

# HUBzero Platform Features

TRADES Proposal Demo  
Oct. 12, 2016

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

# The HUBzero Platform



# CNTbands

Structure: Carbon Nanotube

Simulation Method: Pz orbital

Chirality (n,m)

n: 7

m: 7

Model parameters

Tight Binding Energy: 3eV

Carbon-carbon spacing: 1.42A

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.

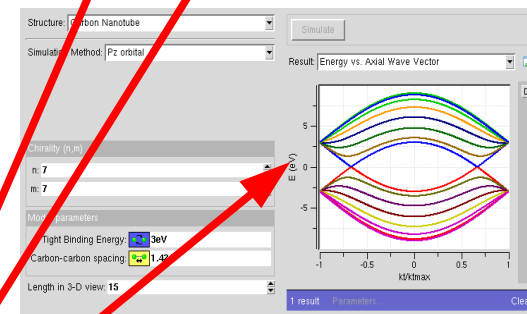
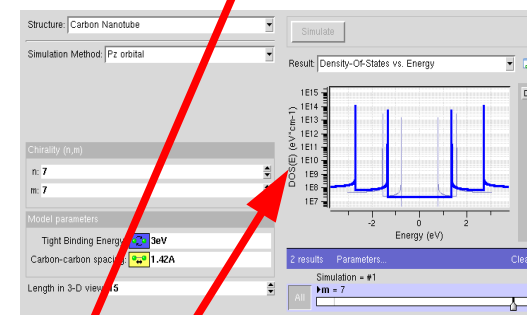
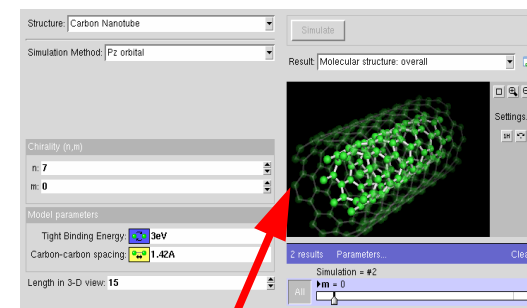
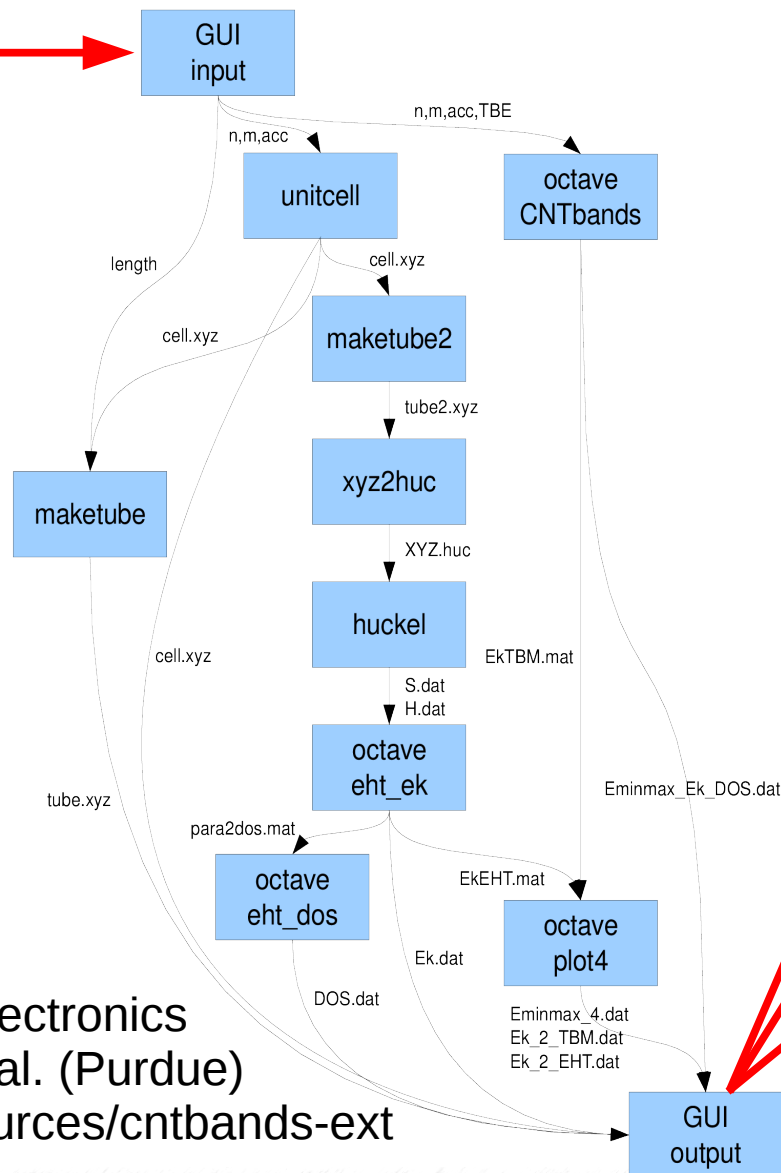
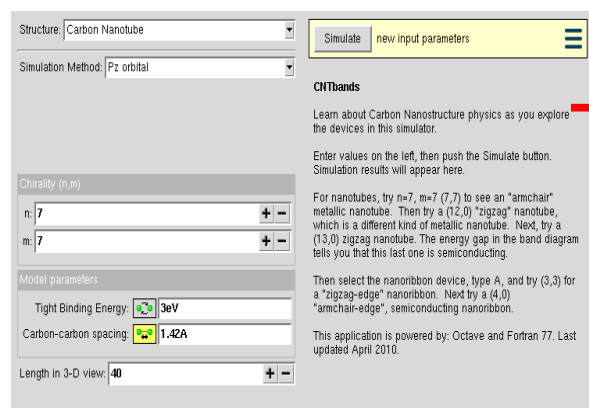
## CNTbands

Science Domain: Nanoelectronics

Scientists: Lundstrom et al. (Purdue)

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

# CNTbands



## CNTbands

Science Domain: Nanoelectronics

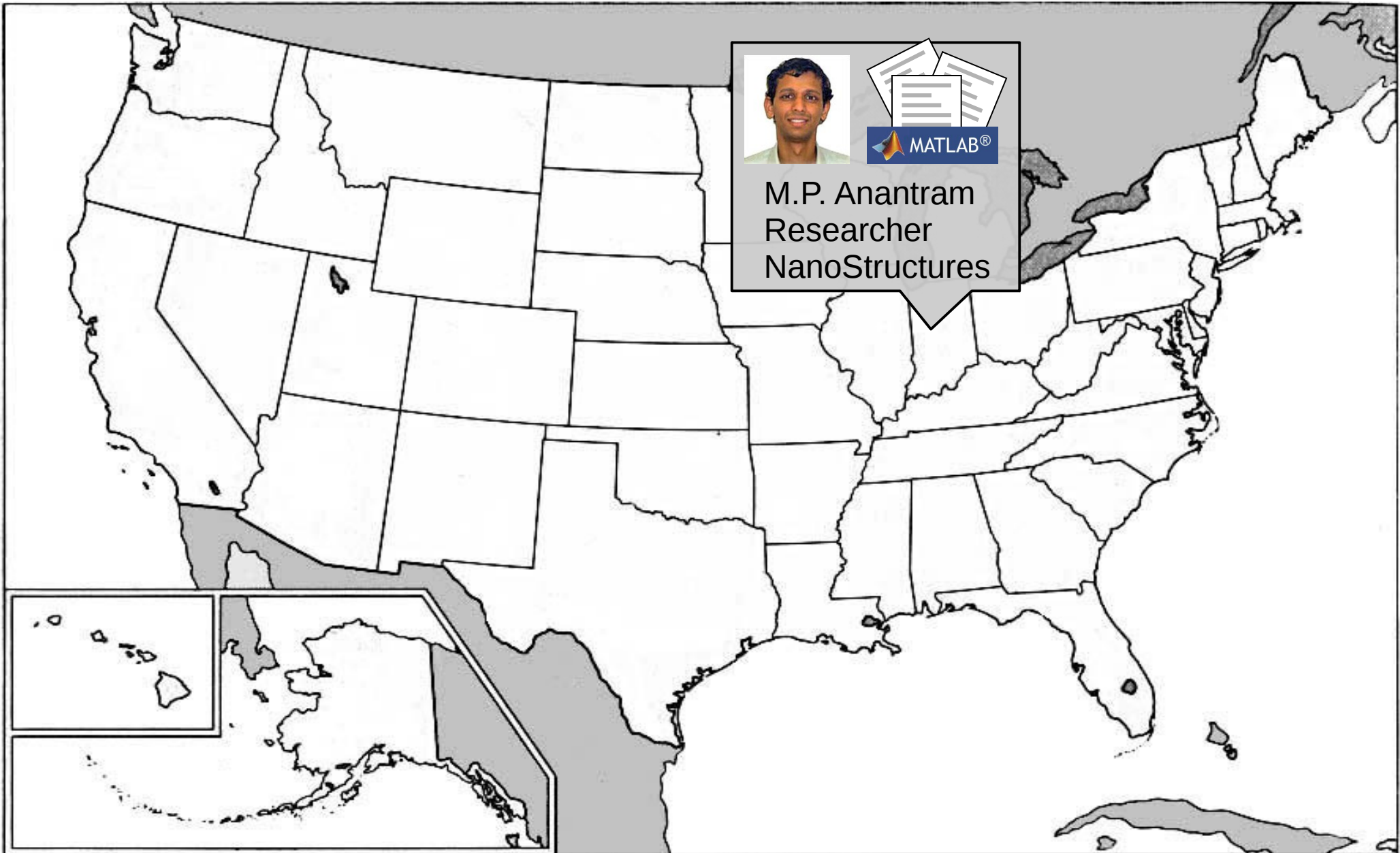
Scientists: Lundstrom et al. (Purdue)

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

# 1990s – Initial Algorithms

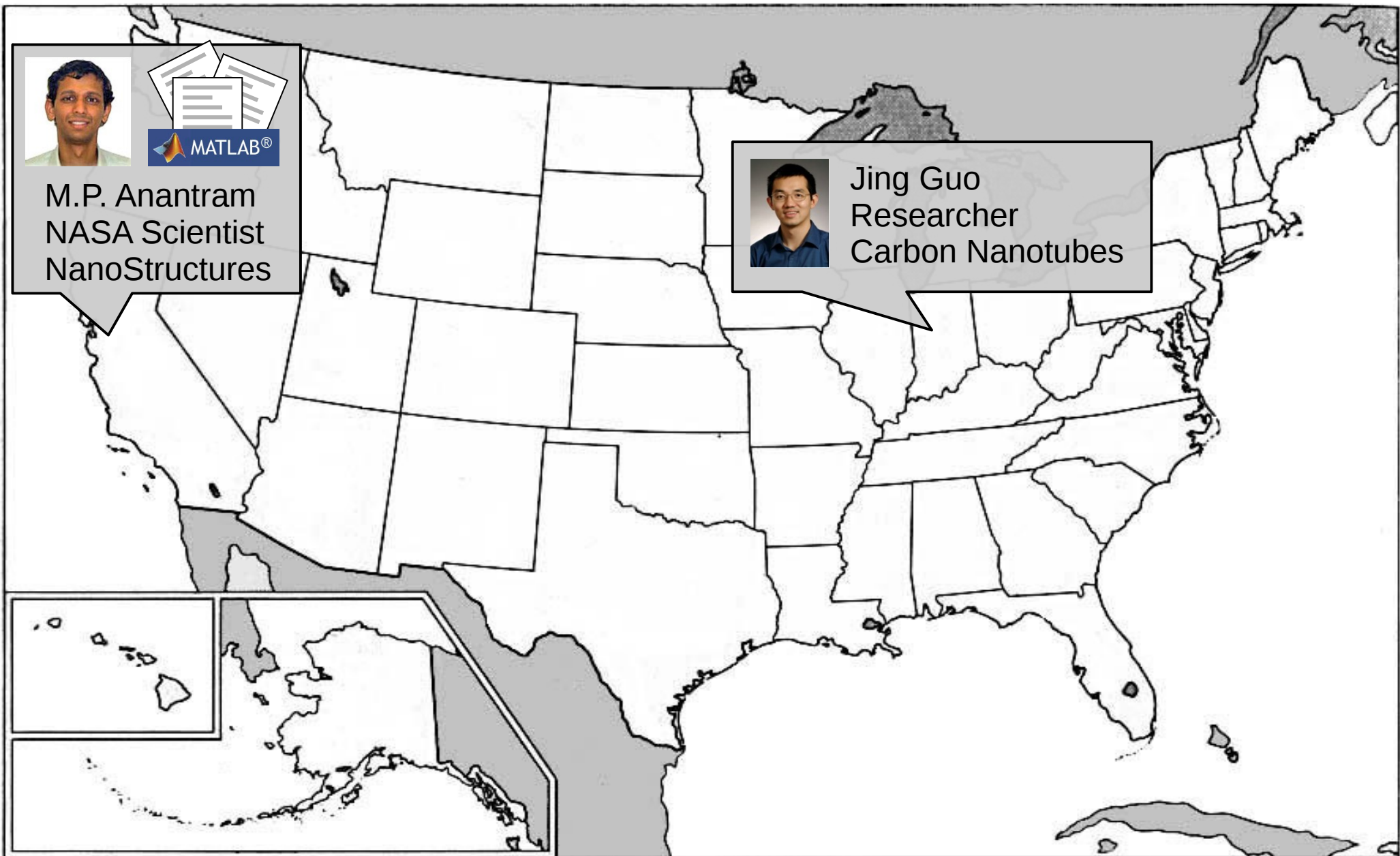


M.P. Anantram  
Researcher  
NanoStructures

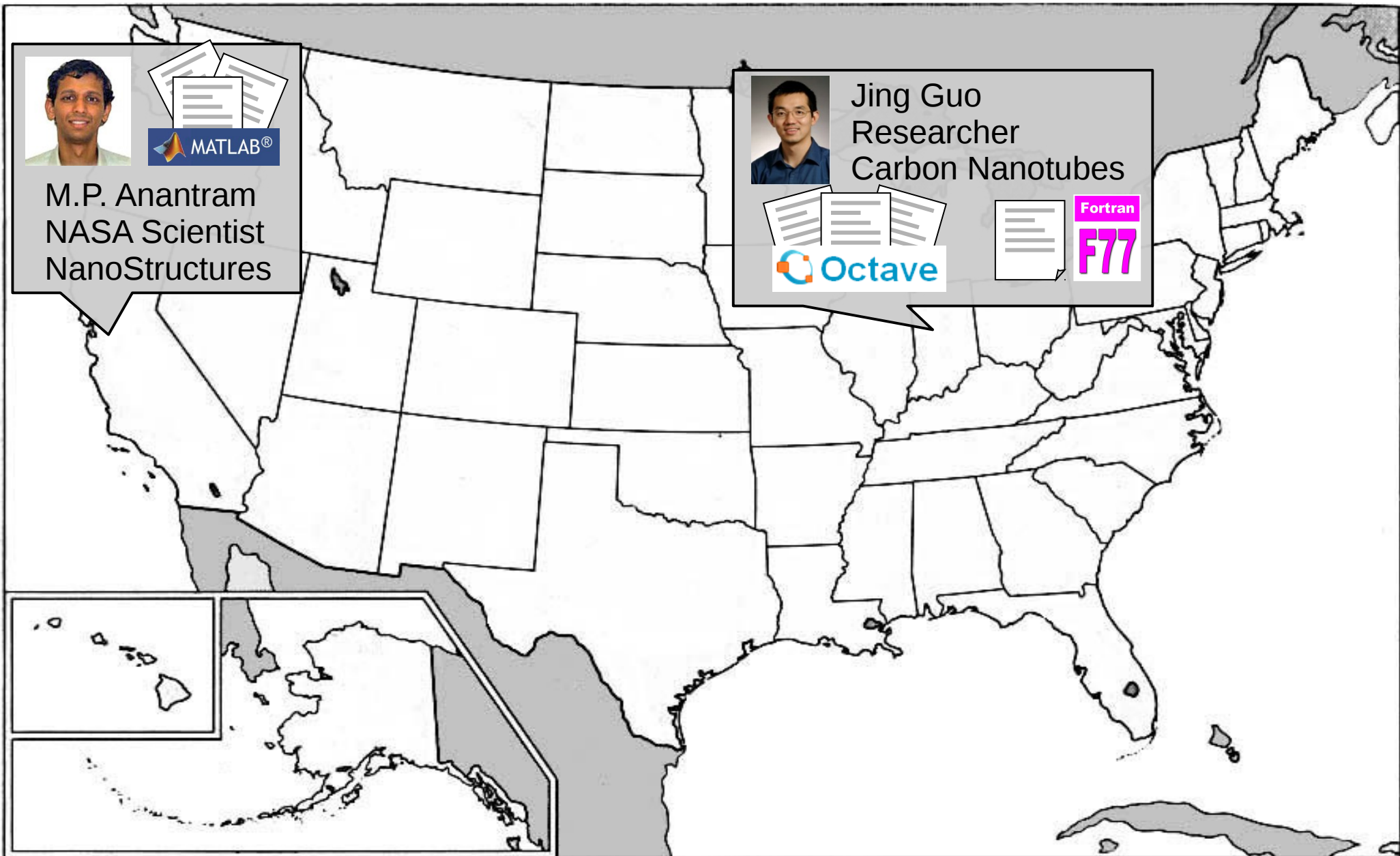




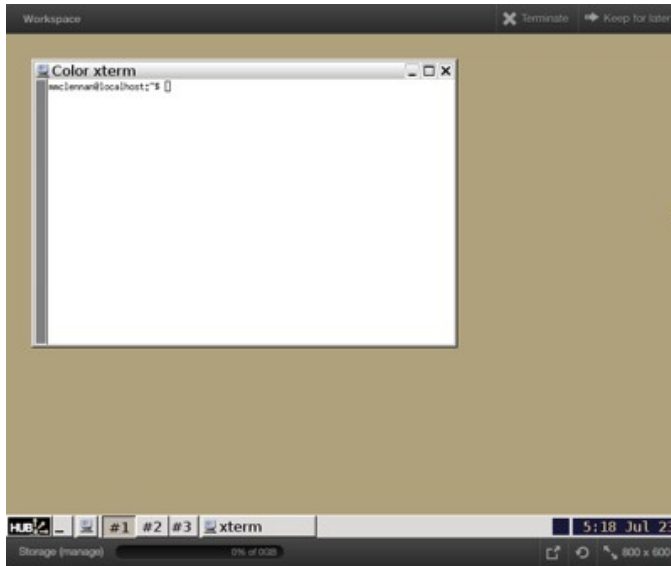
# 2002 – Idea for a Tool



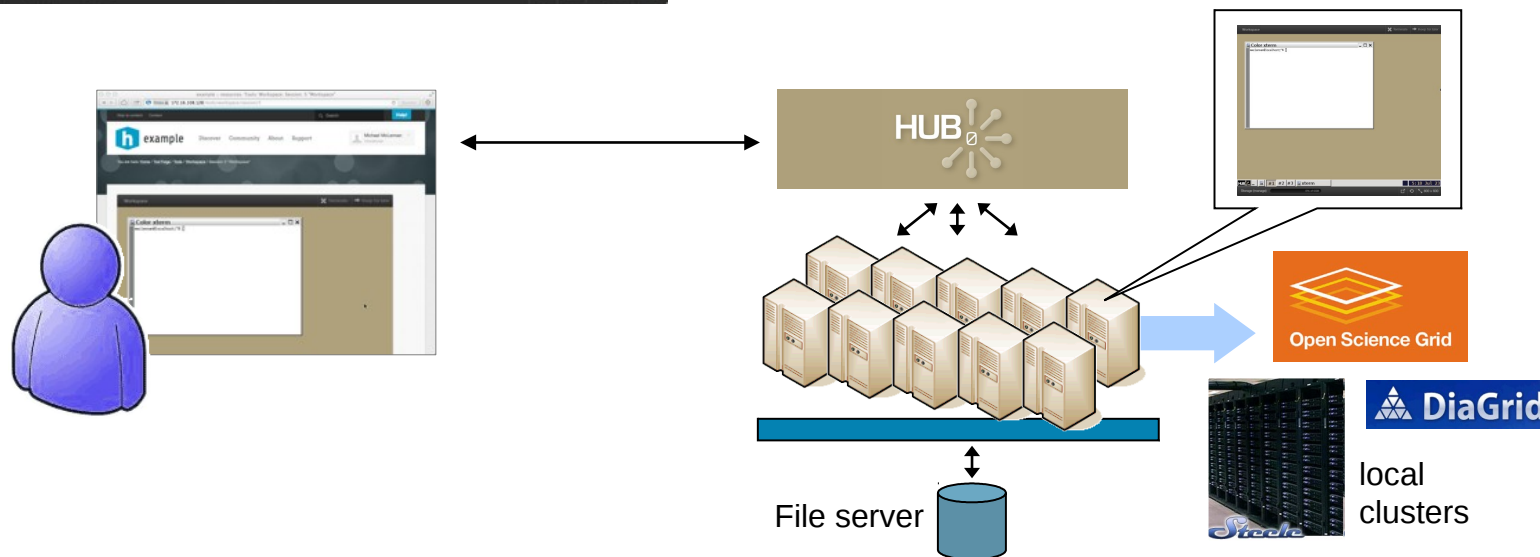
# 2002 – Tool Registered



# What is a Workspace?



- Full-featured Linux or Windows Desktop
- Runs in the Cloud
- For tool developers & researchers
- Accessible from any web browser
- Still running after you close your browser
- Access to computational clusters
- File storage provided by the hub

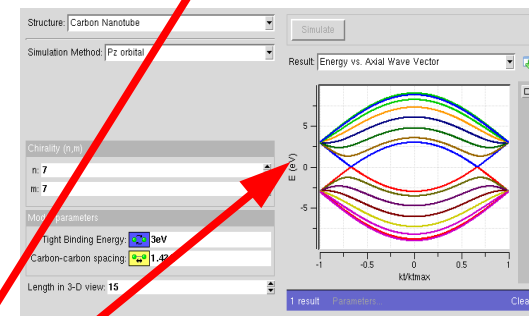
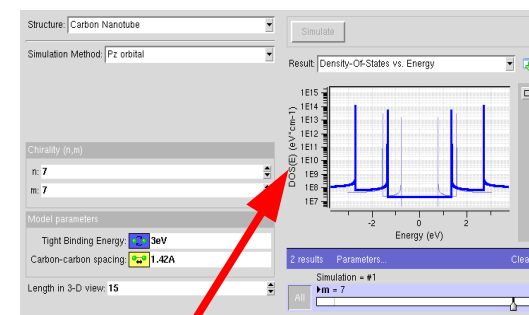
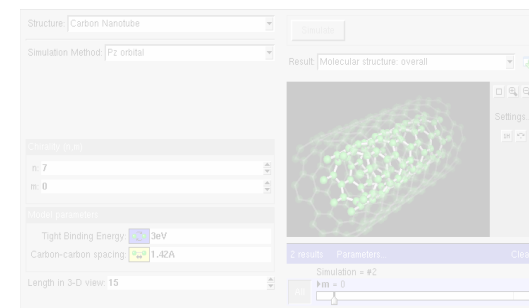
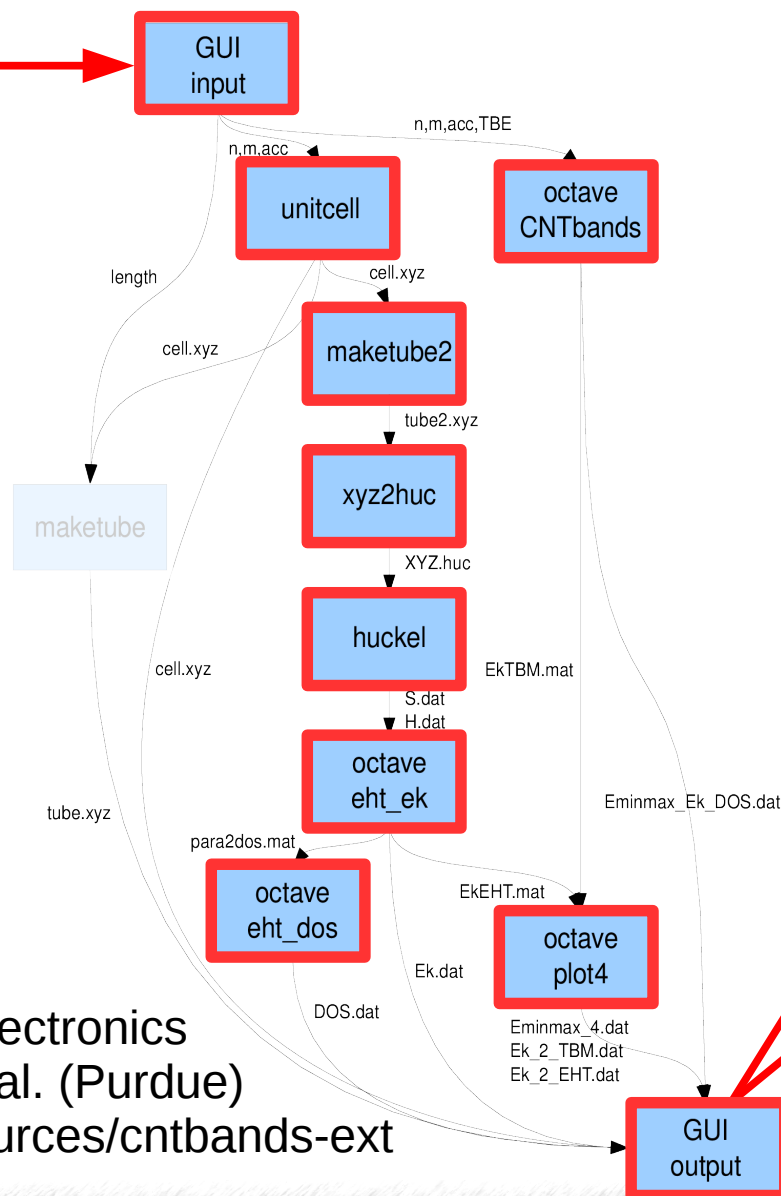
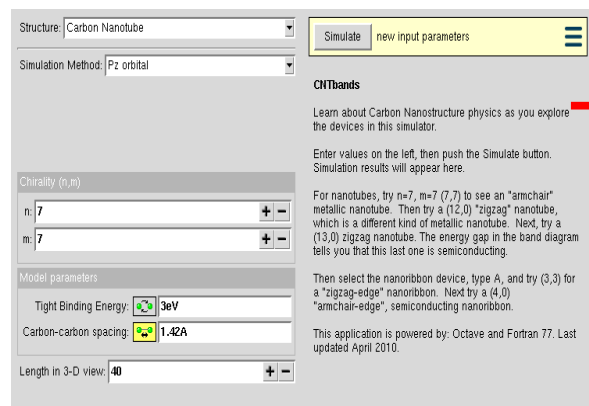




# Collaboration / Groups



# CNTbands



## CNTbands

Science Domain: Nanoelectronics

Scientists: Lundstrom et al. (Purdue)

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

# Installing Applications

## What's next?

Your latest code is installed and ready on nanoHUB. Please test your tool by clicking the button below to ensure that everything is working properly, as well as to make sure that the page describing your tool is created with the correct information:

- ➔ Test your application:

**Launch tool** ➔

- ➔ [Review the page describing your tool](#)

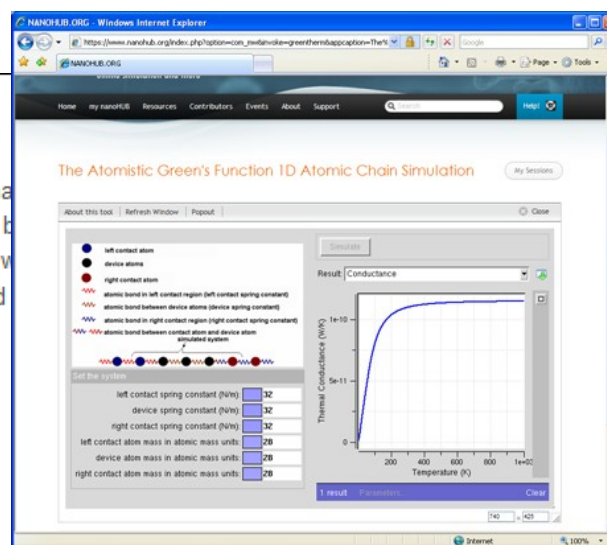
## We are waiting for You

Once you tested your tool and verified that it is working properly, click here to let us know:

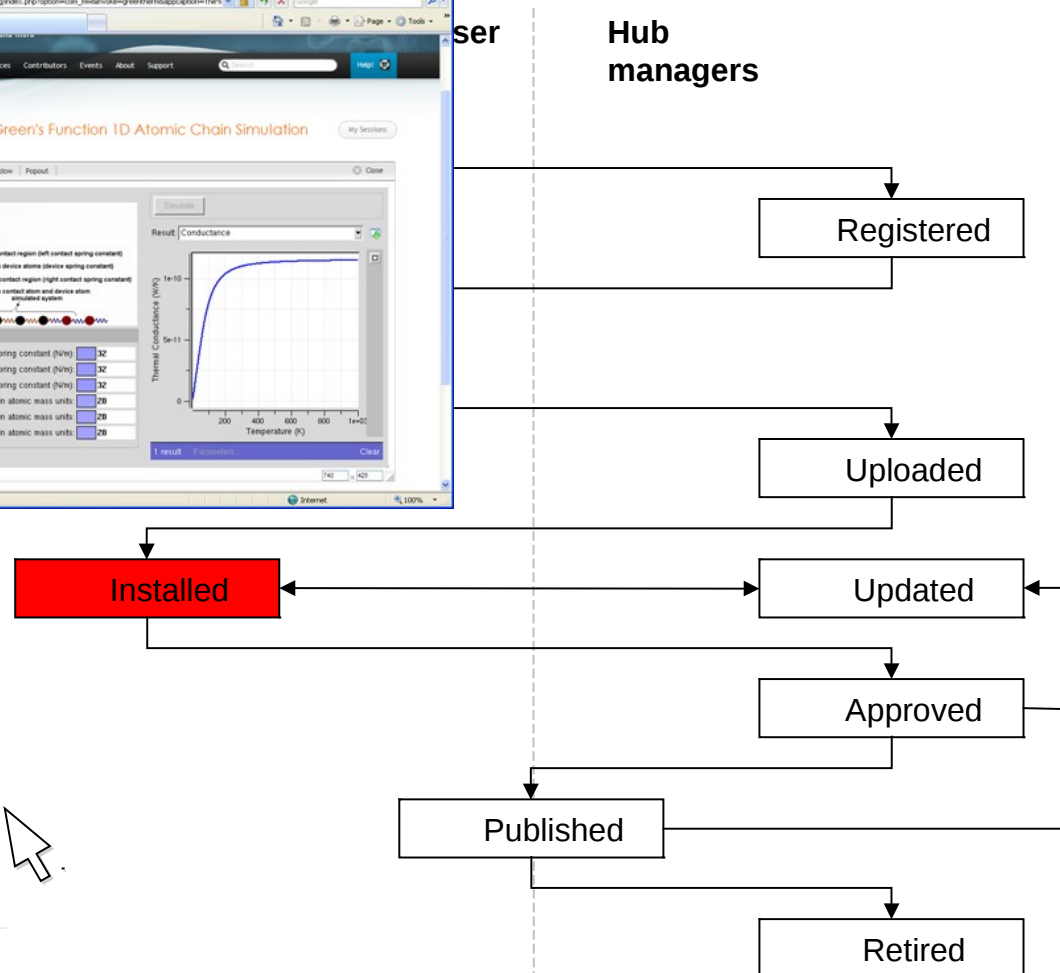
- ➔ [My tool is working properly. I approve it.](#)

Need to make changes? Once you've checked in your latest fixes, click here to let us know:

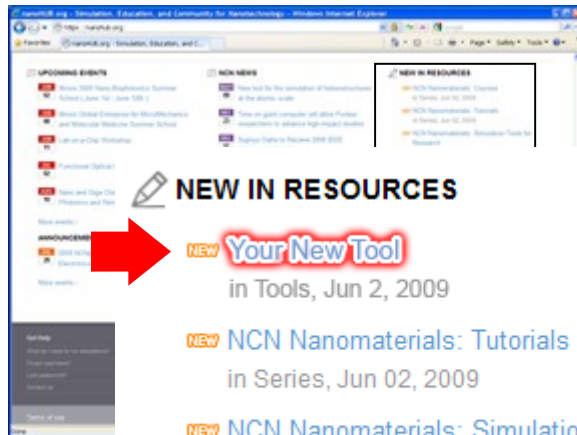
- ➔ [I've fixed my code. Please install the latest updates.](#)



waiting for...



# Publishing Applications



## NEW IN RESOURCES

**NEW Your New Tool**

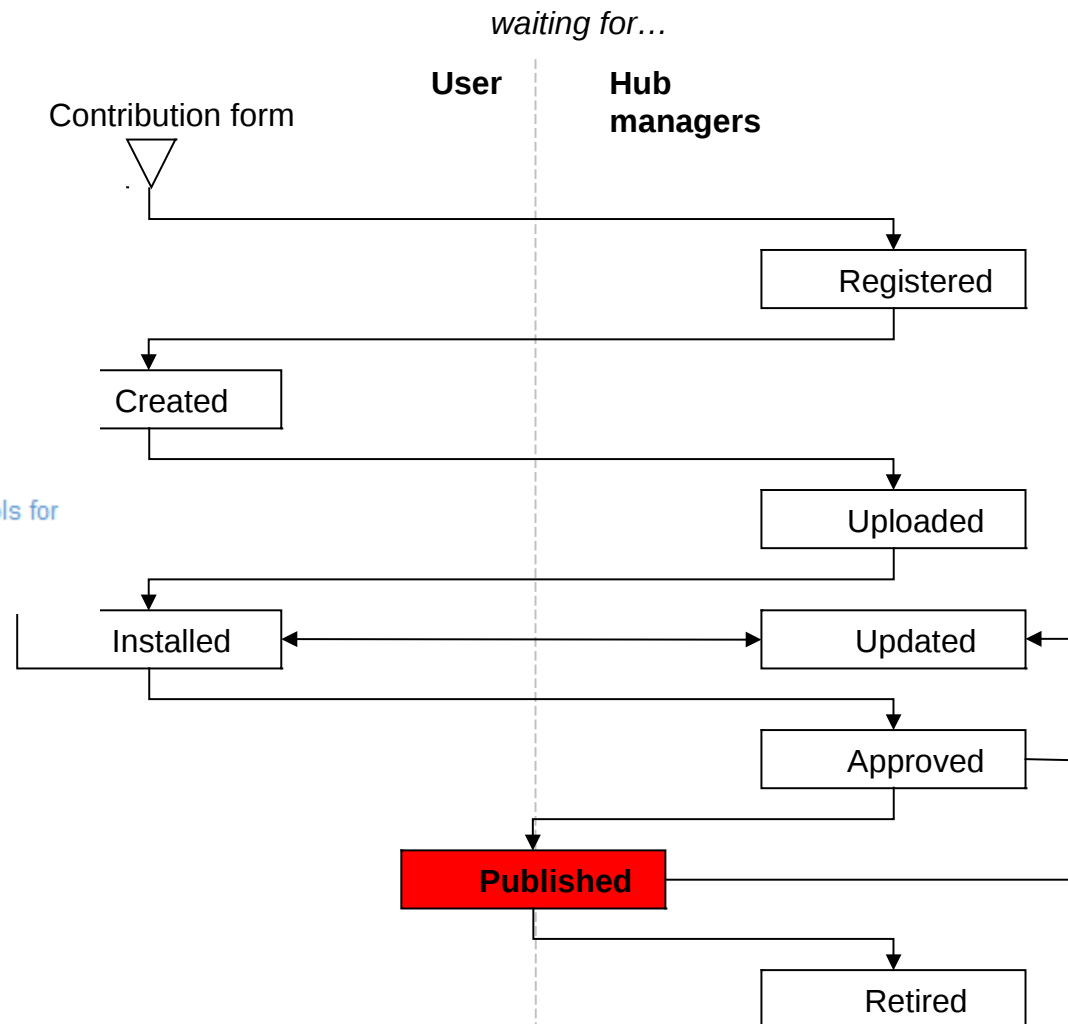
in Tools, Jun 2, 2009

**NEW NCN Nanomaterials: Tutorials**

in Series, Jun 02, 2009

**NEW NCN Nanomaterials: Simulation Tools for Research**

in Series, Jun 02, 2009





# 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: [f](#) [t](#) [s](#) ...

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-Ullah<sup>2</sup>, G. Ibrahim S. 1. University of Shams U


This tool nanoribbon


Easy-Expert


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Versions Supporting Docs Classroom usage

See also

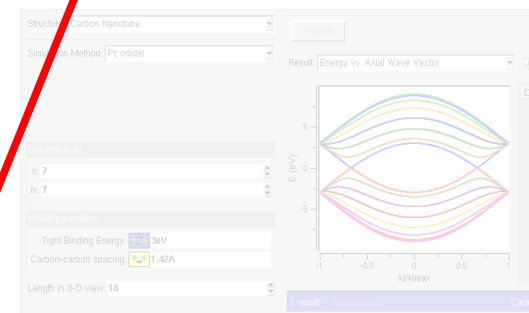
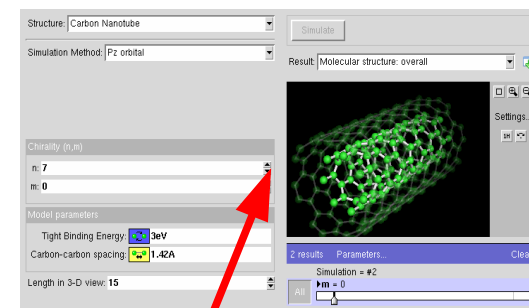
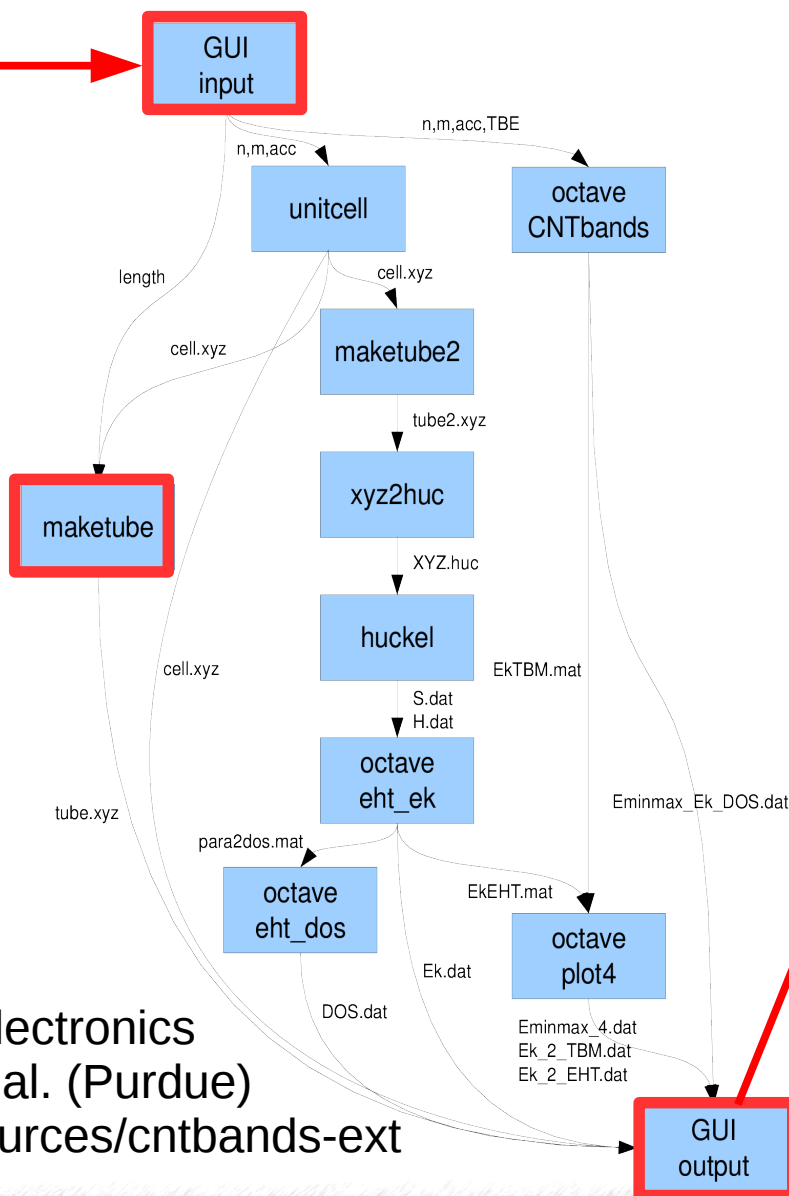
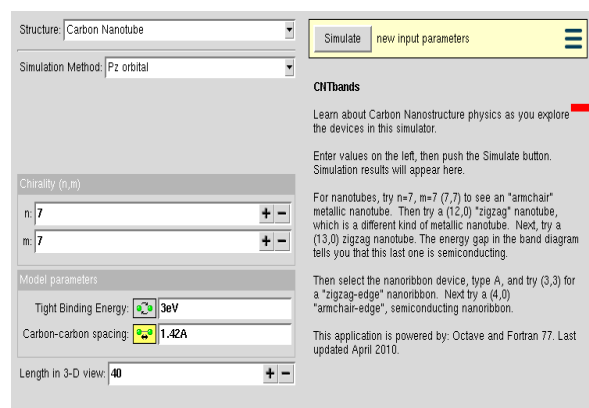
Part of: NCN

Nanoelectronics: Simulation Tools for Education

Part of: NCN

Nanoelectronics:

# Adding New Features



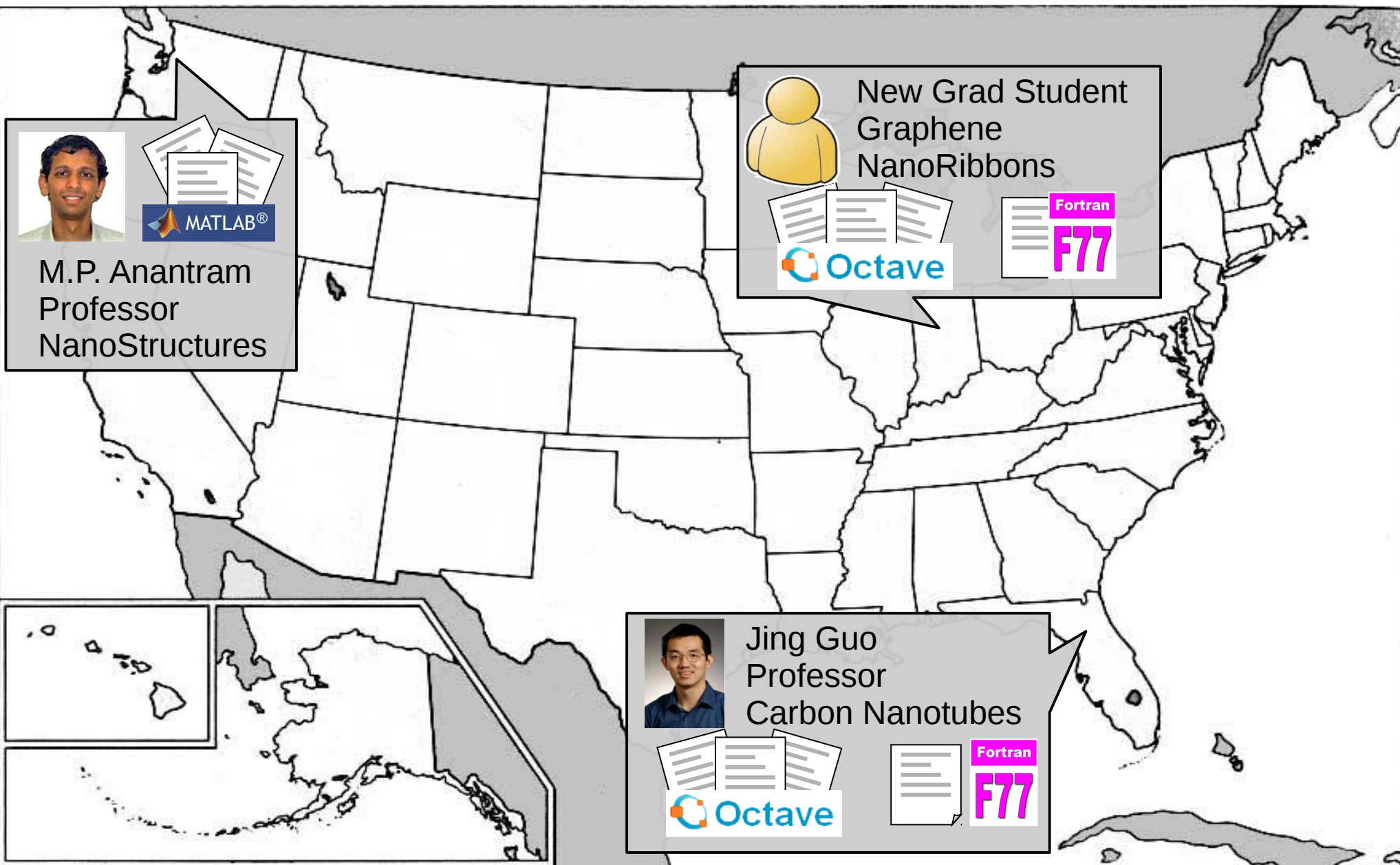
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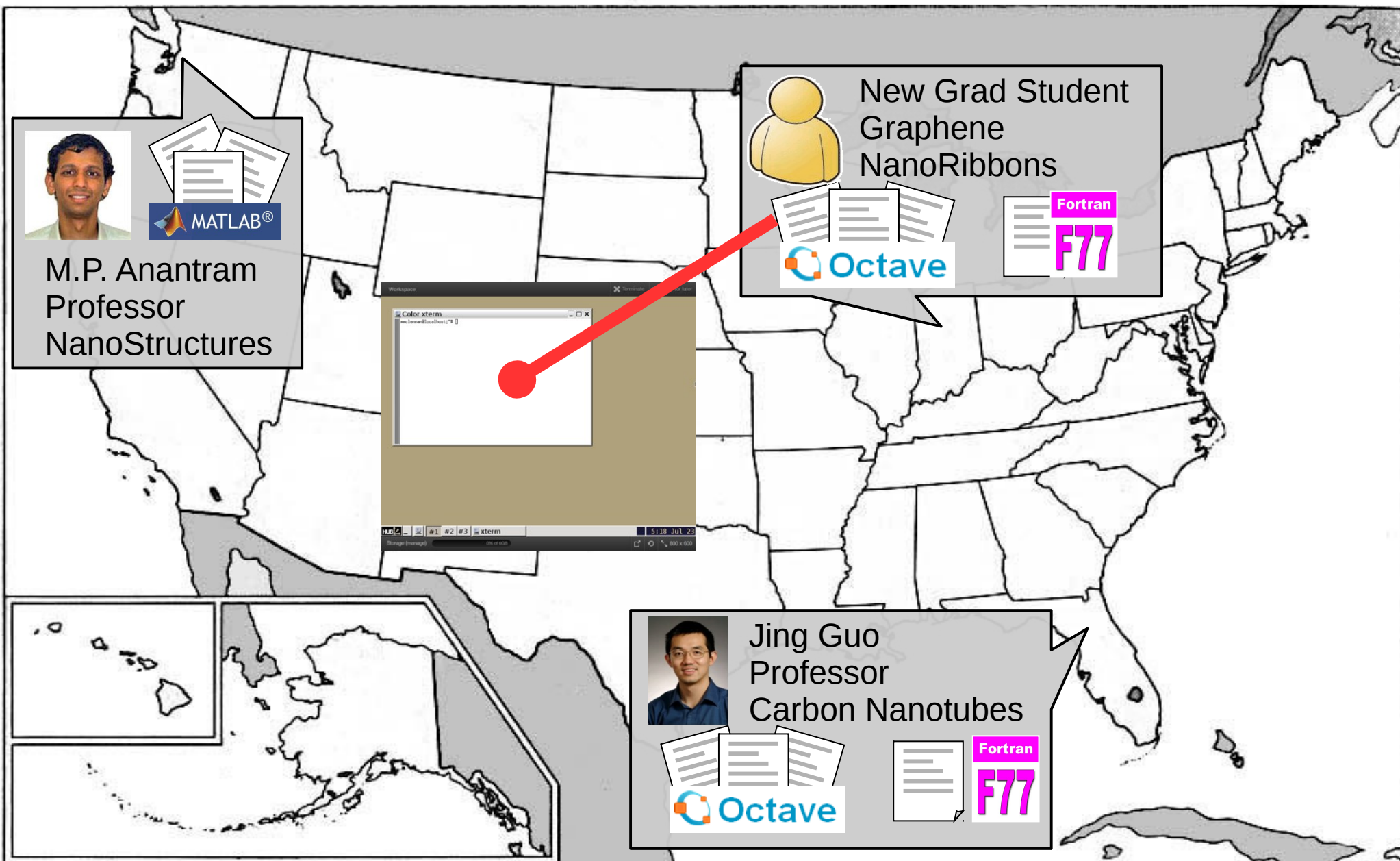
<https://nanohub.org/resources/cntbands-ext>

# 2010 – Introducing New Researchers

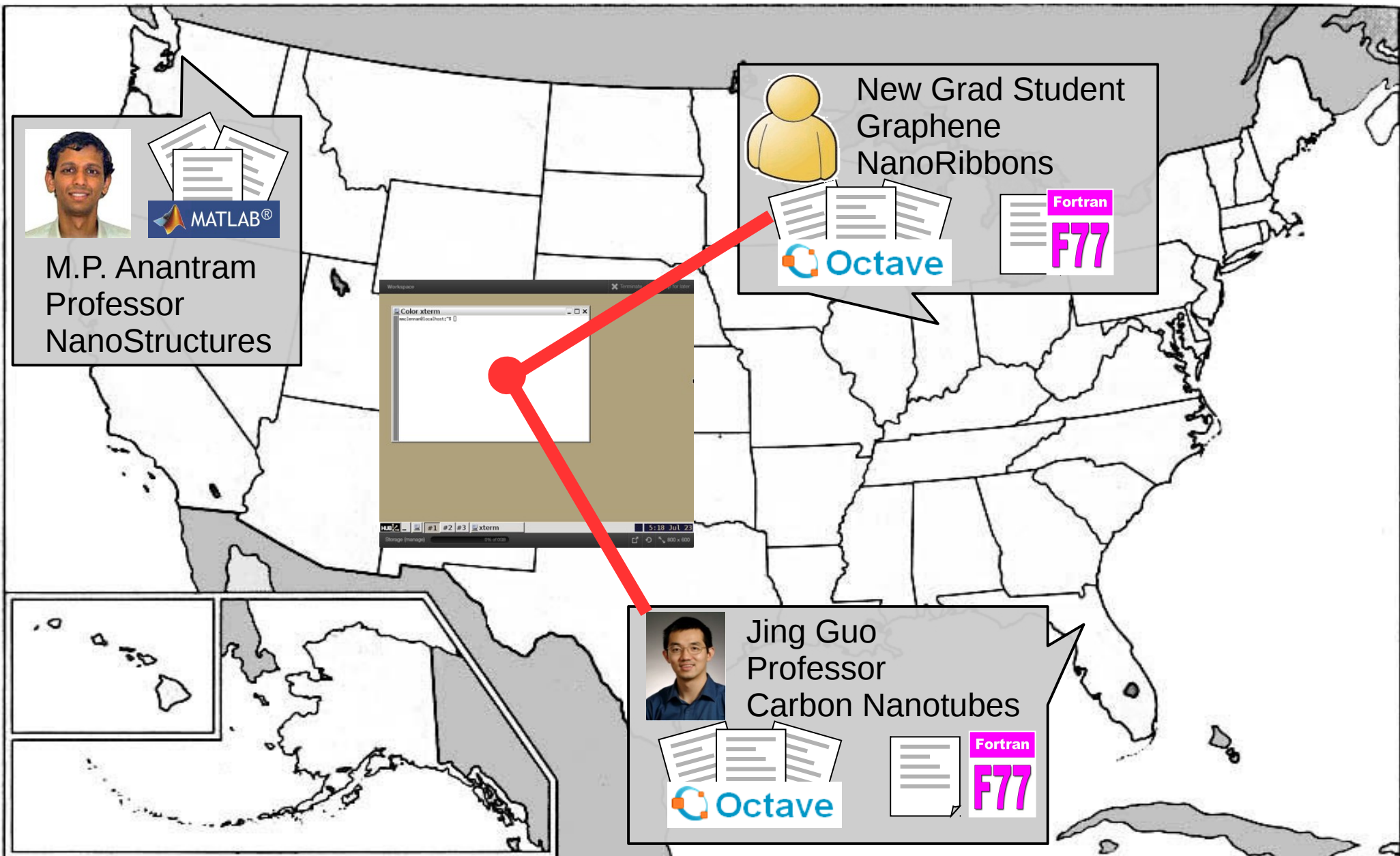




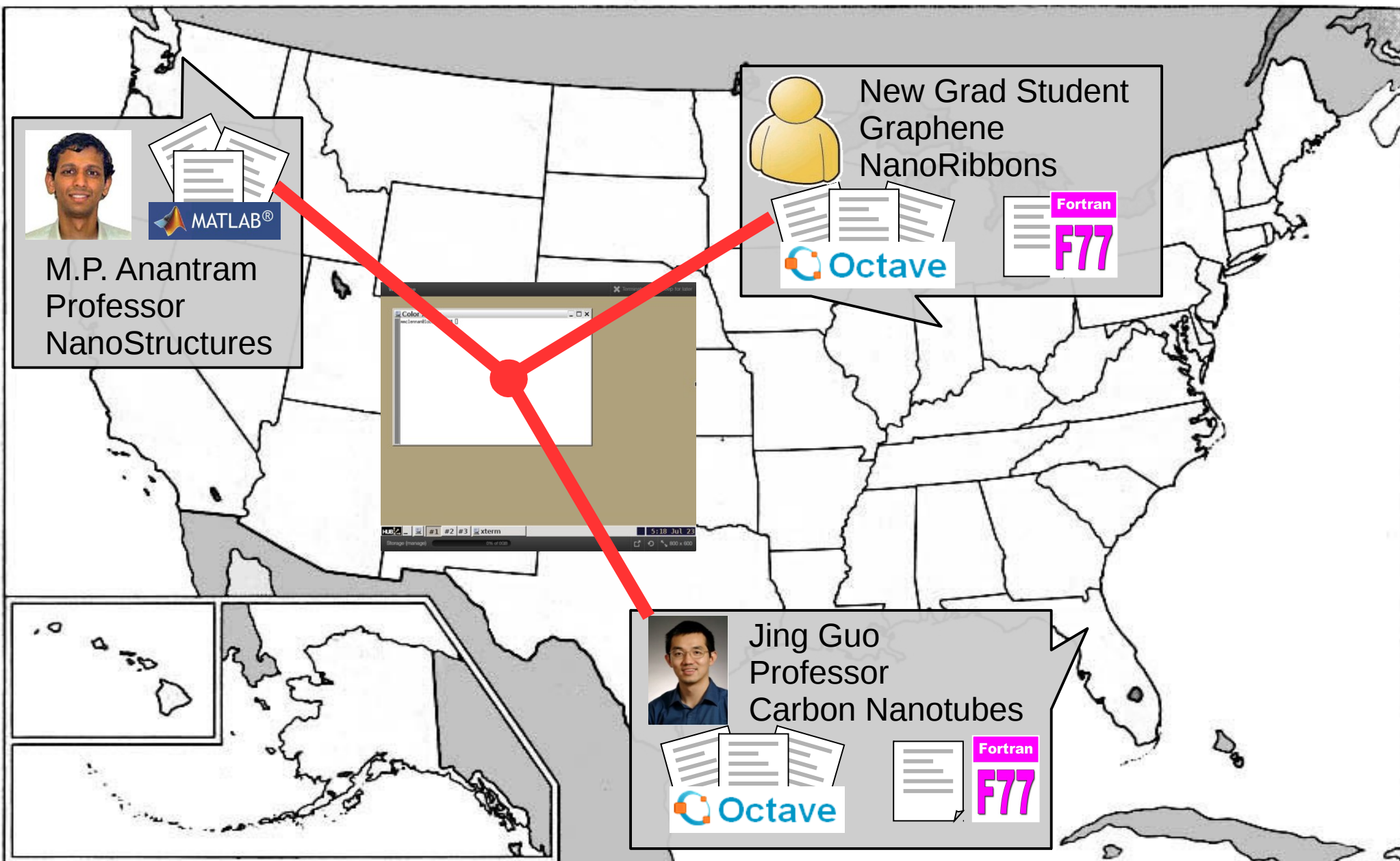
# Collaborate in the Workspace



# Collaborate in the Workspace



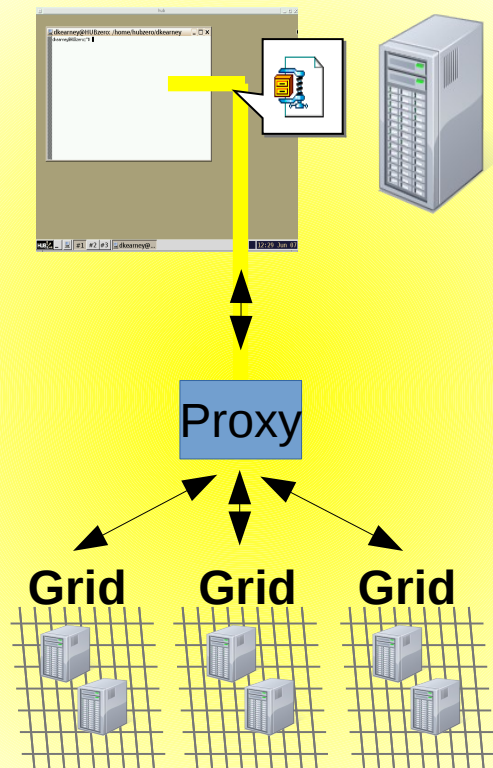
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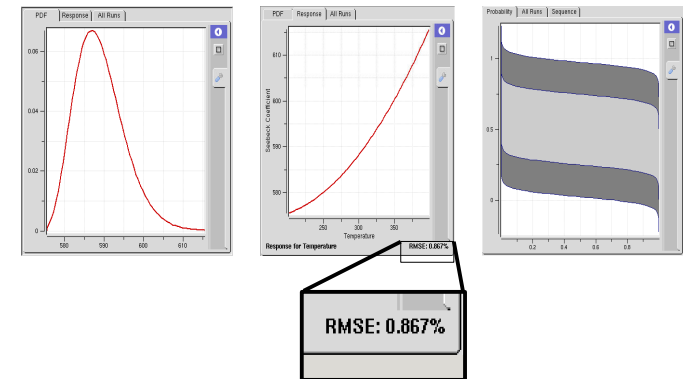
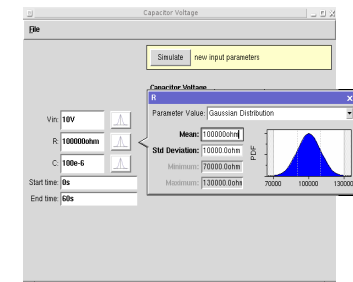
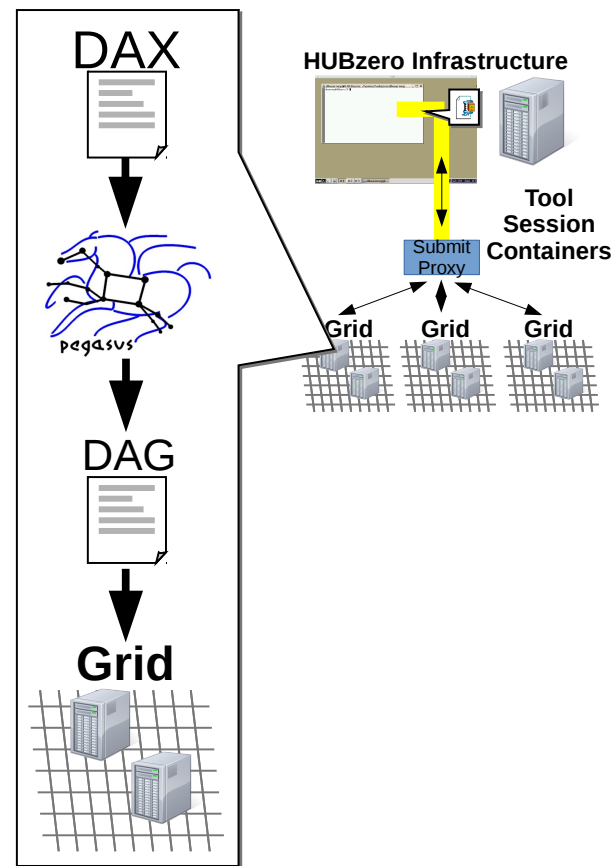


# Productivity in the Workspace

## Submit



## Pegasus Workflows Uncertainty Quantification



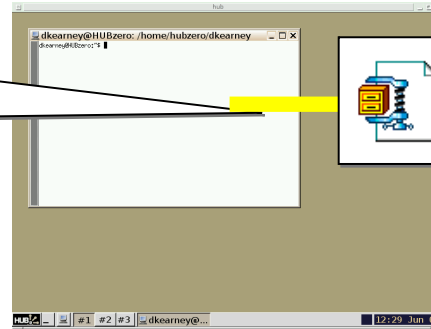


# Run tools locally in Workspace

## User's Workspace Terminal

```
$ echo hi
hi
$
```

## HUBzero Infrastructure



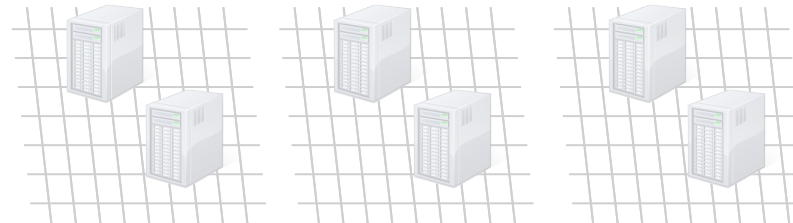
## Tool Session Containers

Submit Proxy

Grid

Grid

Grid

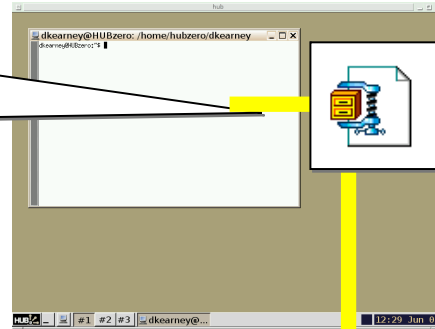


# Submit Jobs to Grid

## User's Workspace Terminal

```
$ submit echo hi
```

## HUBzero Infrastructure



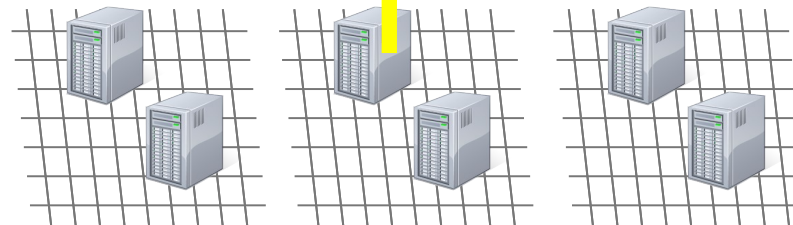
**Tool  
Session  
Containers**

**Submit  
Proxy**

**Grid**

**Grid**

**Grid**

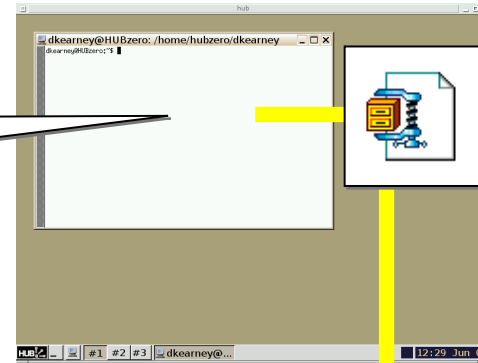


# Let Submit create a workflow ...

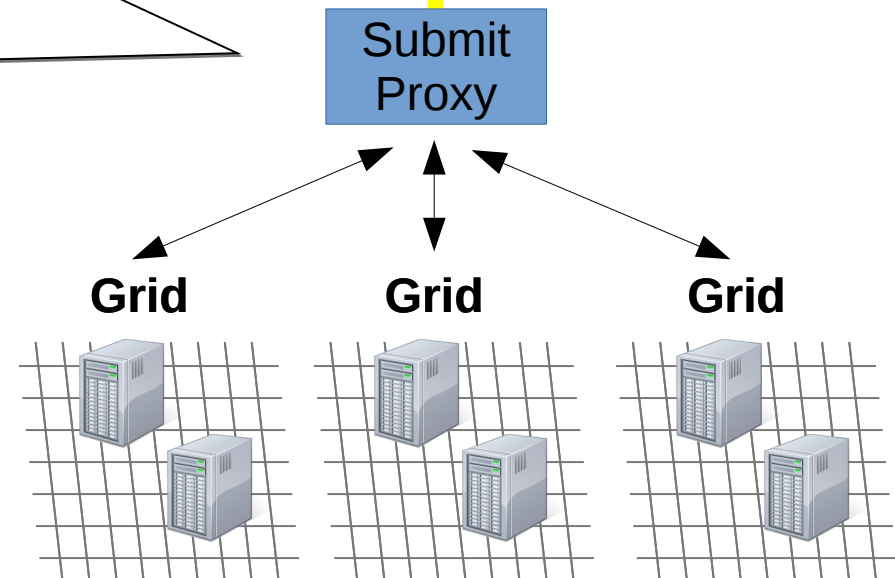
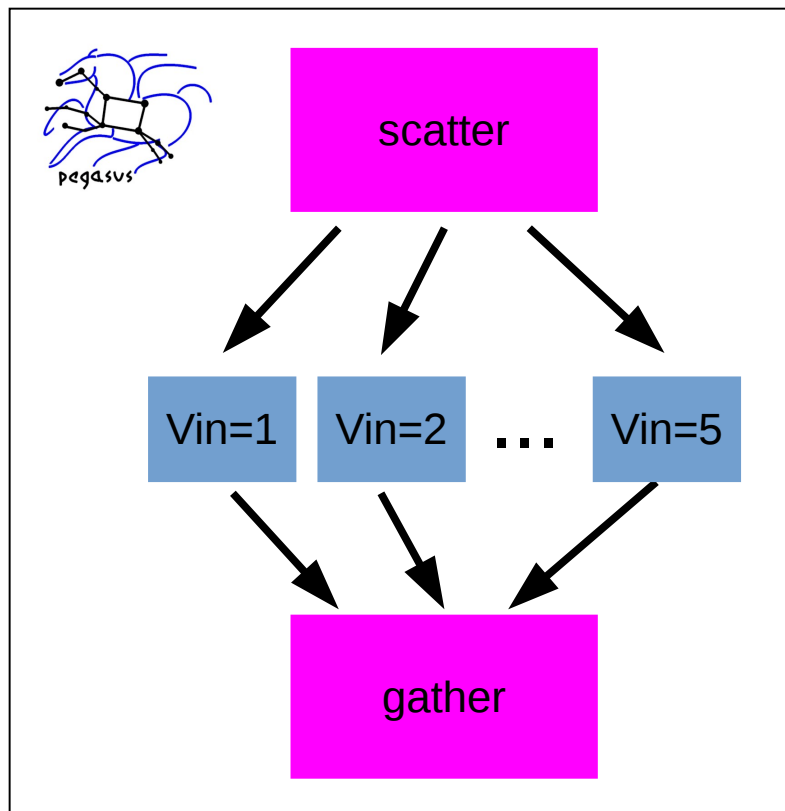
## User's Workspace Terminal

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

## HUBzero Infrastructure



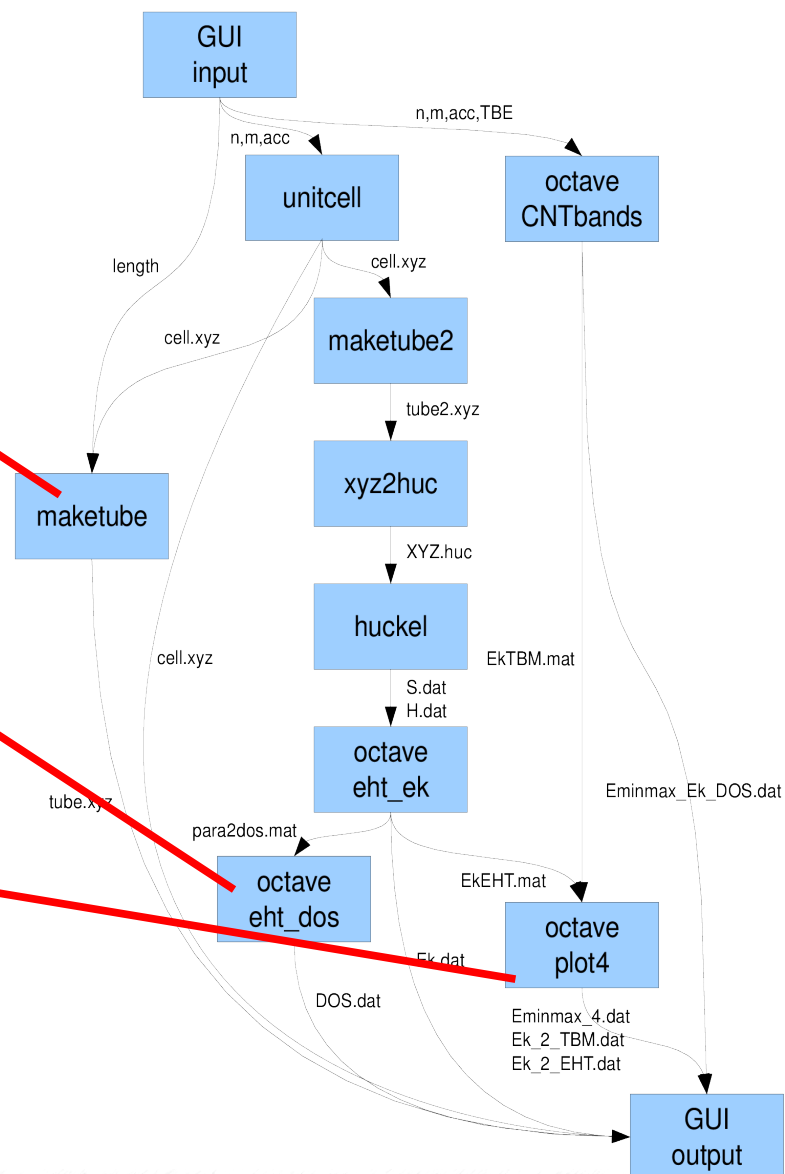
## Tool Session Containers





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

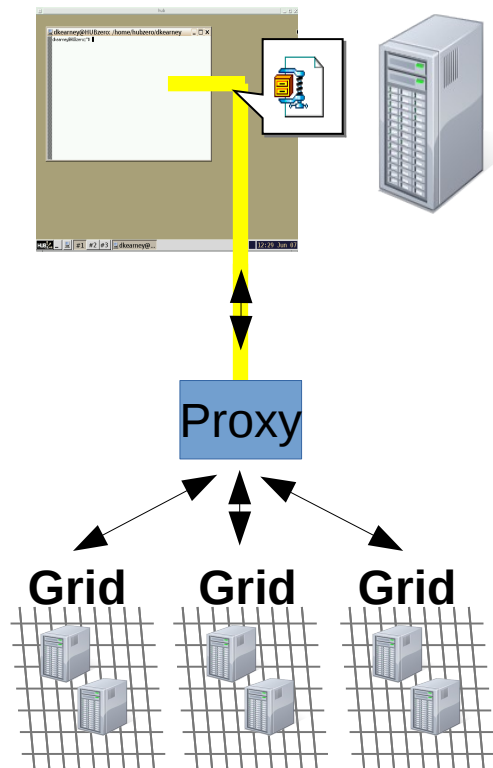
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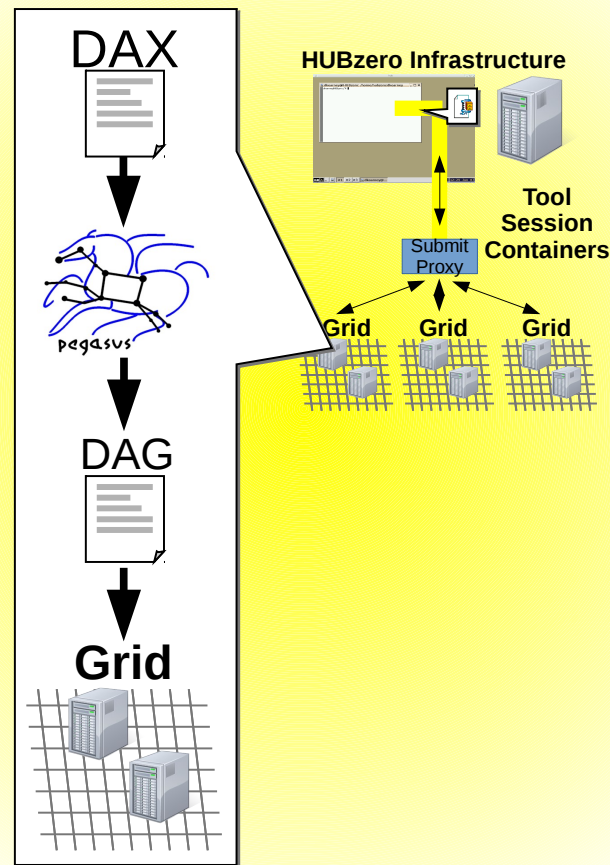


# Productivity in the Workspace

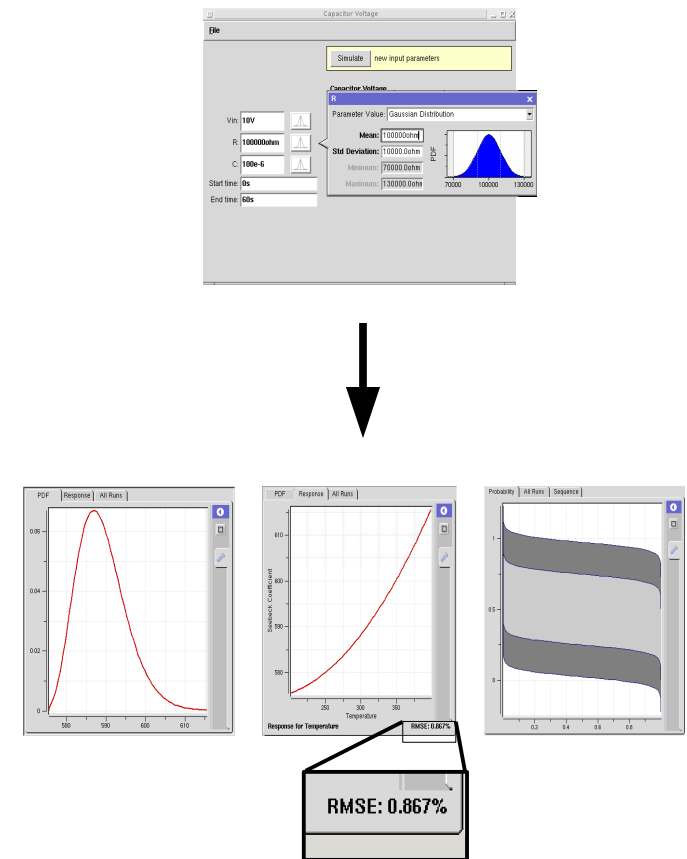
## Submit



## Pegasus Workflows

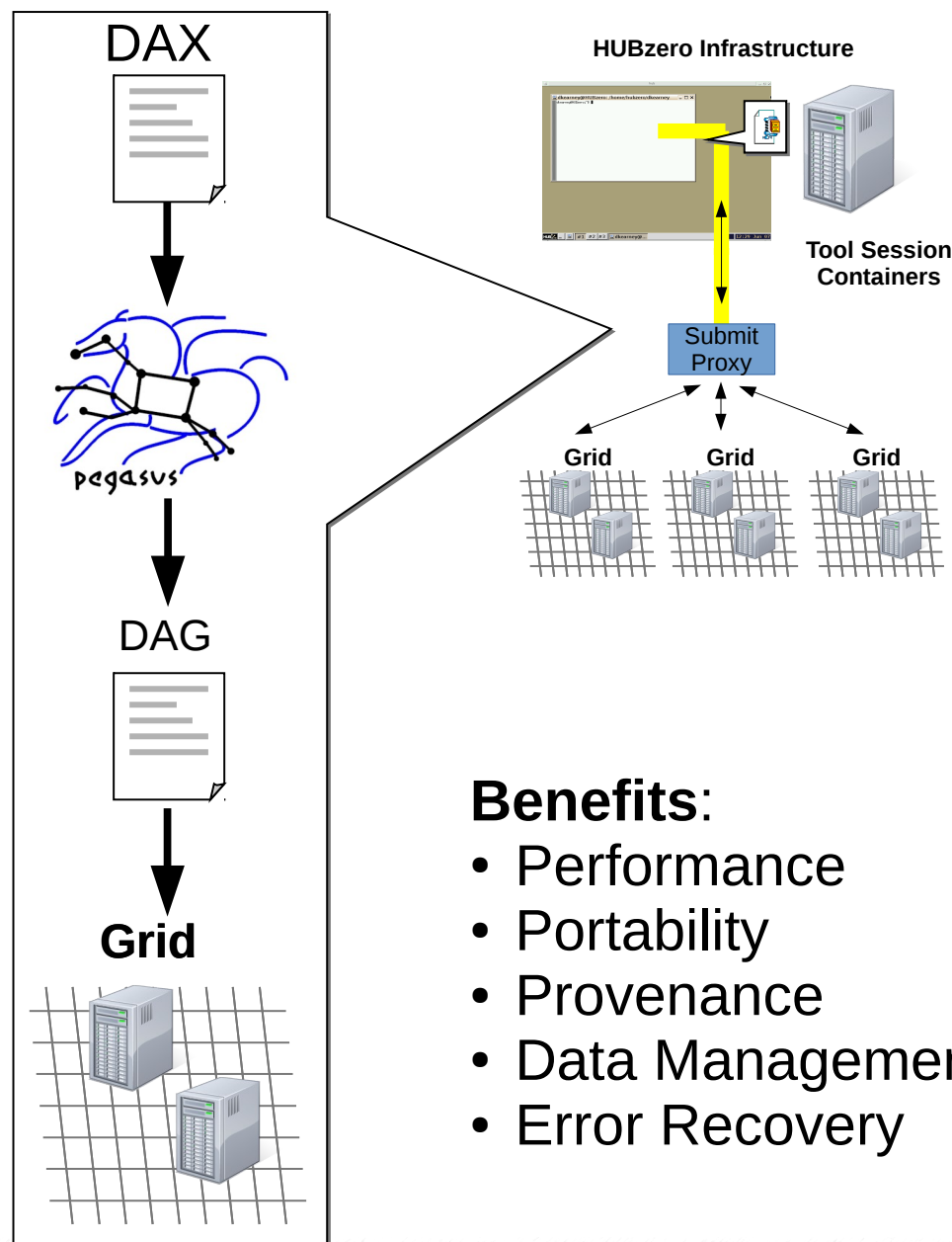
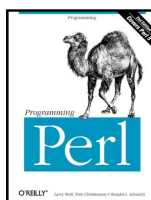
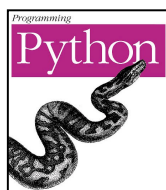


## Uncertainty Quantification



# Pegasus Workflow Management

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

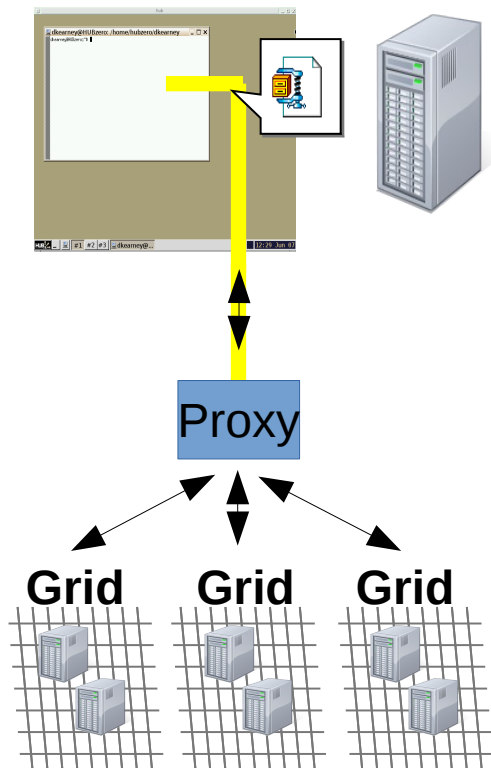


## Benefits:

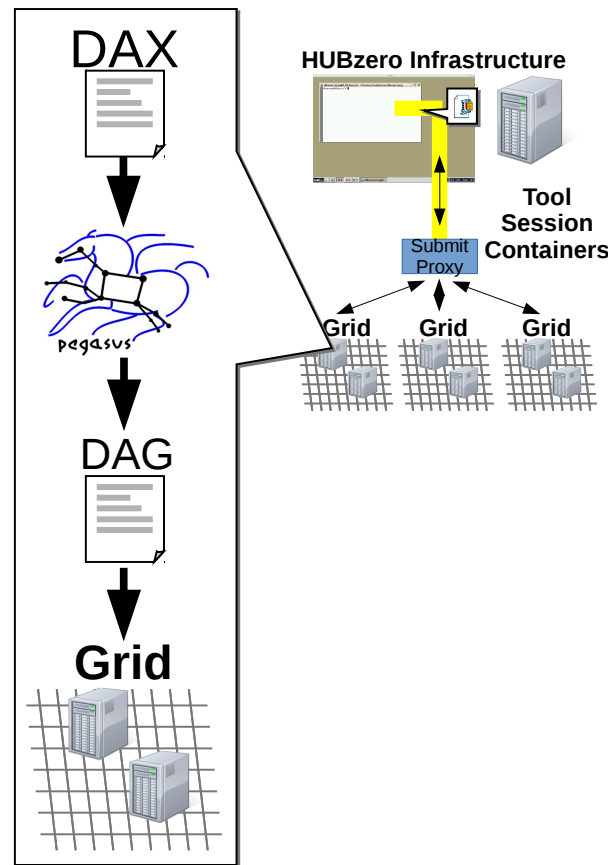
- Performance
- Portability
- Provenance
- Data Management
- Error Recovery

# Productivity in the Workspace

## Submit



## Pegasus Workflows



## Uncertainty Quantification

