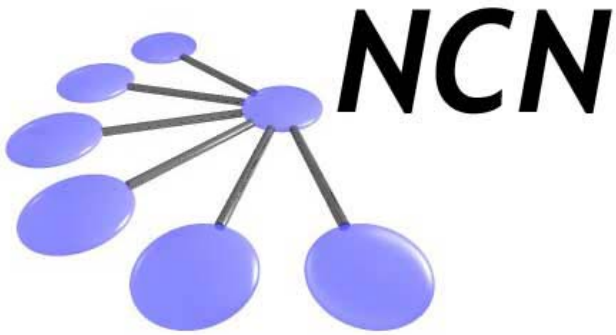
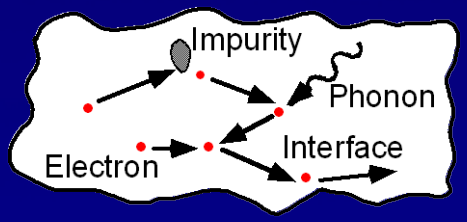
NEMO1D: Software Highlights

Gerhard Klimeck

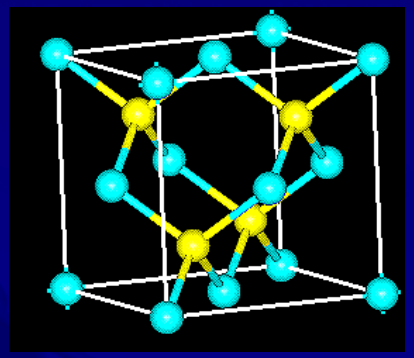


Who are the Users?

Users: Engineers
Interest: Advanced Dev. Design
Shrinking Devices
Problems: Transport with Particle Interaction
Approach: Drift Diffusion, Boltzmann Eq.



Users: Scientists
Interest: Solid State Physics
New Device Materials
Problems: Coherent Quantum Mechanics
Approach: Schrödinger Eq.



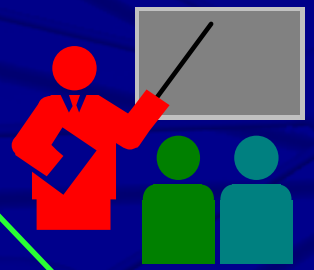
TI, Raytheon, Hughes, Motorola, IBM, Intel

Universities

National Labs.

NEMO

Approach: Non-equilibrium Green Functions
Includes: Quantum Mechanics, Particle Interaction, Transport
Models: Charging
Bandstructure
Scattering
Access: User friendly GUI

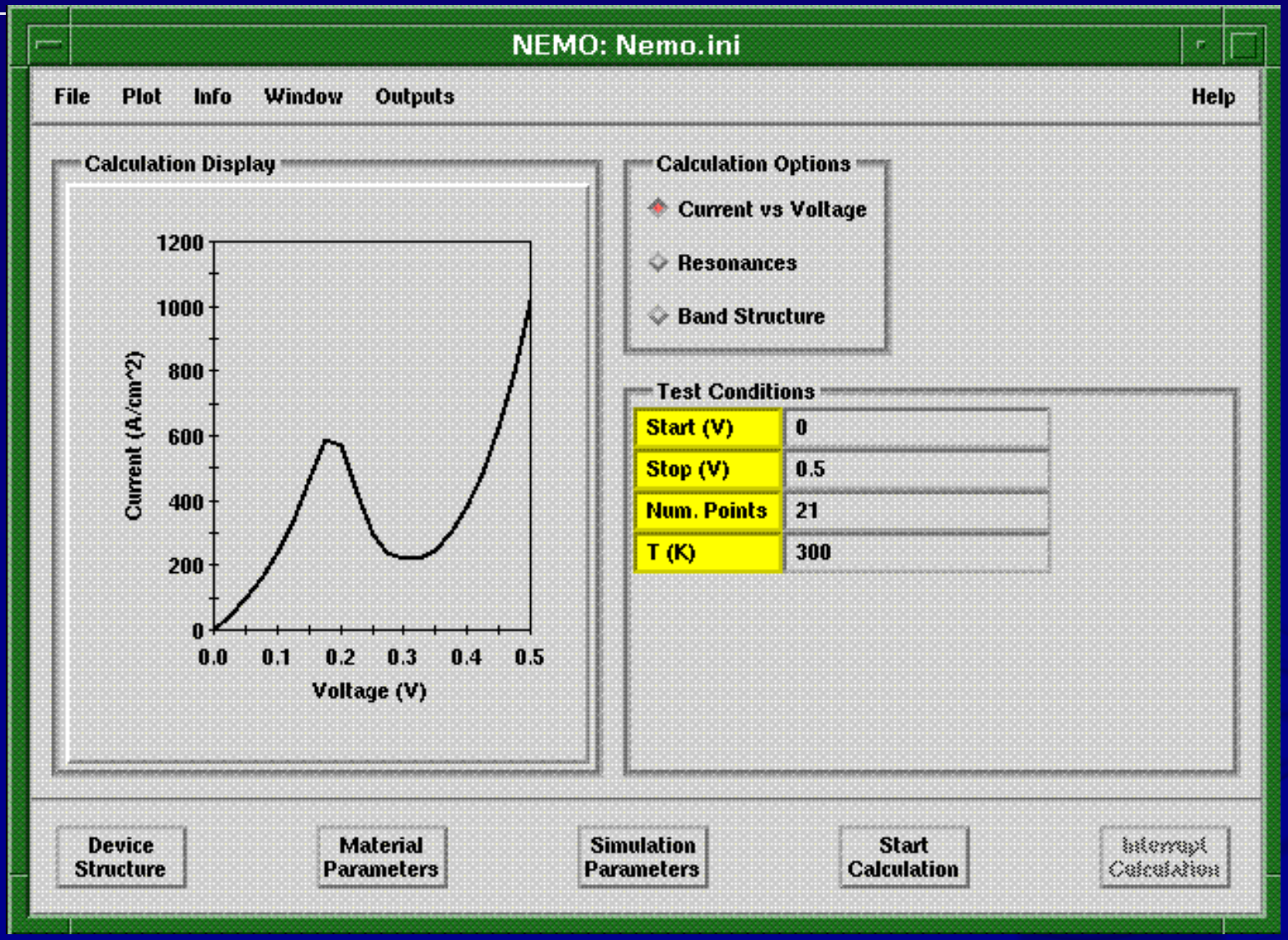


Students
Universities

User Requirements

- Simple Data Input:
  - Device Design
    - No restrictions on geometry.
    - III-V and Si.
  - Material Database
    - Provide material parameters.
    - User can modify material parameters.
    - User can define new materials.
  - Simulation Parameters
    - Guide user through hierarchy during the selection.
- Simple Data Analysis:
  - Built-in graphics plots.
  - Allow access to all computed data.
  - Minimize disk clutter.
- Multiple platforms: SUN, HP, IBM, SGI

NEMO: Current vs. Voltage



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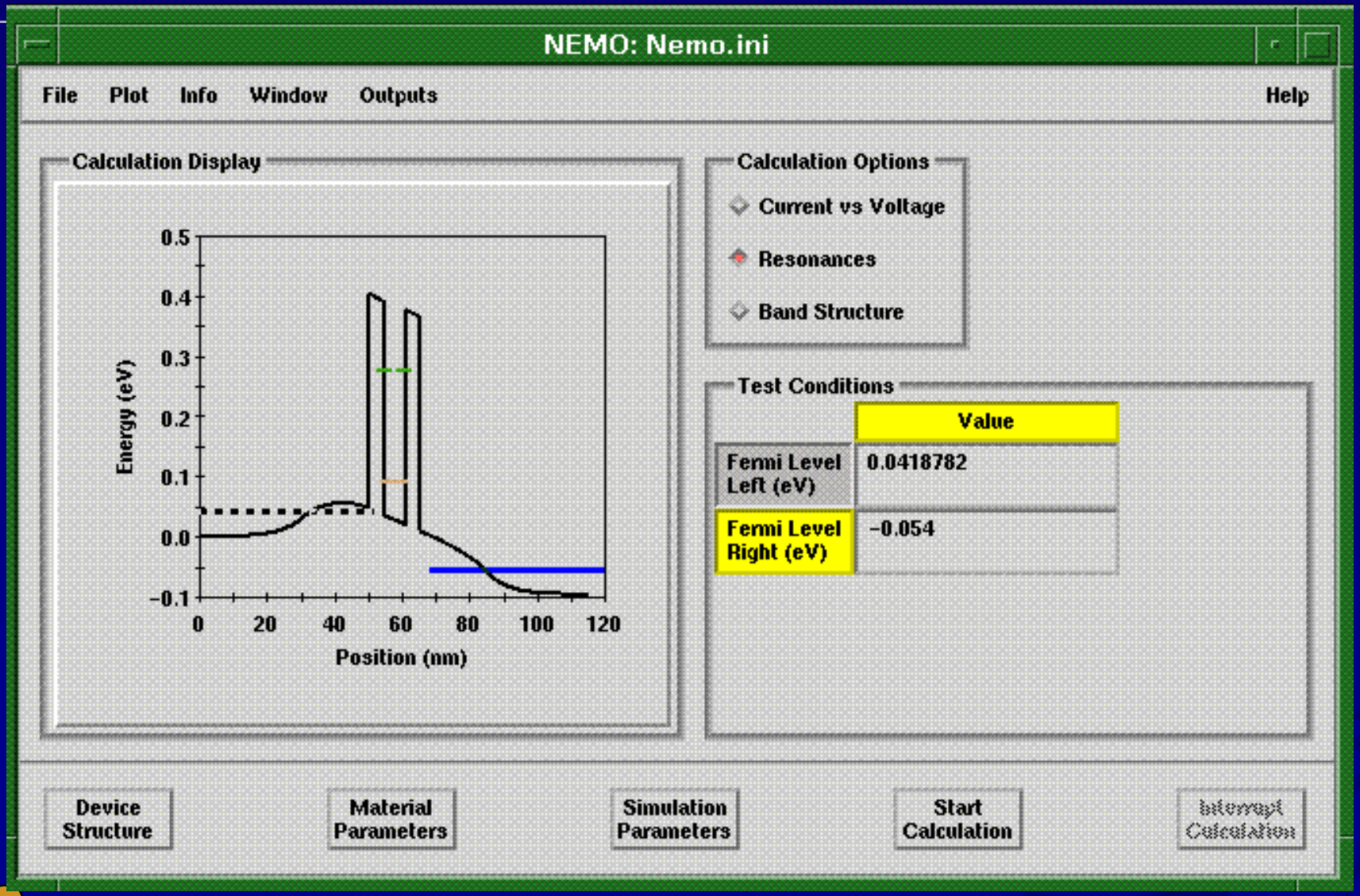
NEMO: Resonances



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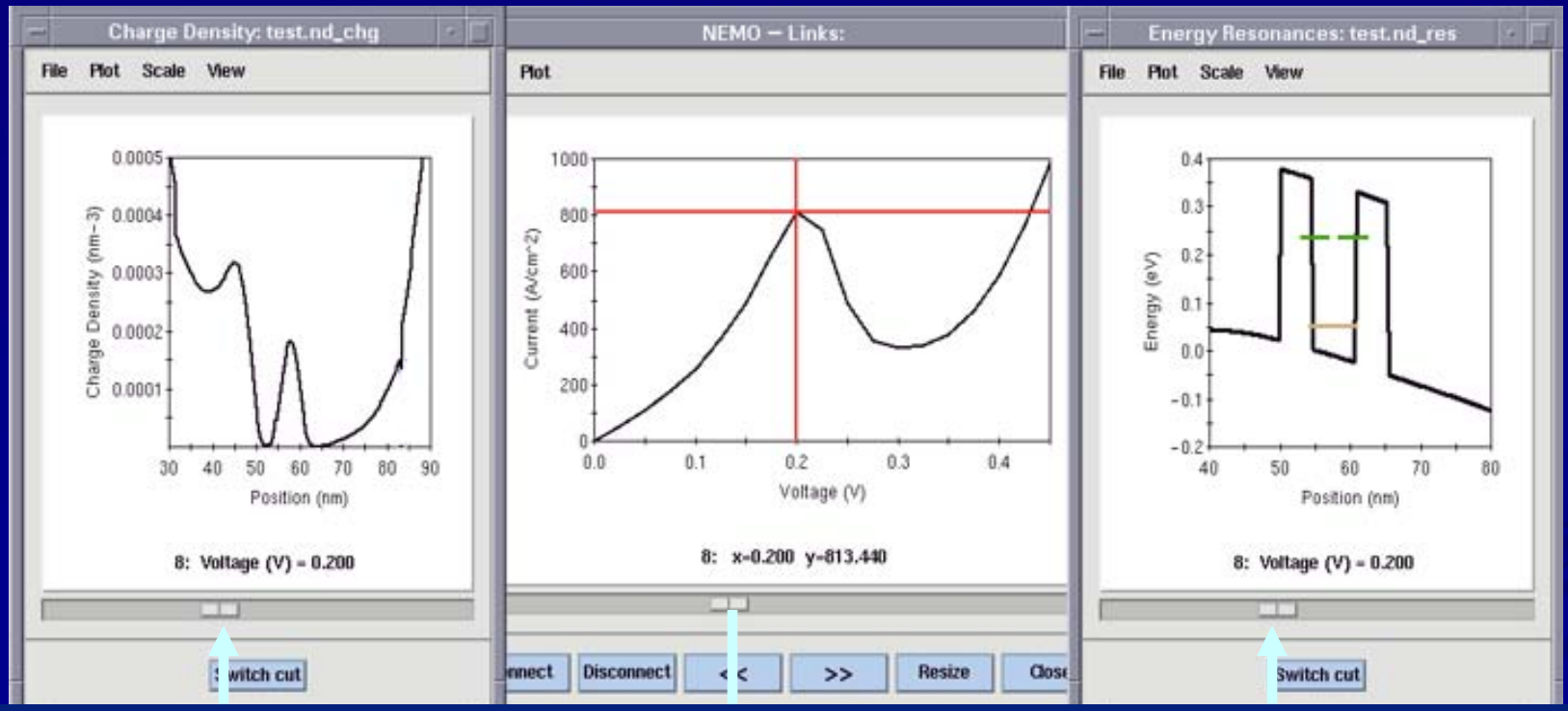
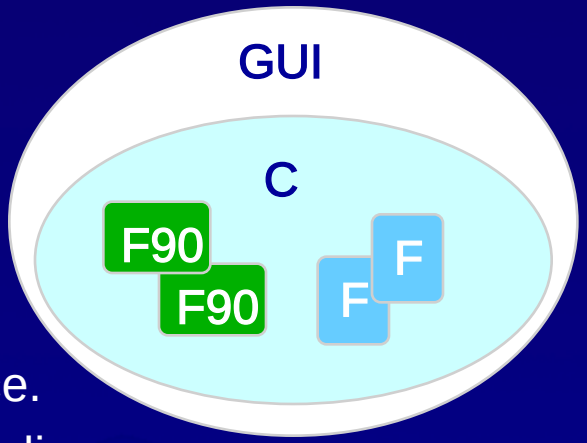
Interactive Data Visualization

- During an I-V run all 2D data files are stored in one “slicer”
- All of the data can be examined after the run.
- All slicers can be linked to examine the correlation of the contained data.
- Hot Buttons Jump to Min/Max Extrema on I-V



Experimentalists Demanded Fast / Interactive Simulation Must Be Faster than Experiment

Software Structure : Hybrid C, FORTRAN, and FORTRAN 90



- Advantages of C:
  - flexible data design, fast prototyping.
  - simple hook-up of the graphical user interface.
  - close to the UNIX system level for job scheduling.
- Advantages of FORTRAN
  - speed for floating point arithmetic.
  - 4x speed-up for the same algorithm comparing C and F77 on HP.
- Advantages FORTRAN90 = FORTRAN + ...
  - standardized vector and matrix arithmetic.
  - data structures.
  - simple parallelization.

Programmer Requirements

- Theory:
  - Fast prototypeing.
  - Change input and output often.
  - Need to visualize detailed (deep down in the code) data.

- GUI:
  - 20/80 rule: 20% of the simulator is used 80% of the time.
    -> Need to put the 20% within easy reach of the user.
  - Keep up with ever changing simulation parameters.
  - Static GUI design is “simple”:
    - Canned software products like X-Designer create a GUI.
    - Windows are defined at compile time.
    - Put in call-backs to the functions which perform a certain action once a button is pushed.
  - Dynamic GUI design is “tough”:
    - Create windows “on-the-fly” depending on the user choices.

Simulation Parameter Entry

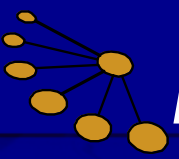
- What are simulation parameters?
  - Current and potential models
  - Energy and momentum grid specifications
  - Iteration numbers, required accuracy, etc.

- Design Premise:
  - Make ALL parameters available to the user

- Problems:
  - User: Large number of parameters
    - not all are needed for a specific simulation
    - they may even be mutually exclusive and conflicting!
    - some of them may only be for expert use

    => Hierarchical Ordering
  - Programmer: Need to be able to add parameters very quickly, painlessly, without reworking the GUI.

    => Dynamic widget creation, reflecting abstract data structures.

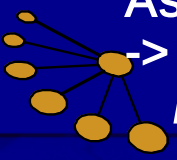


Hierarchical Ordering of User Input

Semi-class. self-cons. pot. & single band current
Specify desired outputs
Quantum region: “Where are wave-functions?”
Non-equilibrium region: “Where are the reservoirs?”
Adaptive energy grid

Quantum self-cons. potential & single band current	exchange & correlation?
	how to go from bias to bias?
Specify desired outputs	
Quantum region: “Where are wave-functions?”	
Non-equilibrium region: “Where are the reservoirs?”	
	Quantum Charge region: “Where is the charge quantum mechanically calculated?”
Resonances-based energy grid	

Ask user for input that is really needed.
-> User input determines the sequence of simulation parameter windows.



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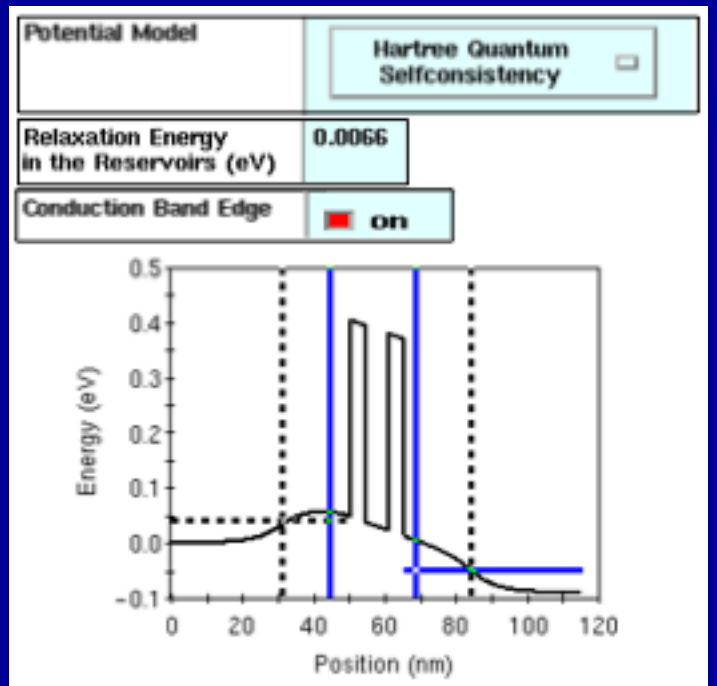
Generic Data Structure I/O

Dynamic GUI Design.
- data structure
- member descriptor

-> I/O for GUI or files



Graphical User Interface

Create

Read

Data Structure

```
PotType potential
real hbarovertau
Boolean Ec
RangeStruct NonEq
```

Translator

Read

Create

File/Batch User Interface

```
potential=Hartree
hbarovertau=0.0066
Ec=FALSE
```

Software

Such Modular Approach is Germaine to Simulation
It Enables Development with Uncertain Specs.

Software Structure : Hybrid C, FORTRAN, and FORTRAN 90

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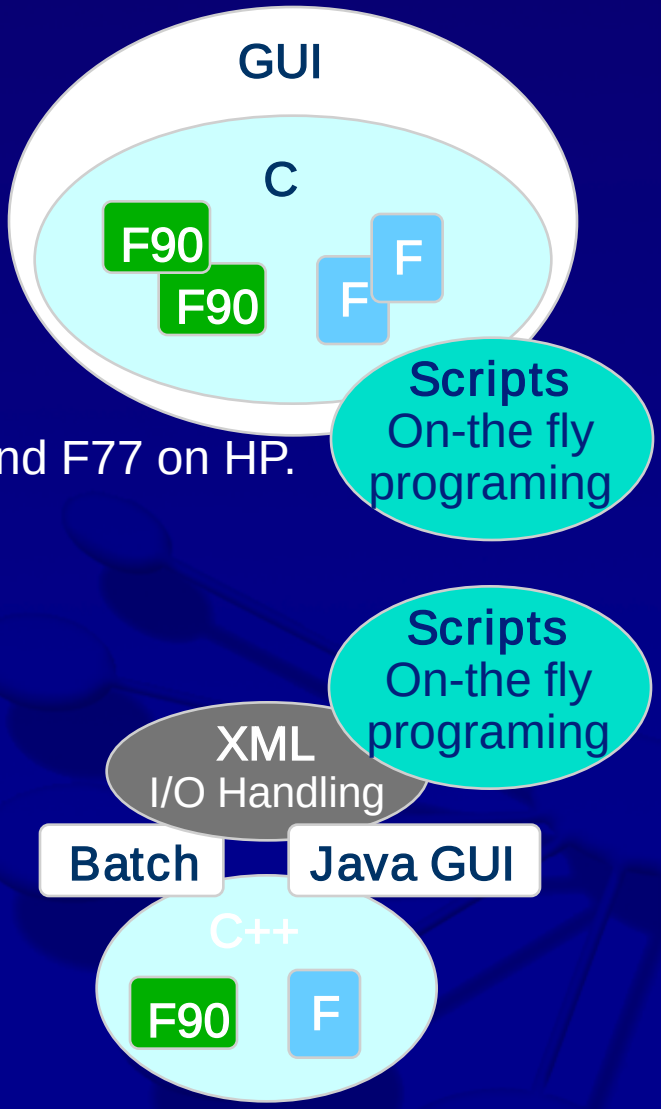
- Advantages FORTRAN90 = FORTRAN + ...
  - standardized vector and matrix arithmetic.
  - data structures.
  - simple parallelization.
- NEMO 3-D design:
  - XML handles all I/O including computational data structures
- Scriptable Interfaces:
  - Key element to integration into other programs



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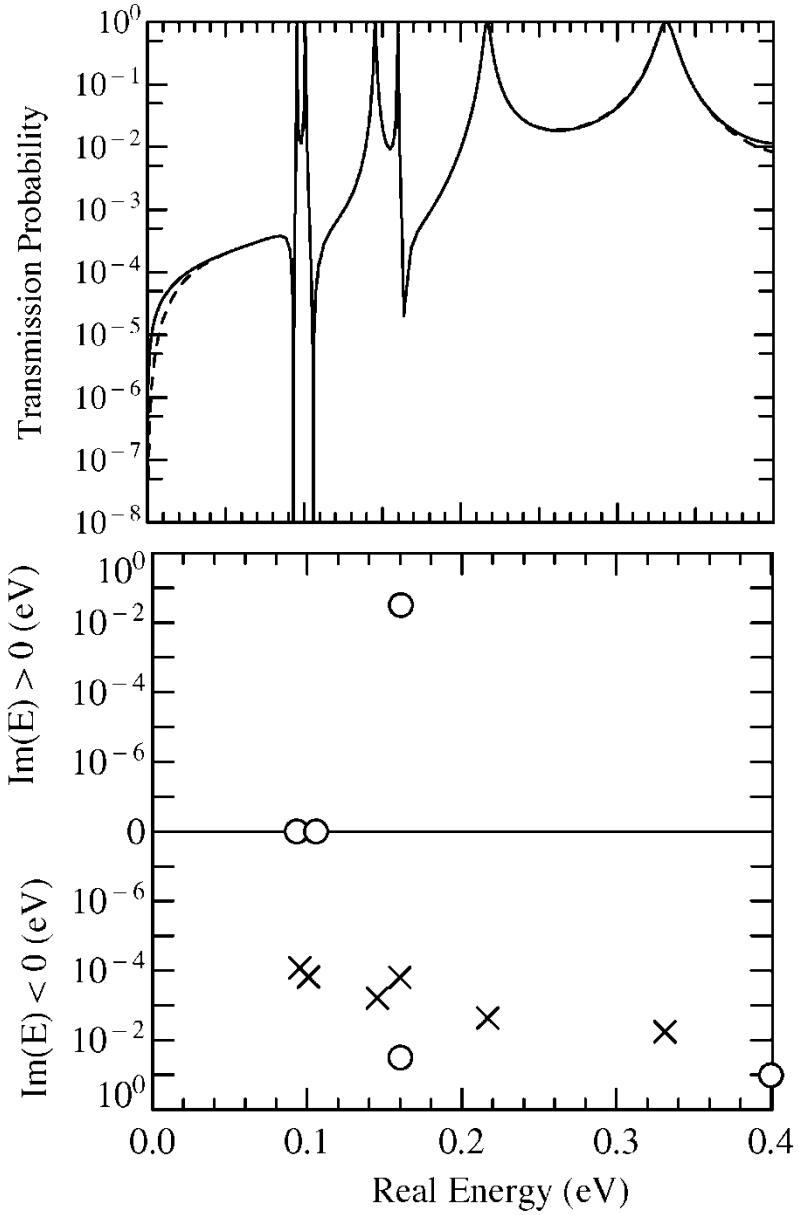
Eigenenergies contain a lot of information!!



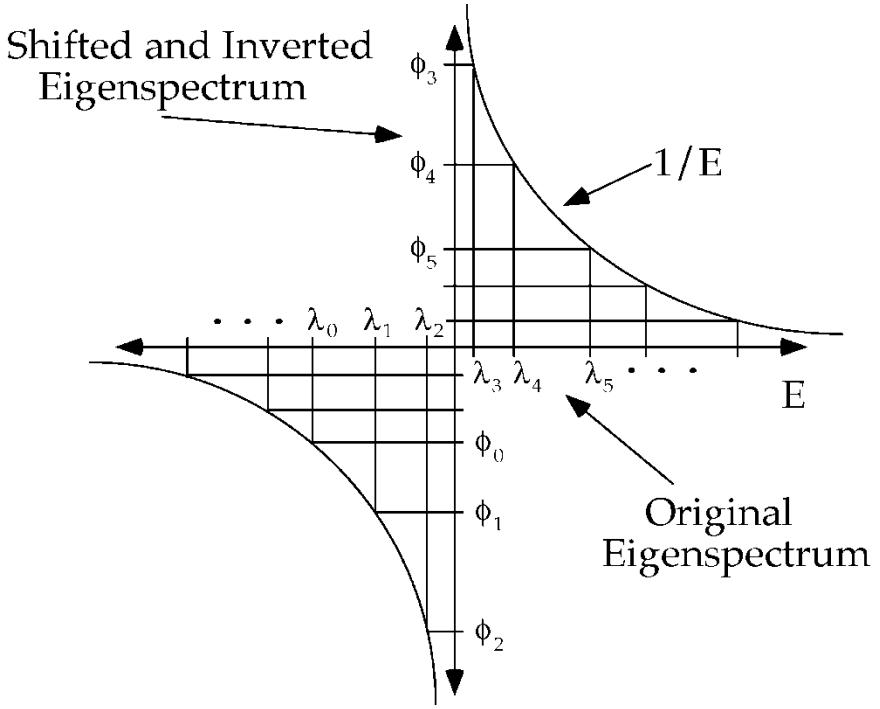
- Poles correspond to resonances
- Zeros correspond to anti-resonances
  - » Real part resonance energy
  - » Imaginary part resonance width

- Resonance width ~ 0.1 meV
- Energy Range 0.4eV
- Each computation of G^R at each energy is expensive
- Need to use an inhomogeneous energy grid.

Shift and Invert Lanczos Solver

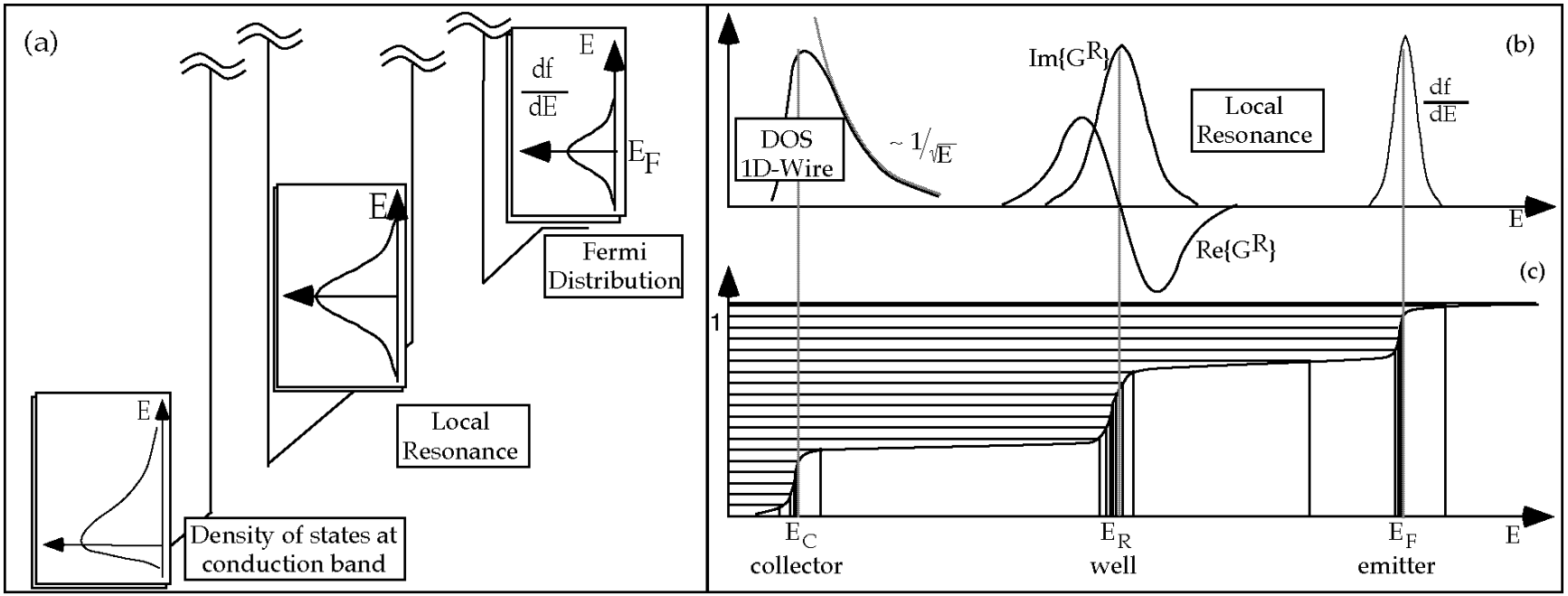
$$\left(E - H - \Sigma^{R}_{bound}(E)\right)\Psi = 0$$

Shifted and Inverted Eigenspectrum



- Hamiltonian is non-Hermitian
- Boundary self-energy is energy dependent
  - » Strong dependence at band edge
  - » Weak dependence between band edges
- Utilize Lanczos on shifted and inverted, energy independent system.
- Refine resonances using Newton iterations on the energy dependent system.

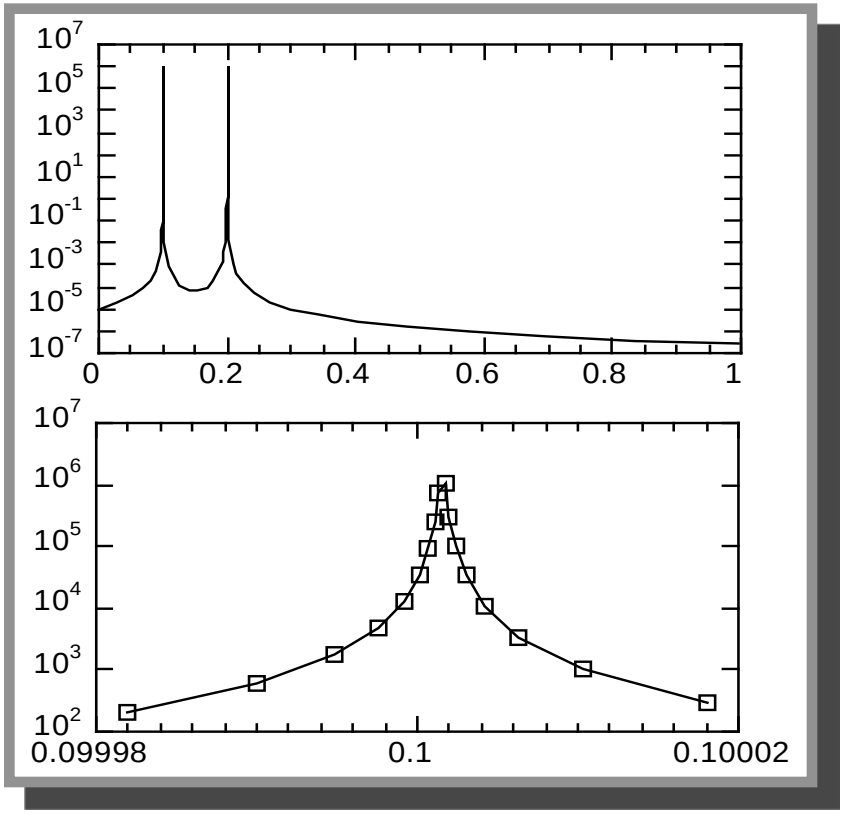
Grid Generation from Projection

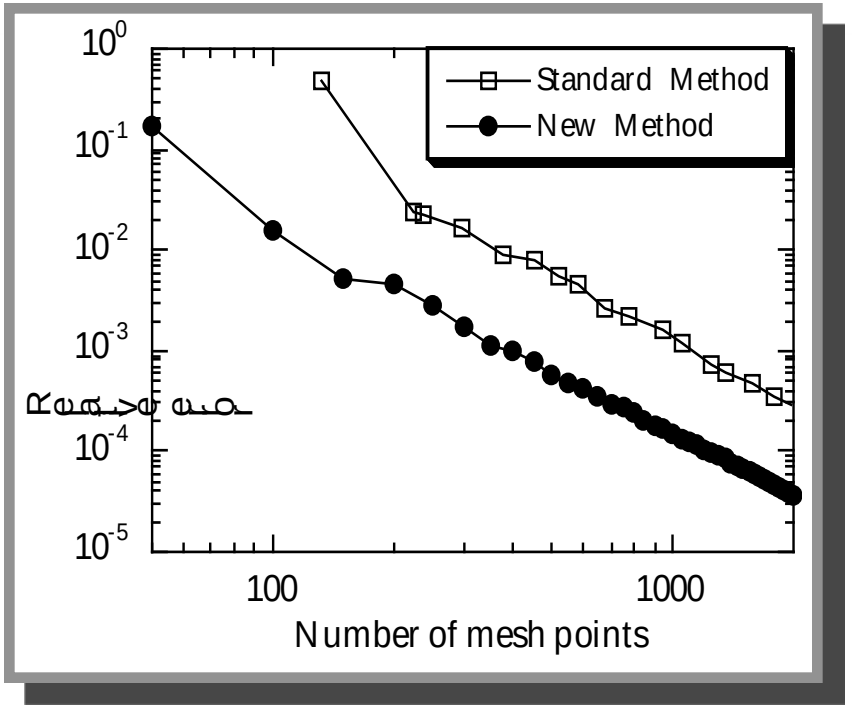


- Utilize eigenvalue solver to locate resonance energies and resonance widths
  - » Need to resolve the real part and imaginary part of the associated Green fct.
  - » Can solve integral analytically for real and imaginary part
- Need to resolve band edges
  - » Integrate over 1-D density of states
- Need to resolve Fermi energies
  - » Utilize Fermi function directly

Novel Energy Grid Generator

- Problem: need to integrate over typically very sharp spectral features
- Assume we know where the resonances are -> toy problem





Reduction of mesh points here: 4x

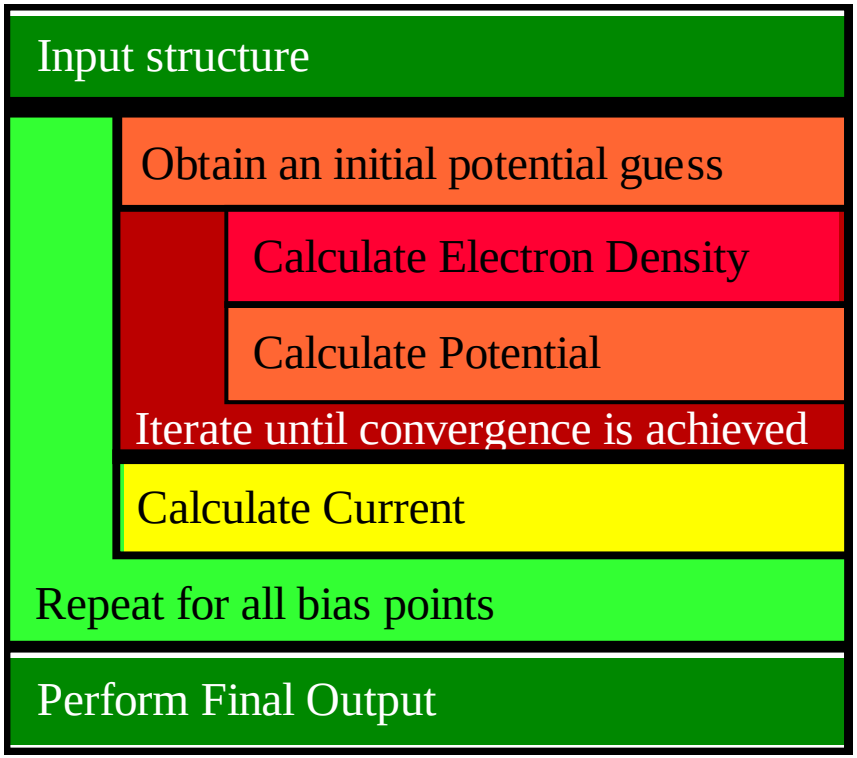
=> Speedup: 4x-16x

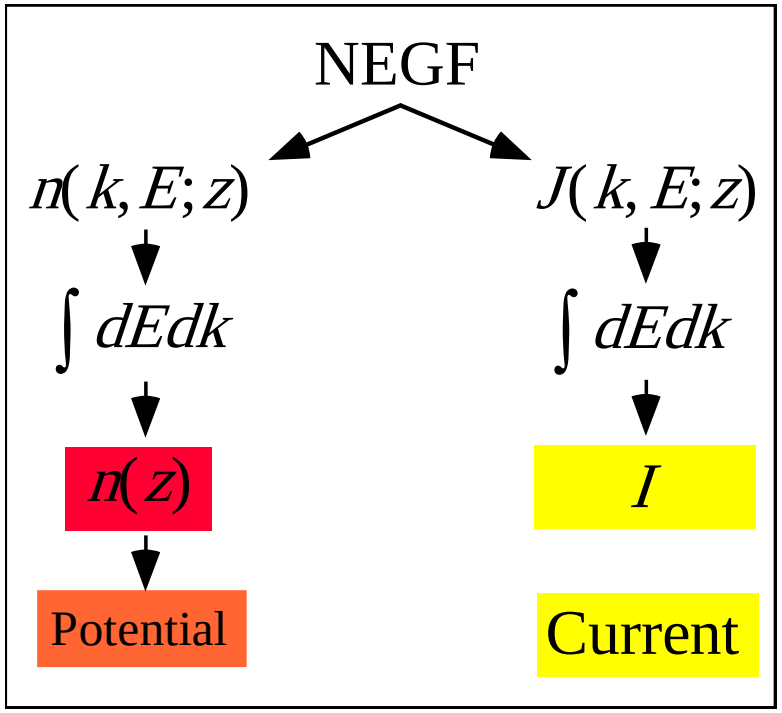
=> Memory Savings: 4x, 16x, 64x

Information Flow in the I-V Simulator

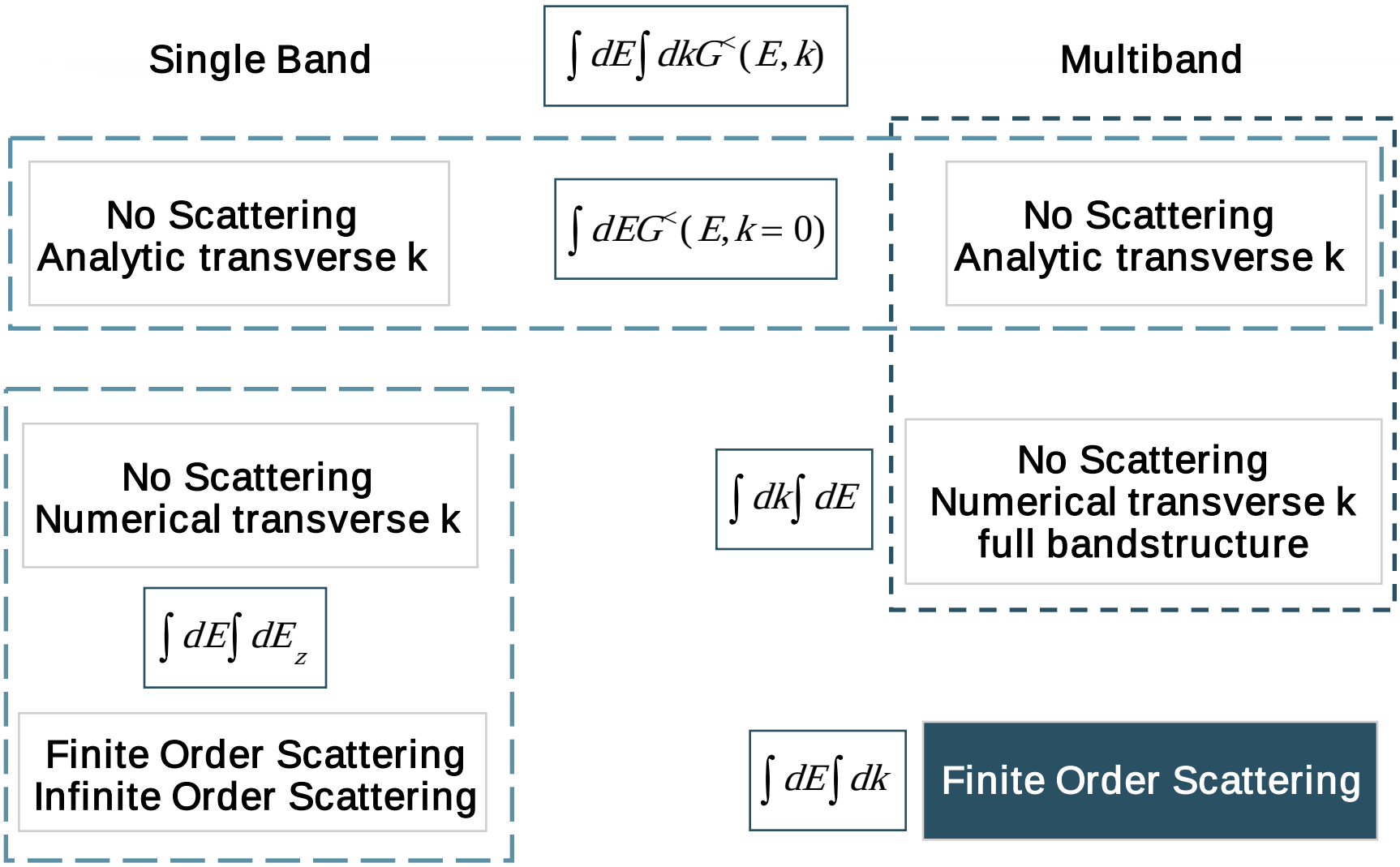
High Level Simulator Tasks:
1) Calculate potential profile:
   charge < -self-cons.- > potential
2) Calculate current:
   may or may not be self-cons. w/ potential.

Low Level Simulator Tasks:
1) Generate microscopic quantity
2) Integrate (1,2,3 dimensions) into observables (charge, current).





How do we Integrate $G^<$? Different Integration Algorithms.

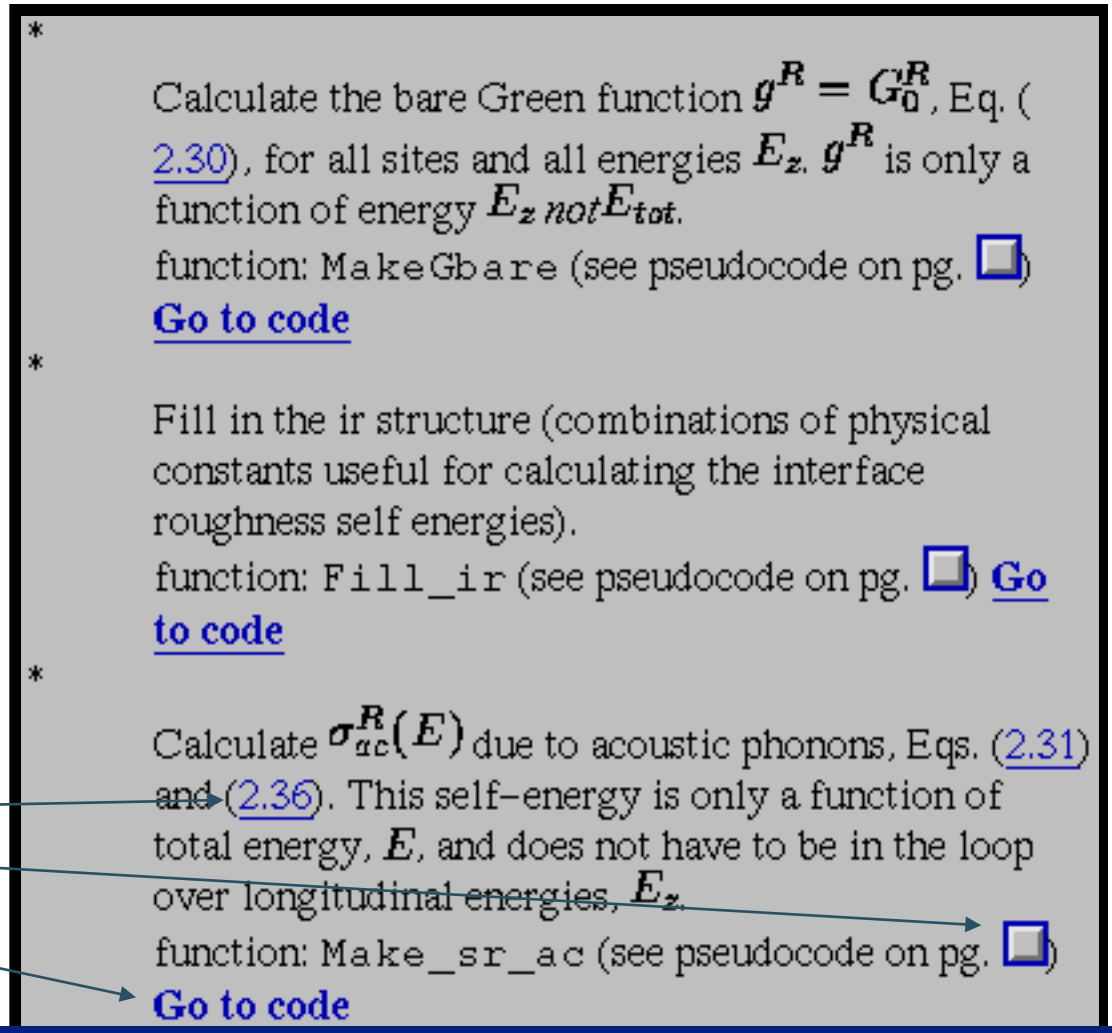


Code Modularity

- Code modularity provides **simulator flexibility.**
- User specifies independently
  - » Model for $G^<(E,k)$
    - ✓ 1,2,10 etc. band model without scattering
  - » Integration target
    - ✓ electron density or current density
  - » Integration Scheme
    - ✓ k=0 analytic transverse integration
    - ✓ full band numerical transverse momentum integration
  - » Energy grid type:
    - ✓ Fixed with resonance finding
    - ✓ Adaptive
    - ✓ Mixed
- Addition of models is as simple as adding a function name to a list.

Novel Interactive Documentation Tool

- **Pseudocode is a step by step description of a program in a natural language (high level and low level)**
- **Maintain pseudocode and code in one document -> easy to keep it up-to-date**
- **Generated automatically from comments in the code**
- **Cross references to**
  - **» theory description**
  - **» further pseudocode**
  - **» the actual code**



Such Documentation Approach is Germaine to Simulation
A Similar Approach is in Wide use in Some Other Tools Now

Revision Control Systems

- Several people - one piece of code ?

- Break up the source code into (many) files.
- Use a central library system.

- All developers can look at the latest versions.
- The files cannot be changed.
- Must check out and lock a file before editing.

FORGET about PRIVATE CODE VERSIONS!!!