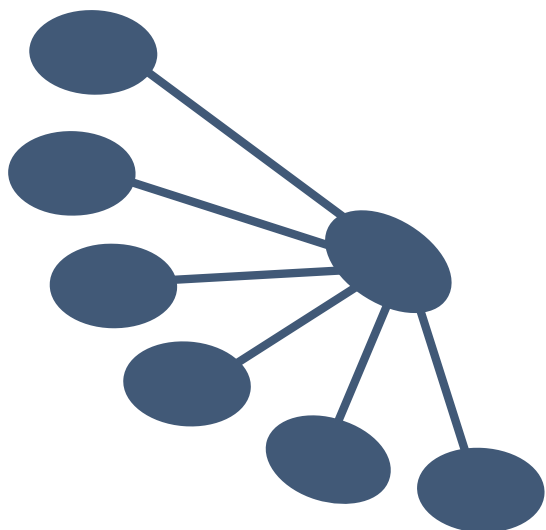




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## *The nanoHUB: A science Gateway for nanotechnology*

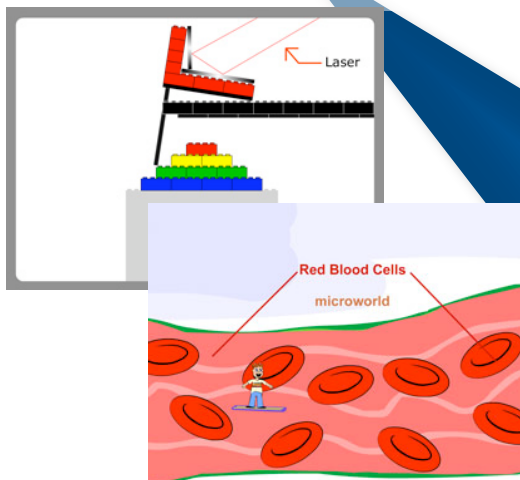
Sebastien Goasguen, Krishna Madhavan, Mike McLennan ,  
Mark S. Lundstrom and Gerhard Klimeck

GGF-14

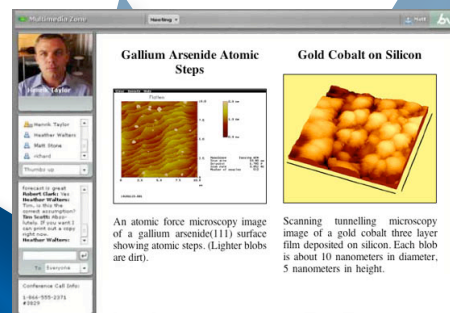
June 28<sup>st</sup> , 2005

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

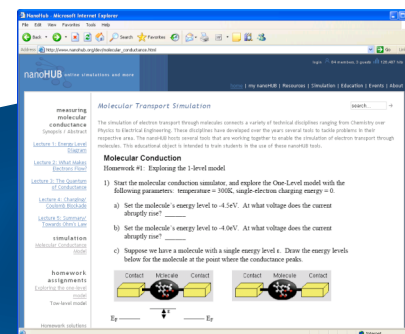
animations



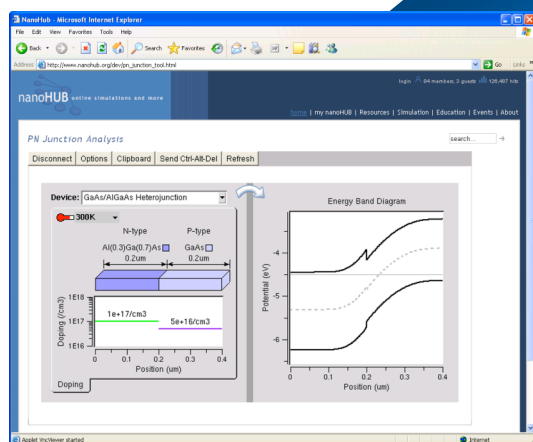
collaboration



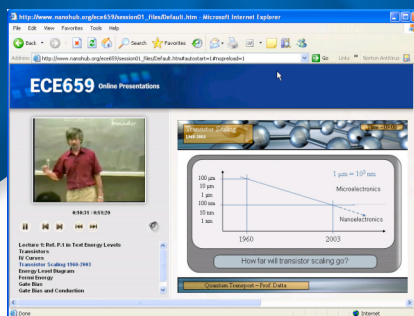
learning modules



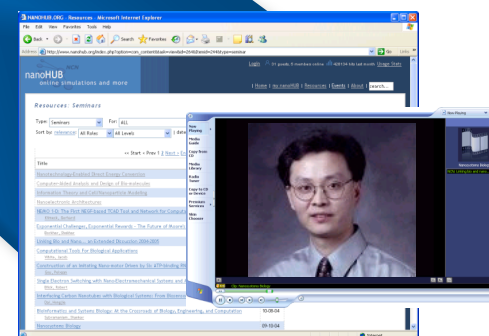
**nanoHUB.org**



online simulations

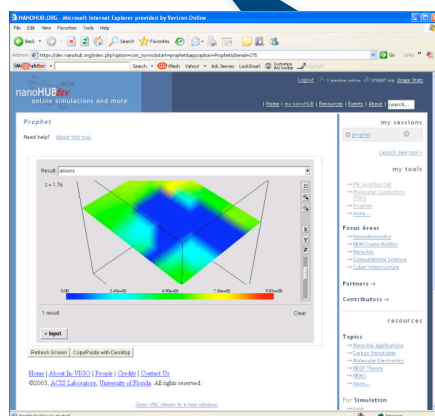


courses, tutorials

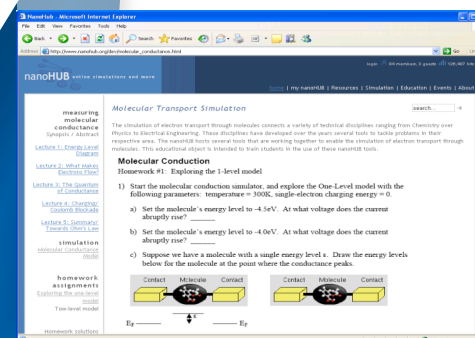


seminars

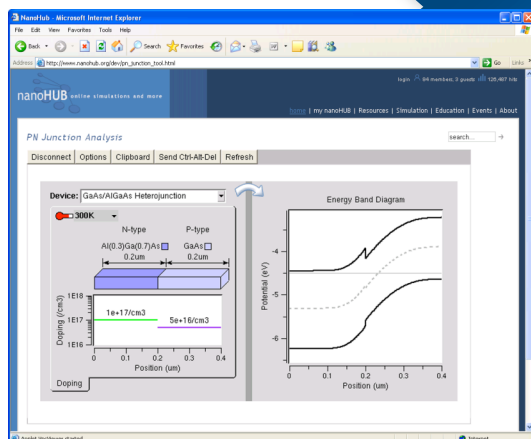
## Applications



## learning modules



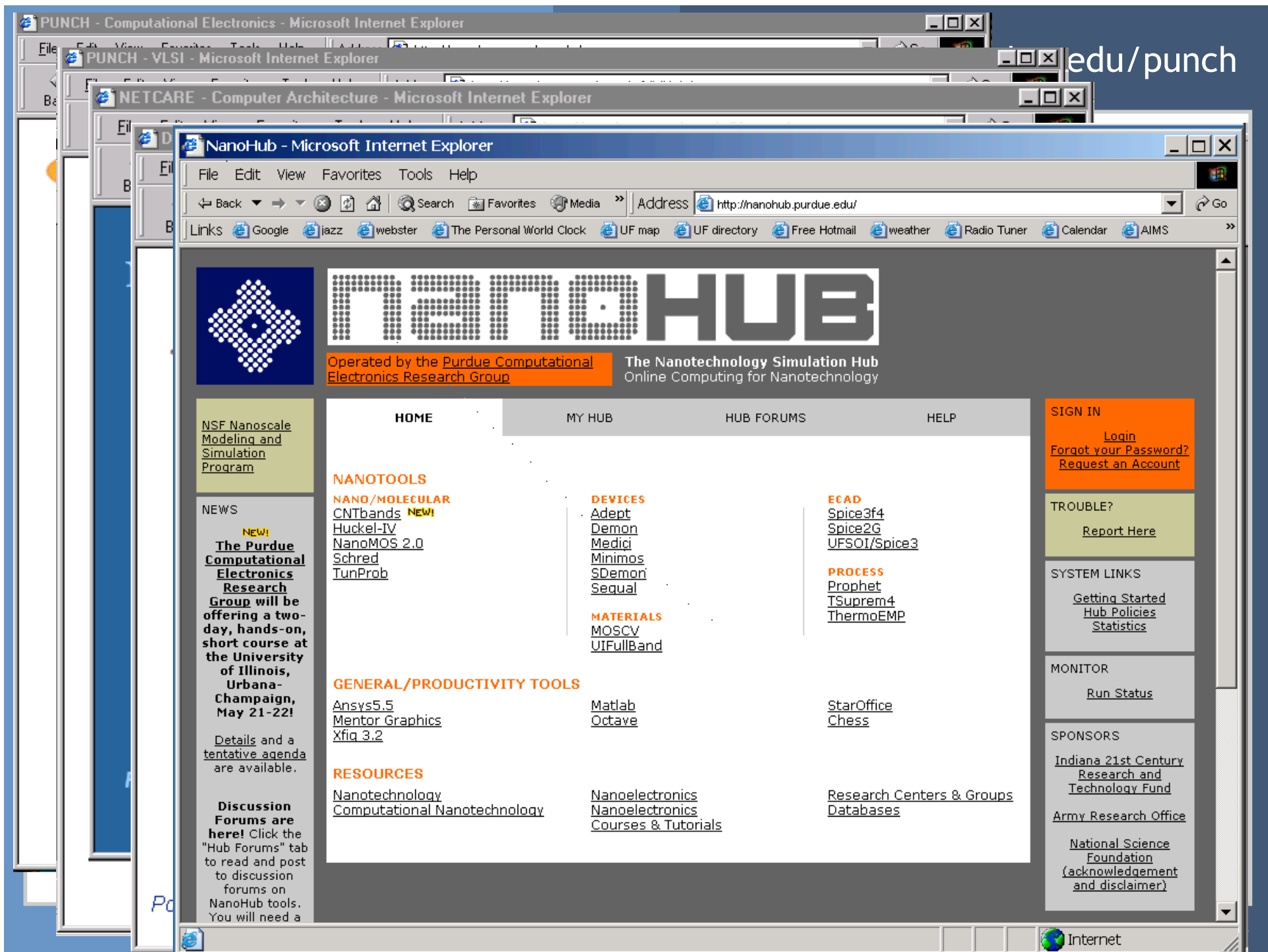
# nanoHUB.org Ecosystem



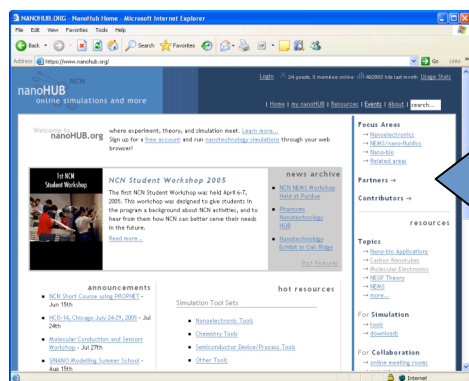
## A middleware



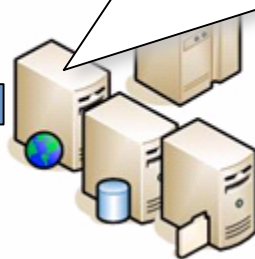
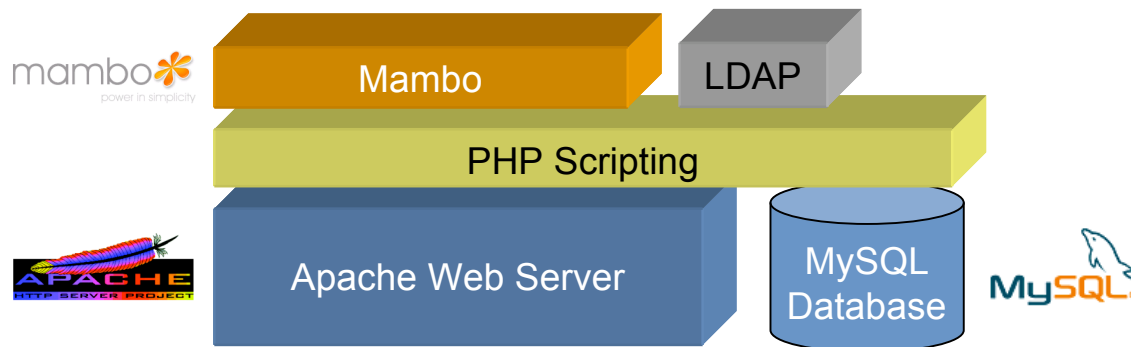
## Resources



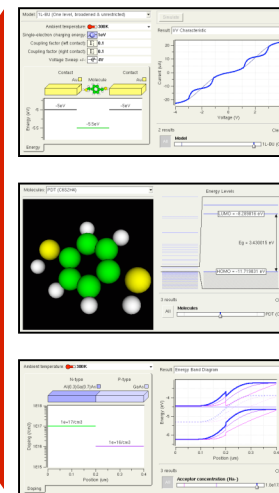




## Web infrastructure



Lots of apps:



How do we serve apps to thousands of users?

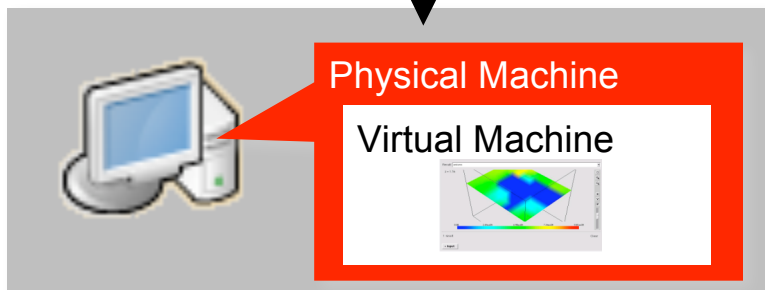
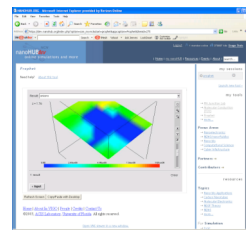


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nanoHUB Architecture

Remote access  
to simulators and  
compute power



PURDUE  
UNIVERSITY

Web Presence



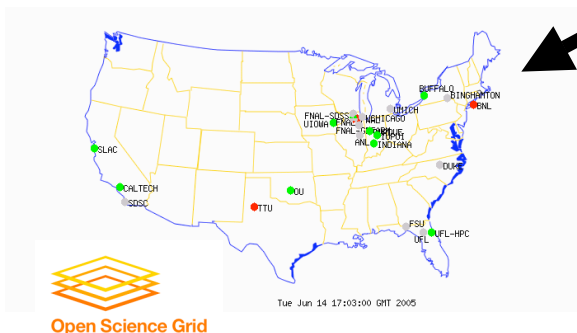
UNIVERSITY OF  
FLORIDA

Appl Middleware



THE UNIVERSITY  
of  
WISCONSIN  
MADISON

Resource Mgmt



Cluster



Network for Computational Nanotechnology





- Fundamental goal of Grid computing:
  - "Flexible, secure, coordinated **resource sharing** among dynamic collections of individuals, institutions, and resources" *[Foster et. al]*
  - **Without** forcing the Grid users to **modify their applications** to make them Grid-aware
- Key challenge to Grid middleware:
  - The provisioning of execution environments that have **flexible, customizable** configurations and allow for **secure** execution of **untrusted** code from Grid users

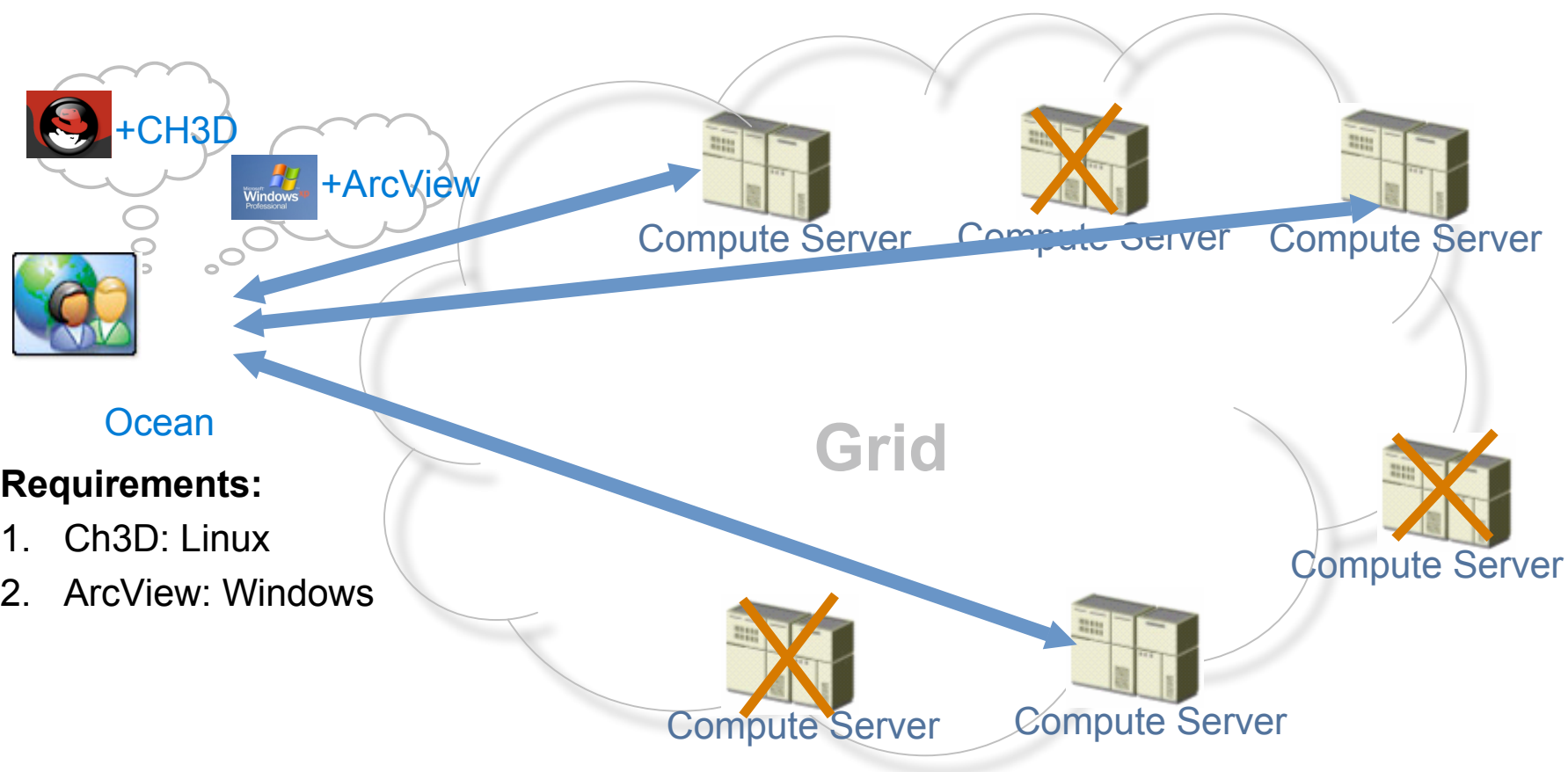
*"The Anatomy of the Grid: Enabling Scalable Virtual Organizations", I. Foster, C. Kesselman, S. Tuecke. International J. Supercomputer Applications, 15(3), 2001*



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## Problems with using physical machines



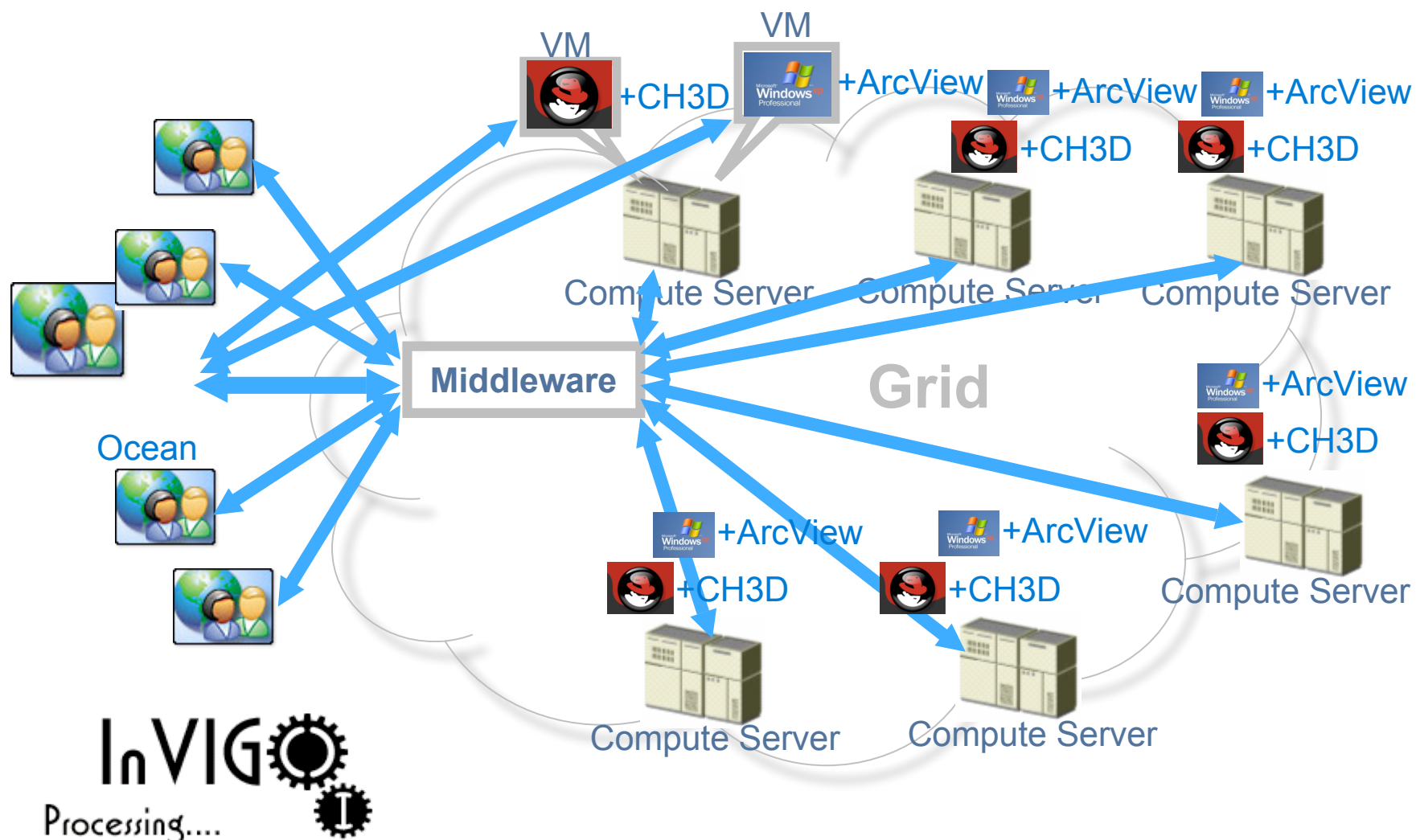
### Requirements:

1. Ch3D: Linux
2. ArcView: Windows



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Our approach: Define once, instantiate on-demand



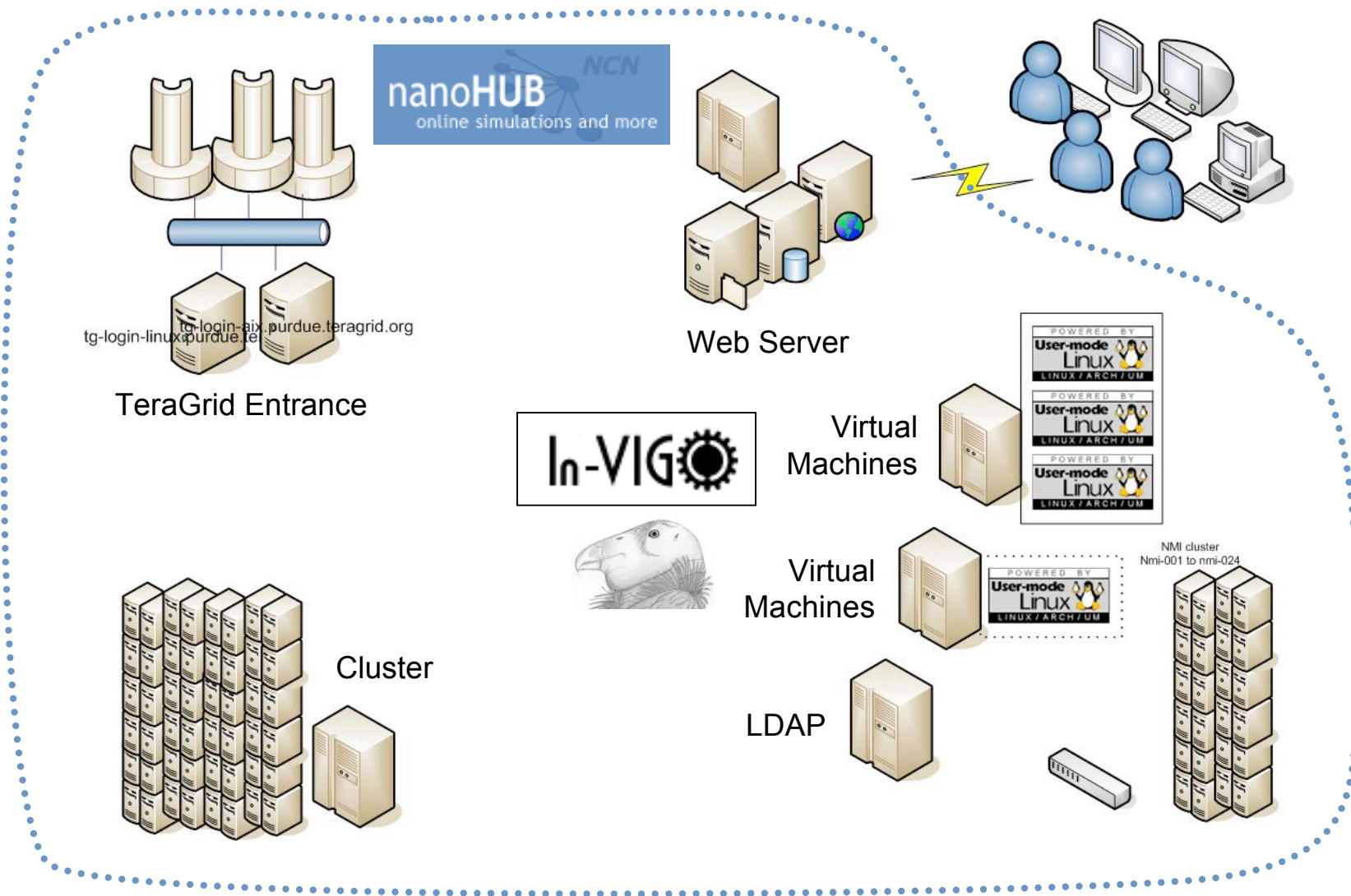
Available at <http://www.acis.ufl.edu/invigo>



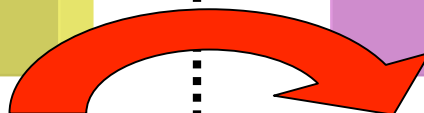
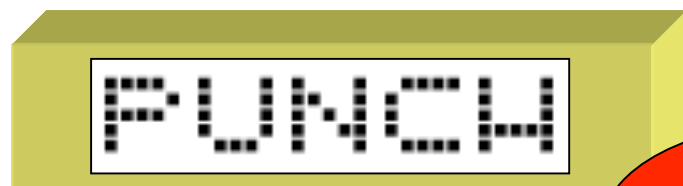
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## Accomplishments







38 apps

- 2DS
- CENEMS
- CNTbands
- FETToy
- MolCToy
- NanoMOS 2.5
- Prophet
- Schred
- SETE
- Spice 2G
- TBGreen
- TunProb
- QNEMS

...

- Abinit
- agere Bipad
- Gamess
- Gromacs
- Huckel-IV
- agere Laser
- Matlab
- Moca
- Molden
- MolCToy
- MSL
- Octave
- agere PADRE
- PN Junctions
- agere Prophet
- Rasmol
- agere SMC
- Spice 2g
- TunProb
- Vtk



= GUI



= Rappture

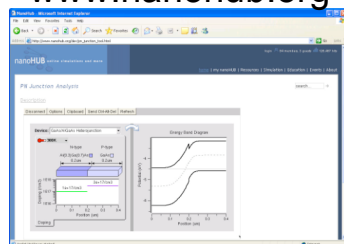


= text interface

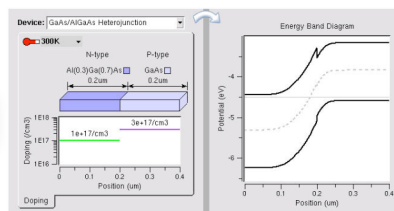


- Scripting languages as a tool development philosophy

www.nanohub.org



In-VIGO

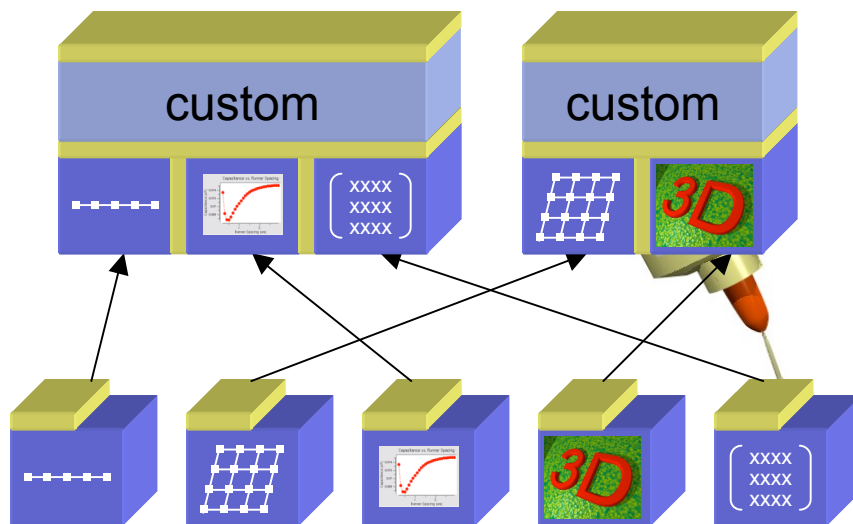


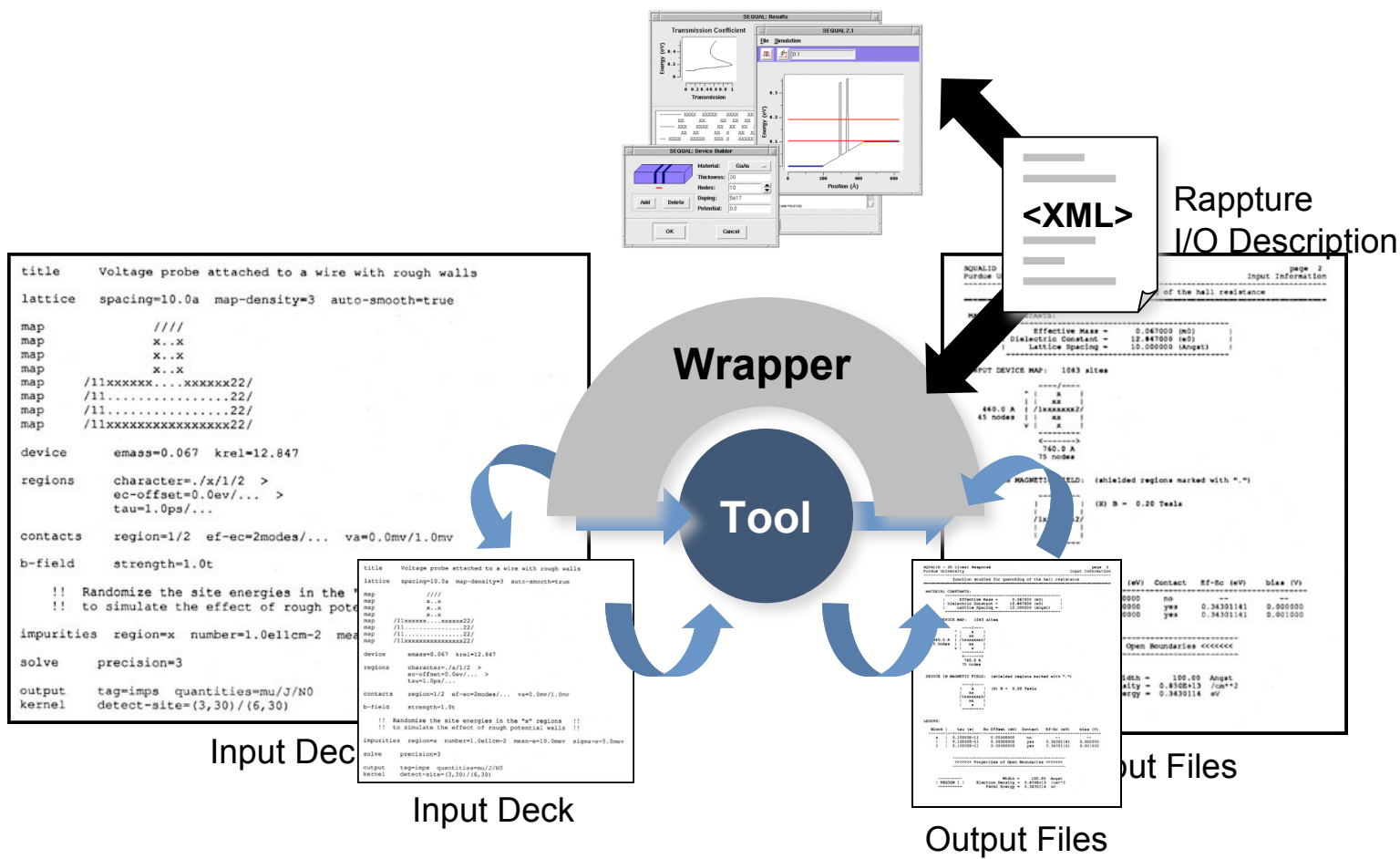
Build interfaces on  
scripting foundation

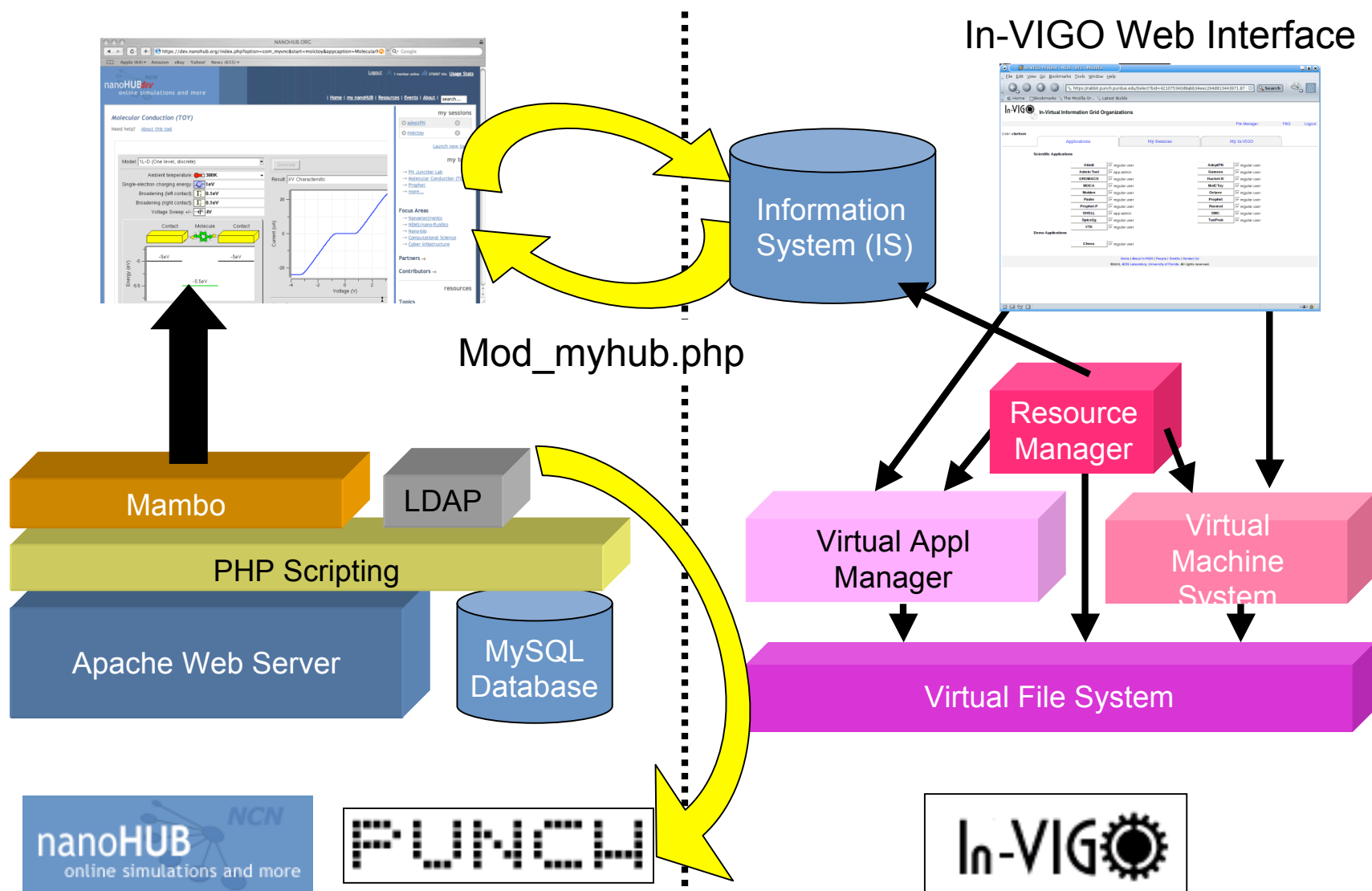
Build tools from  
component parts

Add scripting language  
interface to each component

Components coded  
in C, C++, Fortran









Two virtual machine systems:

*VMware:*

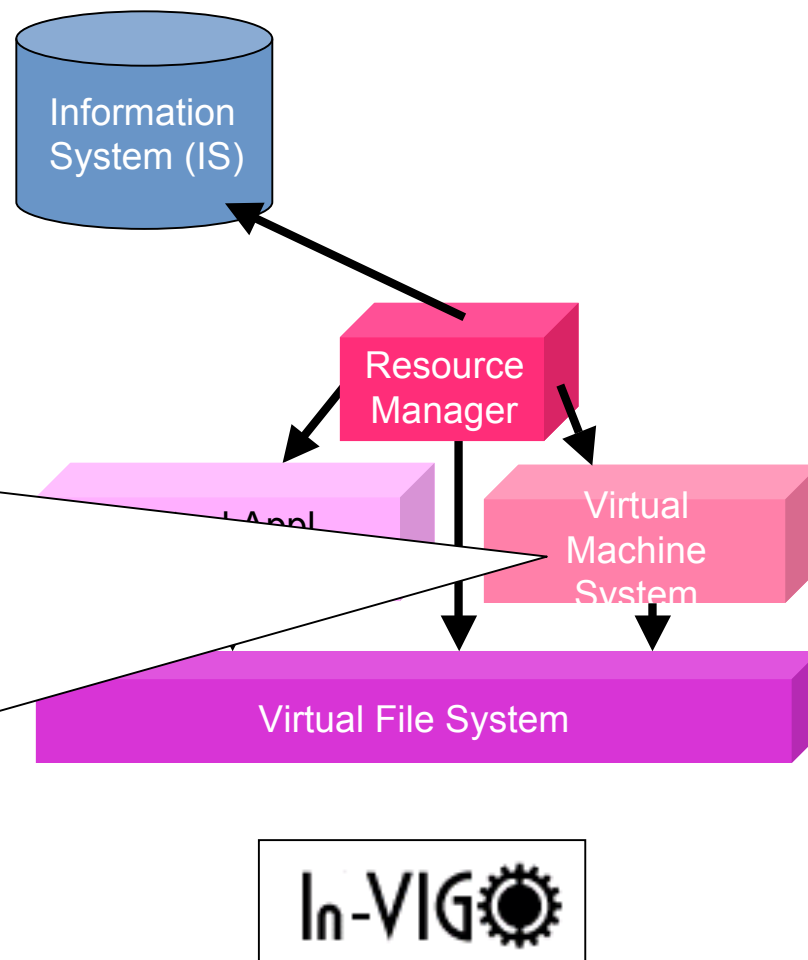
- + Commercial product
- + Mature software
- not open source
- smaller community

*User Mode Linux:*

- + Open Source (hack the code)
- + Large community of developers
- not as mature

*Future with Xen:*

- + Open Source
- + Better performance
- + Collaboration with ANL





*Accomplishments:*

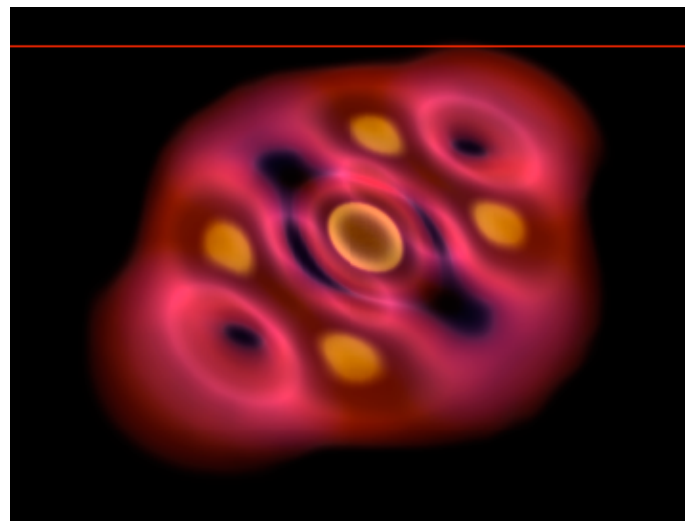
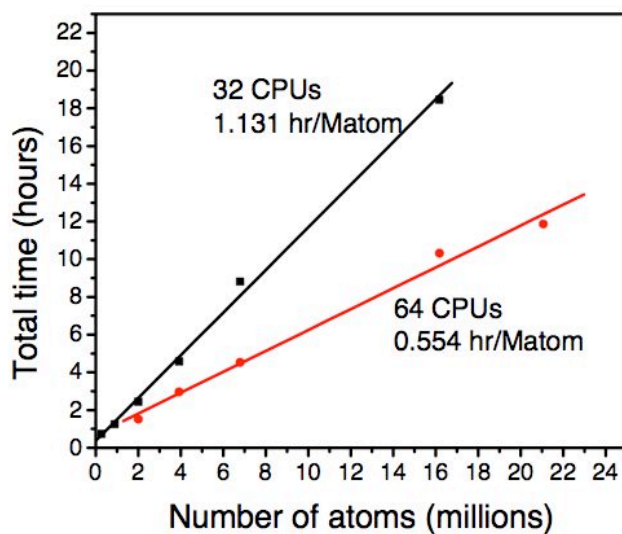
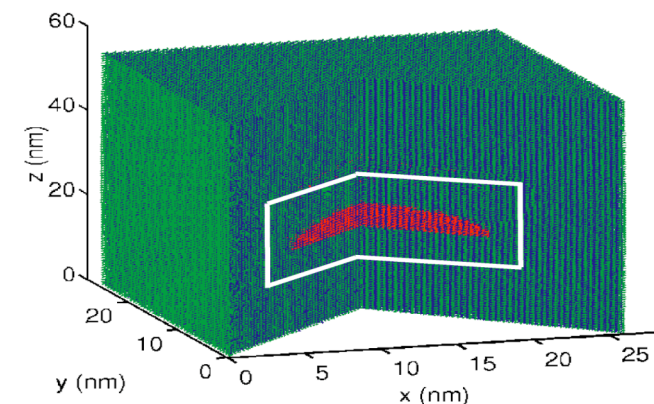
NCN community allocation

NEMO3D ported to TeraGrid

Scaling study

64 Million atoms simulation

~50,000 SUs used on TeraGrid







### *Computational challenge:*

The “window” of observation is on the order of 100 to 1,000 nanoseconds for porin, and from 1,000 to 10,000 nanoseconds for gramicidin.  $\Delta t = 1$  fs

The computational requirement for one data point on the current-voltage curve in porin is estimated between 900 to 6,000 hours of single processor time (Xeon 2.4 GHz, 2GB RAM).

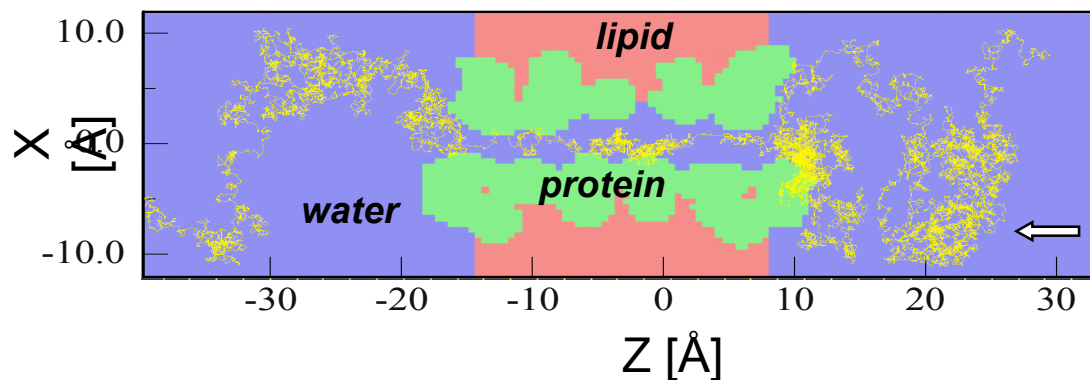
### *Accomplishments:*

NCN student on TeraGrid (Gulzar Kathawala )

MOCA and BioMOCA ported to TeraGrid

~75,000 SUs used on TeraGrid

Permeation trajectory of a “lucky”  $\text{Na}^+$  in a gramicidin A ionic channel  
T. Van der Straaten, G. Kathawala, U. Ravaioli (UIUC)



Expert Introduction by Supriyo Datta

## MolCToy Learning Module

[Abstract](#)

[Opening Remarks on MolCToy](#)

[Introduction to MolCToy](#)

[Special Instructions](#)

[MolCToy Simulation Tool \(New Window\)](#)

[Example 1: Conductance Gap](#)

[Example 2: Charging Energy](#)

[Example 3: Broadening](#)

[Example 4: Asymmetric I-V \(HOMO\)](#)

[Exercise 1: Asymmetric I-V \(LUMO\)](#)

[Solution to Exercise 1](#)

[Exercise 2: Unrestricted Solution](#)

[Solution to Exercise 2](#)

[Exercise 3: Effects of Temperature](#)

[Solution to Exercise 3](#)

[Exercise 4: Tun Level](#)

Opening Remarks on MolCToy

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**Unified Model**

S. Datta, Electrical Resistance:  
An Atomistic View, Nanotechnology,  
15, S 433-451 (2004)

**NANO-ELECTRONICS:  
Unified View**

Devices are described using  
a grid of discrete points.

Grid points can be in real  
space or in an abstract space  
.. They are then called **basis  
functions**.

Size of matrices is  $N \times N$   
where  $N$  is the number of  
basis functions or "grid  
points".

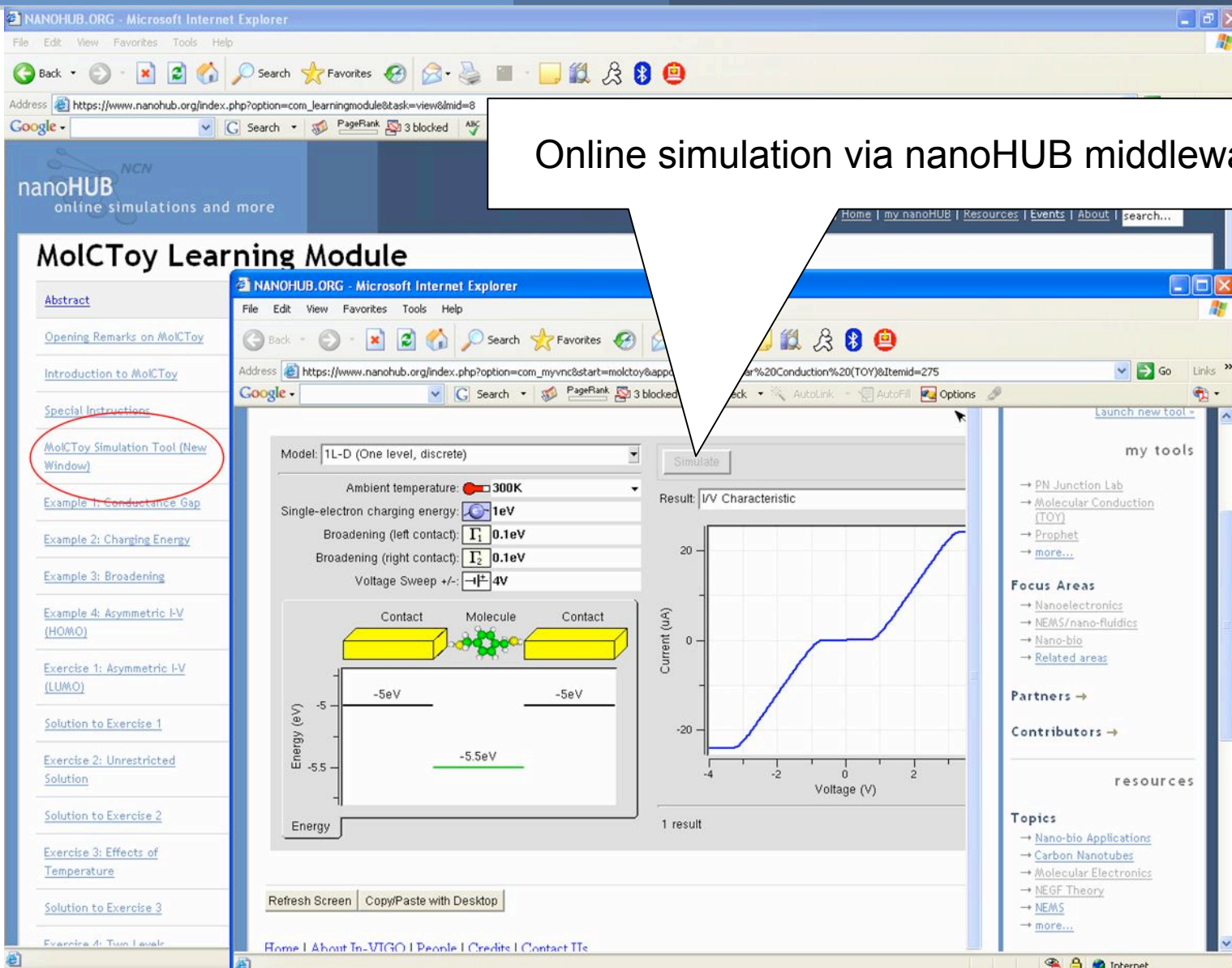
If  $N = 1$ ,  
**Matrices  $\rightarrow$  Numbers**

Opening Remarks on MolCToy

Outline	Thumb	Notes	Search
Slide Title			Duration
MolCToy: Introductory...			01:14
NANO-ELECTRONICS: ...			02:30
What makes electron...			01:02
Escape time			00:49
Toy model: Current			00:60
Current with Broade...			00:41
Broadening + Charging			01:52
MOLCTOY : 1-Level M...			00:29
MOLCTOY : 2-Level M...			00:16
MOLCTOY : Unrestrict...			02:01

8 Minutes 24 Seconds Remaining

Online simulation via nanoHUB middleware



**MolCToy Learning Module**

[Abstract](#)  
[Opening Remarks on MolCToy](#)  
[Introduction to MolCToy](#)  
[Special Instructions](#)  
[MolCToy Simulation Tool \(New Window\)](#)  
[Example 1: Conductance Gap](#)  
[Example 2: Charging Energy](#)  
[Example 3: Broadening](#)  
[Example 4: Asymmetric I-V \(HOMO\)](#)  
[Exercise 1: Asymmetric I-V \(LUMO\)](#)  
[Solution to Exercise 1](#)  
[Exercise 2: Unrestricted Solution](#)  
[Solution to Exercise 2](#)  
[Exercise 3: Effects of Temperature](#)  
[Solution to Exercise 3](#)  
[Exercise 4: Two Levels](#)

**Simulation Parameters:**

- Model: 1L-D (One level, discrete)
- Ambient temperature: 300K
- Single-electron charging energy: 1eV
- Broadening (left contact):  $\Gamma_1$  0.1eV
- Broadening (right contact):  $\Gamma_2$  0.1eV
- Voltage Sweep +/-: 4V

**Molecular Diagram:** A diagram showing a molecule (green spheres) connected to two contacts (yellow rectangles). The energy levels are shown on the left, with a gap of -5.5eV between the HOMO and LUMO levels.

**Results:** I/V Characteristic plot showing Current (uA) vs Voltage (V). The plot shows a non-linear relationship with a plateau around 0V.

**my tools**

- PN Junction Lab
- Molecular Conduction (TOY)
- Prophet
- more...

**Focus Areas**

- Nanoelectronics
- NEMS/nano-fluidics
- Nano-bio
- Related areas

**Partners** →

**Contributors** →

**resources**

**Topics**

- Nano-bio Applications
- Carbon Nanotubes
- Molecular Electronics
- NEGF Theory
- NEMS
- more...

Complete solution explained with voice and PowerPoint

## MolCToy Learning Module

[Abstract](#)

[Opening Remarks on MolCToy](#)

[Introduction to MolCToy](#)

[Special Instructions](#)

[MolCToy Simulation Tool \(New Window\)](#)

[Example 1: Conductance Gap](#)

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[Example 3: Broadening](#)

[Example 4: Asymmetric I-V \(HOMO\)](#)

[Exercise 1: Asymmetric I-V \(LUMO\)](#)

[Solution to Exercise 1](#)

[Exercise 2: Unrestricted Solution](#)

[Solution to Exercise 2](#)

[Exercise 3: Effects of Temperature](#)

[Solution to Exercise 3](#)

[Exercise 4: Two Levels](#)

### Solution to Exercise 1

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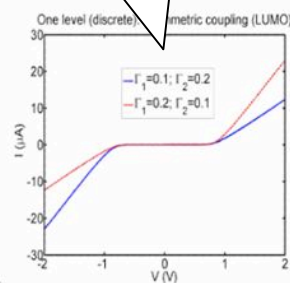
#### Solution of Exercise 1: Asymmetric I-V (LUMO)

**Question 1:**  
What differences do you notice compared to HOMO conduction (example 4)?

**Answer:**  
The direction of asymmetry in the I-V has been reversed.

**Question 2:**  
Explain the reasons for these differences.

**Answer:**  
In the case of LUMO conduction the level is empty at the beginning. Under applied bias the level gets filled up rather than emptied out and this in turn moves level upwards instead of downwards as in the case of HOMO conduction.



#### MolCToy: Solution to Exercise

Outline	Thumb	Notes	Search
Slide Title			Duration
Solution of Exercise 1...			01:24
Solution of Exercise 1...			00:30

0 Minutes 40 Seconds Remaining



NANOHUB.ORG - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Address [https://www.nanohub.org/index.php?option=com\\_learningmodule&task=view&mid=88&resid=23](https://www.nanohub.org/index.php?option=com_learningmodule&task=view&mid=88&resid=23)

Google Search PageRank 3 blocked Check AutoLink AutoFill Options

Introduction to MolCToy

Special Instructions

MolCToy Simulation Tool (New Window)

Example 1: Conductance Gap

Example 2: Charging Energy

Example 3: Broadening

Example 4: Asymmetric I-V (HOMO)

Exercise 1: Asymmetric I-V (LUMO)

Solution to Exercise 1

Exercise 2: Unrestricted Solution

Solution to Exercise 2

Exercise 3: Effects of Temperature

Solution to Exercise 3

Exercise 4: Two Levels

Solution to Exercise 4

Quiz (includes feedback upon completion)

Conductance gap mainly depends on what factor?

- ☐ A) Charging energy
- ☐ B) Broadening
- ☒ C) Distance between Fermi energy and the nearest molecular level
- ☐ D) Temperature

Correct - Click anywhere to continue

Submit Clear

0 Minutes 0 Seconds Remaining

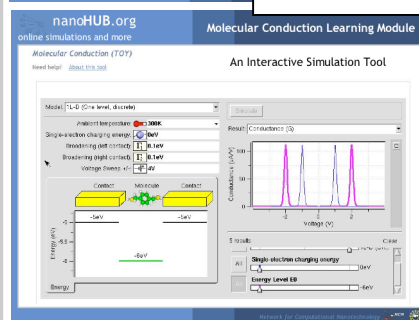
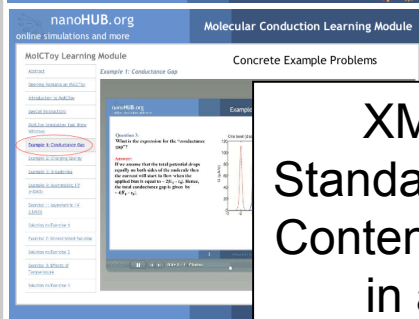
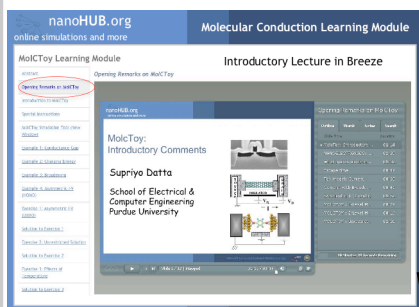
Answer Question 00:00 / 00:00

Usage Statistics | Contact | Report Problems |

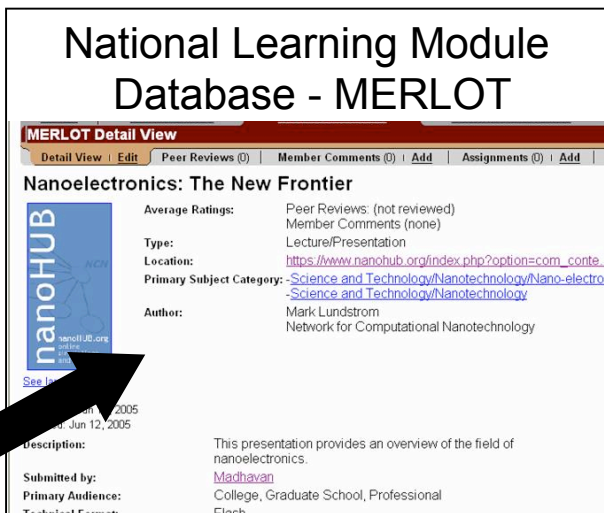
an initiative led by the Network for Computational Nanotechnology and supported by the National Science Foundation, Indiana 21st Century Fund, and ARO

Internet

Quiz that includes feedback

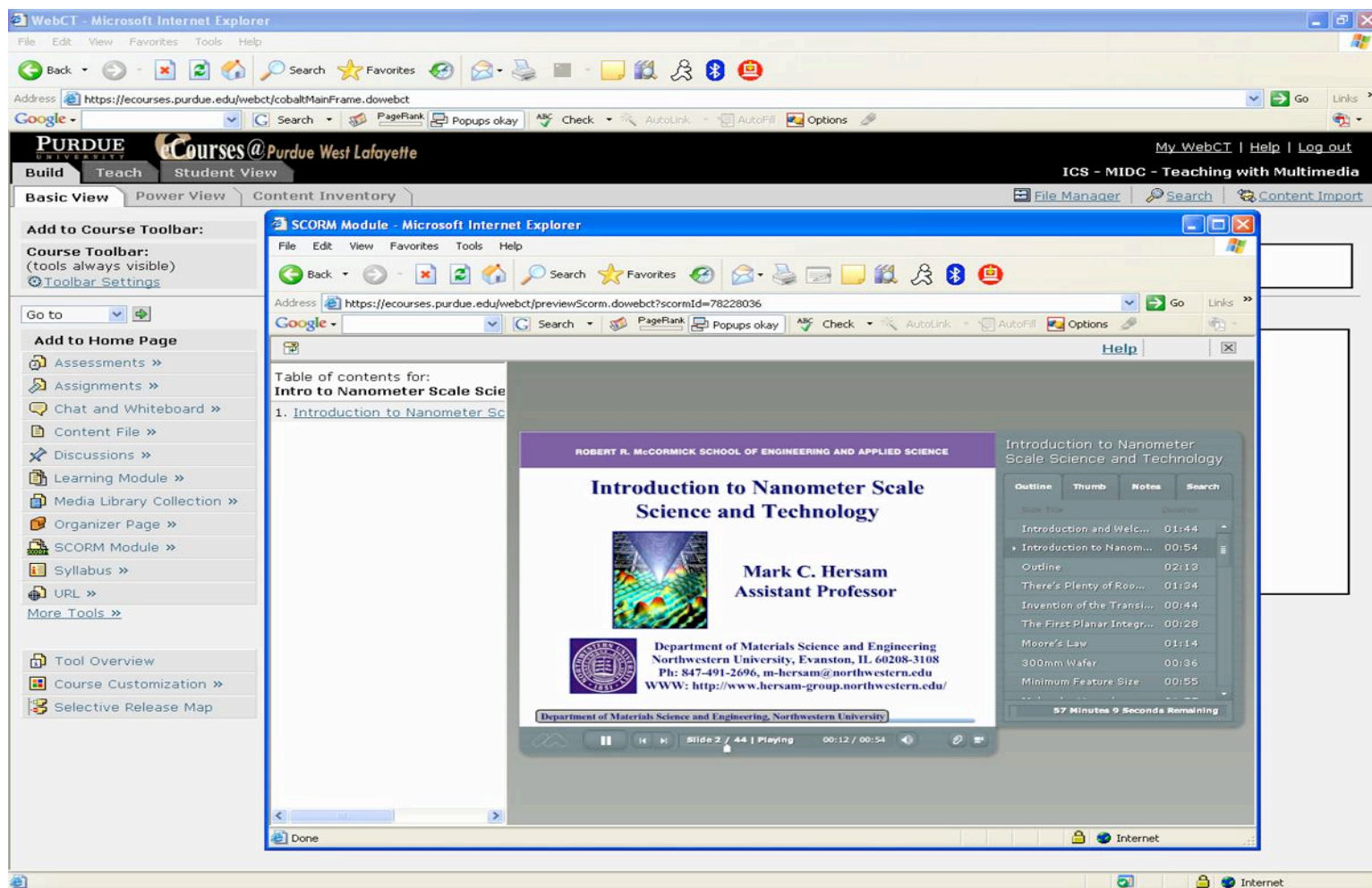


XML-based  
Standard Compliant  
Content Description  
in a ZIP file



Thousands Of Users  
At Most Universities





The screenshot shows a Microsoft Internet Explorer window displaying a Purdue University SCORM module. The browser's address bar shows the URL: <https://ecourses.purdue.edu/webct/cobaltMainFrame.dowebct>. The page features a navigation sidebar on the left with options like 'Add to Course Toolbar', 'Add to Home Page', and 'Tool Overview'. The main content area displays a presentation slide titled 'Introduction to Nanometer Scale Science and Technology' by Mark C. Hersam, Assistant Professor at Northwestern University. A table of contents is visible on the right side of the slide, listing various topics and their durations.

Outline	Thumb	Notes	Search
Introduction and Wel...			01:44
Introduction to Nanom...			00:54
Outline			02:13
There's Plenty of Roo...			01:34
Invention of the Transi...			00:44
The First Planar Integr...			00:28
Moore's Law			01:14
300nm Wafer			00:36
Minimum Feature Size			00:55

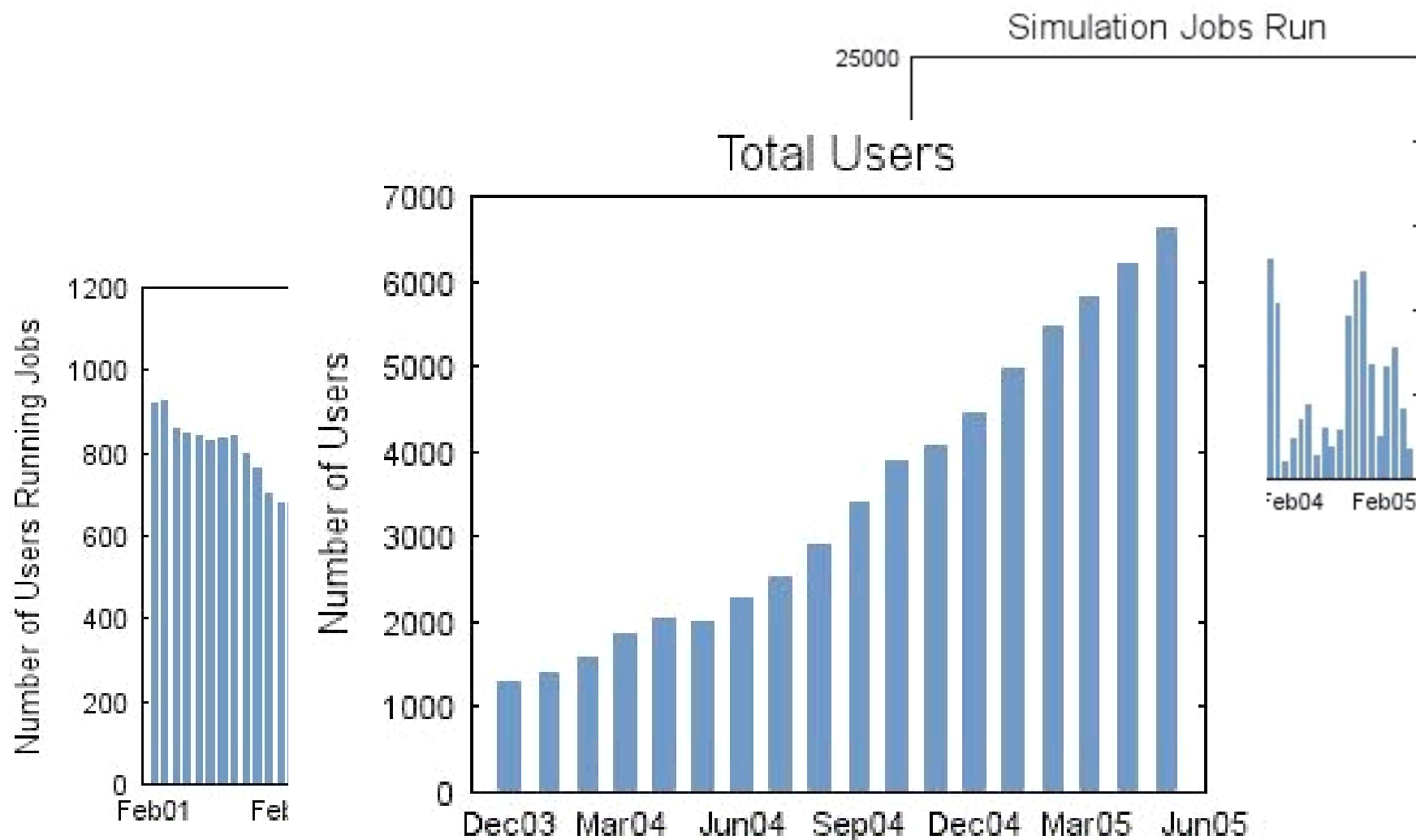
57 Minutes 9 Seconds Remaining



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Users ?





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much, much  
online simulations and more