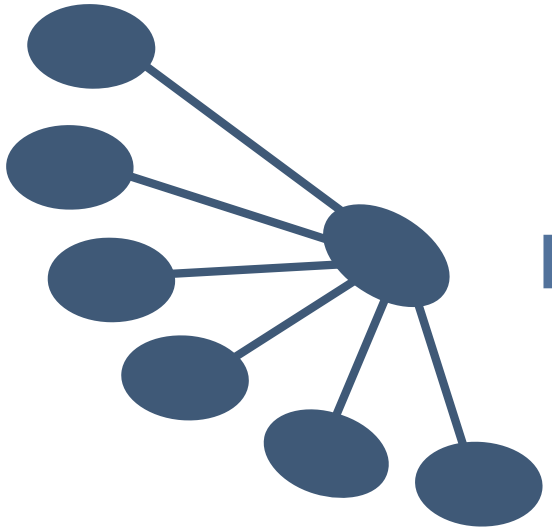


NCN Cyberinfrastructure
or
How can your science software reach thousands of users?

Gerhard Klimeck
NCN Technical Director

April 6, 2005

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

What is Cyberinfrastructure?

Cyberinfrastructure enables discovery and use of services by:

- ***Hardware***
- ***Software***
- ***Personnel***
- ***Organizations***

Concretely for the NCN

- ***Computation:***
  - ***models, user interfaces, compute cycles***
- ***Research and Education:***
  - ***seminars, tutorials, courses, learning objects***
- ***Without ANY user-end software installation***

Simulation is essential for Nanotechnology Development

Hint from the Semiconductor Industry:

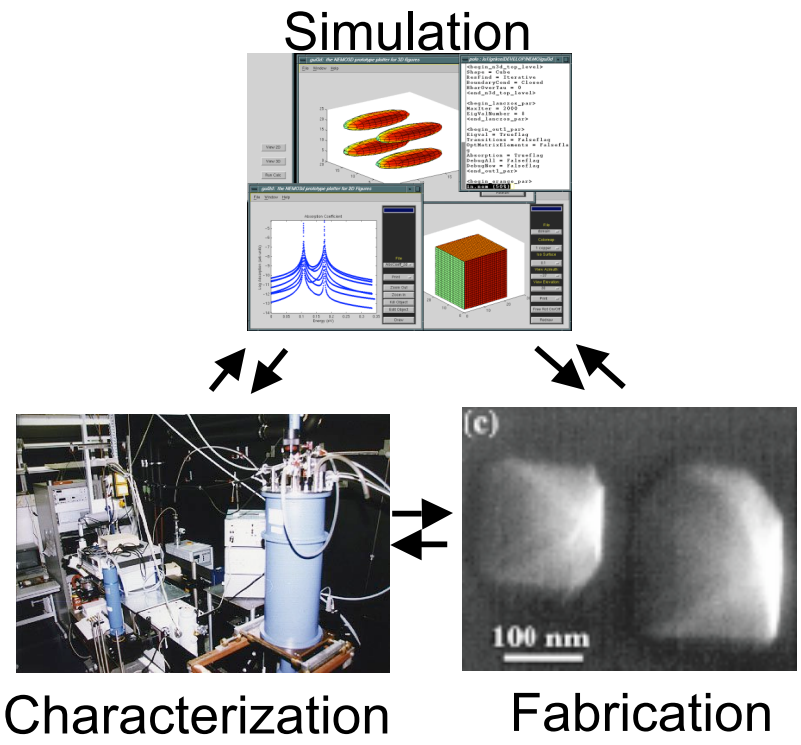
- No new devices / circuits designed without software!

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



The NCN
Research -> Development -> Deployment

www.nanohub.org

web-based simulation, education, collaboration, professional outreach (NSF Cyberinfrastructure)

software development, high-performance computing, course production (NSF-CISE)

research, education, professional leadership

research leverage

The NCN as a Project Organization

Nano Research
- Electronics
- Mechanics
- Bio

Research Deliverables
- Simulation Tools
- Educational Modules

Web-Presence

On-line Simulation

Application Software	Web-Enabled Middleware
21st Century	TeraGrid NMI

Content Management
- Courses
- Homeworks
- Tutorials
- Debates
- Calendar
- Collaboration

Admin.
- Budget
- Reports
- Events
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The NCN is different from any other NSF (Nano) Center

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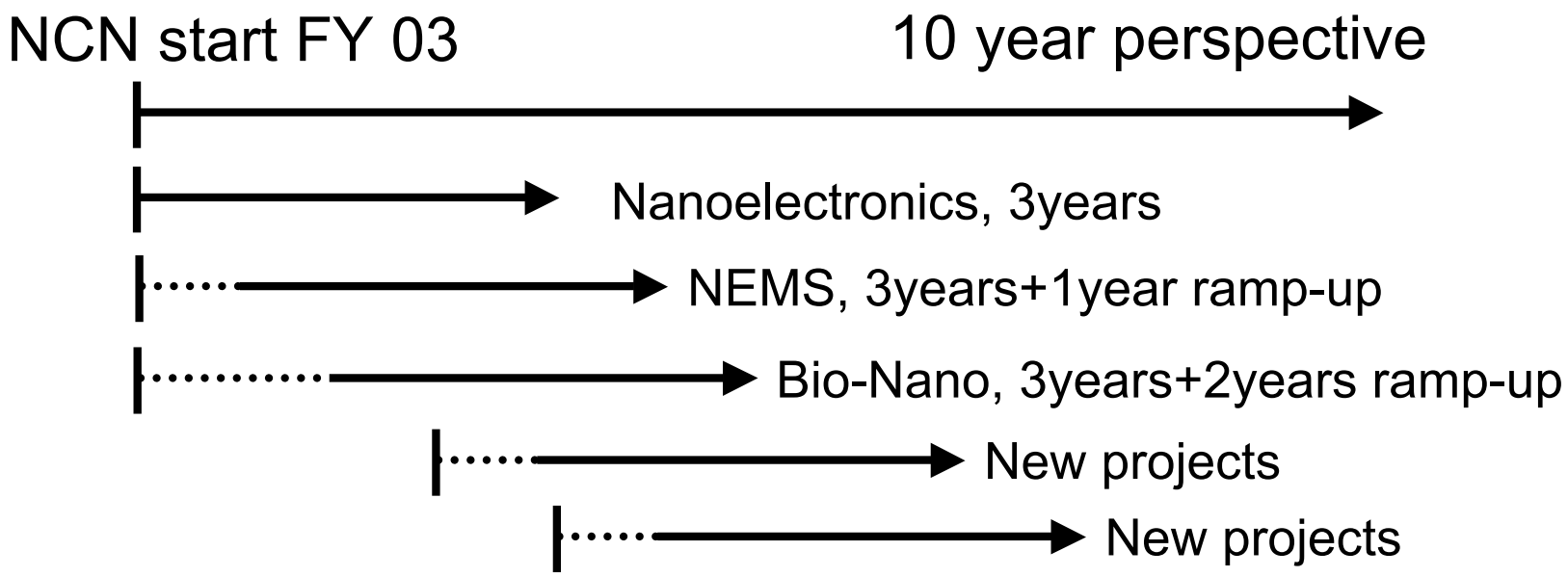
Research Project Transitions

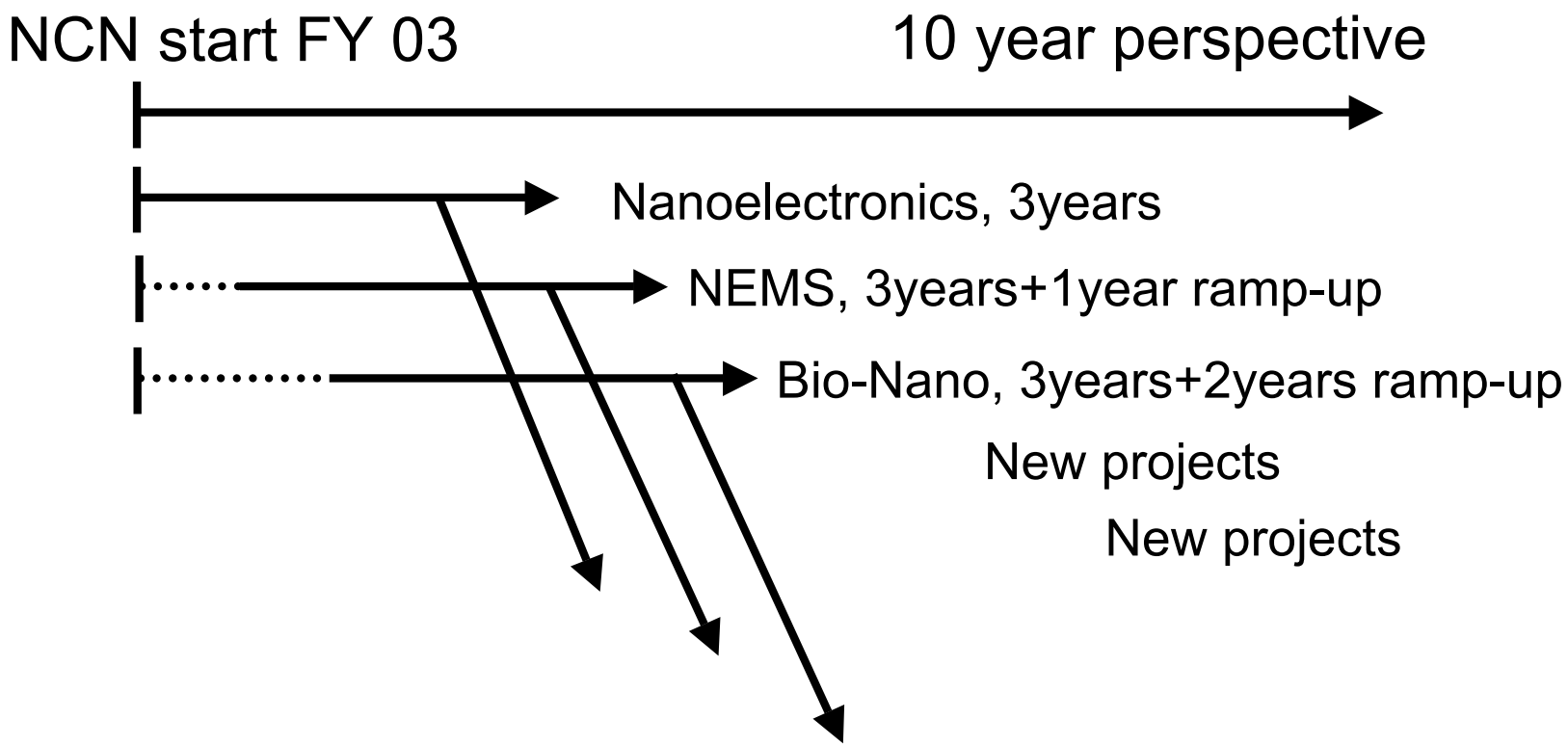


Nanoelectronics project quite mature
=> industrial interest / partners

NEMS - finishing ramp-up

Bio-Nano - extremely exploratory

Research Project Transitions

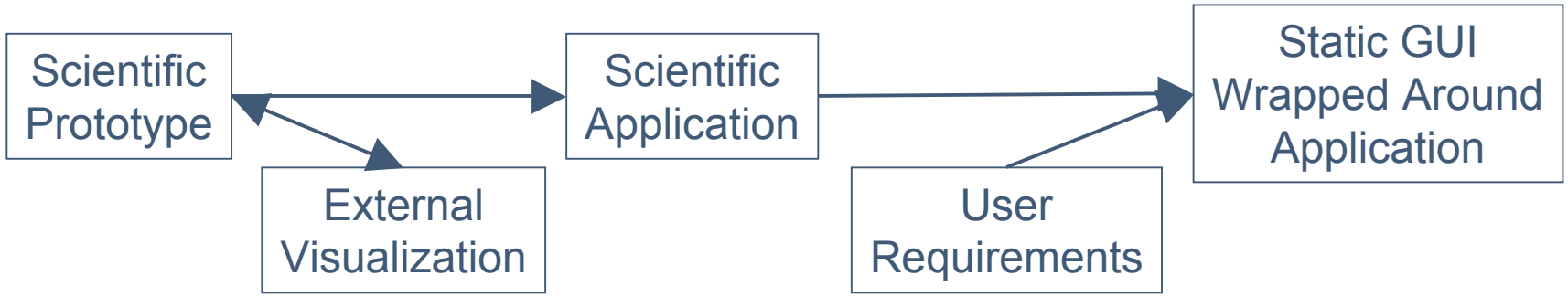


- Expect PI's to deliver modeling software to be disseminated to the Nanotechnology community!
  => web-hosted simulation tools

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.



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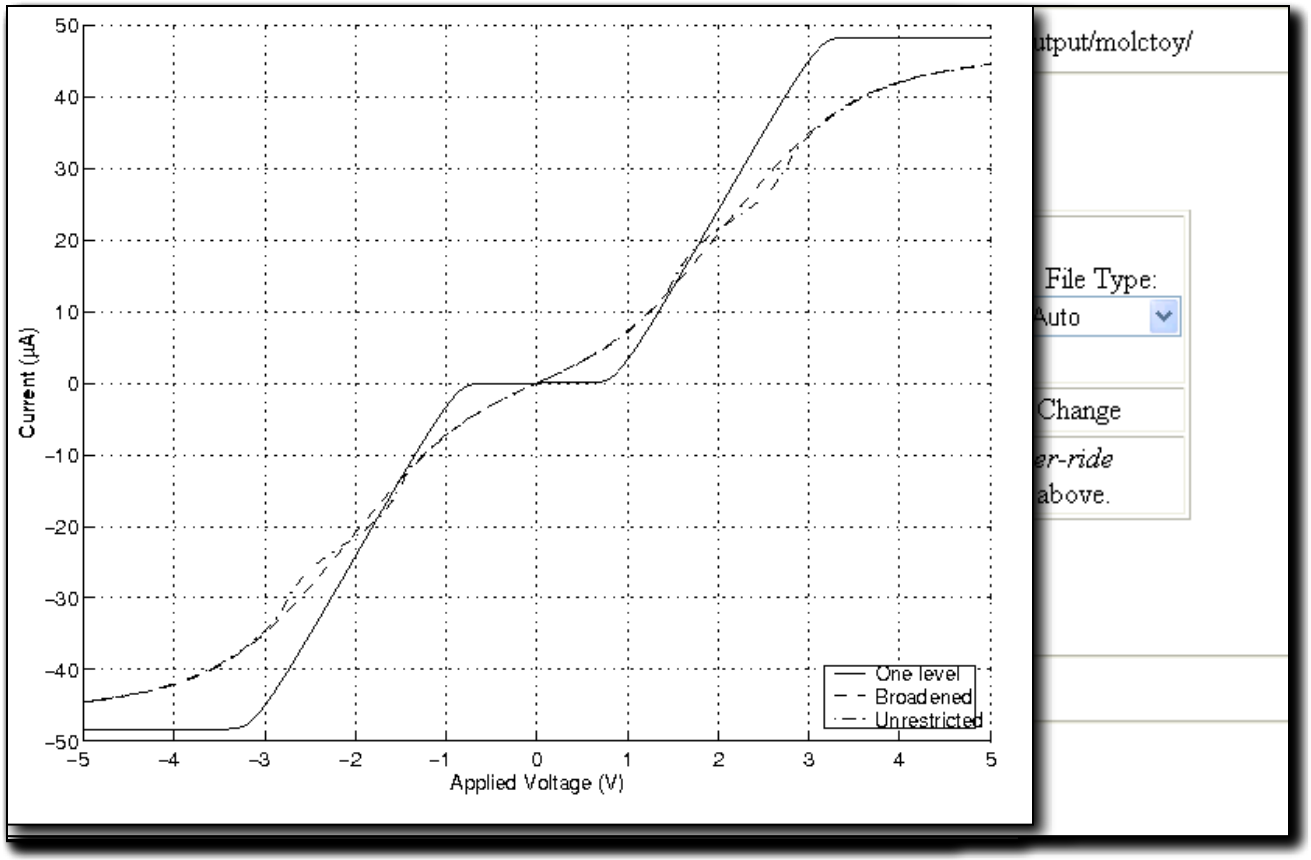


Typical Questions:

- What was my input?
- Did I enter things right?

Symptoms of:

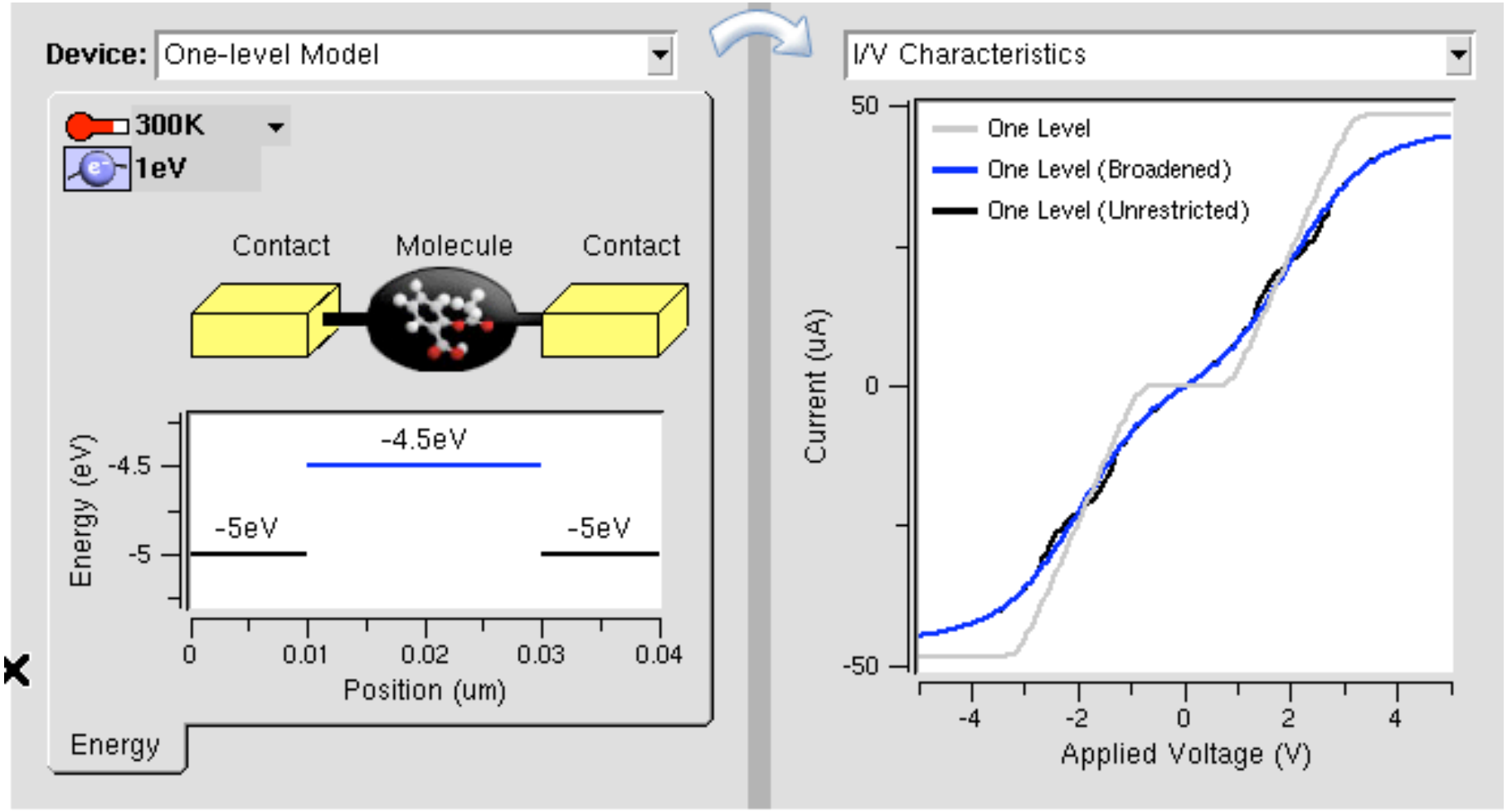
- No VISUAL feedback.
- Not interactive.

MolcToy

An educational tool for Molecular transport Simulations

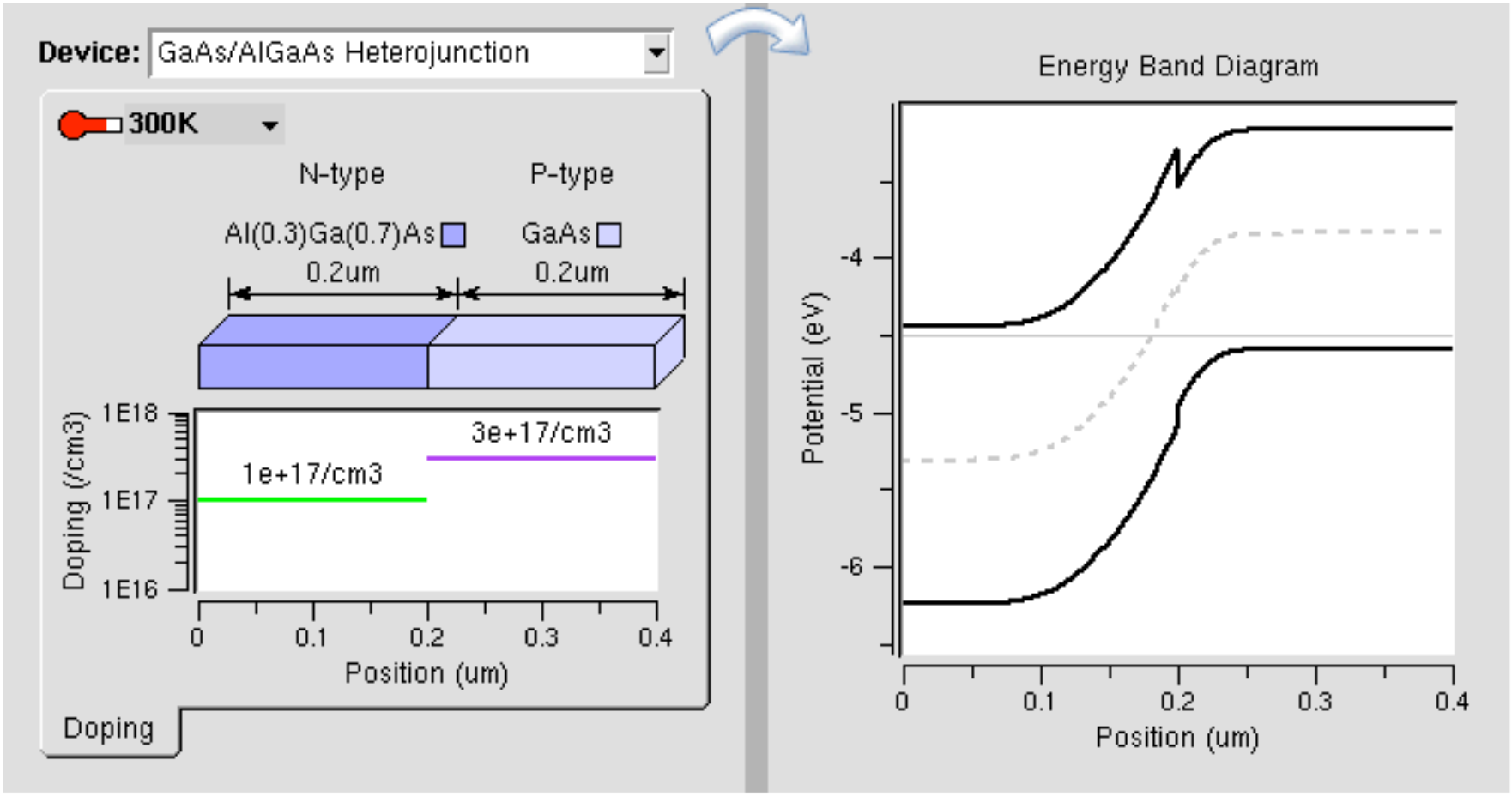
Rapid GUI Deployment!

This Application Integration Required ~1 day of work!!



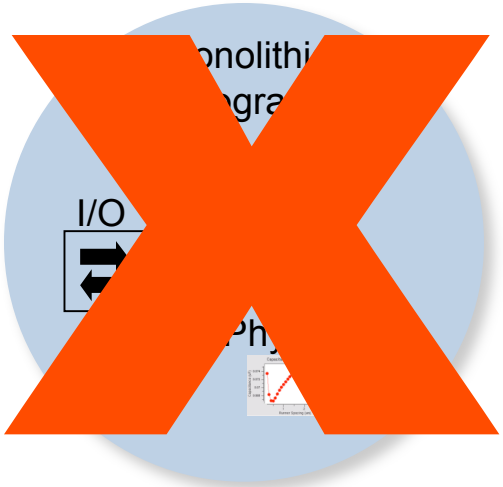
PN - Junctions
ADEPT legacy software

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



A Paradigm Shift Towards Scripting

Traditional Development



Fortran, C/C++

User Issues:
- Not user-friendly
- Not interactive

Development Issues:
- Customized for every application
- Hard to maintain

The rise of scripting

- Computers got faster
- Commercial packages developed
- OpenSource languages developed

Small Script

MATLAB®

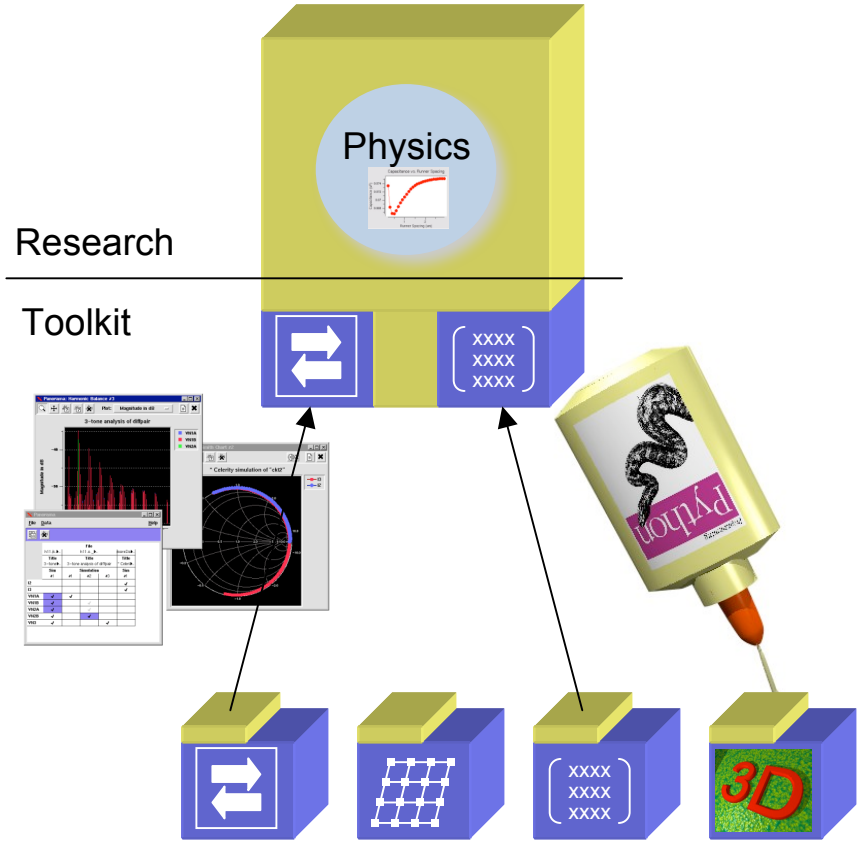
or

python

compiled languages
- low-level
- efficient
- slow development/debugging

interpreted languages
- high-level
- inefficient
- fast development/debugging

Rappture toolkit ➔ Rapid Application Infrastructure toolkit



New tool in short order!

Use toolkit components,
Add unique research

Scripting language interface

Rappture toolkit components

GUI Development Approaches

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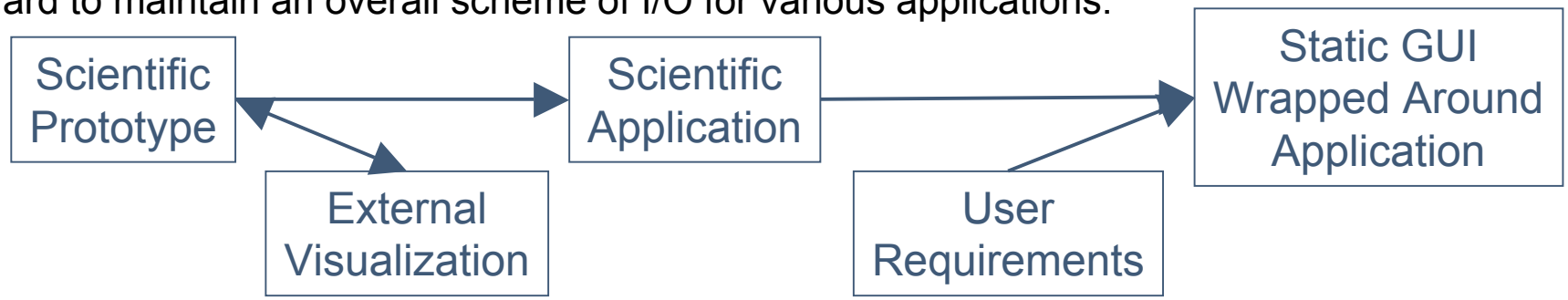
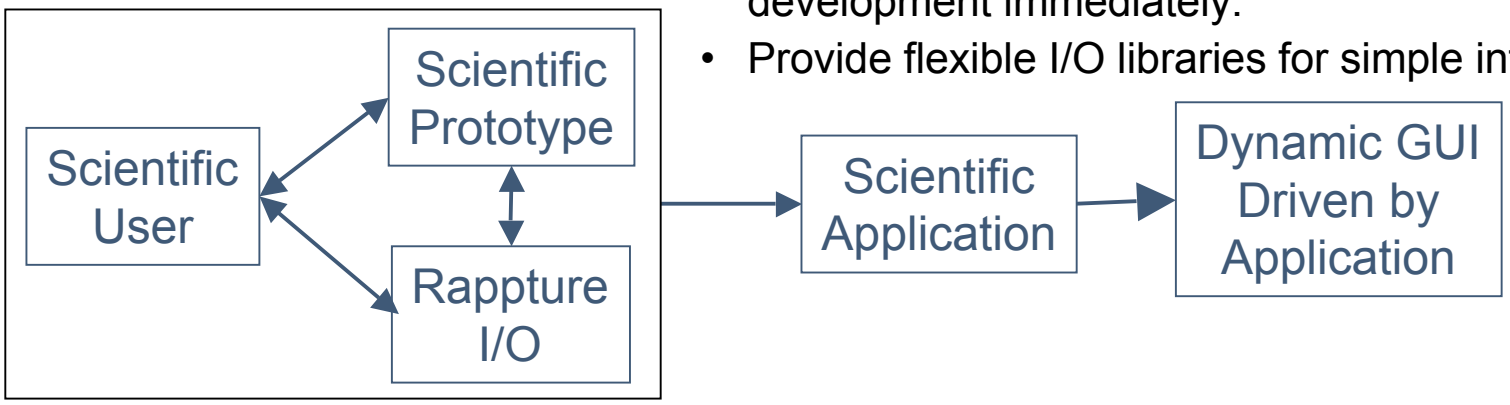


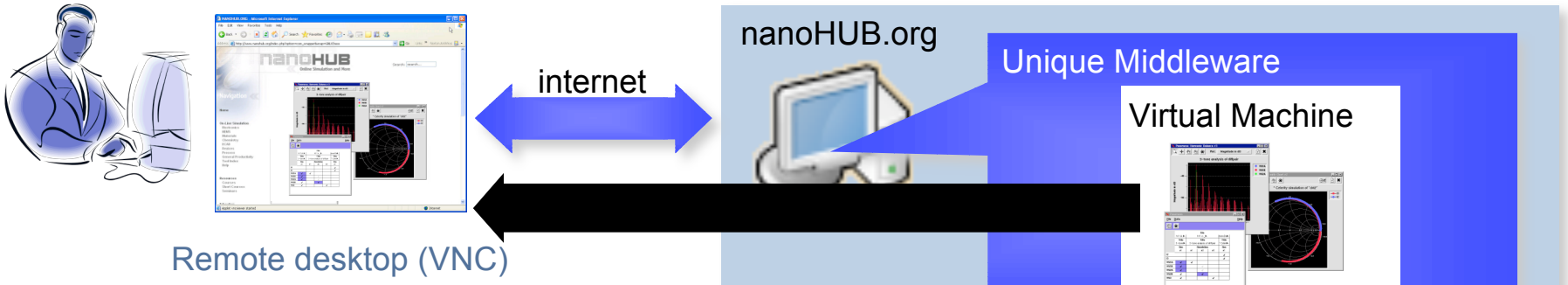
Dynamic Approach:

- Integrate the (student) developer into the GUI development immediately.
- Provide flexible I/O libraries for simple integration



Middleware for Deployment

Remote access to simulators and compute power



This past year:
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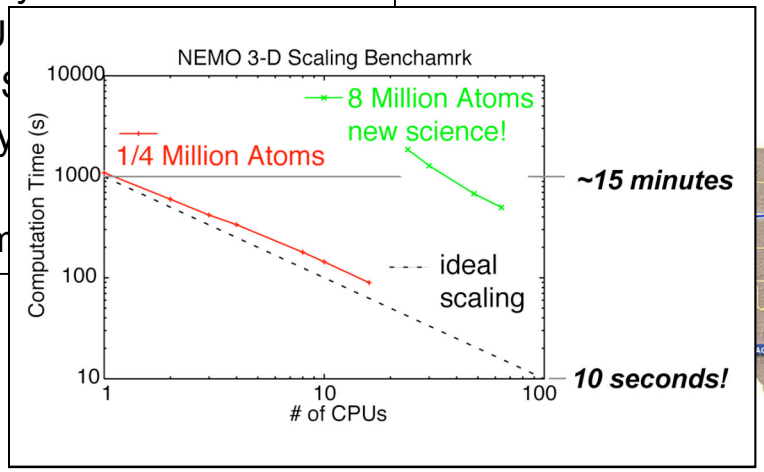


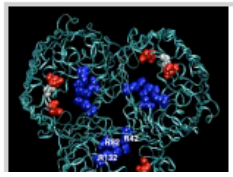
Job Manager

Cluster

nanoHUB.org

online simulations and more

NCN: more than computation

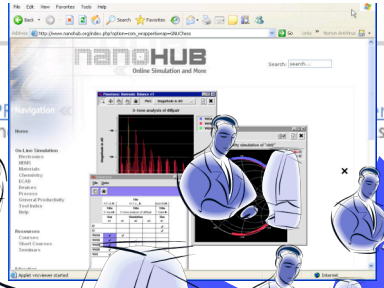


NCN PROPHET Short Course

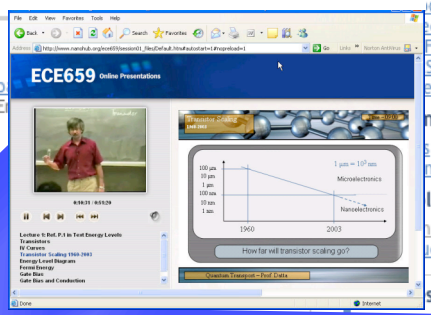
NCN is sponsoring a short course using PR... Champaign. This course will be held Jun... by filling out the online applica...

Read more...

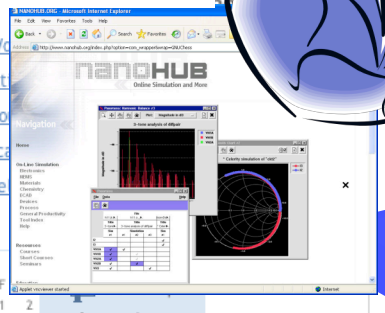
online simulation



courses, tutorials



Your software?



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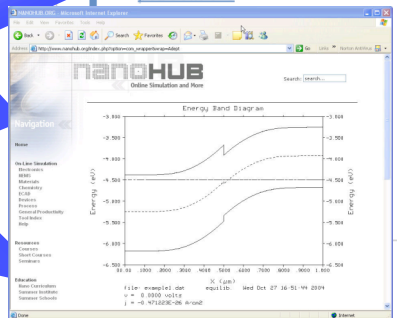
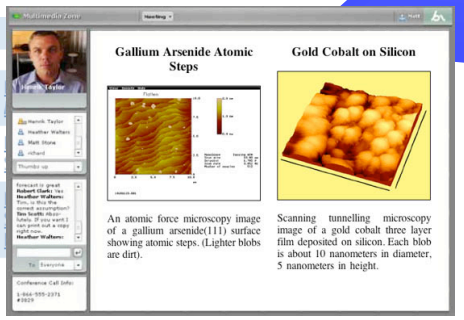
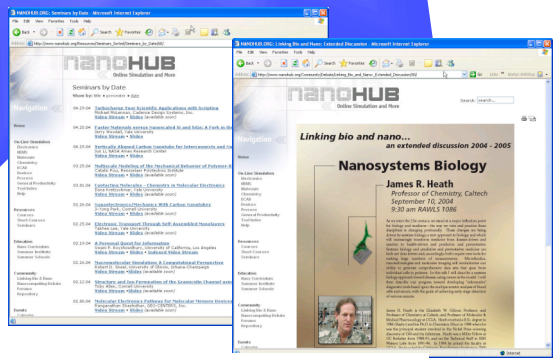


learning modules

collaboration





seminars, themes

Backup

Learning Object: Molecular Transport Simulation

Molecular Transport Simulation

search...

The simulation of electron transport through molecules connects a variety of technical disciplines ranging from Chemistry over Physics to Electrical Engineering. These disciplines have developed over the years several tools to tackle problems in their respective area. The nanoHUB hosts several tools that are working together to enable the simulation of electron transport through molecules. This educational object is intended to train students in the use of these nanoHUB tools.

Learning Object: Molecular Transport Simulation

Molecular Transport Simulation

search...

measuring molecular conductance
Synopsis / Abstract
Lecture 1: Energy Level Diagram
Lecture 2: What Makes Electrons Flow?
Lecture 3: The Quantum of Conductance
Lecture 4: Charging/ Coulomb Blockade
Lecture 5: Summary/ Towards Ohm's Law

simulation
Molecular Conductance Model

homework assignments
Exploring the one-level model
Tow-level model

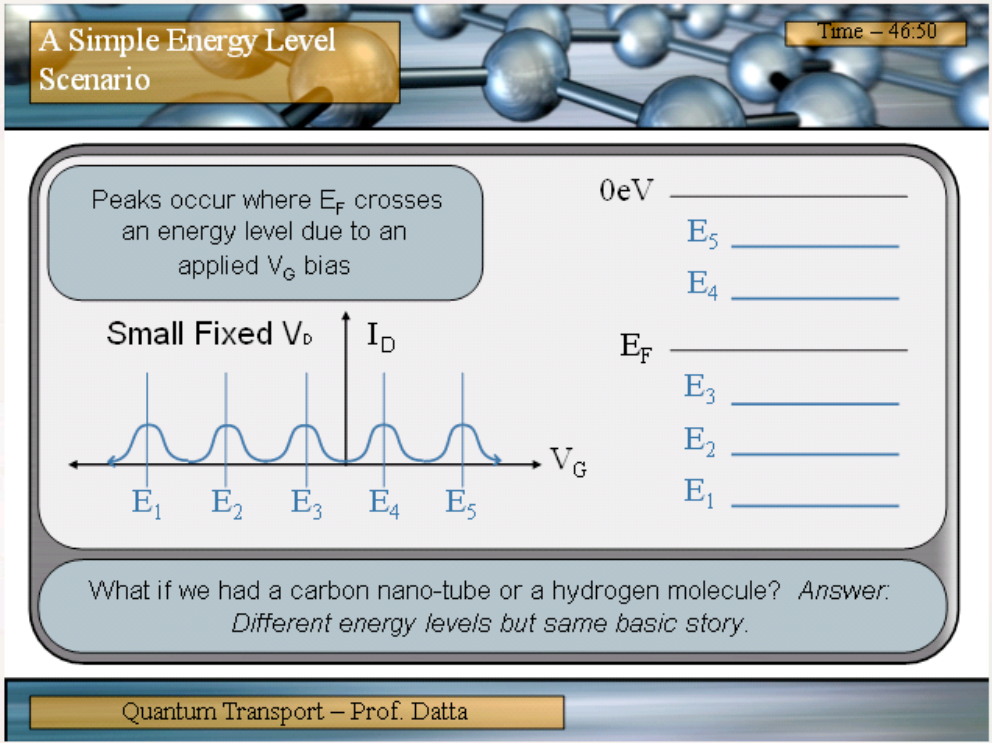
Homework solutions (restricted)

Download learning objects (restricted)

ECE659 Online Presentations

0:47:00 / 0:51:20

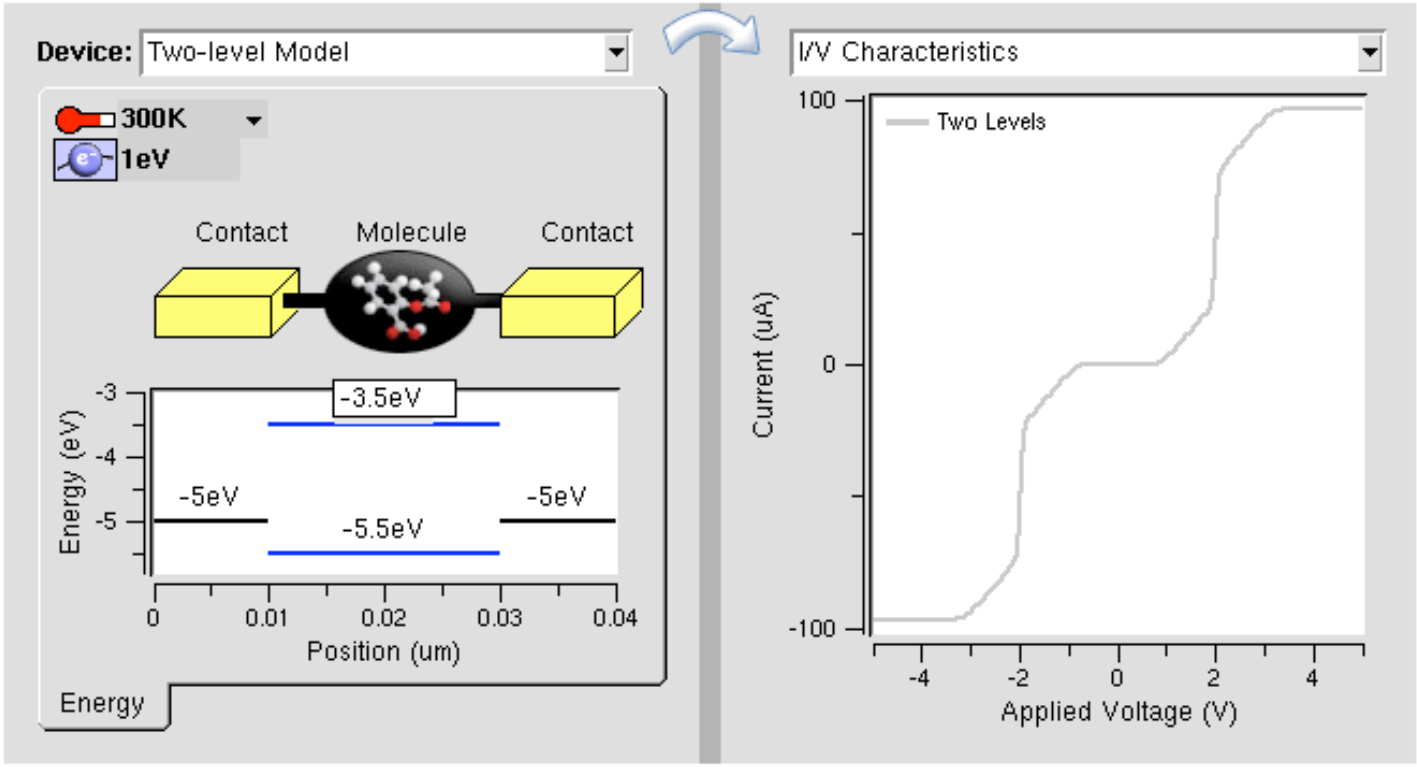
Lecture 1: Ref. P.1 in Text Energy Levels
Transistors
IV Curves
Transistor Scaling 1960-2003
Energy Level Diagram
Fermi Energy
Gate Bias
Gate Bias and Conduction
A Simple Energy Level Scenario



Learning Object: Molecular Transport Simulation

Molecular Transport Simulation

Disconnect | Options | Clipboard | Send Ctrl-Alt-Del | Refresh



Molecular Transport Simulation

Molecular Conduction

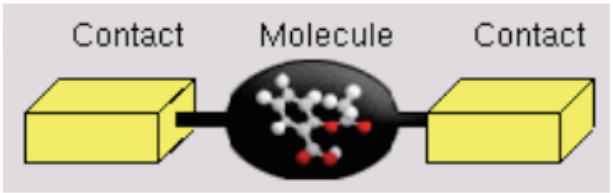
Homework #1: Exploring the 1-level model

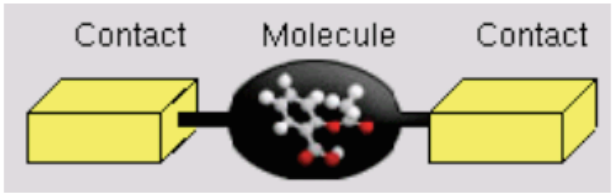
1) Start the molecular conduction simulator, and explore the One-Level model with the following parameters: temperature = 300K, single-electron charging energy = 0.

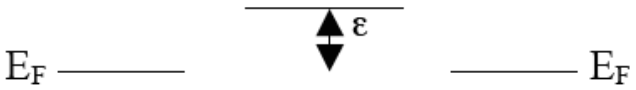
   a) Set the molecule's energy level to -4.5eV. At what voltage does the current abruptly rise? _____

   b) Set the molecule's energy level to -4.0eV. At what voltage does the current abruptly rise? _____

   c) Suppose we have a molecule with a single energy level ε. Draw the energy levels below for the molecule at the point where the conductance peaks.







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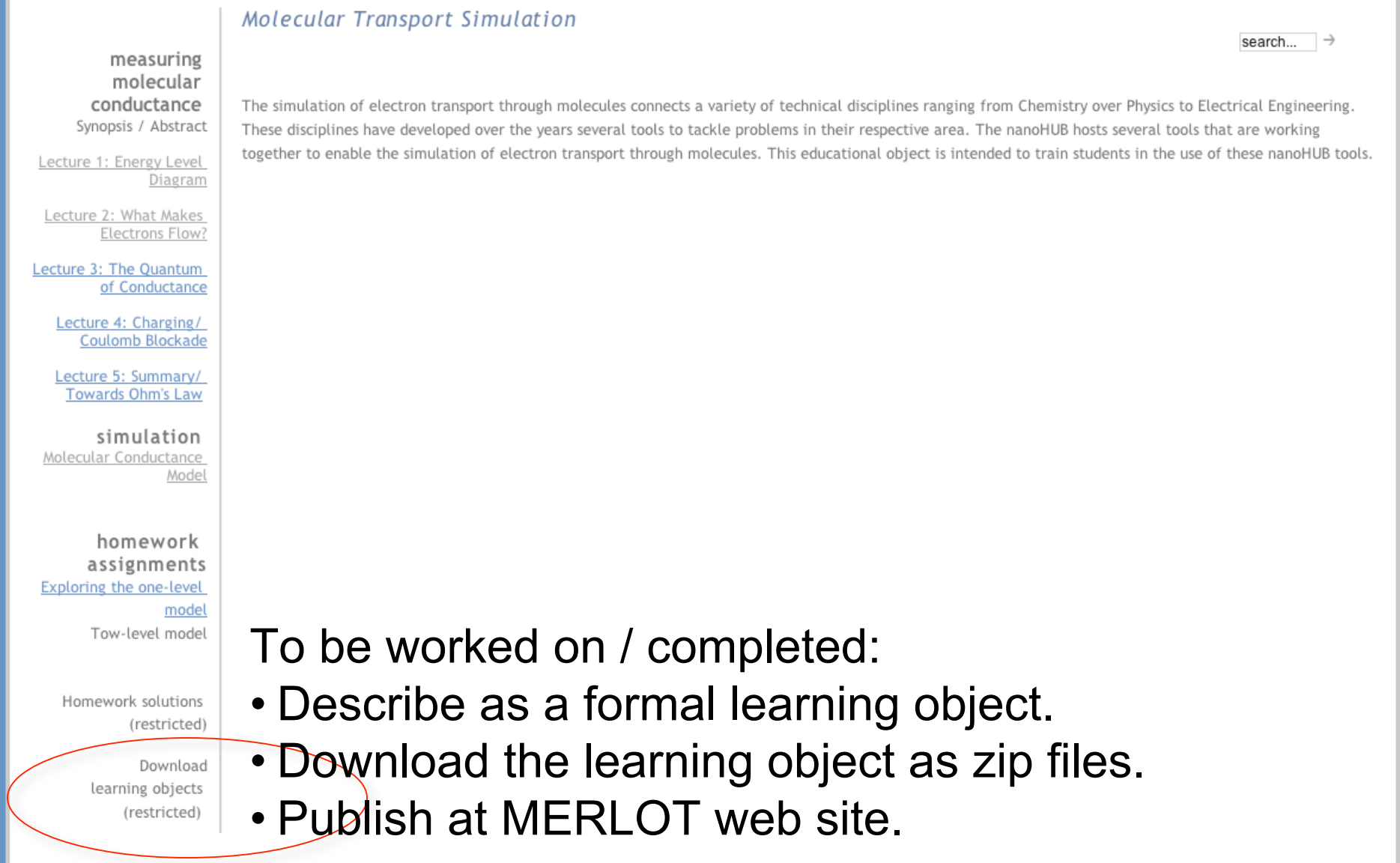

To be worked on / completed:

- Describe as a formal learning object.
- Download the learning object as zip files.
- Publish at MERLOT web site.

Posting nanoHUB learning objects on MERLOT

MERLOT
Multimedia Educational Resource for Learning and Online Teaching

Search Materials: nano GO
advanced search | search more digital libraries | search tips

join now | log in

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MERLOT Search Results: Materials

Your search found 5 materials
Keyword(s): nano
Items 1 - 5 shown.

Default sort order by rating. Resort by: Date Entered Go

Sub-Search: go
Advanced Sub-Search

Title | Author | Date Entered | Rating | Item Type

When Semiconductors Go Nano (Tutorial)
Author: Tony van Buuren
This web site covers the nanoscale properties of semiconductor materials. More specifically, this...
Location: http://www-cms.llnl.gov/s-t/nano-semiconductors.ht...
Added: May 11, 2004
Peer Reviews: (accepted for review)
Member Comments (none)
Assignments (none)
Collections (none)

Exploring the Nanoworld (Reference Material)
Author:
This web site, from the University of Wisconsin - Madison Materials Research Science and Engineering...
Location: http://www.mrsec.wisc.edu/edetc/index.html
Added: May 11, 2004
Peer Reviews: (accepted for review)
Member Comments (none)
Assignments (none)
Collections (none)

NIST Electron Beam Ion Trap (EBIT) Facility (Reference Material)
Peer Reviews: (triaged)
Member Comments (none)

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online simulations and more

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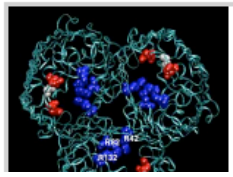

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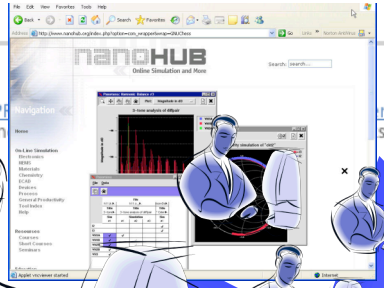

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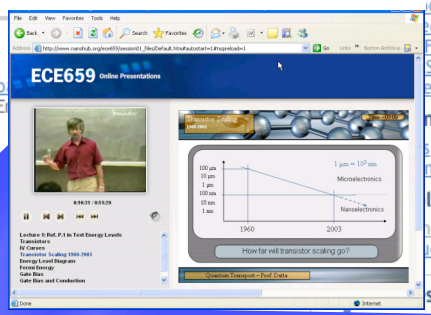

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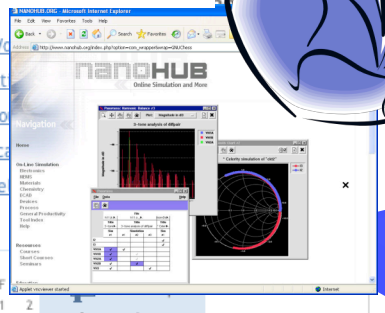

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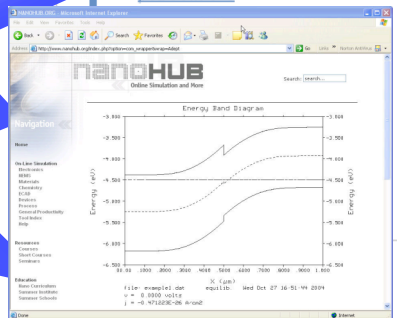

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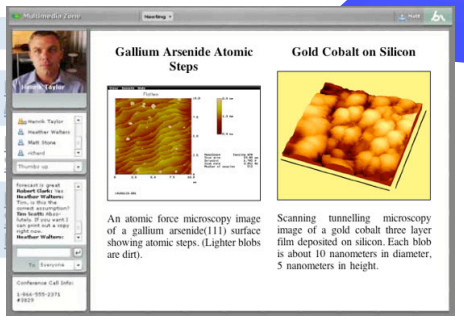

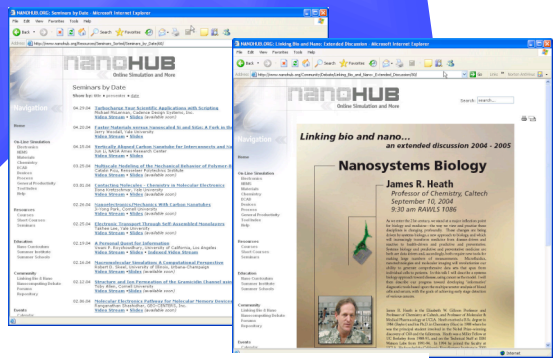

seminars, themes