

# HUBzero Platform Features

TRADES Proposal Demo

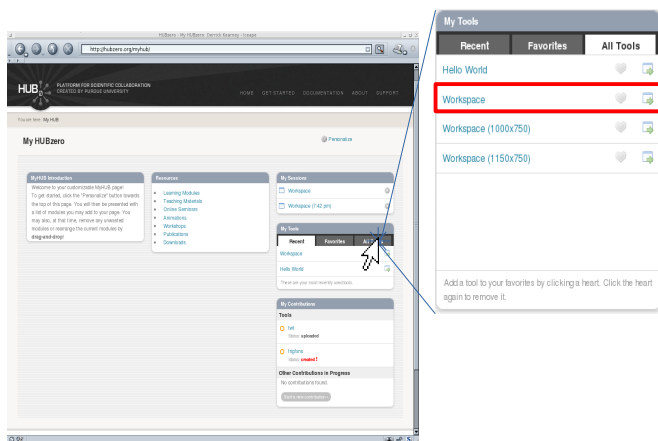
Oct. 12, 2016

Derrick Kearney

[hubzero.org](http://hubzero.org)

# The HUBzero Platform

## User's Web Browser



## HUBzero Infrastructure

Web Server

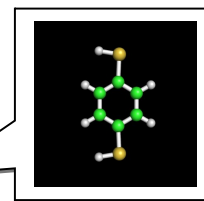
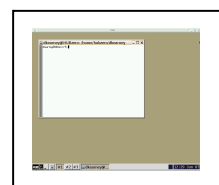
Middleware

## Grid

Submit Proxy

Tool Session Containers

Visualization



# CNTbands

Structure: Carbon Nanotube

Simulation Method: Pz orbital

Chirality (n,m)

n: 7

m: 7

Model parameters

Tight Binding Energy: 3eV

Carbon-carbon spacing: 1.42Å

Length in 3-D view: 40

Simulate

new input parameters

### CNTbands

Learn about Carbon Nanostructure physics as you explore the devices in this simulator.

Enter values on the left, then push the Simulate button. Simulation results will appear here.

For nanotubes, try  $n=7$ ,  $m=7$  (7,7) to see an "armchair" metallic nanotube. Then try a (12,0) "zigzag" nanotube, which is a different kind of metallic nanotube. Next, try a (13,0) zigzag nanotube. The energy gap in the band diagram tells you that this last one is semiconducting.

Then select the nanoribbon device, type A, and try (3,3) for a "zigzag-edge" nanoribbon. Next try a (4,0) "armchair-edge", semiconducting nanoribbon.

This application is powered by: Octave and Fortran 77. Last updated April 2010.

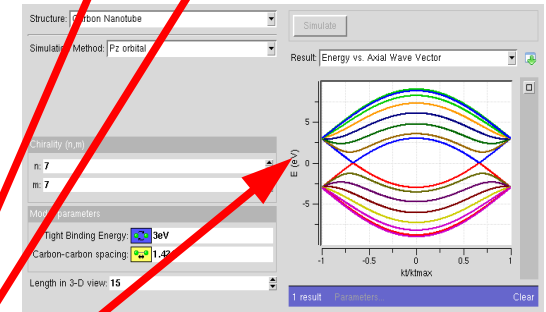
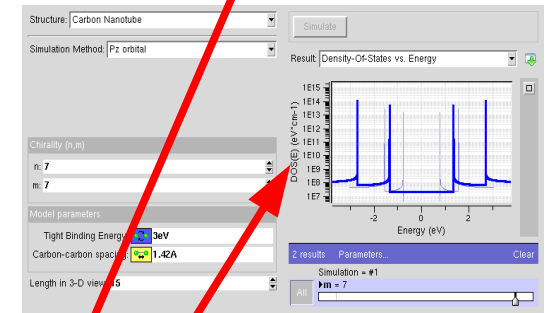
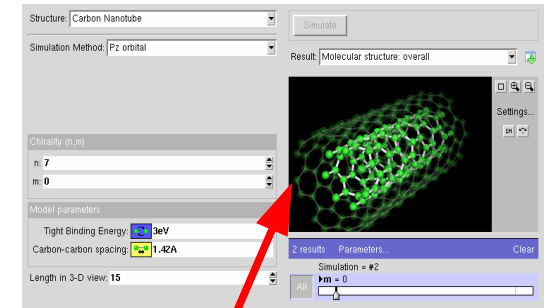
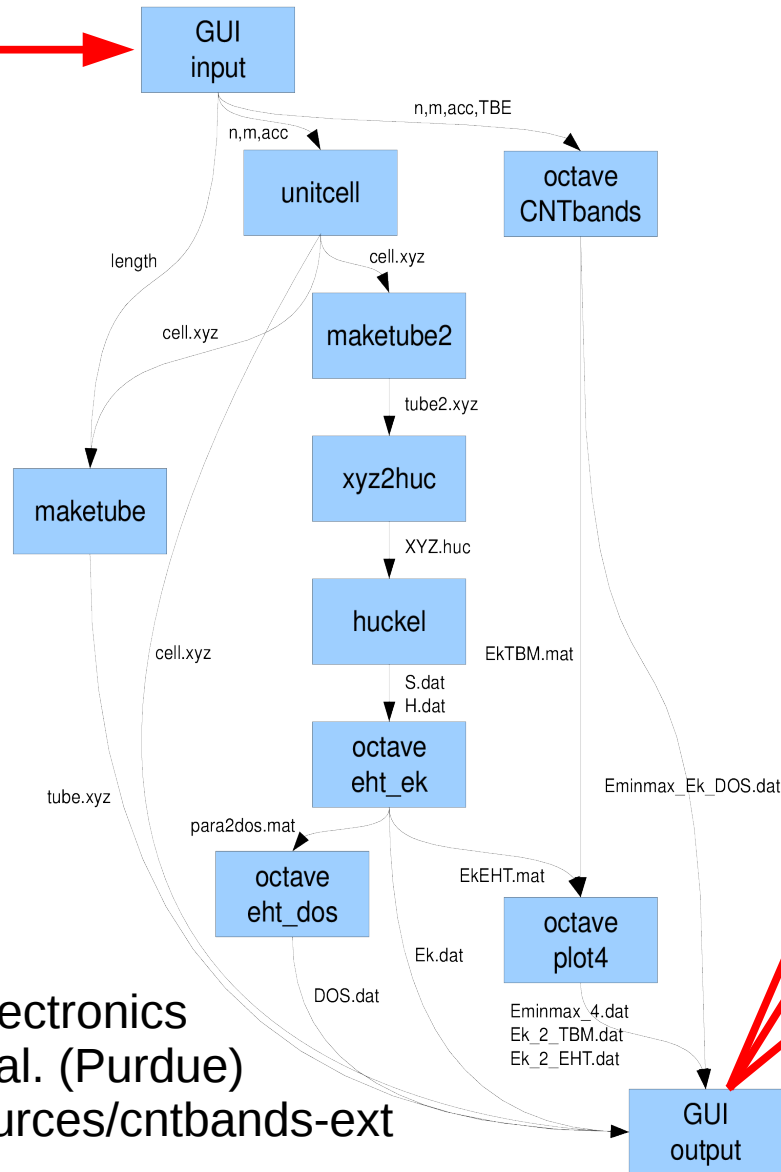
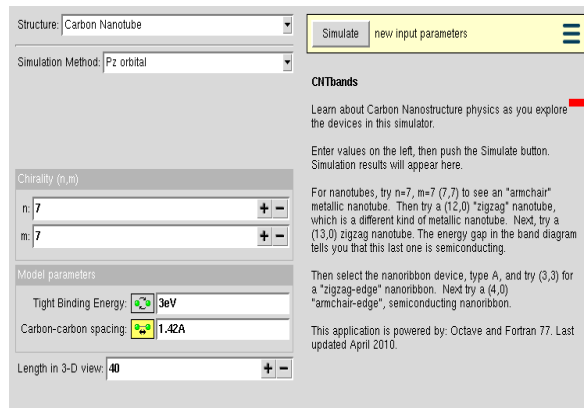
## CNTbands

Science Domain: Nanoelectronics

Scientists: Lundstrom et al. (Purdue)

<https://nanohub.org/resources/cntbands-ext>

# CNTbands



## CNTbands

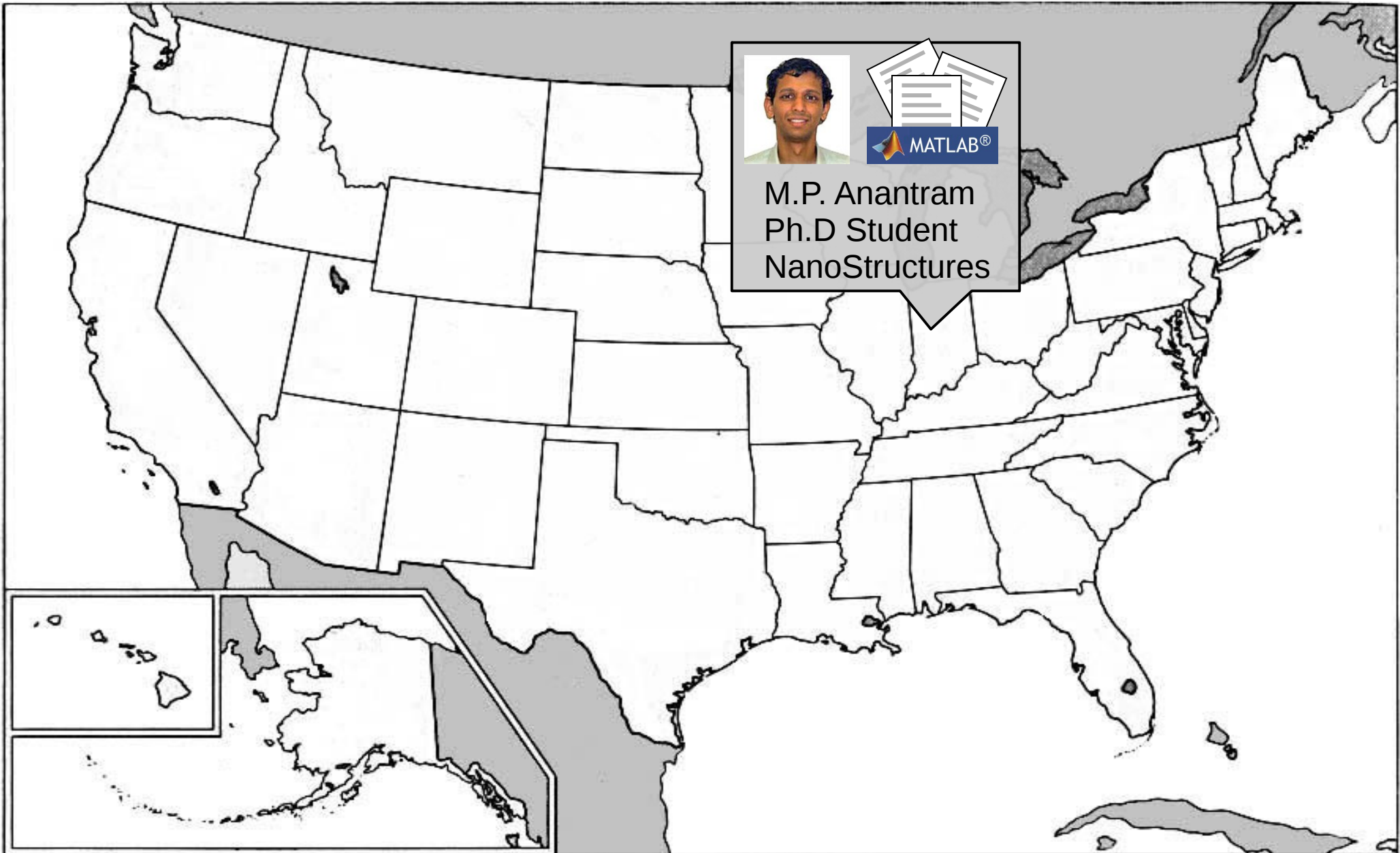
Science Domain: Nanoelectronics  
Scientists: Lundstrom et al. (Purdue)

<https://nanohub.org/resources/cntbands-ext>

# 1990s – Pre CNTbands



M.P. Anantram  
Ph.D Student  
NanoStructures



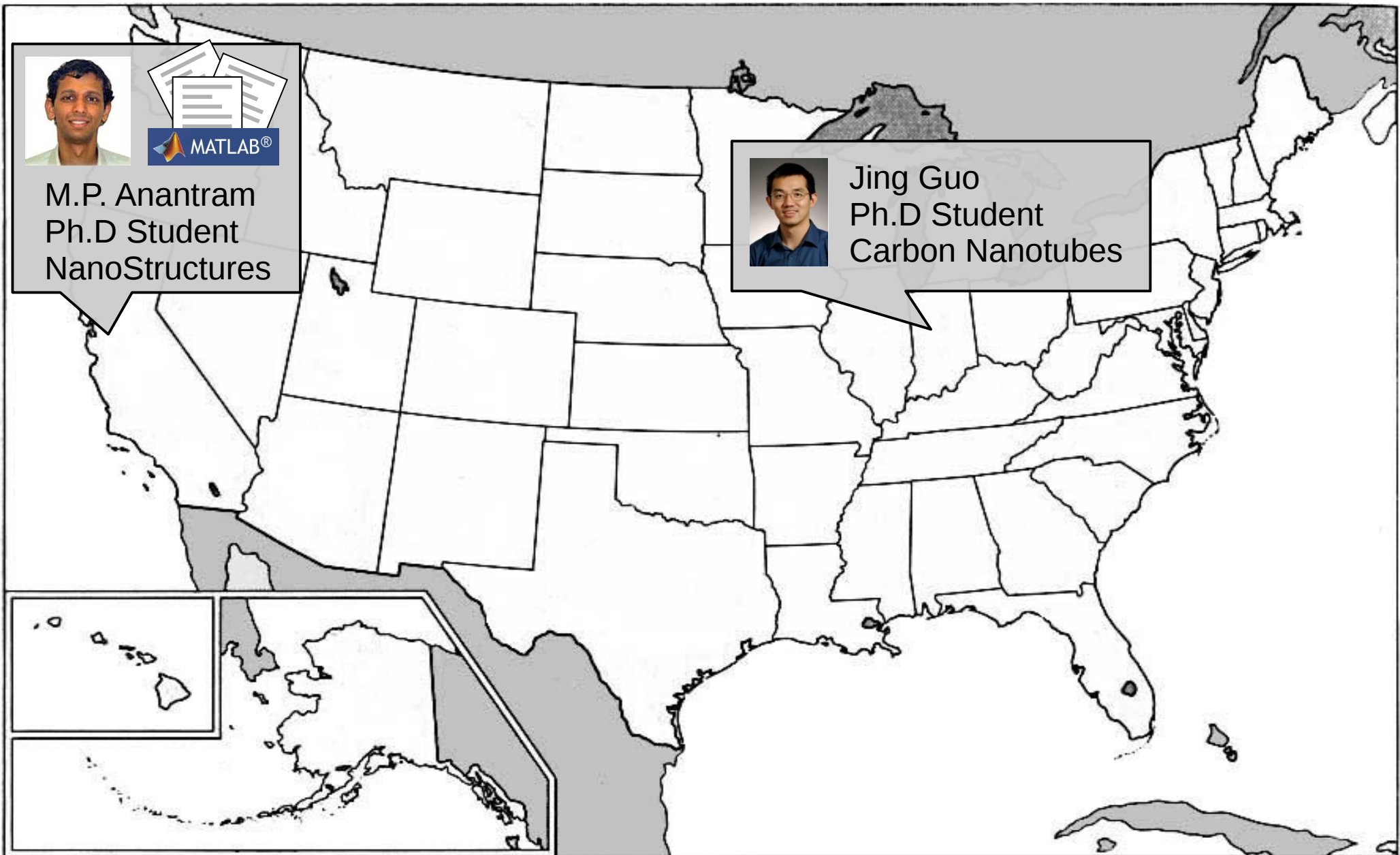
# 2002 – CNTbands Ideas



M.P. Anantram  
Ph.D Student  
NanoStructures



Jing Guo  
Ph.D Student  
Carbon Nanotubes

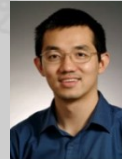




# 2002 – CNTbands Registered



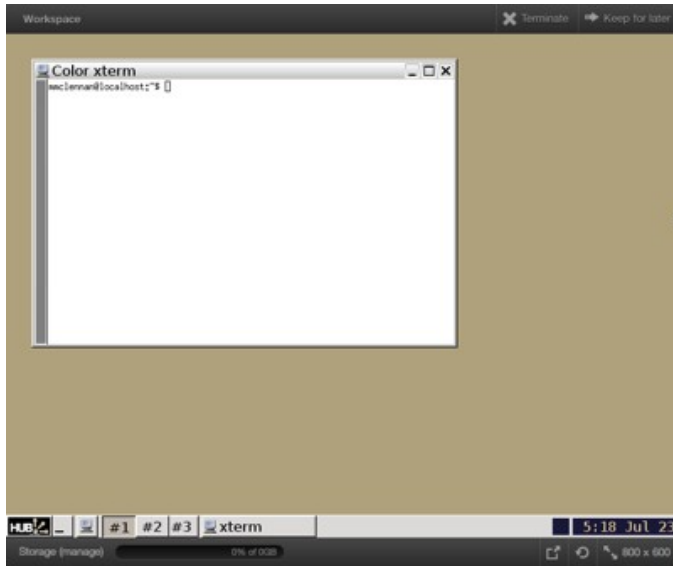
M.P. Anantram  
Ph.D Student  
NanoStructures



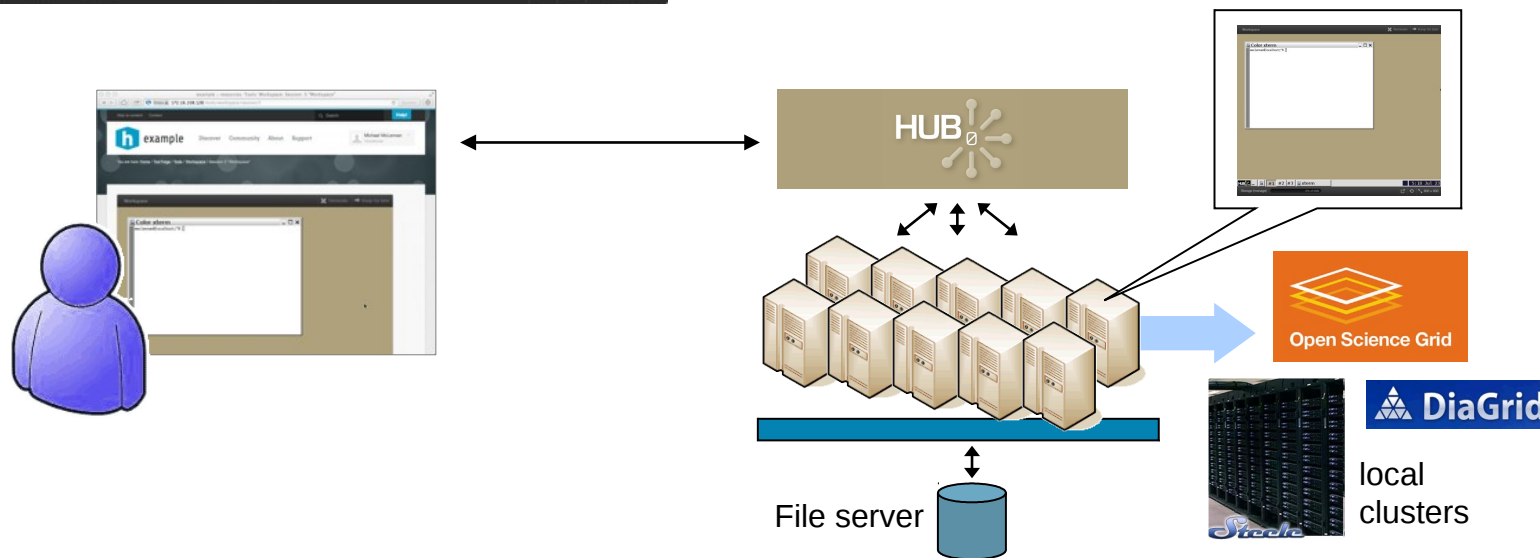
Jing Guo  
Ph.D Student  
Carbon Nanotubes



# What is a workspace?

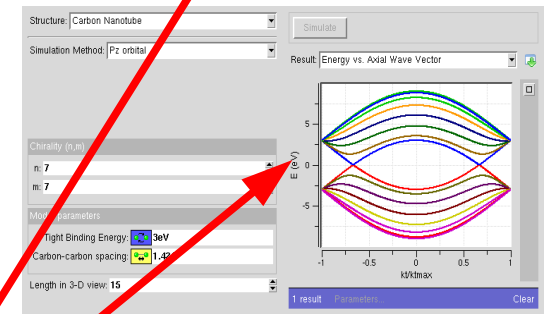
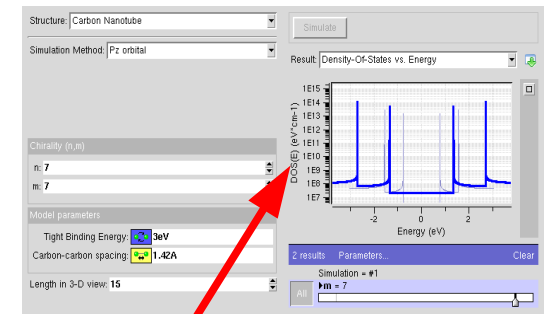
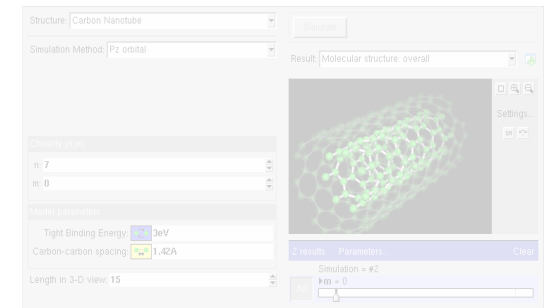
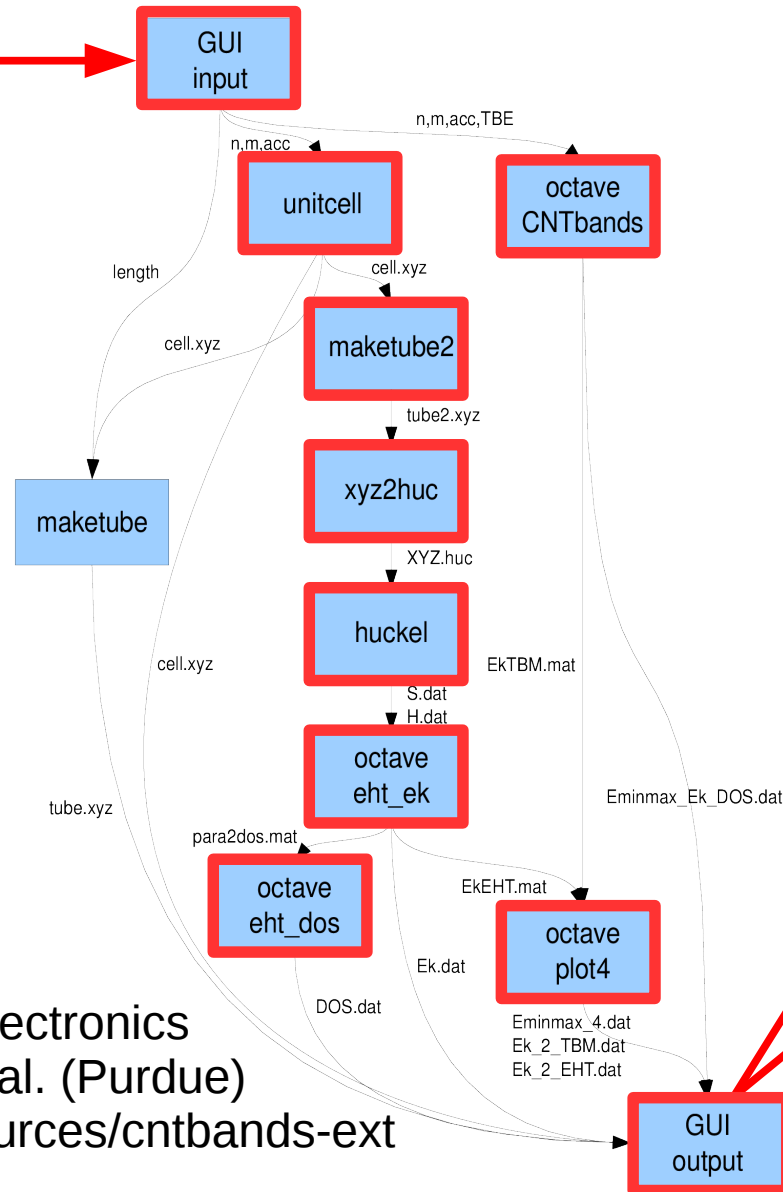
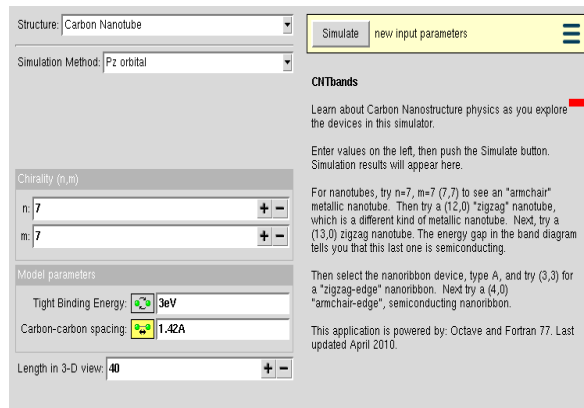


- Full-featured Linux desktop
- For tool developers
- For researchers
- Accessible from any web browser
- Still running after you close your browser
- Access to computational clusters
- File storage provided by the hub





# CNTbands



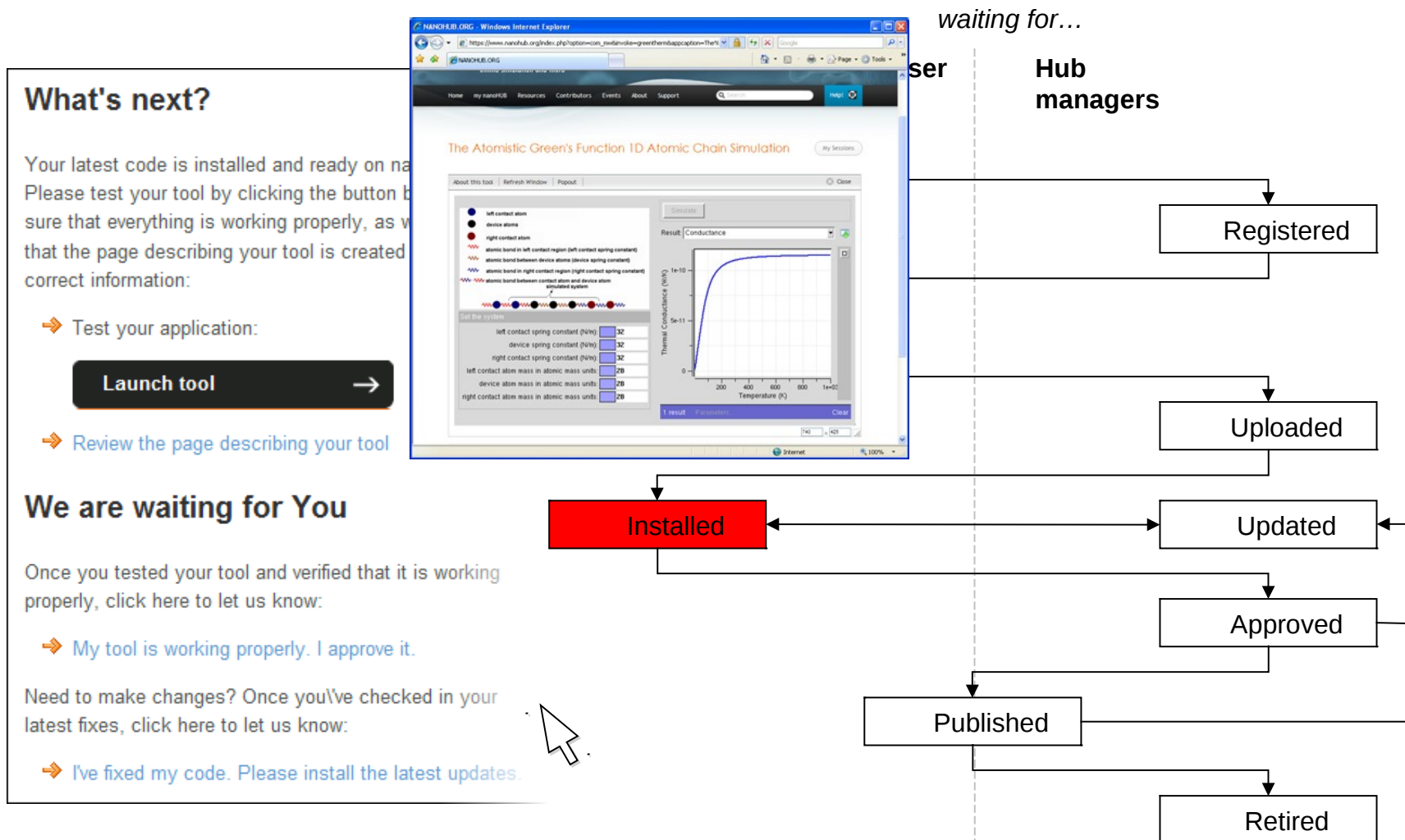
## CNTbands

Science Domain: Nanoelectronics  
Scientists: Lundstrom et al. (Purdue)

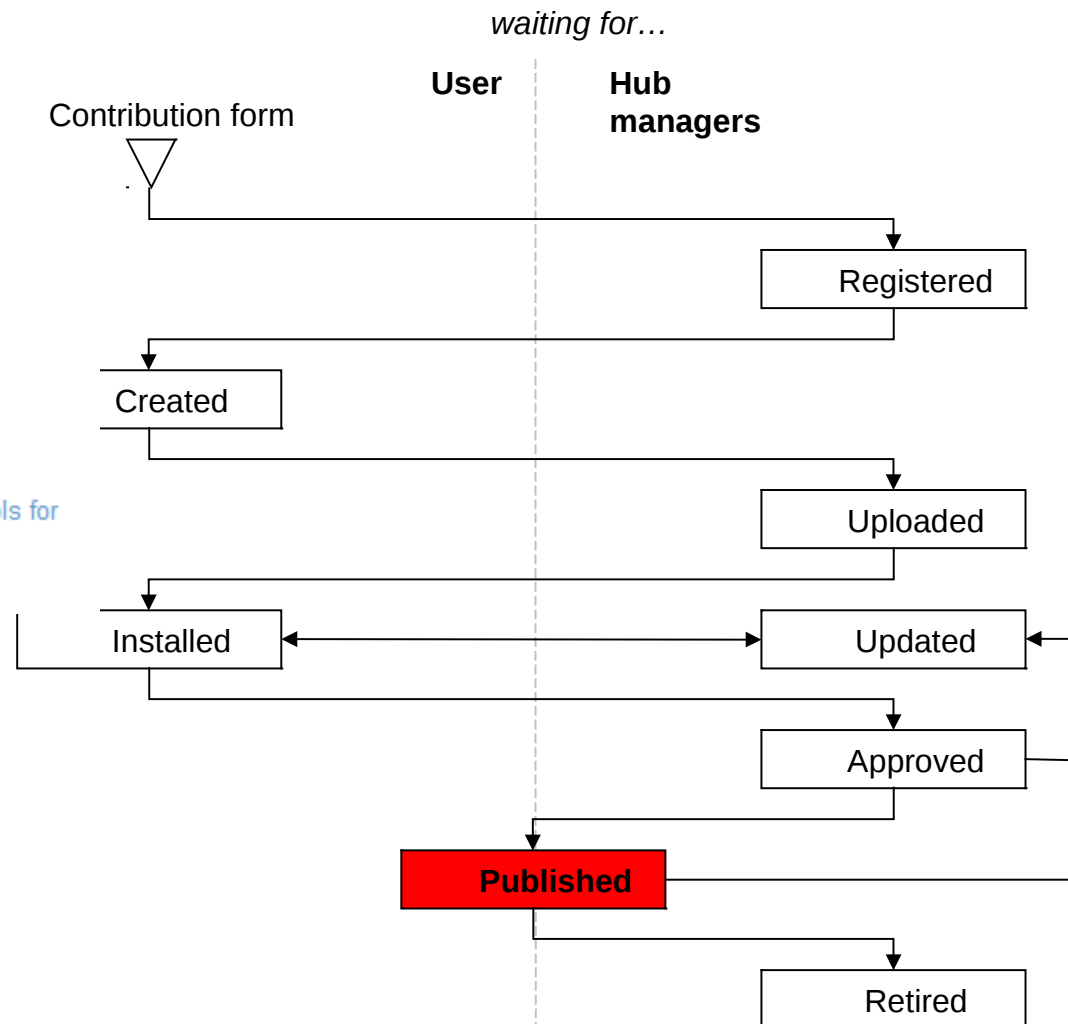
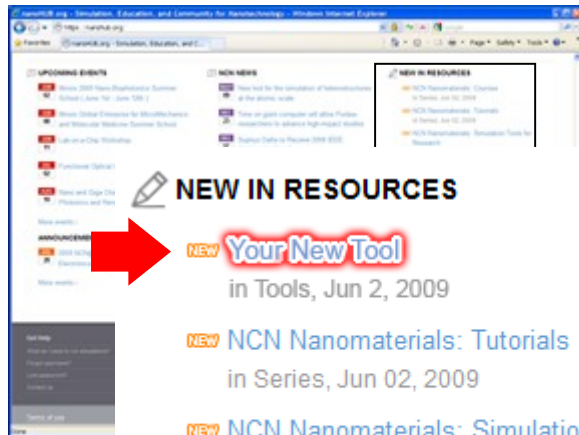
<https://nanohub.org/resources/cntbands-ext>

# Collaboration / Groups

# Installing & Testing Applications



# CNTbands is Published



# Knowing your impact

## CNTbands

By Gyungseon Seol<sup>1</sup>, Youngki Yoon<sup>1</sup>, James K Fodor<sup>1</sup>, Jing Guo<sup>1</sup>, Akira Matsudaira<sup>2</sup>, Diego Kienle<sup>2</sup>, Gengchiao Liang<sup>2</sup>, Gerhard Klimeck<sup>2</sup>, Mark Lundstrom<sup>2</sup>, Ahmed Ibrahim Saeed<sup>3</sup>

1. University of Florida 2. Purdue University 3. Ain Shams University

This tool simulates E-k and DOS of CNTs and graphene nanoribbons.

Edit

Launch Tool

Version 2.7.2 - published on 22 Sep 2014

doi:10.4231/D3GB1XH9j cite this

Open source: license | download



First-Time User Guide  
View All Supporting Documents

● ● ● ● Easy-Expert

★ NCN Supported

5611 users, detailed usage

16 Citation(s)

17 questions (Ask a question)

4 review(s) (Review this)

4 wish(es) (New Wish)

→ Share: ...

About

Usage

Citations

Questions

Reviews

Wishlist

Versions

Supporting Docs

Classroom usage



See also

Part of: NCN  
Nanoelectronics:  
Simulation Tools  
for Education

Part of: NCN  
Nanoelectronics:

# Communicate with users

## CNTbands

By Gyung-Guo<sup>1</sup>, Ali-Liang<sup>2</sup>, Gibraili<sup>3</sup>  
1. University of Shams U  
This tool is  
nanoribbon

Easy-Expert

NCN Supported



5611 users, detailed usage

16 Citation(s)

17 questions (Ask a question)

4 review(s) (Review this)

4 wish(es) (New Wish)

Share:    ...

Published on 22

81XH9j cite

License |

ime User Guide  
will Supporting  
Documents

Easy-Expert

NCN Supported



5611 users, detailed usage

16 Citation(s)

17 questions (Ask a question)

4 review(s) (Review this)

4 wish(es) (New Wish)

Share:    ...

See also

Part of: NCN  
Nanoelectronics:  
Simulation Tools  
for Education

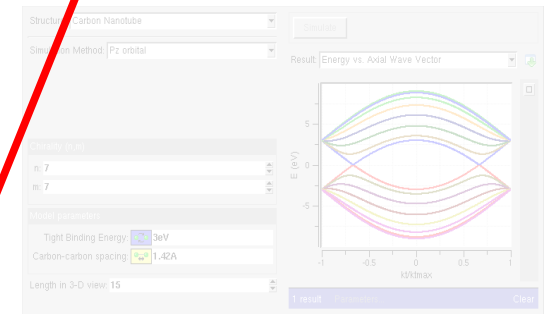
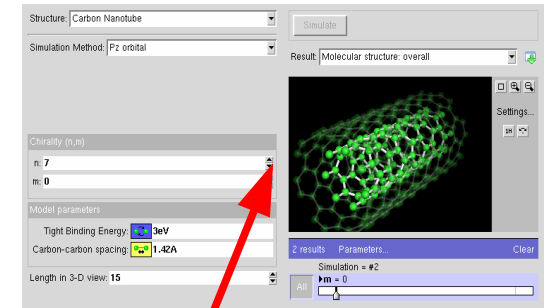
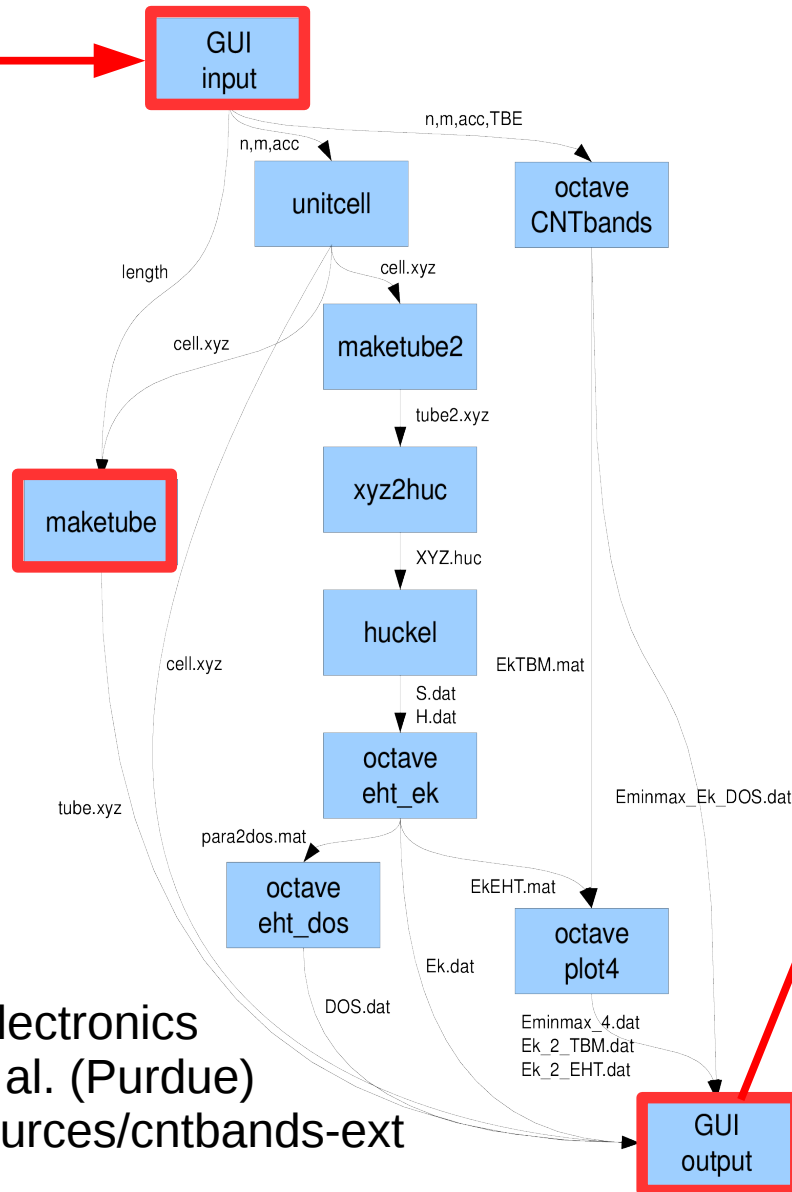
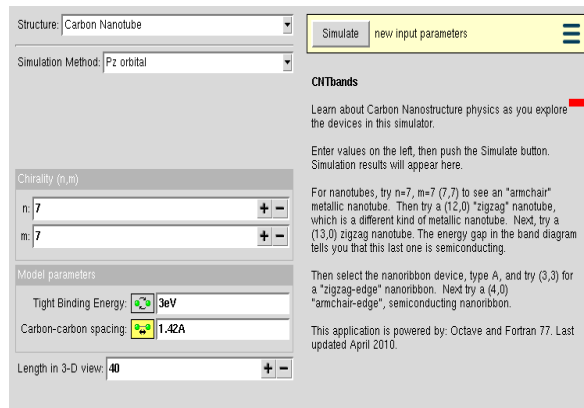
Part of: NCN  
Nanoelectronics:

Versions | Supporting Docs | Classroom usage



# New feature added



## CNTbands

Science Domain: Nanoelectronics  
Scientists: Lundstrom et al. (Purdue)

<https://nanohub.org/resources/cntbands-ext>

# 2010 – New Grad Students



M.P. Anantram  
Ph.D Student  
NanoStructures



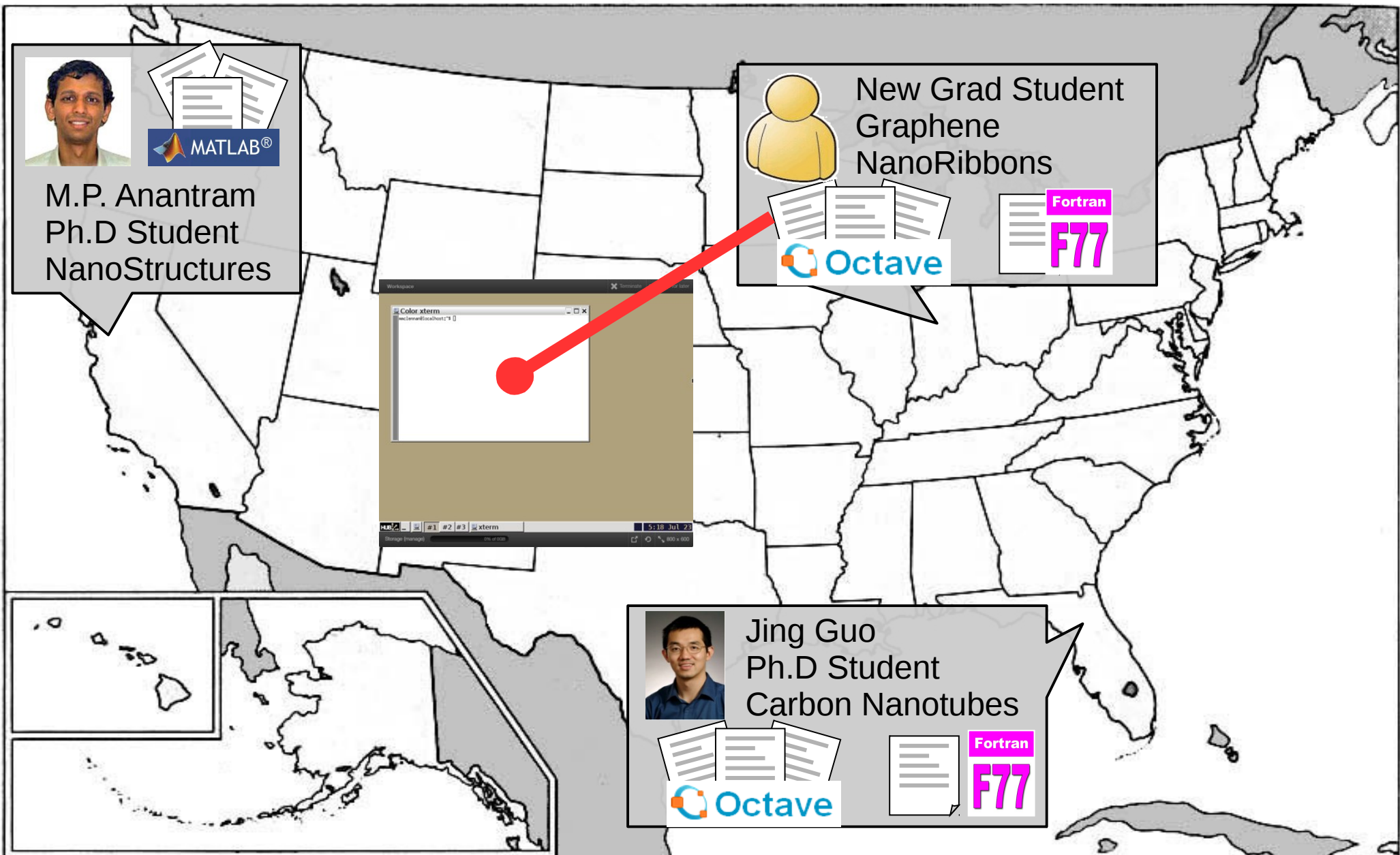
New Grad Student  
Graphene  
NanoRibbons



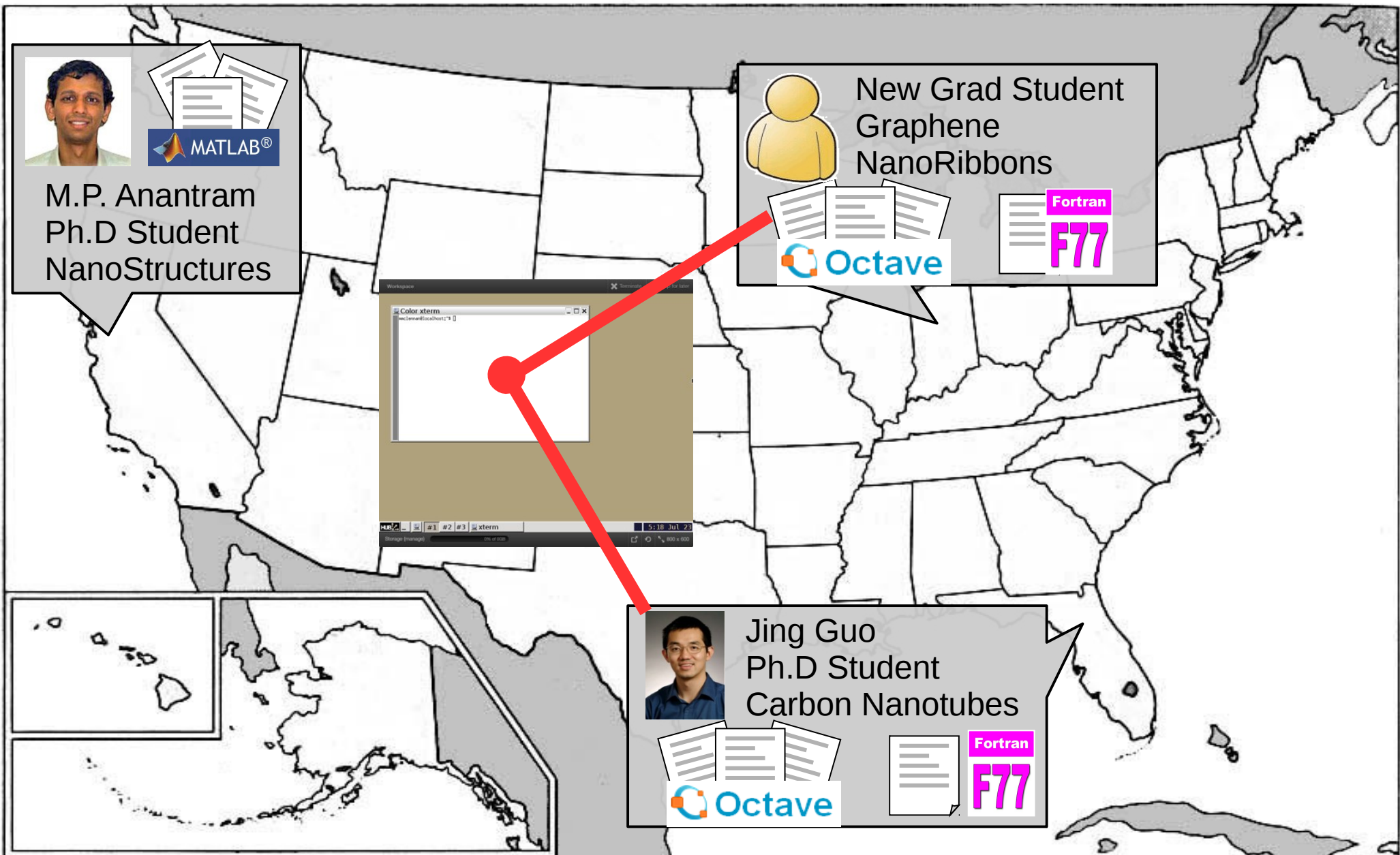
Jing Guo  
Ph.D Student  
Carbon Nanotubes



# Collaboration inside the Workspace

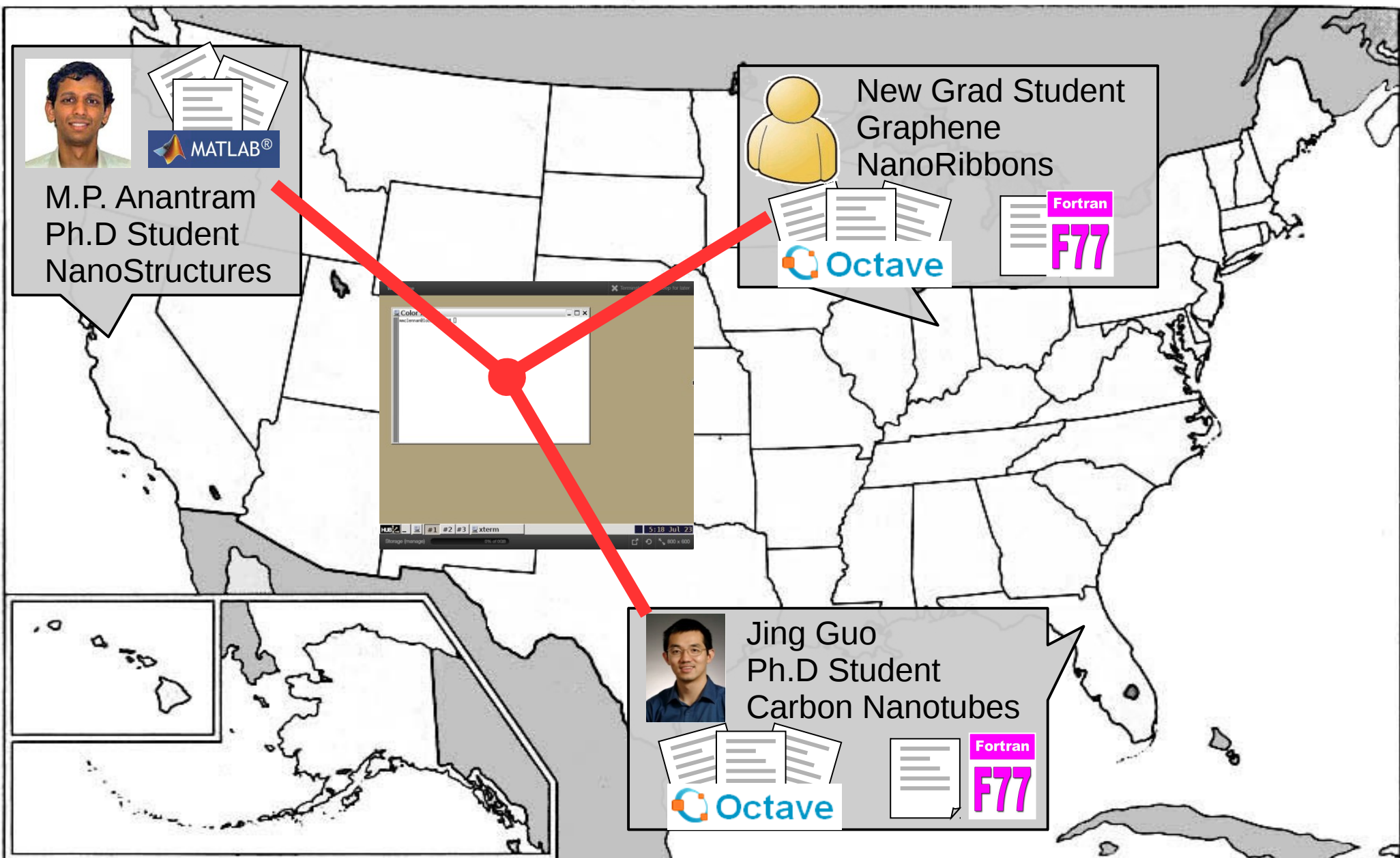


# Collaboration inside the Workspace





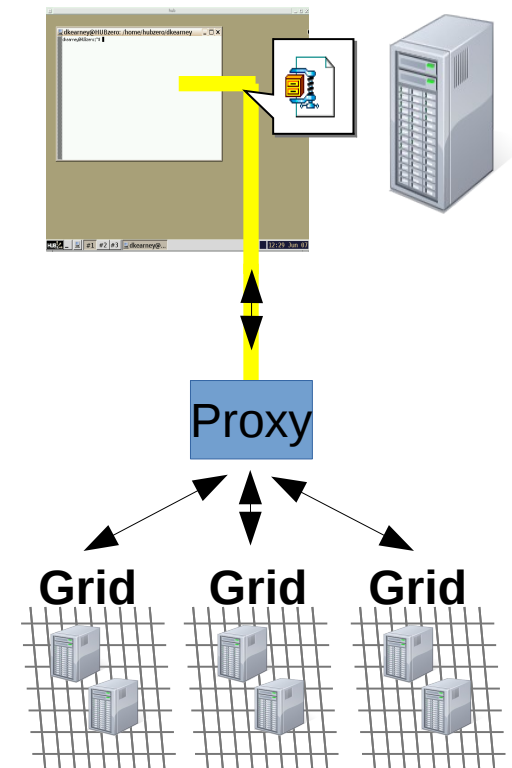
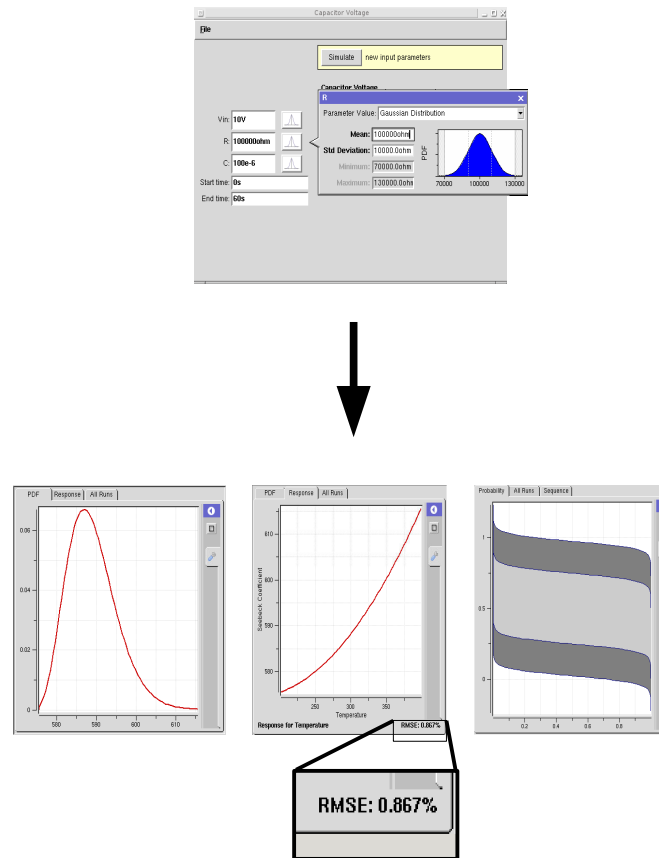
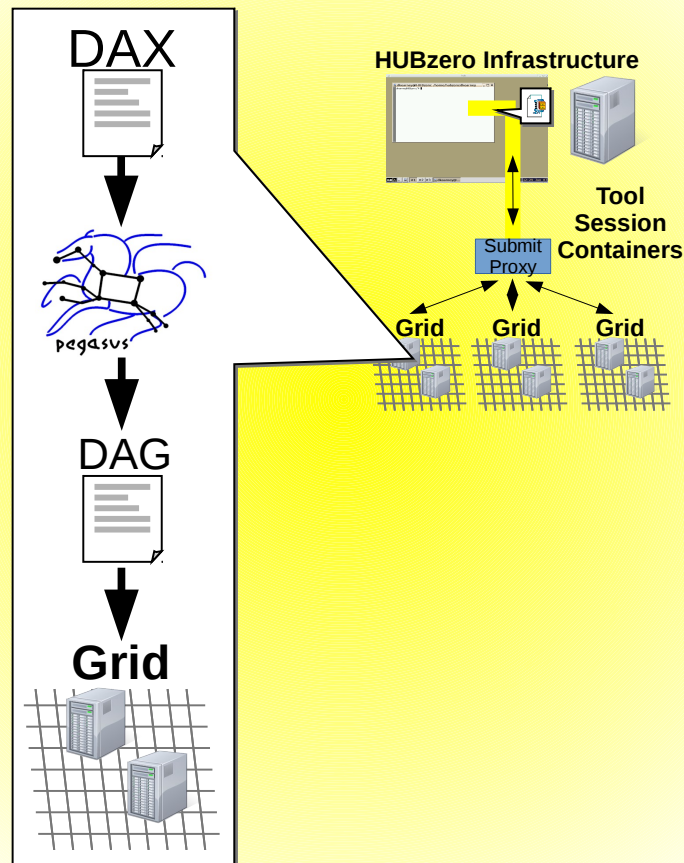
# Collaboration inside the Workspace



# Productivity in the Workspace

Pegasus Workflows    Uncertainty Quantification

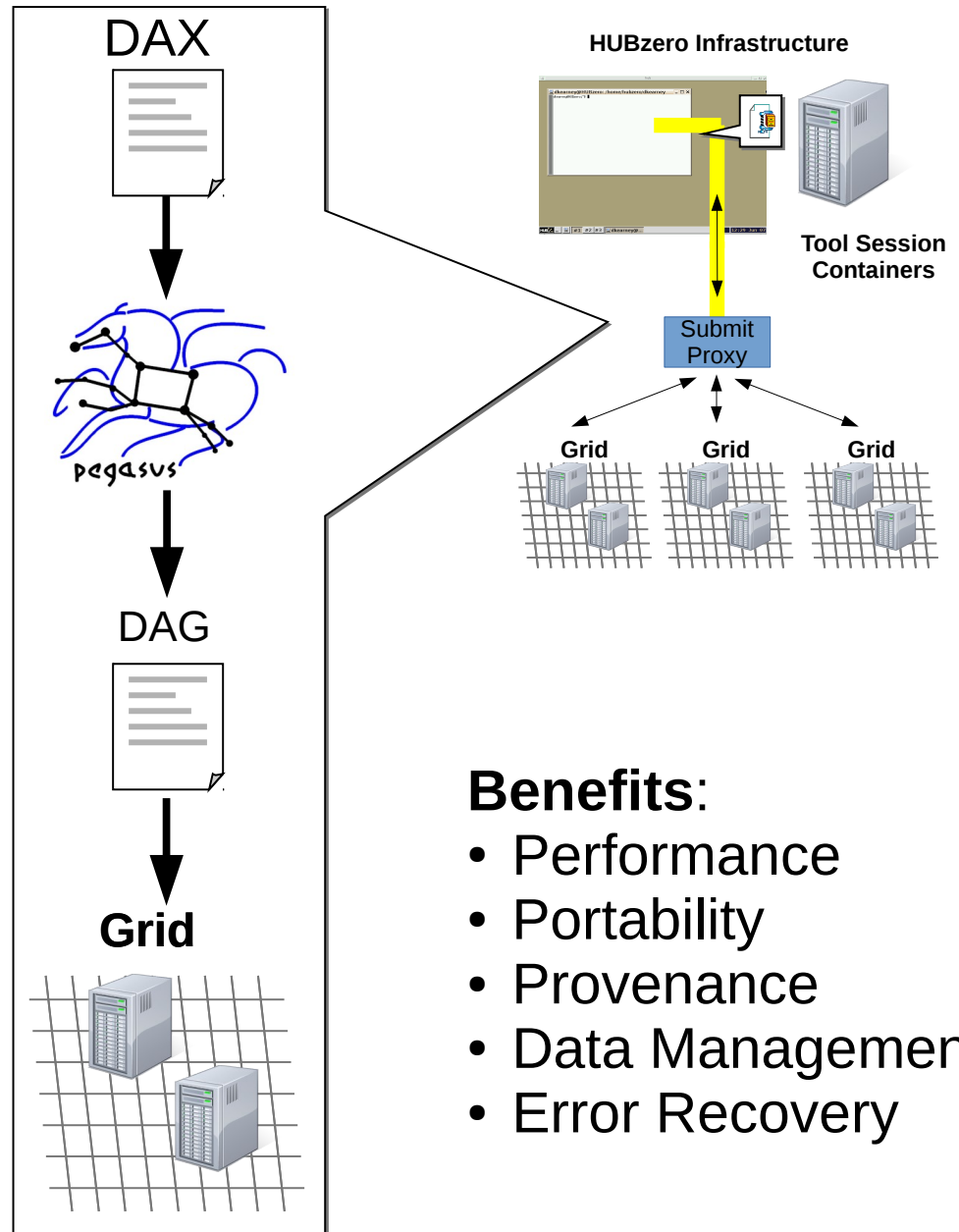
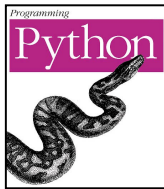
Submit





# Pegasus Workflow Management

- Developed at USC
- Ewa Deelman et al.
- Website: [pegasus.isi.edu](http://pegasus.isi.edu)
- Manage jobs on the grid
- Open Source
- Bindings for your favorite languages:

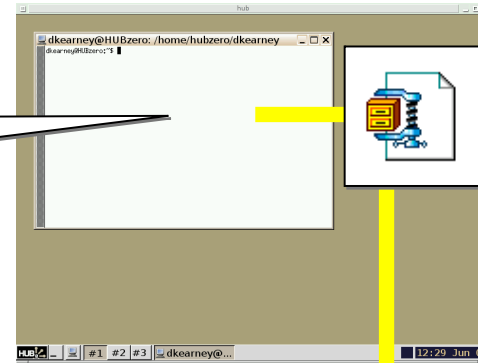


# Let Submit create a workflow ...

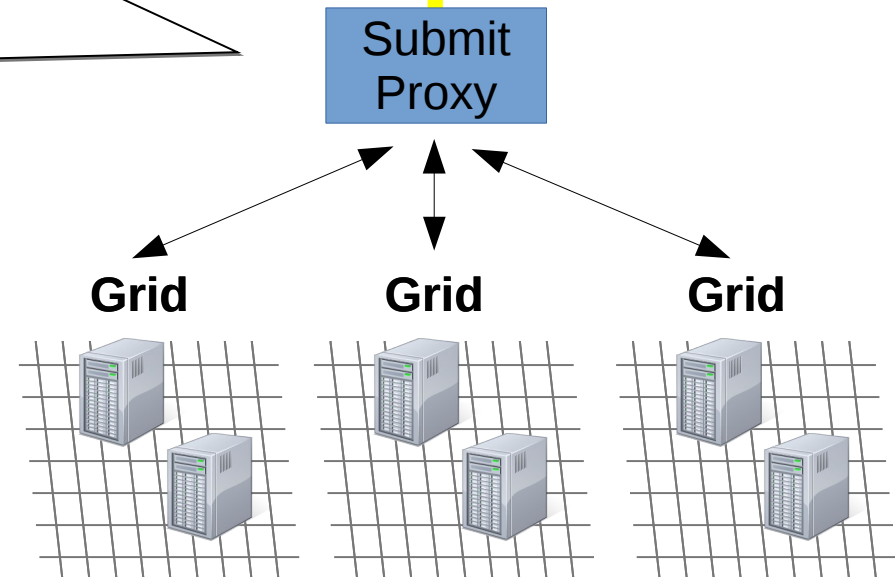
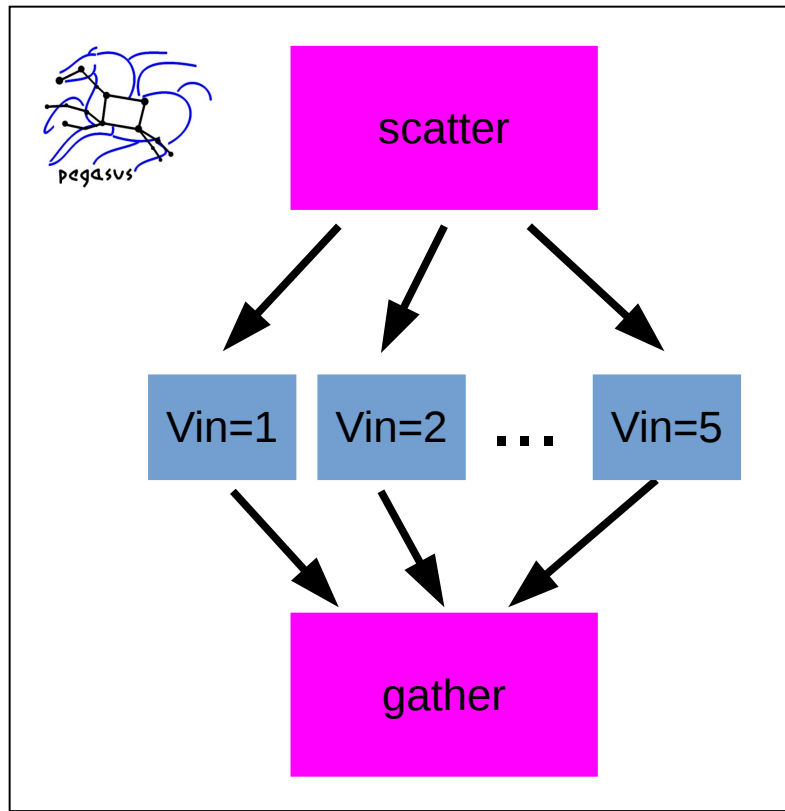
## User's Workspace Terminal

```
$ submit -p @@Vin=1-5 ./sim1.py --Vin @@Vin
```

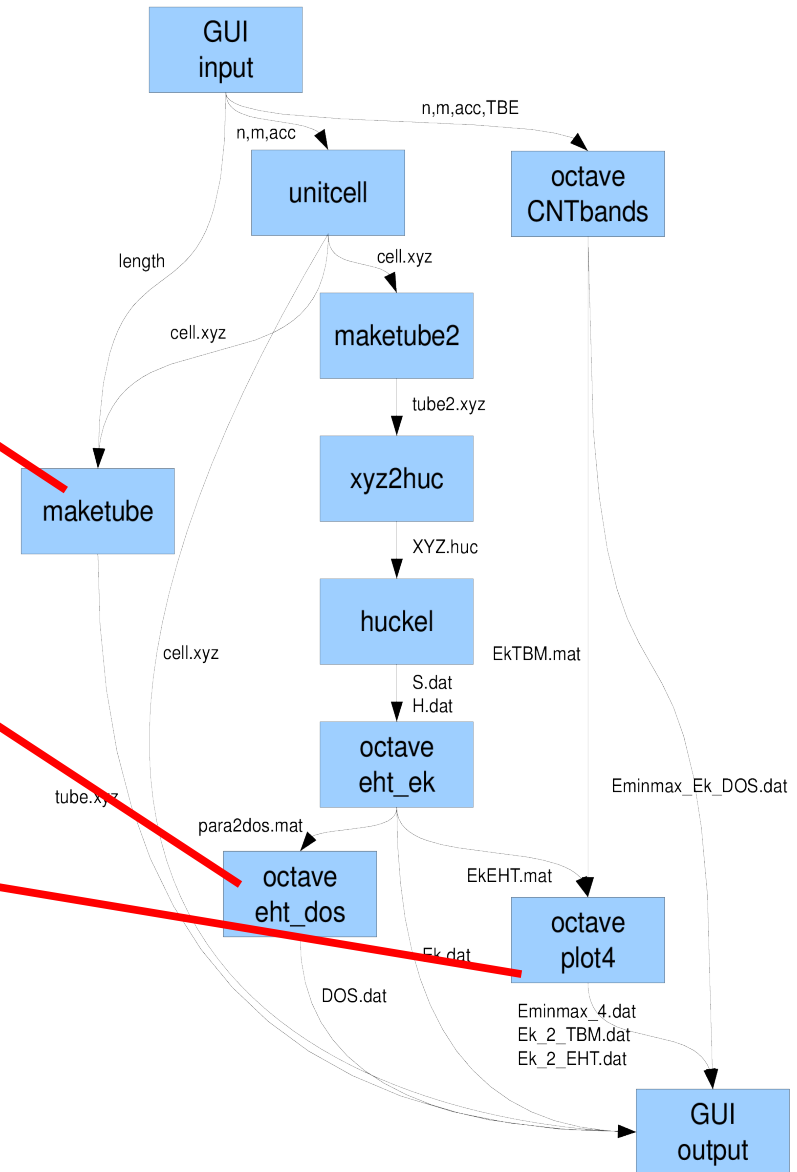
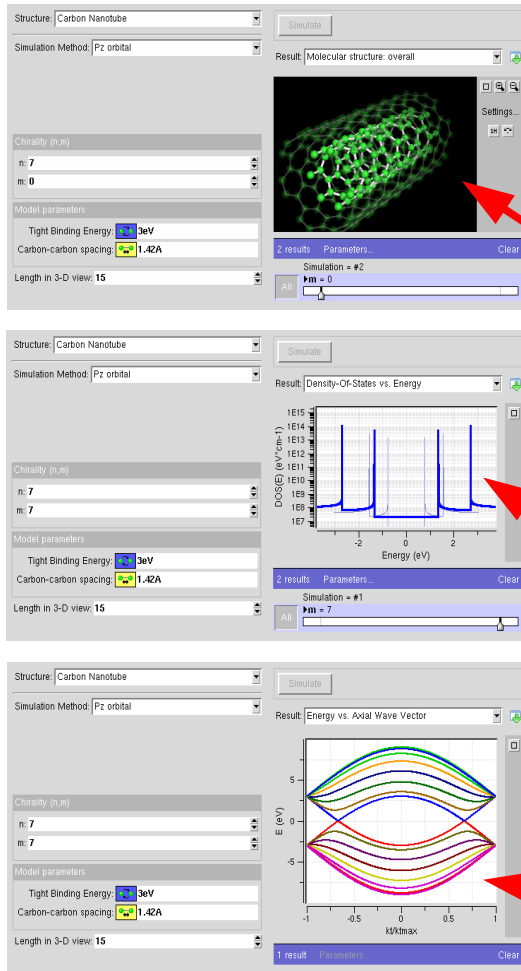
## HUBzero Infrastructure



## Tool Session Containers



# ... or write your own workflow



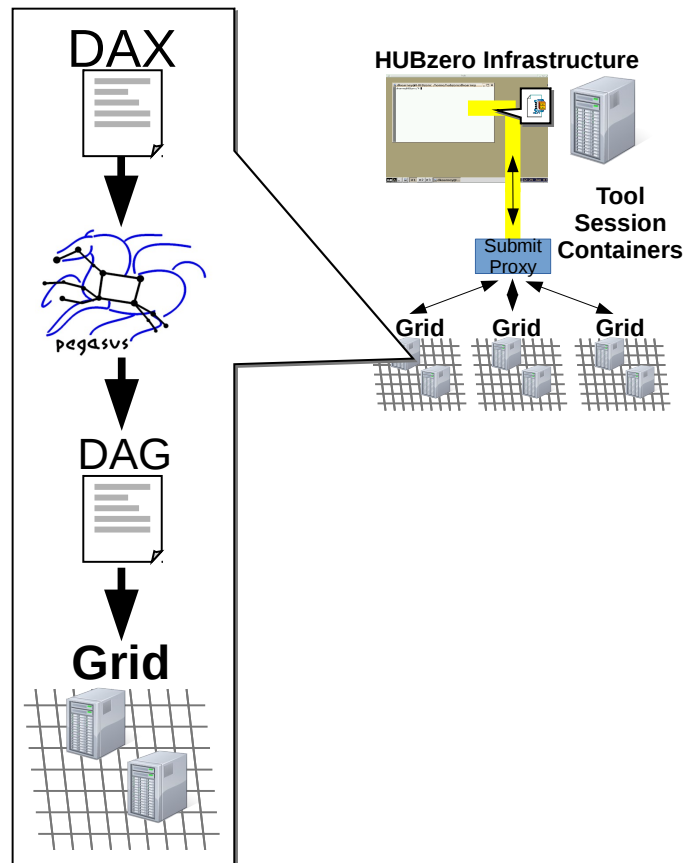
## CNTBands

Science Domain: Nanoelectronics  
Scientists: Lundstrom et al. (Purdue)

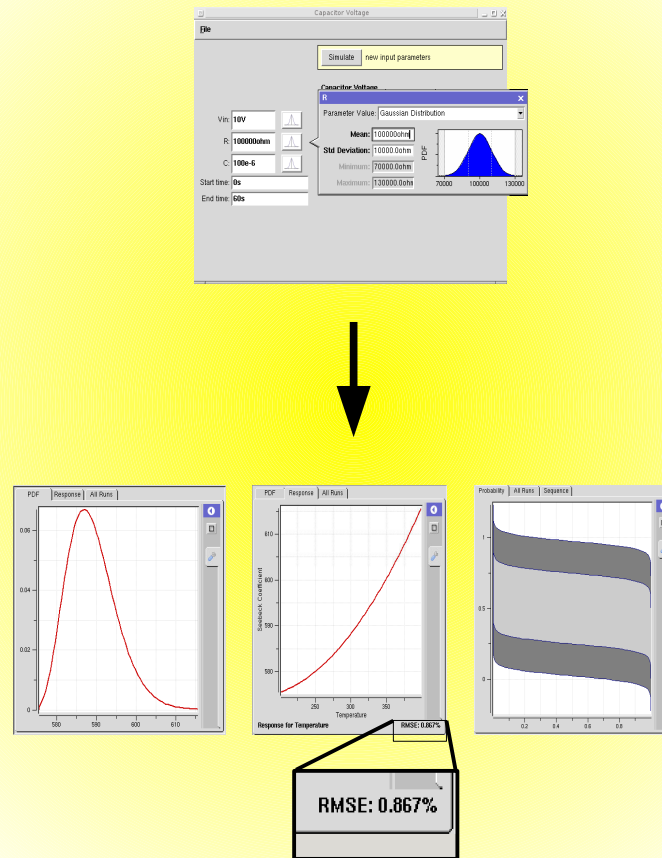
<https://nanohub.org/resources/cntbands-ext>

# Productivity in the Workspace

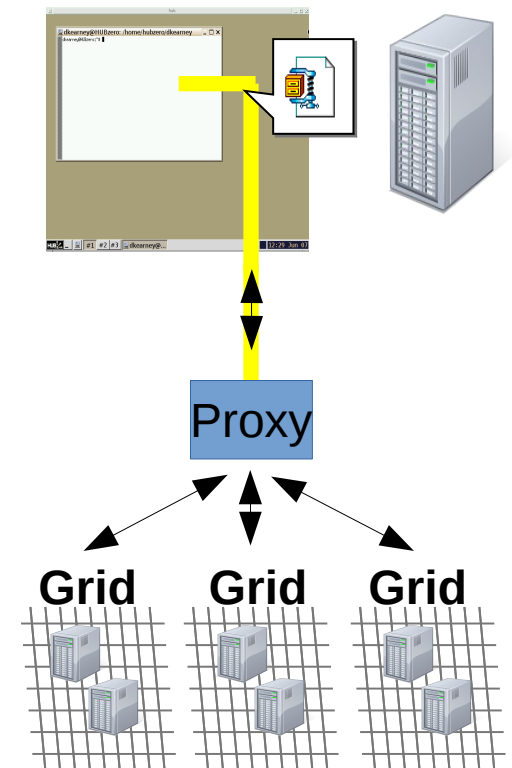
## Pegasus Workflows



## Uncertainty Quantification

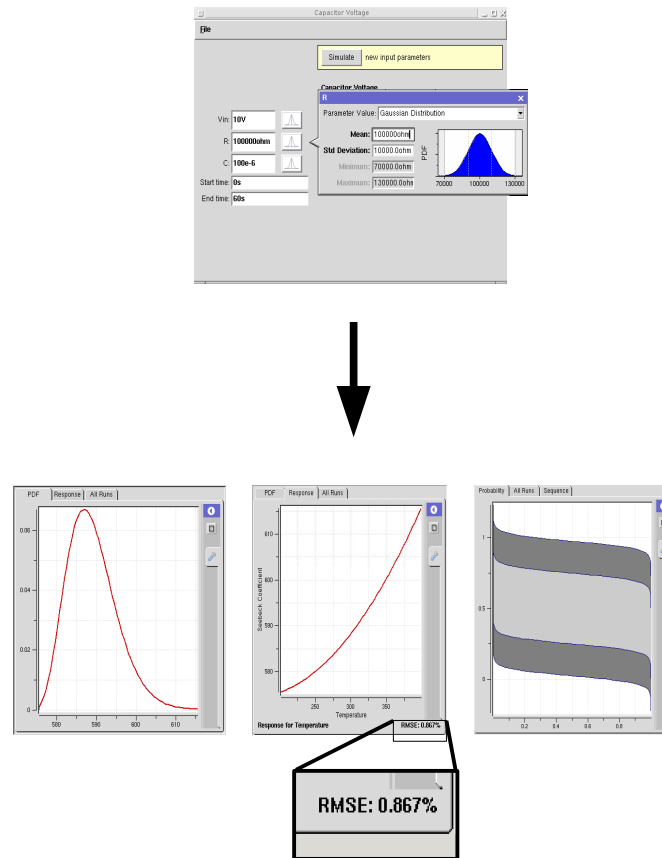
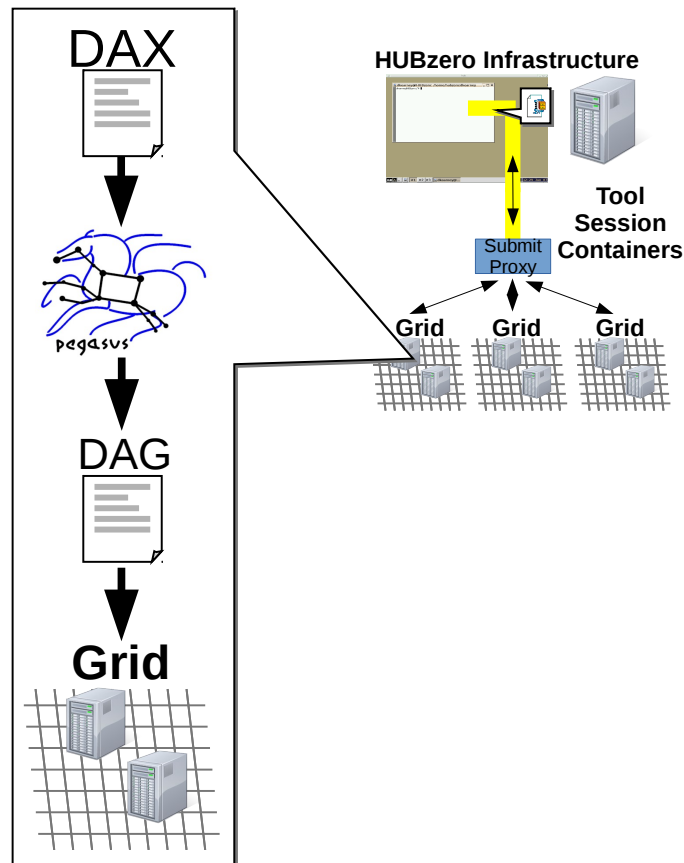


## Submit

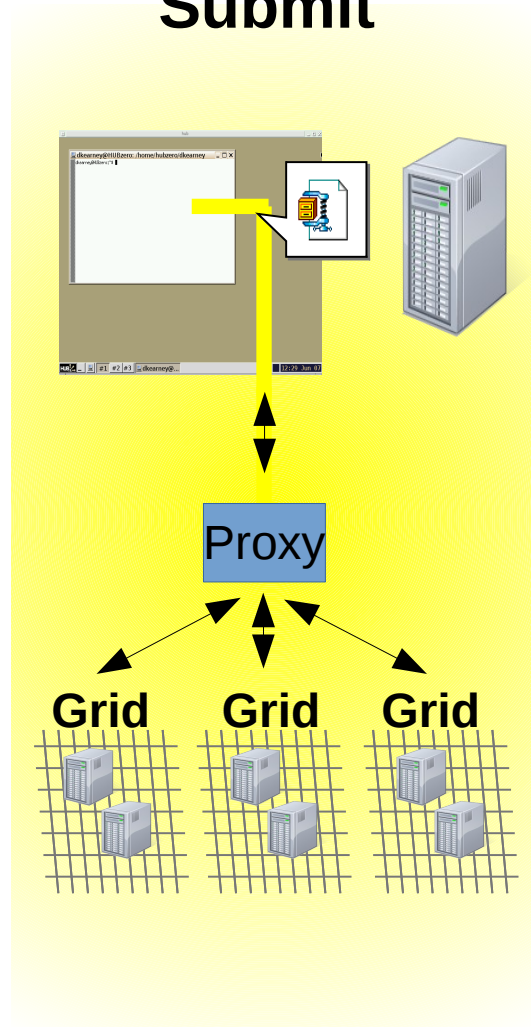


# Productivity in the Workspace

Pegasus Workflows    Uncertainty Quantification



Submit

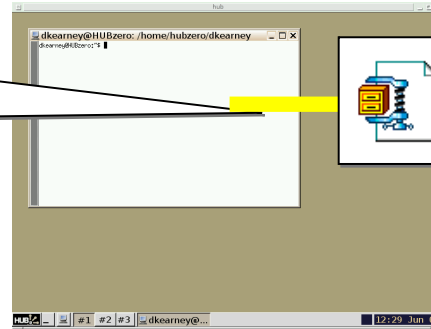


# Running locally in a Workspace

## User's Workspace Terminal

```
$ echo hi  
hi  
$
```

## HUBzero Infrastructure



## Tool Session Containers

Submit  
Proxy

Grid

Grid

Grid



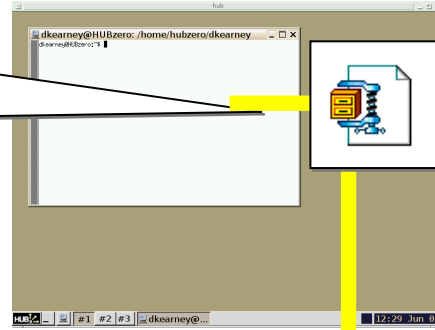


# Submitting from a Workspace

## User's Workspace Terminal

```
$ submit echo hi
```

## HUBzero Infrastructure



## Tool Session Containers

Submit  
Proxy

Grid

Grid

Grid

