The nanoHUB: A science Gateway for nanotechnology

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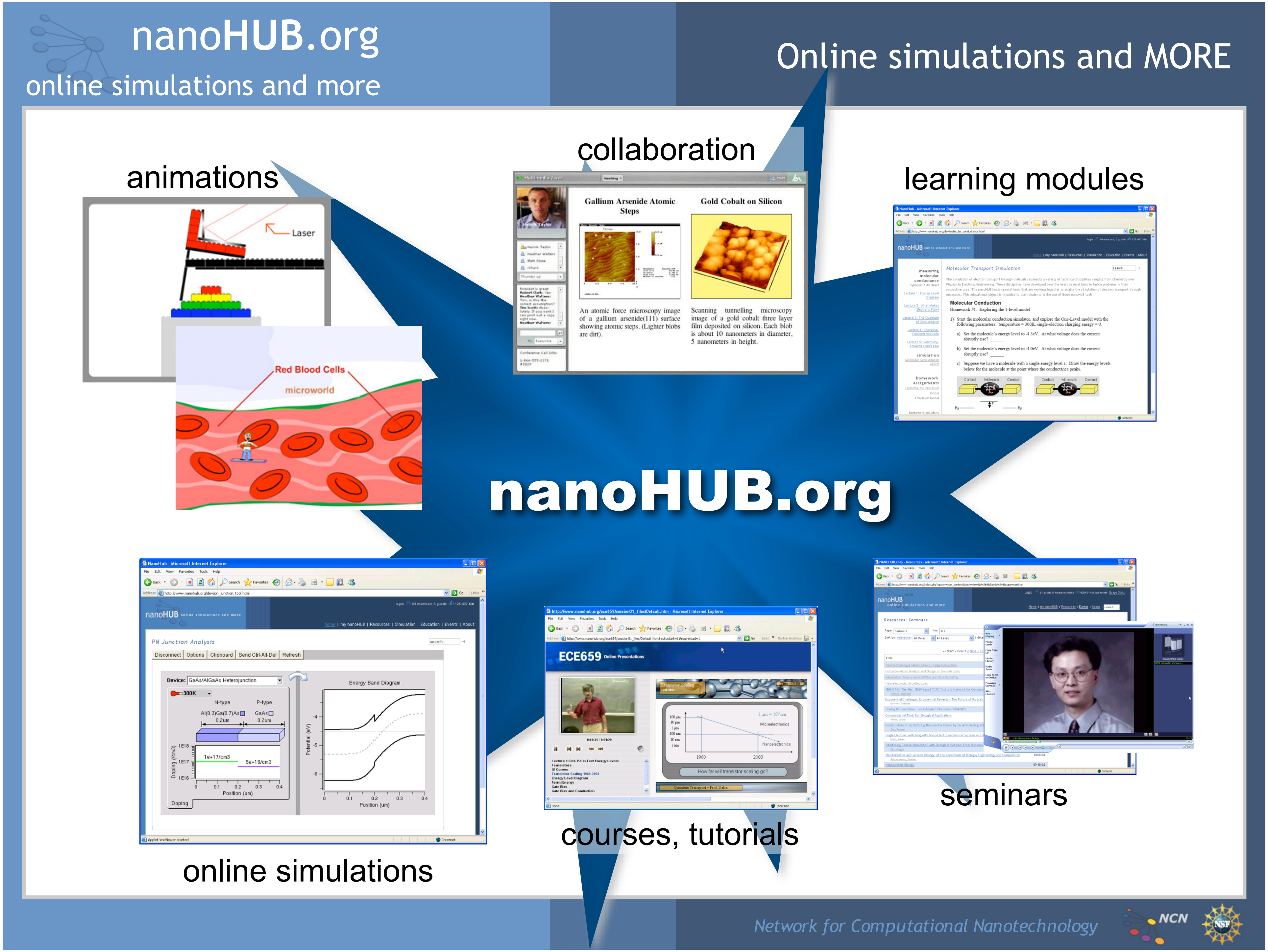
Mark S. Lundstrom and Gerhard Klimeck

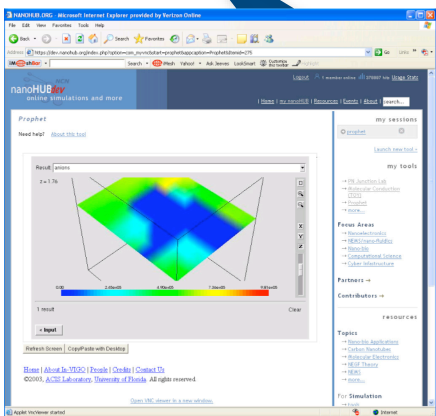
GGF-14
June 28st , 2005

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

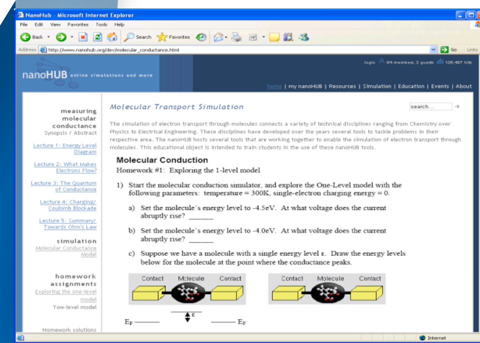

nanoHUB.org
online simulations and more
Online simulations and MORE
animations
Laser
Red Blood Cells
microworld
collaboration
Gallium Arsenide Atomic Steps
Gold Cobalt on Silicon
learning modules
nanoHUB.org
online simulations
courses, tutorials
ECE659
seminars
Network for Computational Nanotechnology
NCN

An Ecosystem

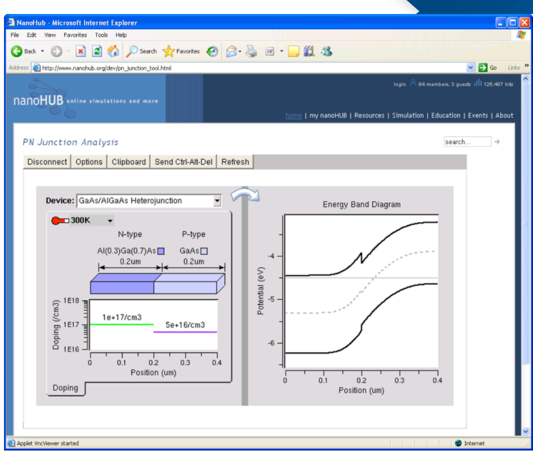
Applications



learning modules



nanoHUB.org Ecosystem

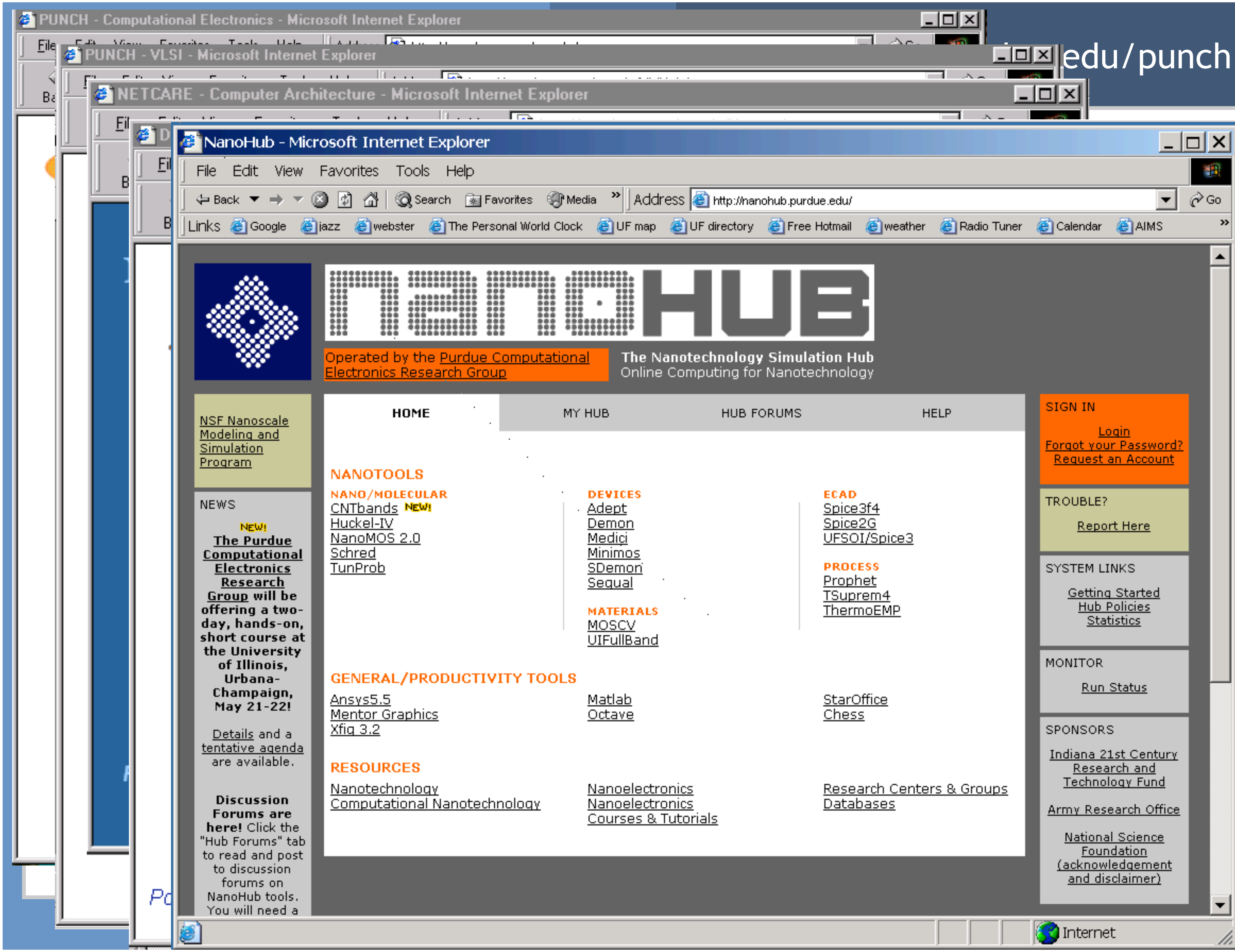


A middleware

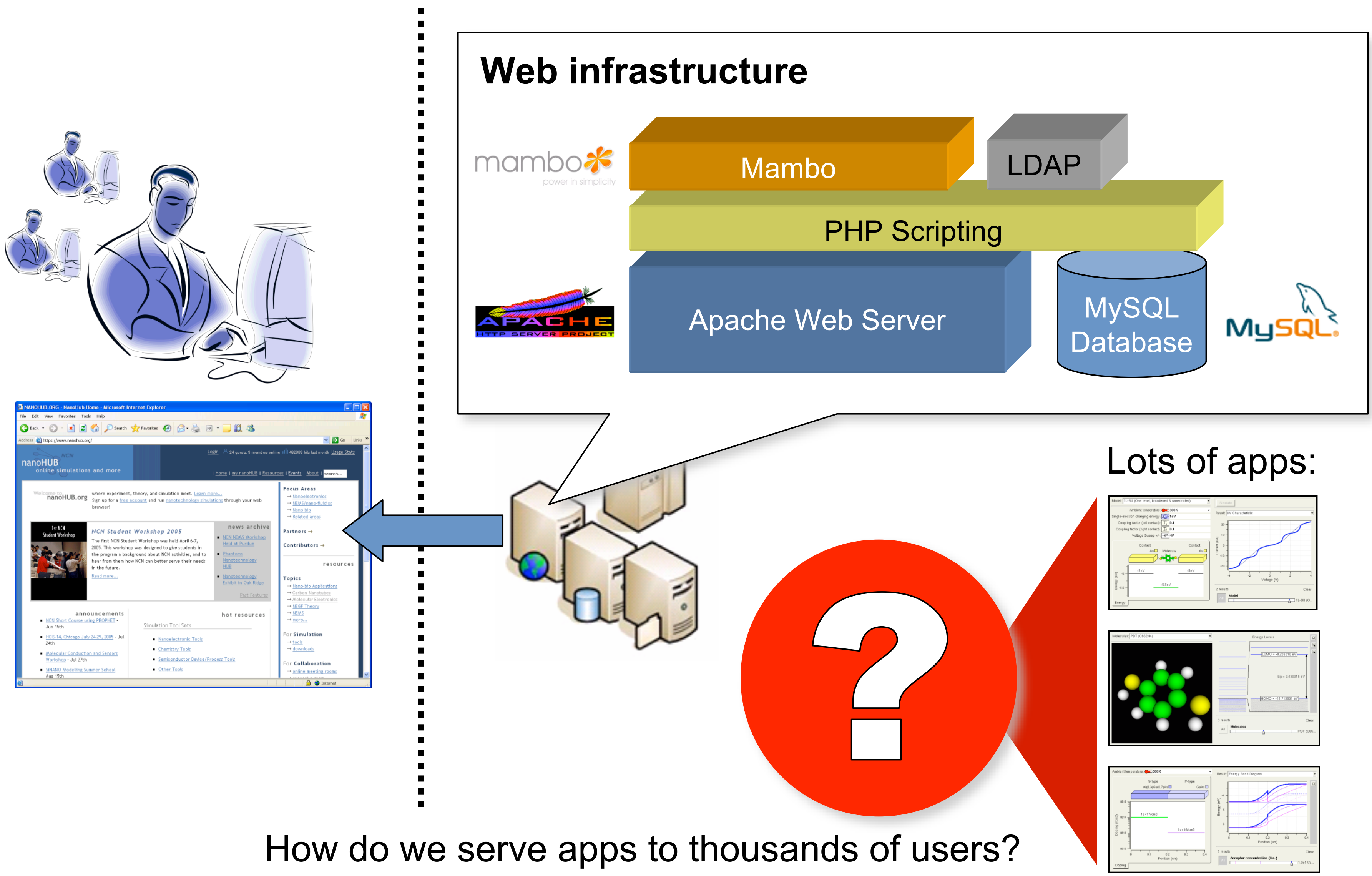
TERAGRID

Resources

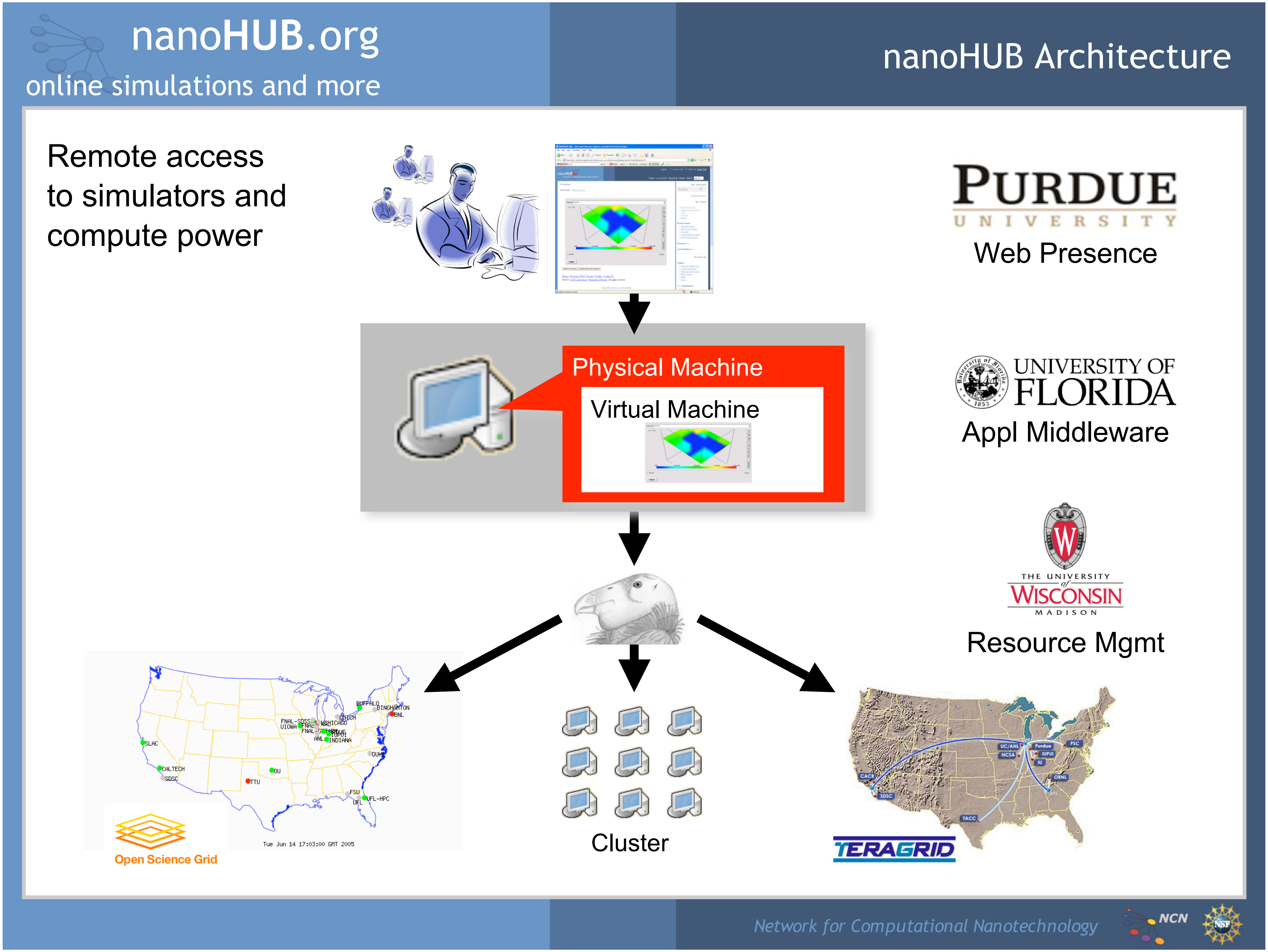
edu/punch


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 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
NSF Nanoscale Modeling and Simulation Program
HOME
MY HUB
HUB FORUMS
HELP
SIGN IN
Login
Forgot your Password?
Request an Account
NANOTOOLS
NANO/MOLECULAR
CNTbands NEW!
Huckel-IV
NanoMOS 2.0
Schred
TunProb
DEVICES
Adept
Demon
Medici
Minimos
SDemon
Sequal
MATERIALS
MOSCV
UIFullBand
ECAD
Spice3f4
Spice2G
UFSOI/Spice3
PROCESS
Prophet
TSuprem4
ThermoEMP
GENERAL/PRODUCTIVITY TOOLS
Ansys5.5
Mentor Graphics
Xfig 3.2
Matlab
Octave
StarOffice
Chess
RESOURCES
Nanotechnology
Computational Nanotechnology
Nanoelectronics
Nanoelectronics
Courses & Tutorials
Research Centers & Groups
Databases
NEWS
NEW!
The Purdue Computational Electronics Research Group will be offering a two-day, hands-on, short course at the University of Illinois, Urbana-Champaign, May 21-22!
Details and a tentative agenda are available.
Discussion Forums are here! Click the "Hub Forums" tab to read and post to discussion forums on NanoHub tools. You will need a
TROUBLE?
Report Here
SYSTEM LINKS
Getting Started
Hub Policies
Statistics
MONITOR
Run Status
SPONSORS
Indiana 21st Century Research and Technology Fund
Army Research Office
National Science Foundation (acknowledgement and disclaimer)
Internet

Why Middleware?



How do we serve apps to thousands of users?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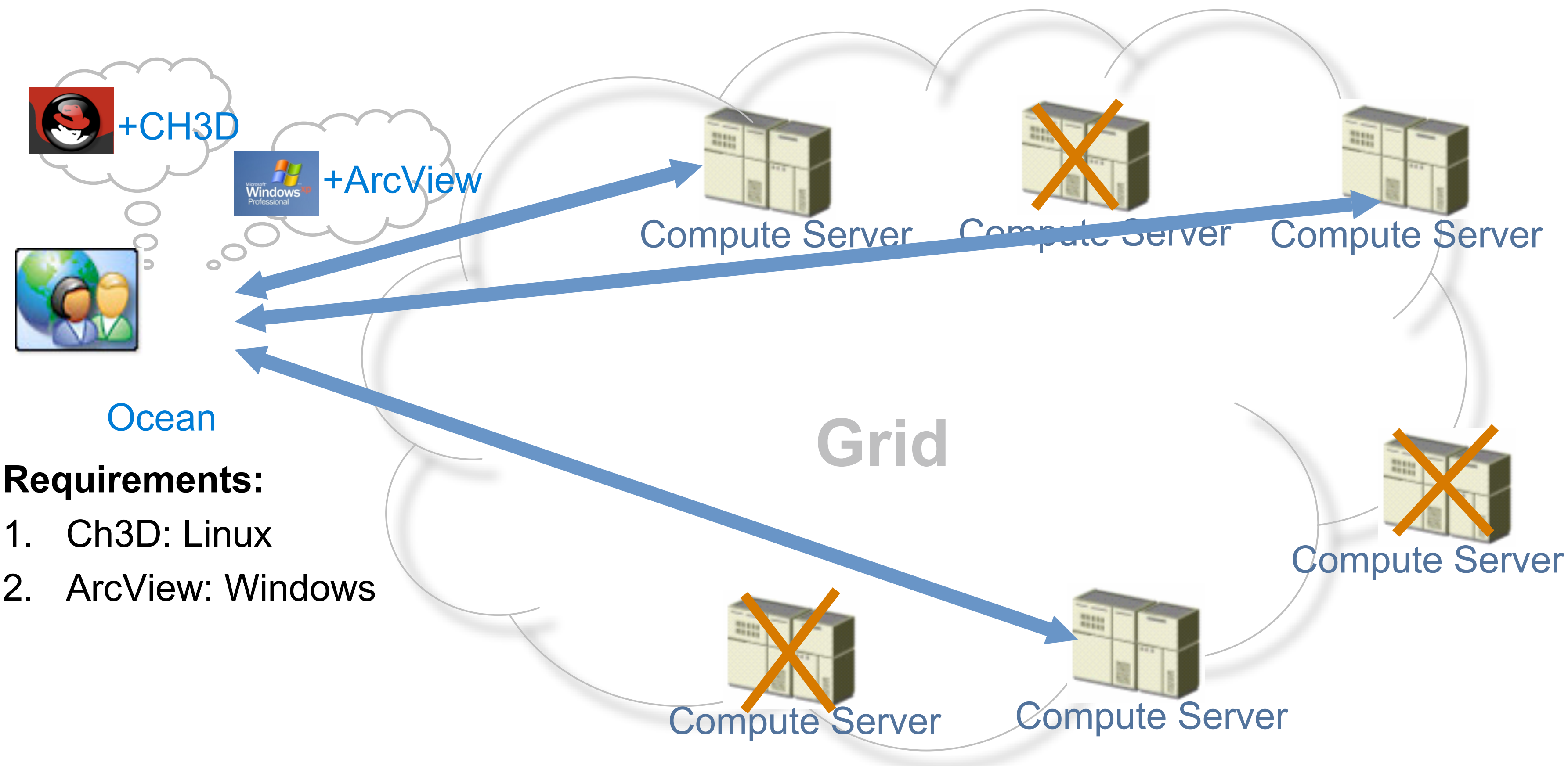
online simulations and more
nanoHUB Architecture
Remote access
to simulators and
compute power
Physical Machine
Virtual Machine
PURDUE
UNIVERSITY
Web Presence
UNIVERSITY OF
FLORIDA
Appl Middleware
THE UNIVERSITY of WISCONSIN MADISON
Resource Mgmt
Cluster
Open Science Grid
Tue Jun 14 17:03:00 GMT 2005
TERAGRID
Network for Computational Nanotechnology
NCN

- 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

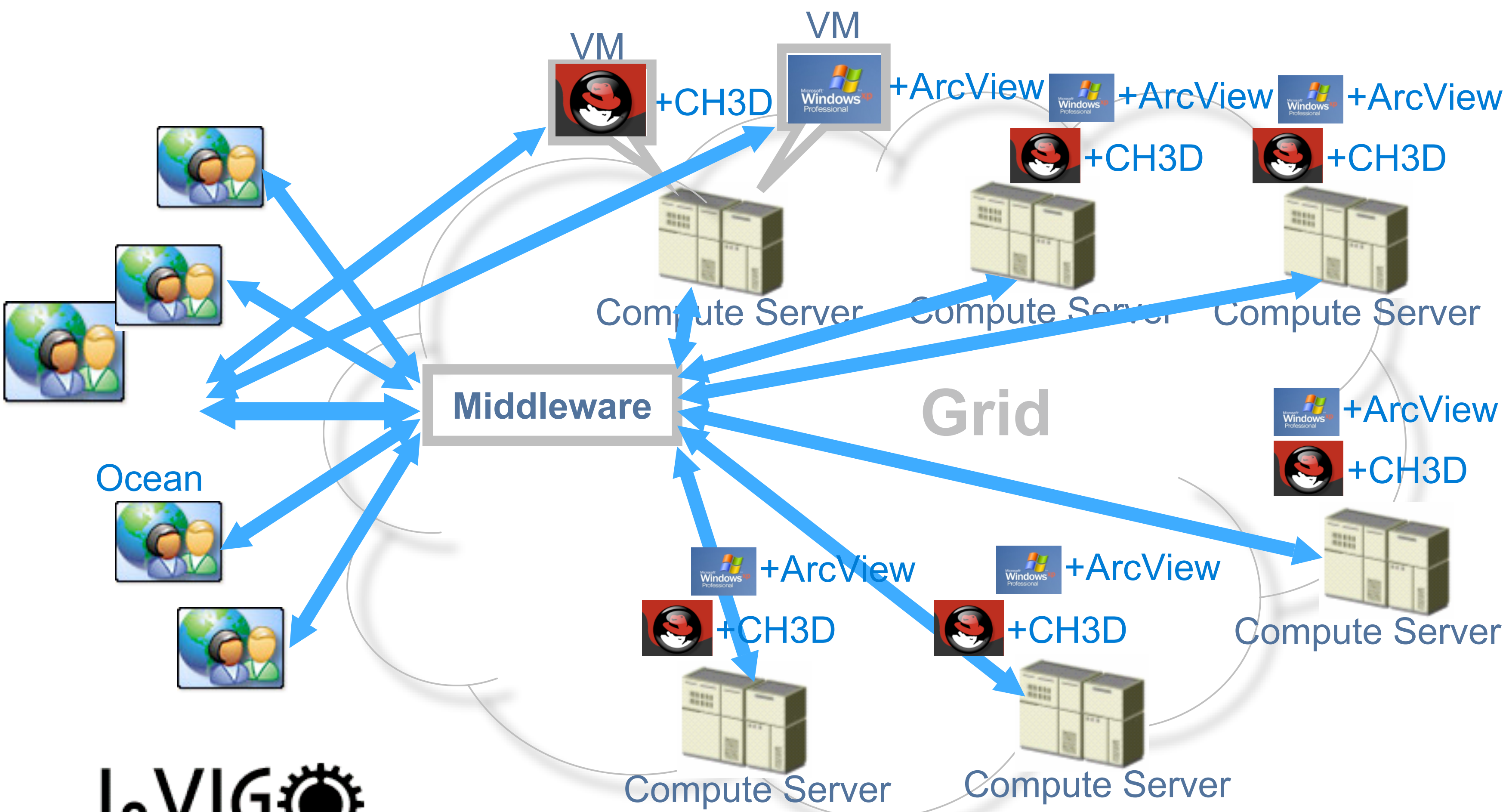
Problems with using physical machines



Requirements:

1. Ch3D: Linux
2. ArcView: Windows

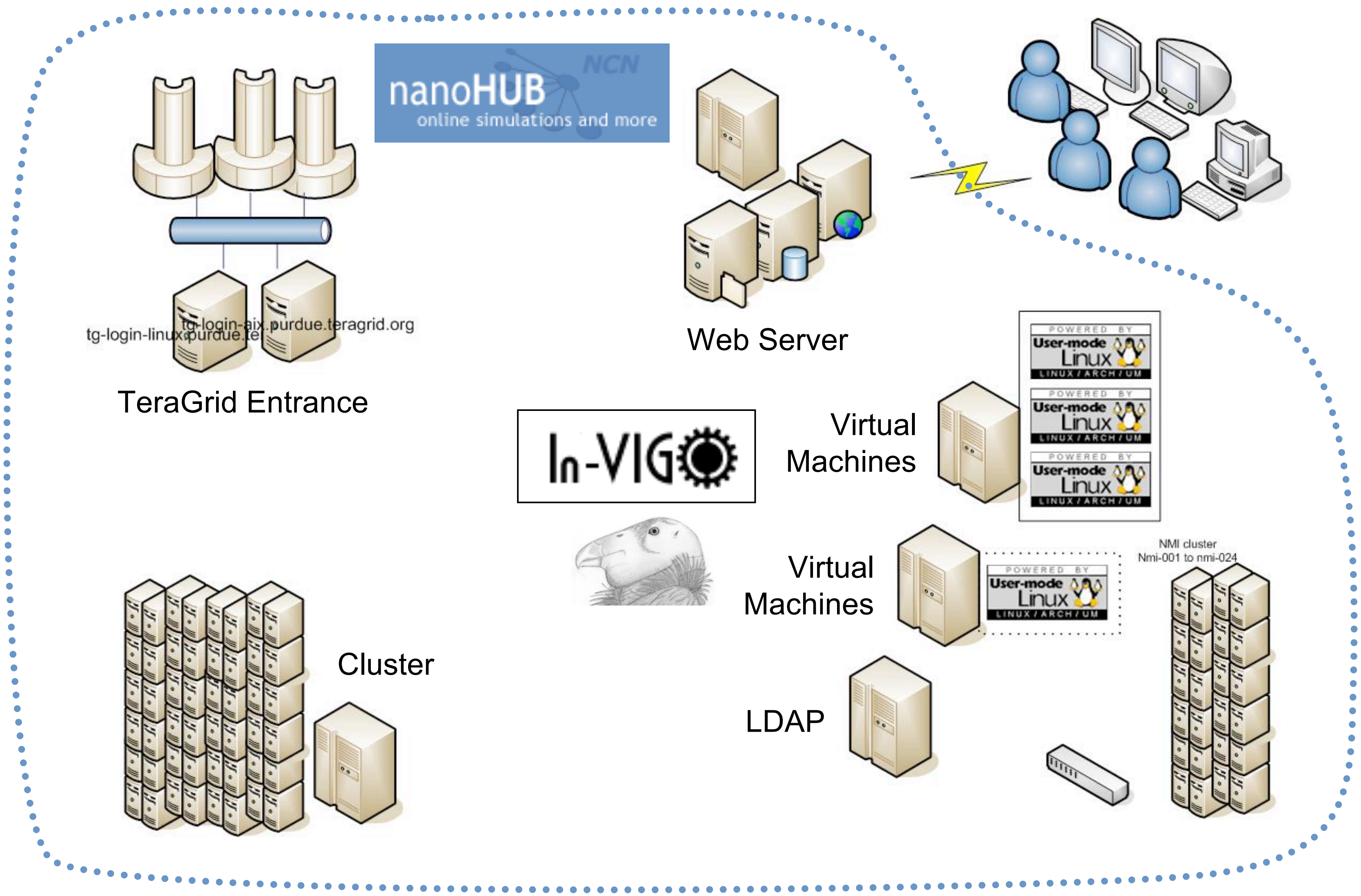
Our approach: Define once, instantiate on-demand



InVIGO
Processing....

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

Accomplishments



Application Deployment

PUNCH

In-VIGO

38 apps

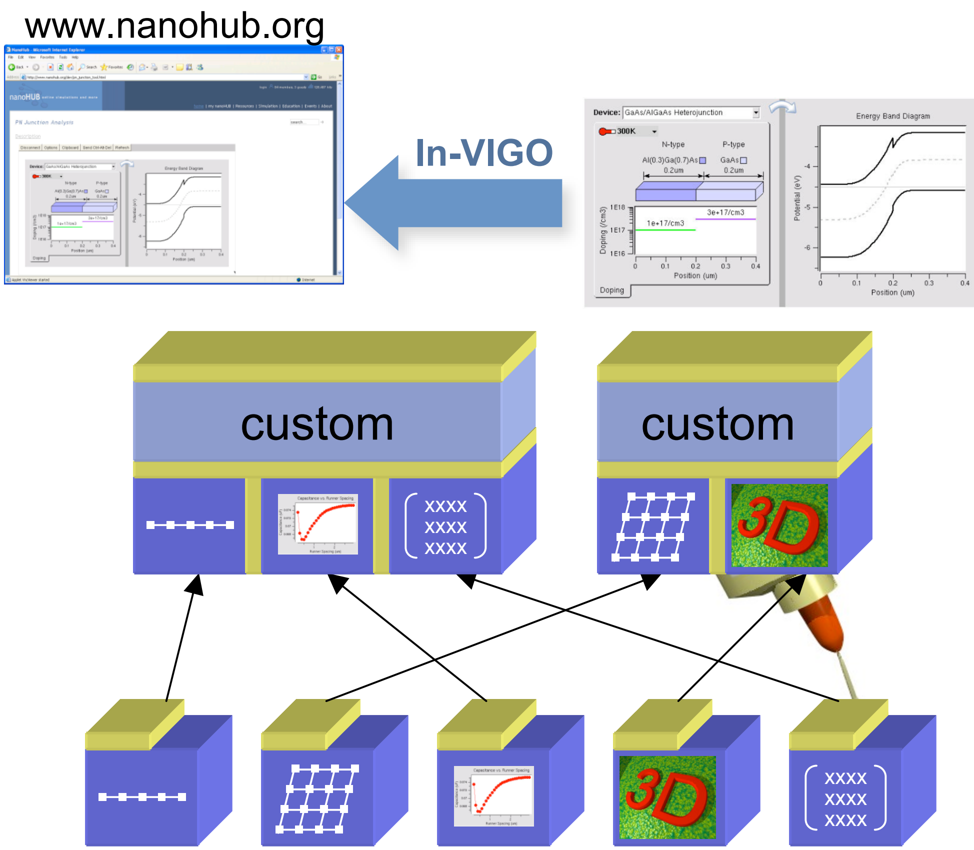
- 2DS
- CENEMS
- CNTbands
- FETToy
- MolCToy
- NanoMOS 2.5
- Prophet
- Schred
- SETE
- Spice 2G
- TBGreen
- TunProb
- QNEMS
- …

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

= GUI = Rappture = text interface

Summary

- Scripting languages as a tool development philosophy



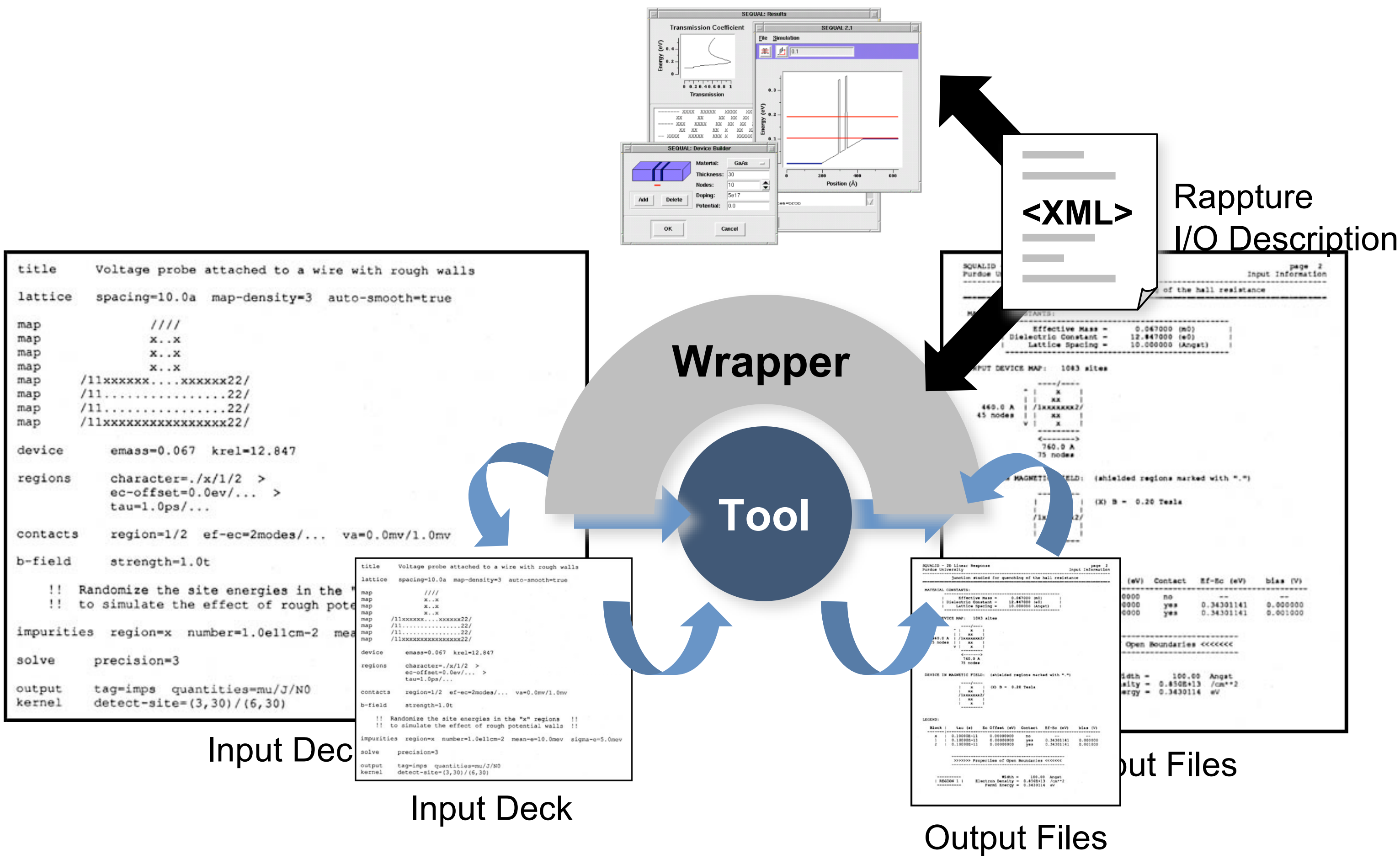
Build interfaces on scripting foundation

Build tools from component parts

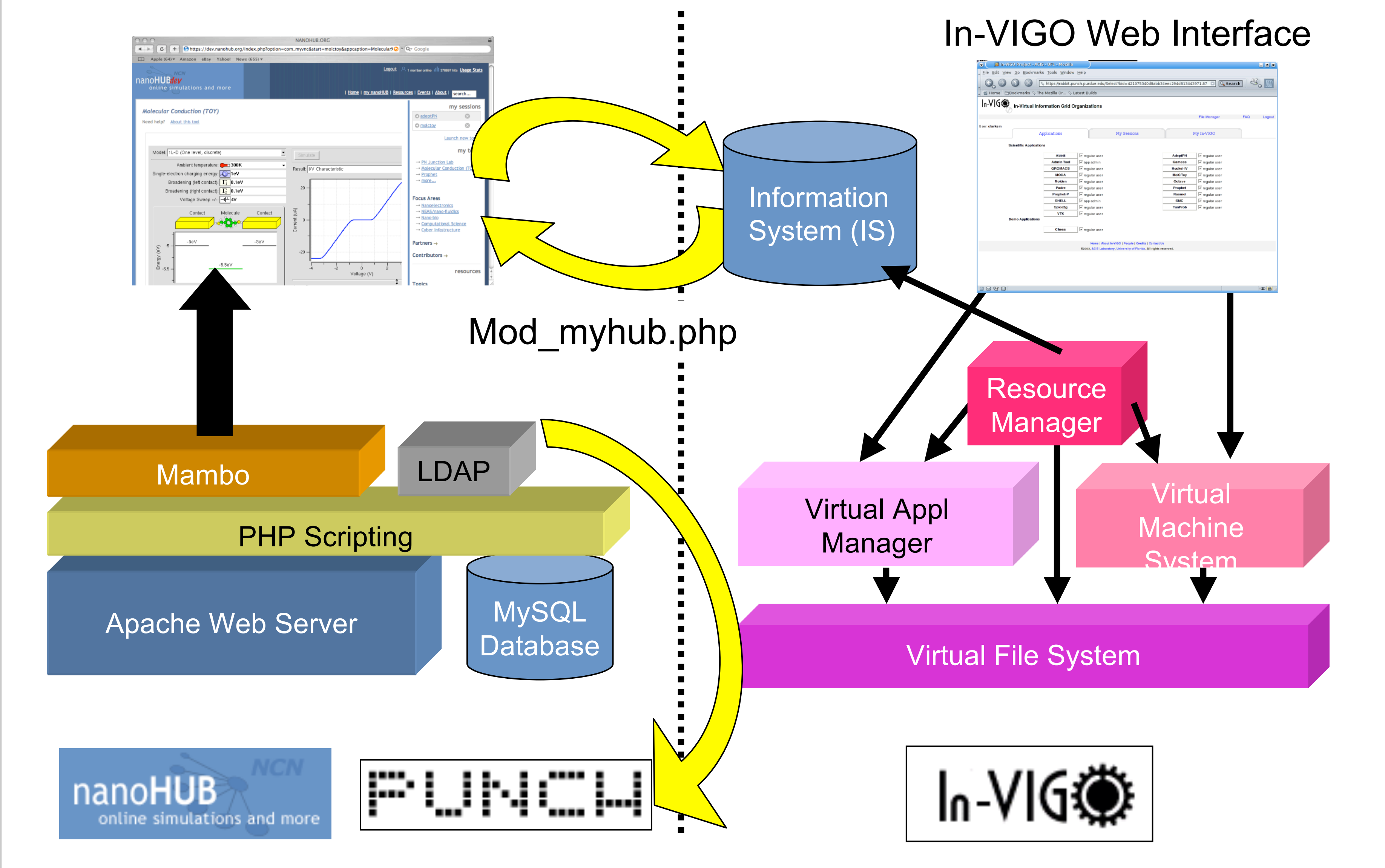
Add scripting language interface to each component

Components coded in C, C++, Fortran

Wrap Existing Tools



nanoHUB and In-VIGO integration



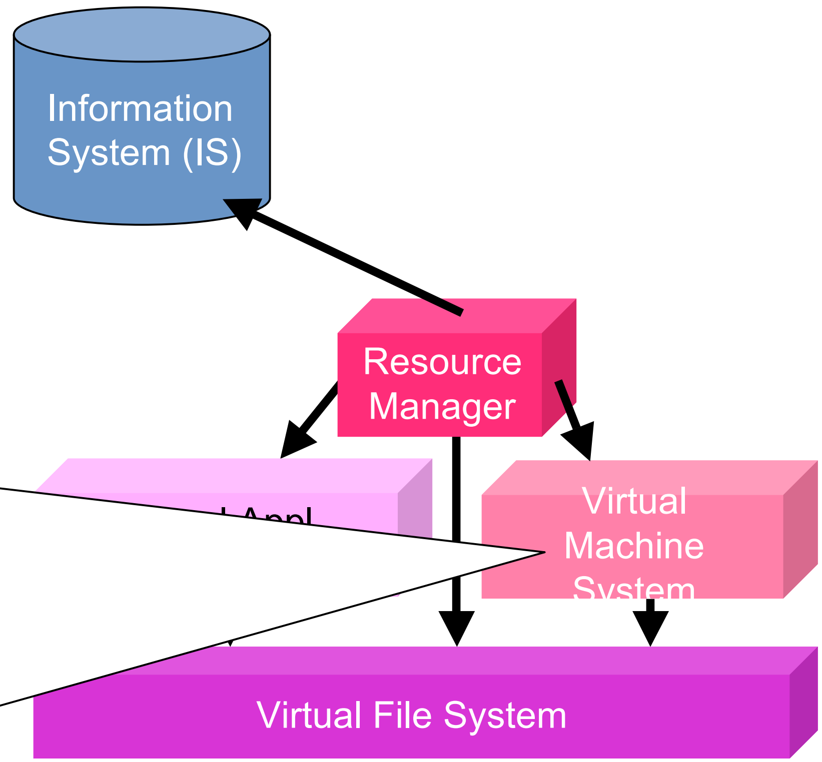
nanoHUB and In-VIGO integration

Two virtual machine systems:

VMware:
+ Commercial product
+ Mature software
– not open source
– smaller community

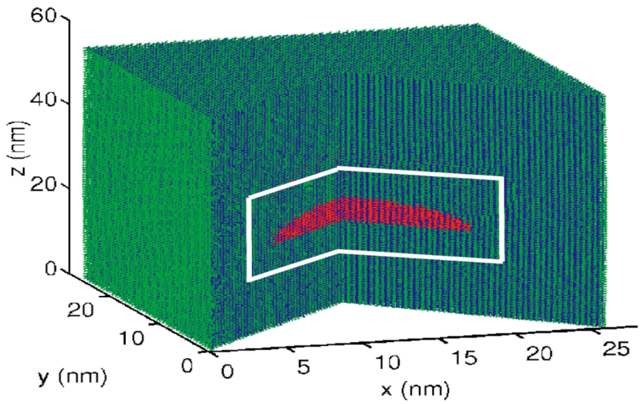
User Mode Linux:
+ Open Source (hack the code)
+ Large community of developers
– not as mature

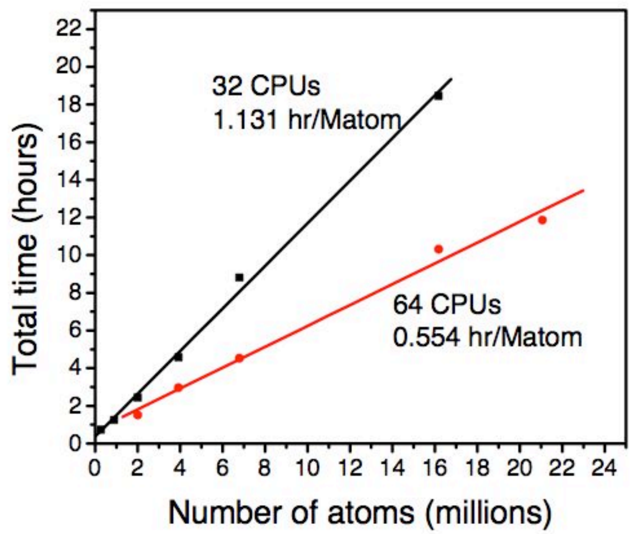
Future with Xen:
+ Open Source
+ Better performance
+Collaboration with ANL



In-VIGO

NEMO3D on TeraGrid





Accomplishments:

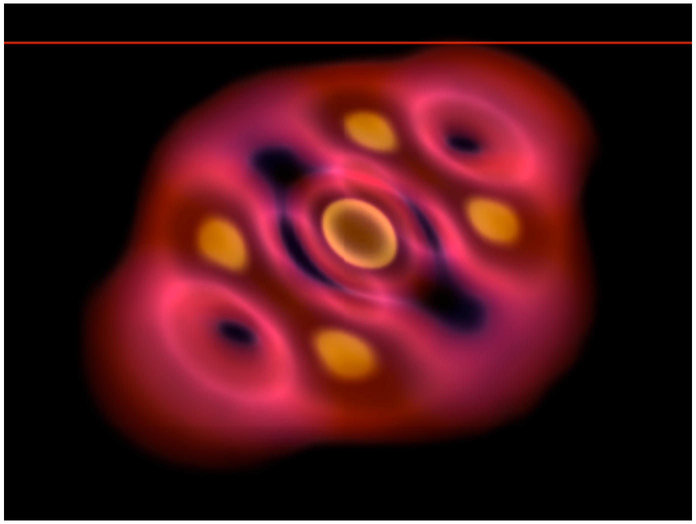
NCN community allocation

NEMO3D ported to TeraGrid

Scaling study

64 Million atoms simulation

~50,000 SUs used on TeraGrid



BioMOCA 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. *Δt=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).

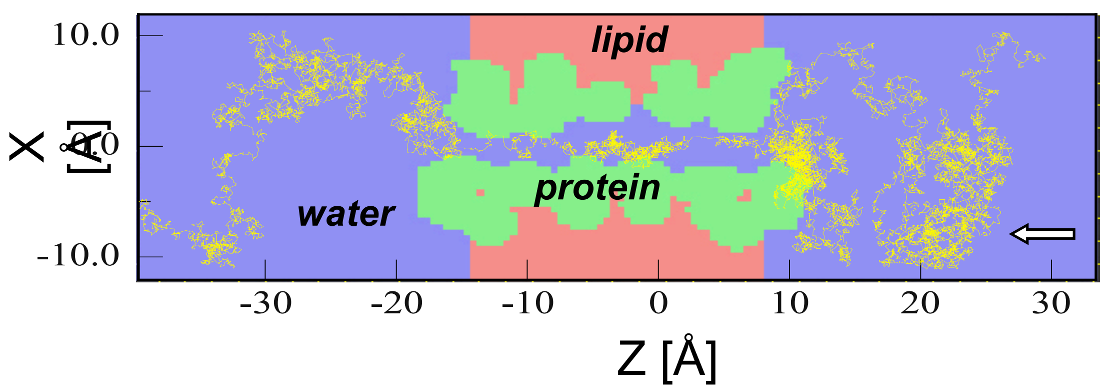
Accomplishments:

NCN student on TeraGrid (Gulzar Kathawala)

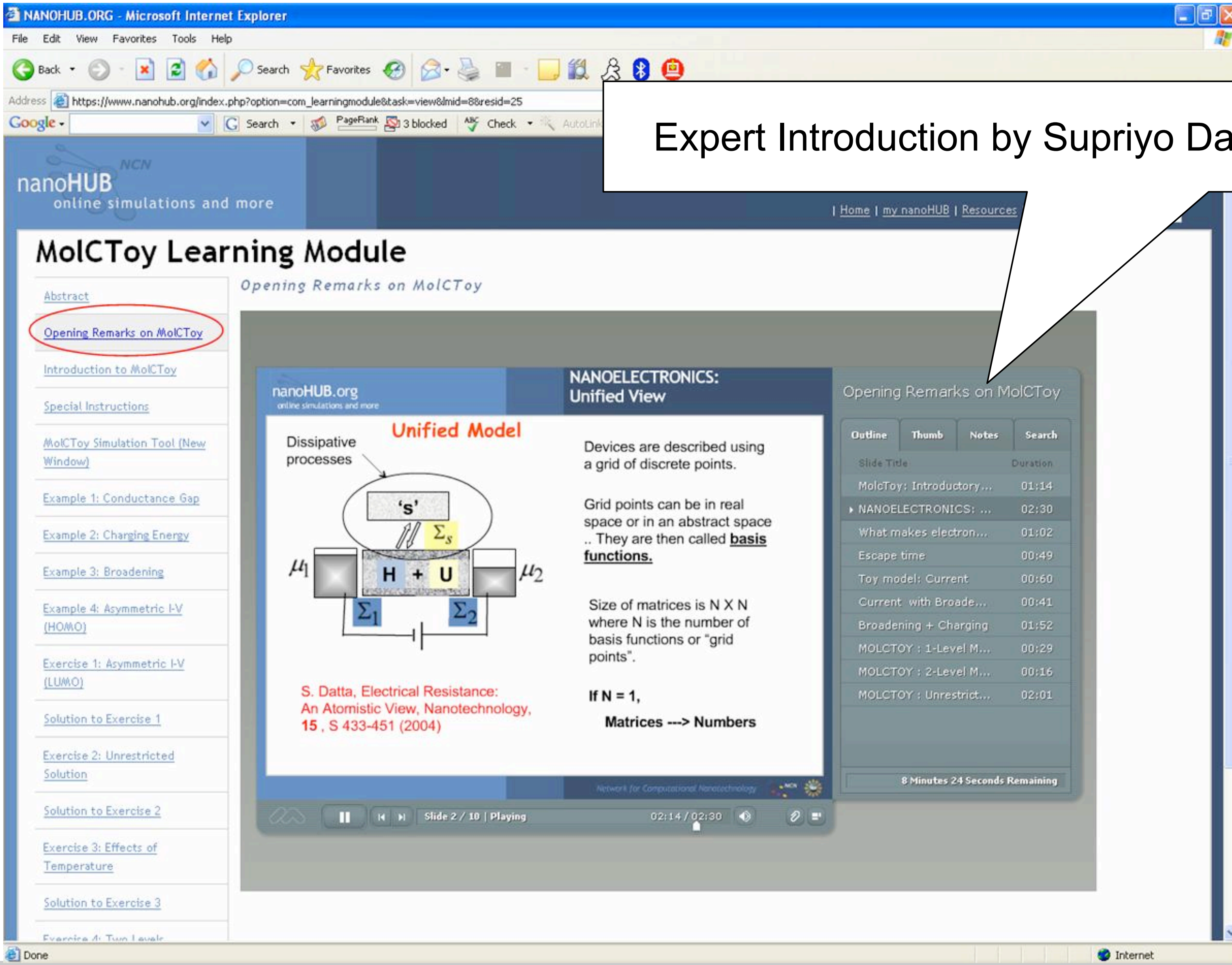
MOCA and BioMOCA ported to TeraGrid

~75,000 SUs used on TeraGrid

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



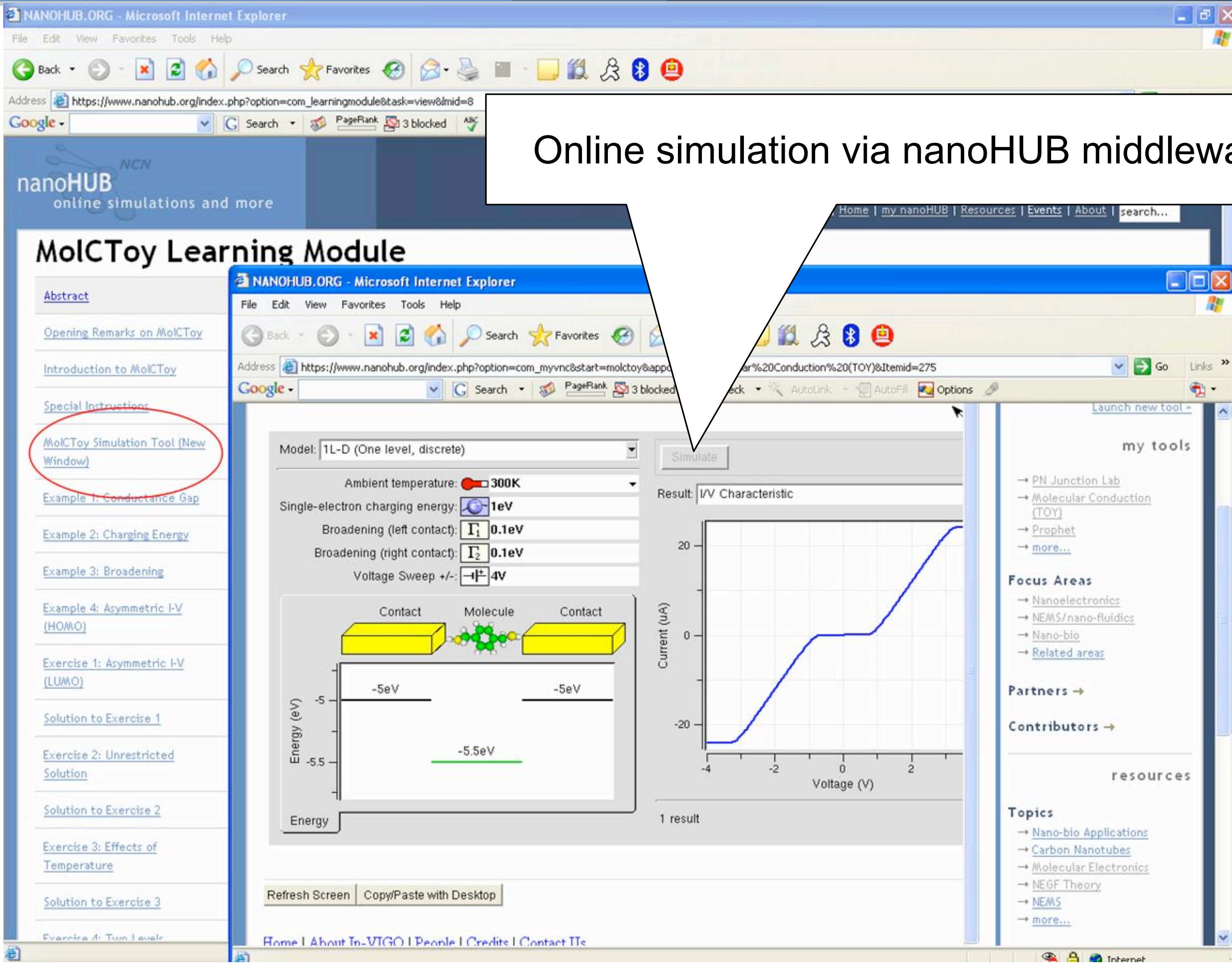
Molecular Conduction Learning Module



Expert Introduction by Supriyo Datta

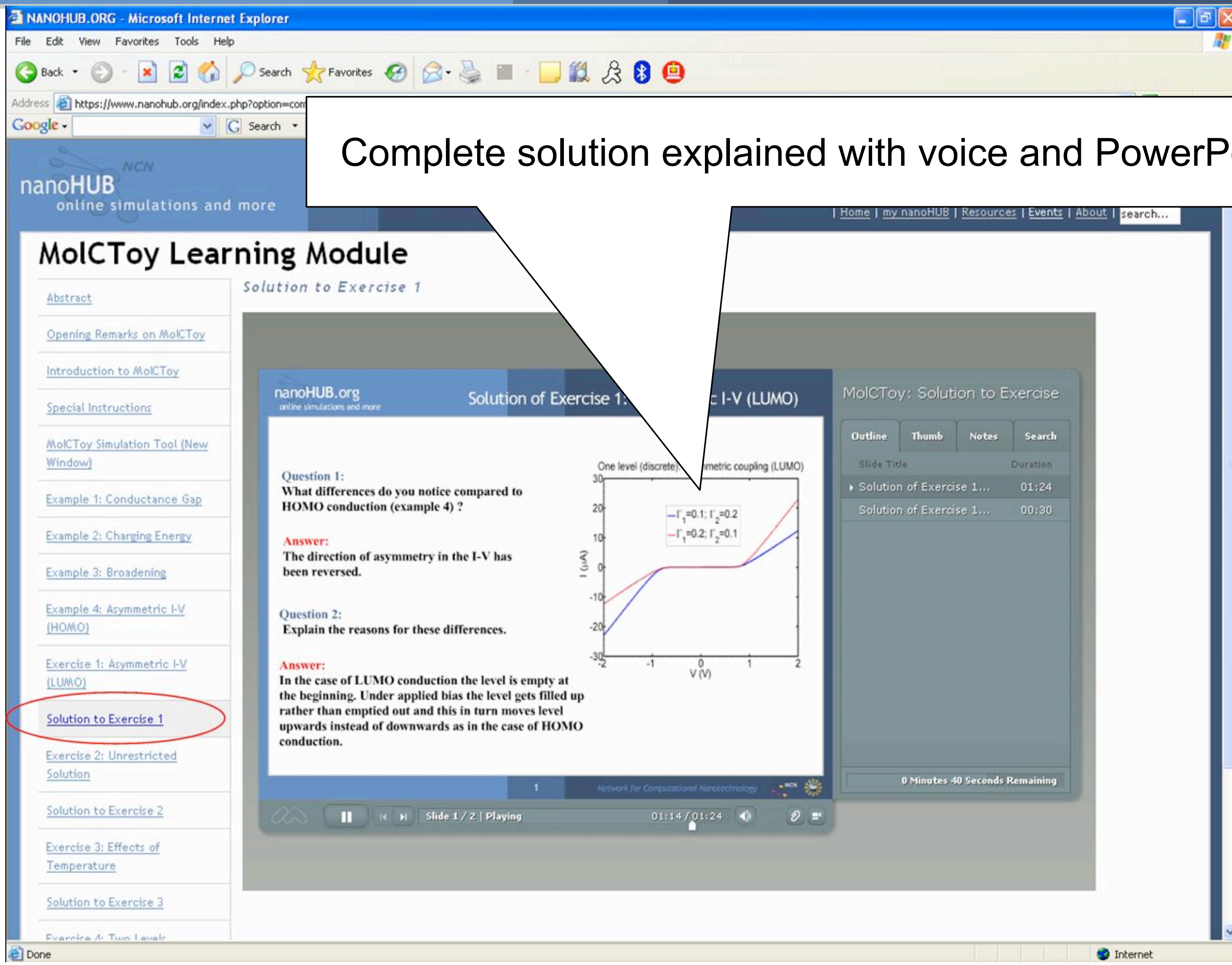
Molecular Conduction Learning Module

Online simulation via nanoHUB middleware

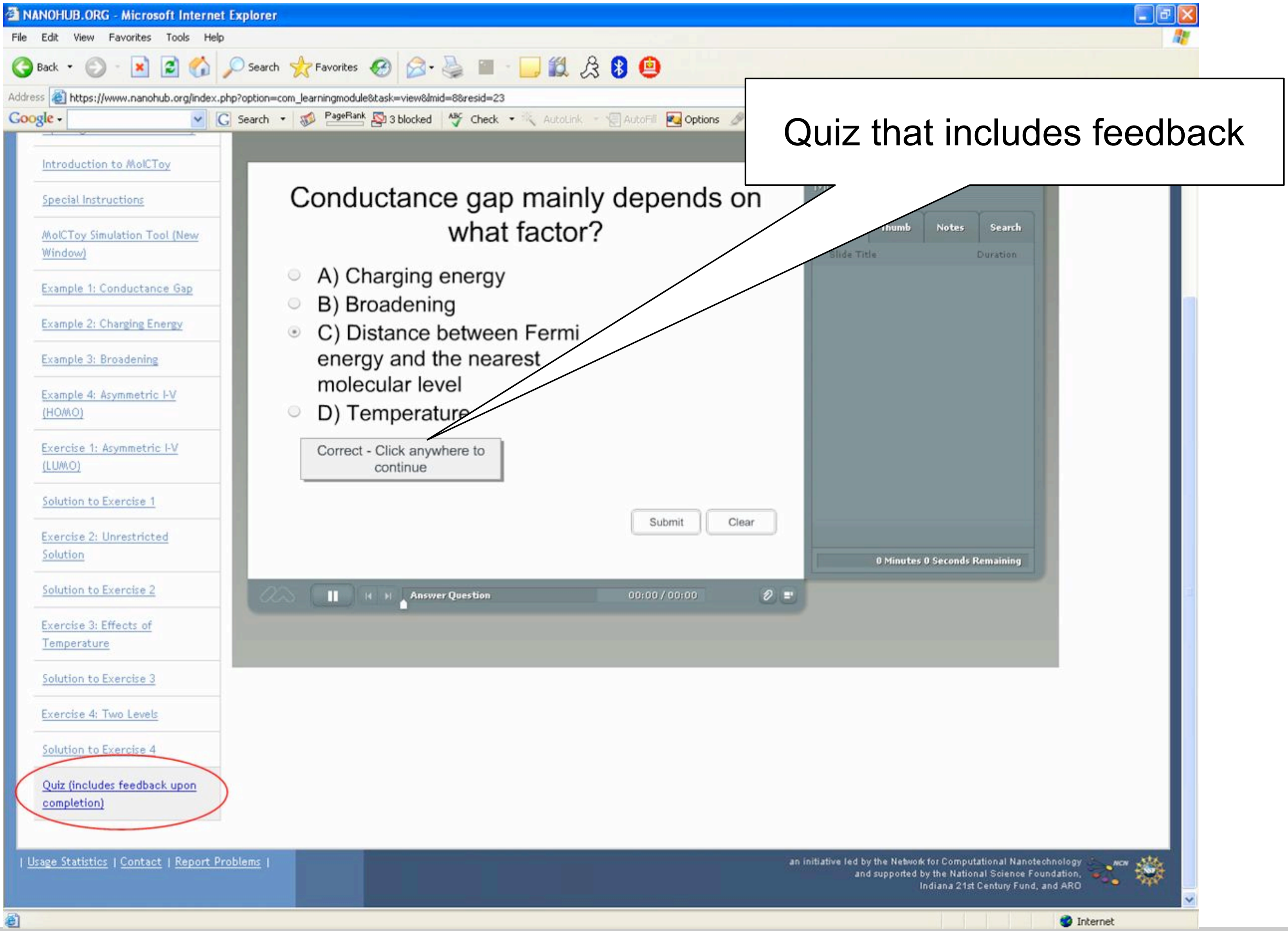


Molecular Conduction Learning Module

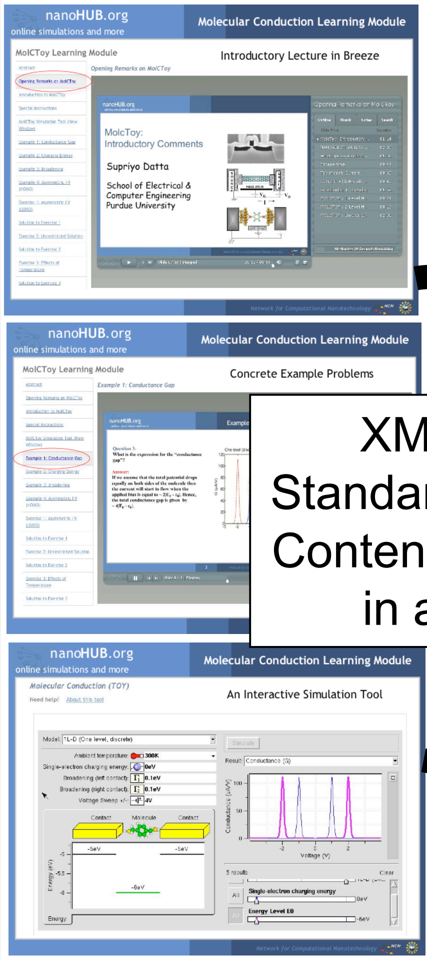
Complete solution explained with voice and PowerPoint



Molecular Conduction Learning Module

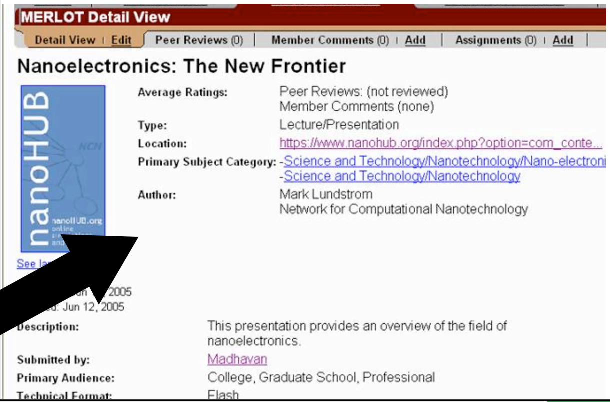


Leveraging Educational Standards



XML-based Standard Compliant Content Description in a ZIP file

National Learning Module Database - MERLOT



Course Management Systems

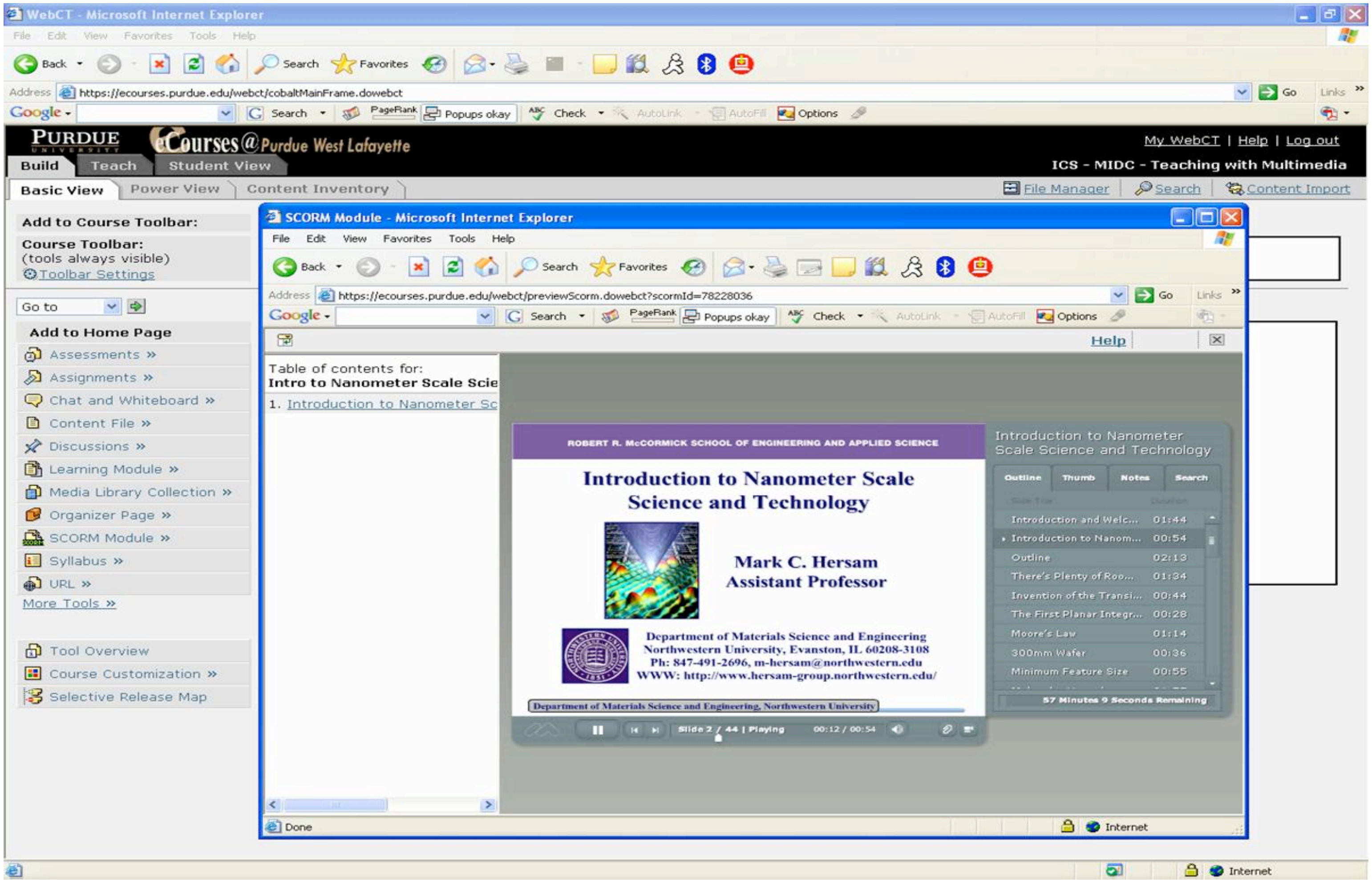
WebCT Vista™

Blackboard

Sakai™

Thousands Of Users At Most Universities

Example of content interoperability



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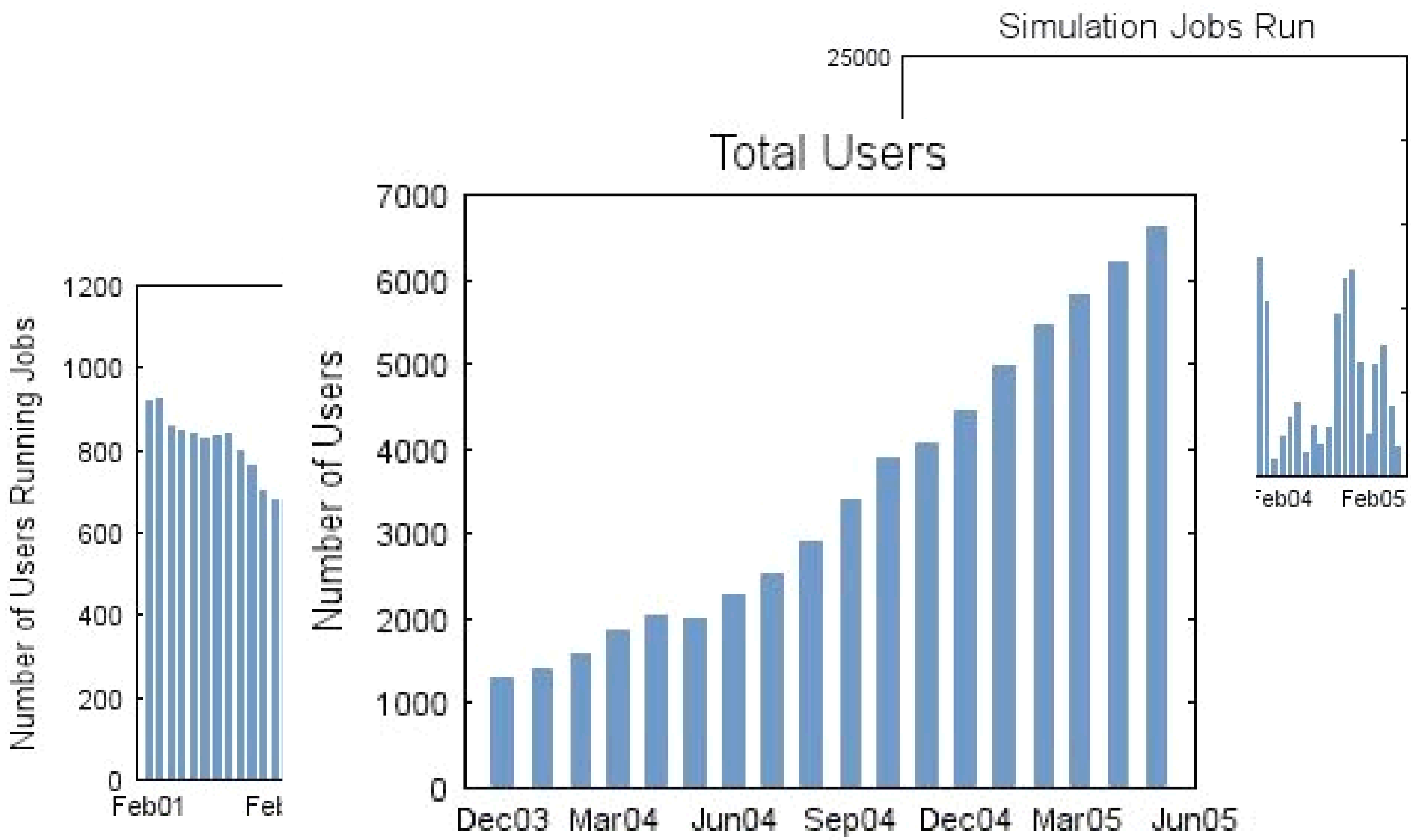
online simulations and more

Users ?



NCN

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online simulations and much, much more