Univ. of Florida, Univ. of Illinois, Morgan State Univ., Northwestern Univ. Purdue Univ. Stanford Univ., UTEP

nanoHUB.org – Toward On-Line Simulation for "Materials and Nanodevices by Design"

[1]Gerhard Klimeck, Mark S Lundstrom,
[1]M Korkusinski, H Xu, F Saied, S Goasguen, A Rahman, J Wang
[2]TB Boykin,
[3]F Oyafuso, S Lee, H Hua, O Lazarankova, RC Bowen, P von Allmen

[1]Network for Computational Nanotechnology (NCN), Purdue University
[2]University of Alabama in Huntsville
[3]NASA Jet Propulsion Laboratory

American Physical Society, March 22, 2005, Los Angeles

The NCN: Mission and Vision

To support the National Nanotechnology Initiative through:

- **research**
- **simulation tools**
- **education and outreach**
- ***web-based services***

"To be the ***place*** where experiment, theory, and simulation meet and move nanoscience to nanotechnology."

Simulation is Essential for Nanotechnology Development

Hint from the Semiconductor Industry:

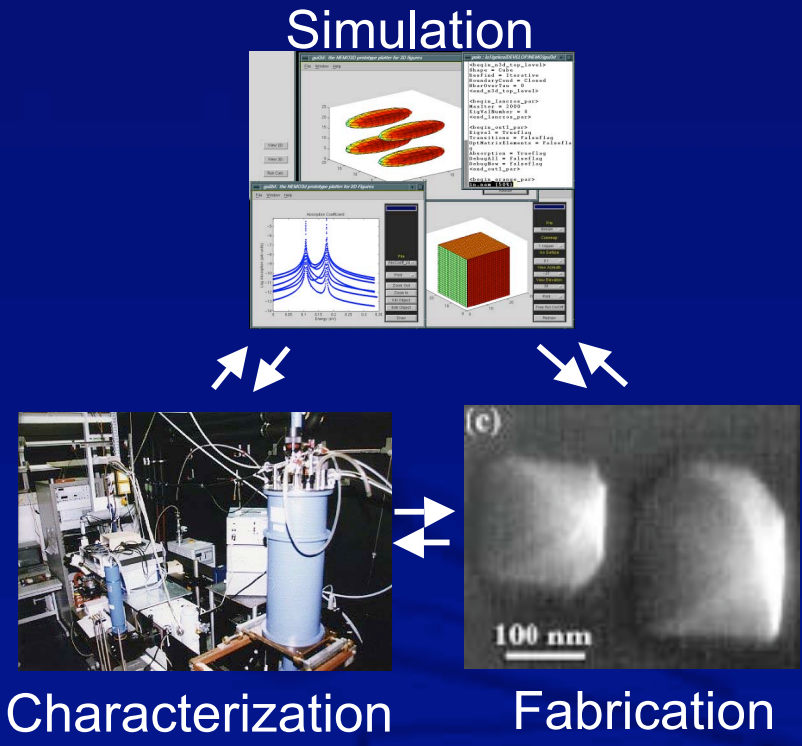
- No new devices / circuits designed without software!

Problem:

- Accepted nano simulation tool suite does NOT exist.

Approach:

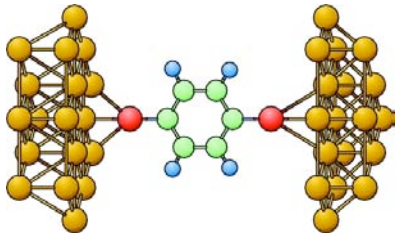
- Conduct research in Modeling and Simulation of:
  - Nanoelectronics
  - Nanoelectromechanics
  - Nano-bio sensors
  - Computational science
- **DEVELOP and DEPLOY** to nanoscience and nanotechnology community



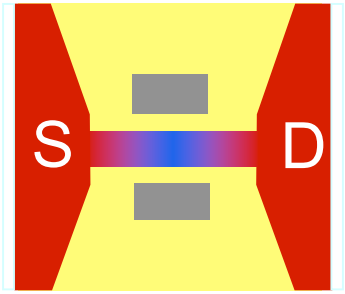
NCN - Research

nanoelectronics:

molecules….



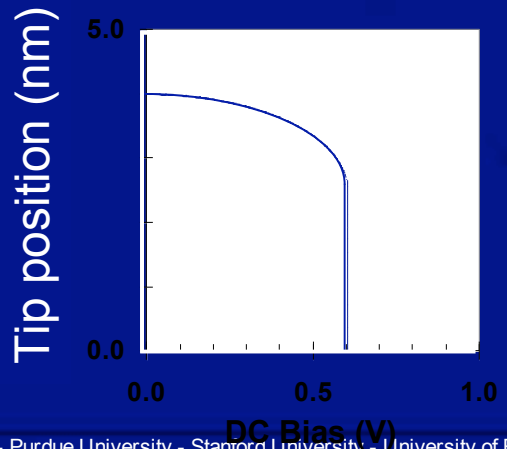
….to MOSFETs



NEMS:

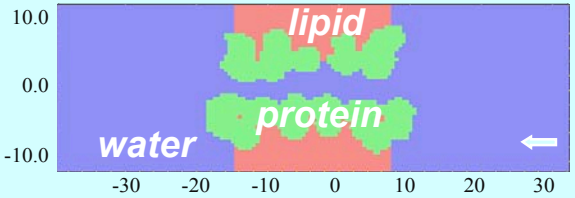
switches and sensors….

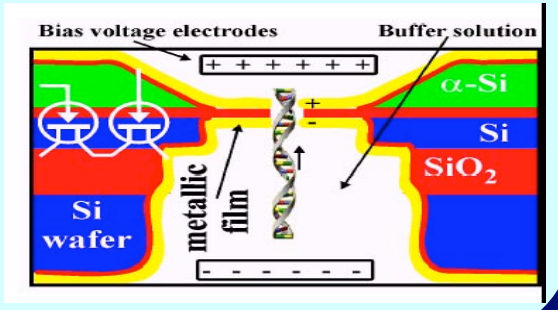
…to compact models



nano-bio:

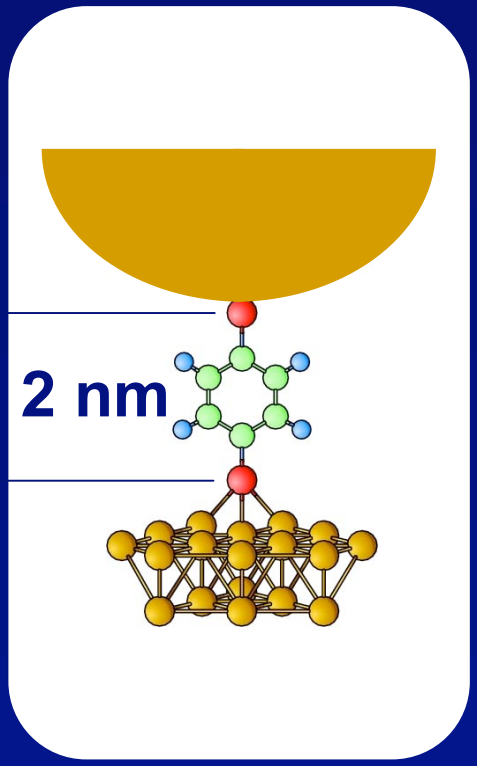
connecting electronics and NEMS to biological systems





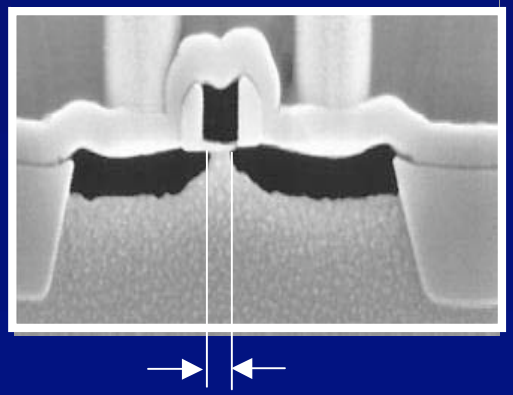
NCN

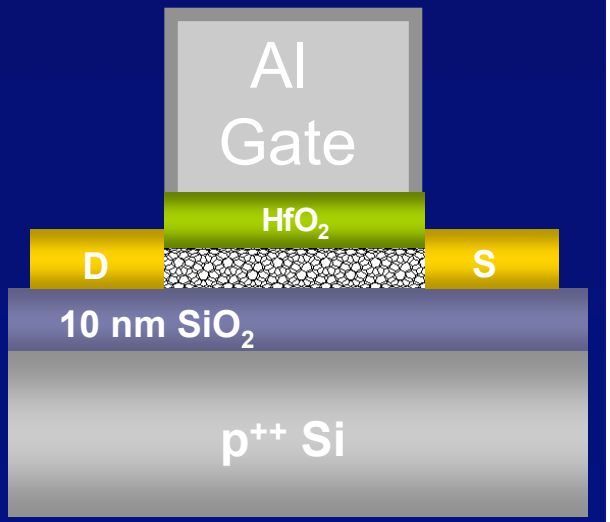
electronics at the molecular scale

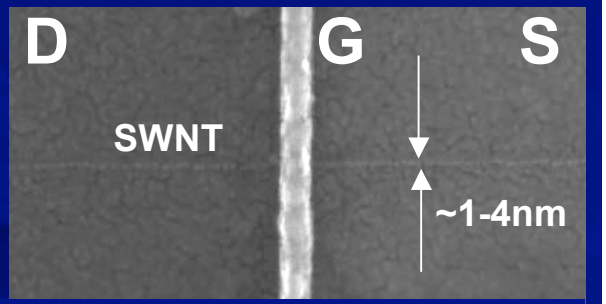


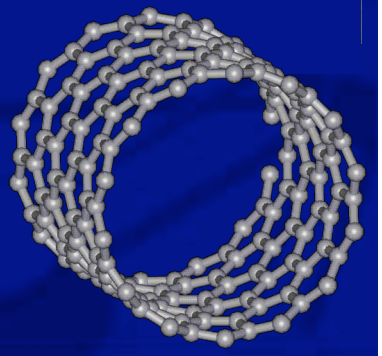
Molecules

Ultra-Scaled CMOS

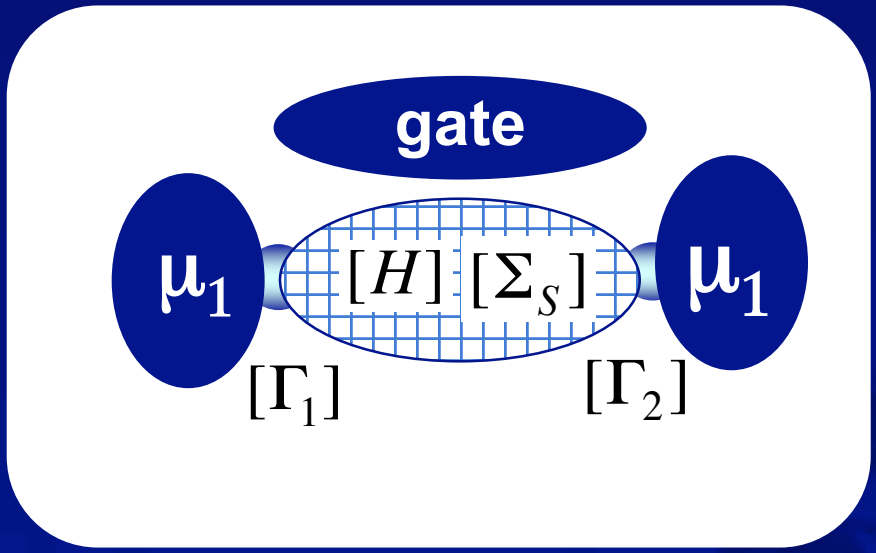








unifying view of small devices



non-equilibrium Green's function approach (NEGF)

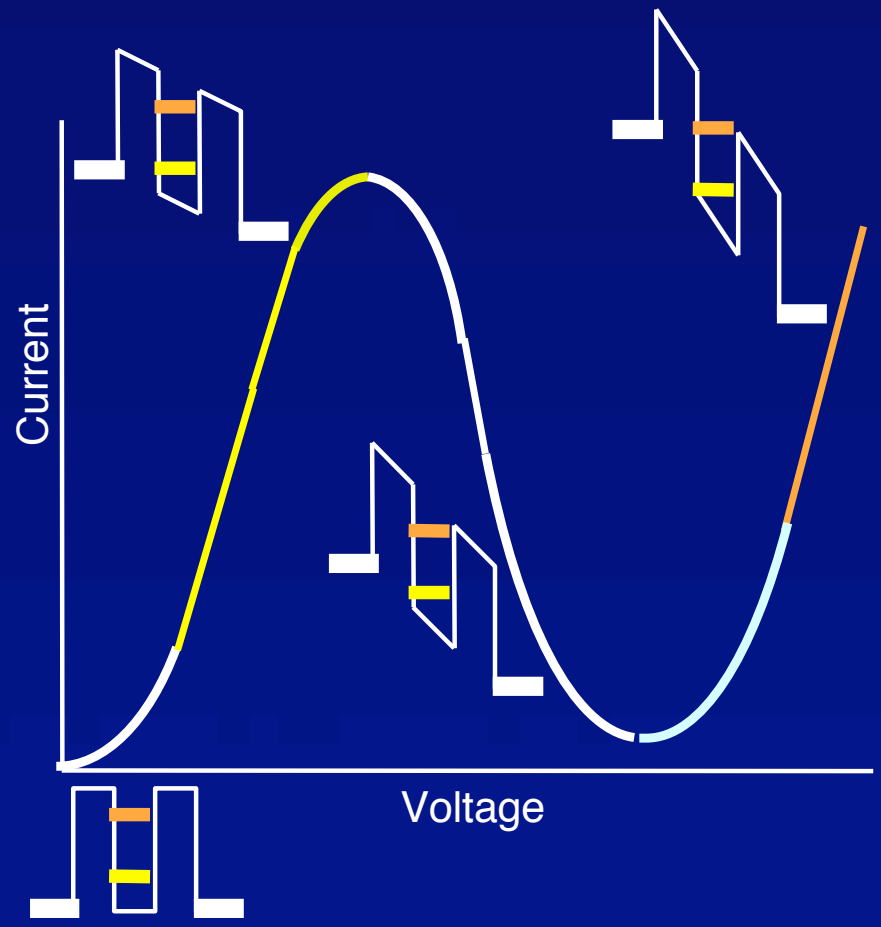
The NCN: Mission and Vision

To support the National Nanotechnology Initiative through:

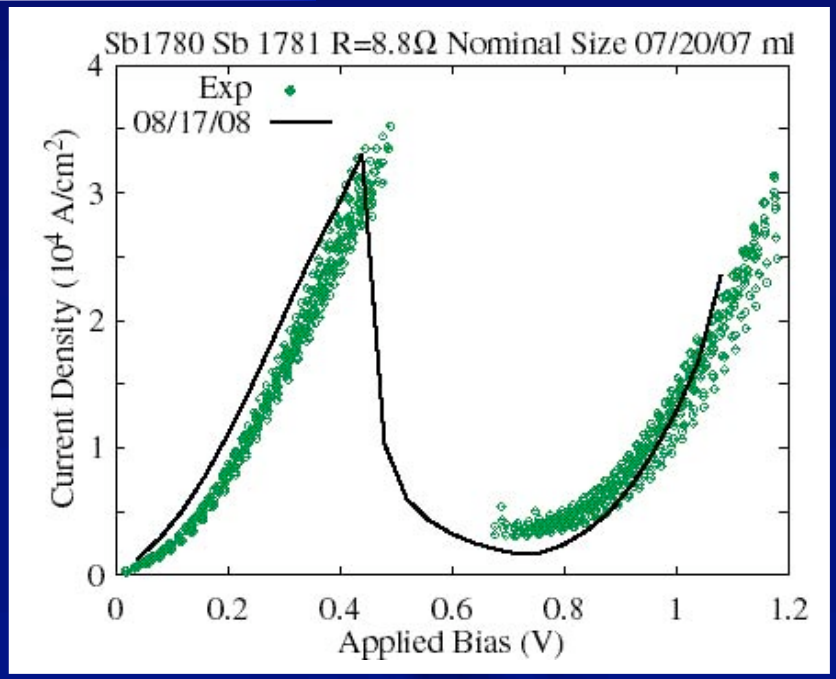
- **research**
- **simulation tools** (1-D transport, 3-D, Synthesis)
- **education and outreach**
- ***web-based services***

"To be the ***place*** where experiment, theory, and simulation meet and move nanoscience to nanotechnology."

Resonant Tunneling Diode



Conduction band diagrams
for different voltages
and the resulting current flow.



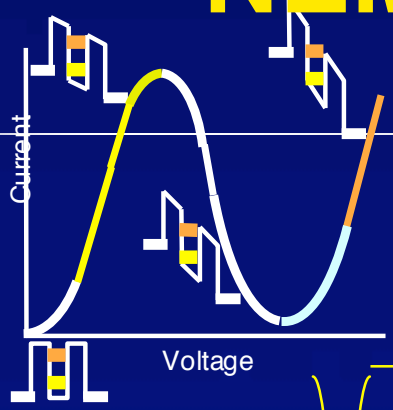
12 different I-V curves: 2 wafers, 3 mesa sizes, 2 bias directions

50nm	1e18	InGaAs
7 ml	nid	InGaAs
7 ml	nid	AlAs
20 ml	nid	InGaAs
7 ml	nid	AlAs
7 ml	nid	InGaAs
50 nm	1e18	InGaAs

NCN

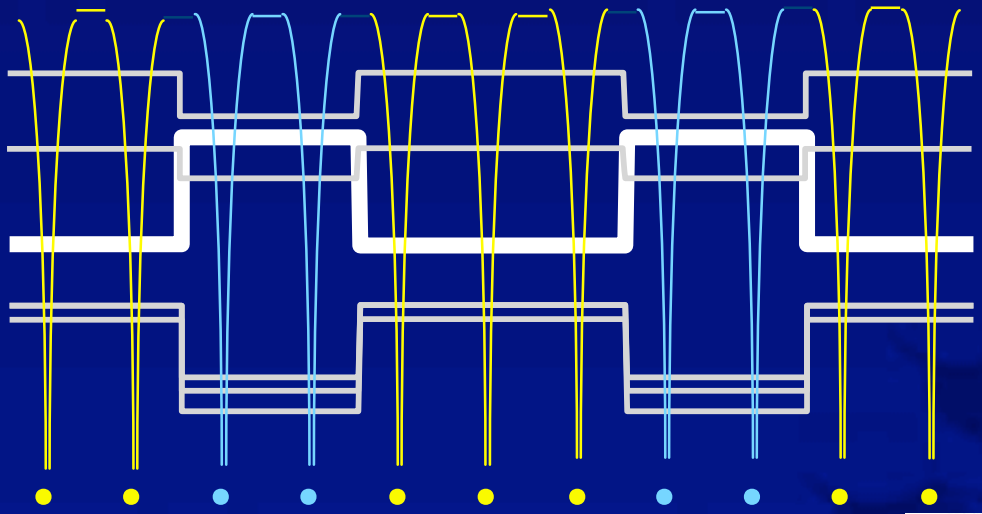
NEMO the first Nano CAD Tool

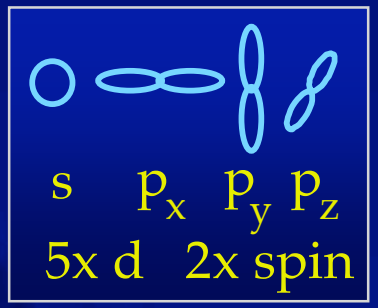
originally developed at Texas Instruments

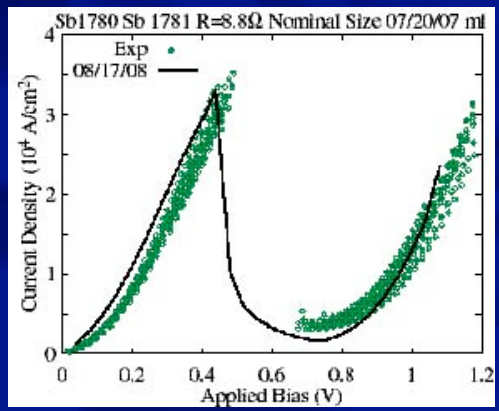


Atomistic Basis Sets

Concepts



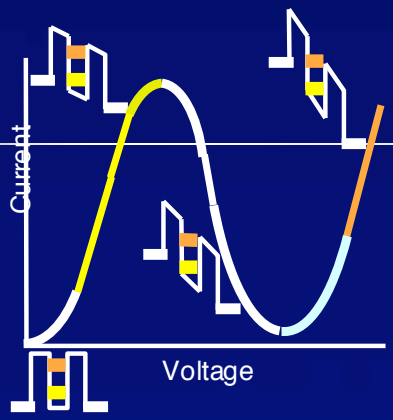




Quantitative
Design, Analysis, Synthesis

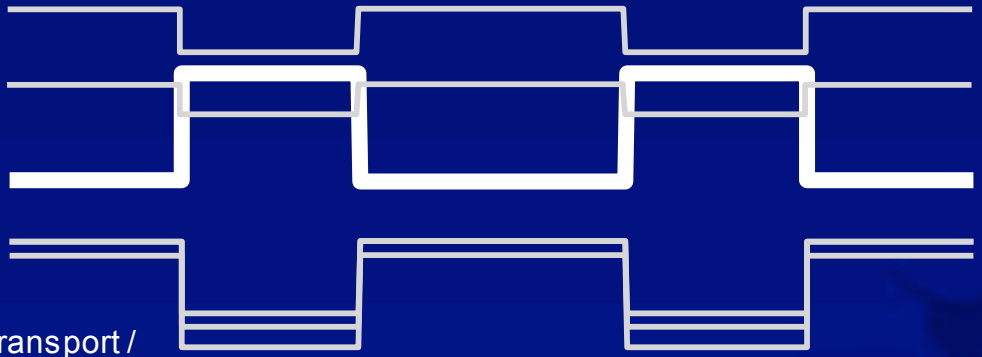
NCN

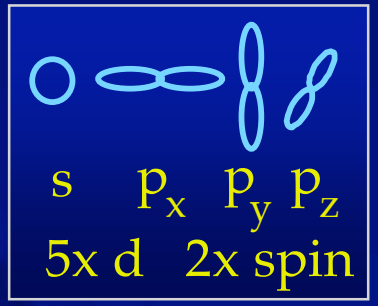
NEMO Key Elements:

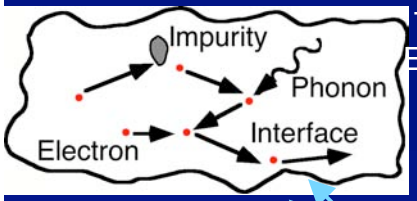


Concepts

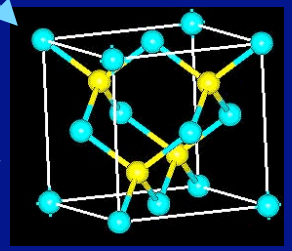
Tight Binding $sp^3d^5s^*$
Realistically Extended Devices
Non-Equilibrium Green Functions





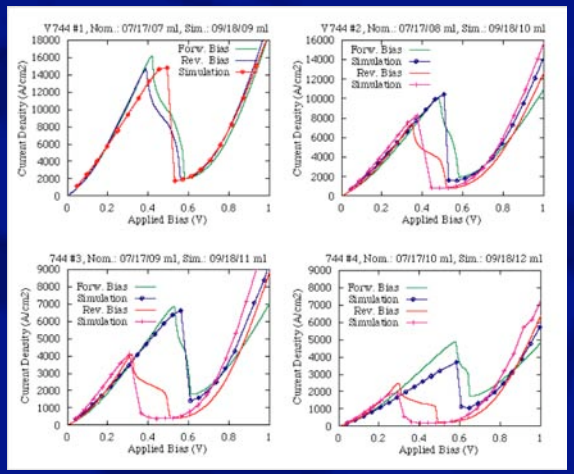


Transport / Engineering



Quantum Mechanics / Physics

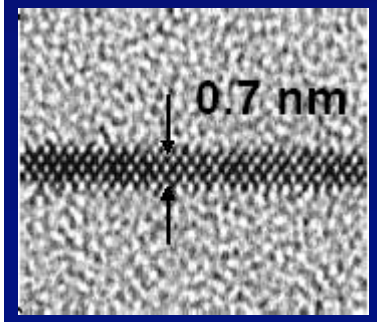
Quantitative
Design, Analysis, Synthesis

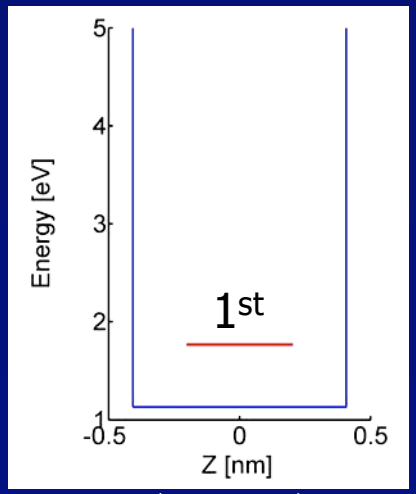


NCN

Ultra Thin Body SOI: A traditional Quantum Well?

Five Atomic Layer
Si (001)
IEDM, Uchida





Most basic quantum mechanical problem: Particle in a box!

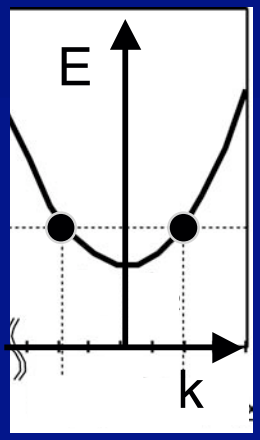
Expect / Remember:
- State quantization
- 2 counter-propagating states
- 1 bound state

Schrödinger Equation

$$\left(E - \frac{\hbar^2}{2m^*}\frac{d^2}{dz^2} - V(z)\right)\Psi(z) = 0$$

$$E = \frac{\hbar^2 k^2}{2m^*}$$

Parabolic Dispersion



$$k_1 = \frac{\pi}{L}$$

quantize k

$$\Psi(z) = e^{-ik_1 z} \quad \Psi(z) = e^{+ik_1 z}$$

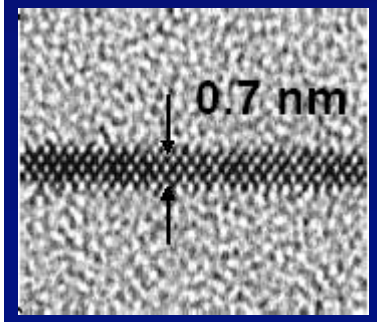
2 propagating states

$$\Psi(z) = \sin(k_1 z)$$

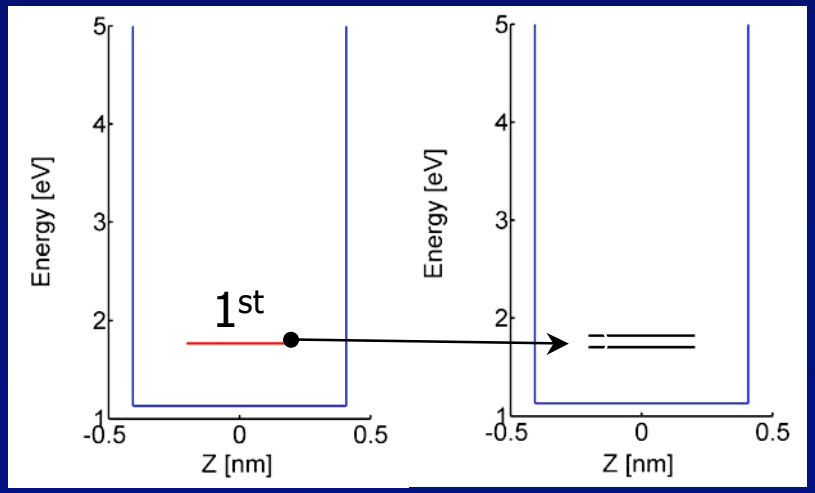
1 bound state

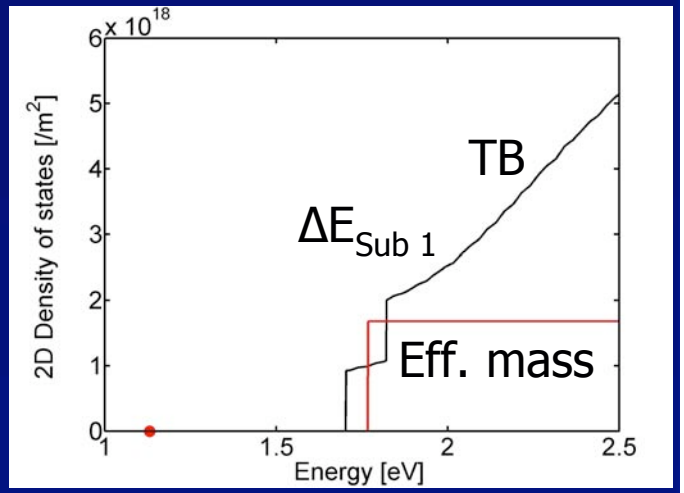
Quantum Wells - Special Considerations in Si

Five Atomic Layer
Si (001)
IEDM, Uchida



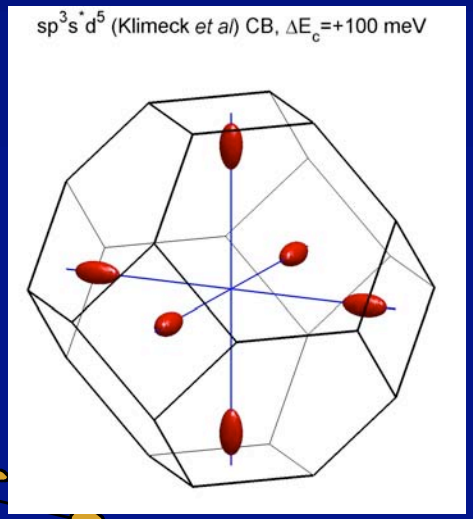
Five Atomic layers

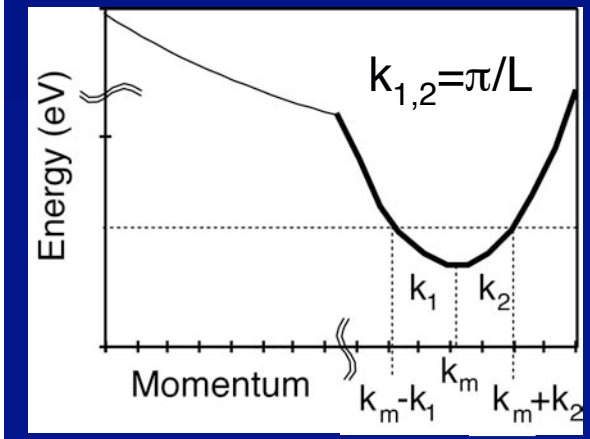




L

ΔE=150meV= 6k$_B$T effect at T=300K

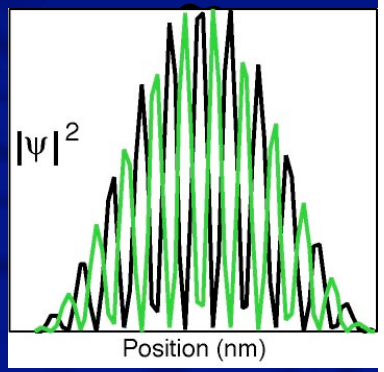




2 valleys
4 propagating states

↓

2 bound states
$k_{1,2}$ envelope
k_m fast oscillations



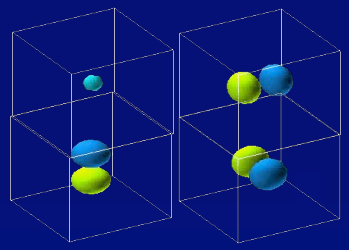
The NCN: Mission and Vision

To support the National Nanotechnology Initiative through:

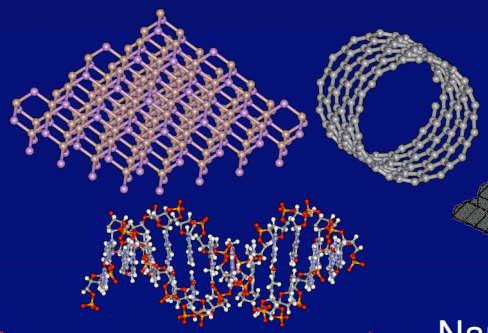
- **research**
- **simulation tools** (1-D transport, **3-D**, Synthesis)
- **education and outreach**
- ***web-based services***

"To be the ***place*** where experiment, theory, and simulation meet and move nanoscience to nanotechnology."

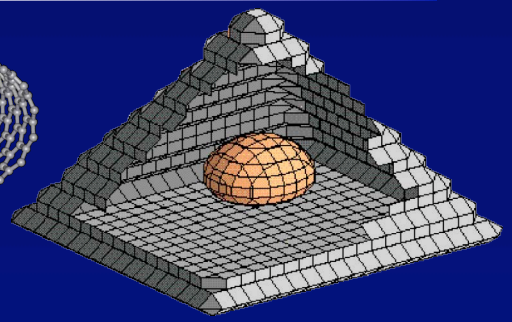
Quantum Dots: A Material / Device Testbed
Multi-Million Atoms Simulations



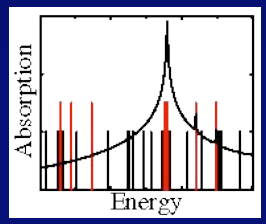
Atomic Orbitals
size: 0.2nm



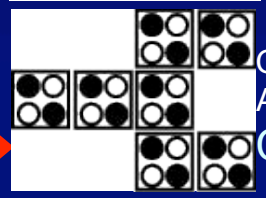
Structure



Nanoscale Quantum States
(Artificial Atoms, size 20nm)



Designed
Optical
Transitions
Sensors



Quantum Dot
Arrays
Computing

Problem:

Nanoscale device simulation requirements:

- Cannot use bulk / jellium descriptions, need description of the material atom by atom
  => use pseudo-potential or local orbitals
- Consider finite extent/transport, not infinitely periodic
  => local orbital approach
- Need to include > 1 million atoms.
  => need massively parallel computers
- The design space is huge: choice of materials, compositions, doping, size, shape. => need a design tool

Approach:

- Use local orbital description for individual atoms in arbitrary crystal / bonding configuration
  - Use s, p, and d orbitals
    Use GA for material parameter fitting
- Strain with VFF
- Custom eigensolver
- **Demonstrated 64 Million Atom System**
  Volume of
  - **110x110x110 nm^3**
  - **15x300x300 nm^3**

NCN

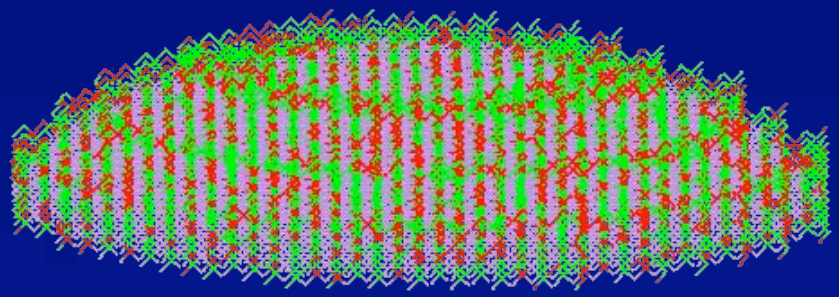
Alloy Disorder

Problem:
- Cations are randomly distributed in alloy dots.
- Does alloy disorder limit electronic structure uniformity for dot ensembles?

Approach:
- Simulate a statistical ensemble of alloyed dots.
- Requires atomistic simulation tool.

Results:
- Simulated >1000 dots with random cation distributions.
- Inhomogeneous broadening factor of ~0.5-5meV due to alloy disorder.

Impact:
- Fundamental uniformity limit for ensemble of alloy-based quantum dots.



$In_{0.6}Ga_{0.4}As$ Lense Shaped Dot

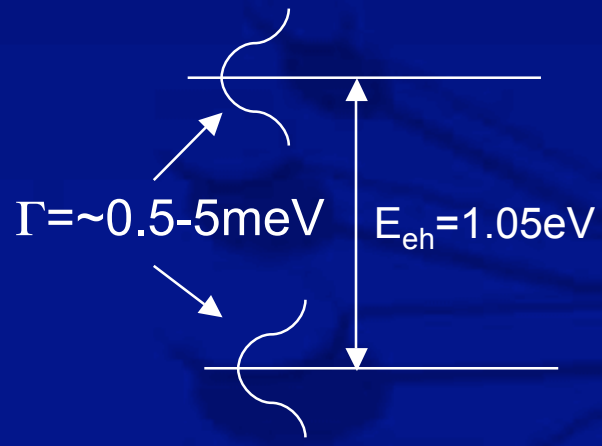
Diameter=30nm,Height=5nm, GaAs embedded

~1,000,000 Atom Simulation, $sp3s^*$ basis

In and Ga atoms are randomly distributed

Inhomegenious Broadening?

Simulation of Alloy Dot Ensemble



Measured Γ=34.6 meV (R. Leon, PRB, **58**, R4262)

Examined Theoretical Lower Limit

NCN

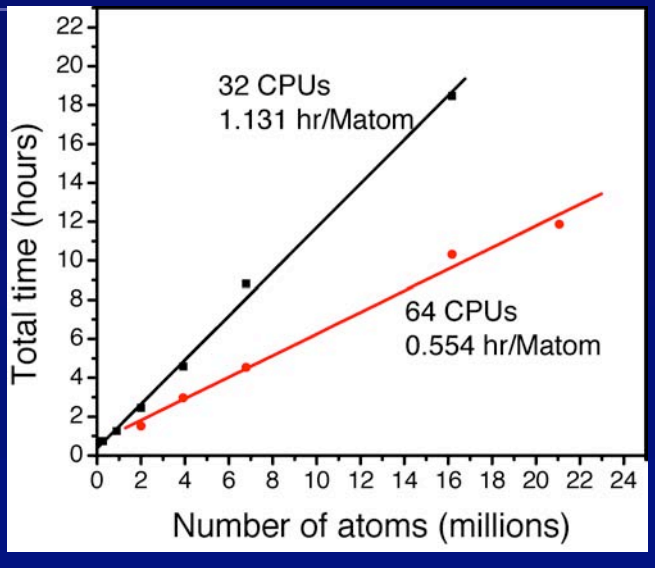
Computational Nanotechnology

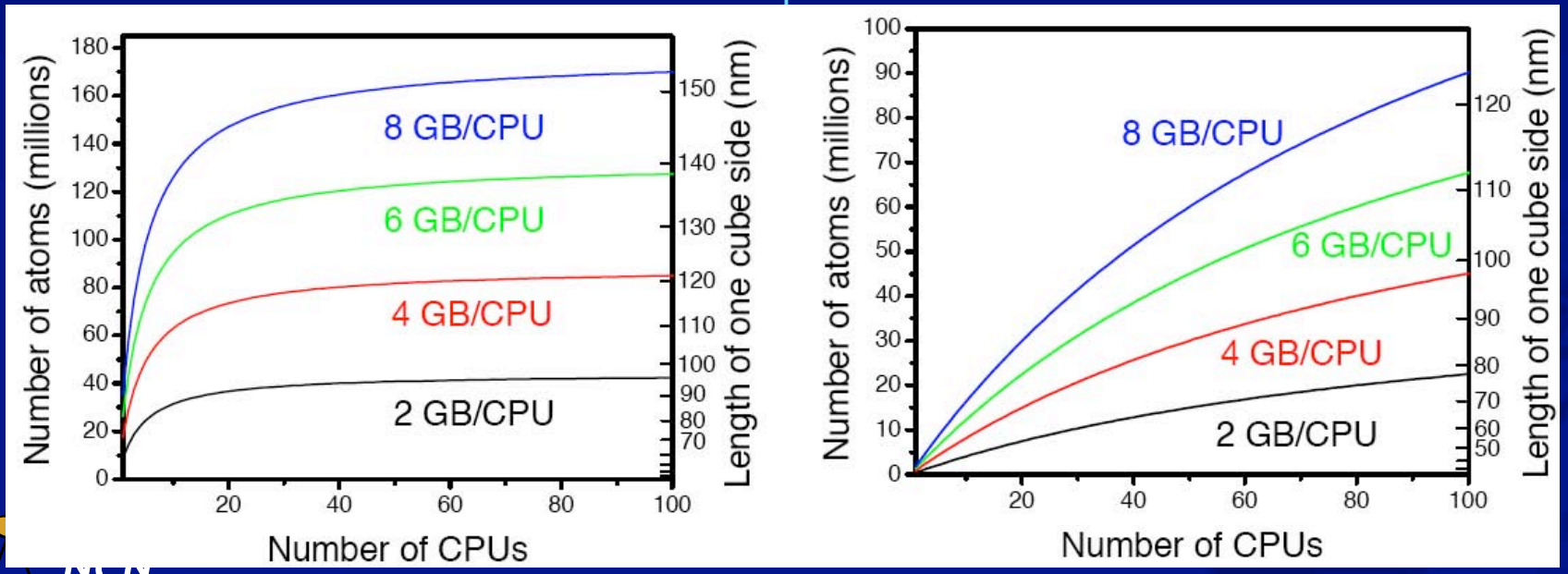
NEMO 3-D: Electronic structure for 23 Million Atoms

Result / Demonstrations / Impact:

- 64 million atom strain - volume $(110nm)^3$
- 23 million atom electronic structure Volume $(78nm)^3$ or $15x178x178nm^3$
- Determined long range extent of strain in self-assembled quantum dots

Performed on NSF Teragrid

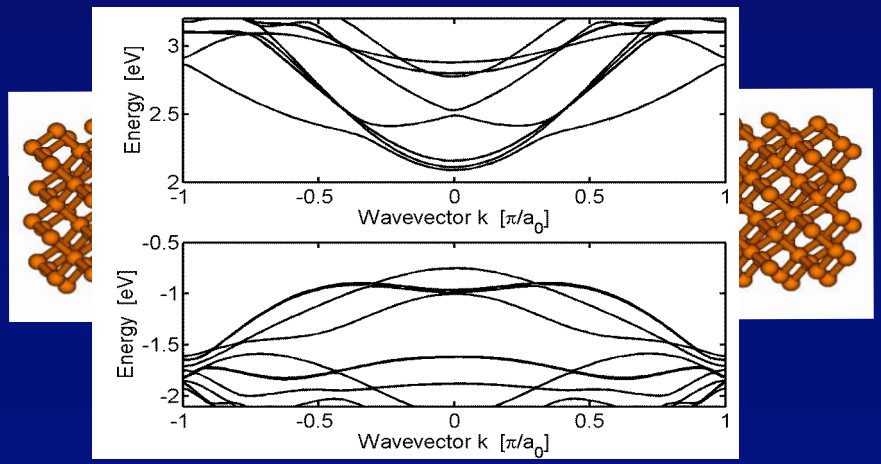




NCN Approach to Simulator Development

Objective:
- Comprehensive nanowire simulator.

Approach:
- Leverage existing theory, tools and s/w approaches
  - •NEGF theory
  - •NASA, JPL, Purdue, and ASU codes
- Utilize post-docs and s/w professionals.
- Deploy the tool to the nanohub.



Design Criteria:

Separate physics from algorithms!
- Generalized numerical algorithms
- General structure descriptions
  - Si wires
  - CNTs
  - Ultra-scaled FET
- Arbitrary materials
- Atomistic and continuum descriptions
- Graphical User Interface

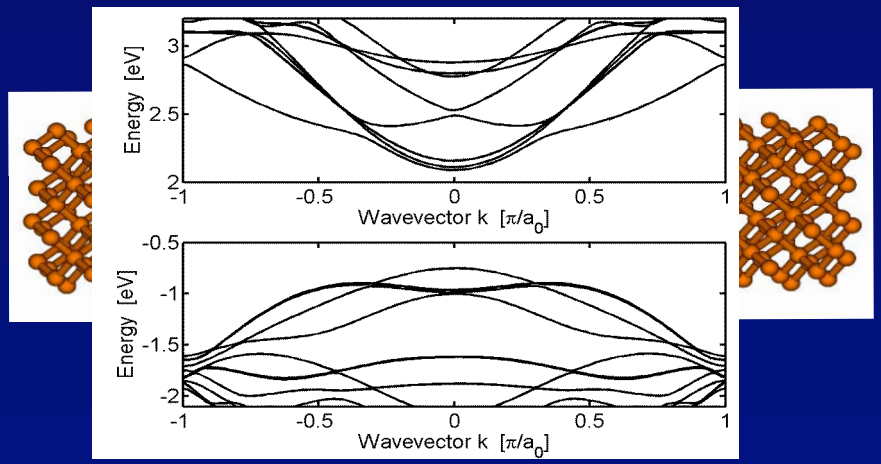
Status:
- Development team in place:
  - 1 S/W architect
  - GUI: 1 s/w professional and 1 post-doc
  - Theory core: 1 post docs
  - Algorithm core: 1 post doc
- Begun Joining NASA transport code and Purdue transport code
- prototype on nanoHUB in May.

Desired Impact:
- Establish community code for community development

NCN Approach to Simulator Development

Objective:
- Comprehensive nanowire simulator.

Approach:
- Leverage existing theory, tools and s/w approaches
  - •NEGF theory
  - •NASA, JPL, Purdue, and ASU codes
- Utilize post-docs and s/w professionals.
- Deploy the tool to the nanohub.



Opportunity for industrial Interaction:
- Become a member of the NCN
- Fund special components of the simulator
- Delegate a guest researcher

Develop real tools for real people!

Status:
- Development team in place:
  - 1 S/W architect
  - GUI: 1 s/w professional and 1 post-doc
  - Theory core: 1 post docs
  - Algorithm core: 1 post doc
- Begun Joining NASA transport code and Purdue transport code
- prototype on nanoHUB in May.

Desired Impact:
- Establish community code for community development

The NCN: Mission and Vision

To support the National Nanotechnology Initiative through:

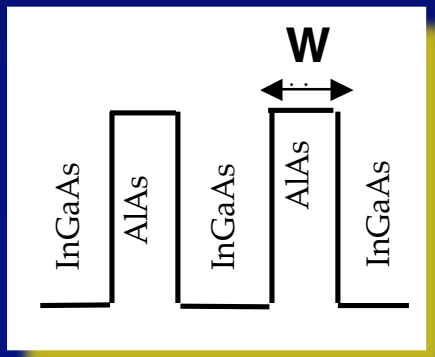
- **research**
- **simulation tools** (1-D transport,3-D, **Synthesis**)
- **education and outreach**
- ***web-based services***

"To be the ***place*** where experiment, theory, and simulation meet and move nanoscience to nanotechnology."

Testmatrix-Based Verification (room temperature)

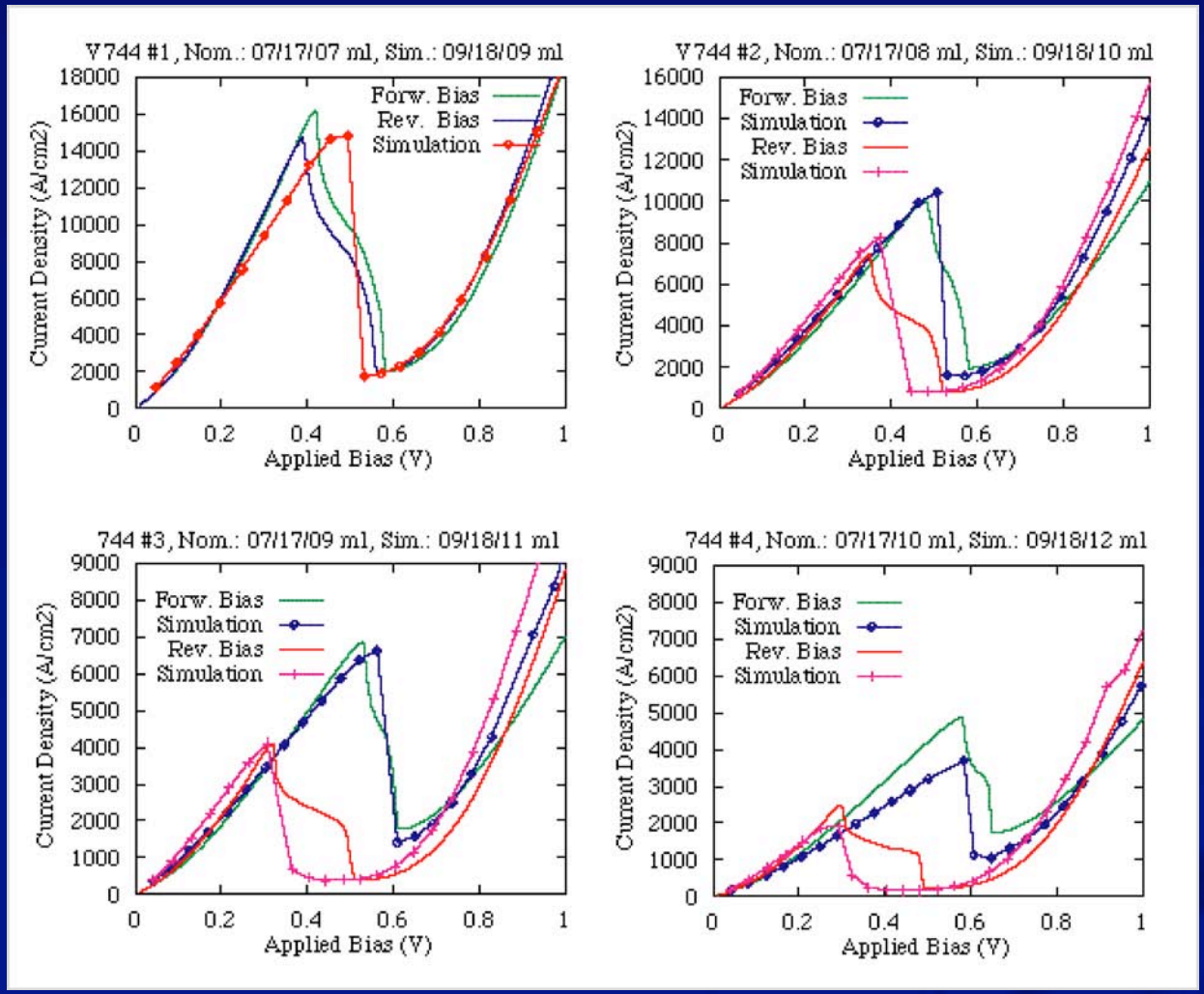
Strained InGaAs/AlAs 4 Stack RTD with Asymmetric Barrier Variation

Vary One Barrier Thickness



Four increasingly asymmetric devices:

20/50/20 Angstrom
20/50/23 Angstrom
20/50/25 Angstrom
20/50/27 Angstrom



Presented at IEEE DRC 1997, work performed at Texas Instrument, Dallas

Genetically Engineered Nanoelectronic Structures (GENES)

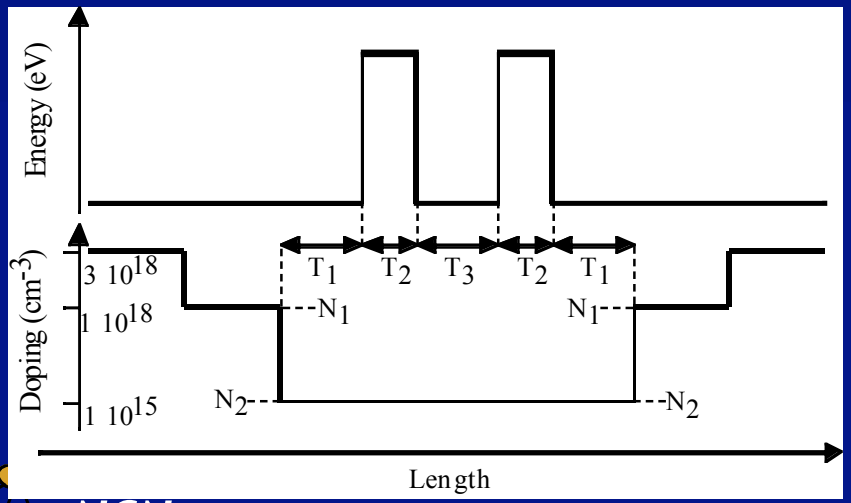
Objectives:

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

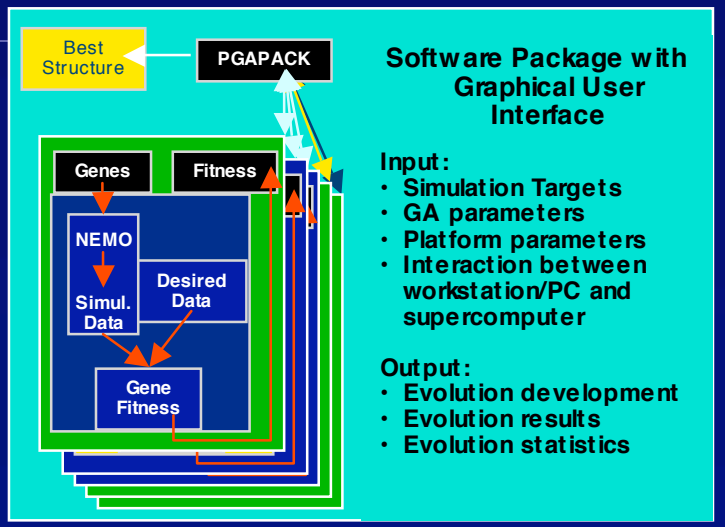
Approach:

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

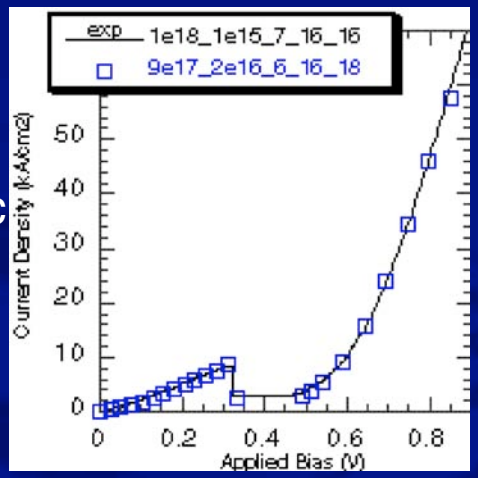
How do you know what you have built?



Architecture



Results:
Nanoelectronic Device Structural analysis



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

NCN

The NCN: Mission and Vision

To support the National Nanotechnology Initiative through:

- **research**
- **simulation tools**
- **education and outreach**
- ***web-based services***

"To be the ***place*** where experiment, theory, and simulation meet and move nanoscience to nanotechnology."

NCN

Network for Computational Nanotechnology

- Community building
- Remote access
- Collaboration
- Education
- "typical" Web-presence
- On-line simulation

- Simulation software
  - Model resource
  - Computer resource
  - Simple interface

- Science applications
  - Electronics
  - Electromechanics
  - Bio

Academics,
Professional,
Teachers,
K-12 Students

WWW Graphical User Interface

Middleware
Hardware and Software Management

Appl… App… …ions …ons
Applications

NCN

NCN
Network for Computational Nanotechnology

- Community building
- Remote access
- Collaboration
- Education
- "typical" Web-presence
- On-line simulation

- Simulation software
  - Model resource
  - Computer resource
  - Simple interface

- Science applications
  - Electronics
  - Electromechanics
  - Bio

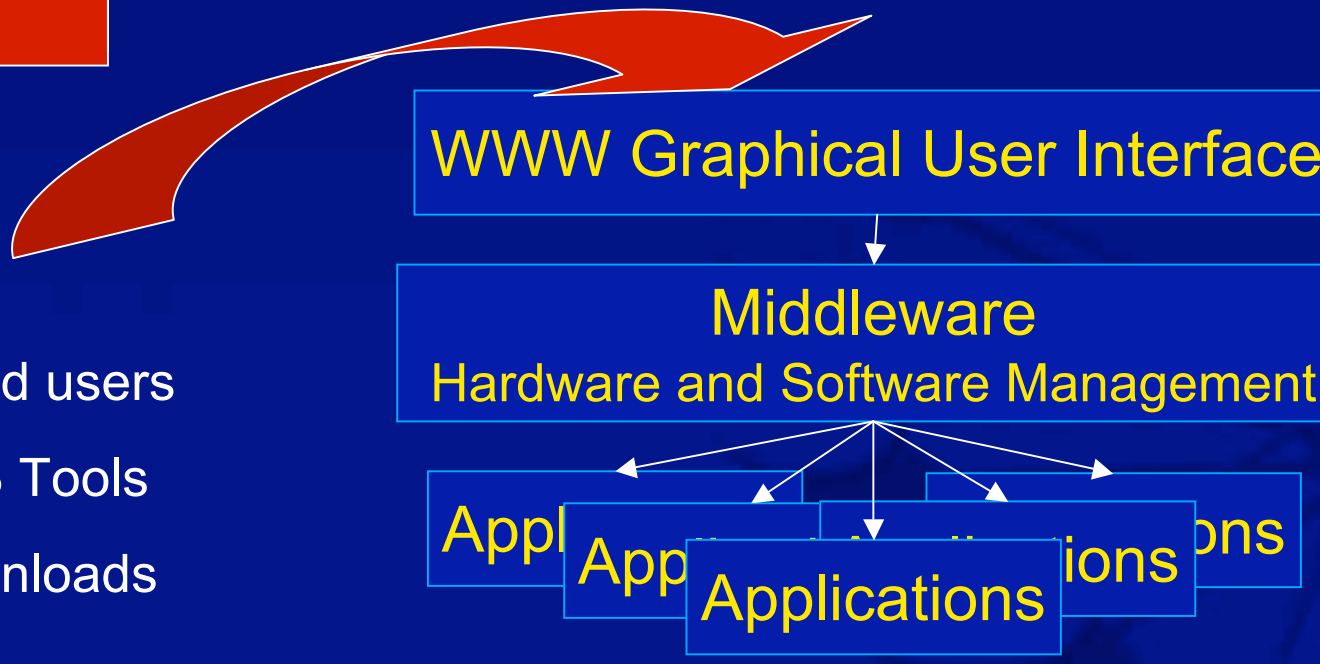
Last year:

>4,500 Users

>1,000 Registered users

>65,000 Jobs, 33 Tools

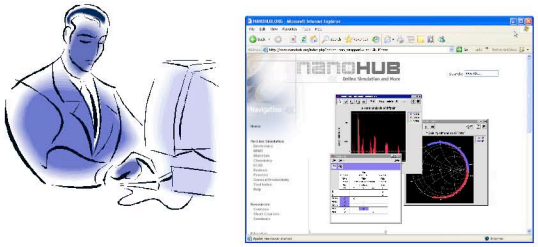
>770 source downloads



NCN

Middleware for Deployment

Remote access to simulators and compute power



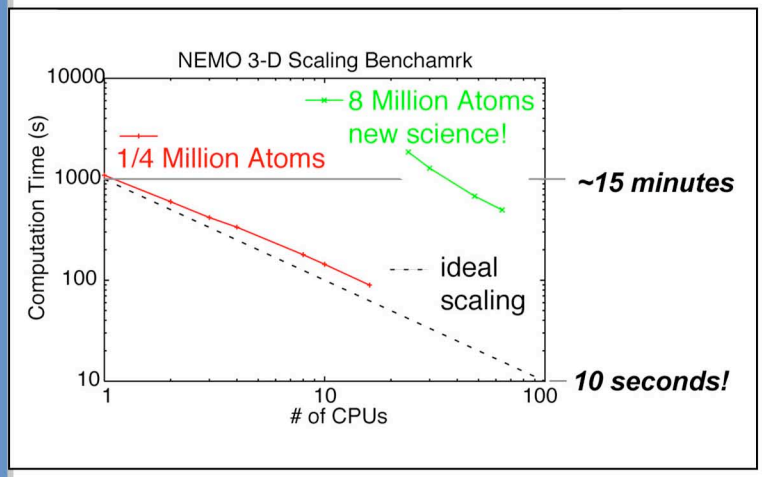
Remote desktop (VNC)

internet

nanoHUB.org

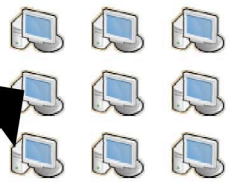
Unique Middleware

Virtual Machine



Job Manager

TeraGrid
(future)



Cluster

Simulation is Essential for Nanotechnology Development

Hint from the Semiconductor Industry:

- No new devices / circuits designed without software!

Problem:

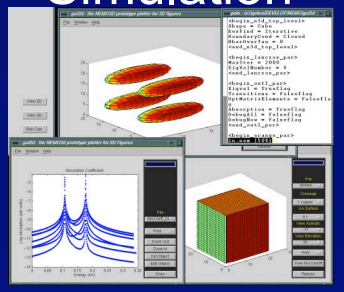
- Accepted nano simulation tool suite does NOT exist.

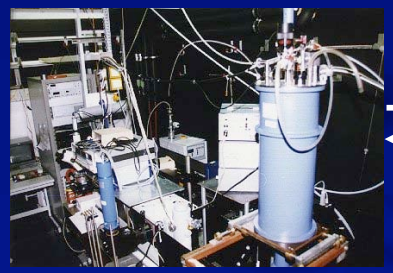
Approach:

- Conduct research in Modeling and Simulation of:
  - Nanoelectronics
  - Nanoelectromechanics
  - Nano-bio sensors
  - Computational science
- **DEVELOP and DEPLOY** to nanoscience and nanotechnology community

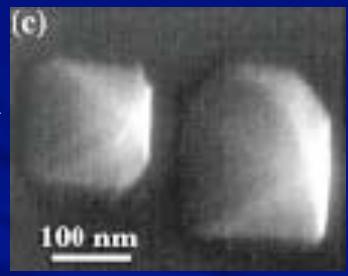
Commonalities:

- Compute platforms (workstation, clusters)
- Structured simulator input.
- Numerical methods.
- Standard output (x-y plots, 3-D data, molecular style visualization)
- **Graphical User Interface**





Characterization



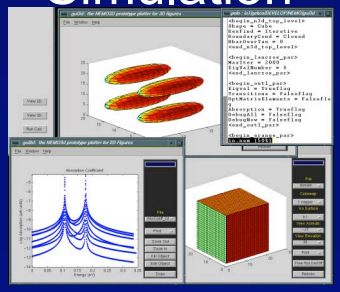
Fabrication

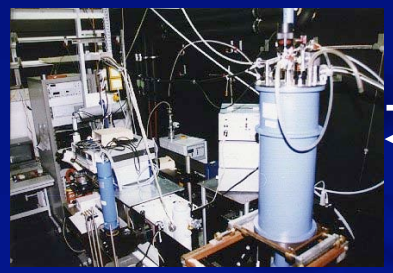
NCN

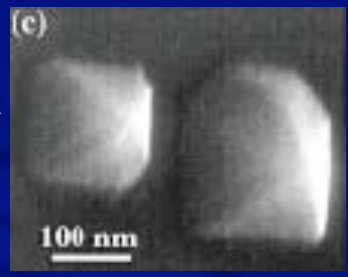
Simulation is Essential for Nanotechnology Development

Software development utilizing generalized approaches enabled the NEMO development and generated new science

Simulation







Characterization

Fabrication

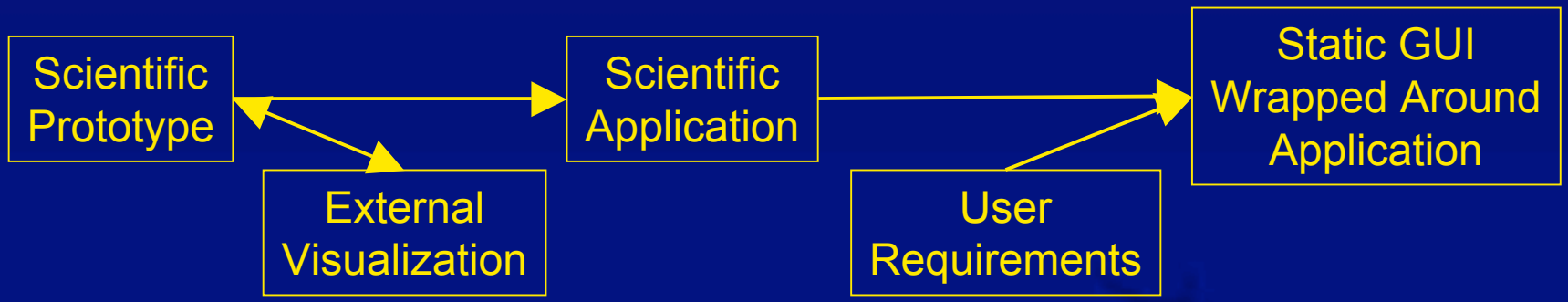
Commonalities:

- Compute platforms (workstation, clusters)
- Structured simulator input.
- Numerical methods.
- Standard output (x-y plots, 3-D data, molecular style visualization)
- **Graphical User Interface**

NCN

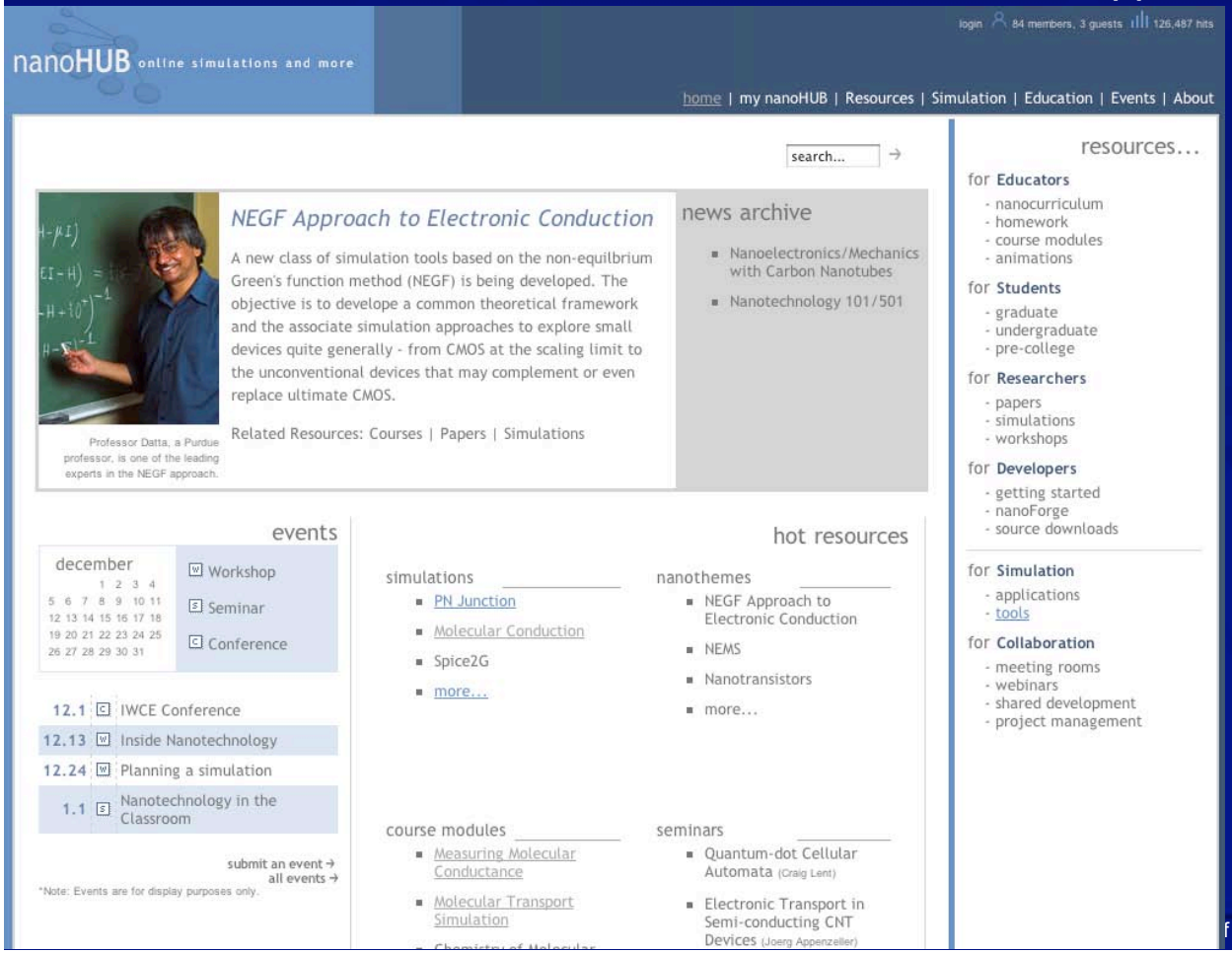
GUI Development Approaches

- **Typical Approach:**
- Scientific programmer is de-coupled from GUI, although that person is the best and most experienced user!
- GUI is static - must be adjusted manually every time for scientific input changes -> maintenance nightmare
- Hard to maintain an overall scheme of I/O for various applications.



GUI Development Approaches

- **Typical Approach:**
- Scientific programmer is de-coupled from GUI, although that person is the best and most experienced user!
- GUI is static - must be adjusted manually every time for scientific input changes -> maintenance nightmare
- Hard to maintain an overall scheme of I/O for various applications.



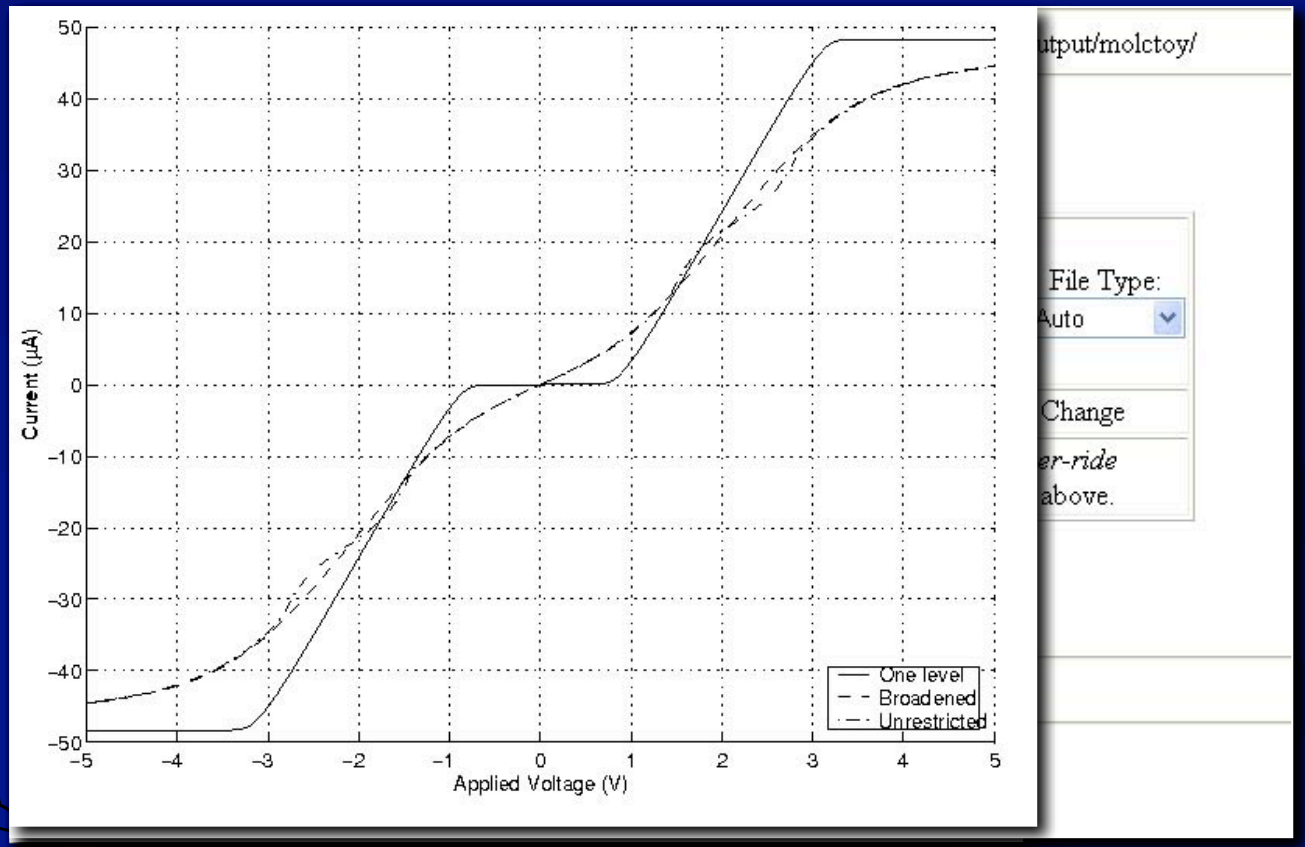
nanoHUB.org

- Current look and feel
- Can perform on-line simulation
- Need to get a (free) login

- Examples in the next slide

GUI Development Approaches

- **Typical Approach:**
- Scientific programmer is de-coupled from GUI, although that person is the best and most experienced user!
- GUI is static - must be adjusted manually every time for scientific input changes -> maintenance nightmare
- Hard to maintain an overall scheme of I/O for various applications.

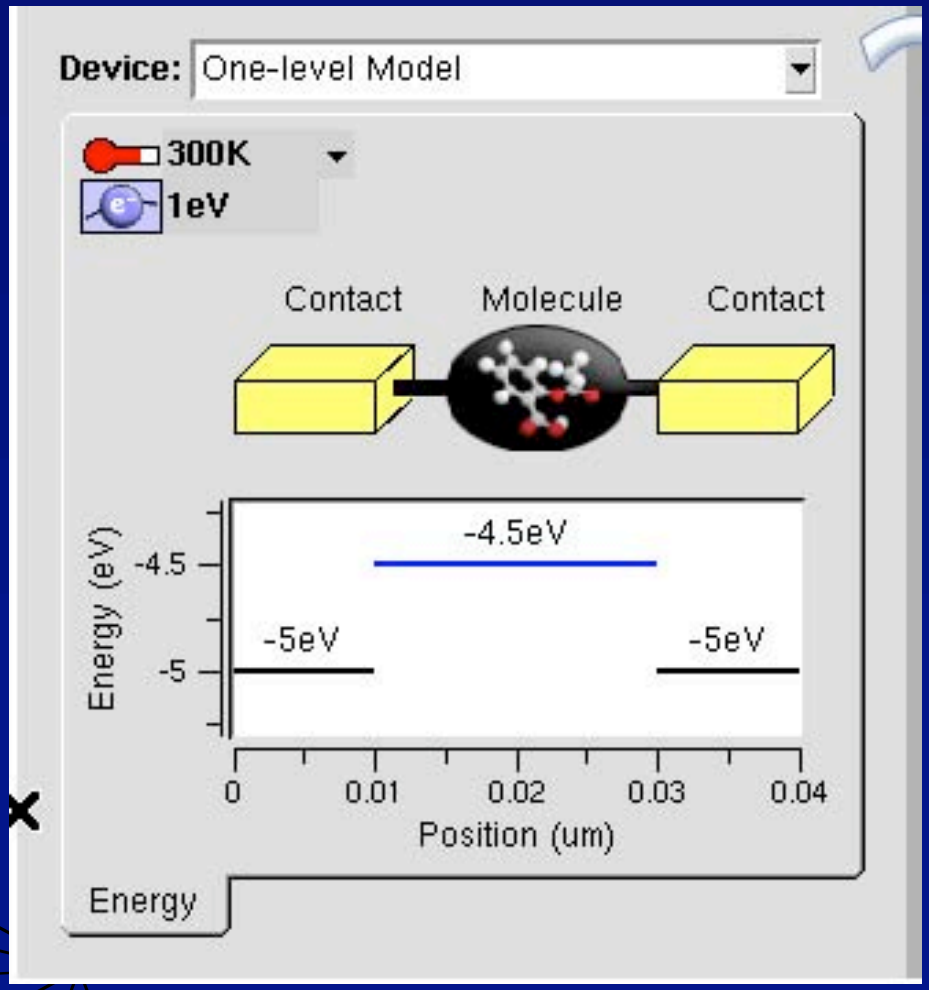


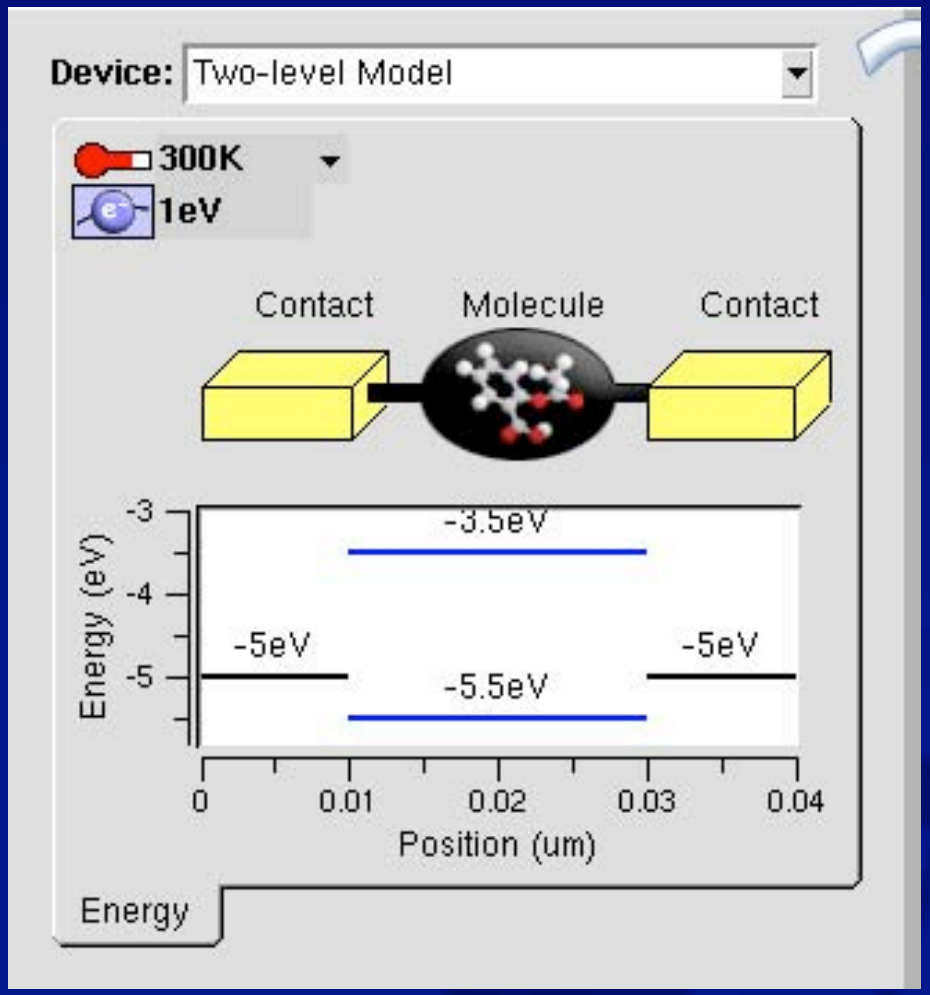
- **Typical Questions:**
- What was my input?
- Did I enter things right?
- **Symptoms of:**
- No VISUAL feedback.
- Not interactive.

MolcToy

An educational tool for Molecular transport Simulations

- ~~**The new interactive MolcToy:**~~
- Visual input



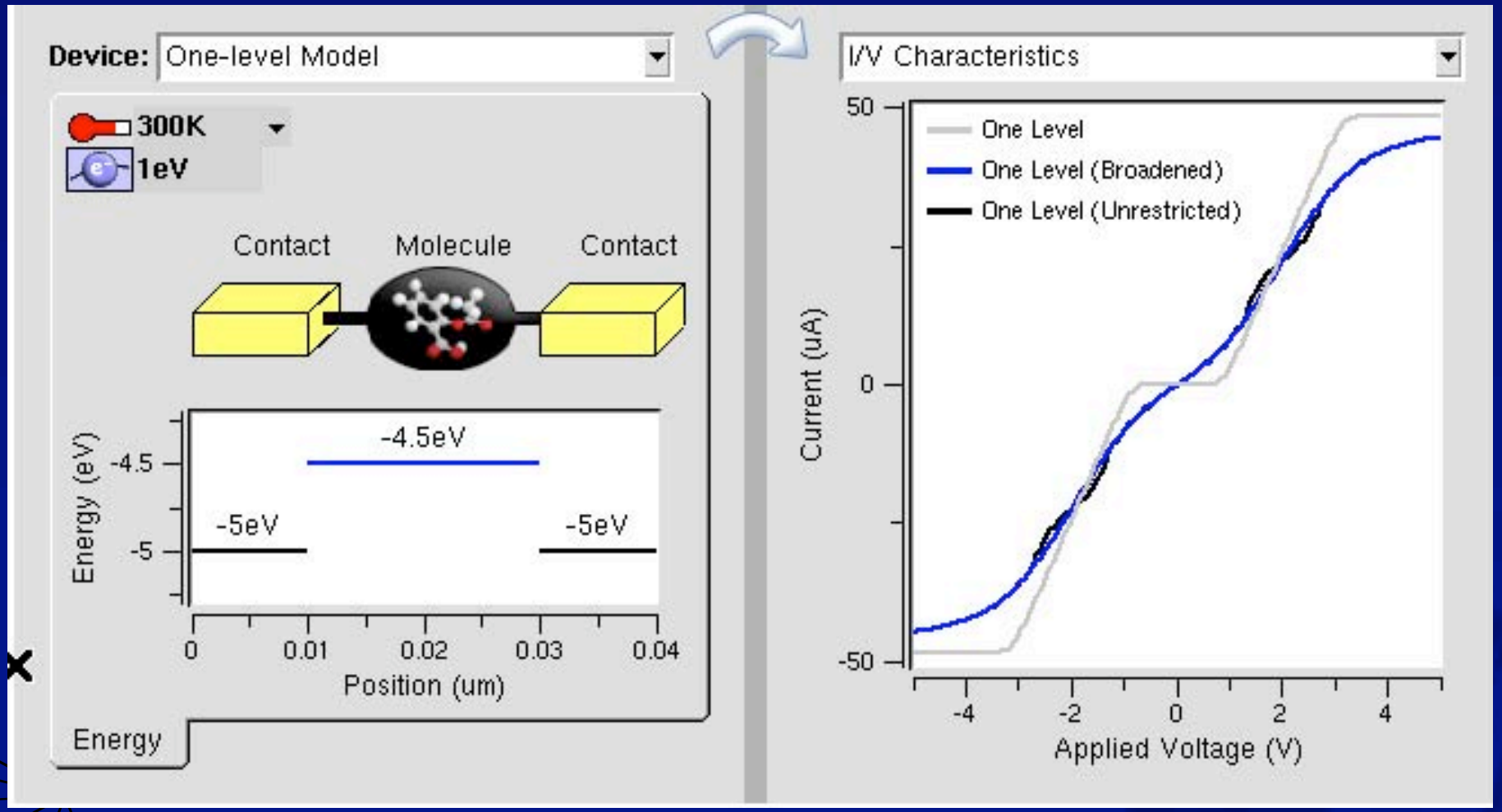


MolcToy

An educational tool for Molecular transport Simulations

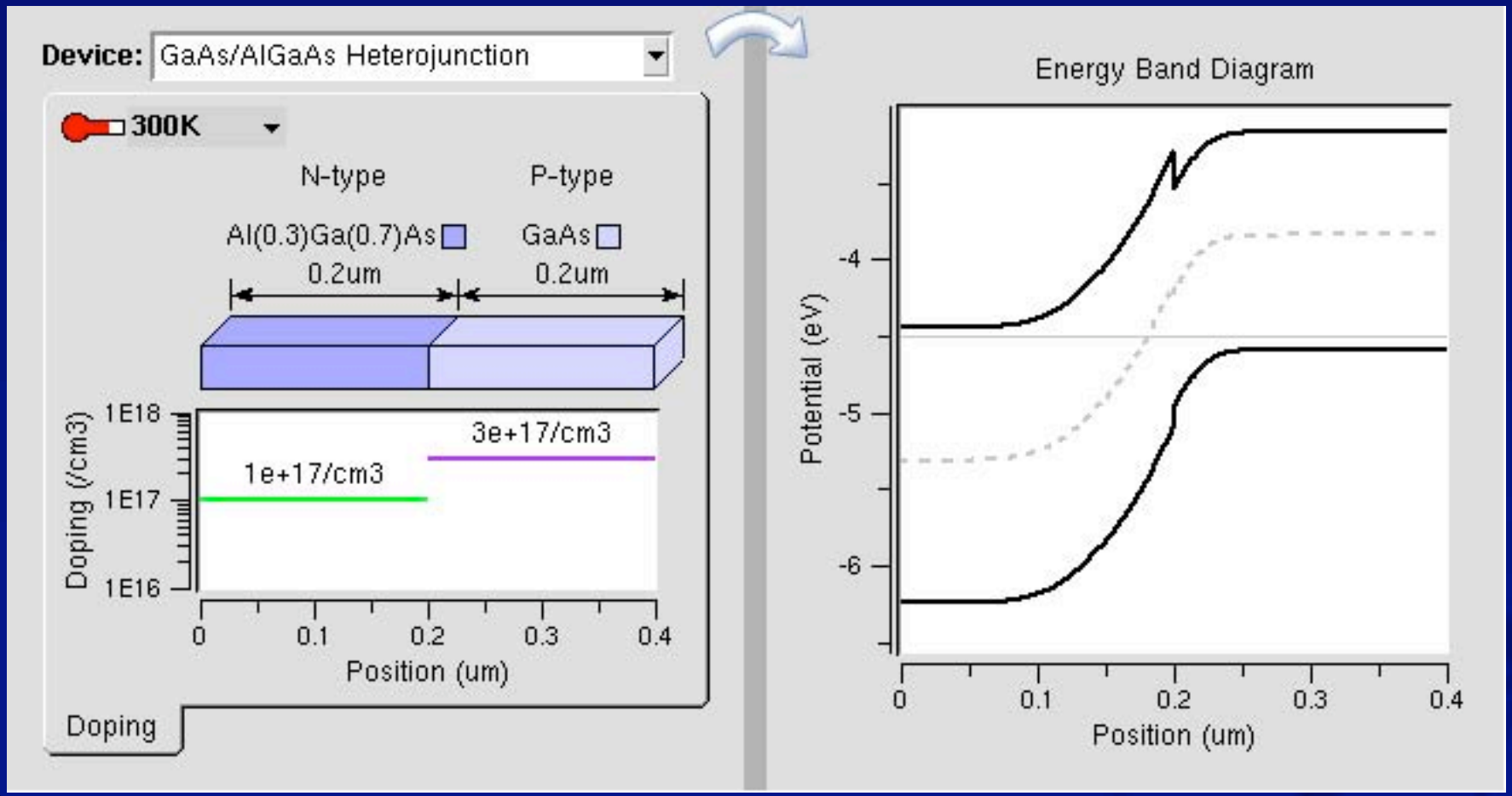
Rapid GUI Deployment!

This Application Integration Required ~1 day of work!!



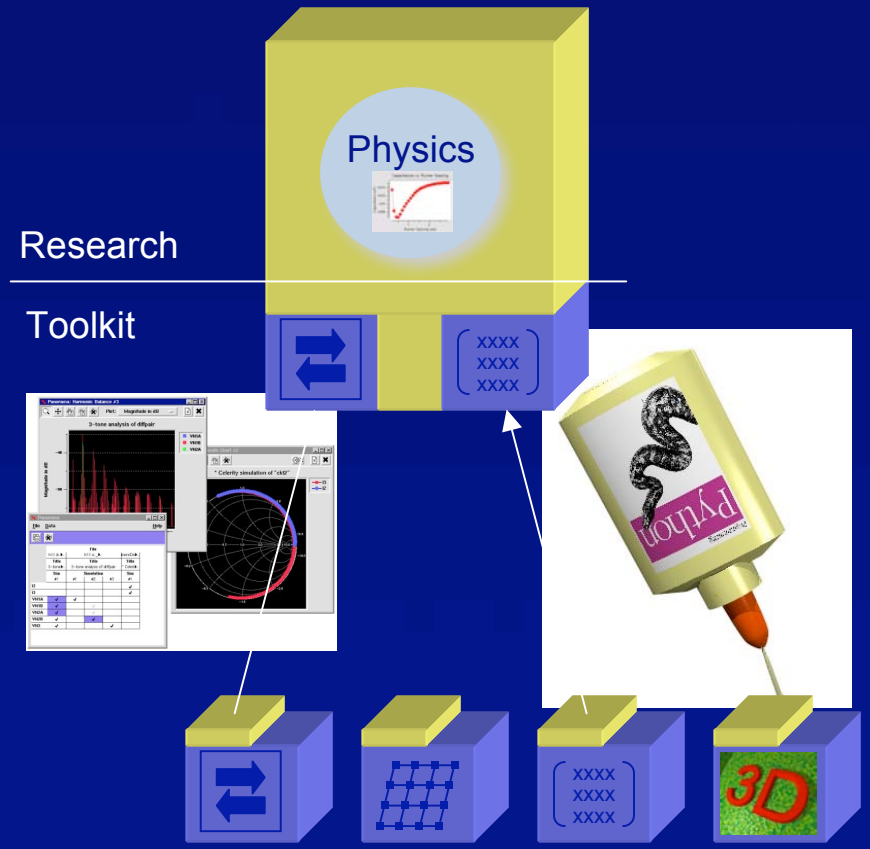
PN - Junctions
ADEPT legacy software

Rapid GUI Deployment!
This approach is NOT custom to one Application!



Software for Simulation

Rappture toolkit ➔ Rapid Application Infrastructure toolkit



New tool in short order!

Use toolkit components,
Add unique research

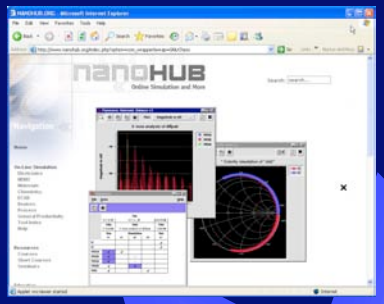
Scripting language interface

Rappture toolkit components

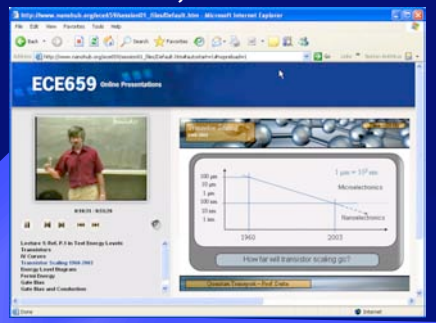
nanoHUB.org: more than computation

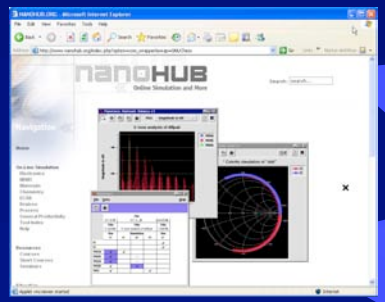
Research, Development, and Deployment

online simulation

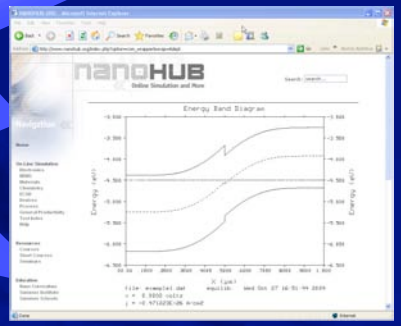


courses, tutorials



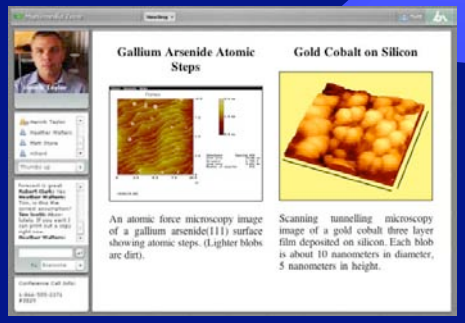


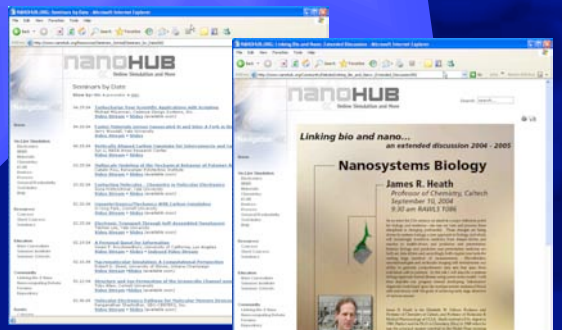
nanoHUB.org



learning objects

collaboration





seminars, themes

NCN

Backup