

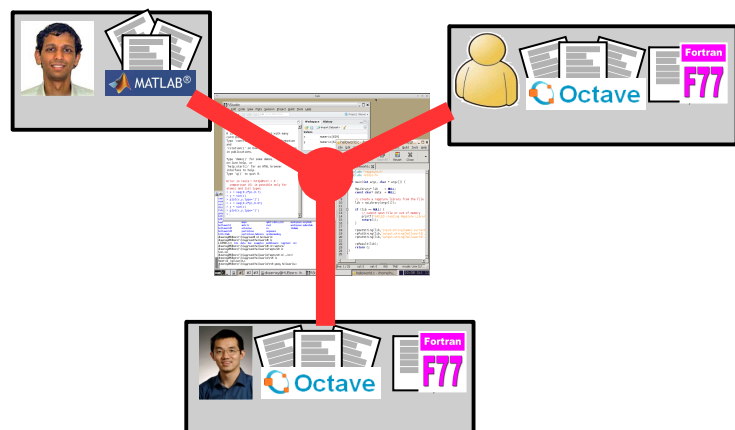
HUBzero Platform Features

Demo of Capabilities for the TRADES Program

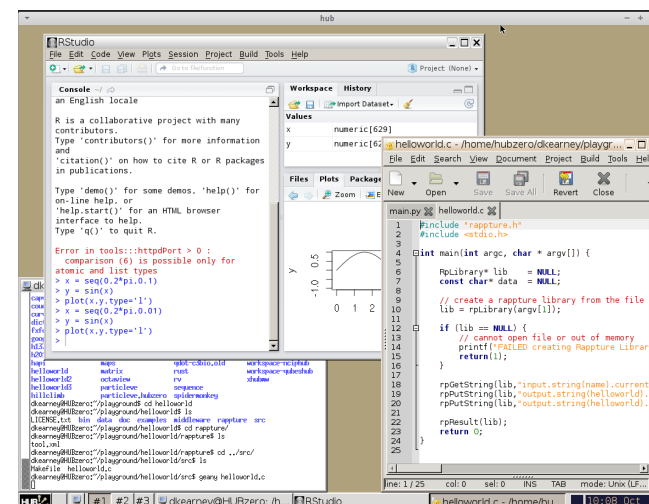
Oct. 12, 2016

Derrick Kearney
hubzero.org

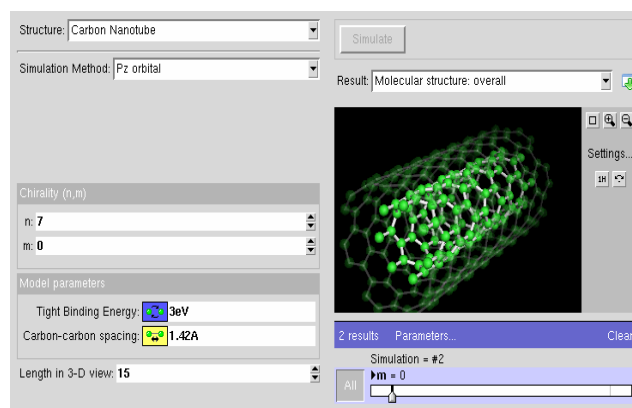
The HUBzero Platform



Perform
Research

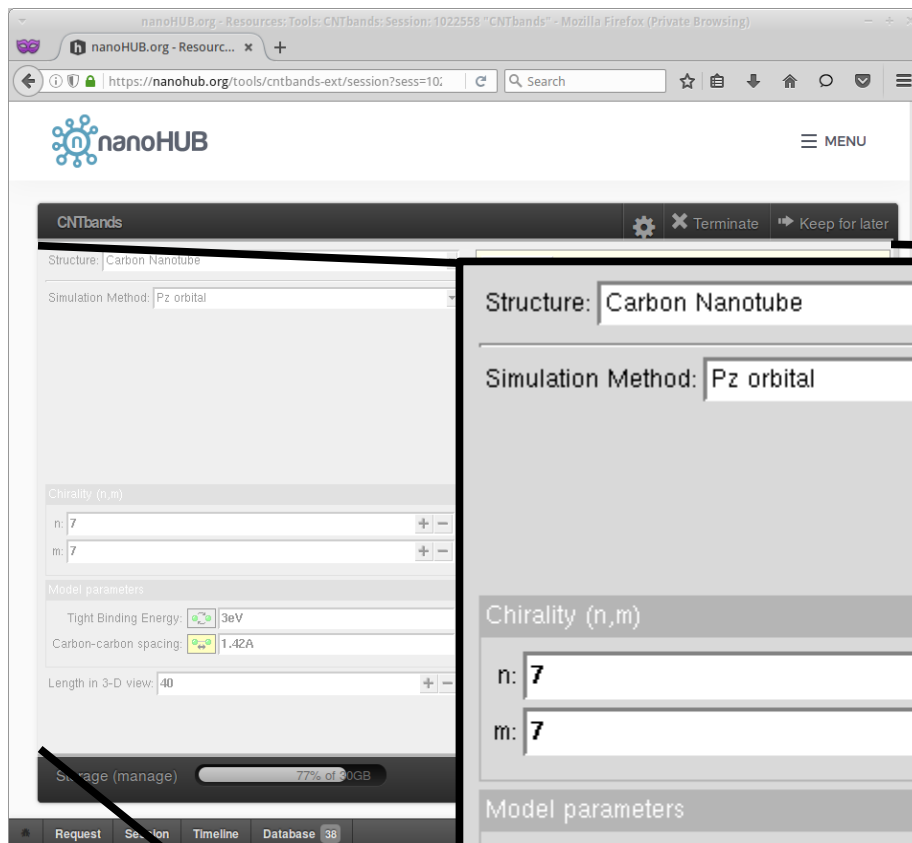


Collaborate
With Others



Secure, Scalable,
Sharable
Dev Environments

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.

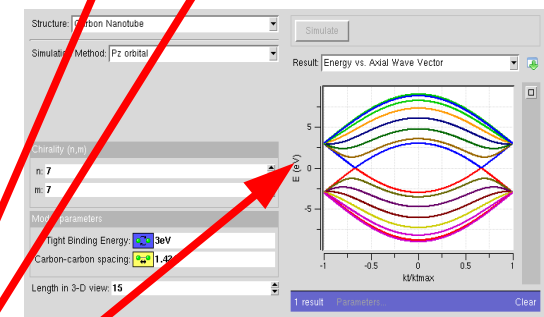
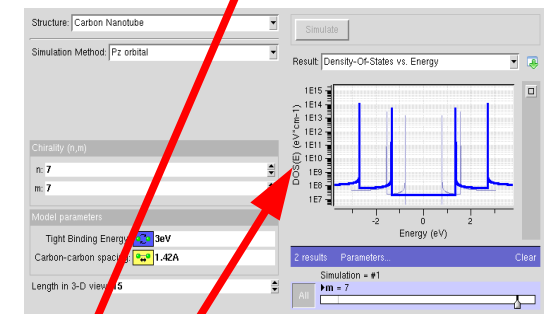
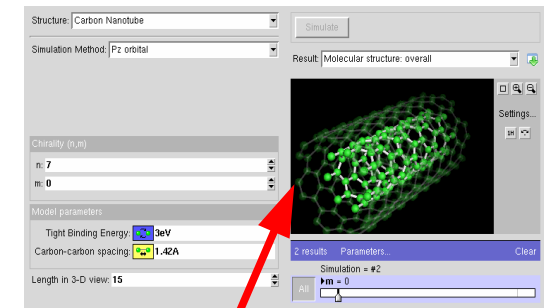
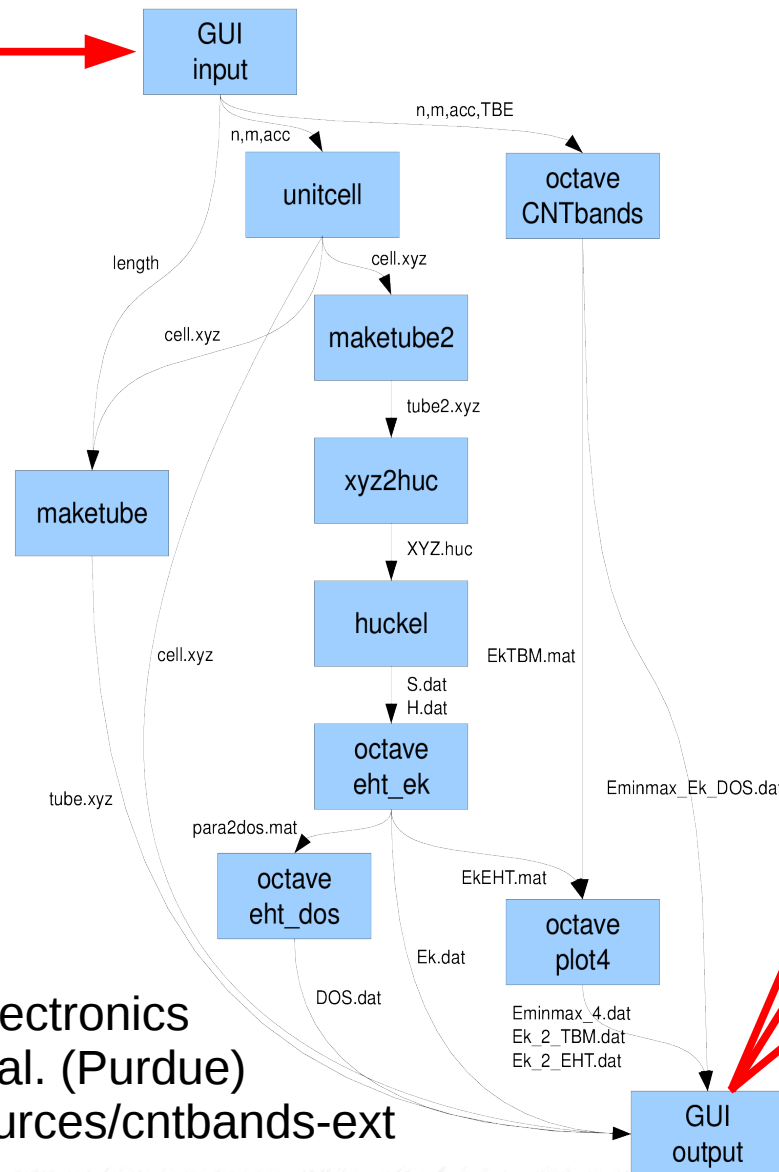
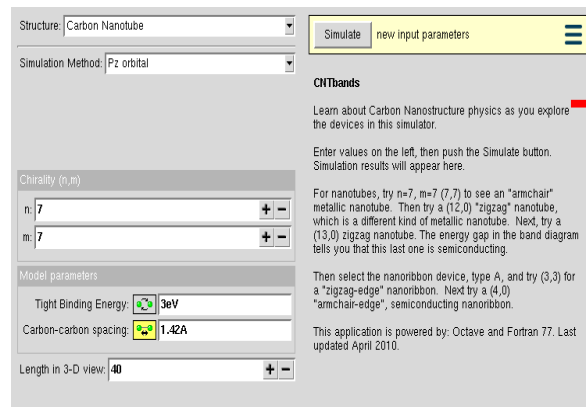
CNTbands

Science Domain: Nanoelectronics

Scientists: Lundstrom et al. (Purdue)

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

Many Pieces by Different Developers



CNTbands

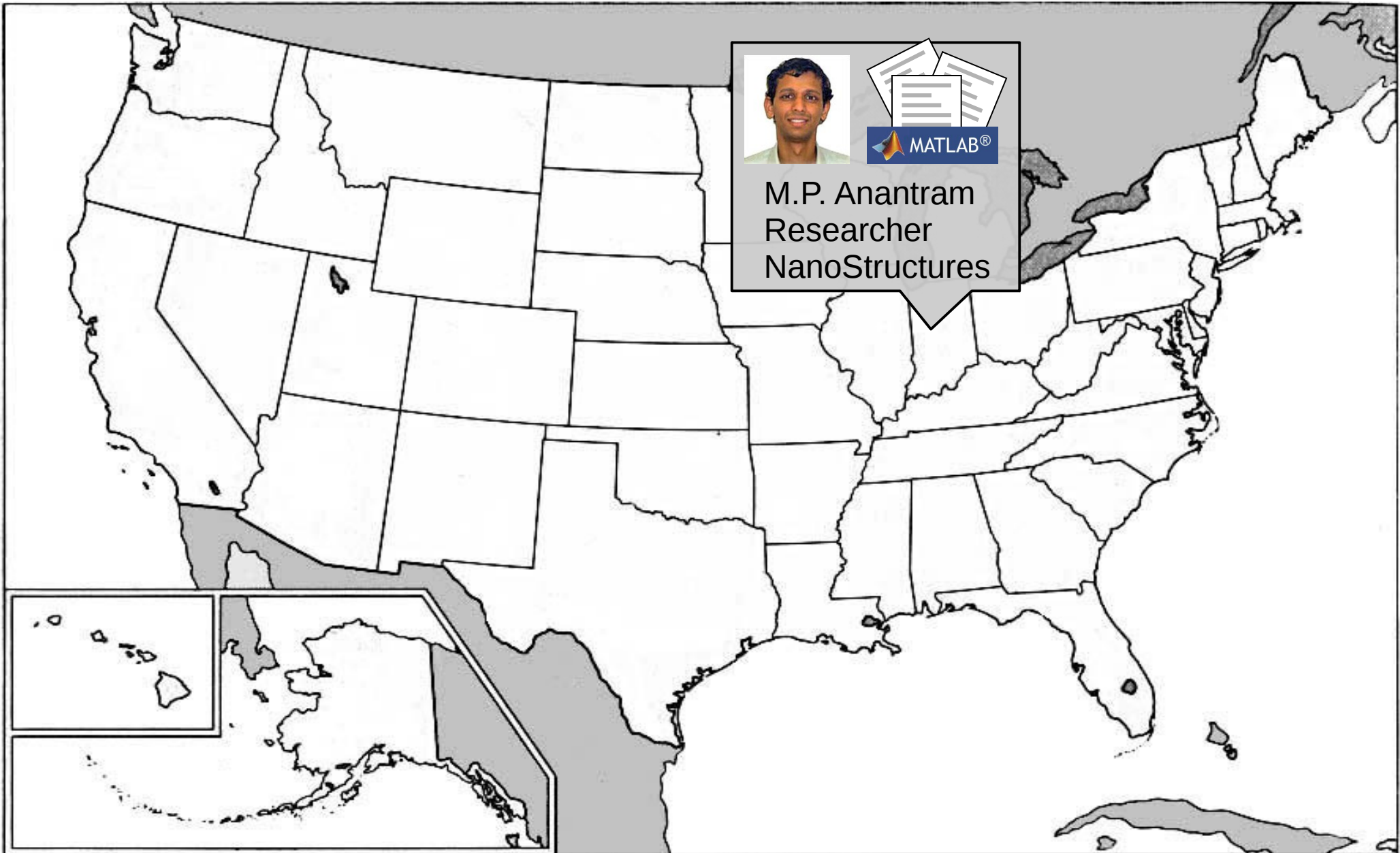
Science Domain: Nanoelectronics
Scientists: Lundstrom et al. (Purdue)

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

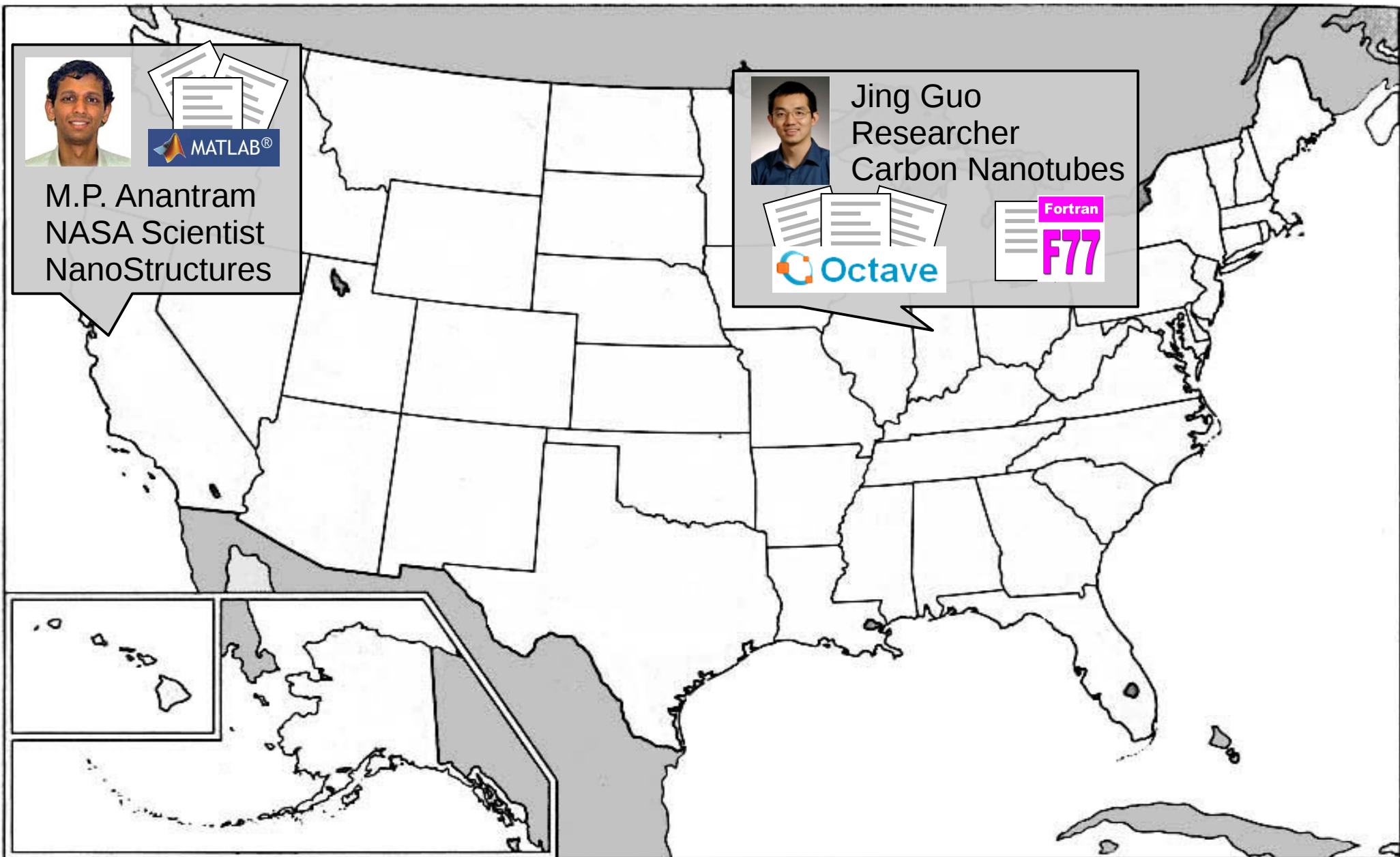
1990s – Initial Algorithms



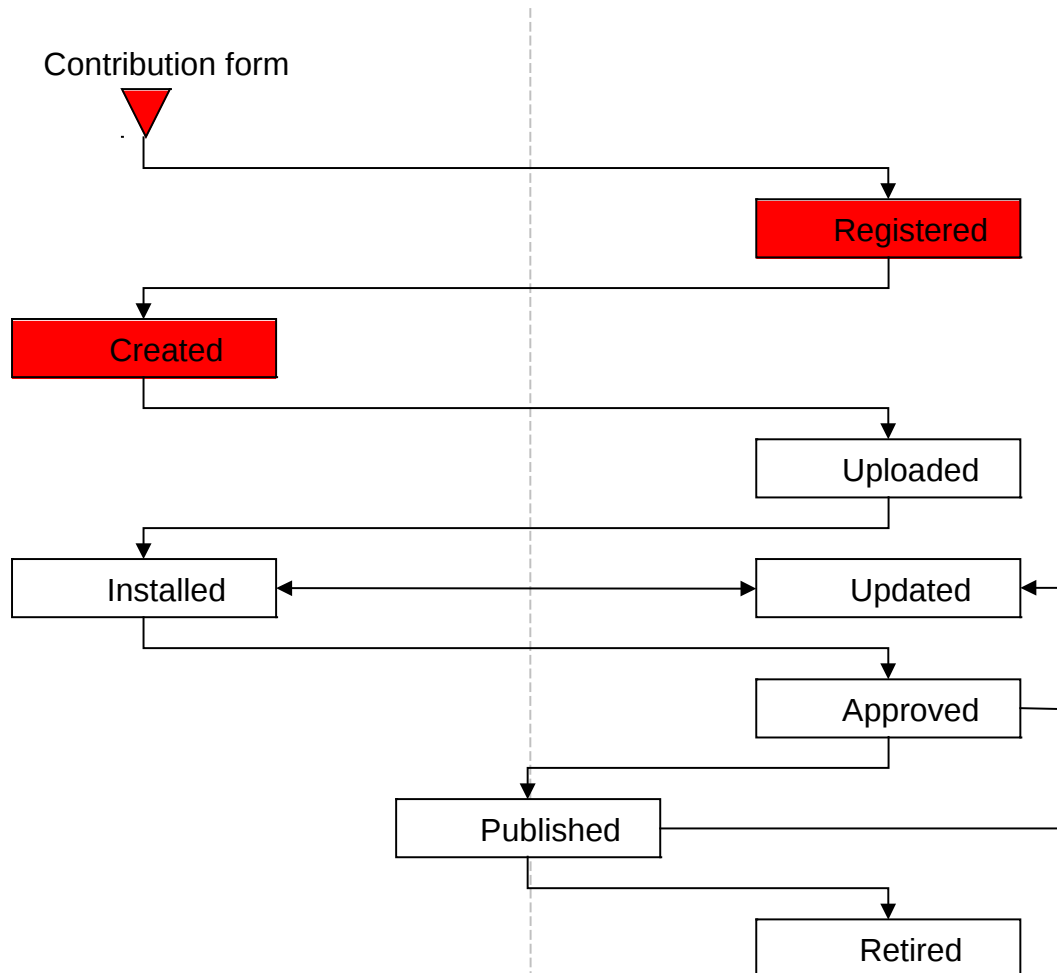
M.P. Anantram
Researcher
NanoStructures



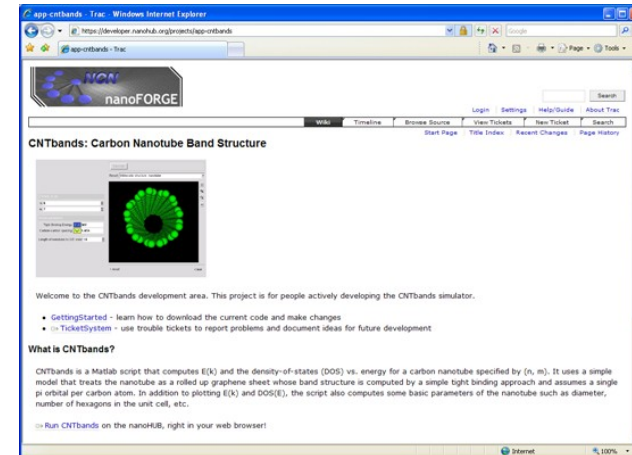
2002 – Idea for a Tool



Tool Registered



<https://yourhub.org/tools>

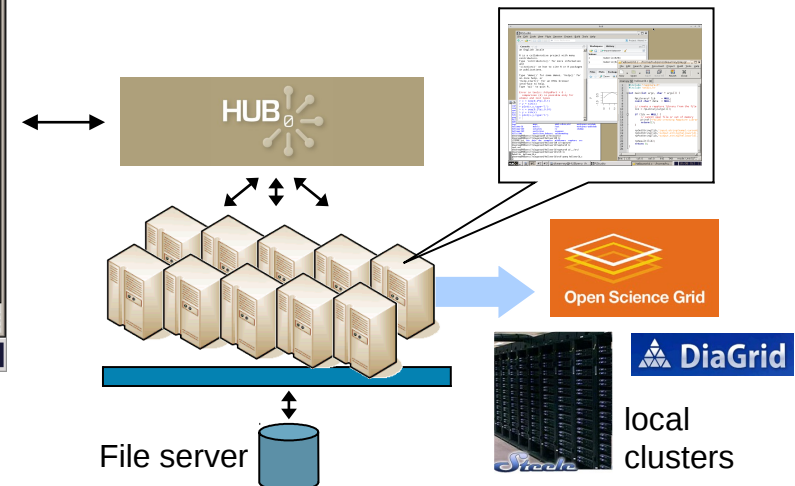
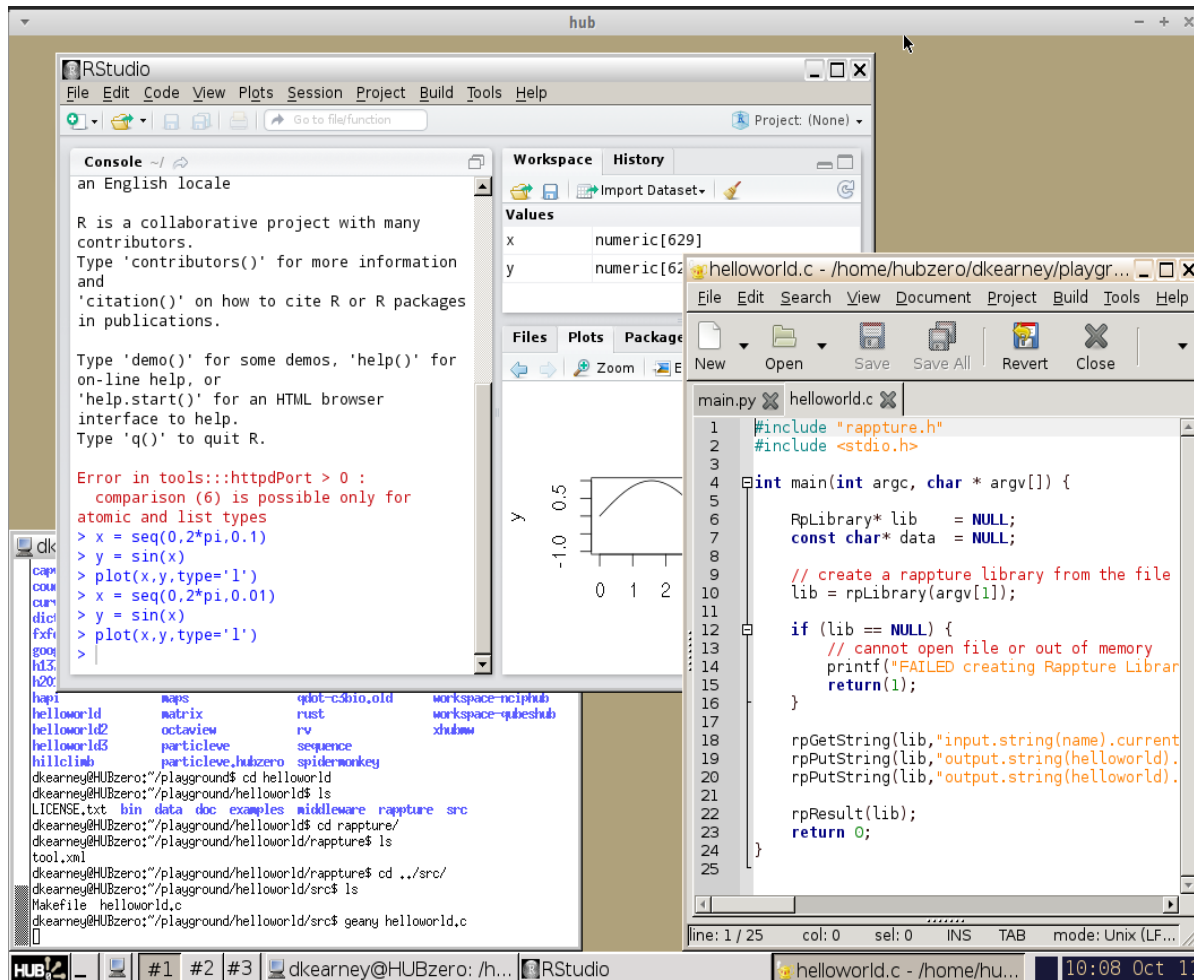


Provides:

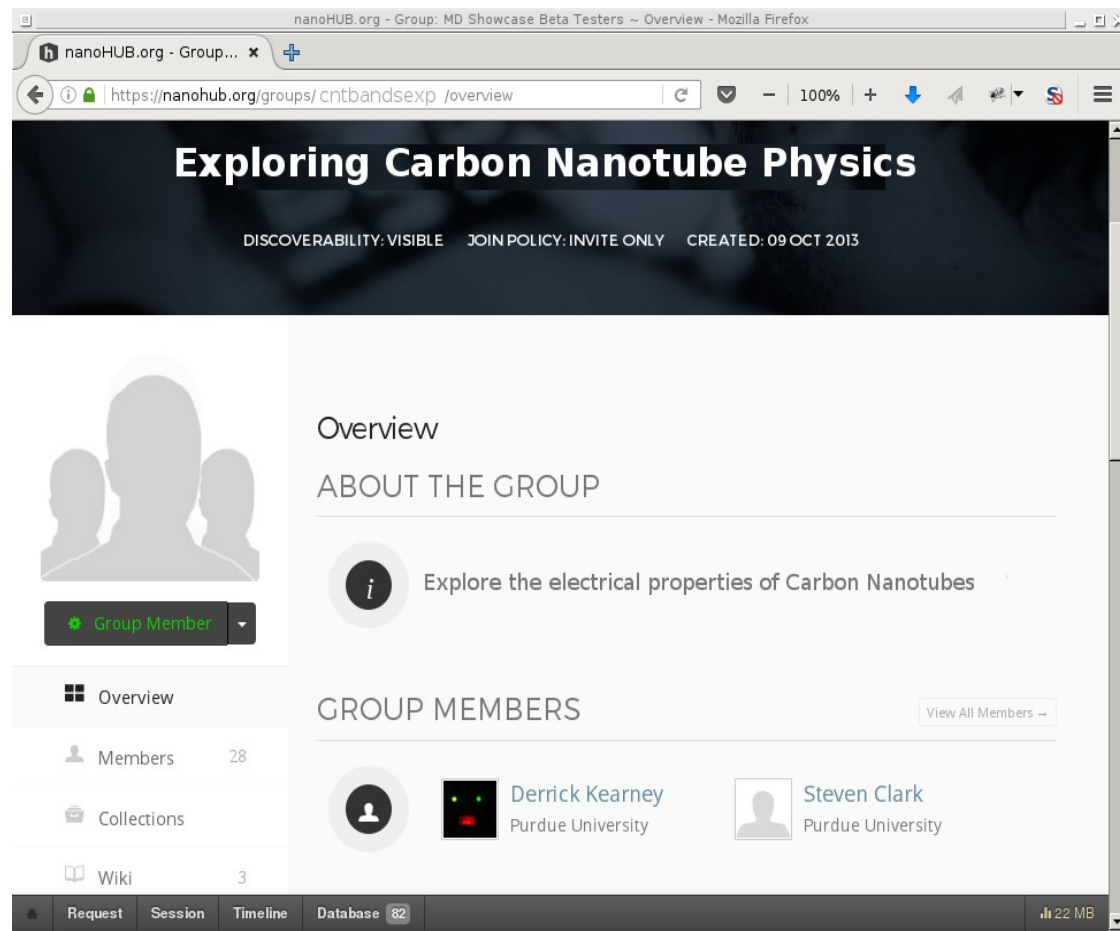
- Source code repository
- Wiki for project documentaton
- Placeholder for publishing tool
- Access to HUB Workspace

What is a Workspace?

- Full-featured Desktop
- Runs in the Cloud
- For Developers & Researchers
- Accessible from any web browser
- Still running after you close browser
- File storage provided by the HUB

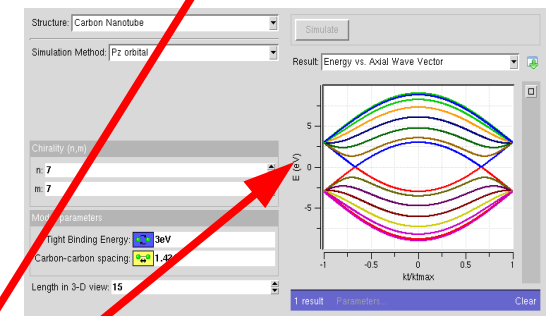
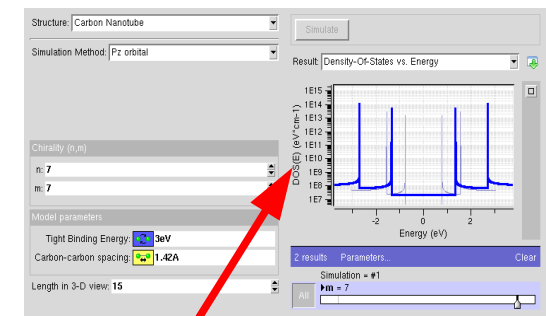
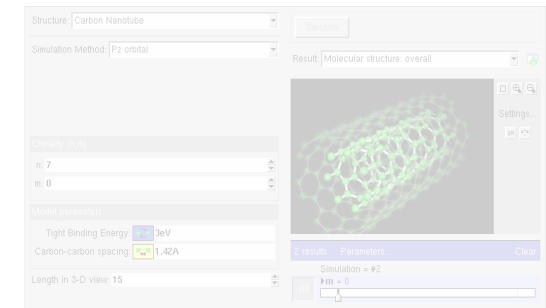
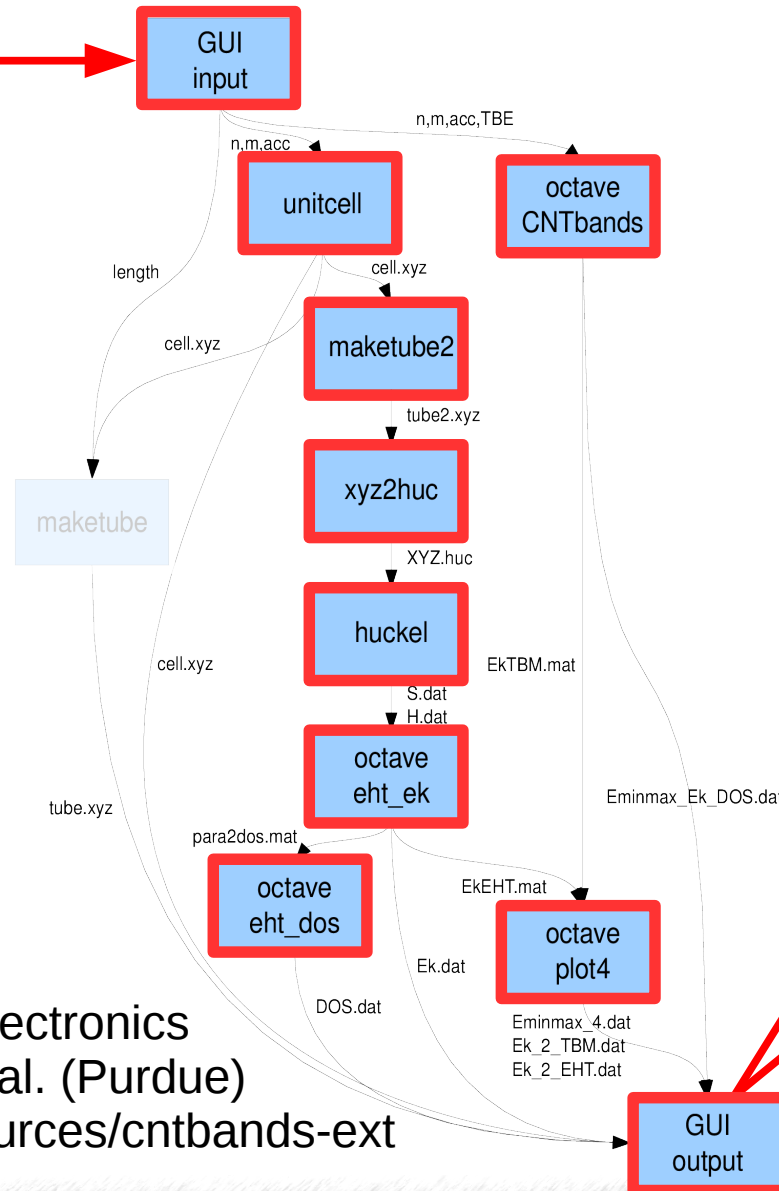
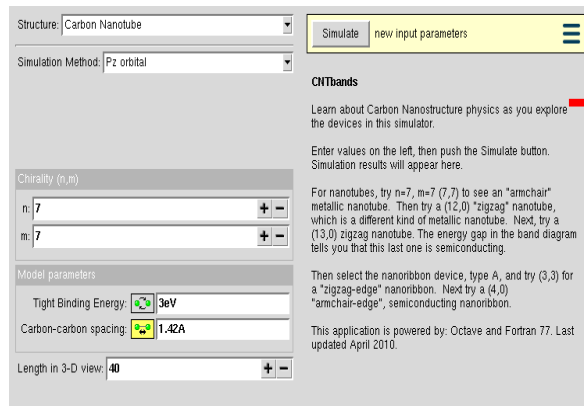


Collaborate within a Group



- Build a community around your research
- Share links, papers, and data
- Forums encourage discussion
- Create how-tos with wiki pages
- Keep everyone informed with Announcements

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 that the page describing your tool is created with correct information:

→ Test your application:

Launch tool →

→ Review the page describing your tool

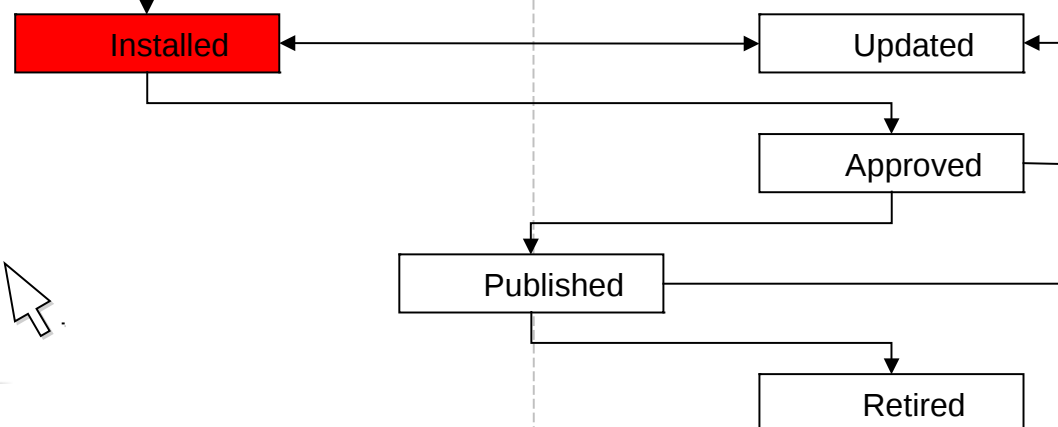
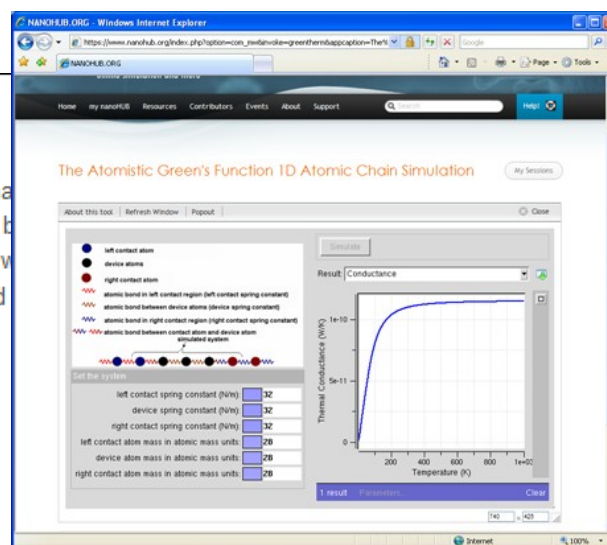
We are waiting for You

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

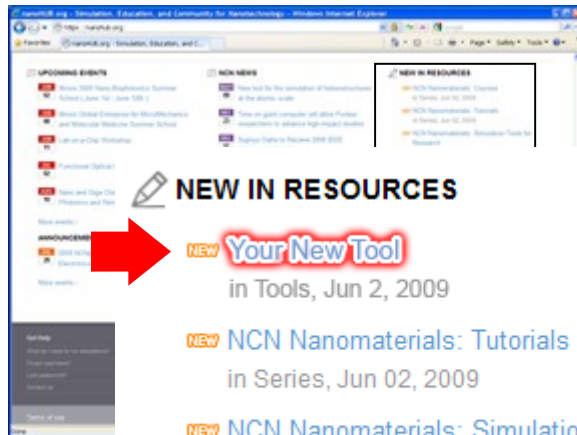
→ My tool is working properly. I approve it.

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.



Publishing Applications



NEW IN RESOURCES

NEW Your New Tool

in Tools, Jun 2, 2009

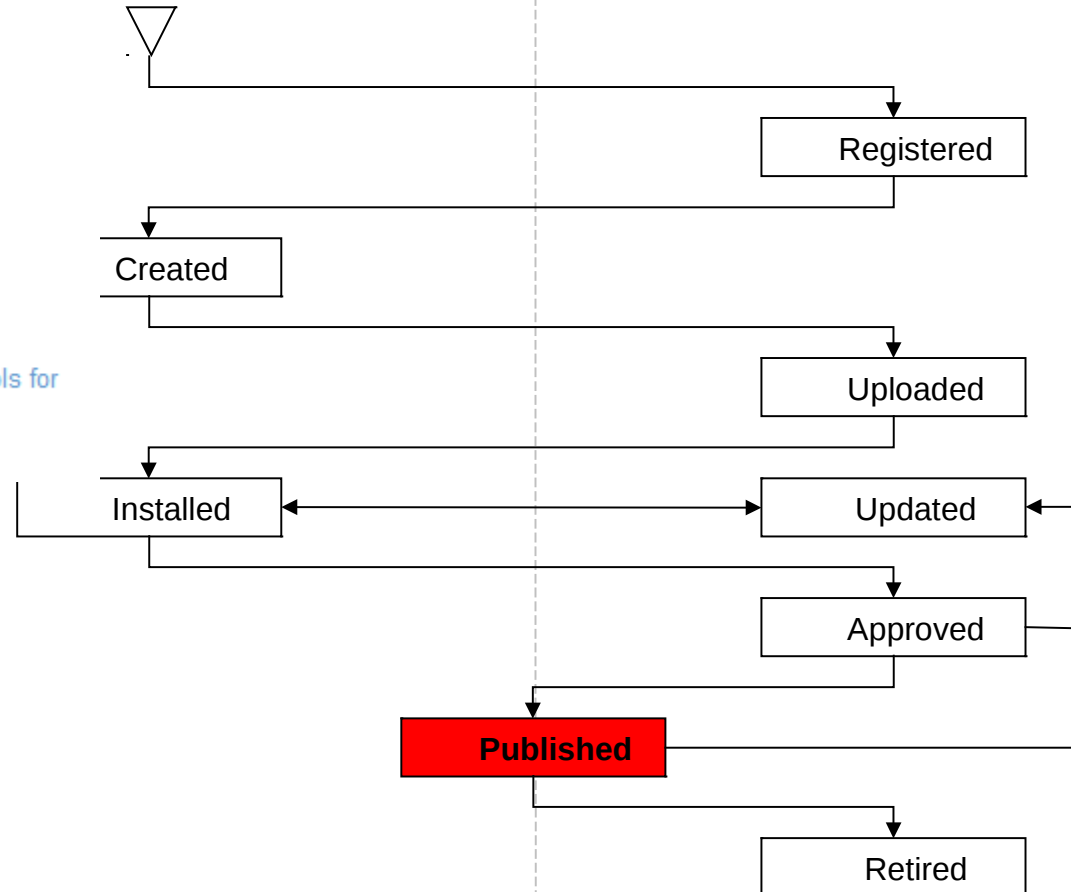
NEW NCN Nanomaterials: Tutorials

in Series, Jun 02, 2009

NEW NCN Nanomaterials: Simulation Tools for Research

in Series, Jun 02, 2009

Contribution form



Knowing Your Impact

CNTbands

By Gyungseon Seol¹, Youngki Yoon¹, James K Fodor¹, Jing Guo¹, Akira Matsudaira², Diego Kienle², Gengchiao Liang², Gerhard Klimeck², Mark Lundstrom², Ahmed Ibrahim Saeed³

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

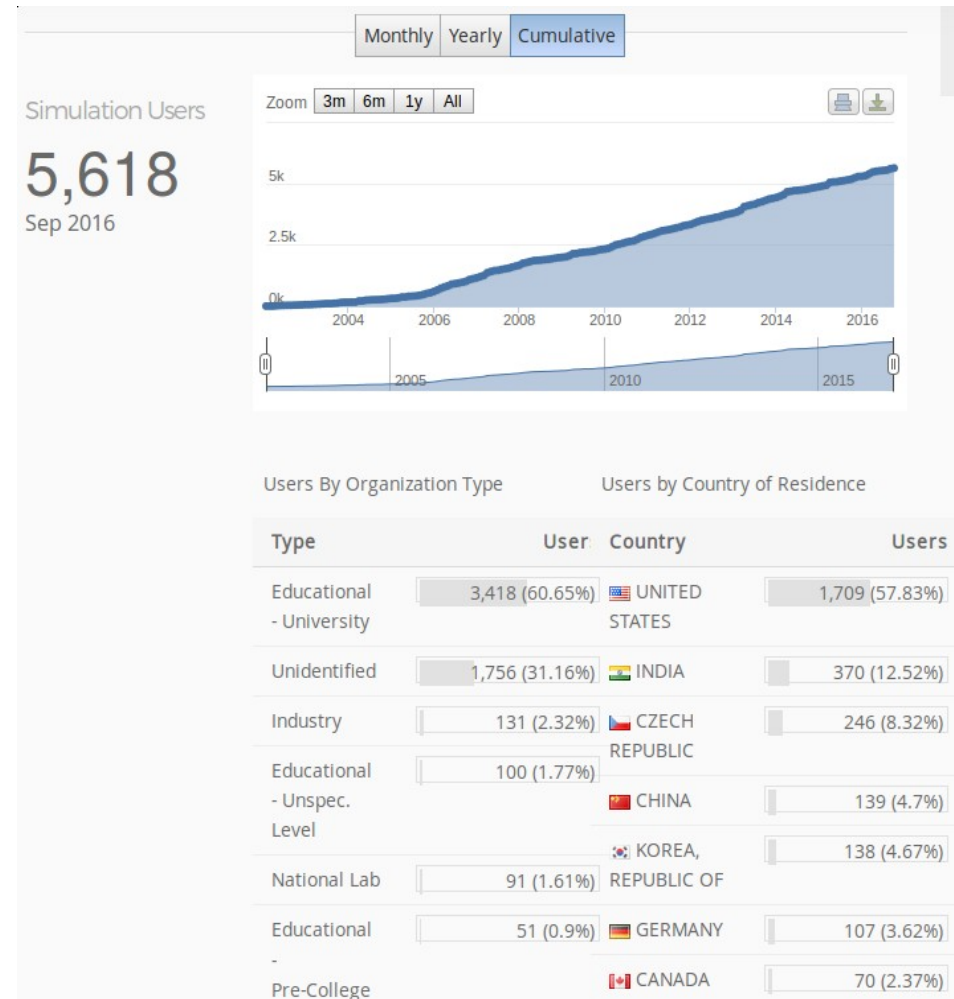
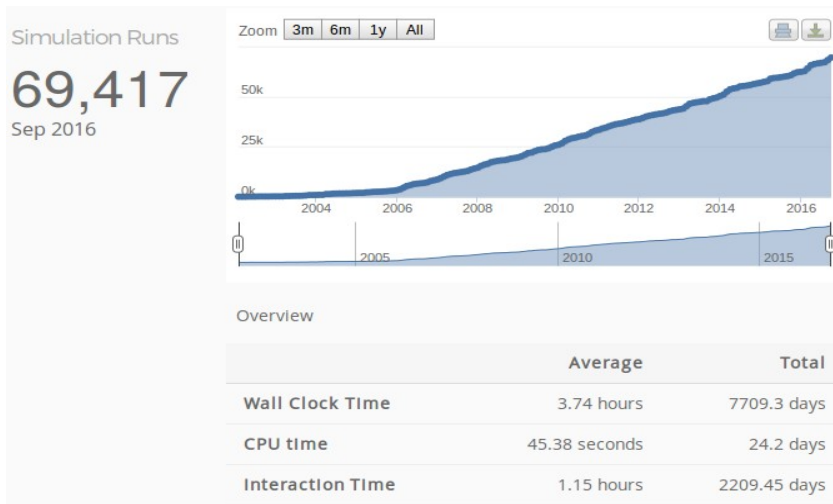
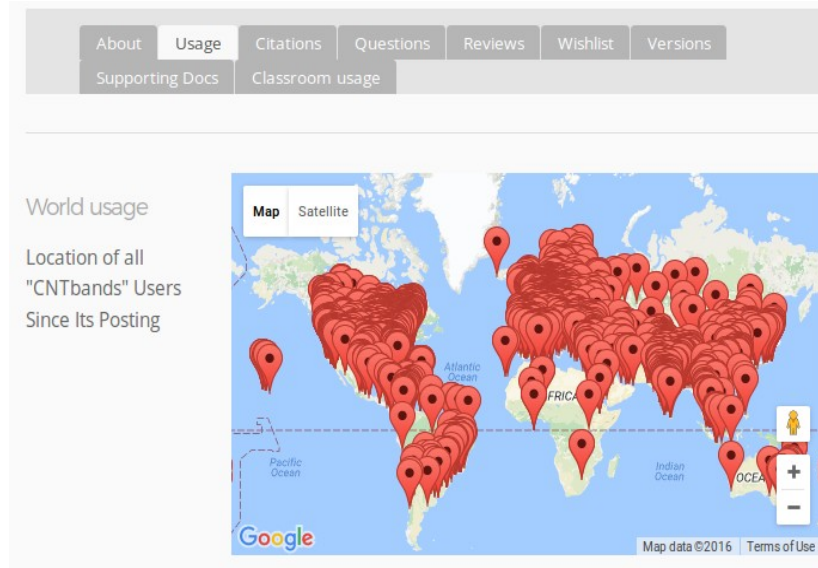
Supporting Docs

Classroom usage

See also

Part of: NCN
Nanoelectronics:
Simulation Tools
for Education
Part of: NCN
Nanoelectronics:

Track Usage Metrics




Communicate With Users


CNTbands


By Gyung-Guo¹, Ali-Ullah², G. Ibrahim S. 1. University of Shams U


This tool 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


31XHG site


License


the User Guide


the 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:    ...

Versions Supporting Docs Classroom usage

See also

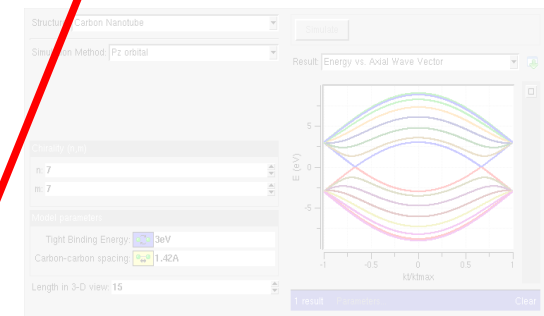
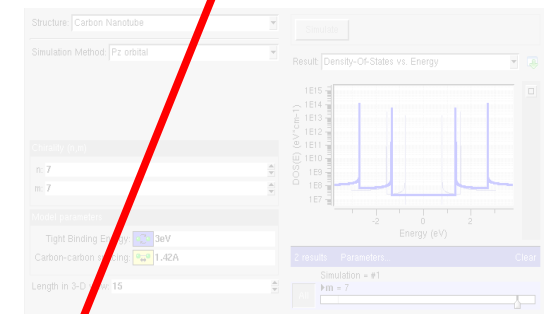
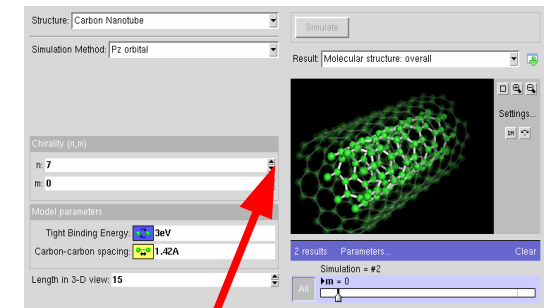
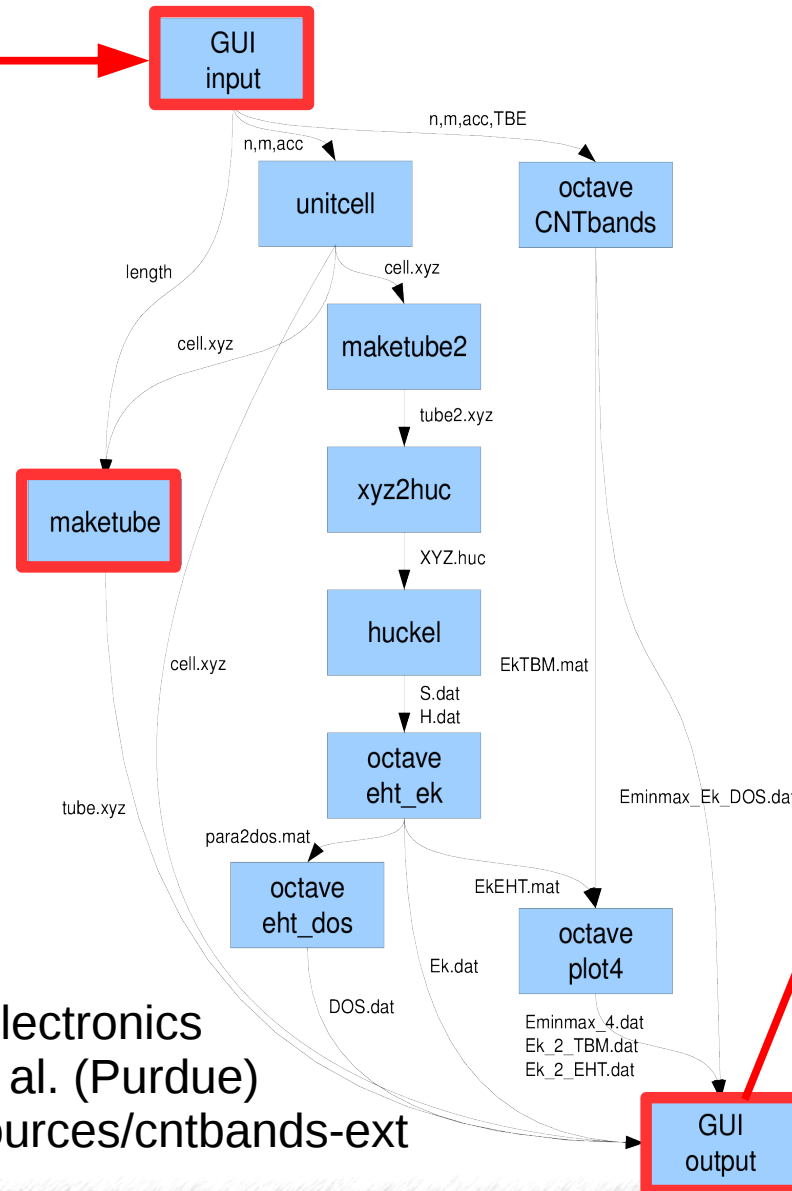
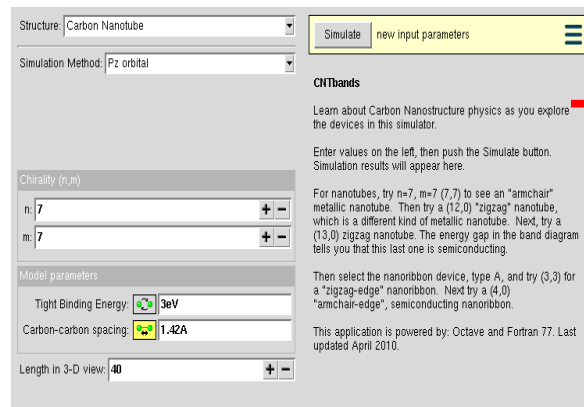
Part of: NCN

Nanoelectronics: Simulation Tools for Education

Part of: NCN

Nanoelectronics:

Adding New Features

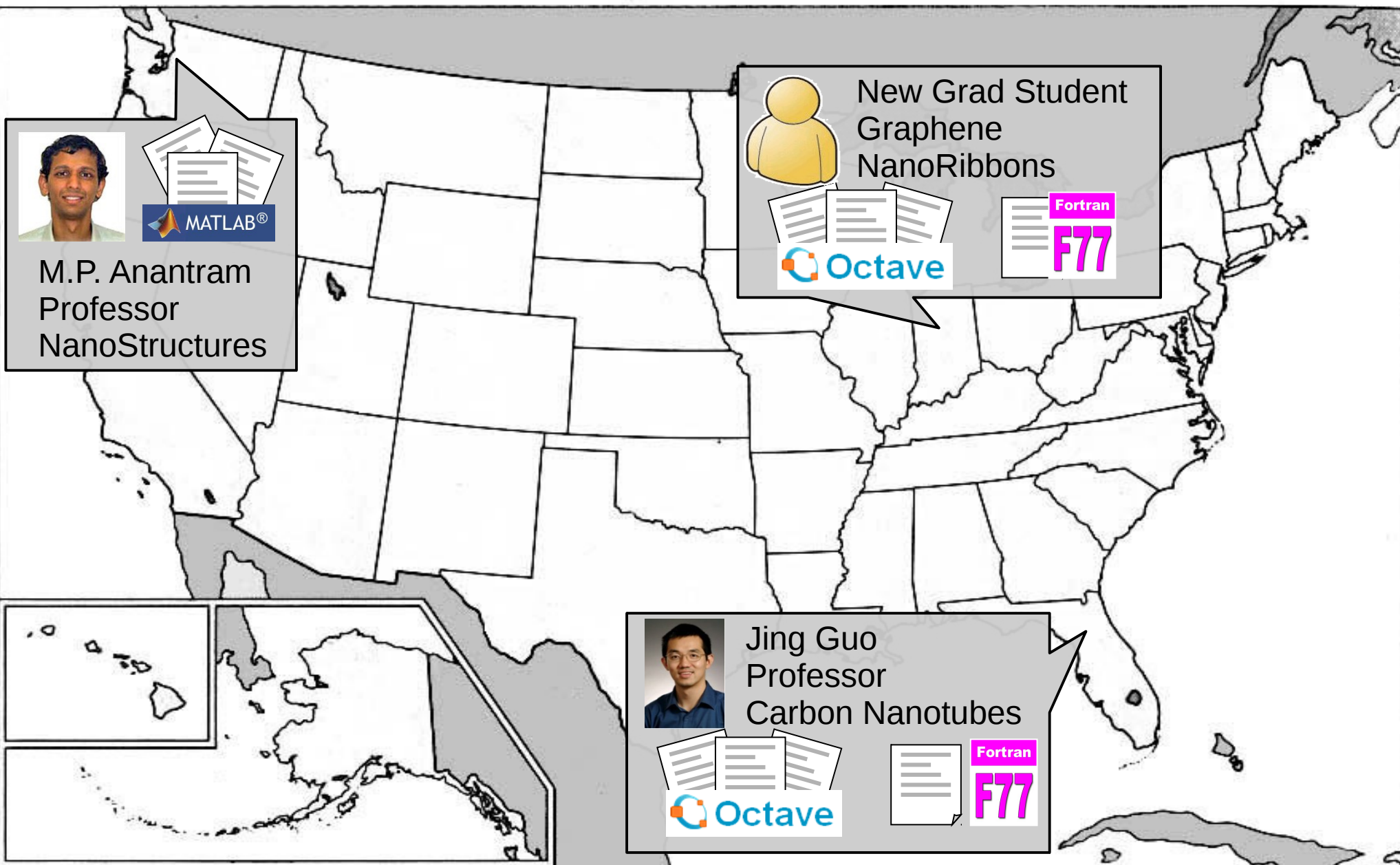


CNTbands

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

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

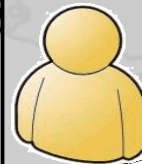
2010 – Introducing New Researchers



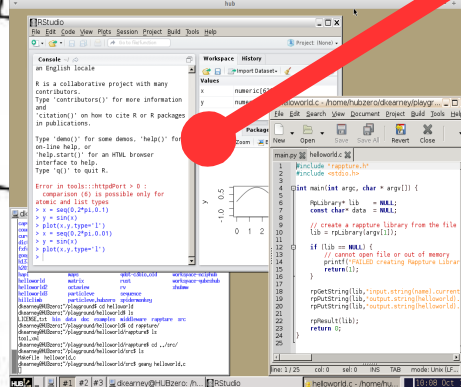
Collaborate in the Workspace



M.P. Anantram
Professor
NanoStructures



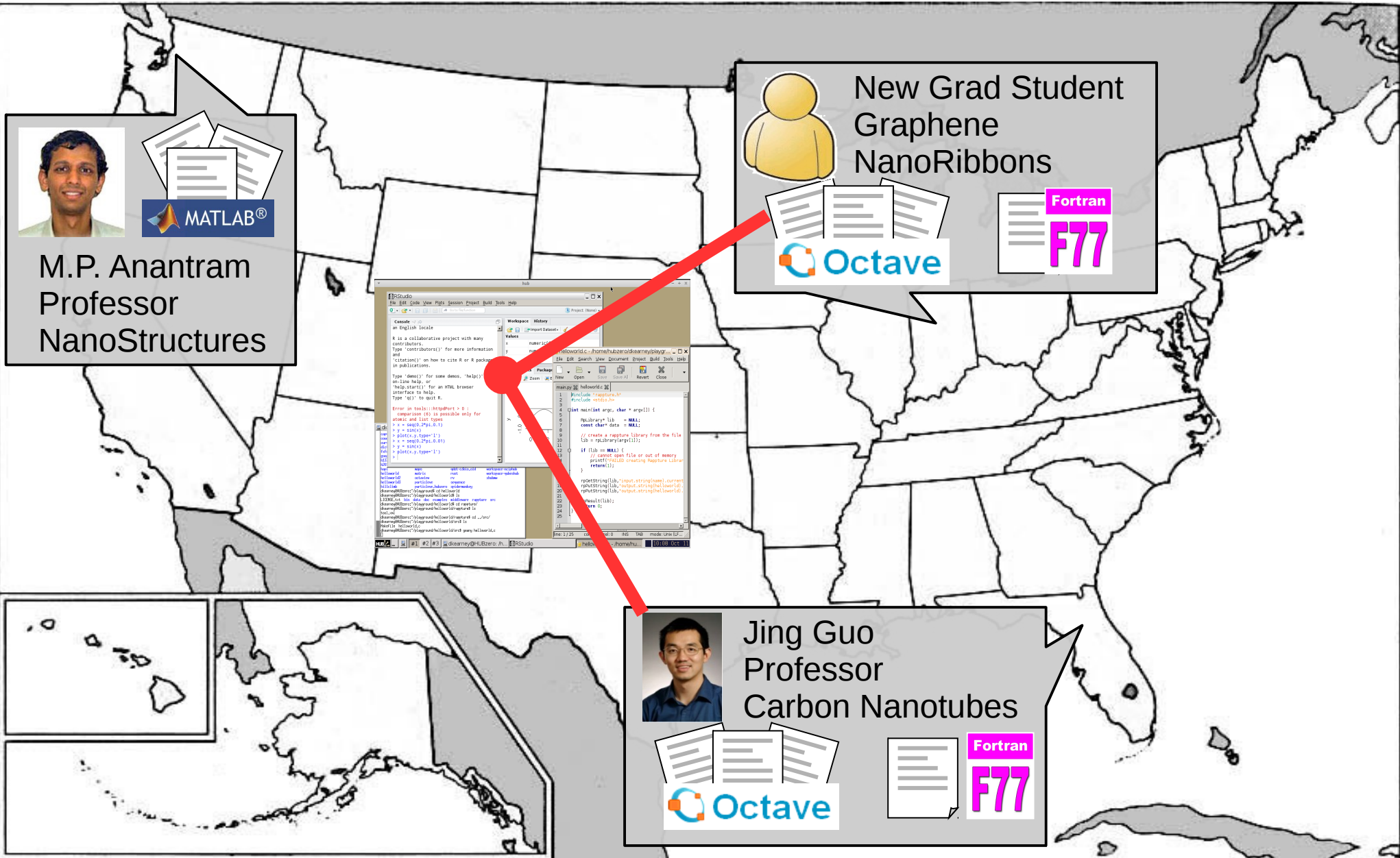
New Grad Student
Graphene
NanoRibbons



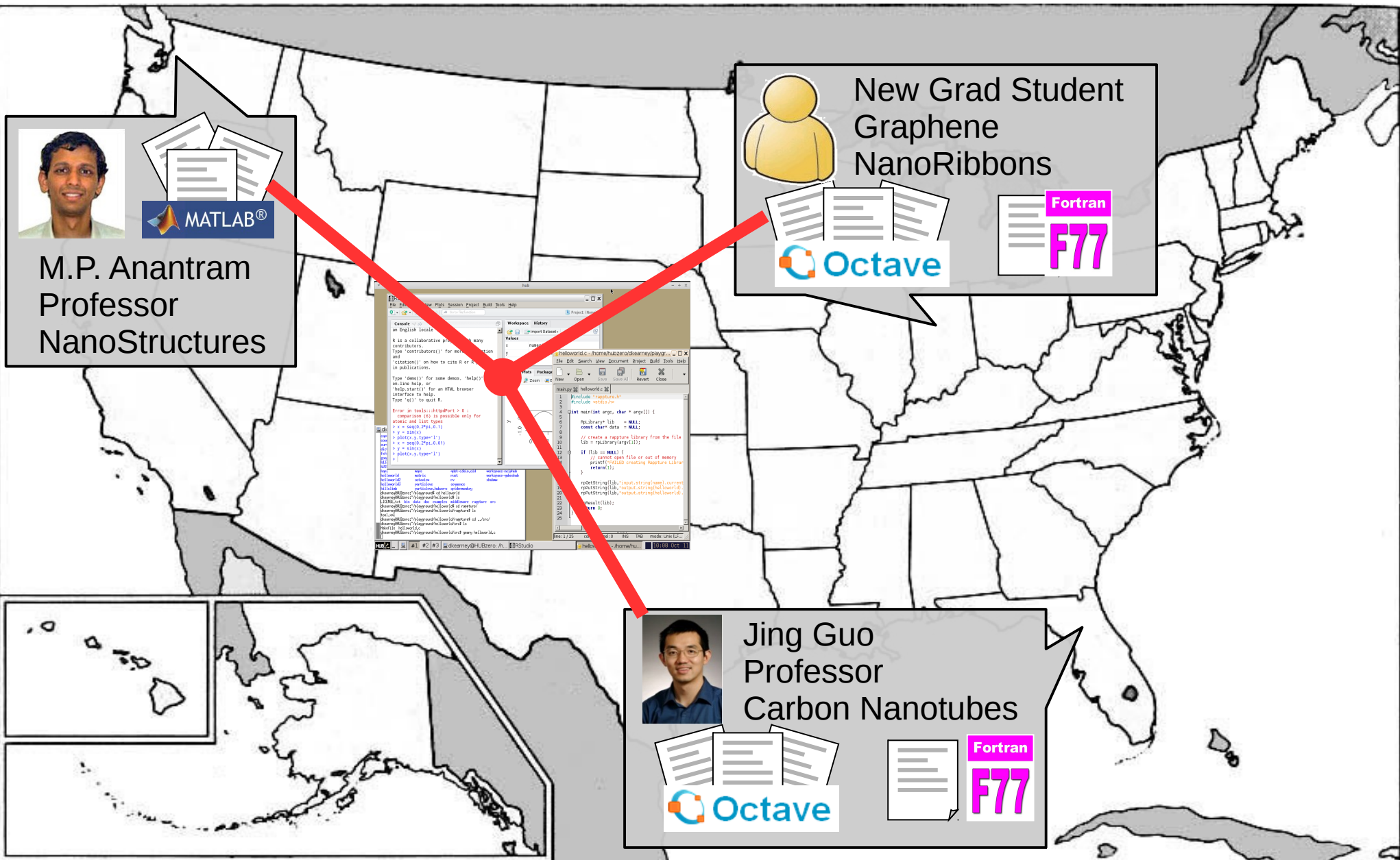
Jing Guo
Professor
Carbon Nanotubes



Collaborate in the Workspace

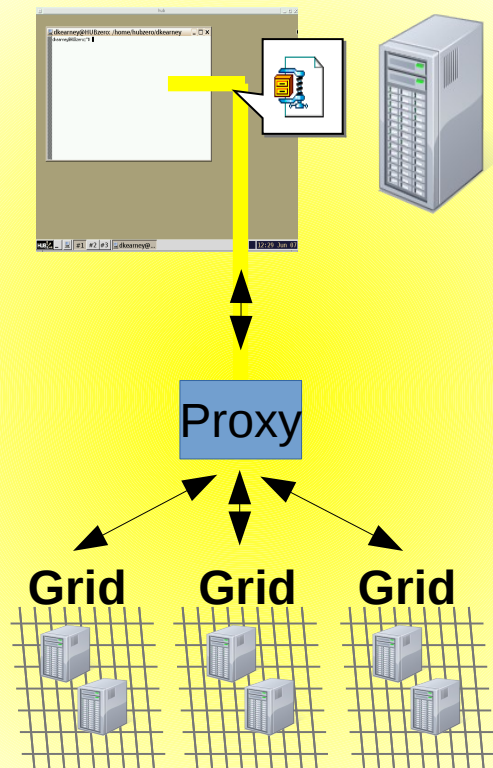


Collaborate in the Workspace

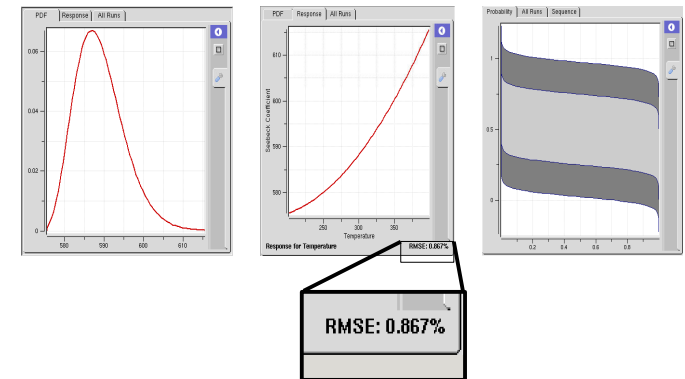
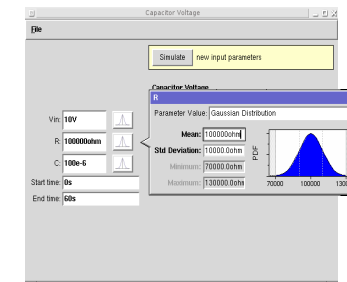
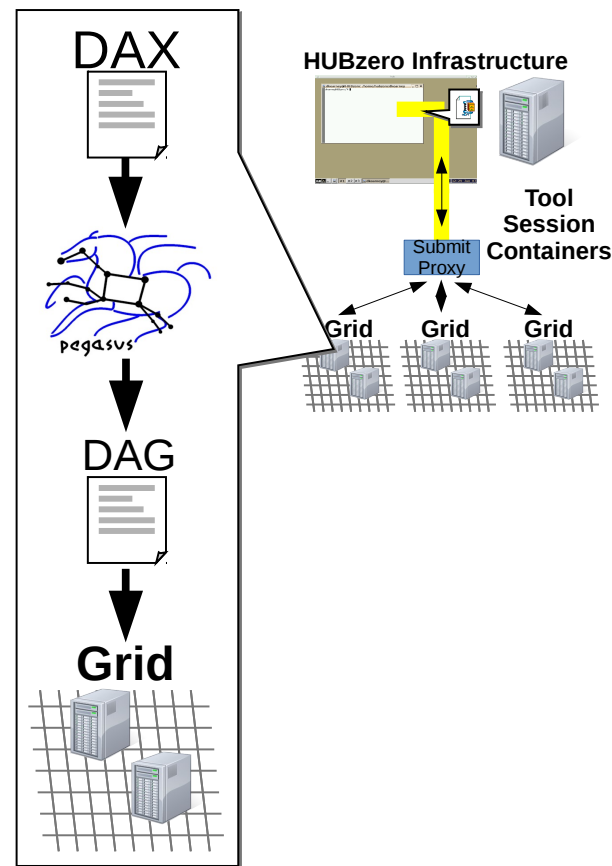


Productivity in the Workspace

Submit



Pegasus Workflows Uncertainty Quantification

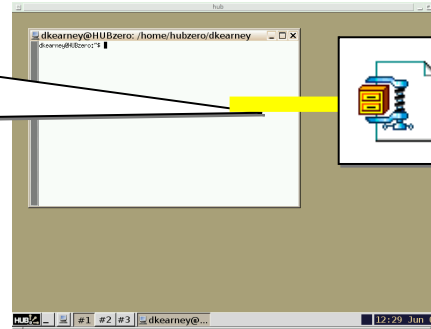


Run tools locally in Workspace

User's Workspace Terminal

```
$ echo hi
hi
$
```

HUBzero Infrastructure



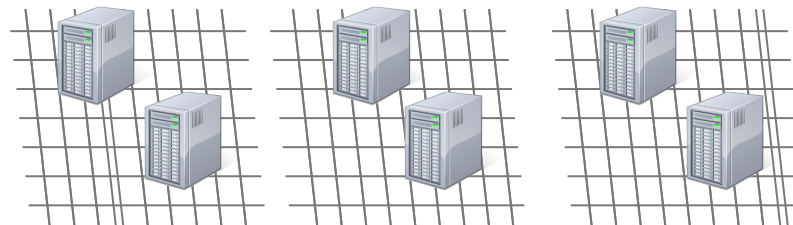
**Tool
Session
Containers**

**Submit
Proxy**

Grid

Grid

Grid

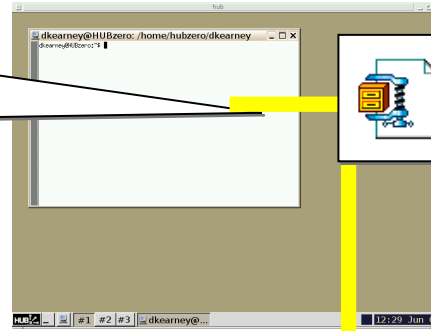


Submit Jobs to Grid

User's Workspace Terminal

```
$ submit echo hi
```

HUBzero Infrastructure



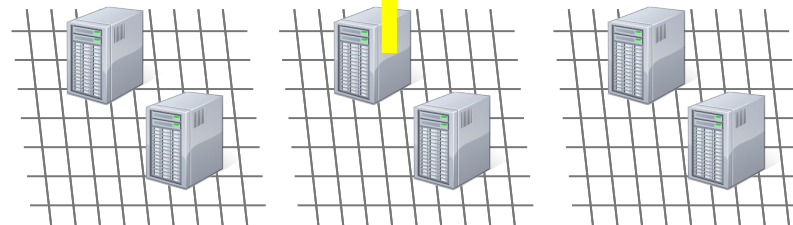
**Tool
Session
Containers**

**Submit
Proxy**

Grid

Grid

Grid

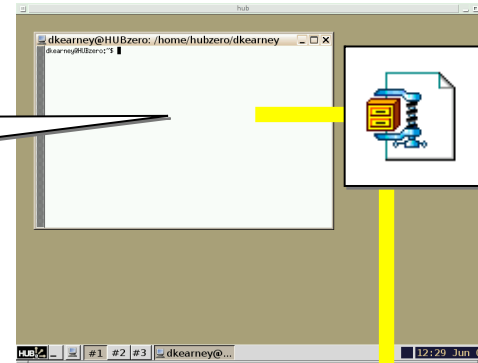


Let Submit create a workflow ...

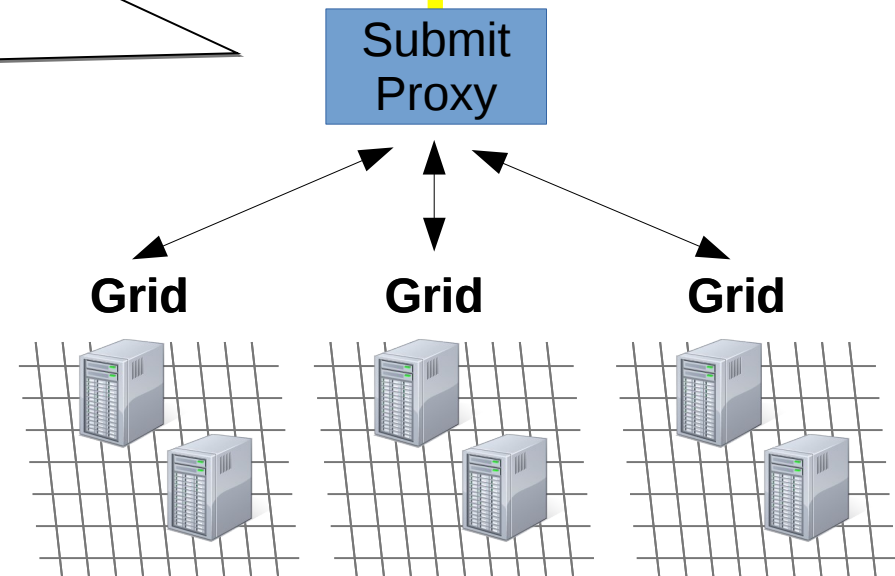
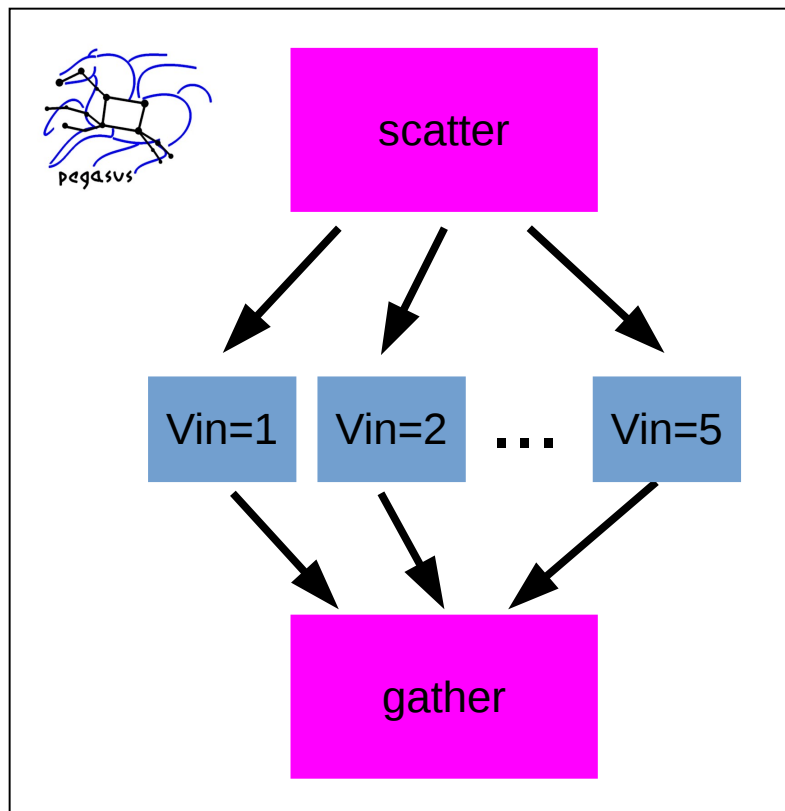
User's Workspace Terminal

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

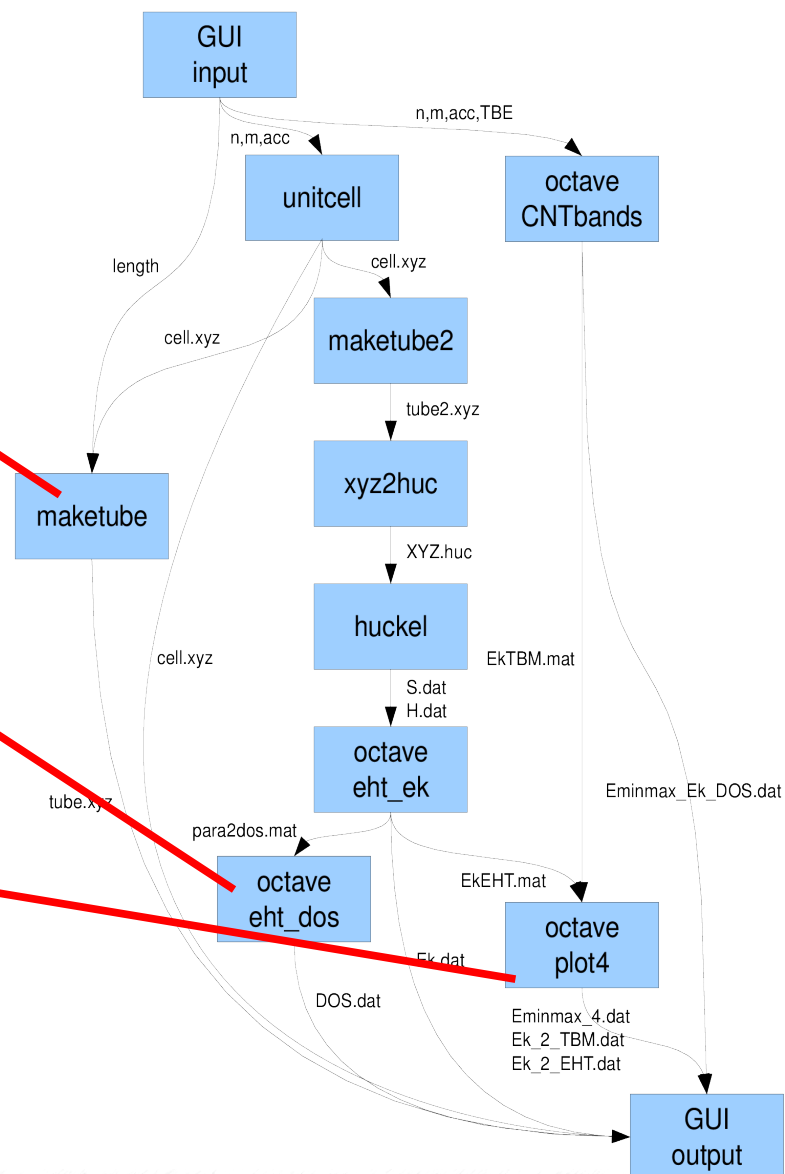
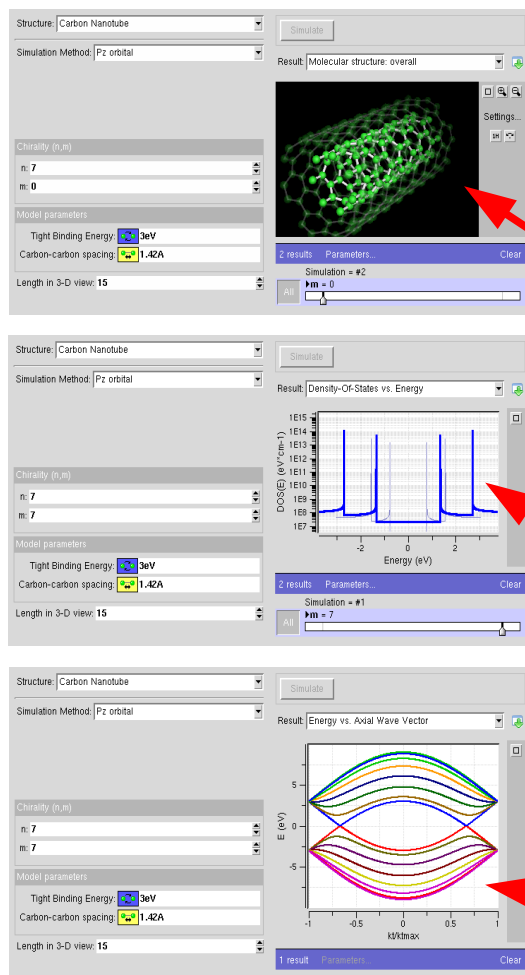
HUBzero Infrastructure



Tool Session Containers



... or write your own workflow



CNTBands

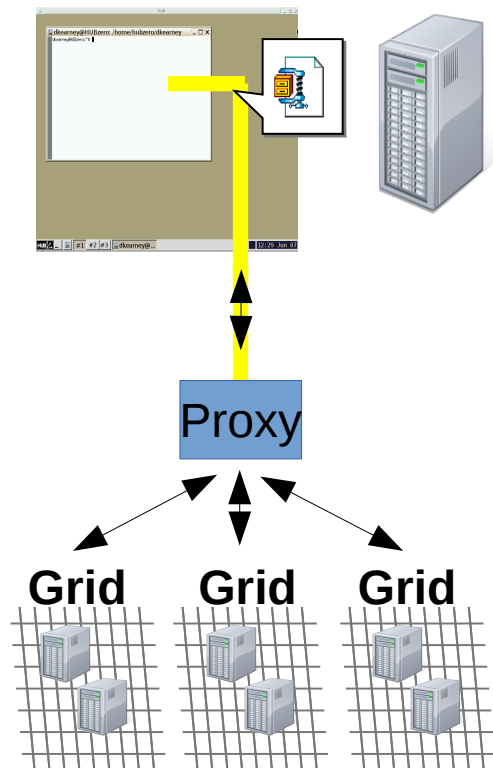
Science Domain: Nanoelectronics

Scientists: Lundstrom et al. (Purdue)

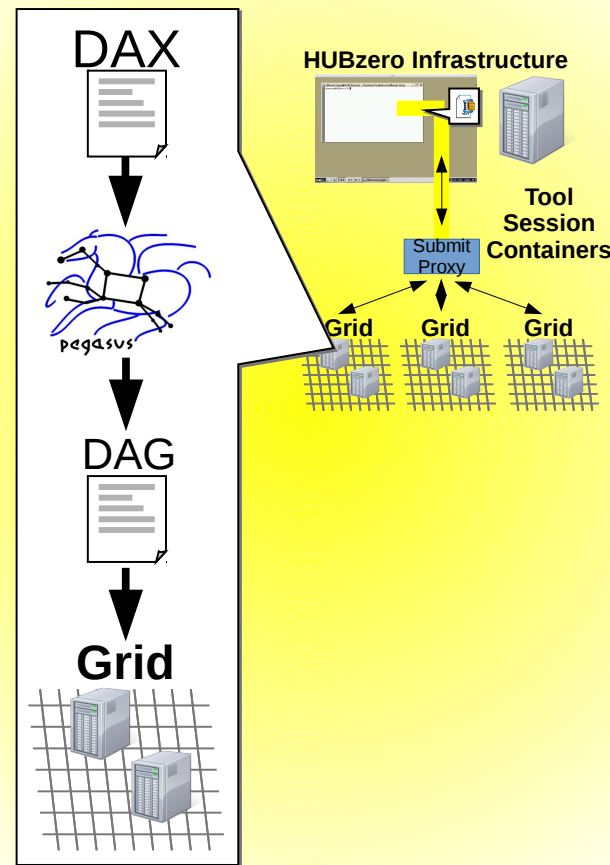
<https://nanohub.org/resources/cntbands-ext>

Productivity in the Workspace

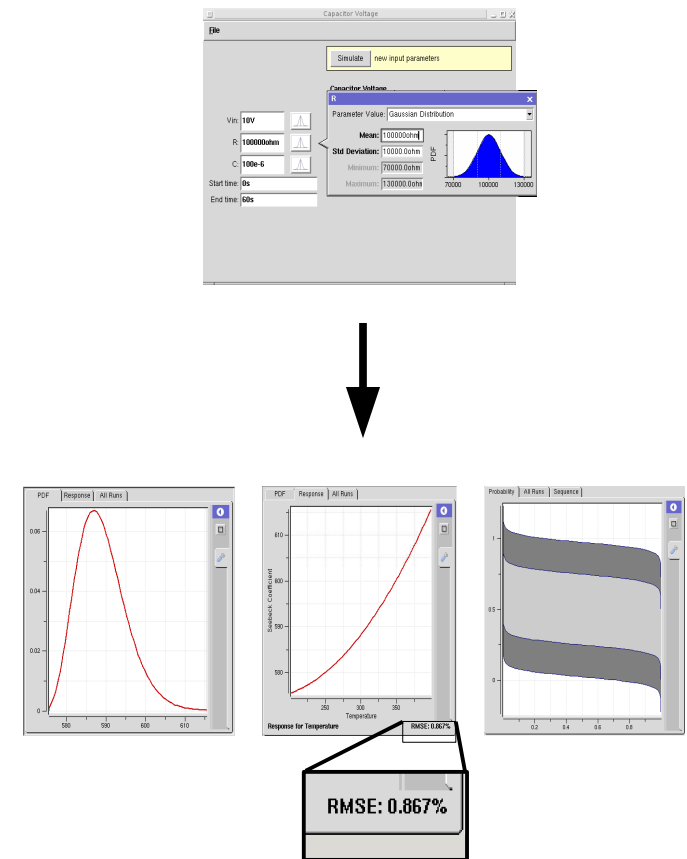
Submit



Pegasus Workflows

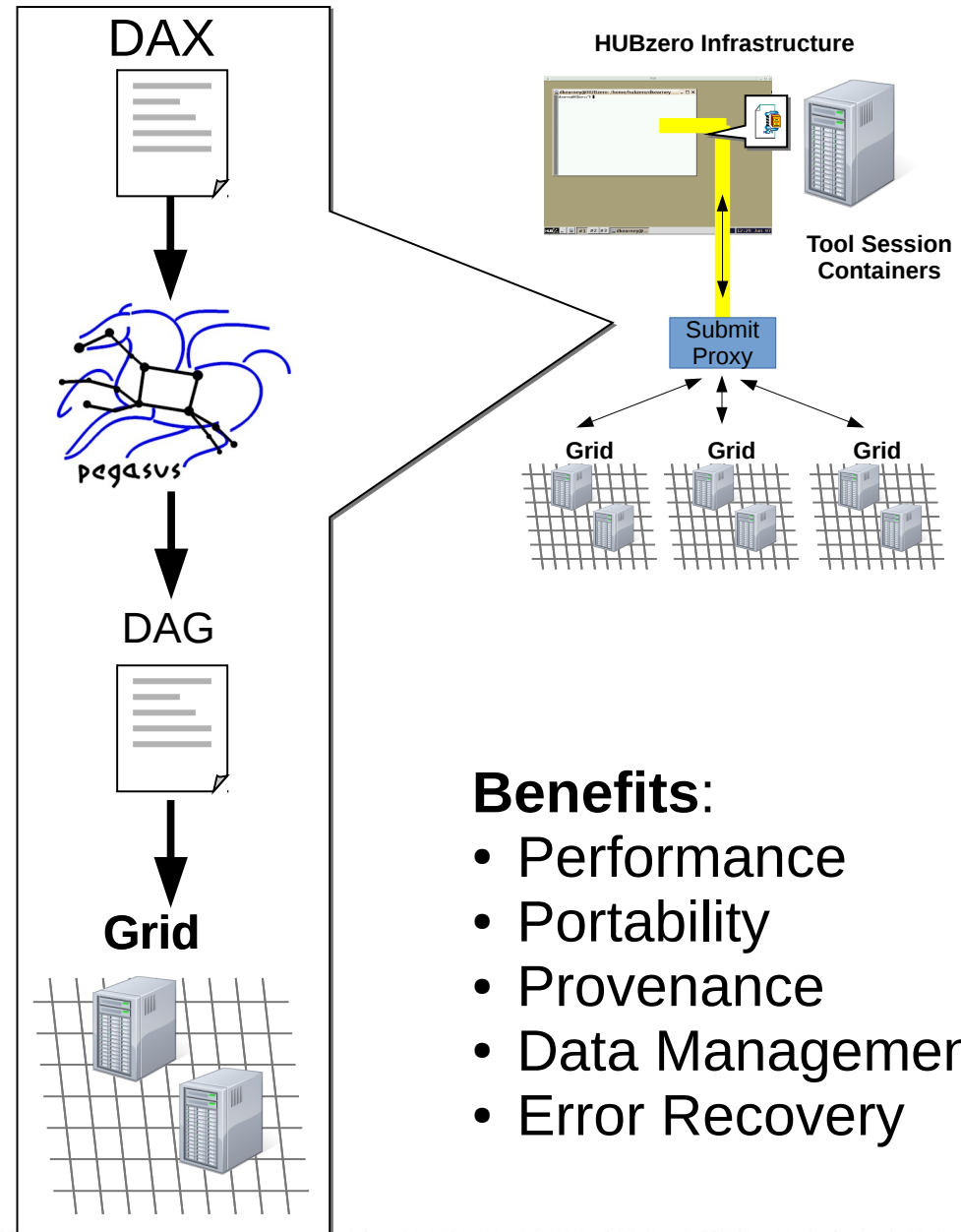
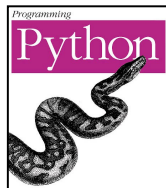


Uncertainty Quantification



Pegasus Workflow Management

- Developed at USC
- Ewa Deelman et al.
- Website: pegasus.isi.edu
- Open Source
- Bindings for your favorite languages:

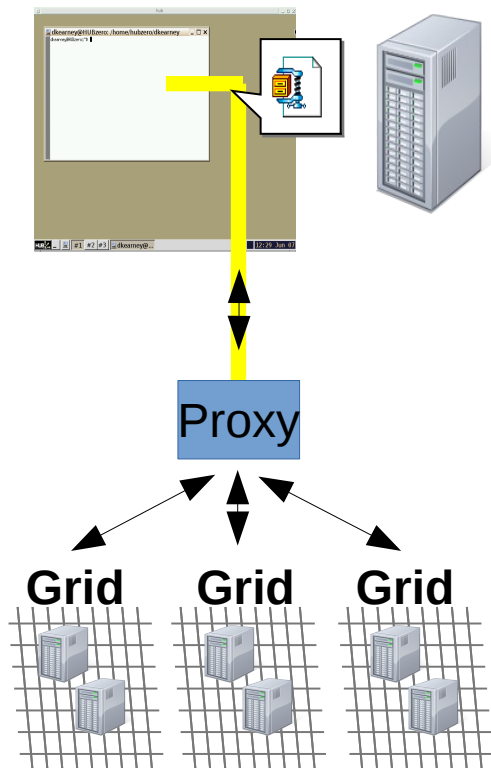


Benefits:

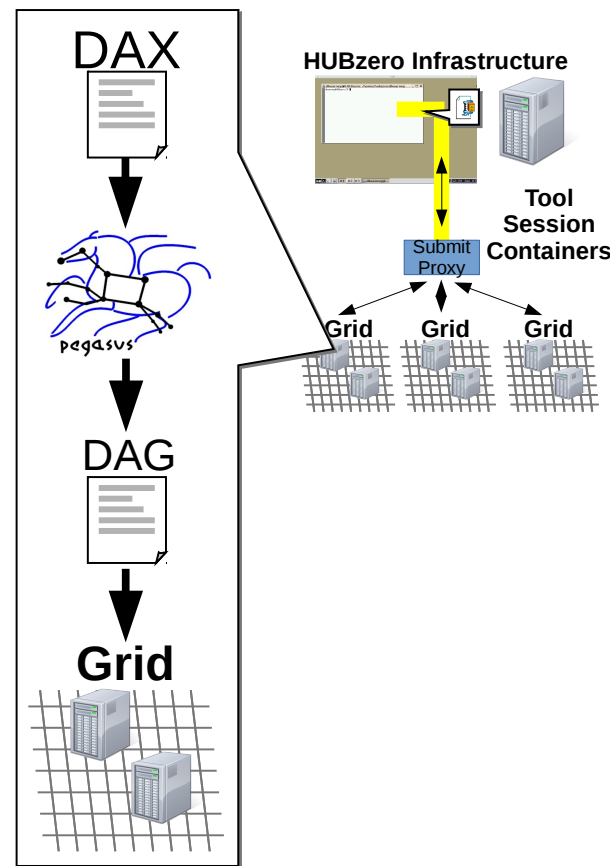
- Performance
- Portability
- Provenance
- Data Management
- Error Recovery

Productivity in the Workspace

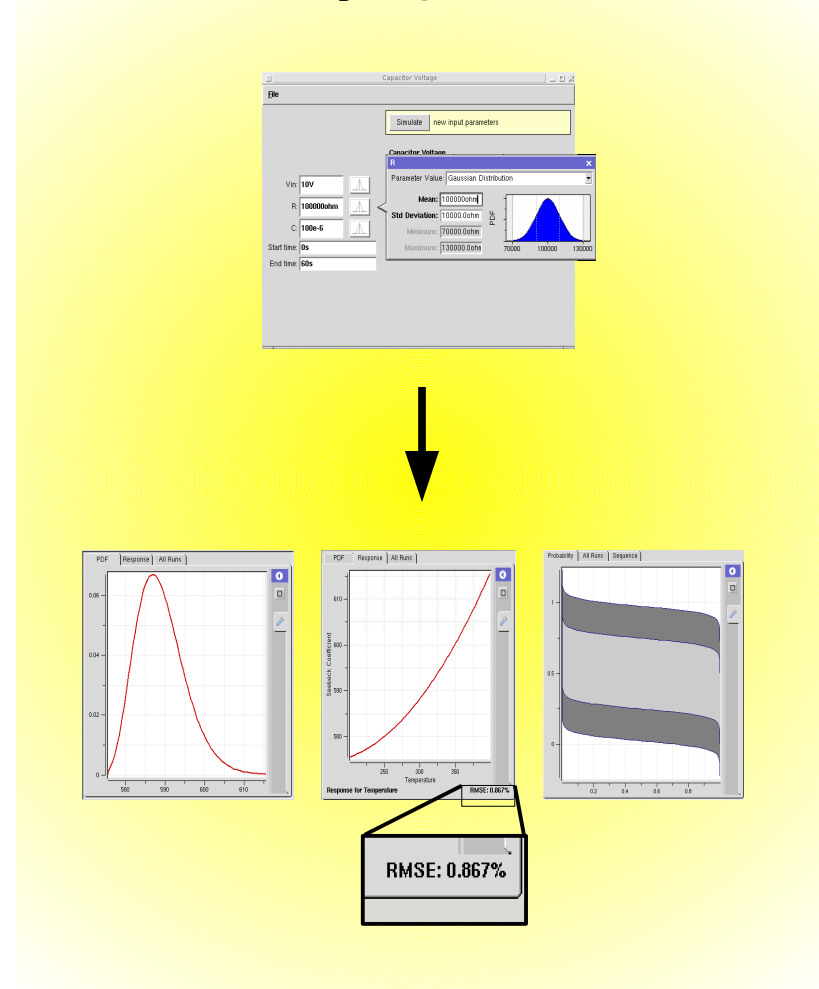
Submit



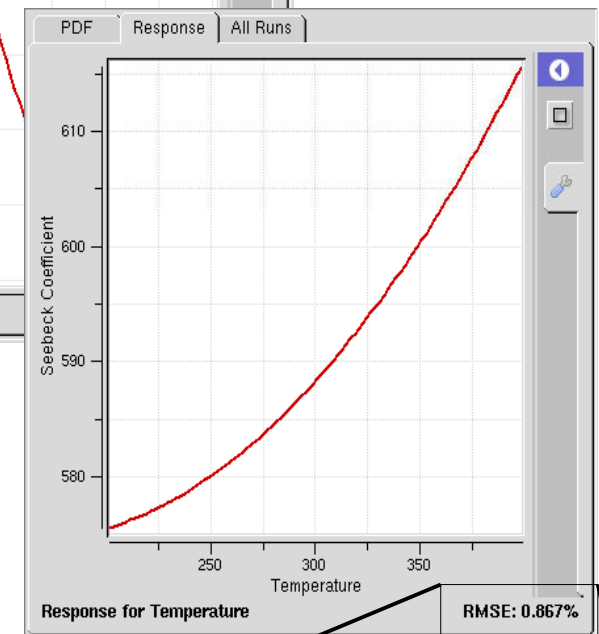
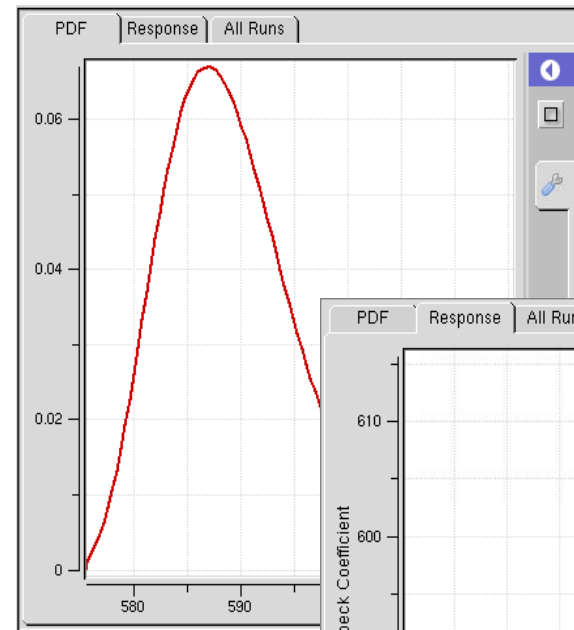
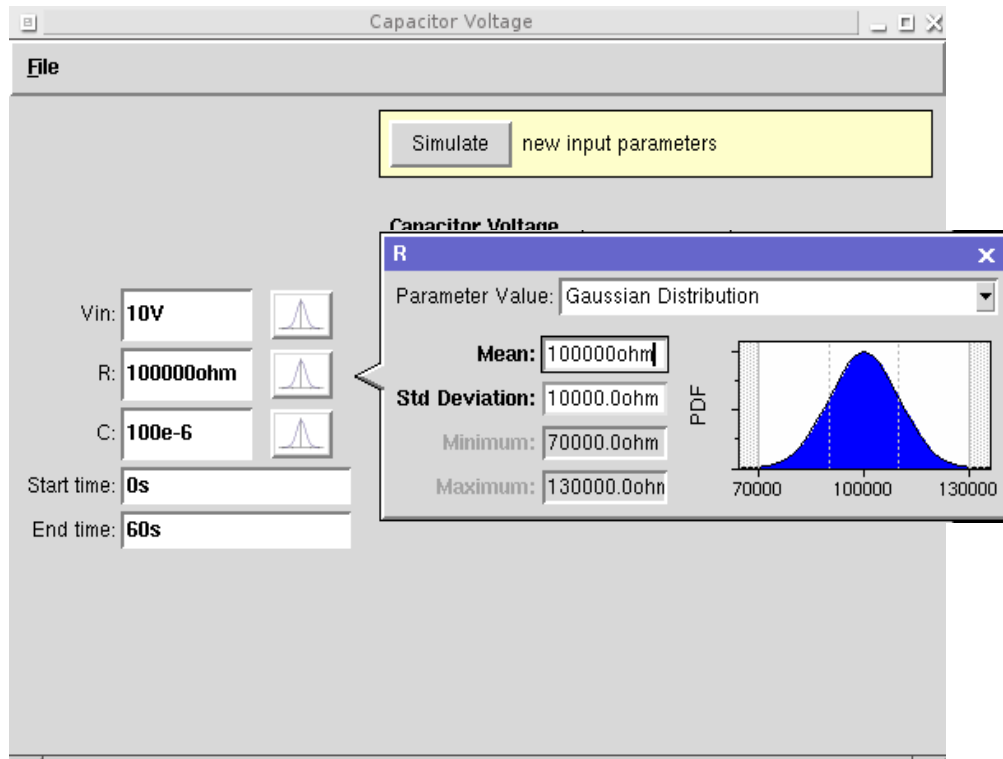
Pegasus Workflows



Uncertainty Quantification



Inputs and Outputs as Distributions

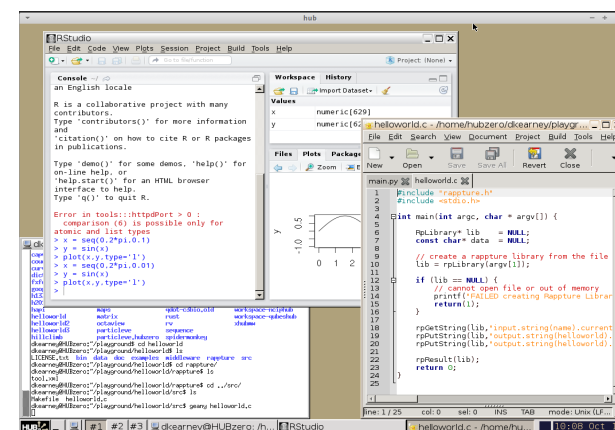
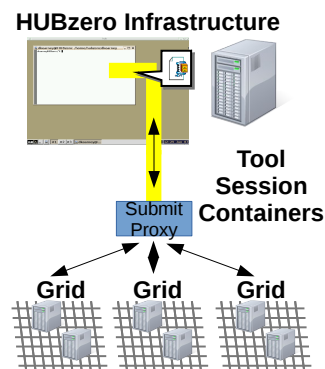
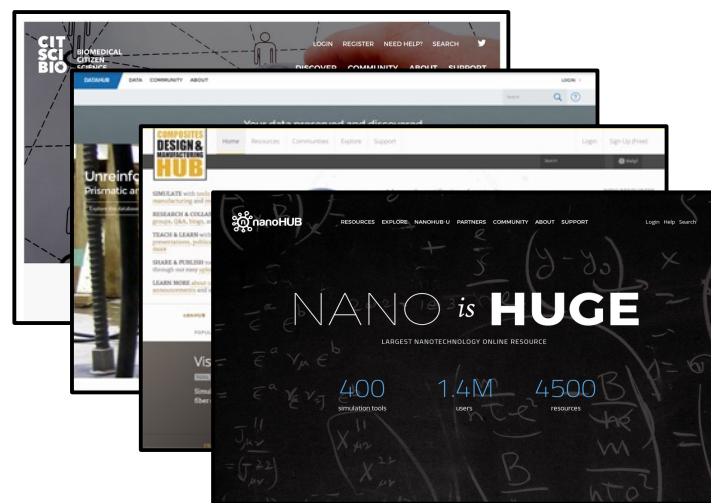


RMSE: 0.867%

27 FTEs
18 Developers
5 Support/Training

10+ Years
Supporting Research
And Collaboration

2+M
Visits

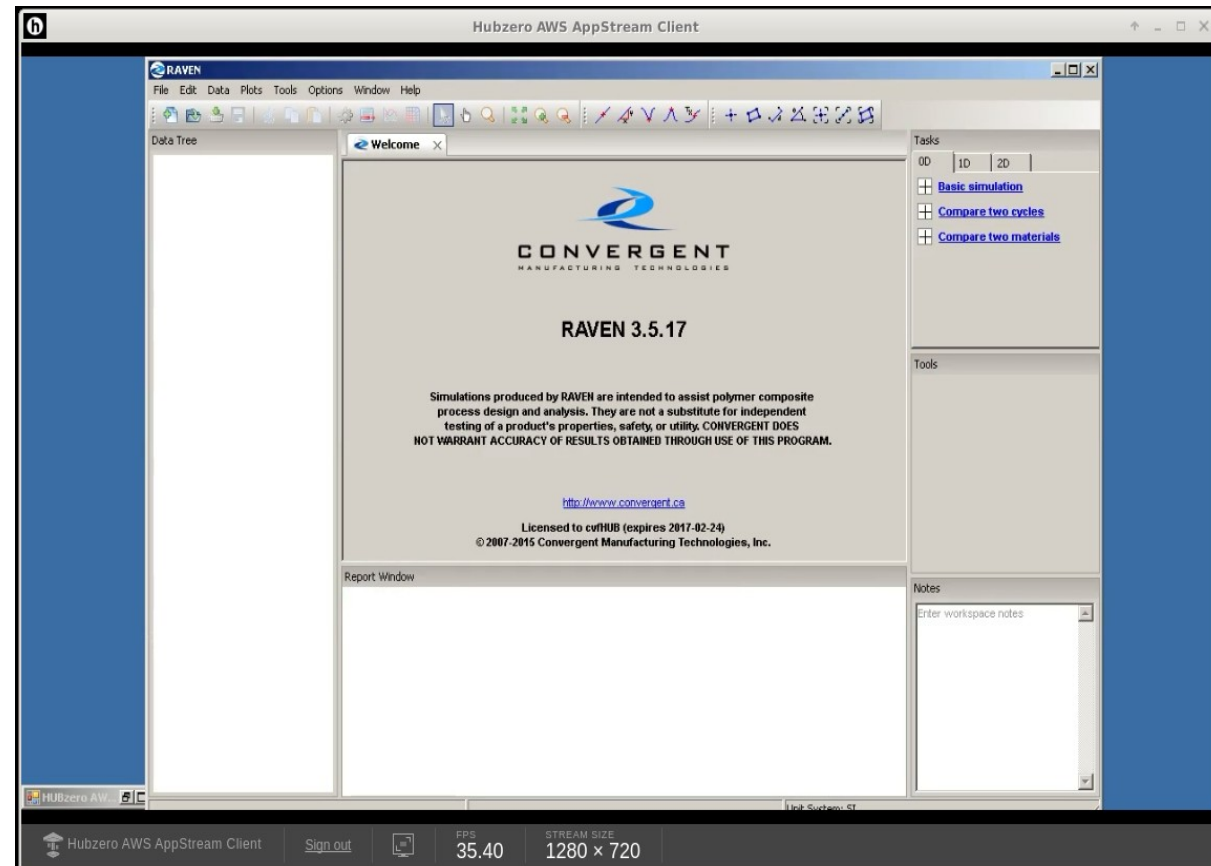


Secure, Scalable, Sharable
Dev Environments

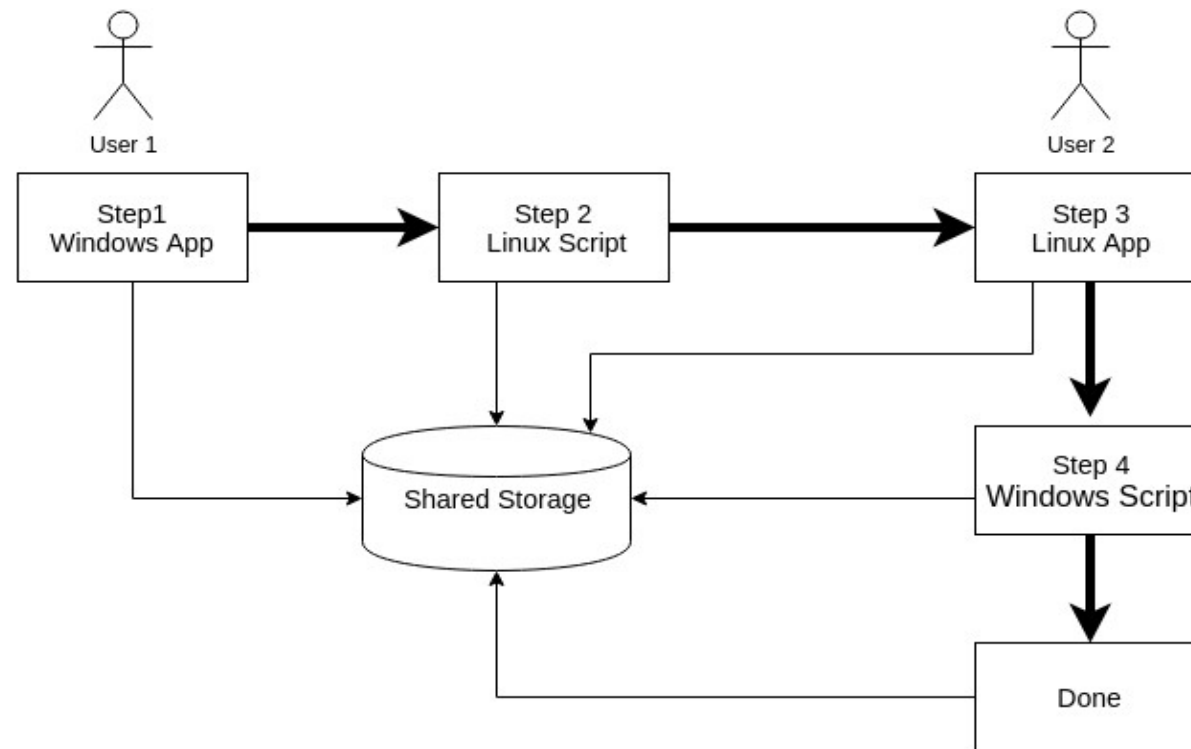


Windows tools and HUBzero

- Newer feature to complement our Linux Tool functionality
- Explore cloud based resources
- Initial implementation utilizes AWS Appstream, a highly optimized video intensive Windows deployment platform
- Overall effort focuses more on end user application deployment and collaboration than tool development.
- Use of commercial tools
- Strict licensing requirements
- Heavy single workstation requirements



“Macro” level workflow



- Pegasus is one of many granular scientific workflow management tools
 - Highly automated workflows
 - Specializes in task partition and scheduling in HPC environments
- We're also working on higher level workflow – Business Rules Engine
 - Focuses more on higher level tasks
 - Higher degree of user interaction
 - Use a mix of workflows at several different levels
 - Use of heterogeneous operating systems