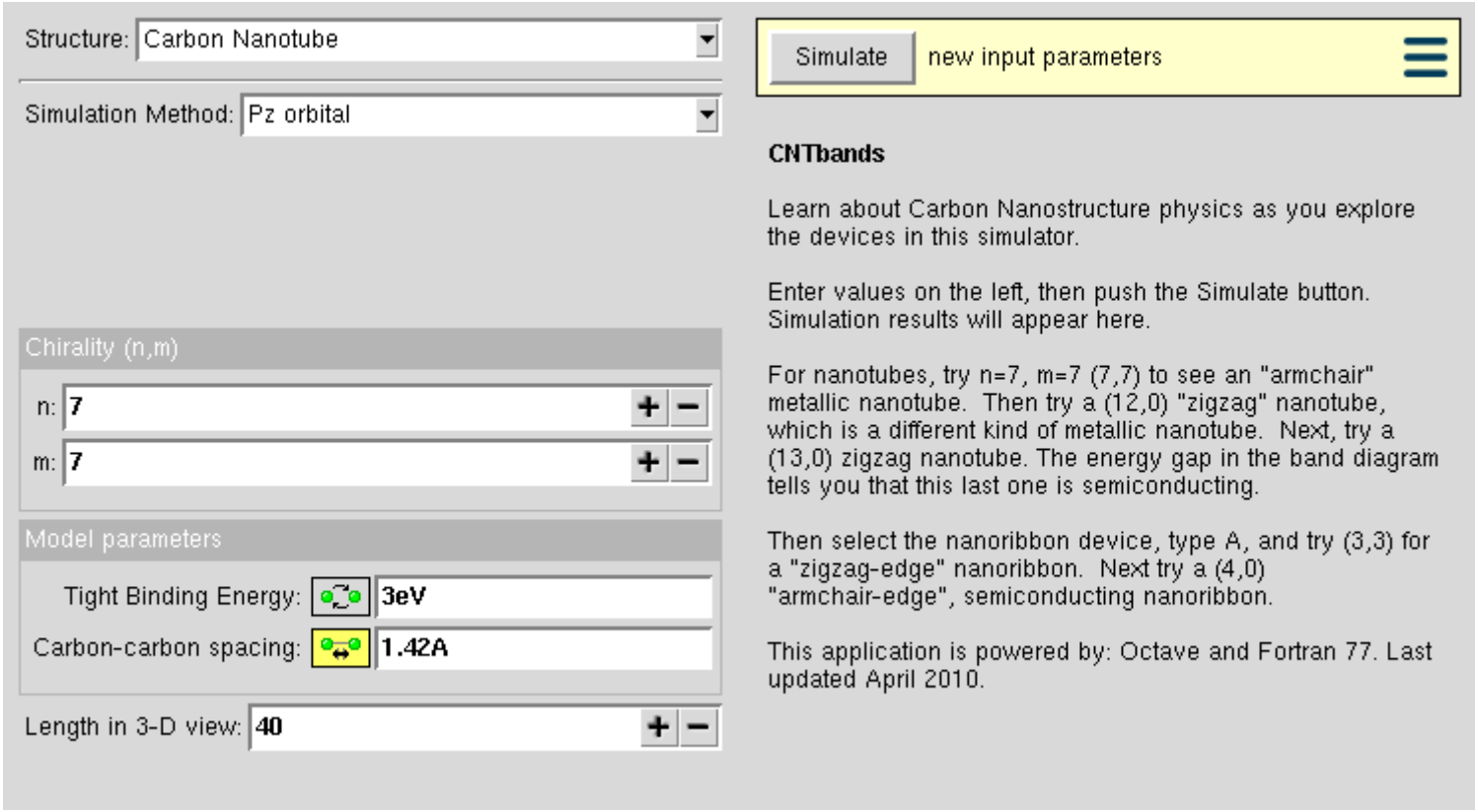
HUBzero Platform Features

TRADES Proposal Demo
Oct. 12, 2016

Derrick Kearney
hubzero.org

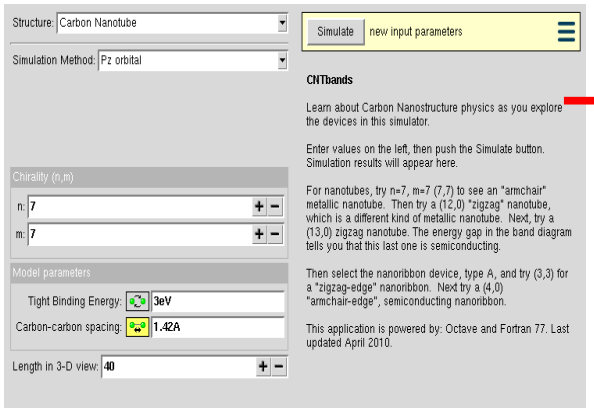
The HUBzero Platform

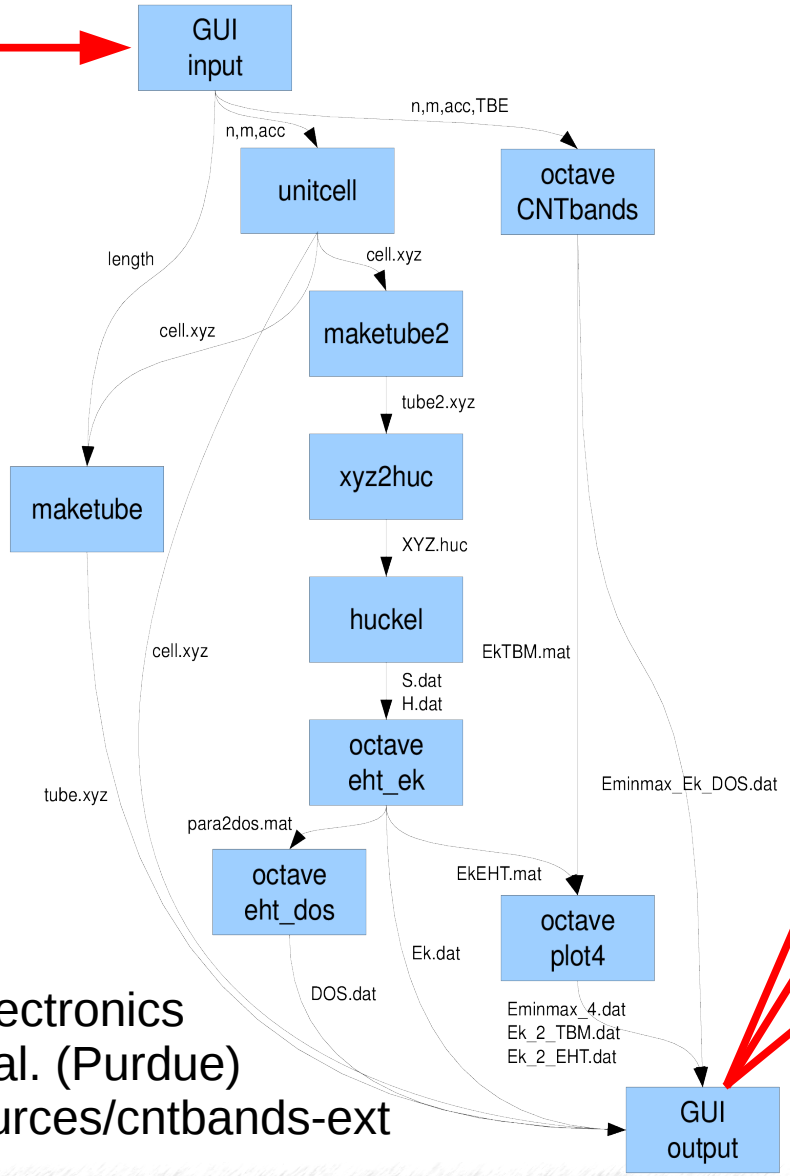
CNTbands

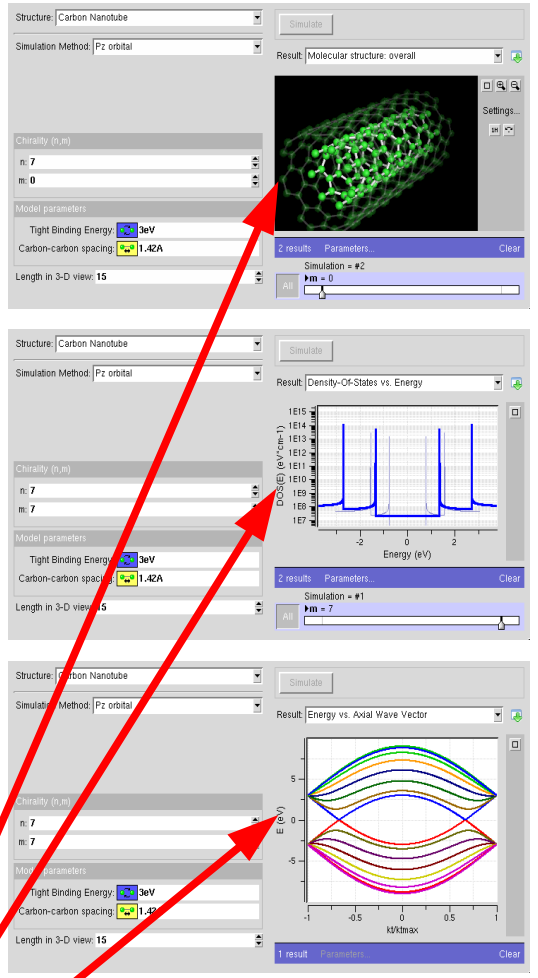


CNTbands
Science Domain: Nanoelectronics
Scientists: Lundstrom et al. (Purdue)
https://nanohub.org/resources/cntbands-ext

CNTbands







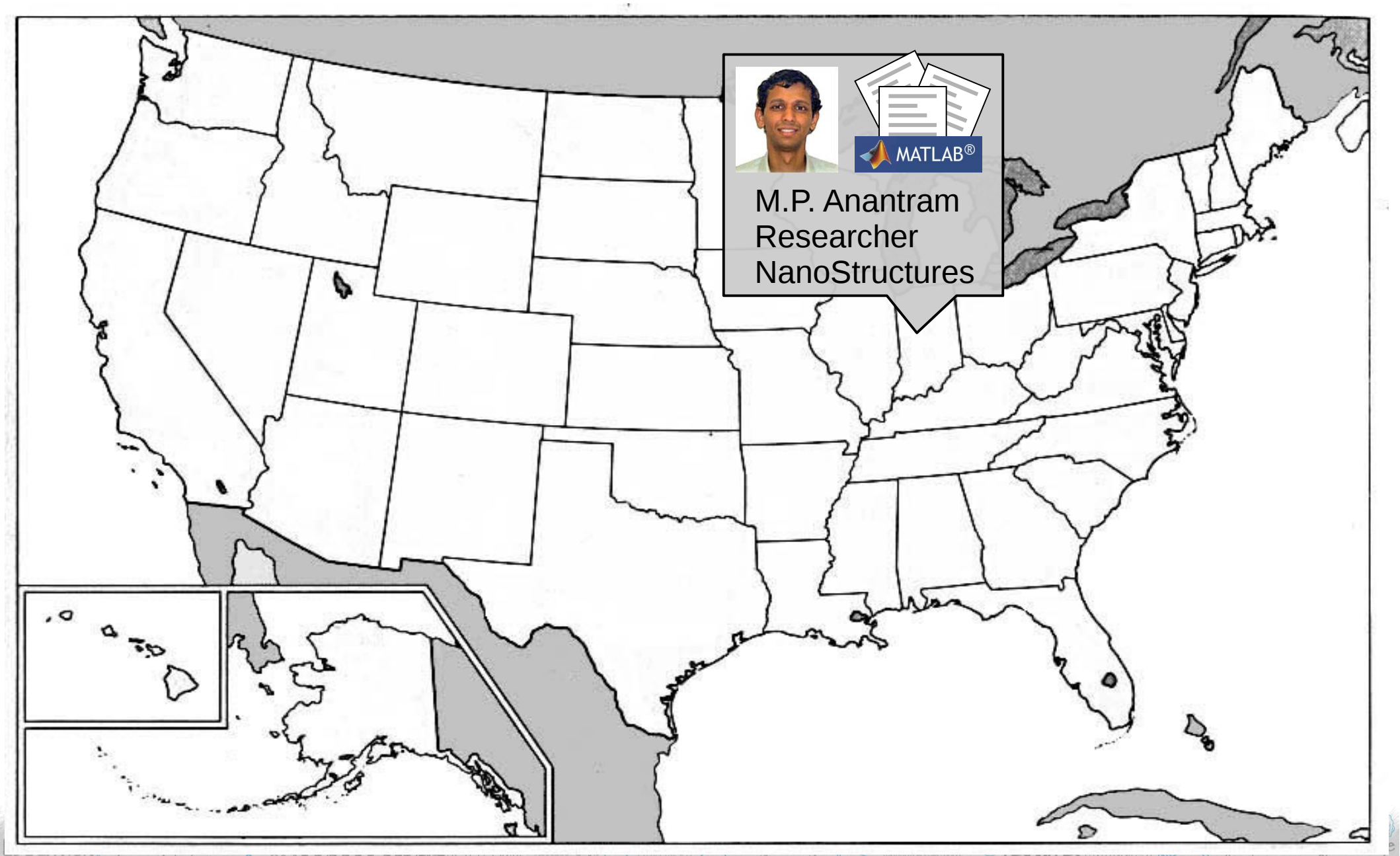
CNTbands

Science Domain: Nanoelectronics

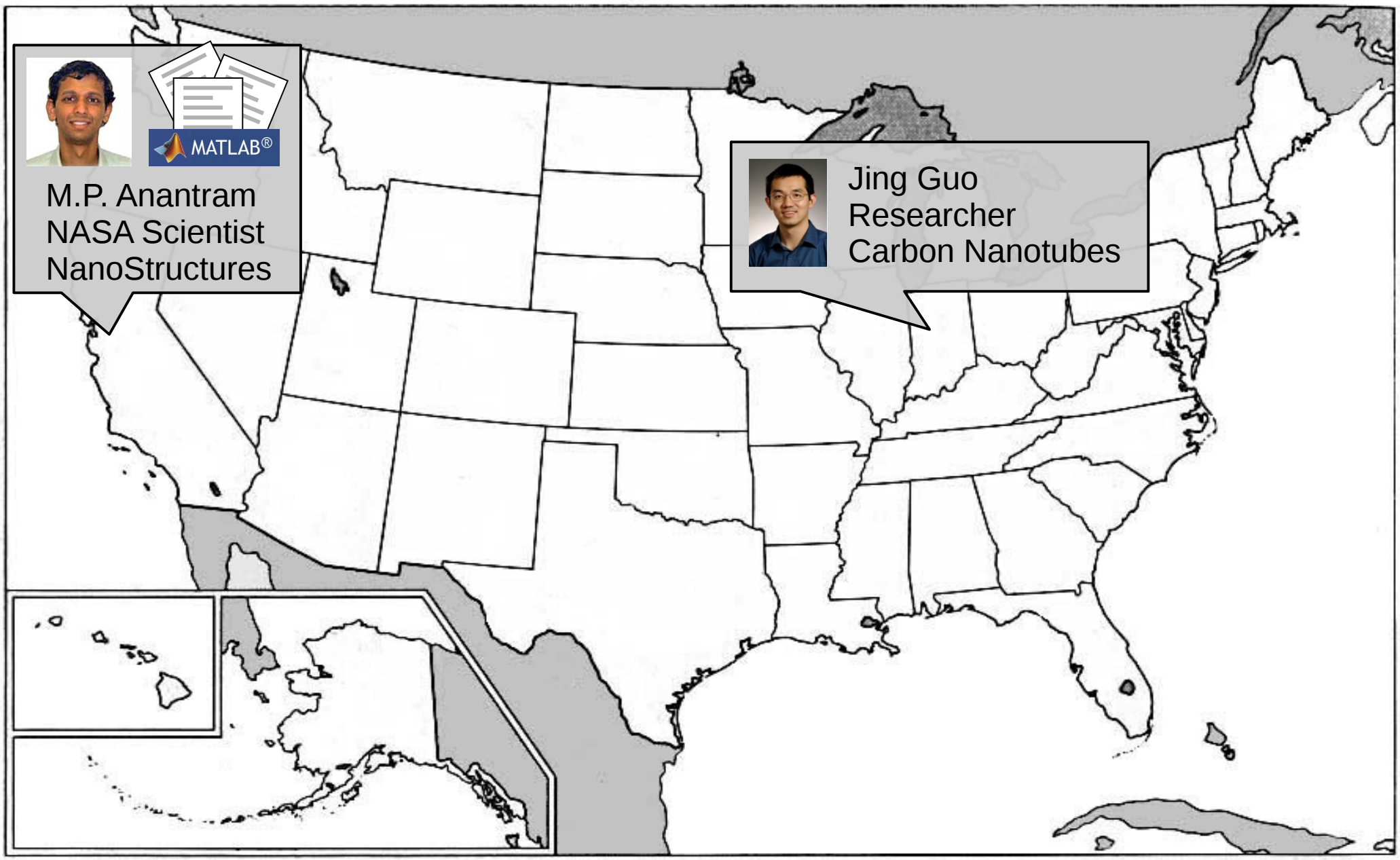
Scientists: Lundstrom et al. (Purdue)

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

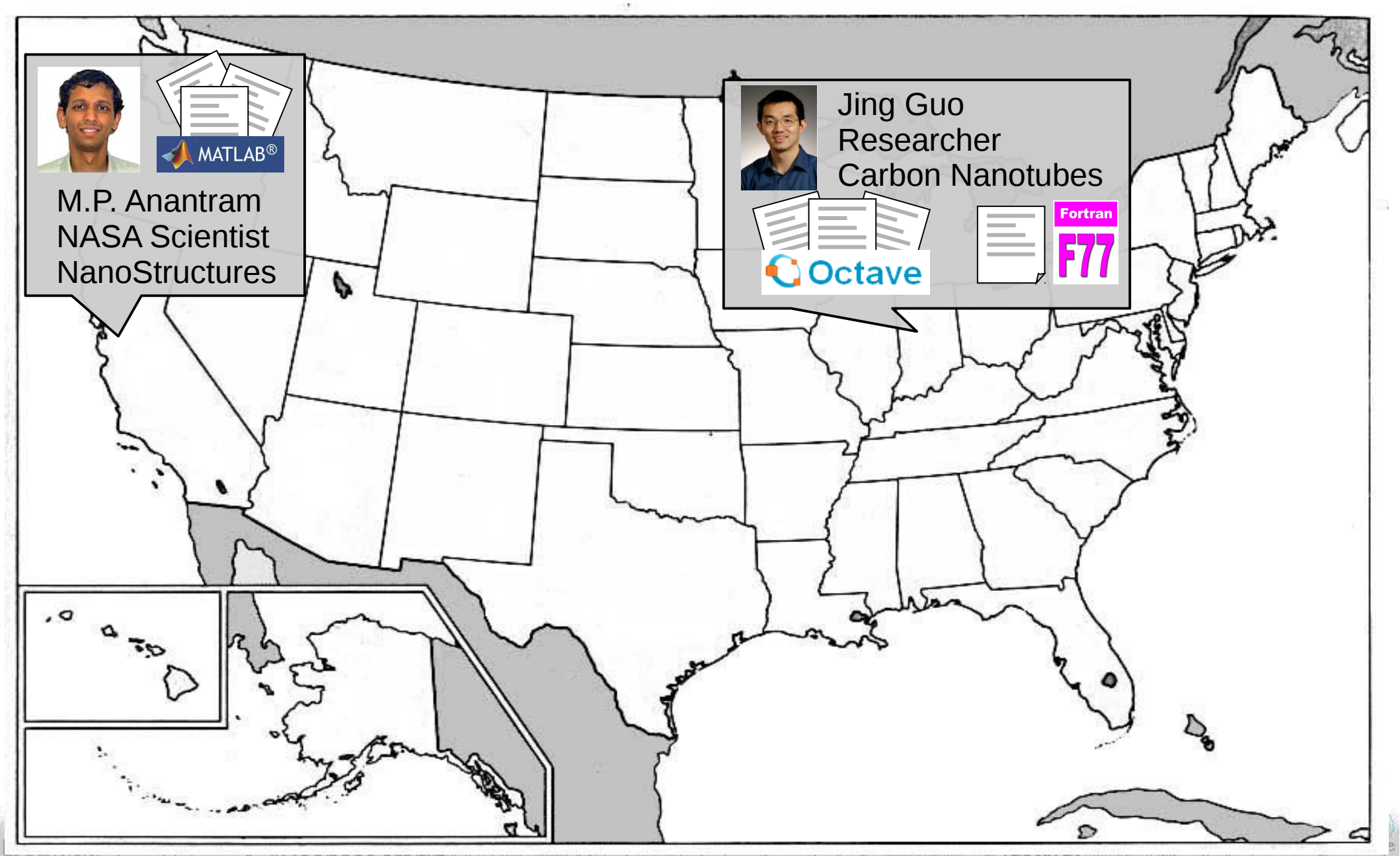
1990s – Initial Algorithms



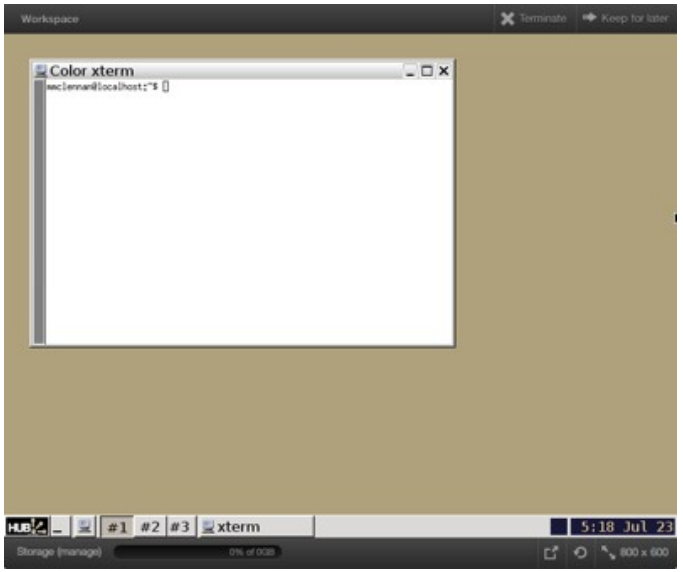
2002 – Idea for a Tool



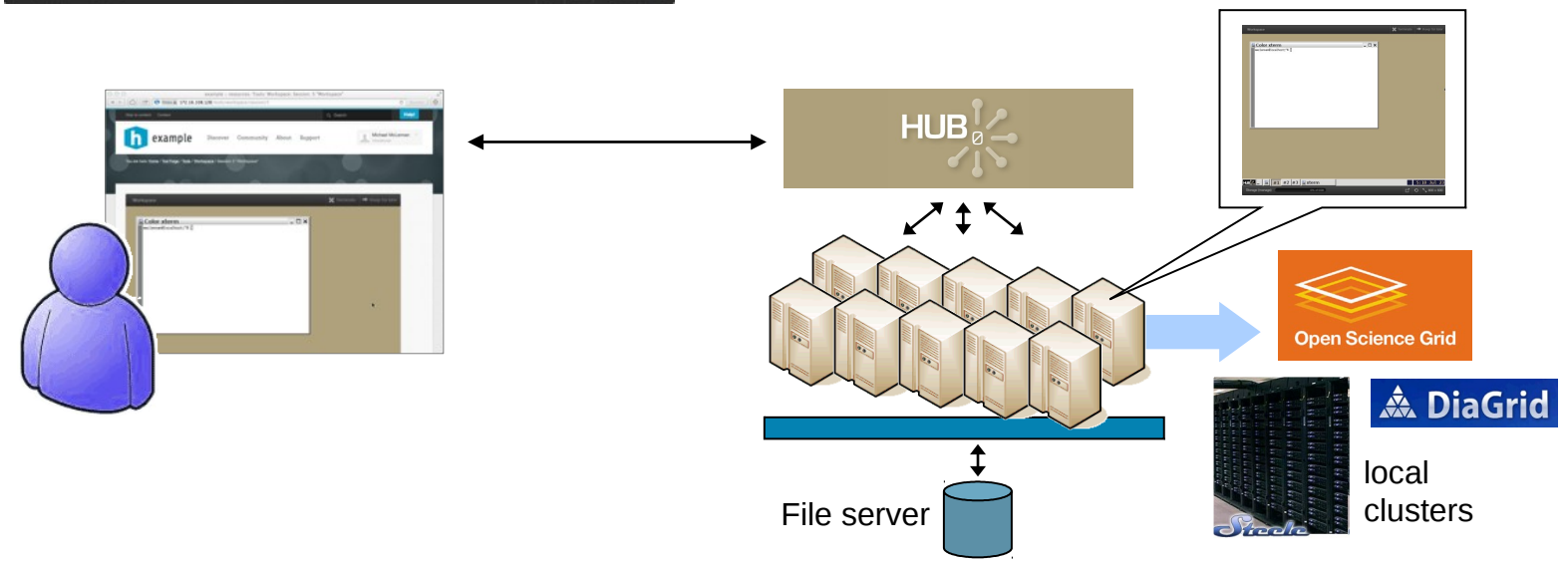
2002 – Tool Registered



What is a Workspace?

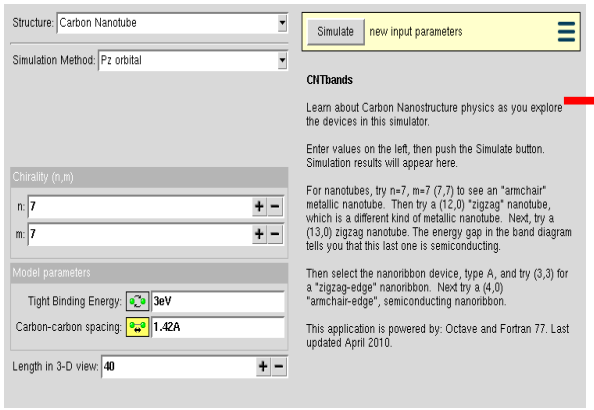


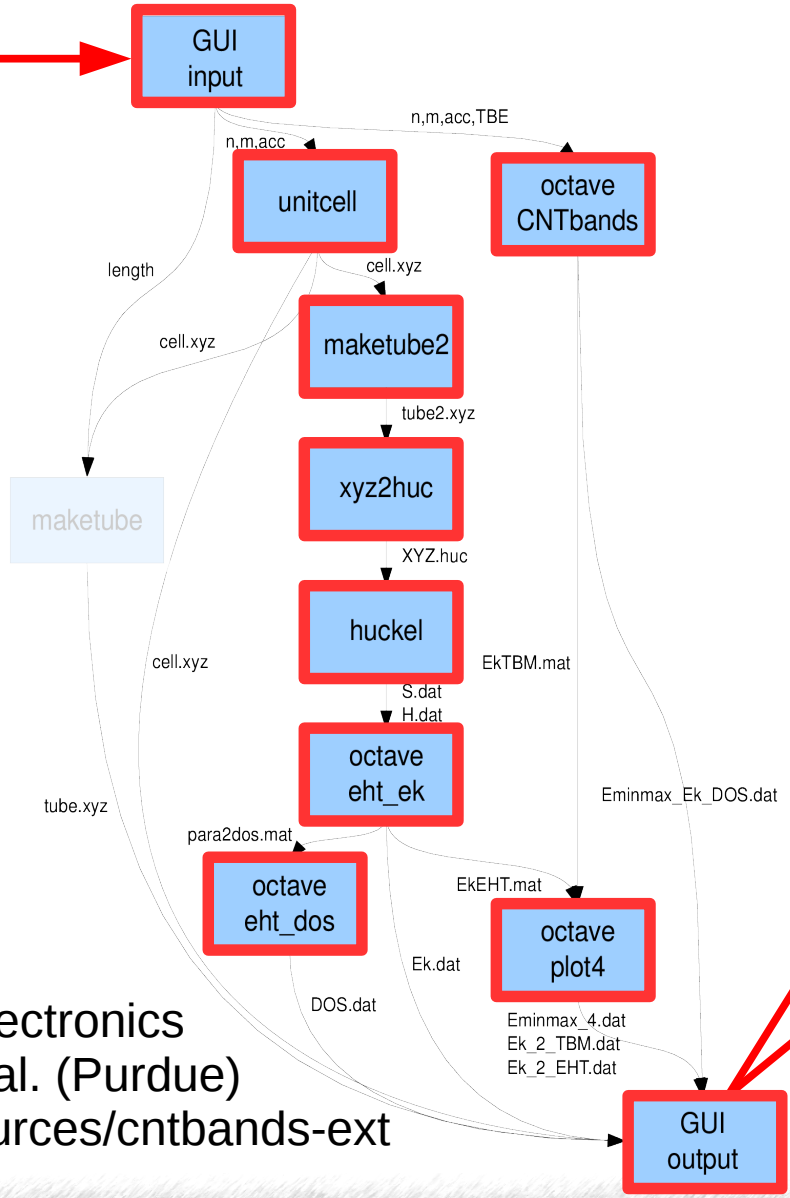
- Full-featured Linux or Windows Desktop
- Runs in the Cloud
- For tool developers & researchers
- Accessible from any web browser
- Still running after you close your browser
- Access to computational clusters
- File storage provided by the hub

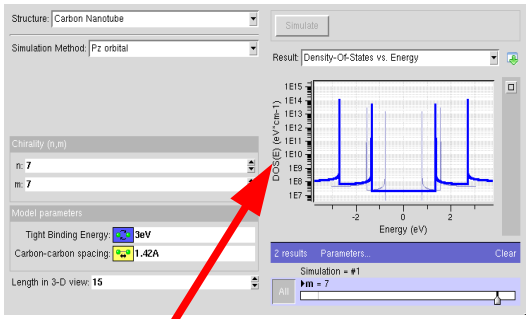


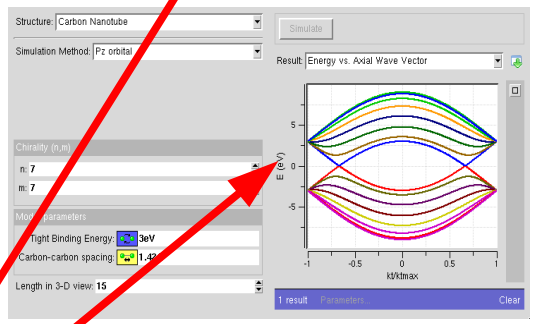
Collaboration / Groups

CNTbands









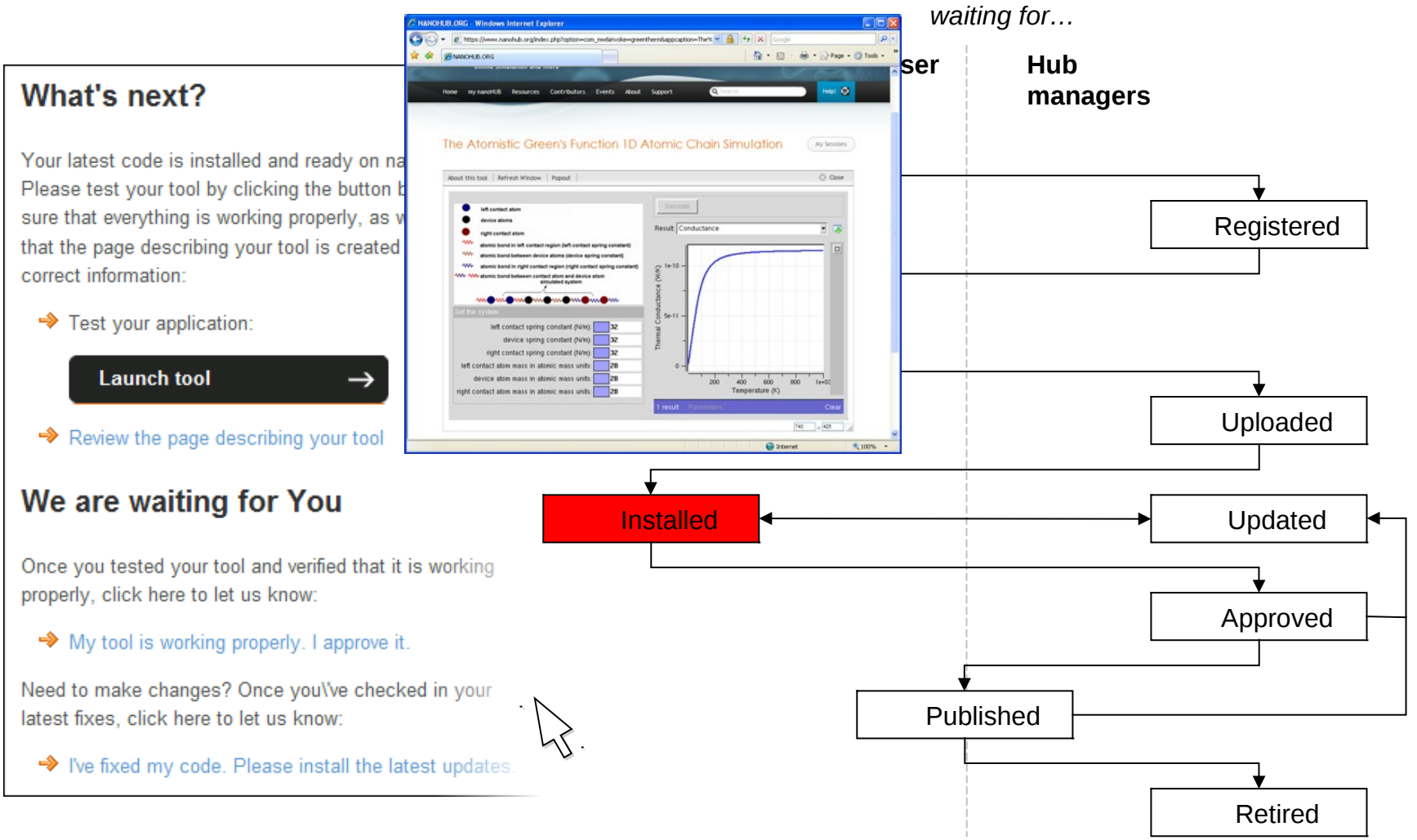
CNTbands

Science Domain: Nanoelectronics

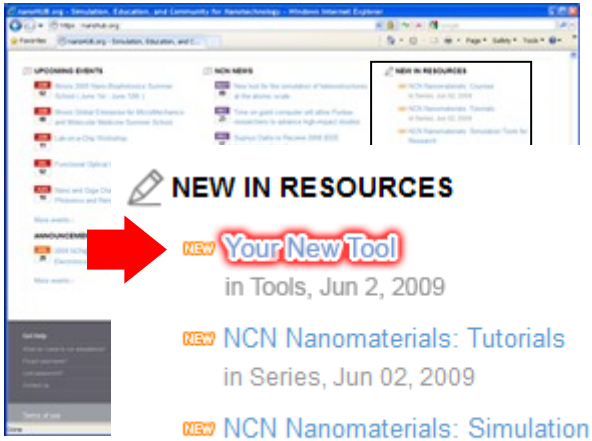
Scientists: Lundstrom et al. (Purdue)

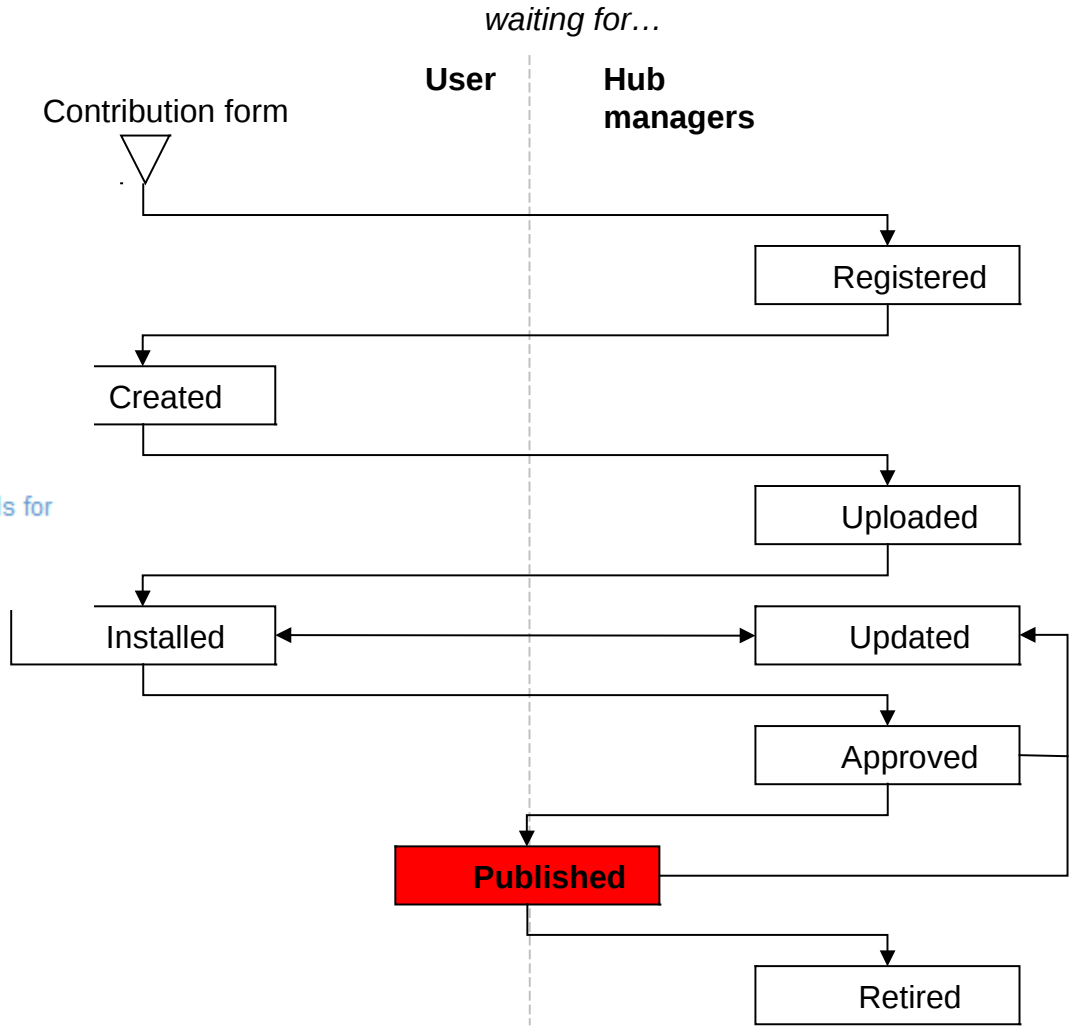
https://nanohub.org/resources/cntbands-ext

Installing Applications



Publishing Applications





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:

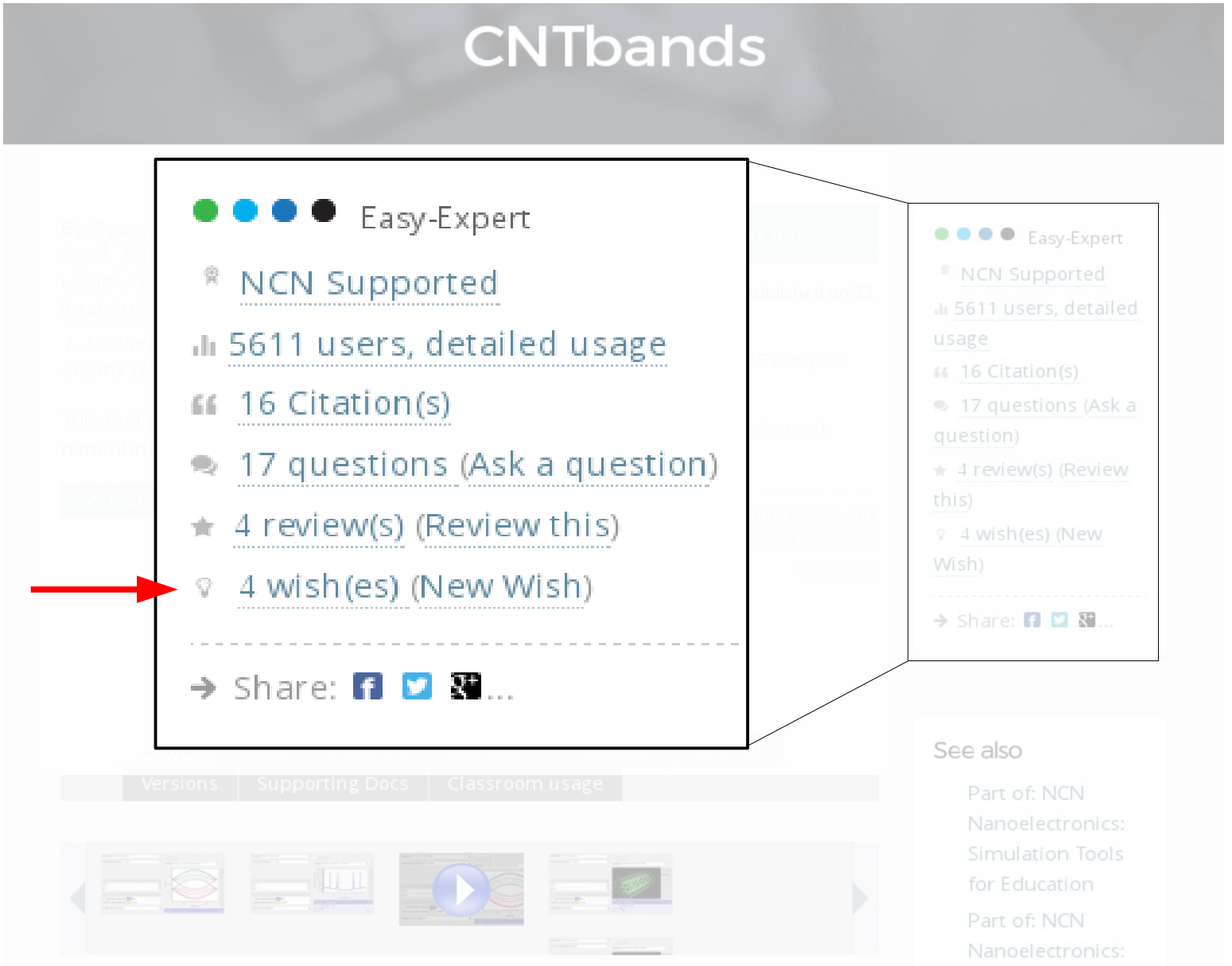
About | Usage | Citations | Questions | Reviews | Wishlist | Versions | Supporting Docs | Classroom usage

See also

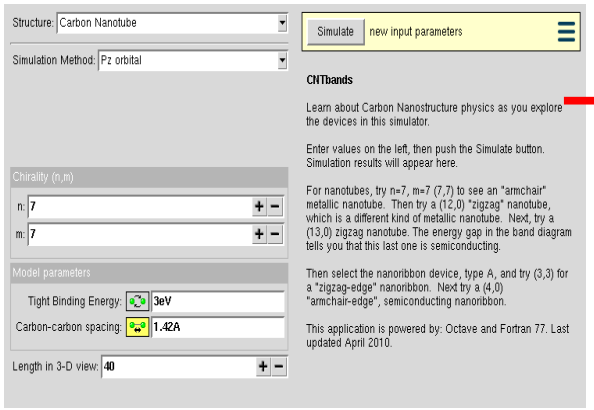
Part of: NCN Nanoelectronics: Simulation Tools for Education

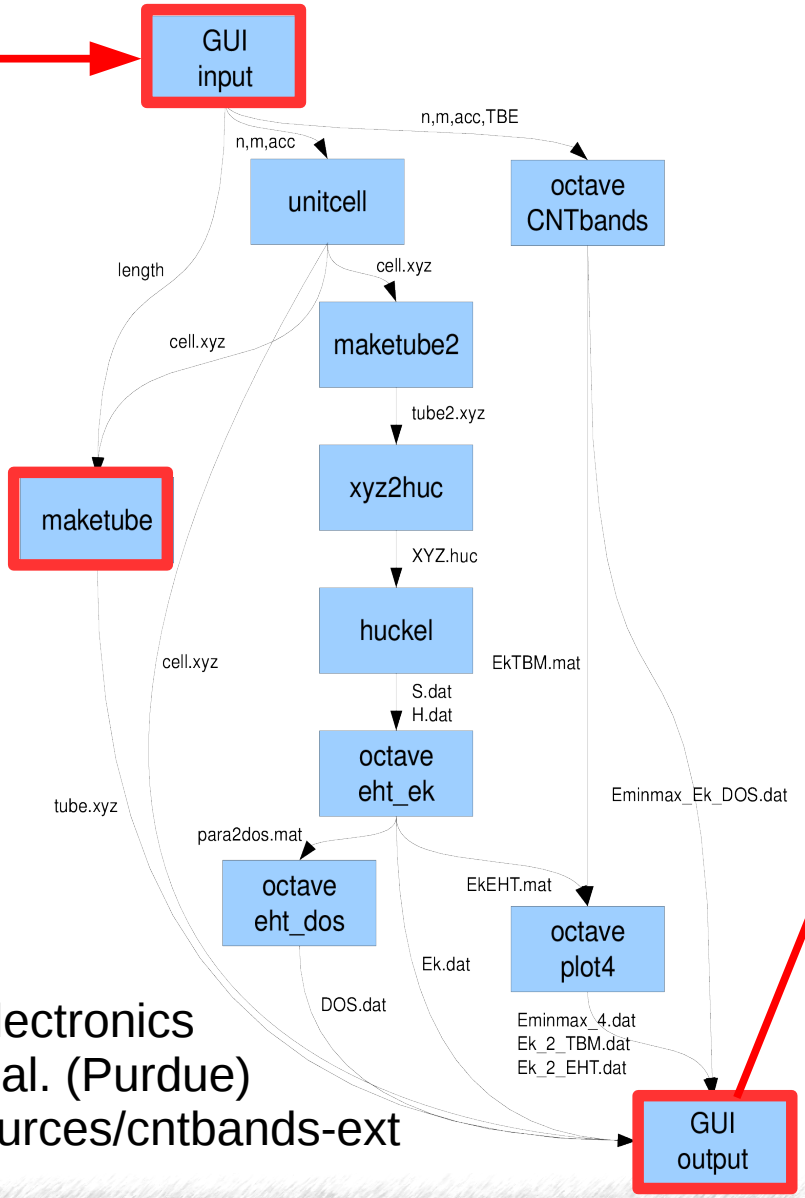
Part of: NCN Nanoelectronics:

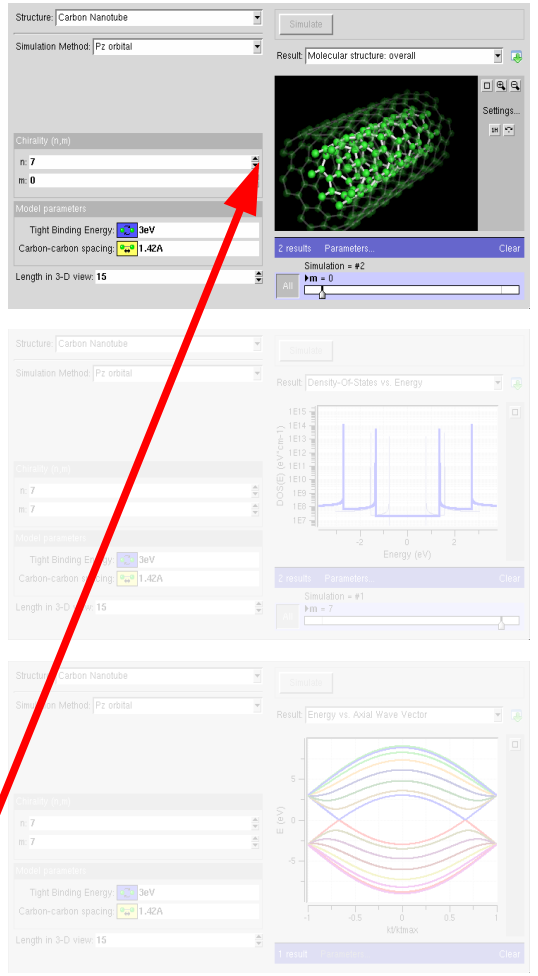
Communicate with users



Adding New Features







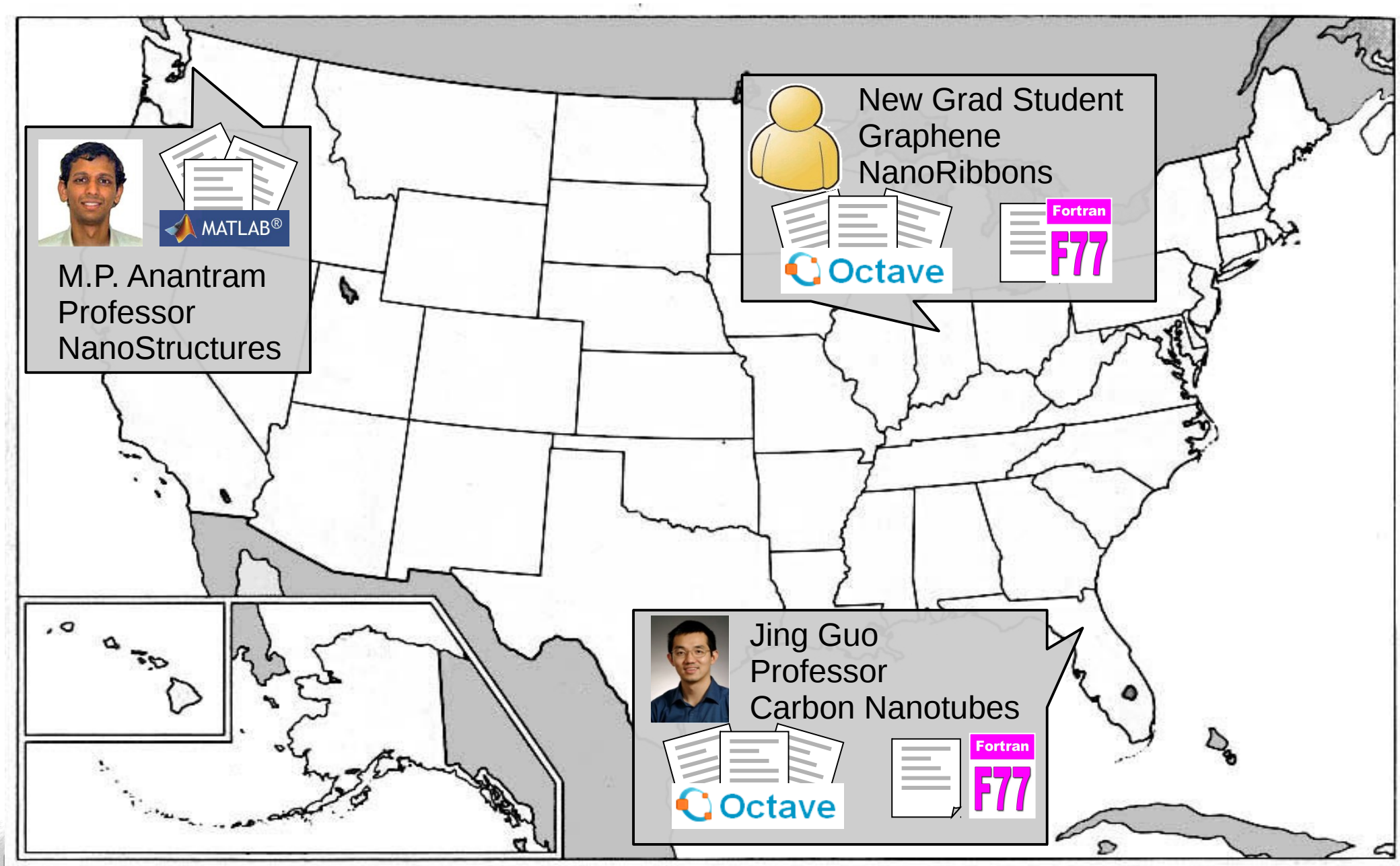
CNTbands

Science Domain: Nanoelectronics

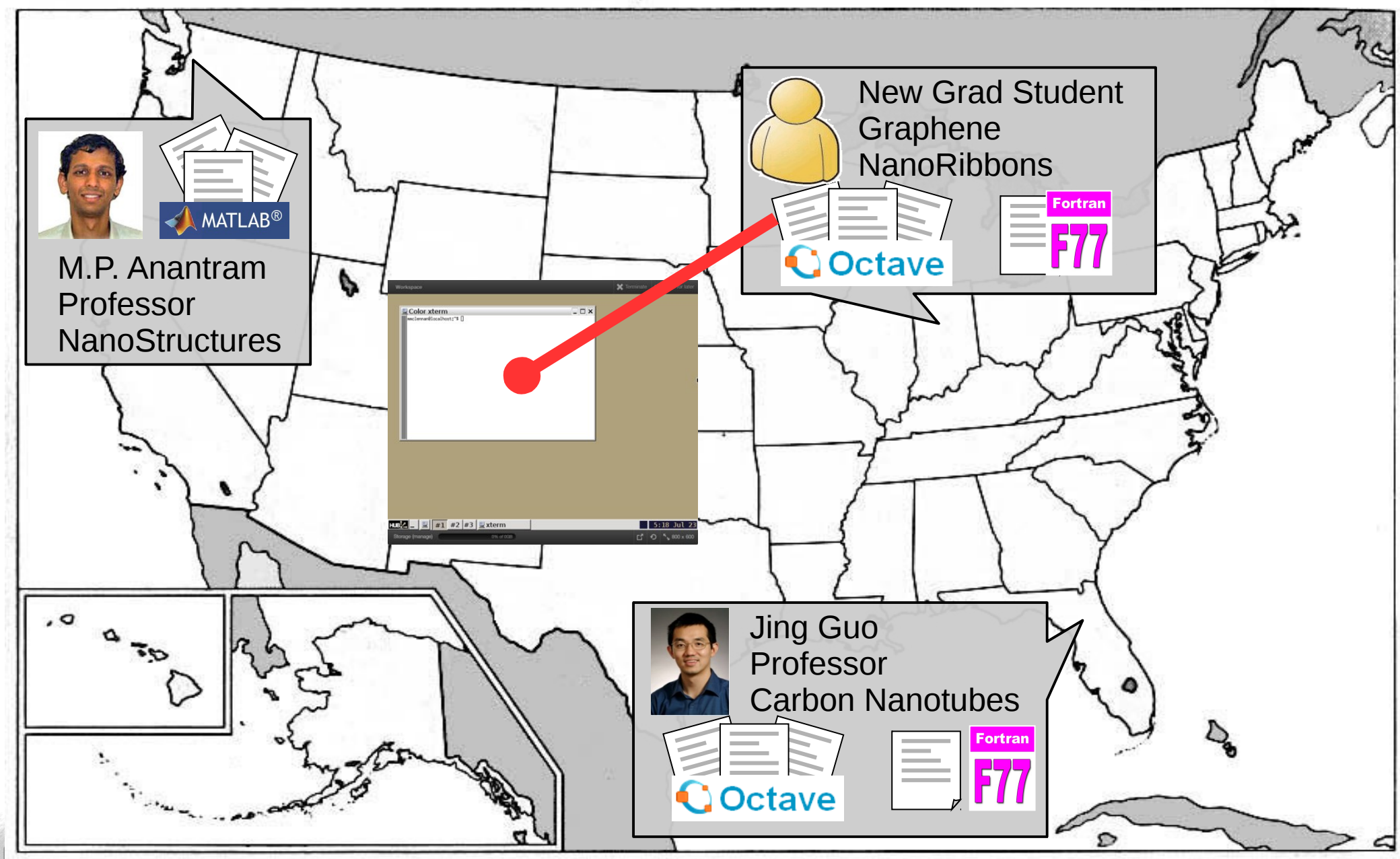
Scientists: Lundstrom et al. (Purdue)

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

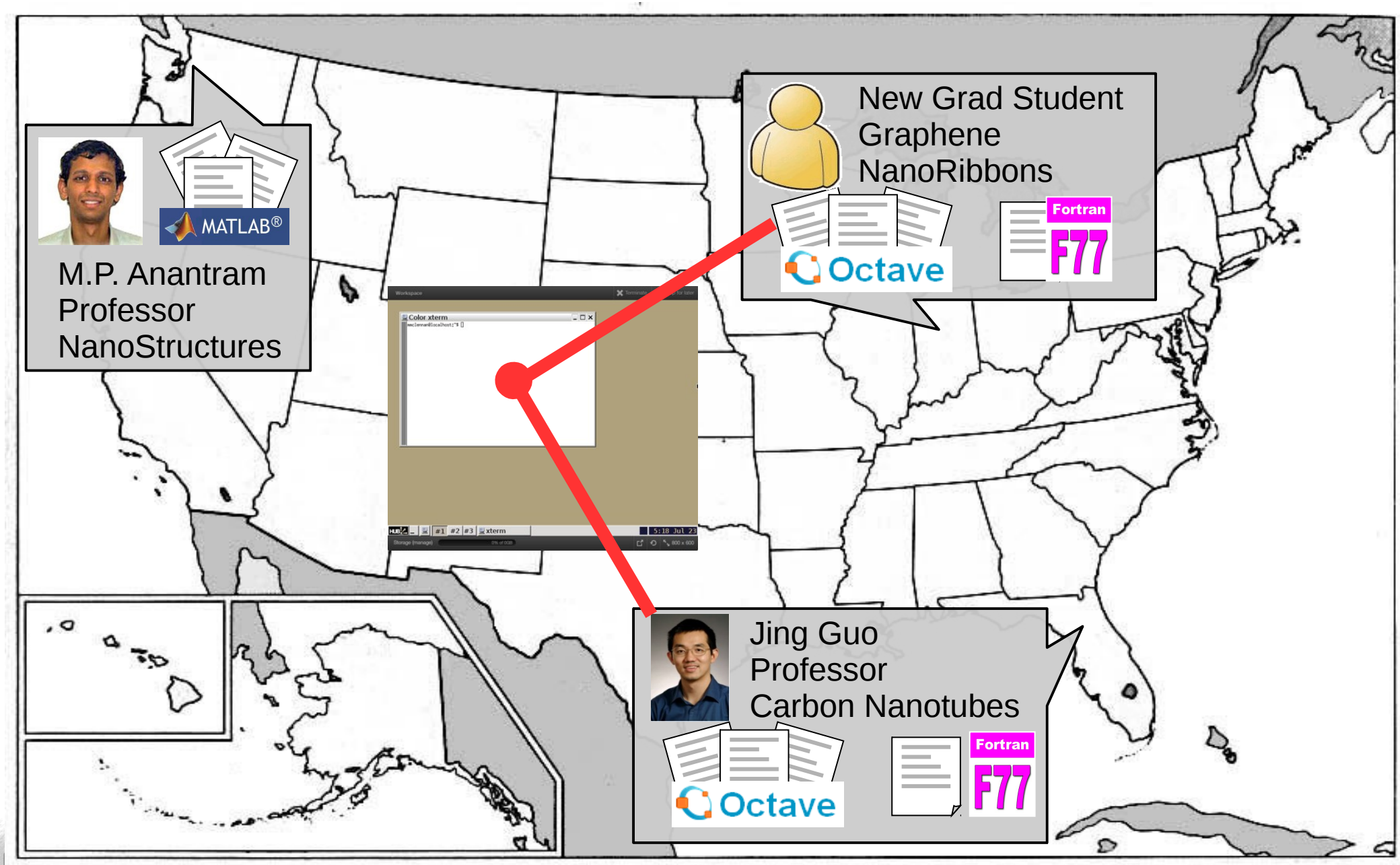
2010 – Introducing New Researchers



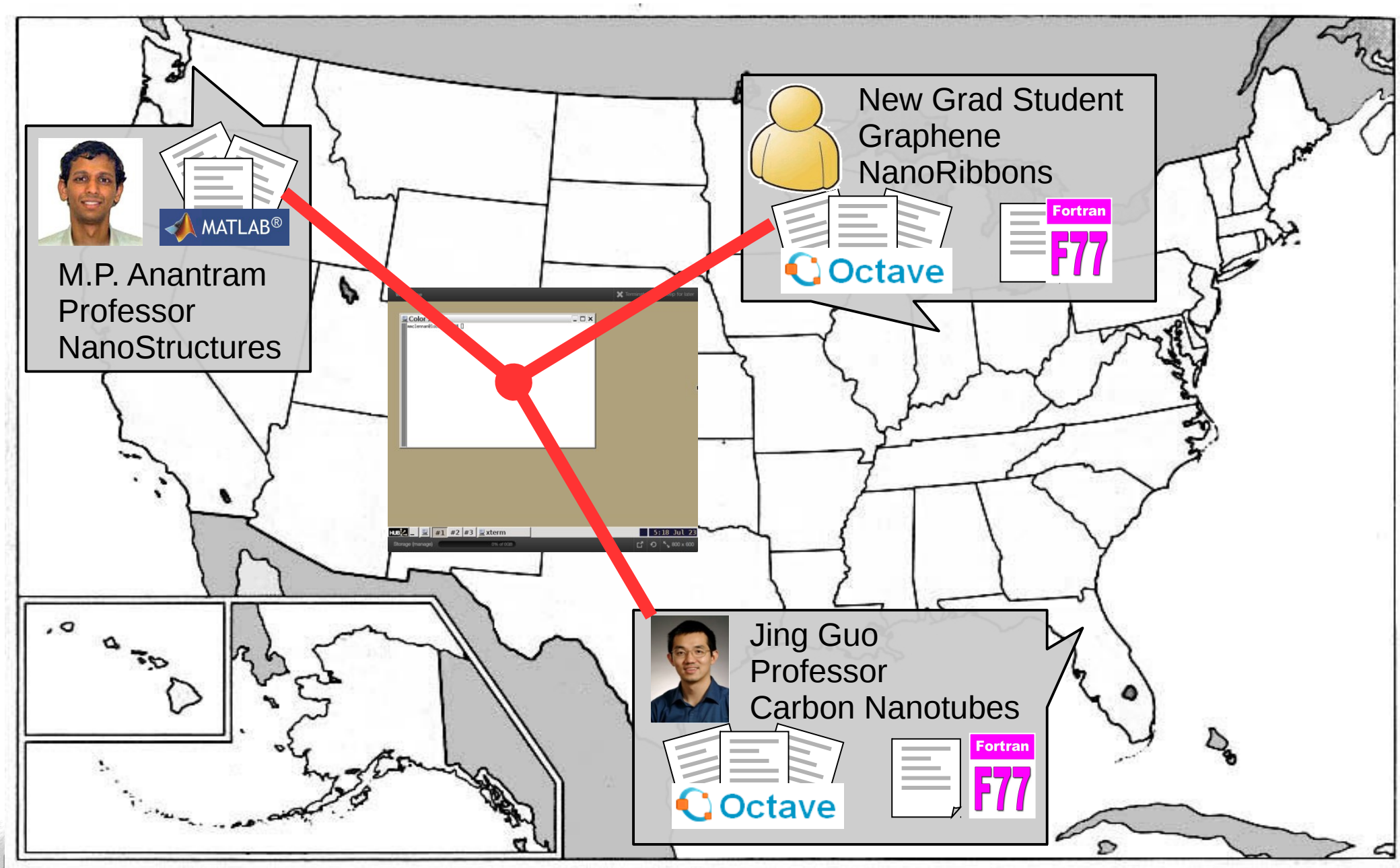
Collaborate in the Workspace



Collaborate in the Workspace

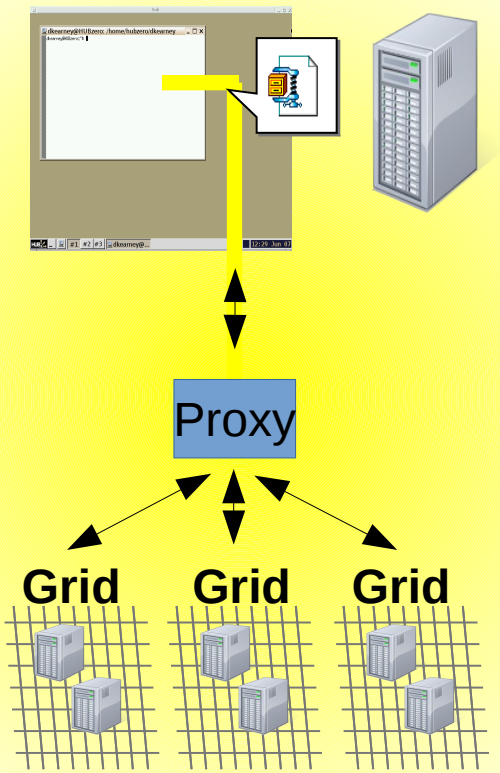


Collaborate in the Workspace

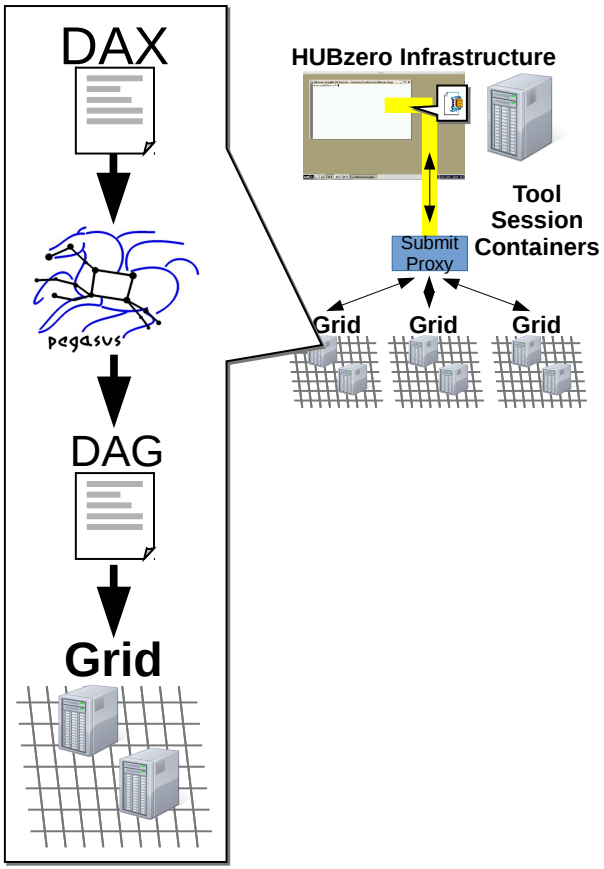


Productivity in the Workspace

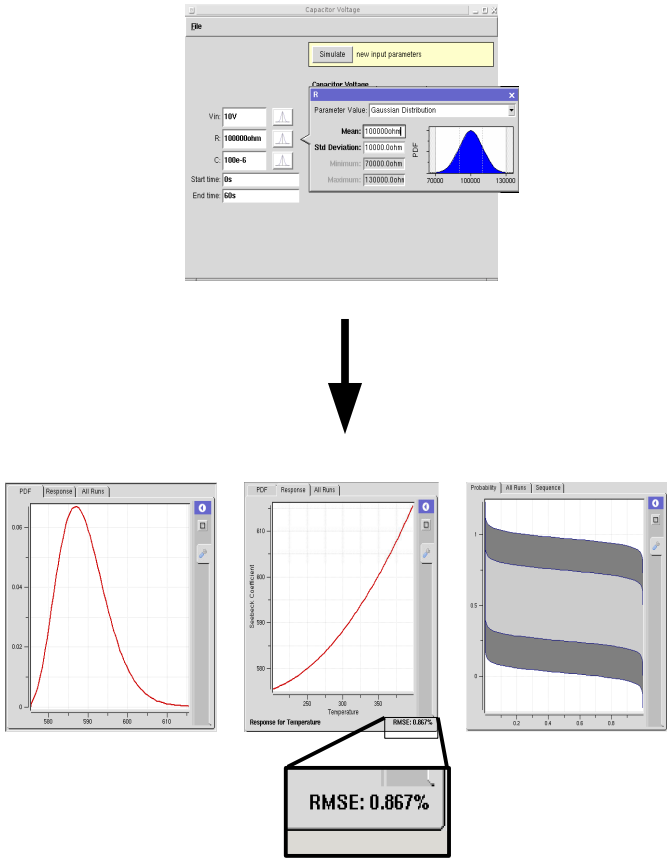
Submit



Pegasus Workflows



Uncertainty Quantification

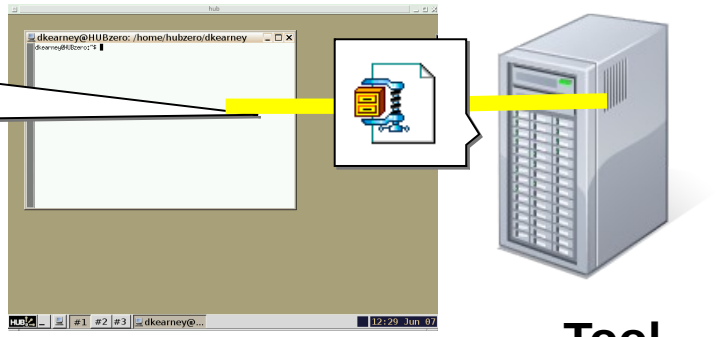


Run tools locally in Workspace

User's Workspace Terminal

```
$ echo hi
hi
$
```

HUBzero Infrastructure



Tool Session Containers

Submit Proxy

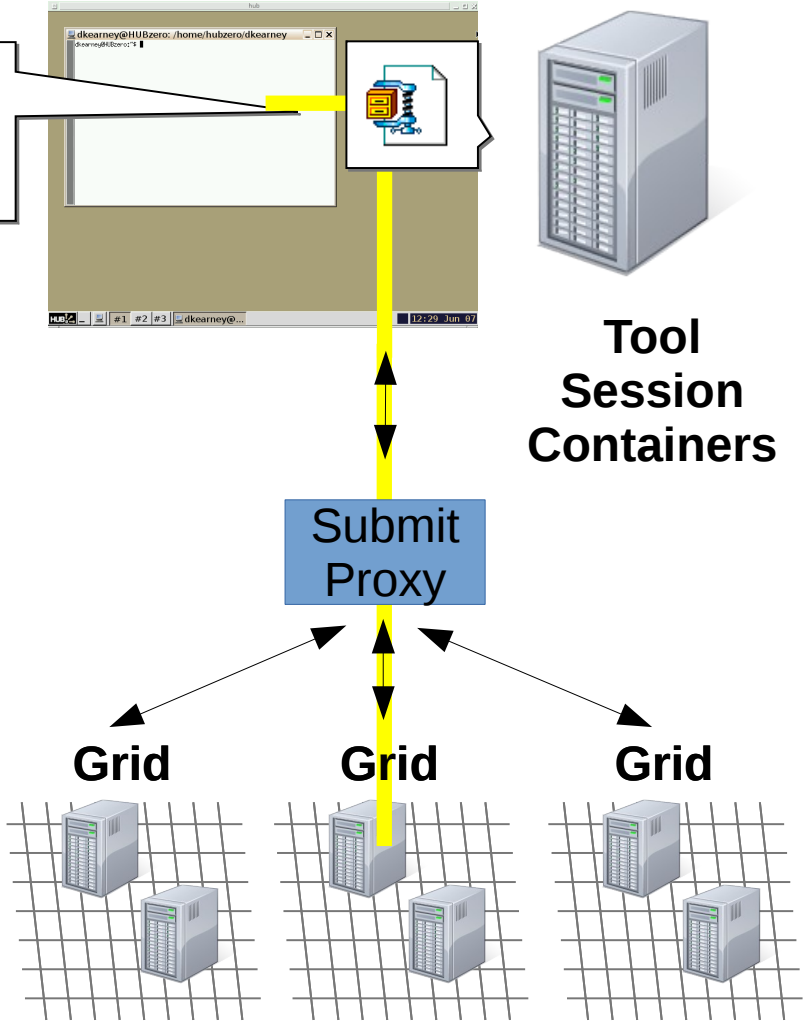
Grid Grid Grid

Submit Jobs to Grid

User's Workspace Terminal

```
$ submit echo hi
```

HUBzero Infrastructure

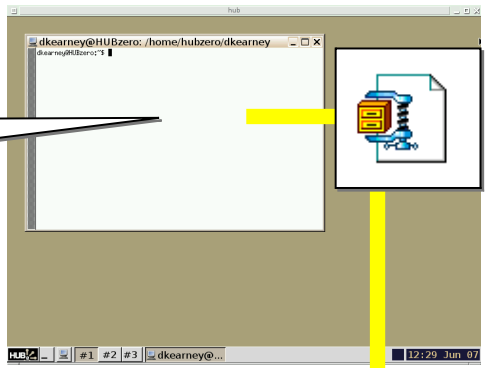


Let Submit create a workflow ...

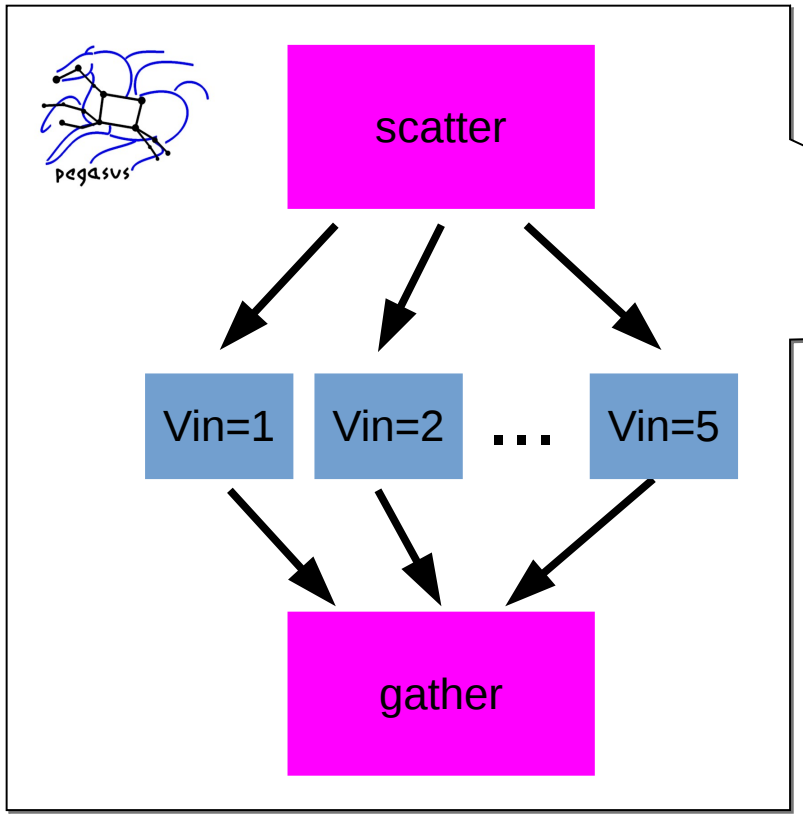
User's Workspace Terminal

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

HUBzero Infrastructure

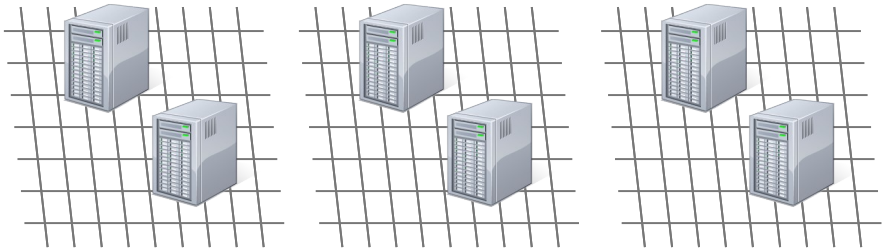


Tool Session Containers

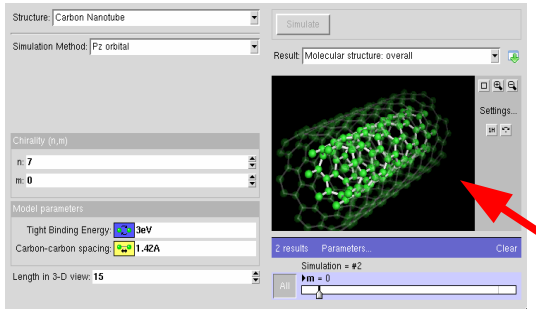


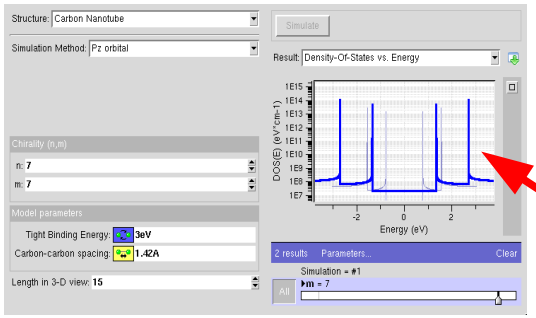
Submit Proxy

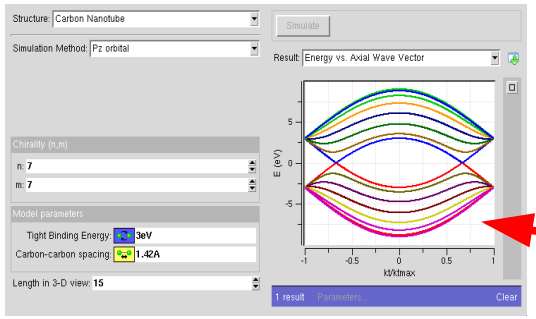
Grid **Grid** **Grid**

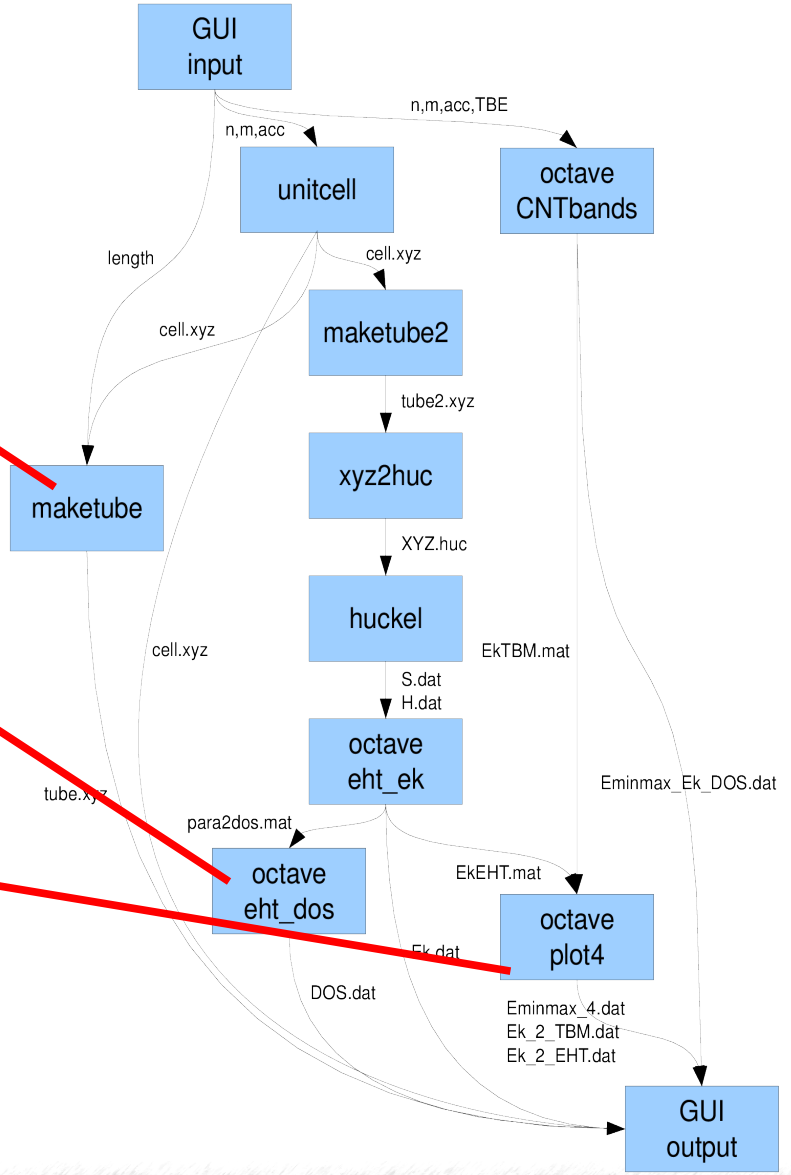


… or write your own workflow









CNTBands

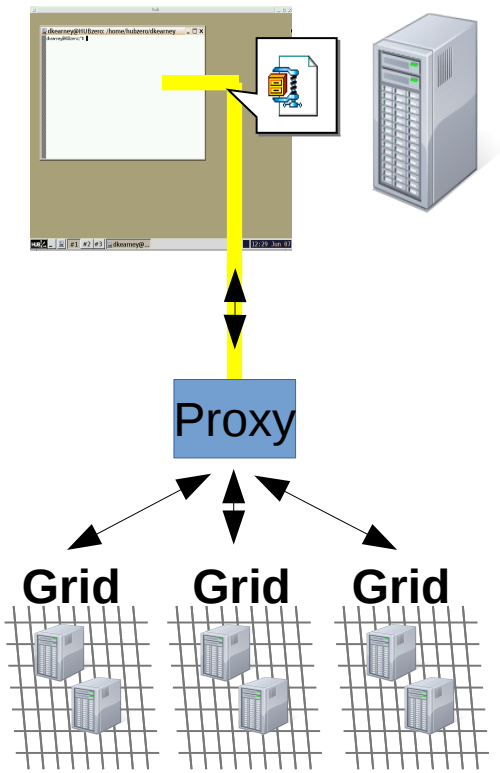
Science Domain: Nanoelectronics

Scientists: Lundstrom et al. (Purdue)

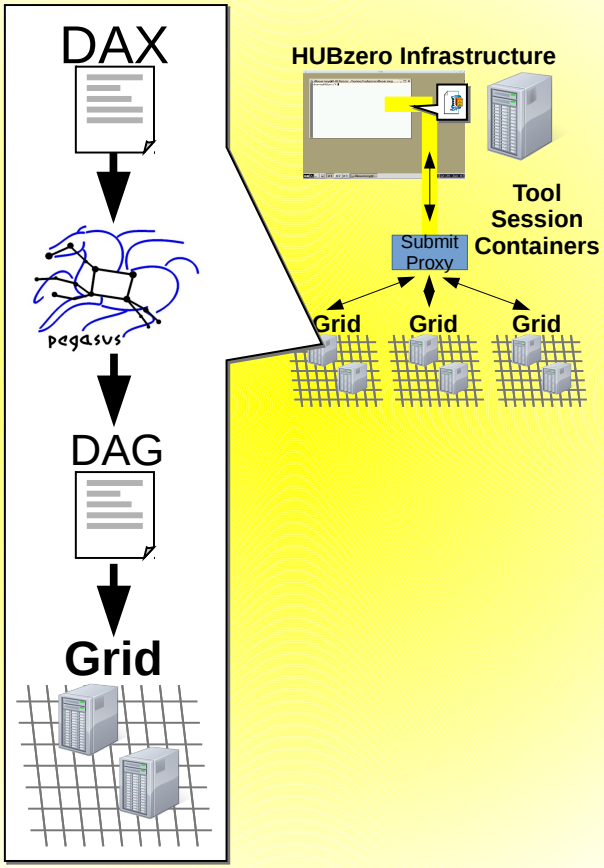
https://nanohub.org/resources/cntbands-ext

Productivity in the Workspace

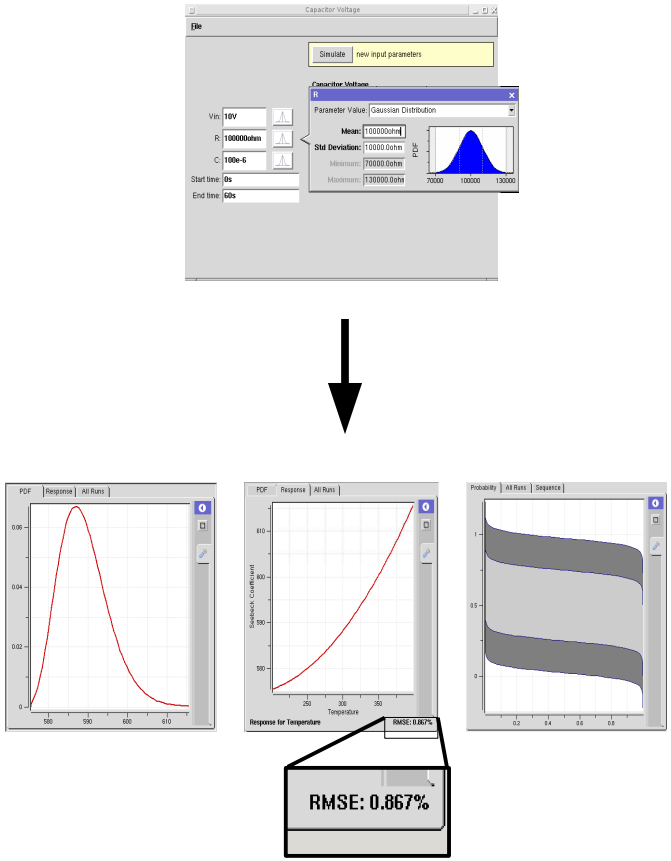
Submit



Pegasus Workflows

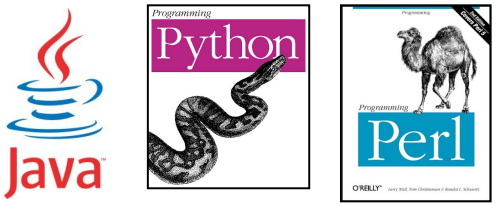


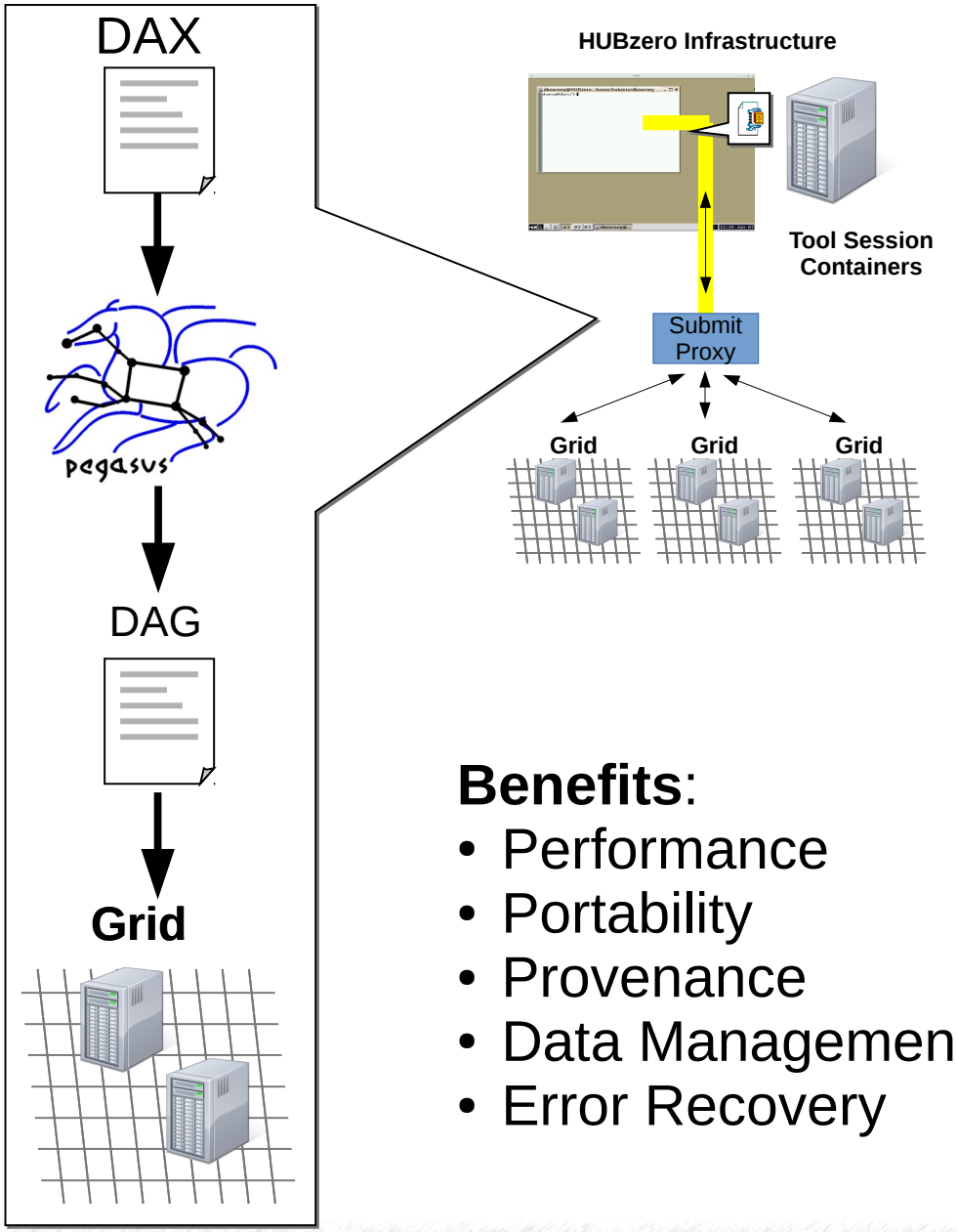
Uncertainty Quantification



Pegasus Workflow Management

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



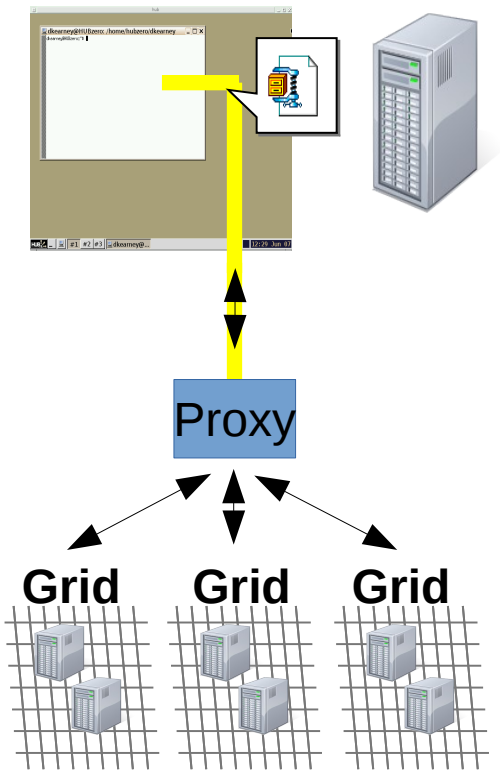


Benefits:

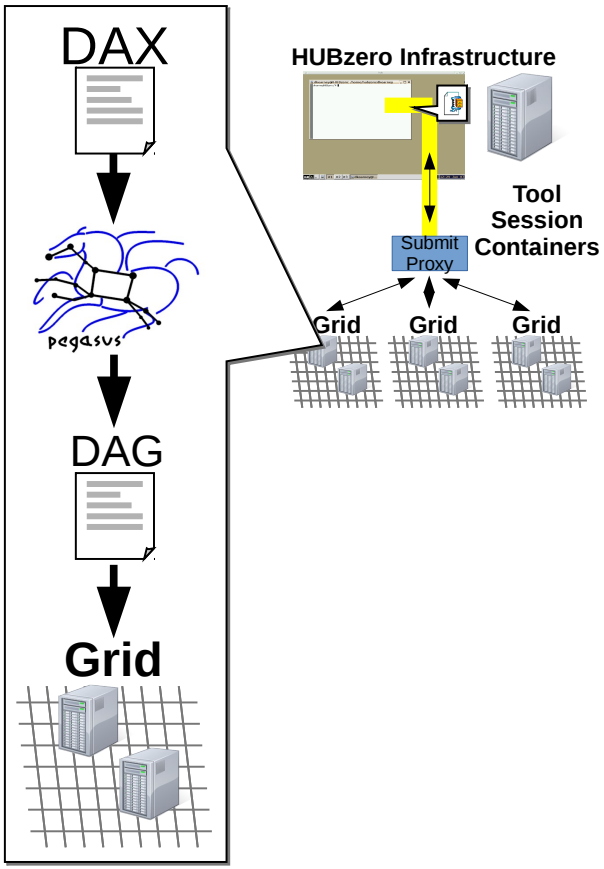
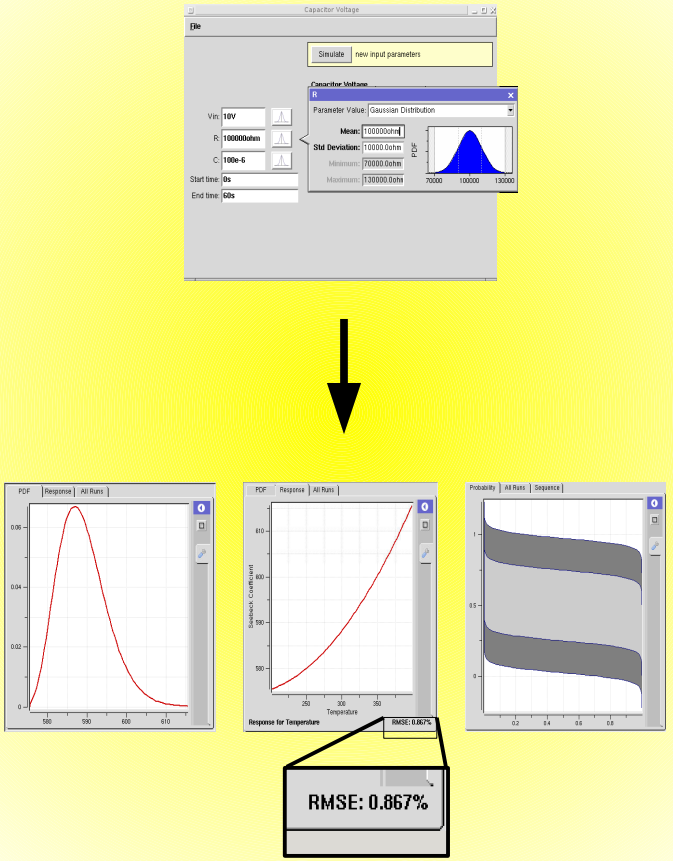
- Performance
- Portability
- Provenance
- Data Management
- Error Recovery

Productivity in the Workspace

Submit



Pegasus Workflows



Uncertainty Quantification