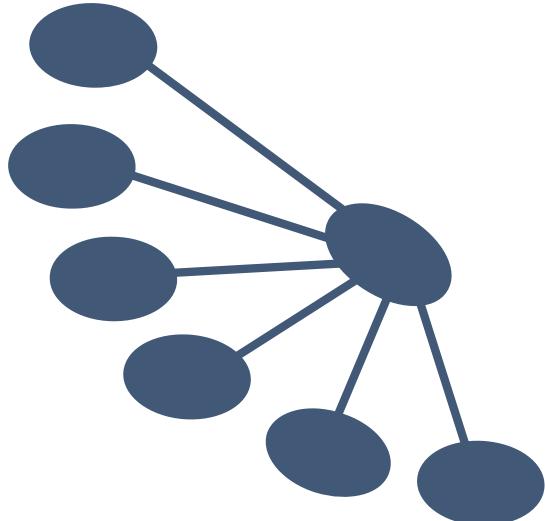




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online simulations and more



The nanoHUB: A science Gateway for nanotechnology

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

GGF-14
June 28st , 2005

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

Network for Computational Nanotechnology

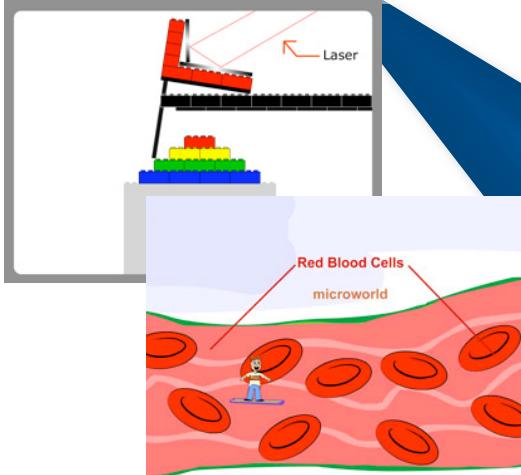




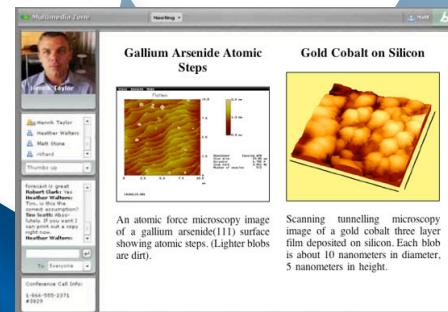
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Online simulations and MORE

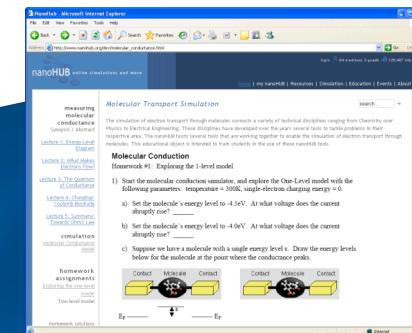
animations



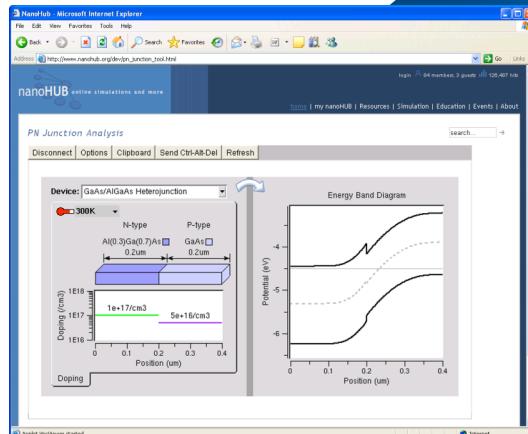
collaboration



learning modules

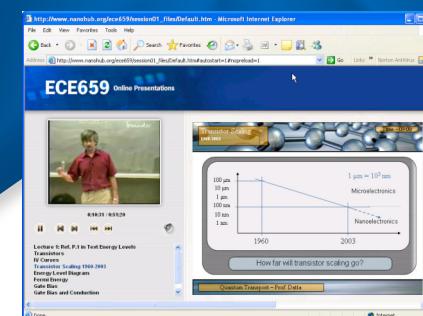


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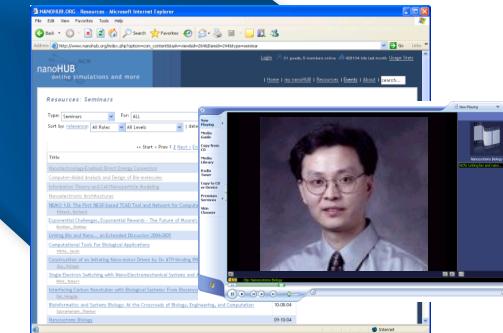


online simulations

courses, tutorials



seminars



Network for Computational Nanotechnology



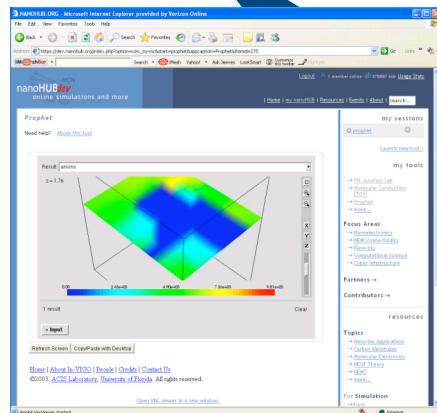


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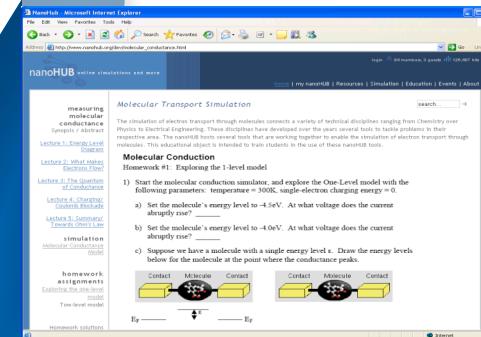
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An Ecosystem

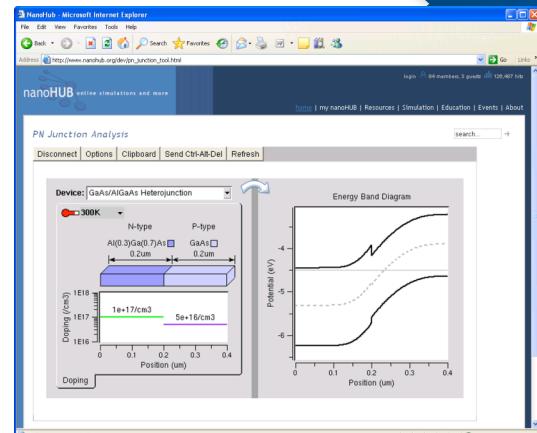
Applications



learning modules



nanoHUB.org Ecosystem



A middleware



TERAGRID

Resources

Network for Computational Nanotechnology



edu/punch

PUNCH - Computational Electronics - Microsoft Internet Explorer

PUNCH - VLSI - Microsoft Internet Explorer

NETCARE - Computer Architecture - Microsoft Internet Explorer

NanoHub - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Back Forward Stop Refresh Home Search Favorites Media Address http://nanohub.purdue.edu/ Go

Links Google jazz webster The Personal World Clock UF map UF directory Free Hotmail weather Radio Tuner Calendar AIMS

 **NanoHub**
Operated by the Purdue Computational Electronics Research Group

The Nanotechnology Simulation Hub
Online Computing for Nanotechnology

HOME MY HUB HUB FORUMS HELP SIGN IN

[NSF Nanoscale Modeling and Simulation Program](#)

NANOTOOLS

NANO/MOLECULAR
[CNTbands](#) NEW!
[Huckel-IV](#)
[NanoMOS 2.0](#)
[Schred](#)
[TunProb](#)

DEVICES
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[Demon](#)
[Medici](#)
[Minimos](#)
[SDemon](#)
[Sequal](#)

ECAD
[Spice3f4](#)
[Spice2G](#)
[UFSOI/Spice3](#)

PROCESS
[Prophet](#)
[TSuprem4](#)
[ThermoEMP](#)

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[UIFullBand](#)

GENERAL/PRODUCTIVITY TOOLS

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[Mentor Graphics](#)
[Xfig 3.2](#)

[Matlab](#)
[Octave](#)

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[Chess](#)

RESOURCES

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[Computational Nanotechnology](#)

[Nanoelectronics](#)
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TROUBLE?
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SYSTEM LINKS
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[Hub Policies](#)
[Statistics](#)

MONITOR
[Run Status](#)

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[Army Research Office](#)
[National Science Foundation \(acknowledgement and disclaimer\)](#)

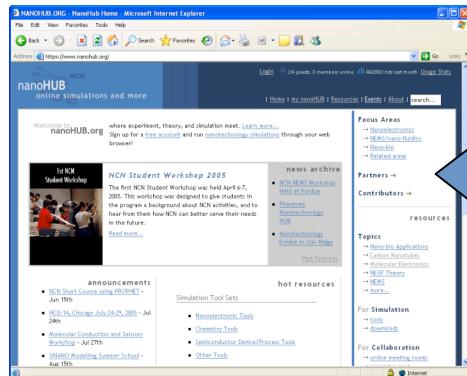
Internet



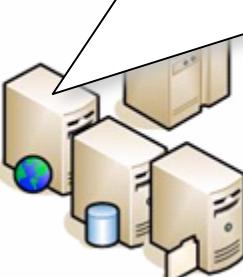
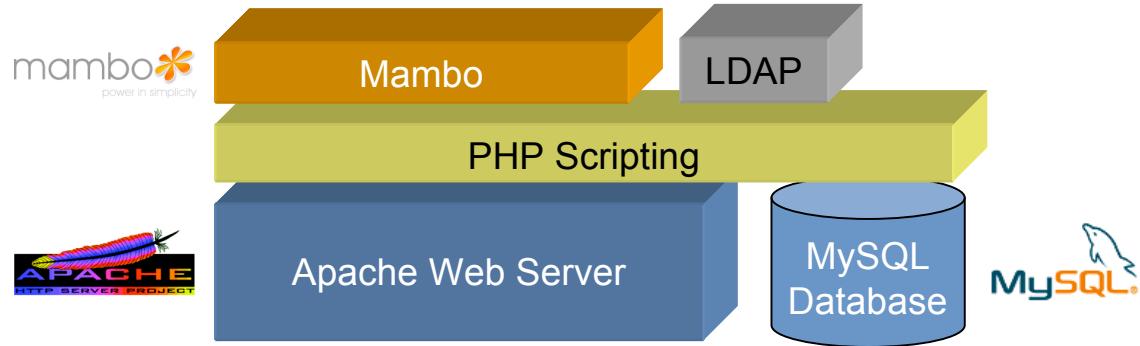
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Why Middleware?

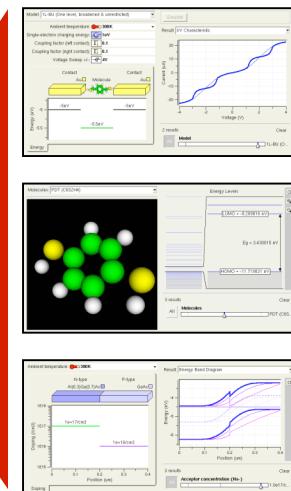


Web infrastructure



How do we serve apps to thousands of users?

Lots of apps:

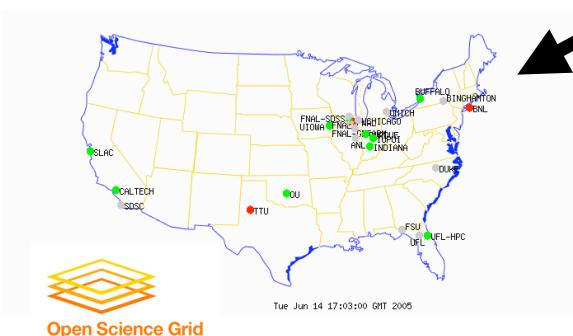
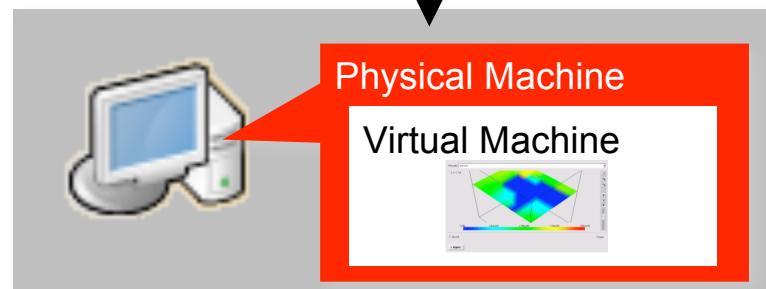
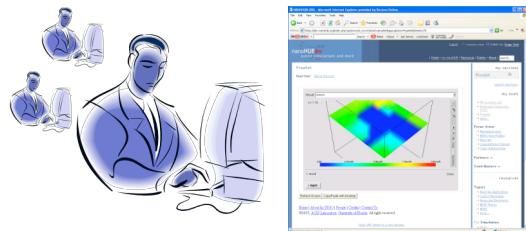




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Remote access
to simulators and
compute power



Cluster



nanoHUB Architecture



 UNIVERSITY OF
FLORIDA
Appl Middleware



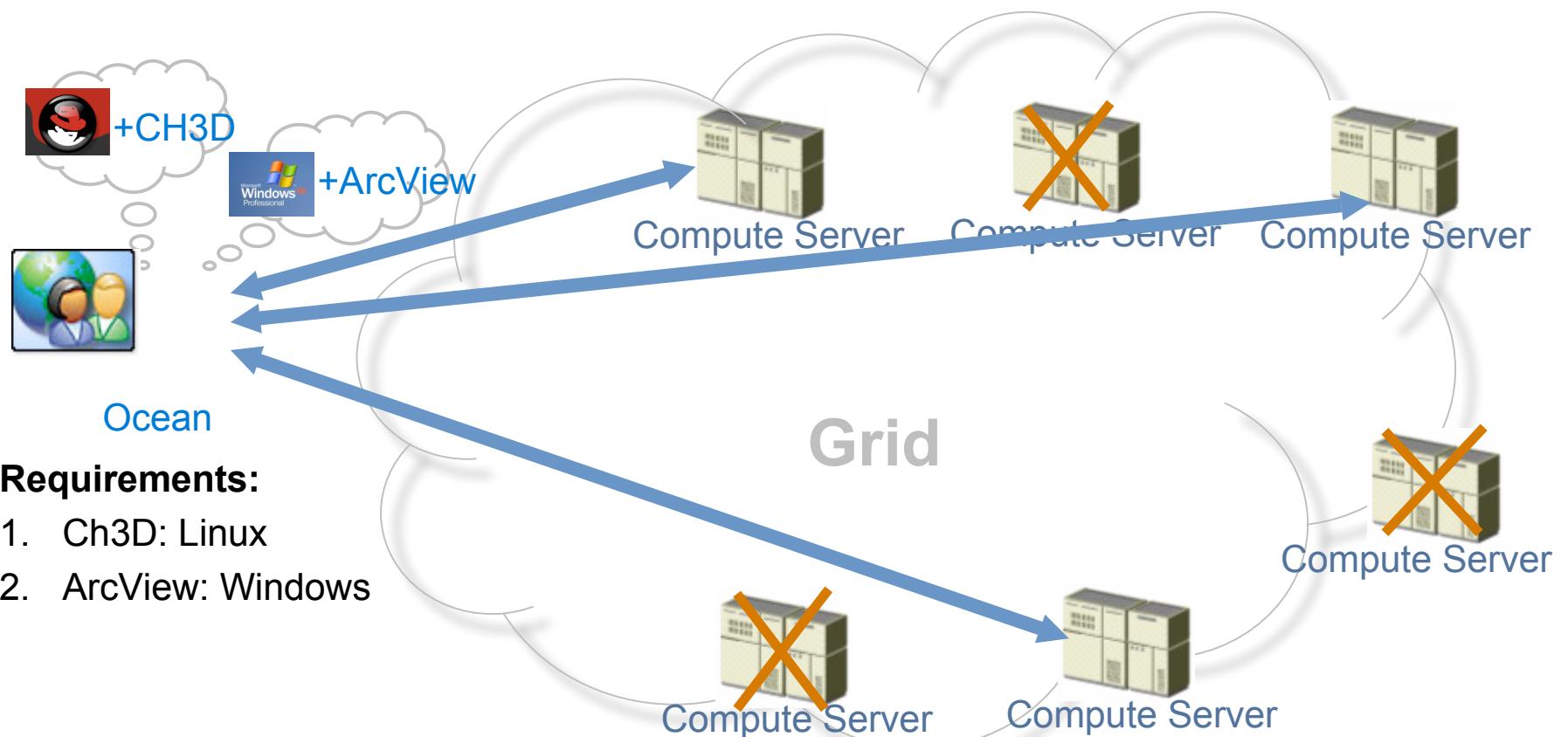
Resource Mgmt





- 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

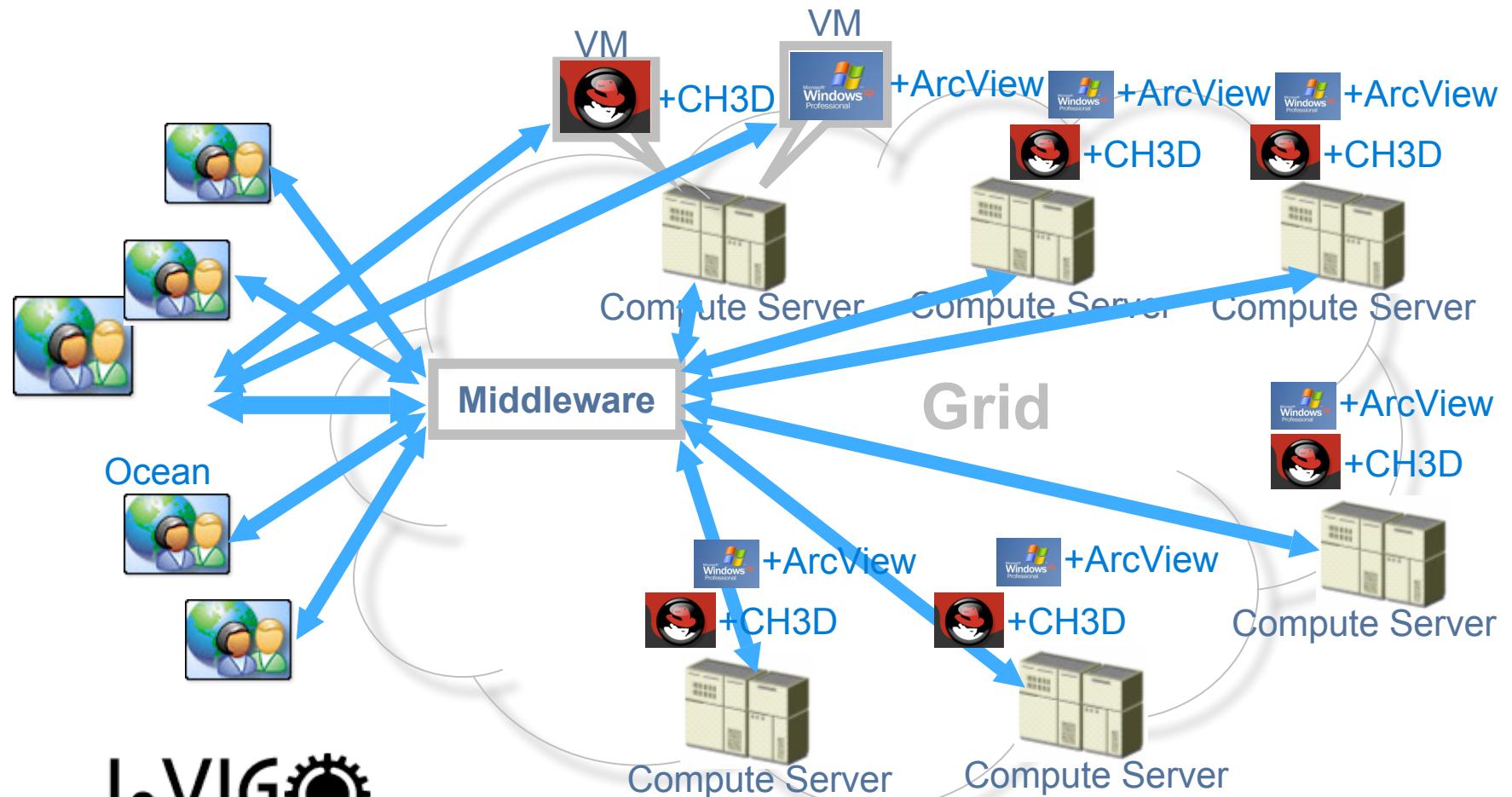
"The Anatomy of the Grid: Enabling Scalable Virtual Organizations", I. Foster, C. Kesselman, S. Tuecke. International J. Supercomputer Applications, 15(3), 2001





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Our approach: Define once, instantiate on-demand



InVIGO
Processing....

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

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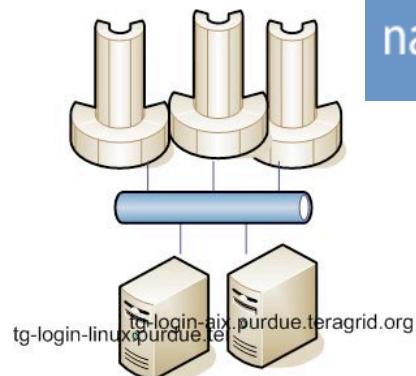




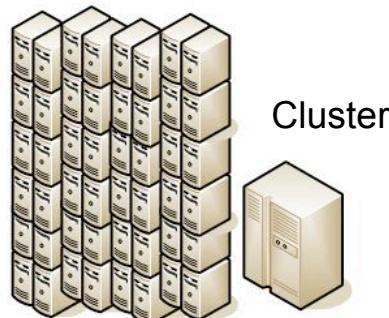
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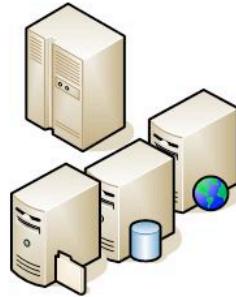
Accomplishments



TeraGrid Entrance



Cluster



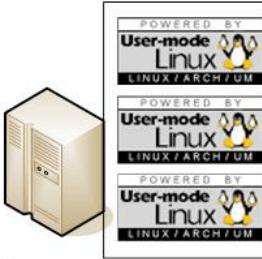
Web Server



Virtual
Machines

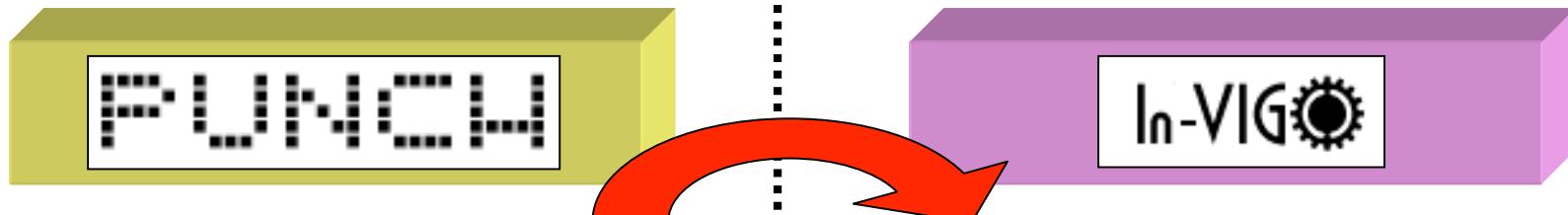
Virtual
Machines

LDAP



NMI cluster
Nmi-001 to nmi-024





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

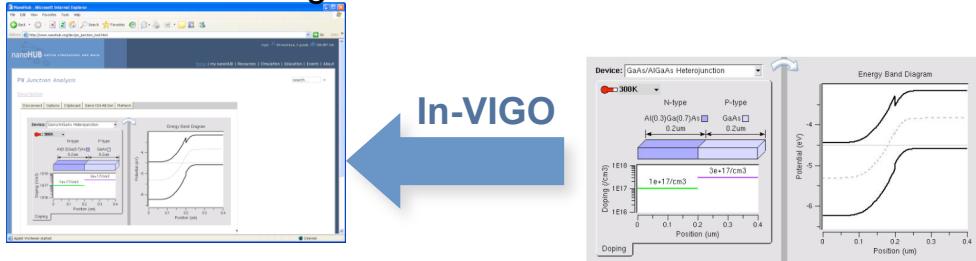
- Abinit
 - Bipad
 - Gamess
 - Gromacs
 - Huckel-IV
 - Laser
 - Matlab
 - Moca
 - Molden
 - MolCToy
- agere** **agere** **agere**
- MSL
 - Octave
 - PADRE
 - PN Junctions
 - Prophet
 - Rasmol
 - SMC
 - Spice 2g
 - TunProb
 - Vtk

= GUI = Rappture = text interface

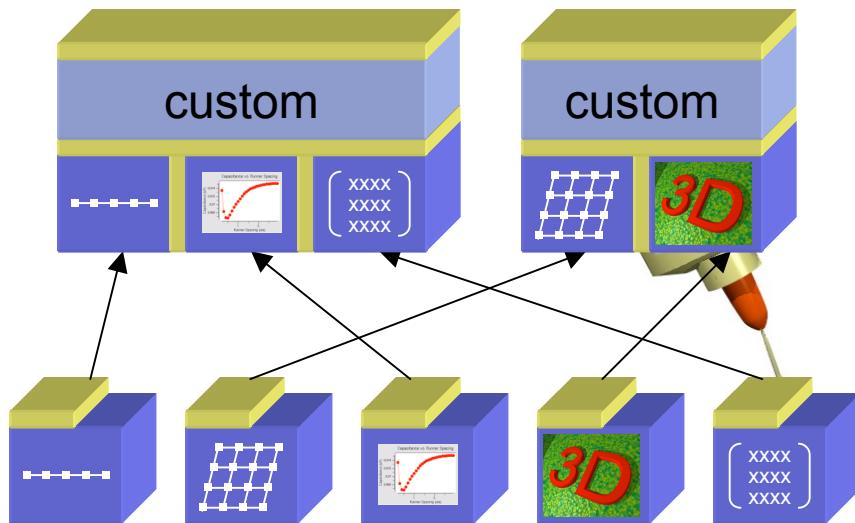


- Scripting languages as a tool development philosophy

www.nanohub.org



In-VIGO

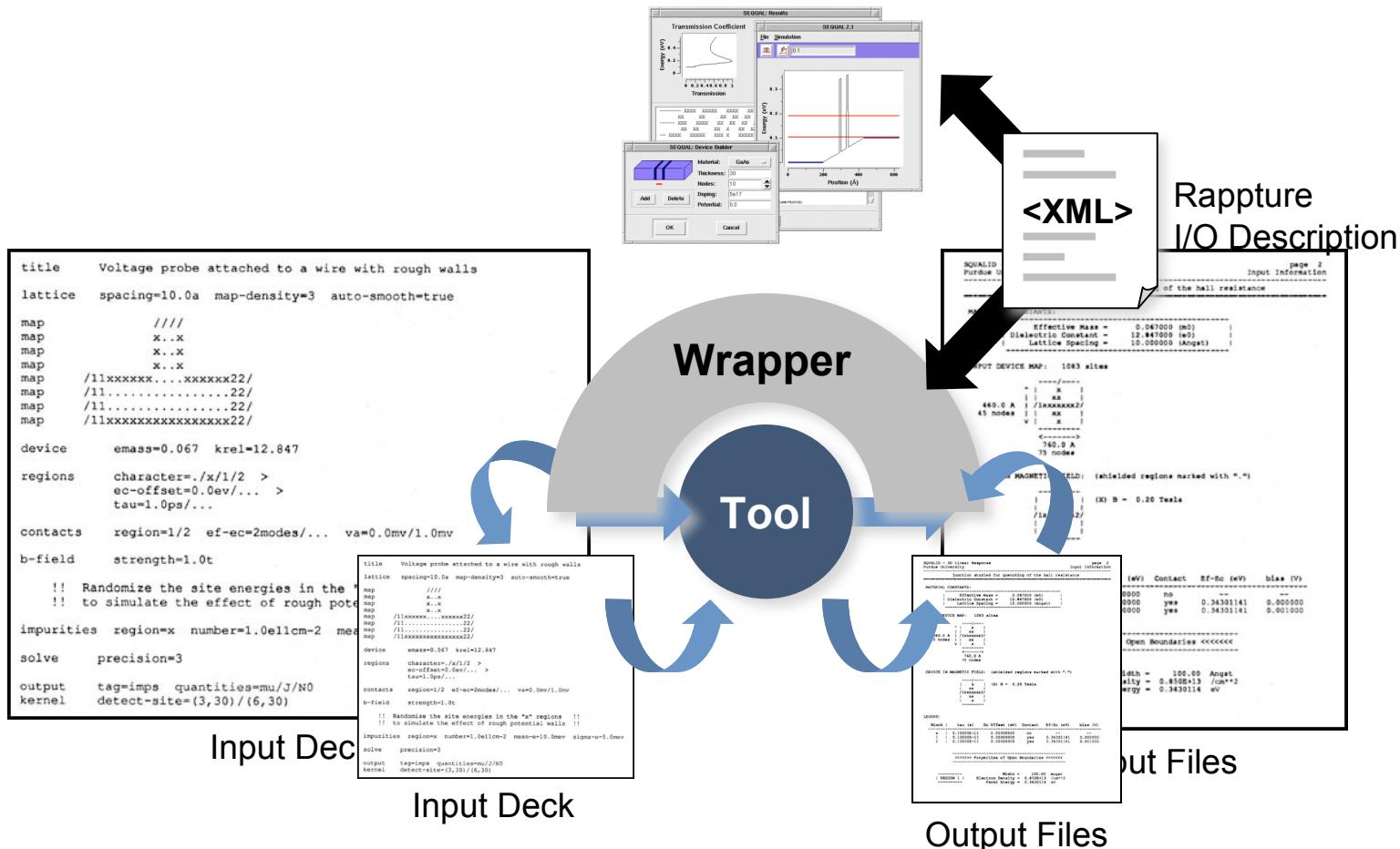


Build interfaces on scripting foundation

Build tools from component parts

Add scripting language interface to each component

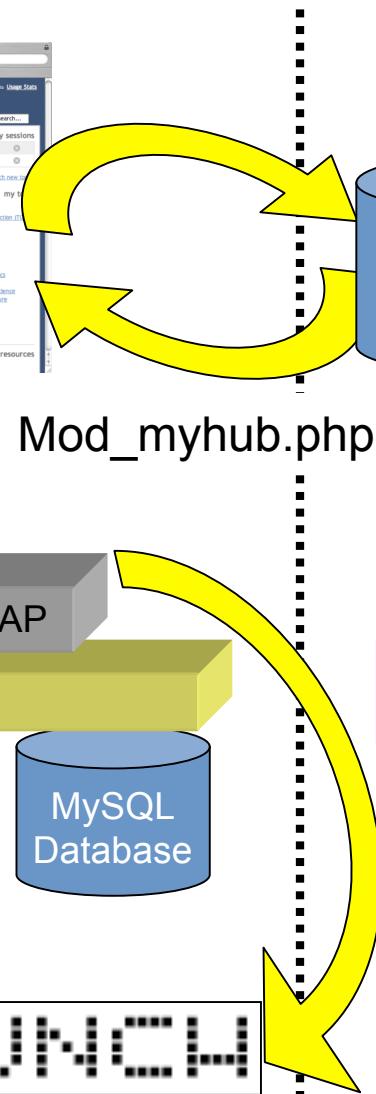
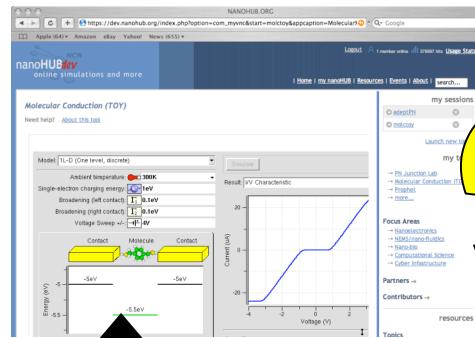
Components coded in C, C++, Fortran



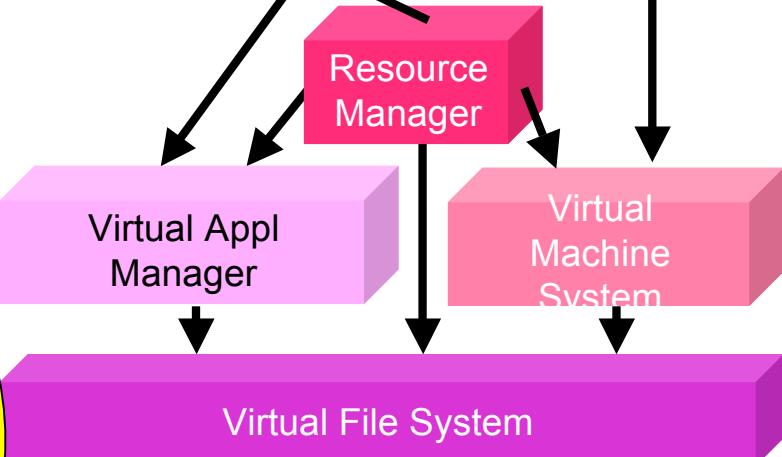
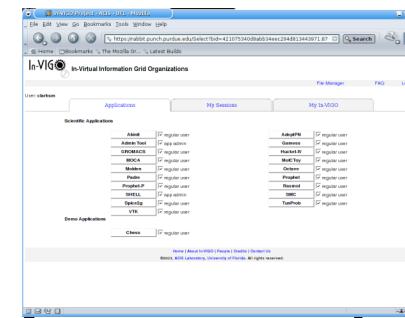


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nanoHUB and In-VIGO integration



In-VIGO Web Interface



PUNCH



Network for Computational Nanotechnology





Two virtual machine systems:

VMware:

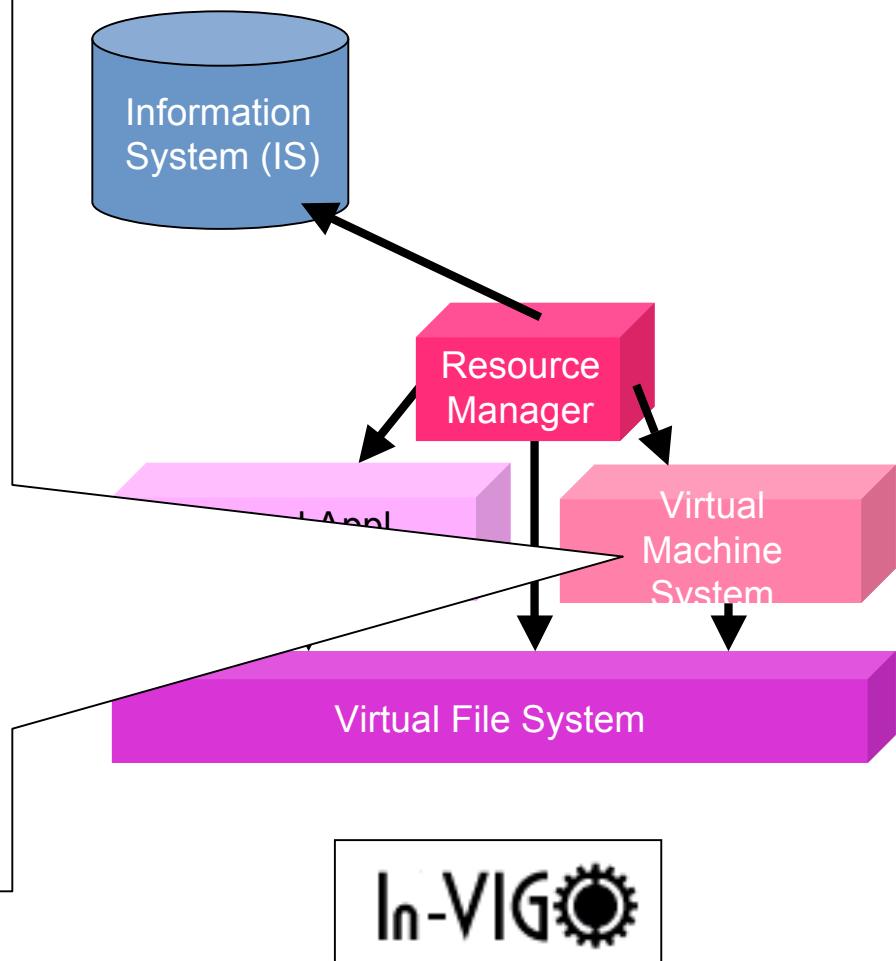
- + Commercial product
- + Mature software
- not open source
- smaller community

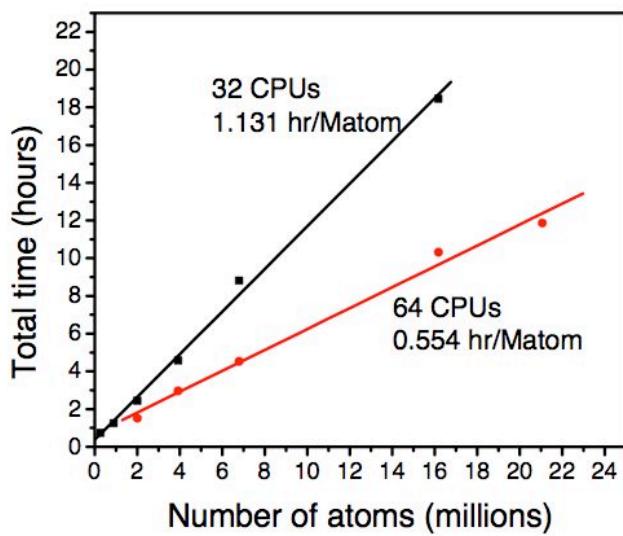
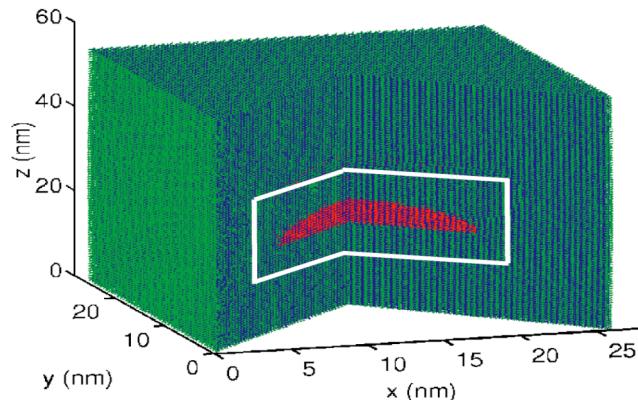
User Mode Linux:

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

Future with Xen:

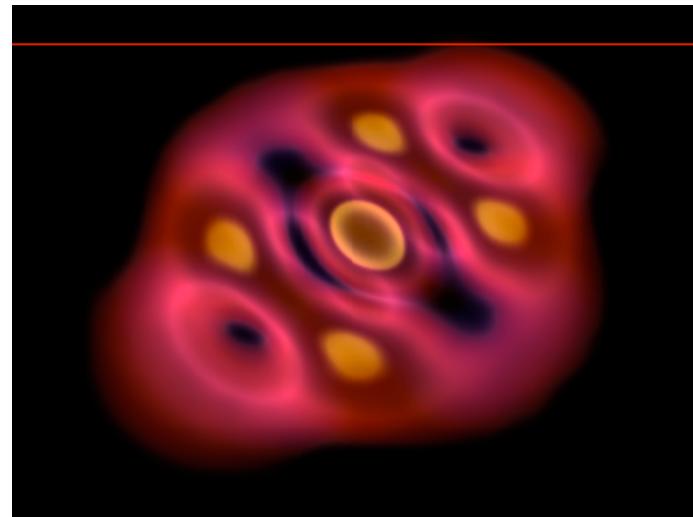
- + Open Source
- + Better performance
- + Collaboration with ANL





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. $\Delta t = 1 \text{ fs}$

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:

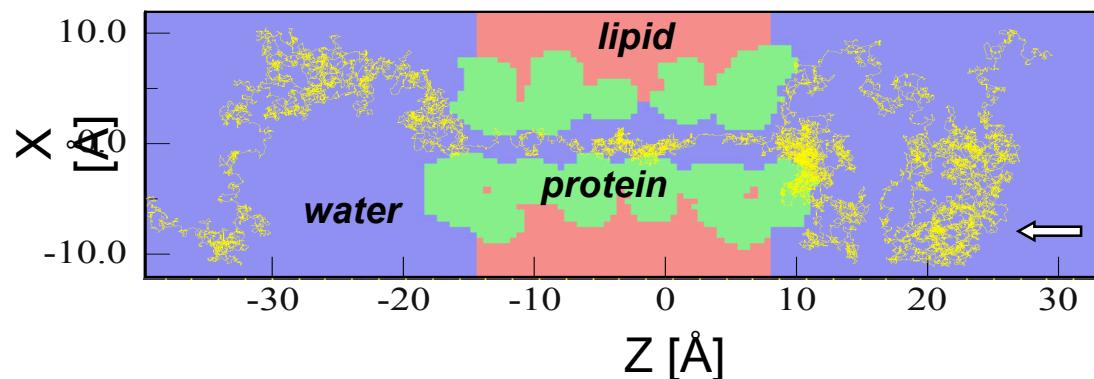
NCN student on TeraGrid (Gulzar Kathawala)

MOCA and BioMOCA ported to TeraGrid

~75,000 SUs used on TeraGrid

Permeation trajectory of a “lucky” Na^+ in a gramicidin A ionic channel

T. Van der Straaten, G. Kathawala, U. Ravaioli (UIUC)





Expert Introduction by Supriyo Datta

The screenshot shows a Microsoft Internet Explorer window displaying the nanoHUB.org website. The main content area is titled "MolCToy Learning Module". On the left, a sidebar lists various learning resources. A red circle highlights the link "Opening Remarks on MolCToy". The central content area features a diagram of a "Unified Model" for nanoelectronics, showing a system with contacts μ_1 and μ_2 , a source S , and a scattering region $H + U$. The diagram is labeled "Unified Model" and "Dissipative processes". To the right of the diagram, text explains that devices are described using a grid of discrete points, and that grid points can be in real space or abstract space, called basis functions. It also notes that the size of matrices is $N \times N$ where N is the number of basis functions or "grid points". If $N = 1$, matrices are reduced to numbers. A citation from S. Datta's work is provided. A video player interface is overlaid on the text, showing a list of video clips related to the module. The video player interface includes a title bar, a list of video thumbnails, and a progress bar indicating "8 Minutes 24 Seconds Remaining". The bottom status bar of the browser window shows "Internet" and the NCN (Network for Computational Nanotechnology) logo.



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online simulations and more

Molecular Conduction Learning Module

Online simulation via nanoHUB middleware

The screenshot shows two windows. The left window is the 'MolCToy Learning Module' with a sidebar of links like 'Abstract', 'Introduction to MolCToy', and 'MolCToy Simulation Tool (New Window)' which is circled in red. The right window is a simulation interface titled 'I/V Characteristic' showing a plot of Current (A) versus Voltage (V). The plot shows a non-linear relationship, characteristic of molecular conduction. The simulation parameters include Ambient temperature (300K), Single-electron charging energy (1eV), Broadening (left contact) (0.1eV), Broadening (right contact) (0.1eV), and a Voltage Sweep from -4V to 4V. Below the plot is a diagram of a molecule between two contacts, with energy levels labeled at -5eV, -5.5eV, and -5eV.



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Molecular Conduction Learning Module

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](#)

[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: Turn 1 level](#)

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.

One level (discrete) symmetric coupling (LUMO)

I (μA)

V (V)

$\Gamma_1=0.1; \Gamma_2=0.2$

$\Gamma_1=0.2; \Gamma_2=0.1$

Slide 1 / 2 | Playing 01:14 / 01:24

Network for Computational Nanotechnology NCN

0 Minutes 40 Seconds Remaining

Internet

Done

MolCToy: Solution to Exercise

Outline Thumb Notes Search

Slide Title Duration

Solution of Exercise 1... 01:24

Solution of Exercise 1... 00:30

6 Minutes 40 Seconds Remaining



Quiz that includes feedback

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

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 \(includes feedback upon completion\)](#)

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 ARD

NCN

Internet



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Leveraging Educational Standards

XML-based Standard Compliant Content Description in a ZIP file

National Learning Module Database - MERLOT

MERLOT Detail View

Nanoelectronics: The New Frontier

Average Ratings: Peer Reviews: (not reviewed)
Member Comments: (none)

Type: Lecture/Presentation
Location: https://www.nanohub.org/index.php?option=com_content&task=view&id=10
Primary Subject Category: Science and Technology/Nanotechnology/Nano-electronics
Author: Mark Lundstrom
Network for Computational Nanotechnology

This presentation provides an overview of the field of nanoelectronics.

Submitted by: Madhavan
Primary Audience: College, Graduate School, Professional
Technical Format: Flash

Course Management Systems

WebCT Vista™

Blackboard

Sakai™

Thousands Of Users
At Most Universities



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Example of content interoperability

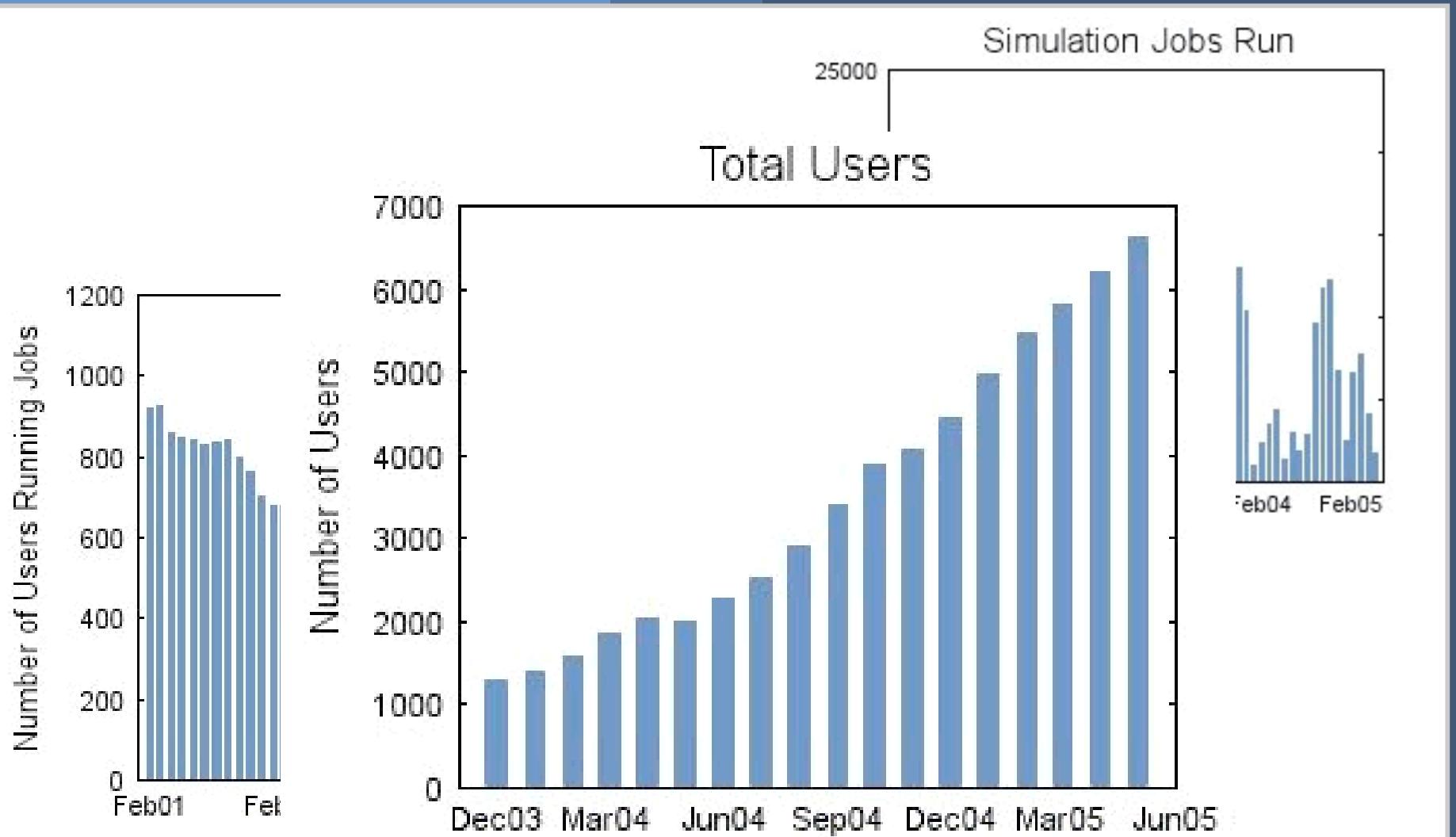
The screenshot shows a Microsoft Internet Explorer window with two overlapping windows. The background window is the Purdue WebCT course page, and the foreground window is a SCORM module player.

Purdue WebCT Course Page (Background):

- Address: <https://ecourses.purdue.edu/webct/cobaltMainFrame.dowebct>
- Toolbar: Back, Forward, Stop, Refresh, Search, Favorites, Print, E-mail, etc.
- Menu: File, Edit, View, Favorites, Tools, Help
- Links: My WebCT, Help, Log out, ICS - MIDC - Teaching with Multimedia, File Manager, Search, Content Import
- Content Area: Basic View, Power View, Content Inventory, Add to Course Toolbar, Course Toolbar (tools always visible), Toolbar Settings, Go to, Add to Home Page, Assessments, Assignments, Chat and Whiteboard, Content File, Discussions, Learning Module, Media Library Collection, Organizer Page, SCORM Module, Syllabus, URL, More Tools, Tool Overview, Course Customization, Selective Release Map.

SCORM Module Player (Foreground):

- Address: <https://ecourses.purdue.edu/webct/previewScorm.dowebct?scormId=78228036>
- Toolbar: Back, Forward, Stop, Refresh, Search, Favorites, Print, E-mail, etc.
- Menu: File, Edit, View, Favorites, Tools, Help
- Links: Help
- Content Area:
 - Table of contents for: **Intro to Nanometer Scale Sci**
 - 1. Introduction to Nanometer Sc
 - ROBERT R. MCCORMICK SCHOOL OF ENGINEERING AND APPLIED SCIENCE
 - Introduction to Nanometer Scale Science and Technology**
 - Mark C. Hersam, Assistant Professor
 - Department of Materials Science and Engineering
Northwestern University, Evanston, IL 60208-3108
Ph: 847-491-2696, m-hersam@northwestern.edu
WWW: <http://www.hersam-group.northwestern.edu/>
 - Outline, Thumb, Notes, Search
 - Slide Title Duration
 - Introduction and Welcom... 01:54
 - Introduction to Nanom... 00:54
 - Outline 02:13
 - There's Plenty of Room... 01:54
 - Invention of the Transi... 00:44
 - The First Planar Integr... 00:28
 - Moore's Law 01:14
 - 300mm Wafer 00:36
 - Minimum Feature Size 00:55
 - 57 Minutes 9 Seconds Remaining
- Player Controls: Previous, Next, Stop, Play, Volume, etc.
- Status Bar: Slide 2 / 44 | Playing 00:12 / 00:54
- Bottom Bar: Done, Internet





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Questions?

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much, much

