



nanoHUB



The Nanotechnology Simulation Hub
Online computing for Nanotechnology
Operated by the Computational Electronics Lab at
Purdue University.

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5/24/2002

1



Summary



- n What is the nanoHUB ?
- n What's behind the nanoHUB ?
- n A bit of History
- n Running a simulation
- n Some statistics
- n Usage policies
- n Links

5/24/2002

2



What is the nanoHUB ?

- n A web-site for online computing through the web.
- n A repository of open source research codes for the nanotechnology community (nanoMOS...)
- n A place to find information and share knowledge about nanotechnology challenges (Forums)
- n The place to go to learn and do research on new techniques and new devices (NEGF...carbon nanotubes...).
- n A portal for high-performance computing in nanotechnology (parallel computing using clusters).

5/24/2002

3

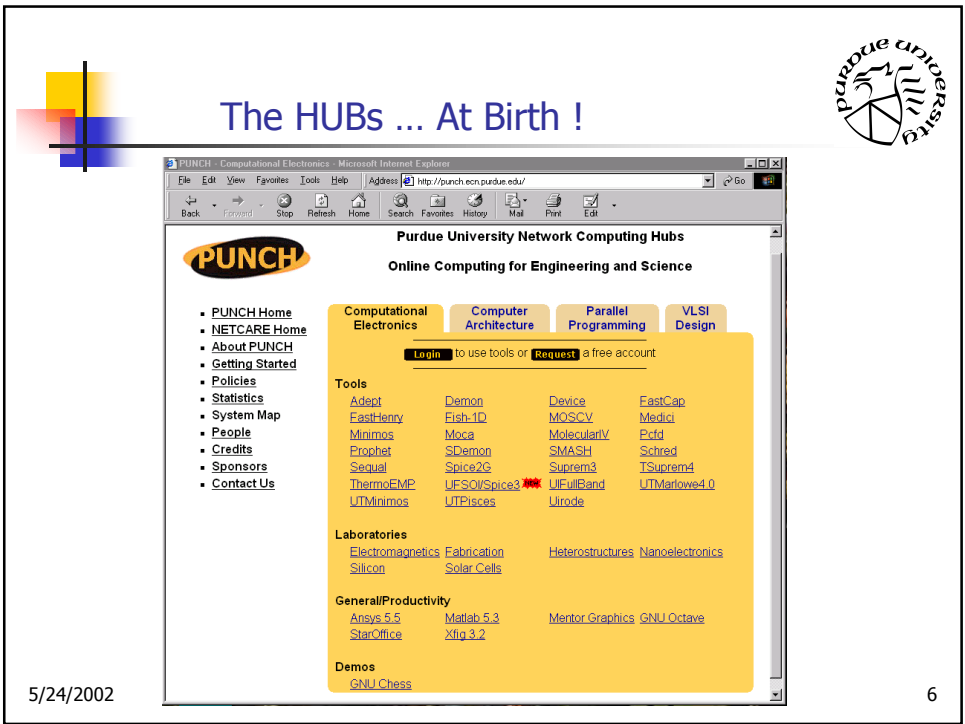
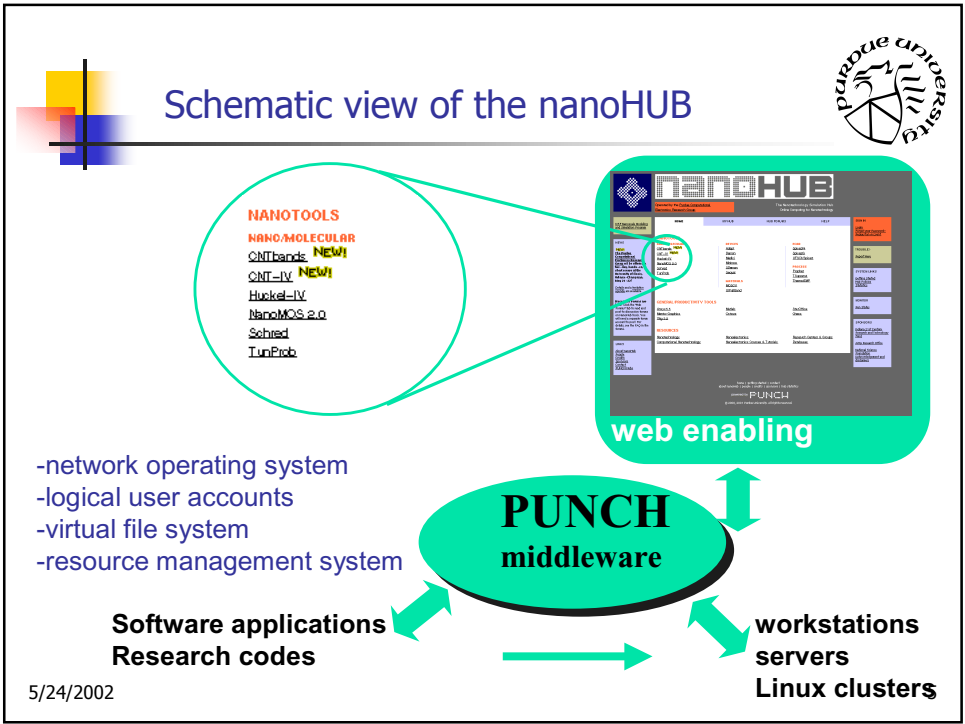



What is behind the nanoHUB ?

- n A regular web-site.....
- n Powered by a powerful interface to ship computing jobs to the appropriate computer...PUNCH !
- n PUNCH is what allows us/you to run jobs (interactive or not) through the nanoHUB.
- n A pool of machines is available for jobs submitted through the nanoHUB, resources are allocated depending on usage and job requirements.
- n This allows transparent use of workstations, supercomputers, linux clusters.

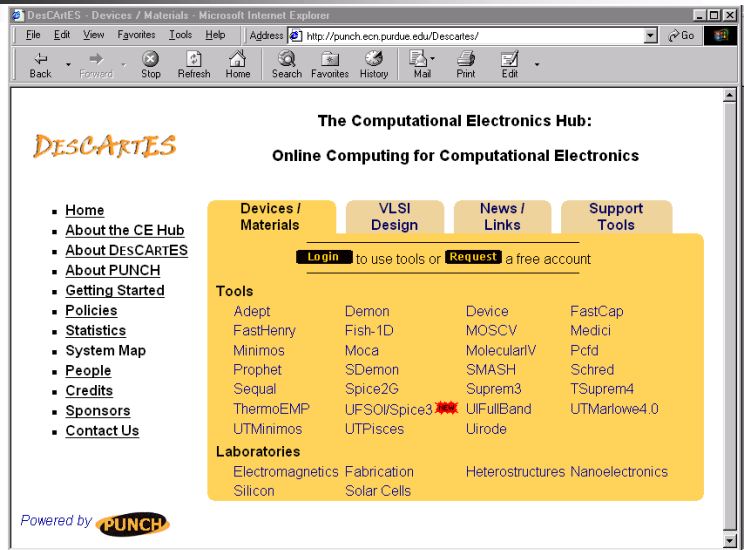
5/24/2002

4






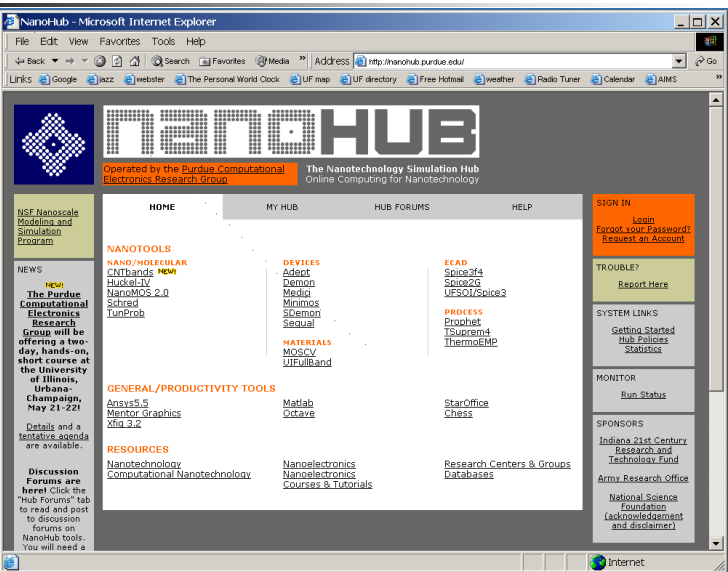
The HUBs...Yesterday !





5/24/2002 7




The nanoHUBtoday !



5/24/2002 8

A matlab script for DOS calculations of carbon nanotubes


CNTbands

[Hub Directory](#)

User: hundstro | Run CNTbands [Help](#) Available.



CNTbands-Related Information

[Description](#)
[Source](#)
[Questions](#)
[Run Status](#)


Run CNTbands

- [Execute CNTbands](#)
- [View/Download CNTbands Output Files](#)

5/24/2002 11

In the execute page you define the CNT


CNTbands: Execute

[Hub Directory](#) | [CNTbands](#) | [Step1:Execute](#) | [Step2:Output](#)

[Help](#) for Step2:Execute | User: hundstro

Carbon Nanotube Type	
n:	<input type="text" value="10"/>
m:	<input type="text" value="0"/>
Tight Binding Energy	
t (eV):	<input type="text" value="3"/>
Plot Options	
DOS Energy Range (eV): <i>(from -x to +x)</i>	<input type="text" value="2.5"/>
Normalized Axial Wavevector [kt/ktmax]: <i>(from -x to +x)</i>	<input type="text" value="1"/>
Number of Unit Cell Atoms for 3-D Plot	<input type="text" value="10"/>
Plot Format(s)	
<input checked="" type="checkbox"/> GIF (Graphic Interchange Format)	
<input type="checkbox"/> PDF (Portable Document Format)	
<input type="checkbox"/> PS (PostScript)	
Output Folder:	<input type="text" value="cntbands"/>

5/24/2002 12



Then you run it ...!



Program Status

[Hub Directory](#) | [CNTbands](#) | [Step1.Execute](#) | [Step2.Output](#)

You are currently running 1 program(s) (Maximum Allowed: 3).

Update Status Info OR Abort Selected Program(s) ...

cntbands (process #86). Status: running. Elapsed time: 14 seconds.
Machine: four-processor 296MHz Sun Enterprise server.
Credits: made possible by grants from the National Science Foundation.

[Hub Directory](#) | [CNTbands](#) | [Step1.Execute](#) | [Step2.Output](#)

5/24/2002

13



When done, you check the output files



CNTbands: Output

[Hub Directory](#) | [CNTbands](#) | [Step1.Execute](#) | [Step2.Output](#)

[Help](#) for Step3:Output | User: hndstro | Working Folder: /cntbands/Output/cntbands/

1. Select one of the commands from the categories a, b, or c.

	<input checked="" type="radio"/> View File OR Open Folder	<input type="text" value="j"/>	File Type:
a	<input type="radio"/> Delete File OR Folder	DOS.dat	Auto
	<input type="radio"/> Download File to Your Disk	DOS.gif	
		Ek.dat	
b	<input type="radio"/> Go To Examples Folder	Working Folder Will Not Change	
c	<input type="text"/>	Commands typed here <i>override</i> the check-box selections above.	

2. Execute the selected command

[Hub Directory](#) | [CNTbands](#) | [Step1.Execute](#) | [Step2.Output](#)

Nanotechnology Simulation Hub
[PUNCH User's Manual](#) | [PUNCH-Related Questions/Comments](#)

5/24/2002

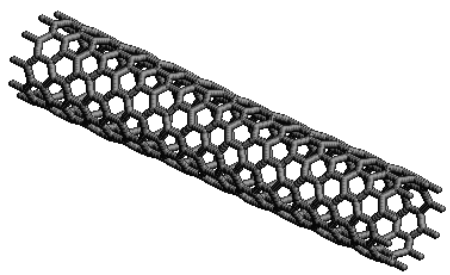
14



You can get a molecular view of the CNT !



Use RasMol to view the .pdb file



5/24/2002

15



The nanoHUB, some statistics



PUNCH: ~ 2500 users in 35 countries
>7M hits / almost 400,000 simulations
3 Hubs, nanoHUB, Netcare, EDASHub

nanoHUB: 74 users in 22 countries
>2000 simulations
>150 source downloads

5/24/2002

16



Usage Policy



- n Only one account !
- n 5 simulations allowed at once !
- n Request a separate account for the forums.
- n Some tools are public, some are not !
- n If your are not from Purdue you can only use public tools – all nanotools developed by the CELAB are public/open source.

5/24/2002

17



Tips for using the nanoHUB



- n Some file downloads do not have the proper name....Internal problem of PUNCH.
- n Rename file name at download !
- n Try different browser if you experience problems viewing pages.
- n Use the forums, so we can grow the nanoHUB community !

5/24/2002

18



More tips...



- n You login.....but there is no logout !
- n Interactive tools request your password...VNC authentication...this is the same password.
- n You can find help on the Forums, or by sending email to punch@purdue.edu or by sending email to the author of the tool directly.
- n Download the manuals
- n Check out the examples folder
- n Do not forget that you can use the command line !

5/24/2002

19



Links



- n PUNCH (portal to Netcare,EDAHub and nanoHUB, more information about the nanoHUB internals)
<http://punch.purdue.edu>
- n nanoHUB (nanotools and standard microelectronics tools, codes download, links, forums)
<http://www.nanohub.purdue.edu>
- n CELAB (The team behind the nanoHUB and the nanotools, more paper/presentation/Ph-d thesis downloads)
<http://ece.purdue.edu/celab>

5/24/2002

20