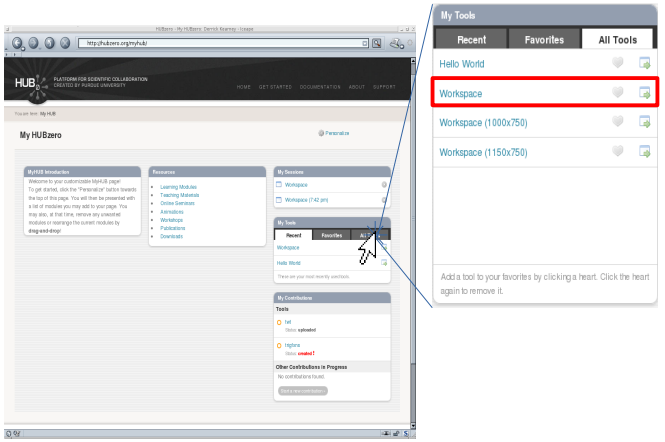
HUBzero Platform Features

TRADES Proposal Demo
Oct. 12, 2016

Derrick Kearney
hubzero.org

The HUBzero Platform

User's Web Browser



HUBzero Infrastructure

Web Server

Middleware

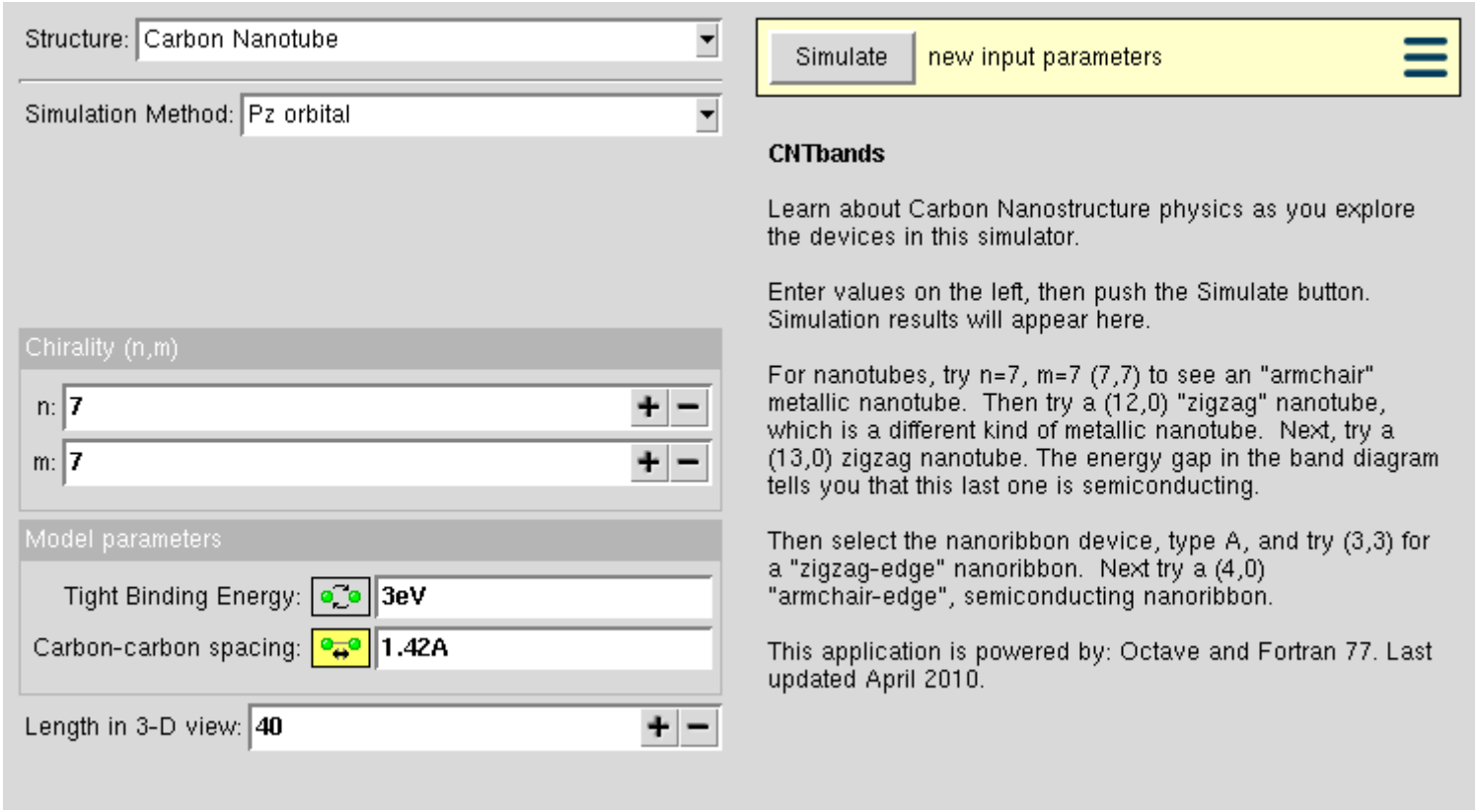
Submit Proxy

Grid

Tool Session Containers

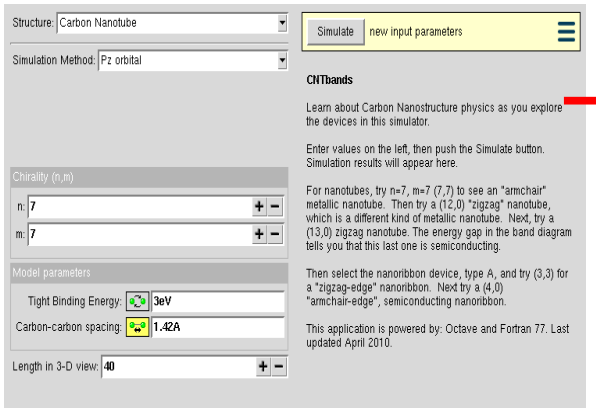
Visualization

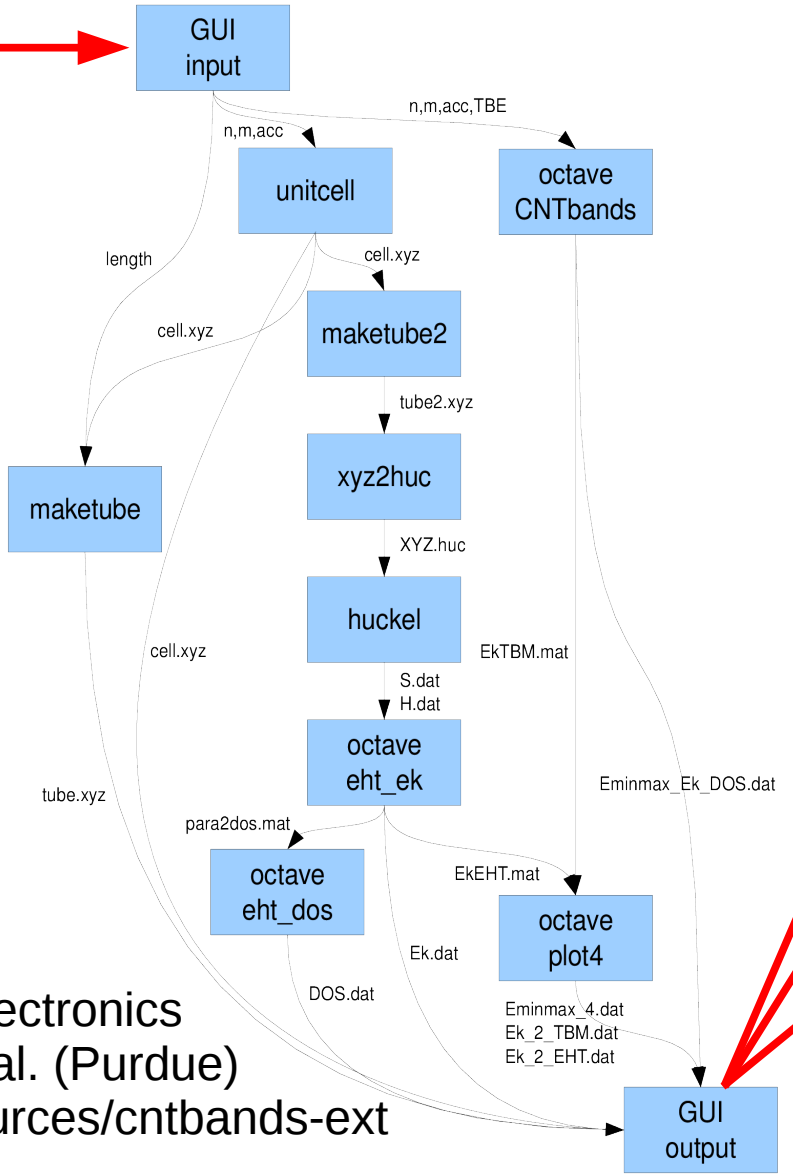
CNTbands

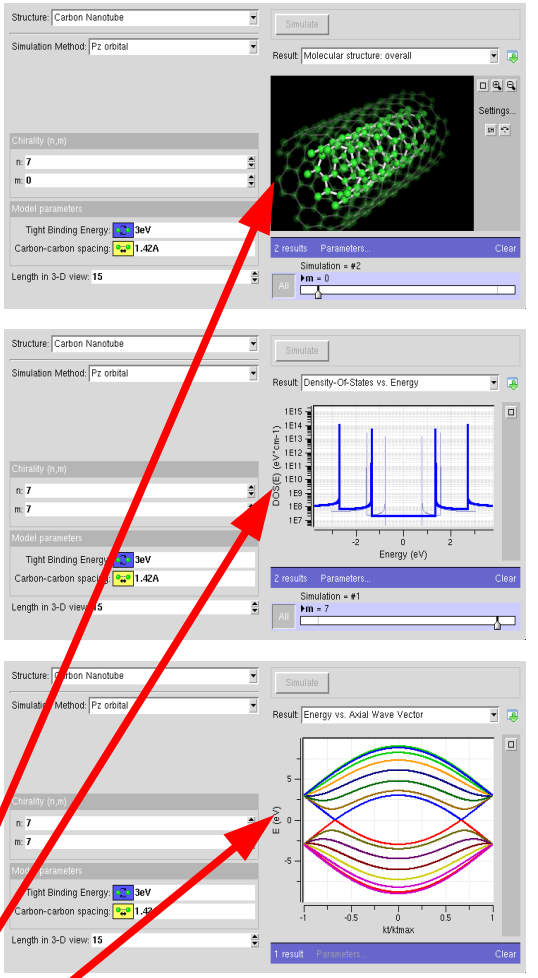


CNTbands
Science Domain: Nanoelectronics
Scientists: Lundstrom et al. (Purdue)
https://nanohub.org/resources/cntbands-ext

CNTbands







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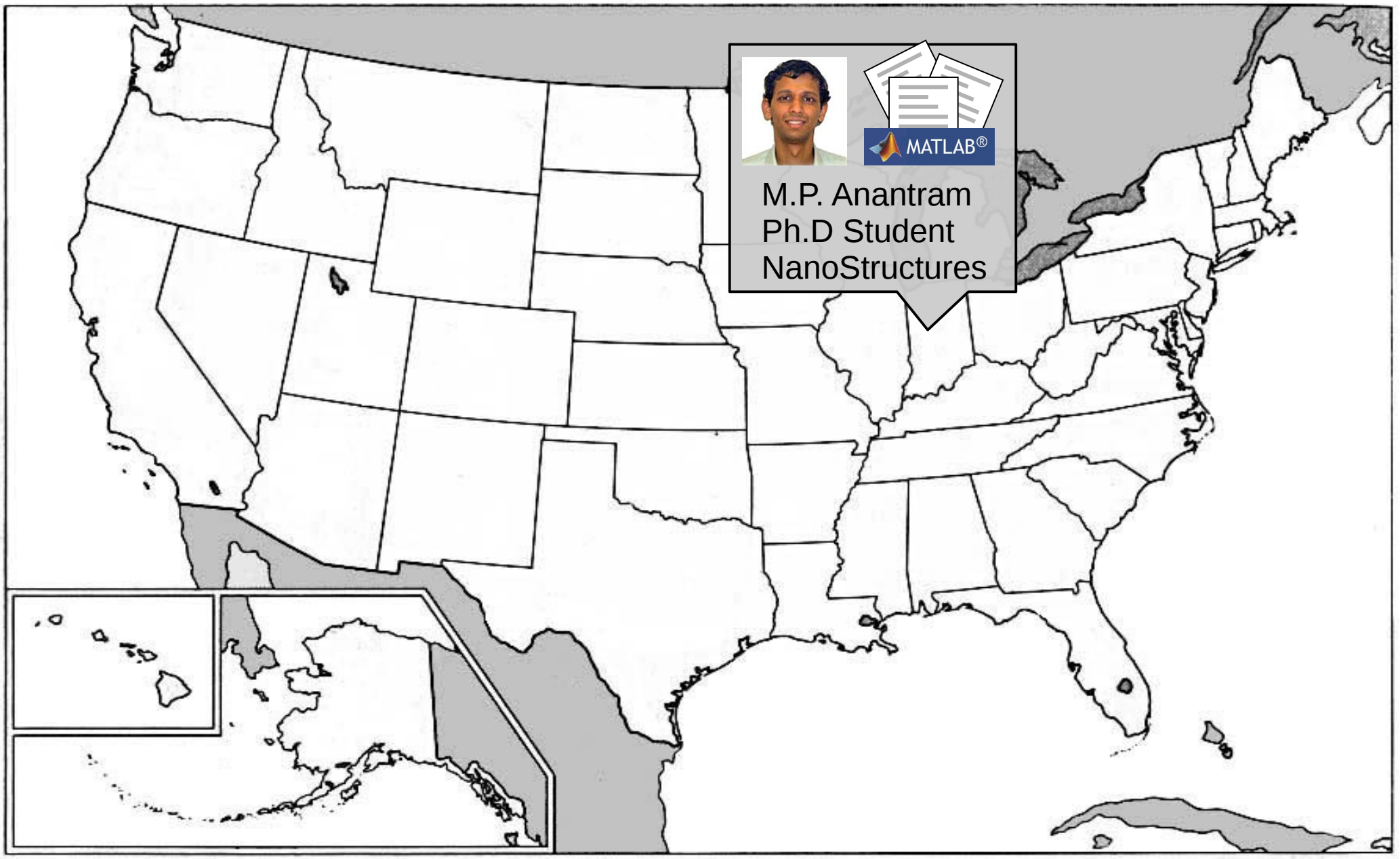
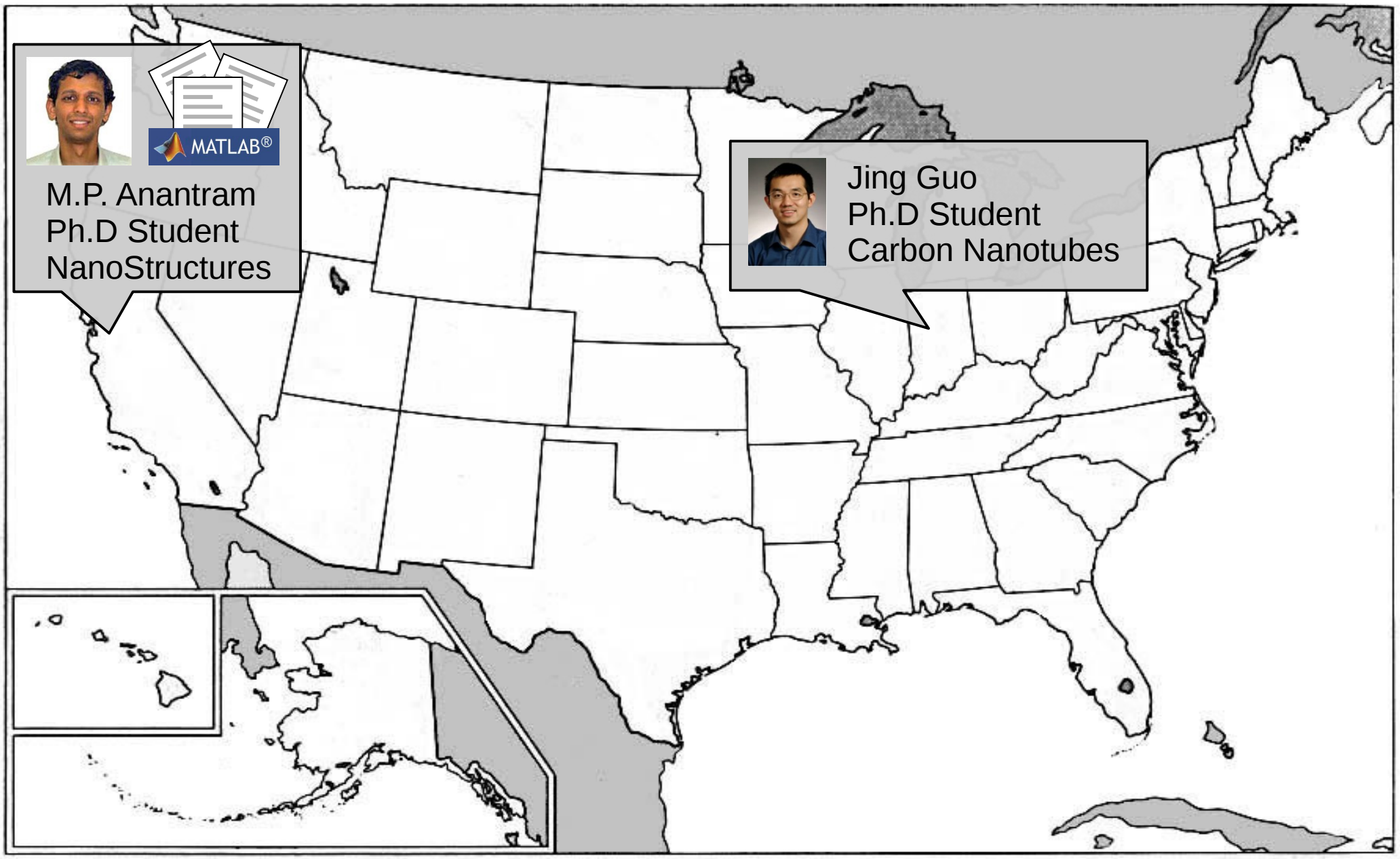
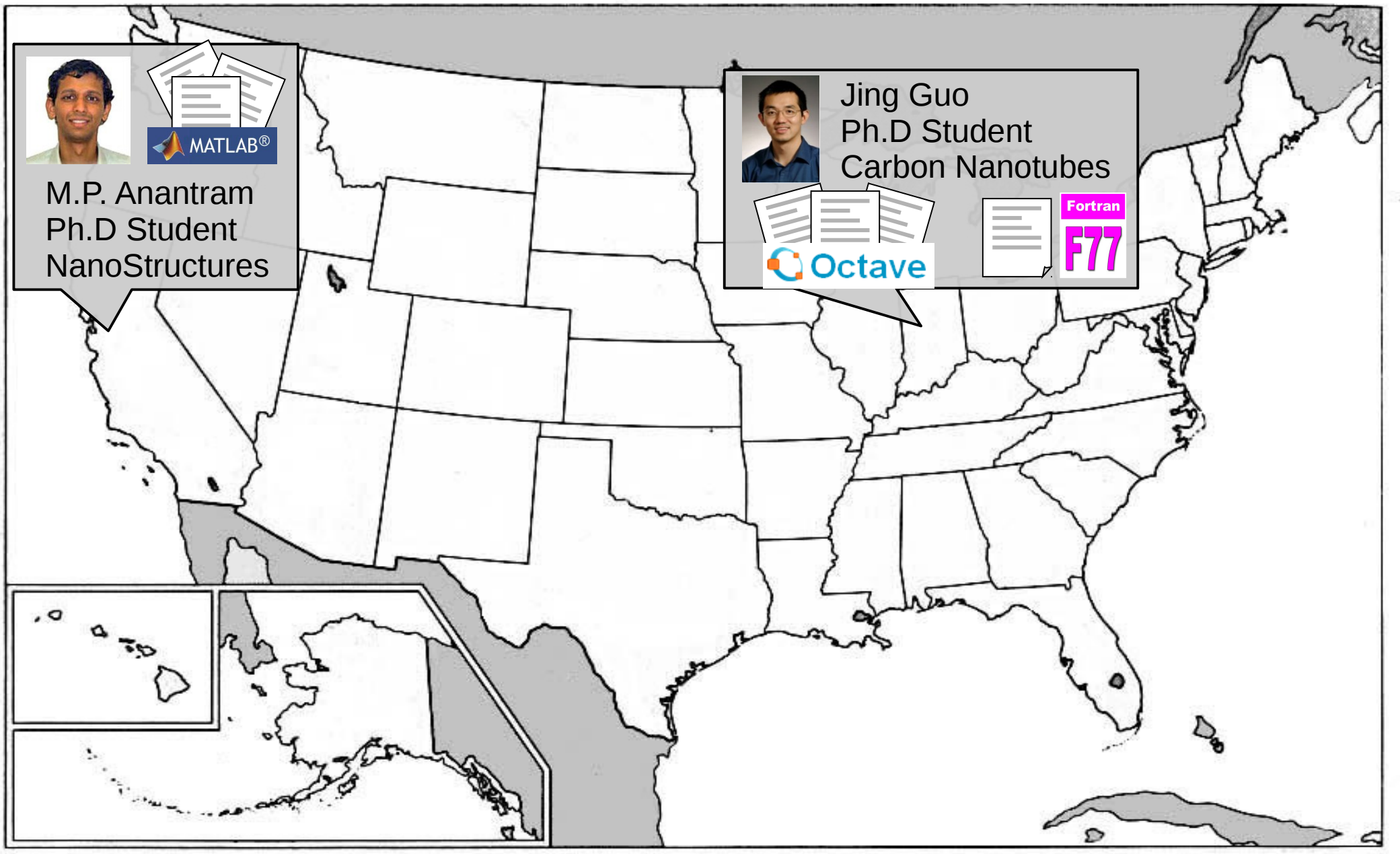
1990s – Pre CNTbands



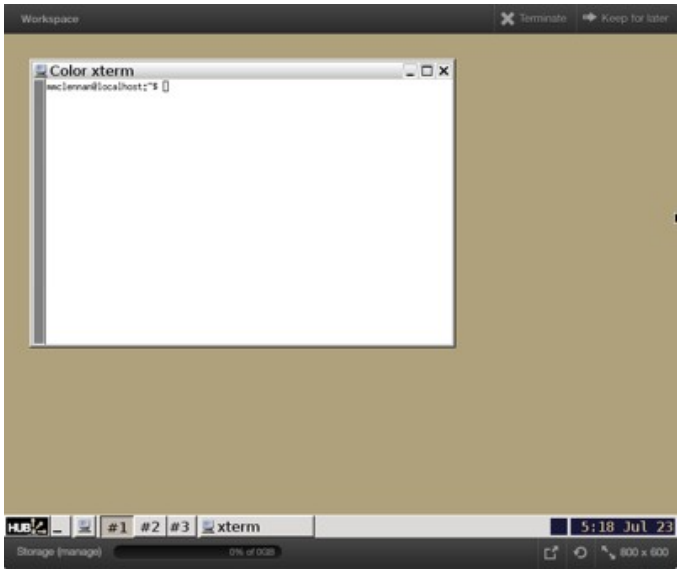
2002 – CNTbands Ideas



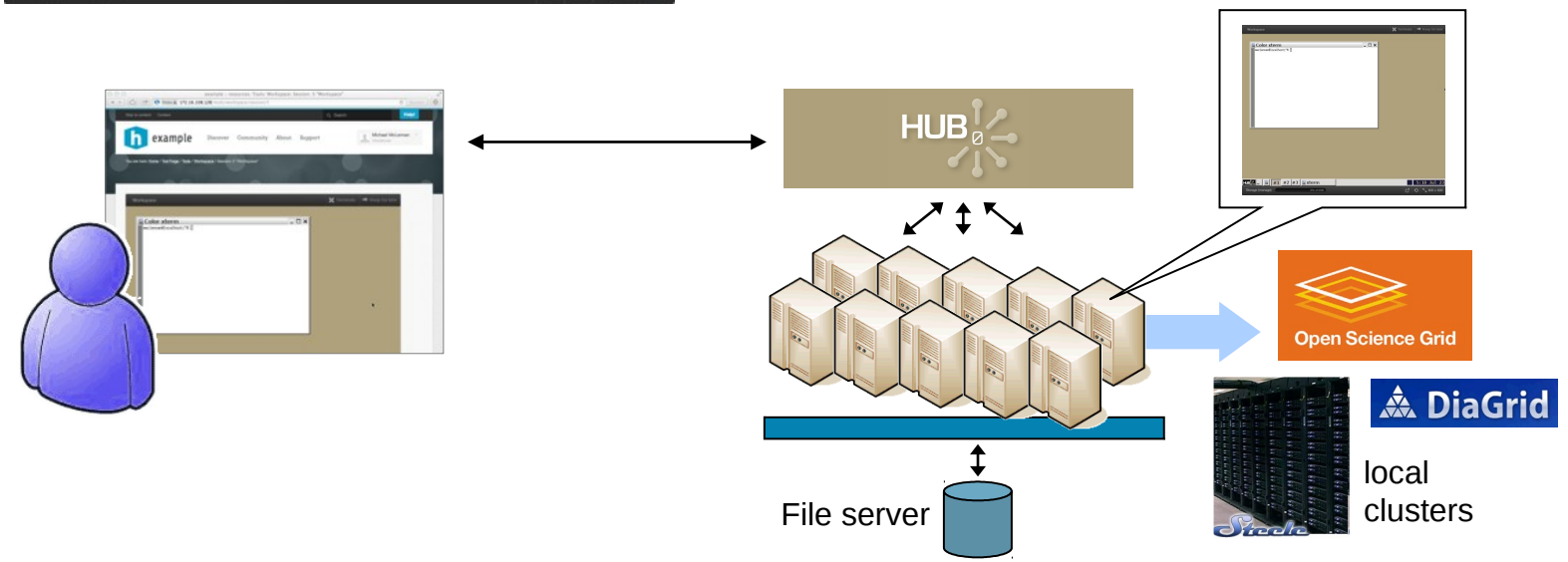
2002 – CNTbands Registered



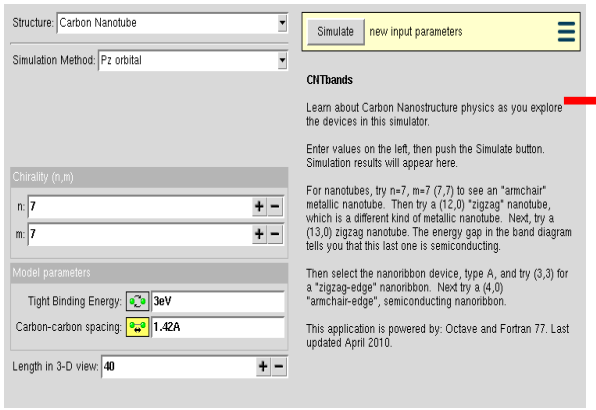
What is a workspace?

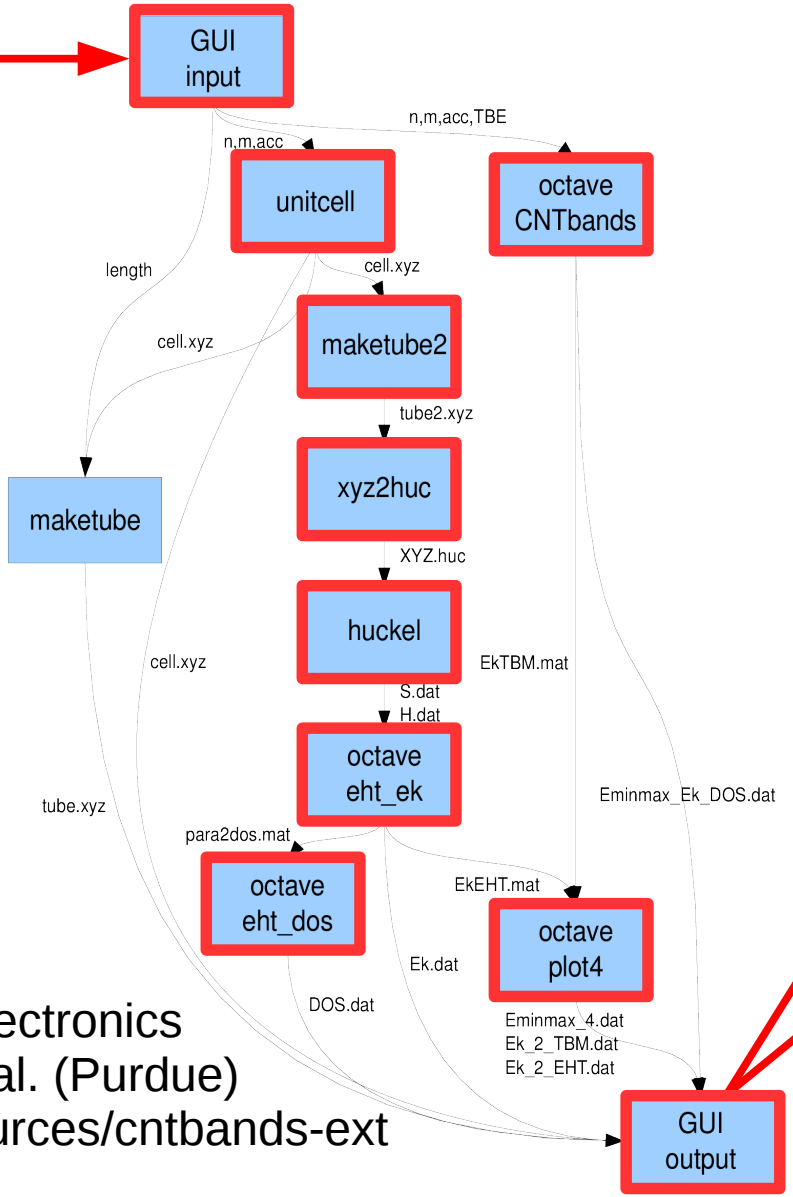


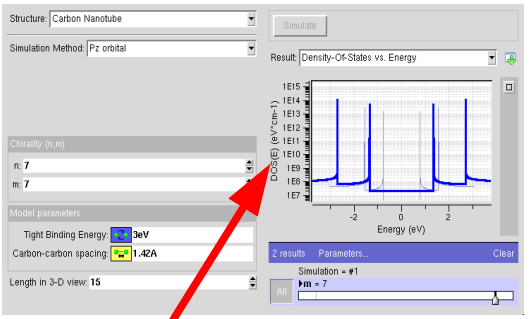
- Full-featured Linux desktop
- For tool developers
- For researchers
- Accessible from any web browser
- Still running after you close your browser
- Access to computational clusters
- File storage provided by the hub

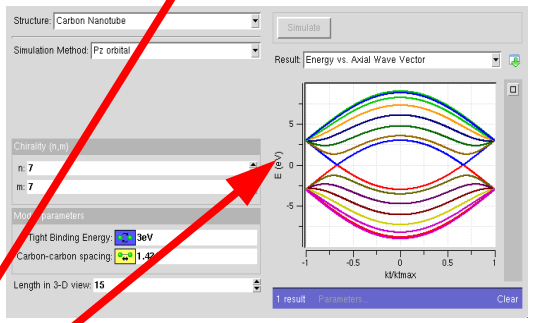


CNTbands









CNTbands
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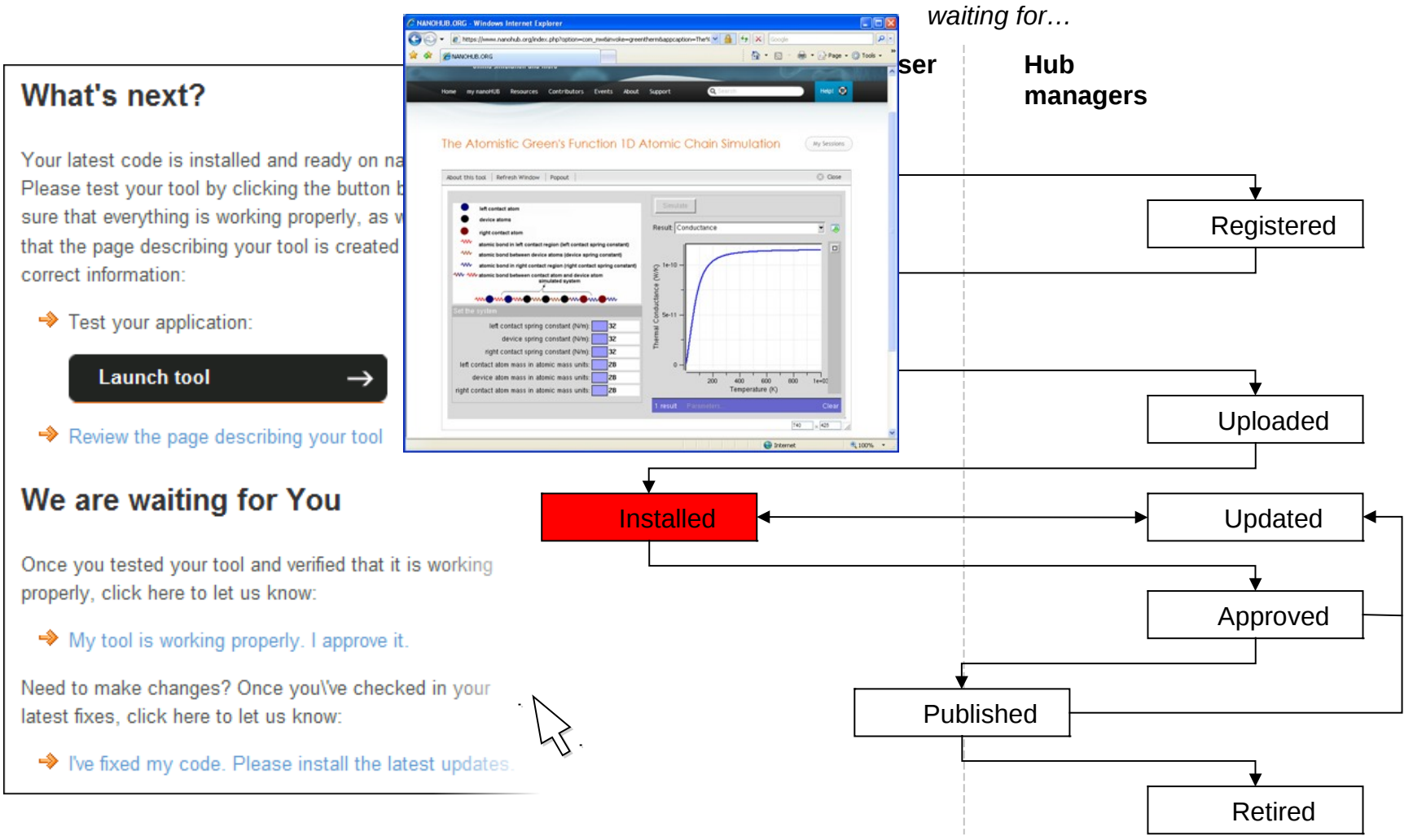
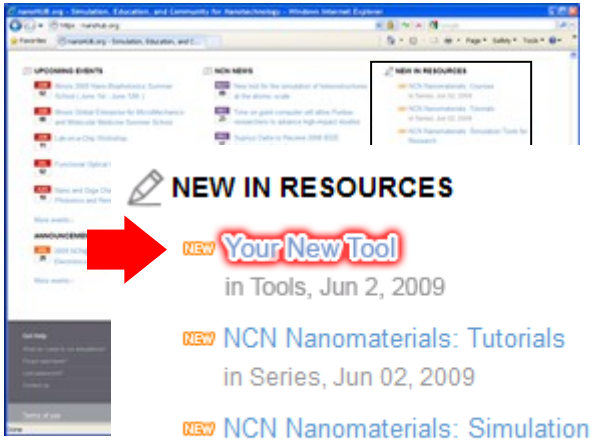
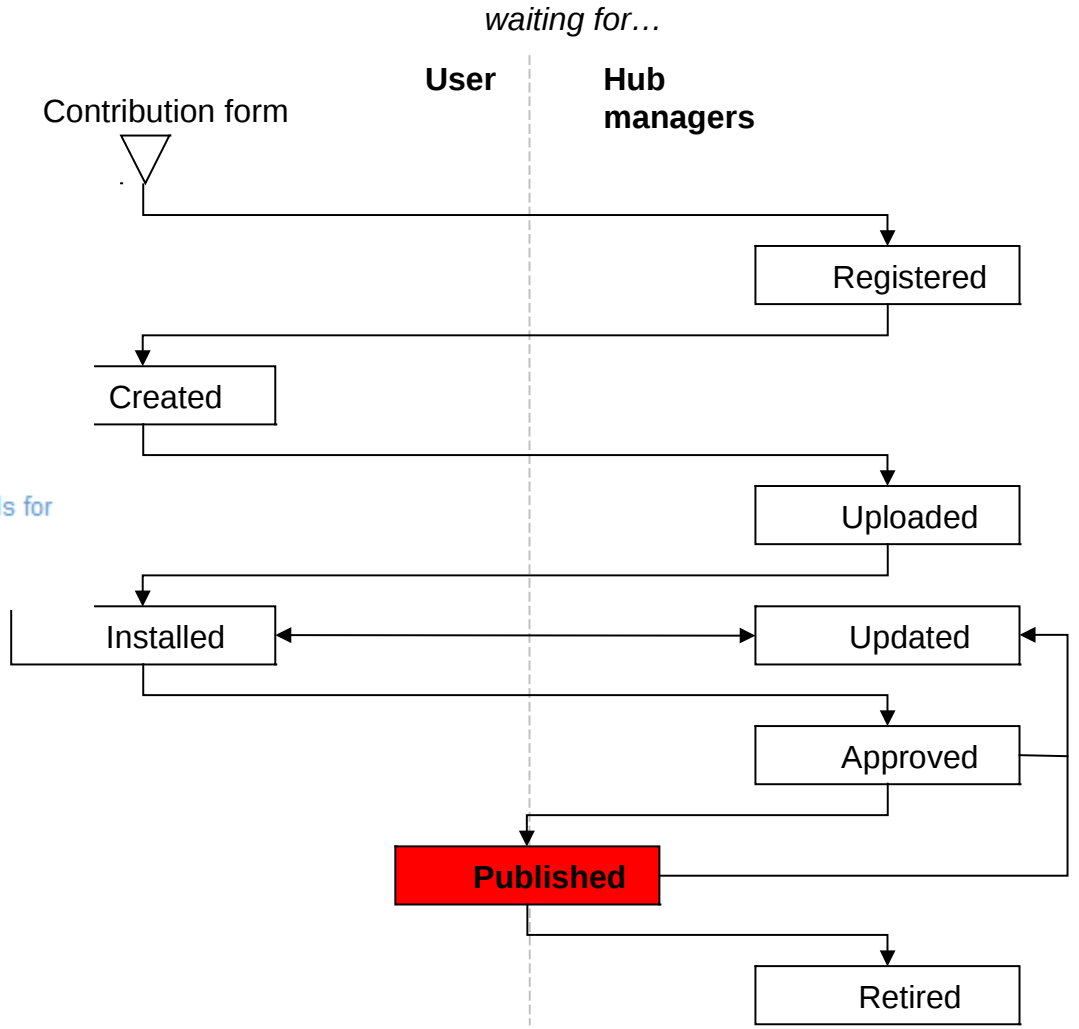
Collaboration / Groups

Installing & Testing Applications



CNTbands is Published





Knowing your impact

CNTbands

By Gyungseon Seol[1], Youngki Yoon[1], James K Fodor[1], Jing Guo[1], Akira Matsudaira[2], Diego Kienle[2], Gengchiau Liang[2], Gerhard Klimeck[2], Mark Lundstrom[2], Ahmed Ibrahim Saeed[3]

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:

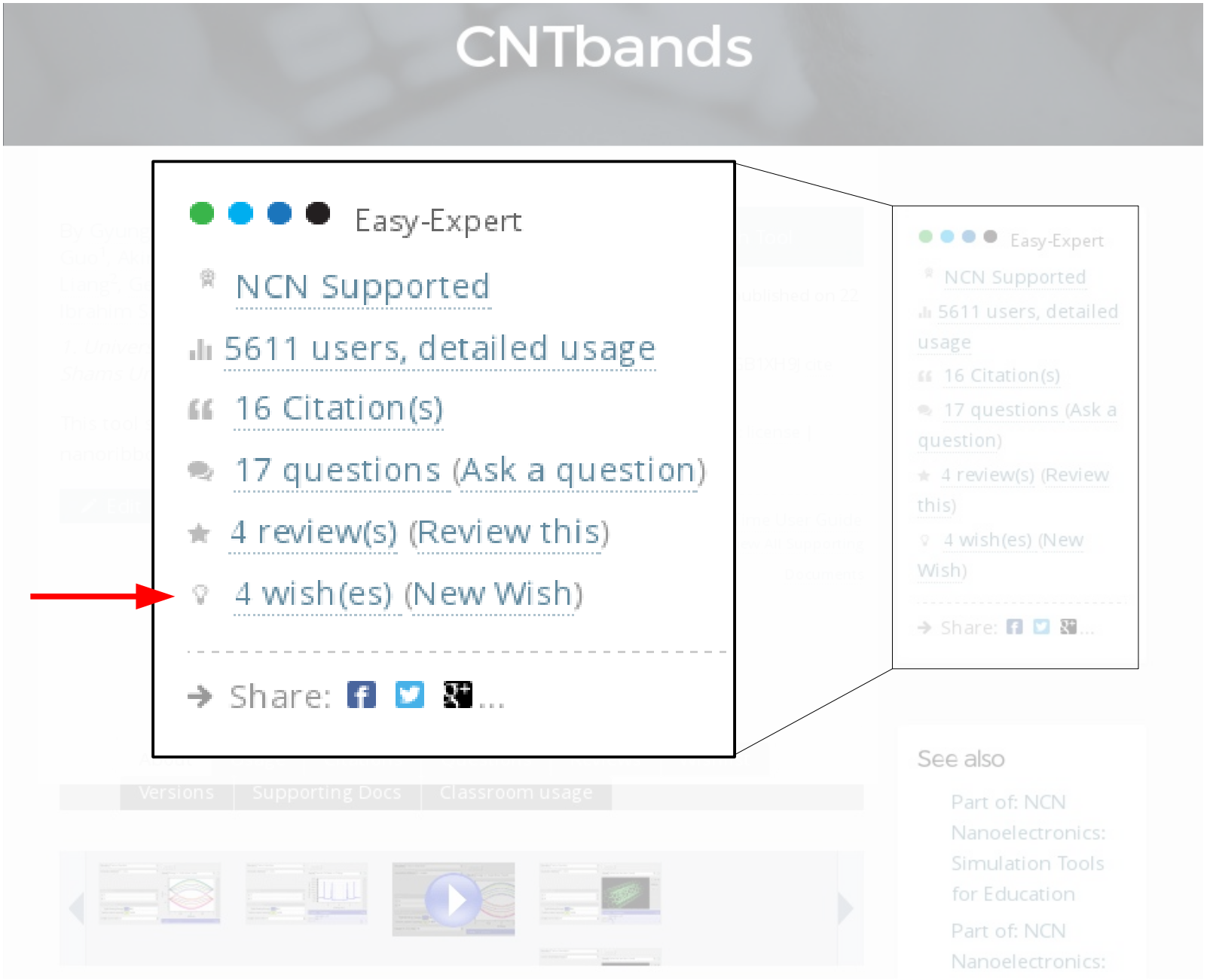
About | Usage | Citations | Questions | Reviews | Wishlist | Versions | Supporting Docs | Classroom usage

See also

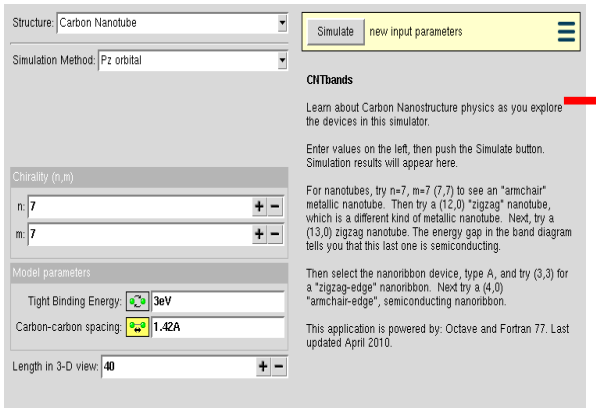
Part of: NCN Nanoelectronics: Simulation Tools for Education

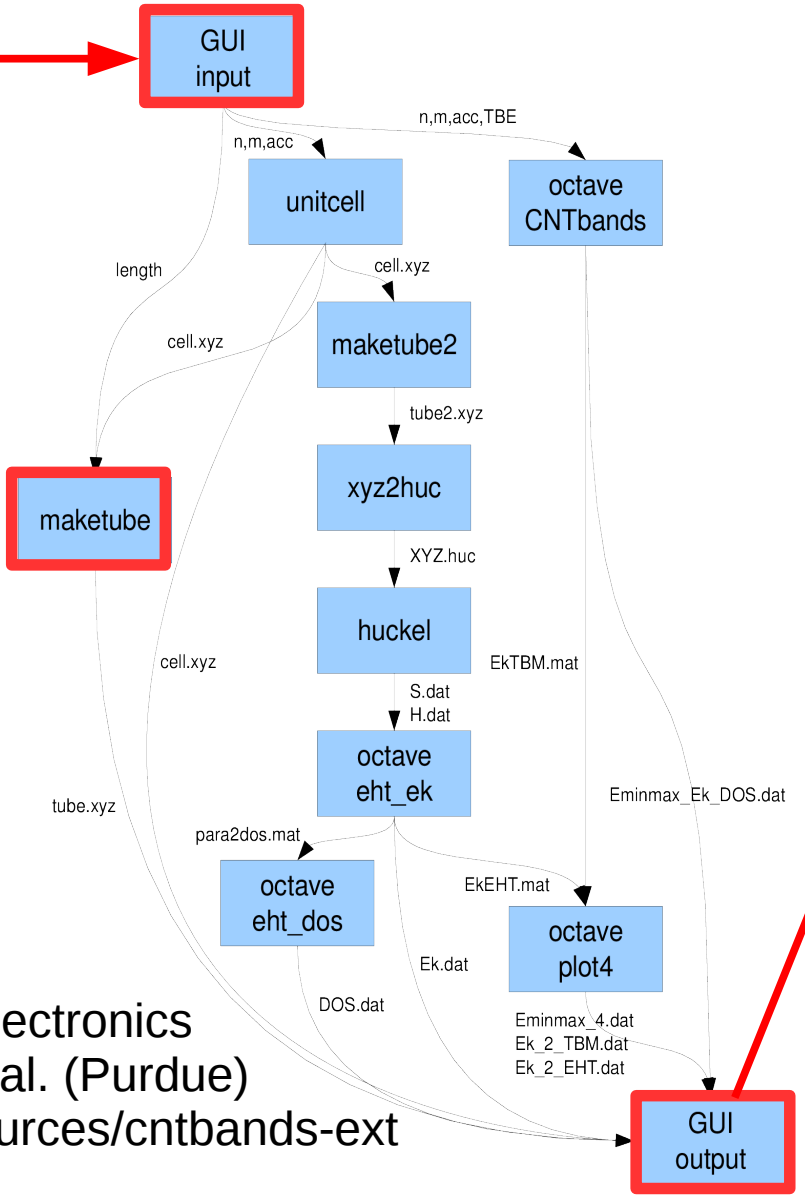
Part of: NCN Nanoelectronics:

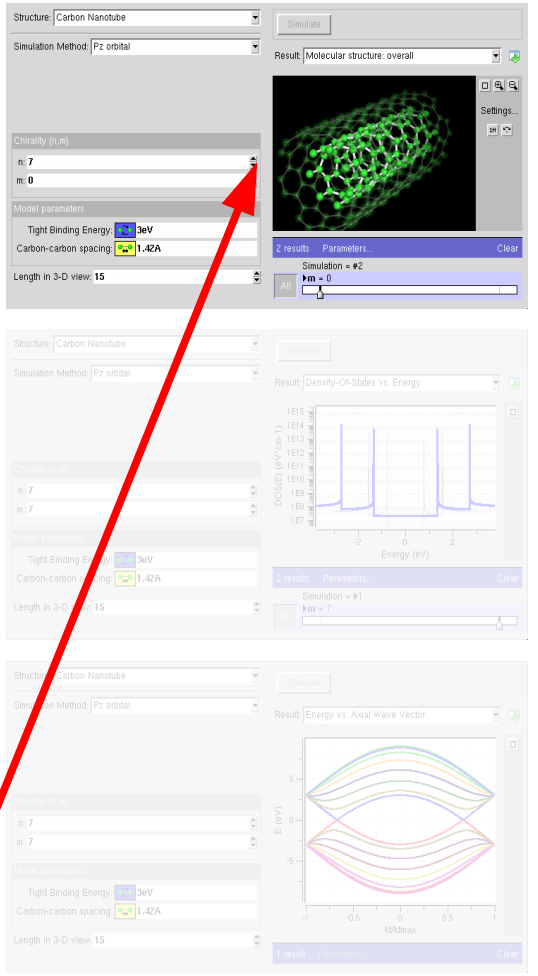
Communicate with users



New feature added







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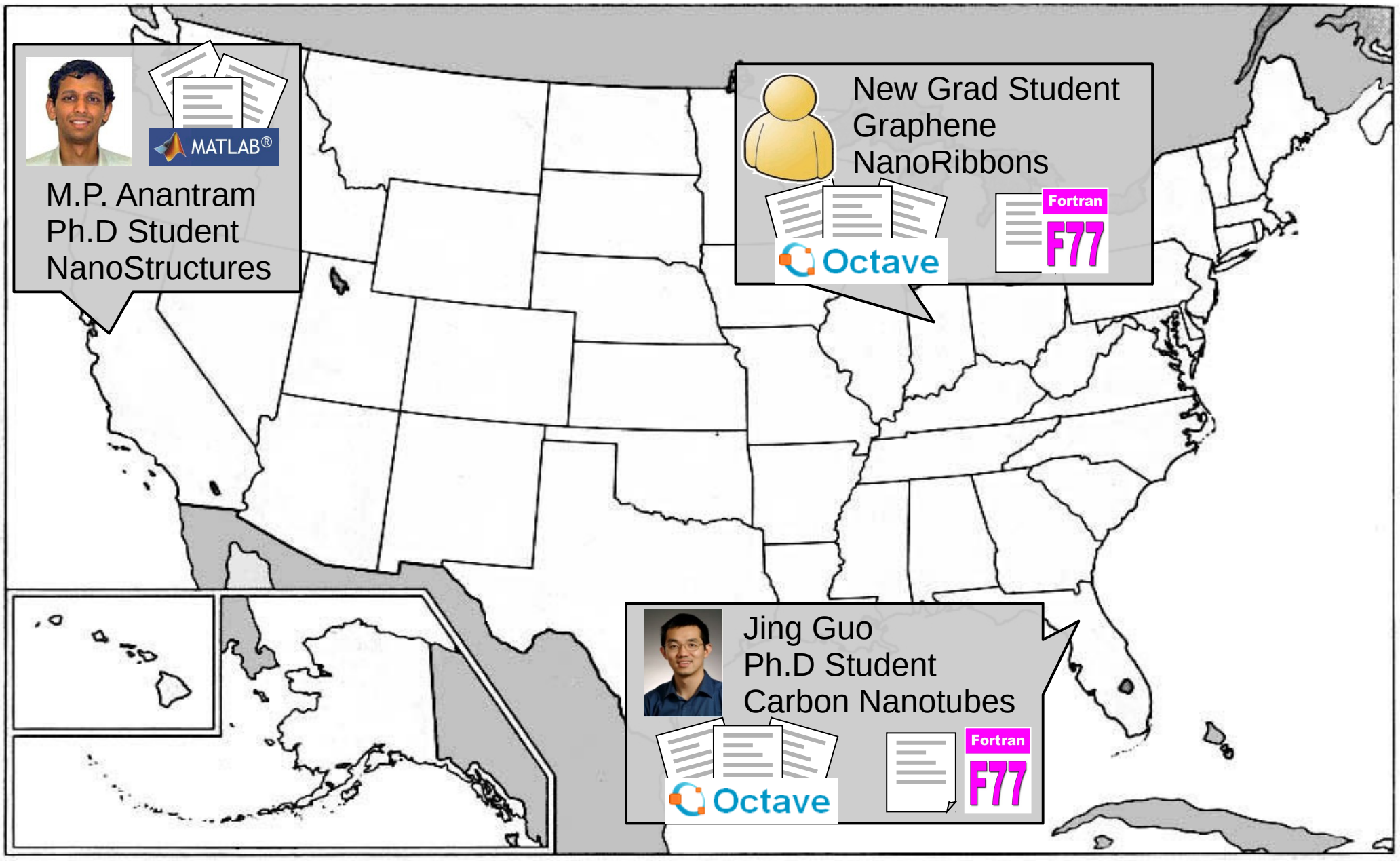
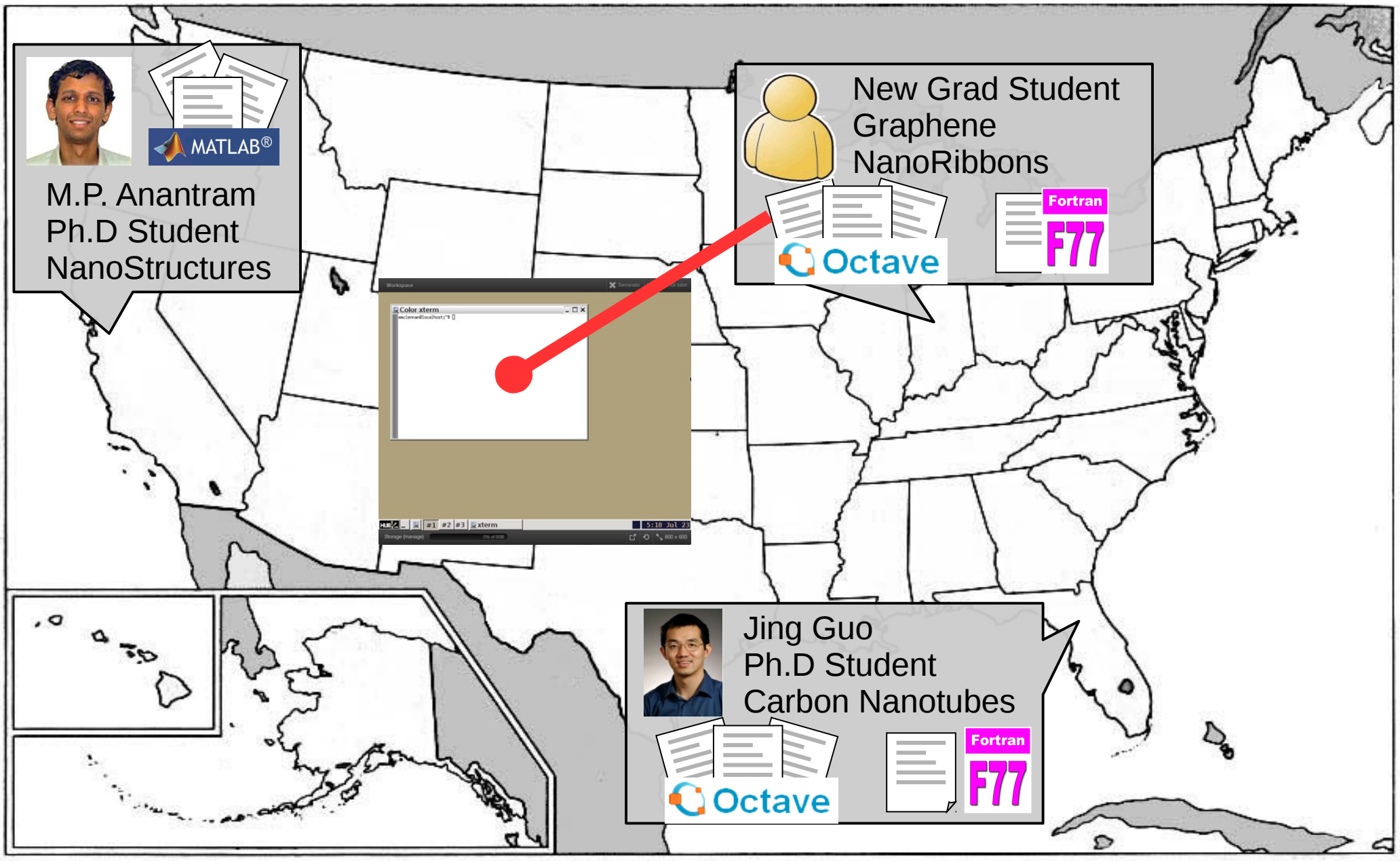
2010 – New Grad Students



Collaboration inside the Workspace



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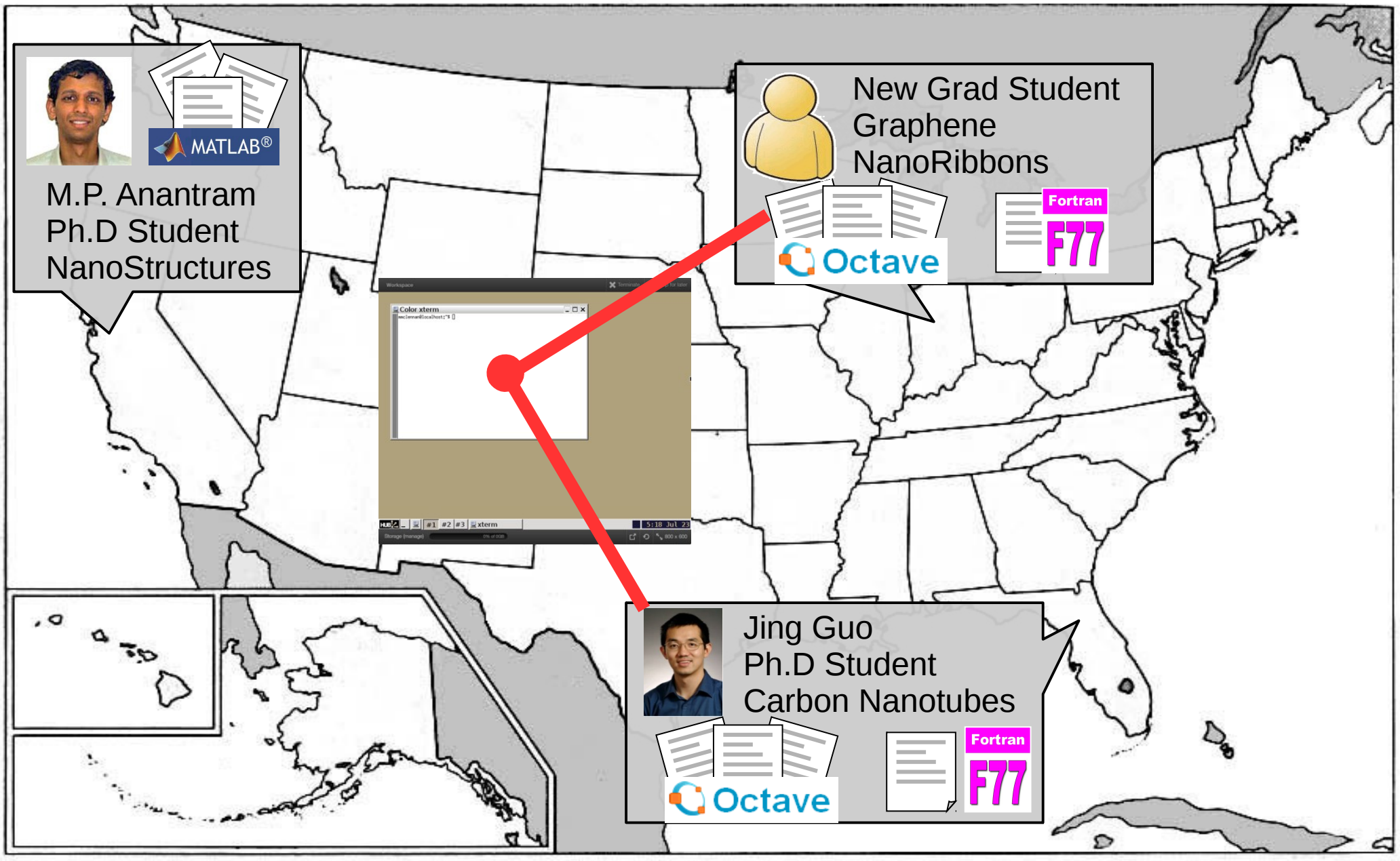
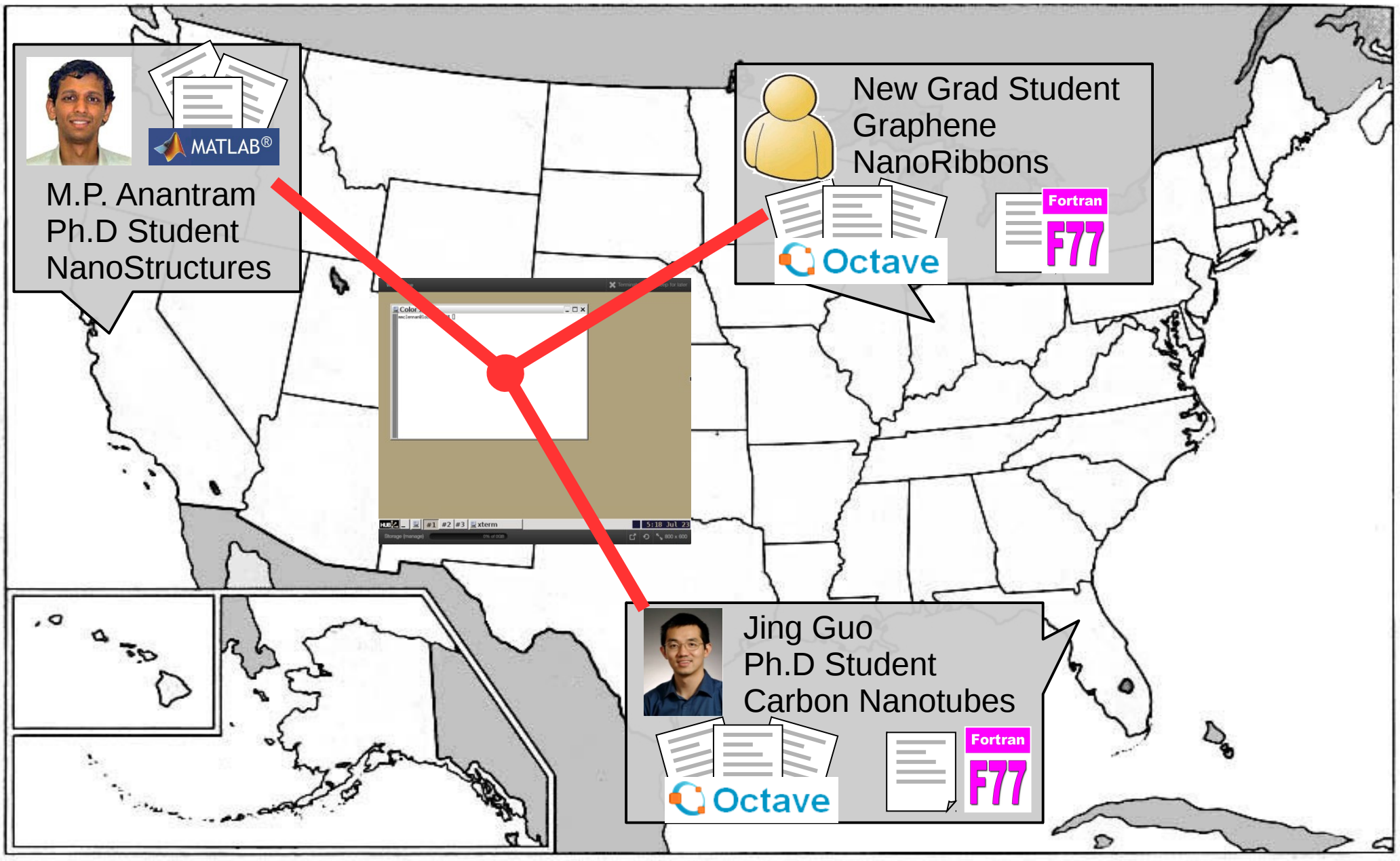
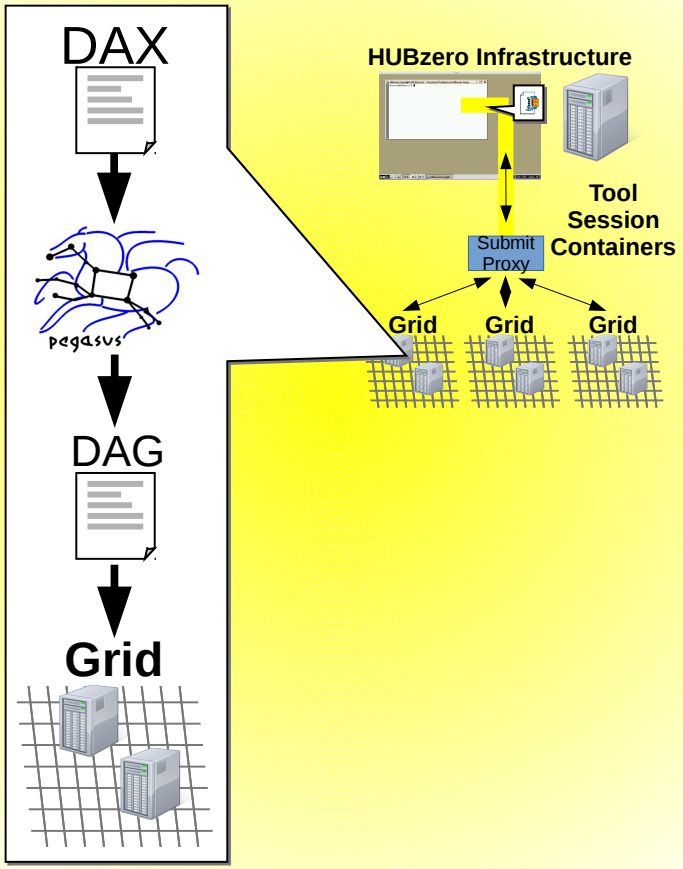


Collaboration inside the Workspace

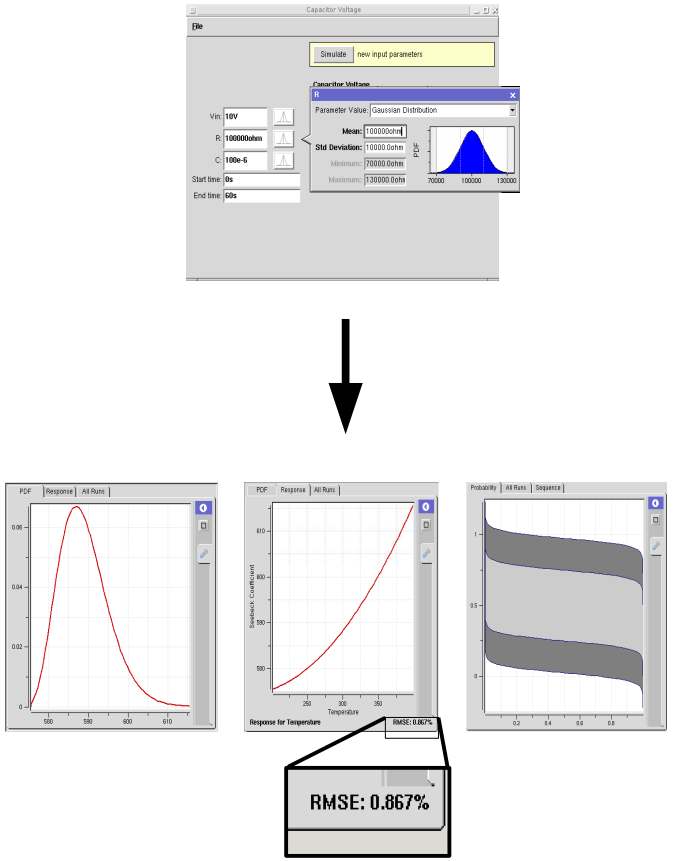


Productivity in the Workspace

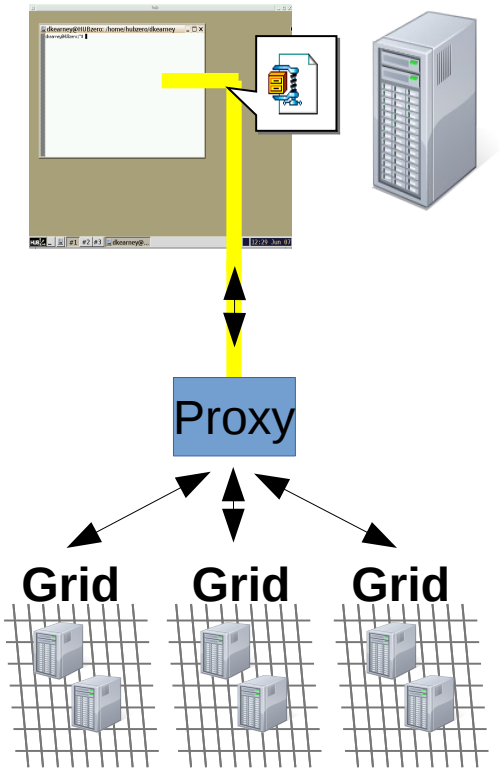
Pegasus Workflows



Uncertainty Quantification

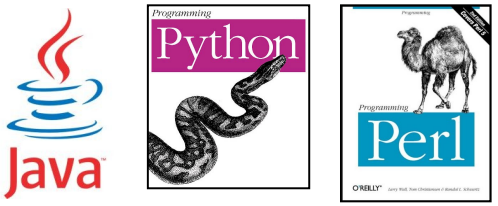


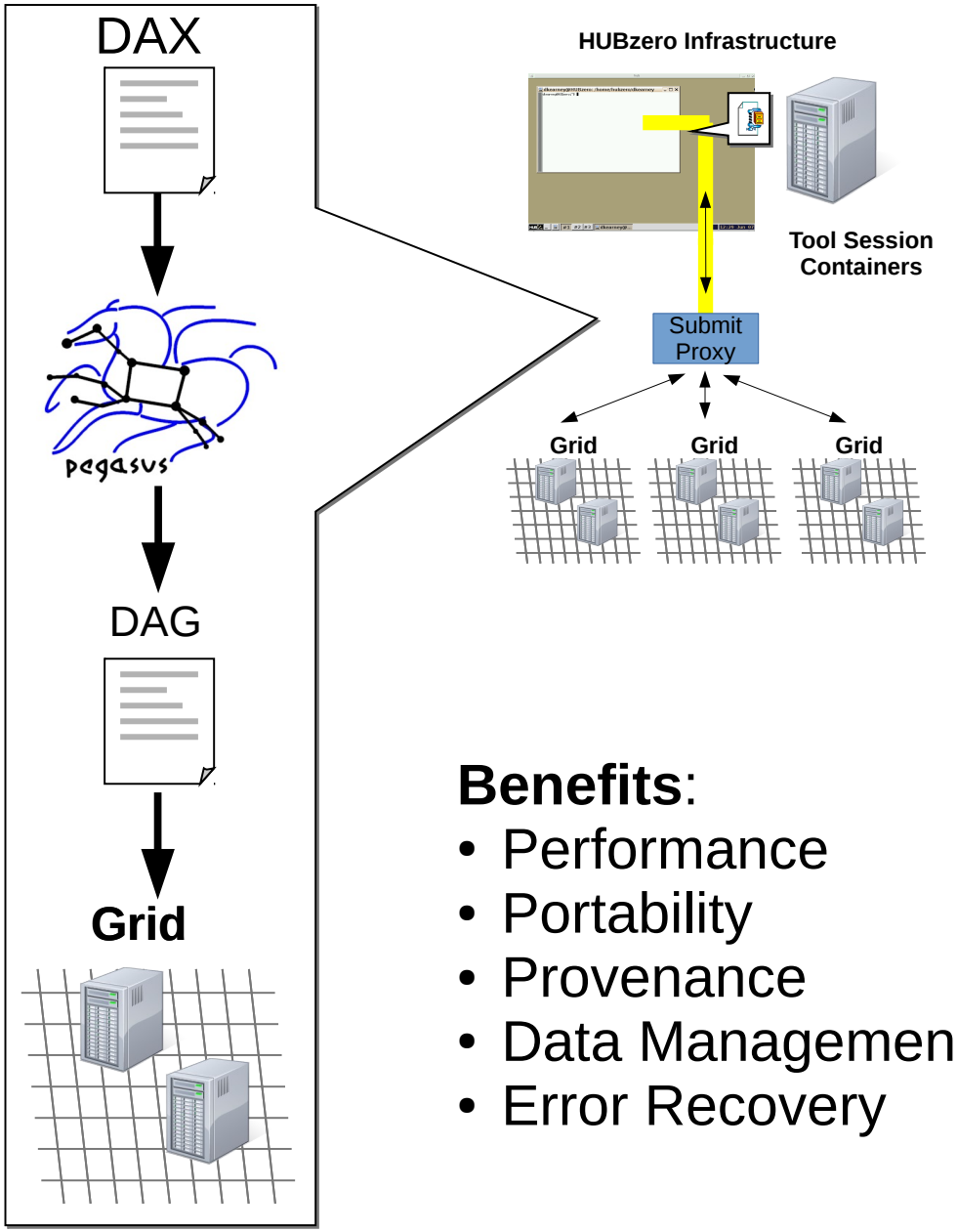
Submit



Pegasus Workflow Management

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





Benefits:

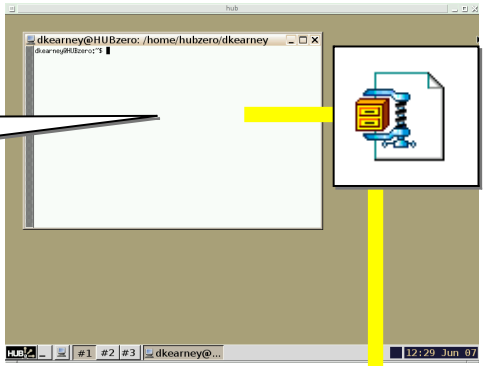
- Performance
- Portability
- Provenance
- Data Management
- Error Recovery

Let Submit create a workflow ...

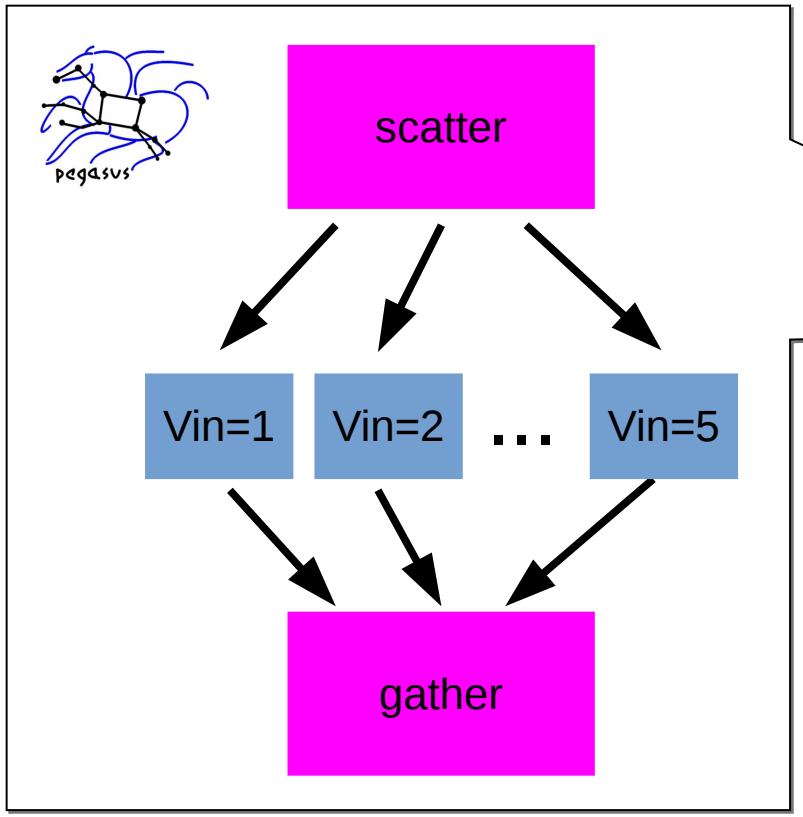
User's Workspace Terminal

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

HUBzero Infrastructure

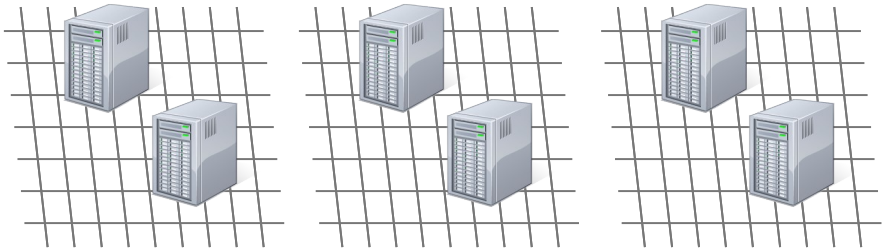


Tool Session Containers

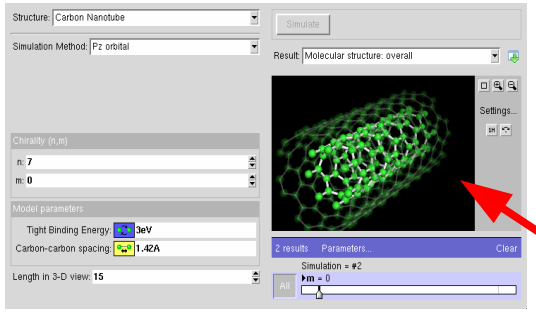


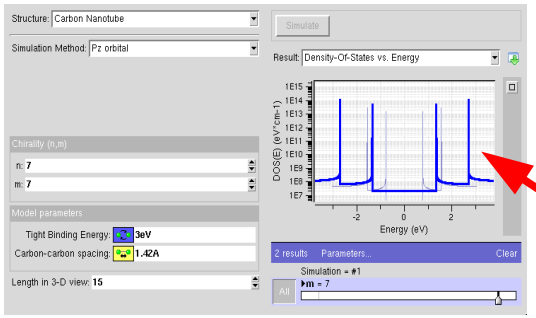
Submit Proxy

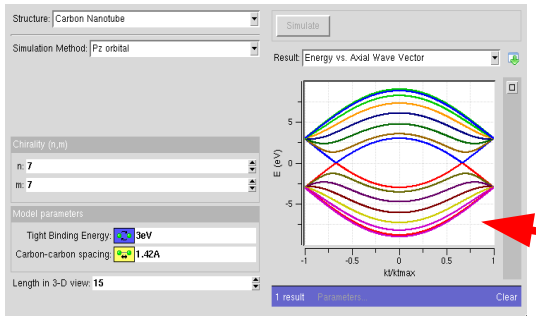
Grid **Grid** **Grid**

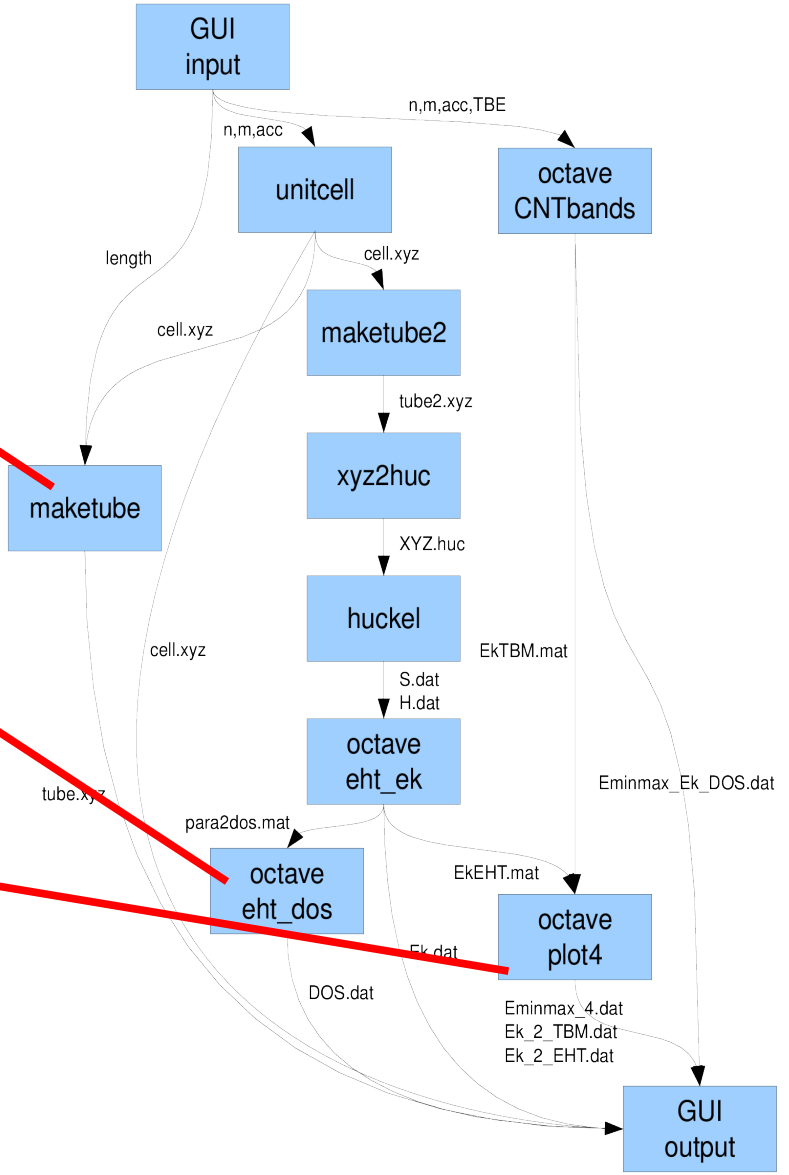


… or write your own workflow









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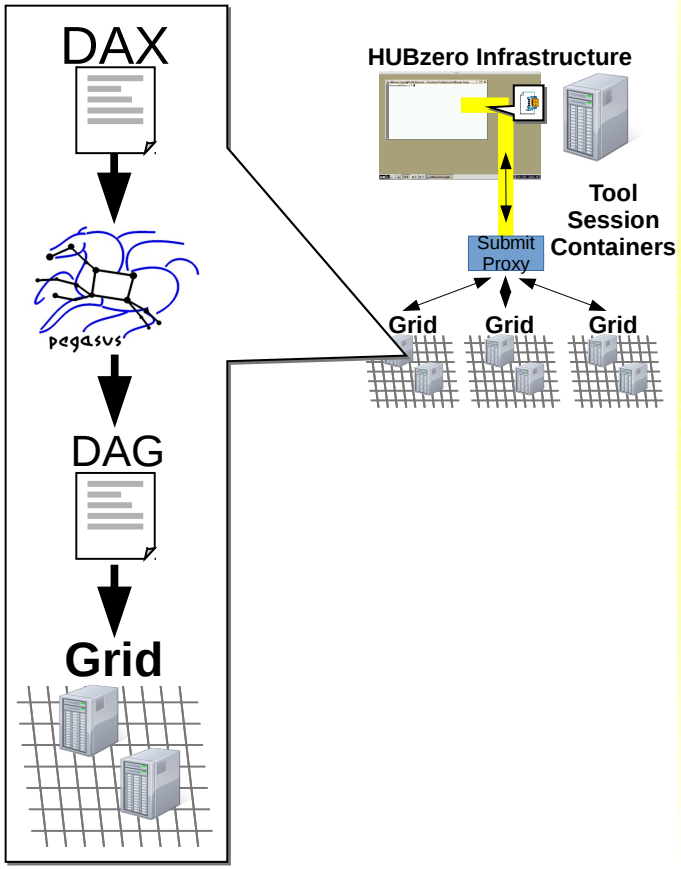
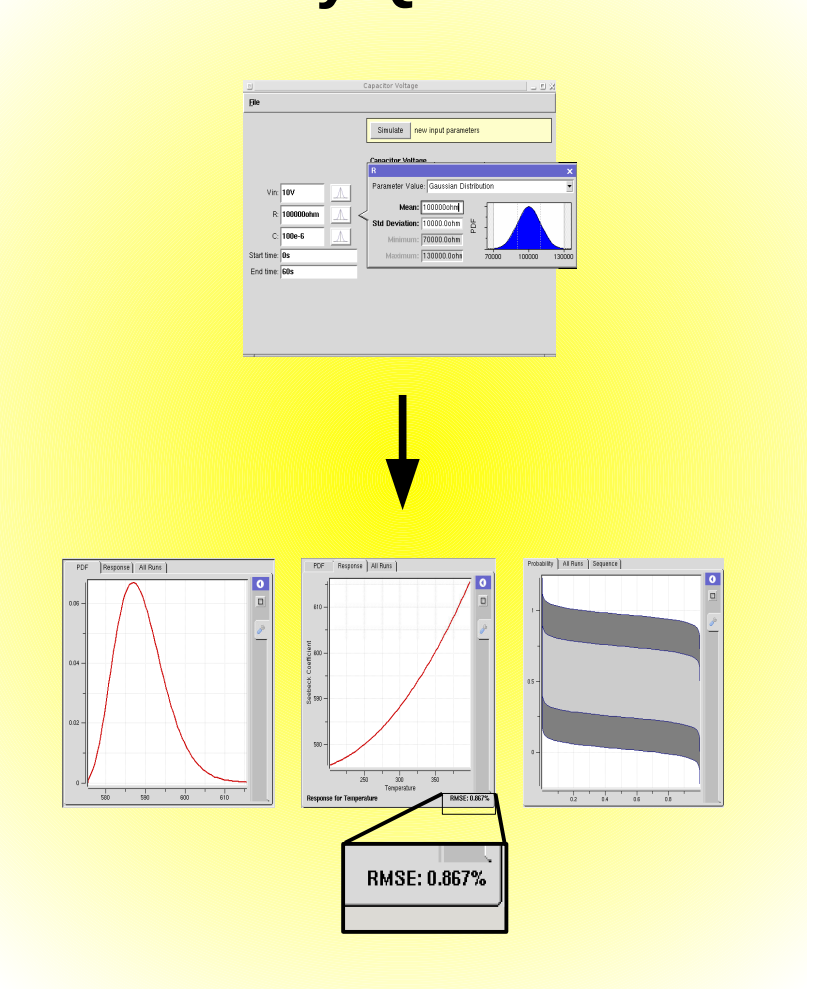


Uncertainty Quantification



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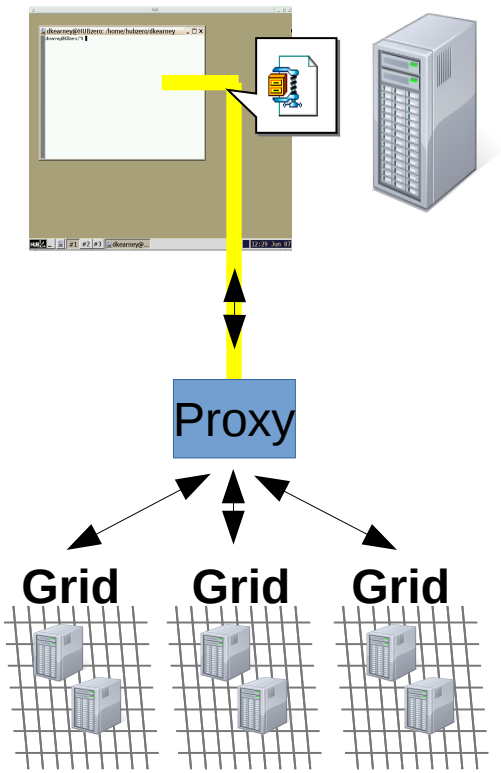

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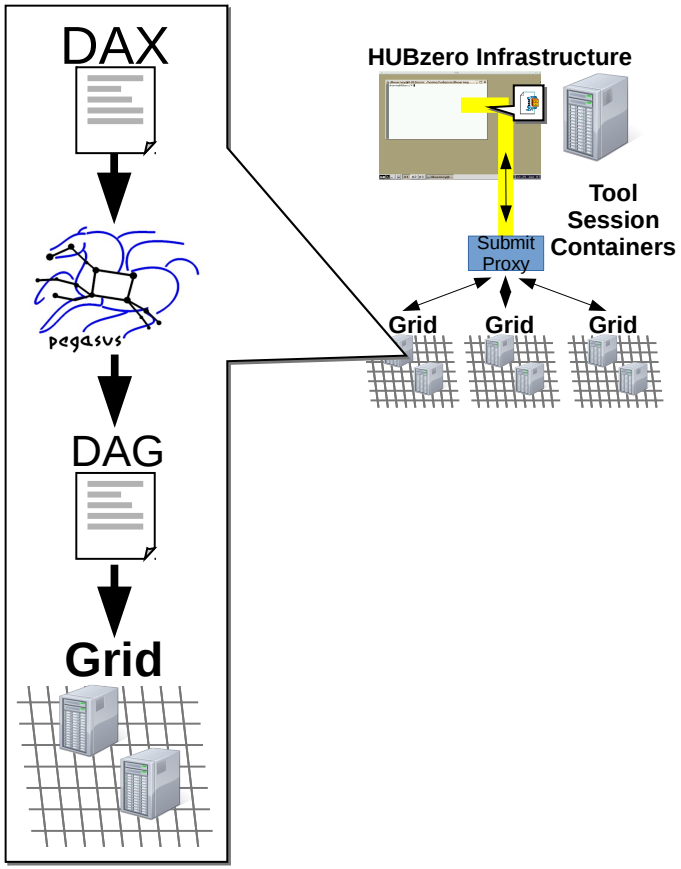

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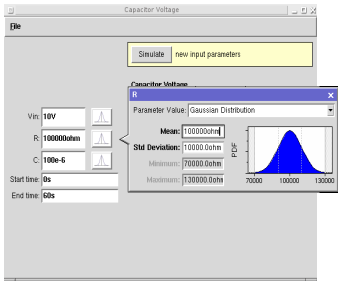

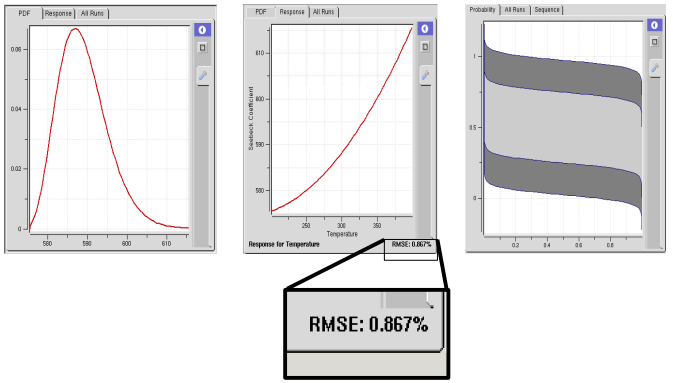

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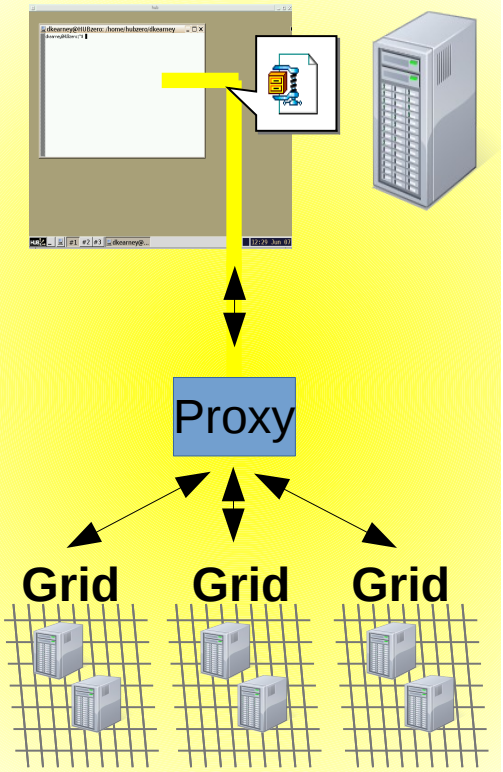
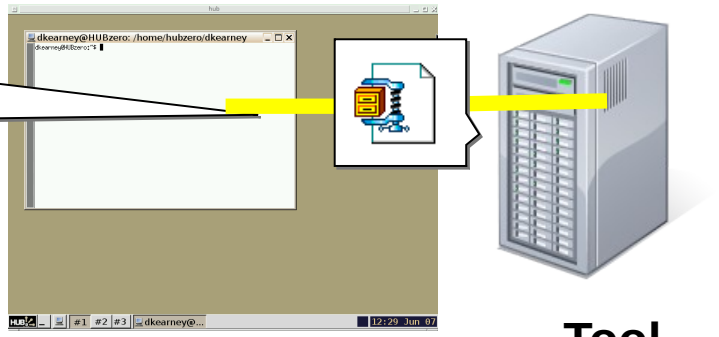


Running locally in a Workspace

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