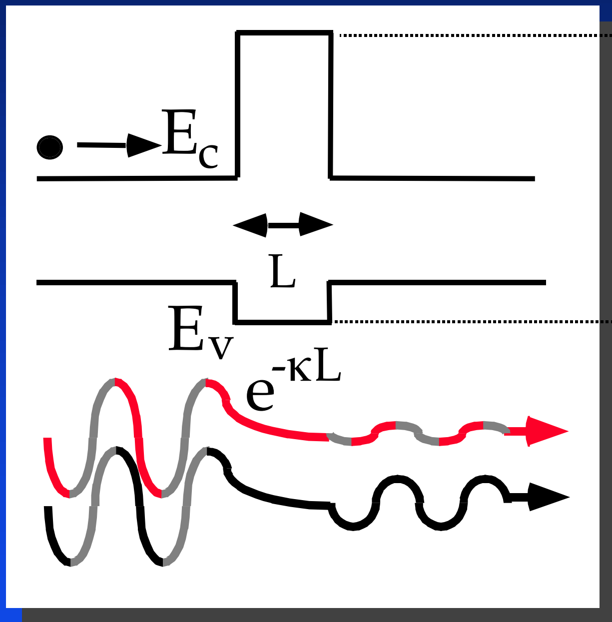


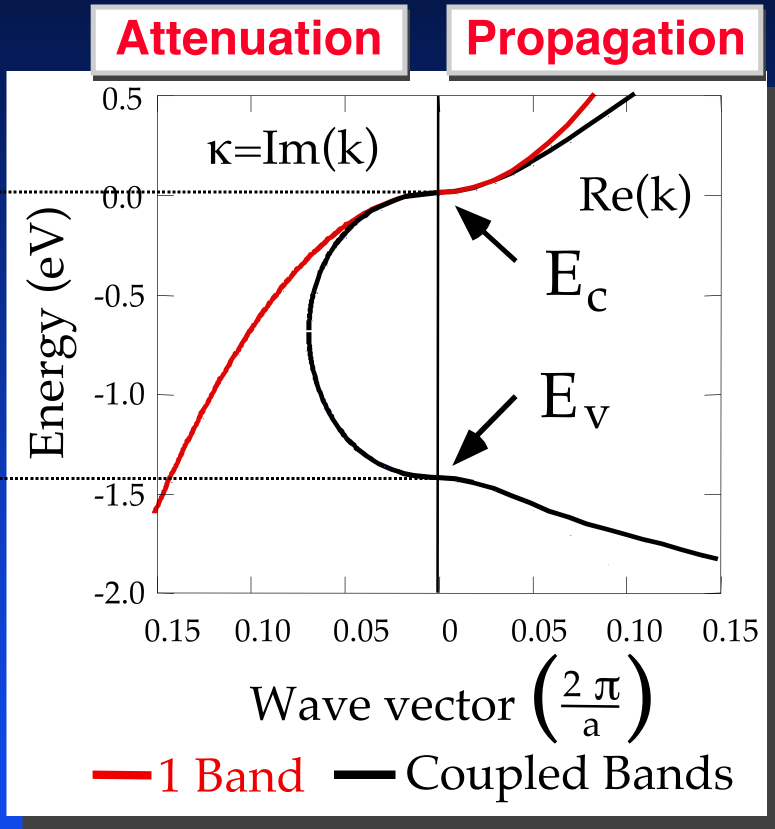
Dispersion E(k)



Second diode turn-on at lower voltages.

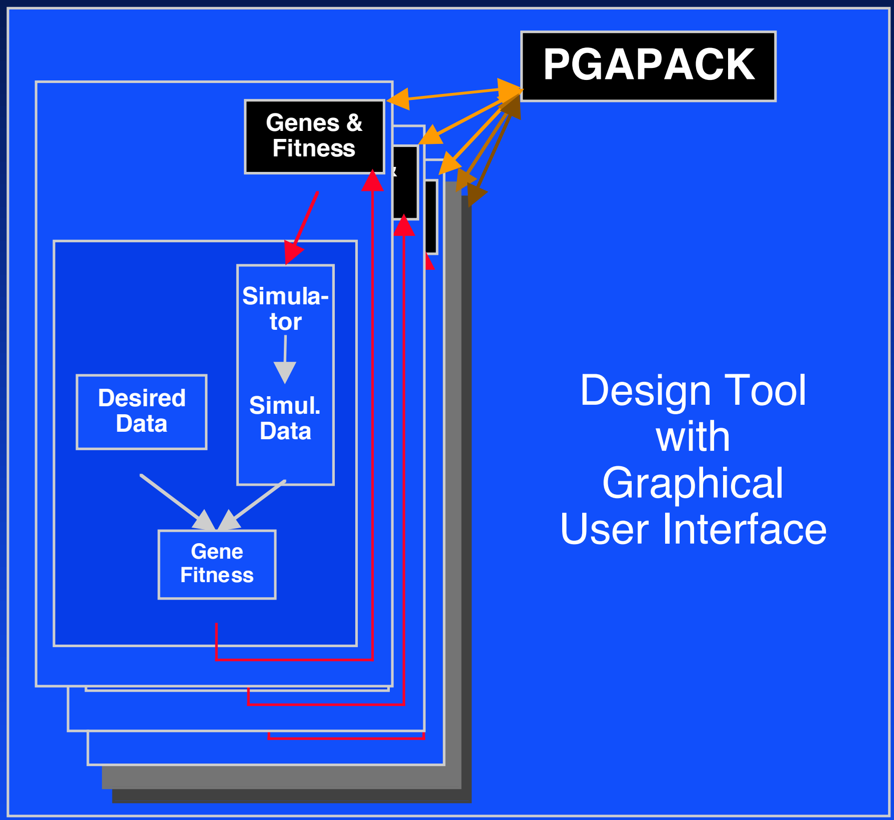
Wave Attenuation in Barriers





- Attenuation is smaller with coupled bands
- Tunneling probability increases
- Current increases

Future Interest



- Analyze material parameter influence on overall device performance
  -> material spectroscopy

- Implement general architecture such that a variety of different simulation tools can be plugged into an optimization tool.

- Explore other optimization algorithms, such as simulated annealing or directive approaches within the same framework.

  -> scripting tools that can link different tools

  -> Tcl/Tk