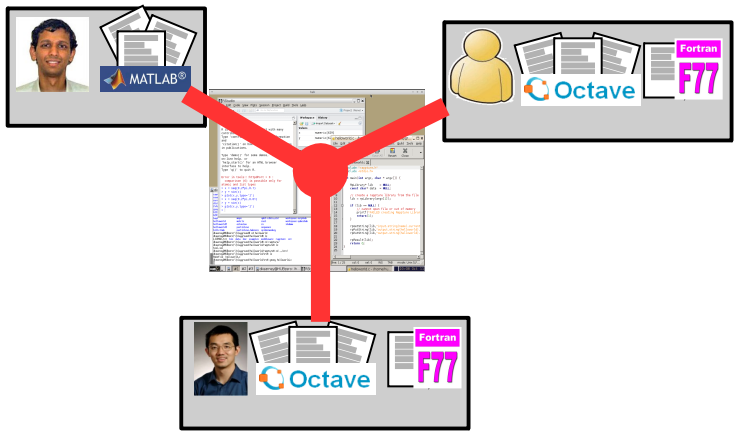
HUBzero Platform Features

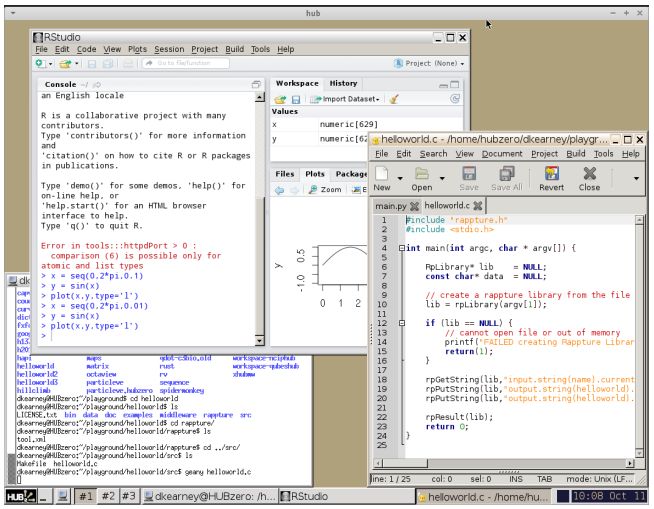
Demo of Capabilities for the TRADES Program
Oct. 12, 2016

Derrick Kearney
hubzero.org

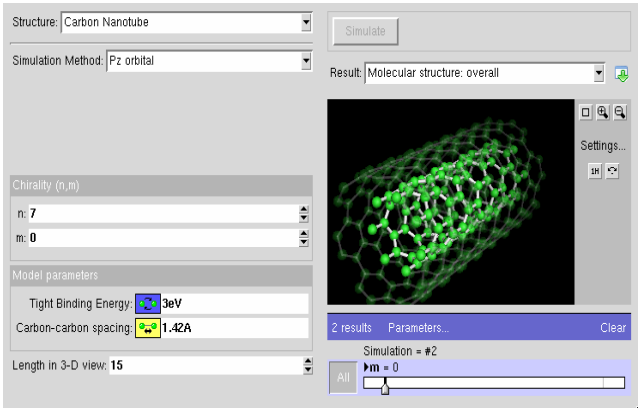
The HUBzero Platform



Perform
Research

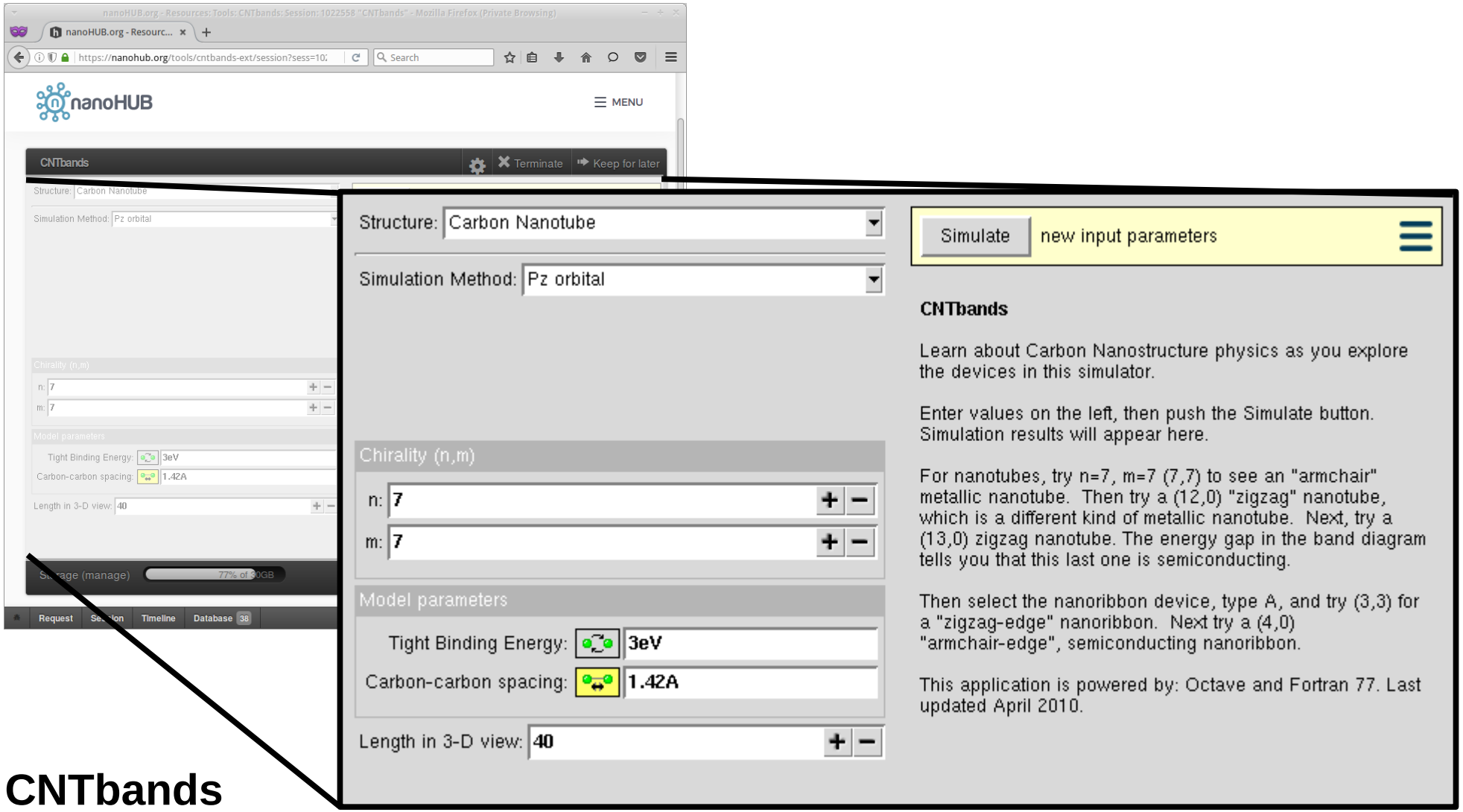


Collaborate
With Others



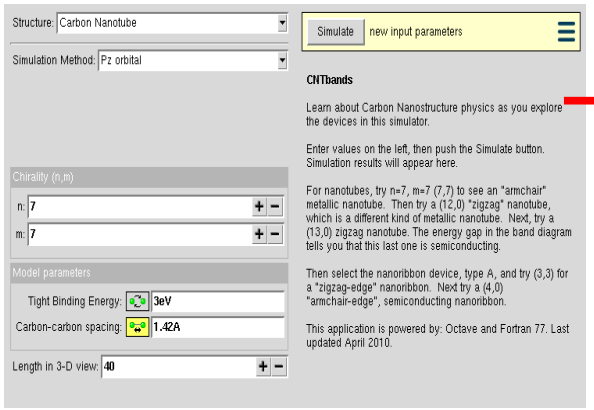
Secure, Scalable,
Sharable
Dev Environments

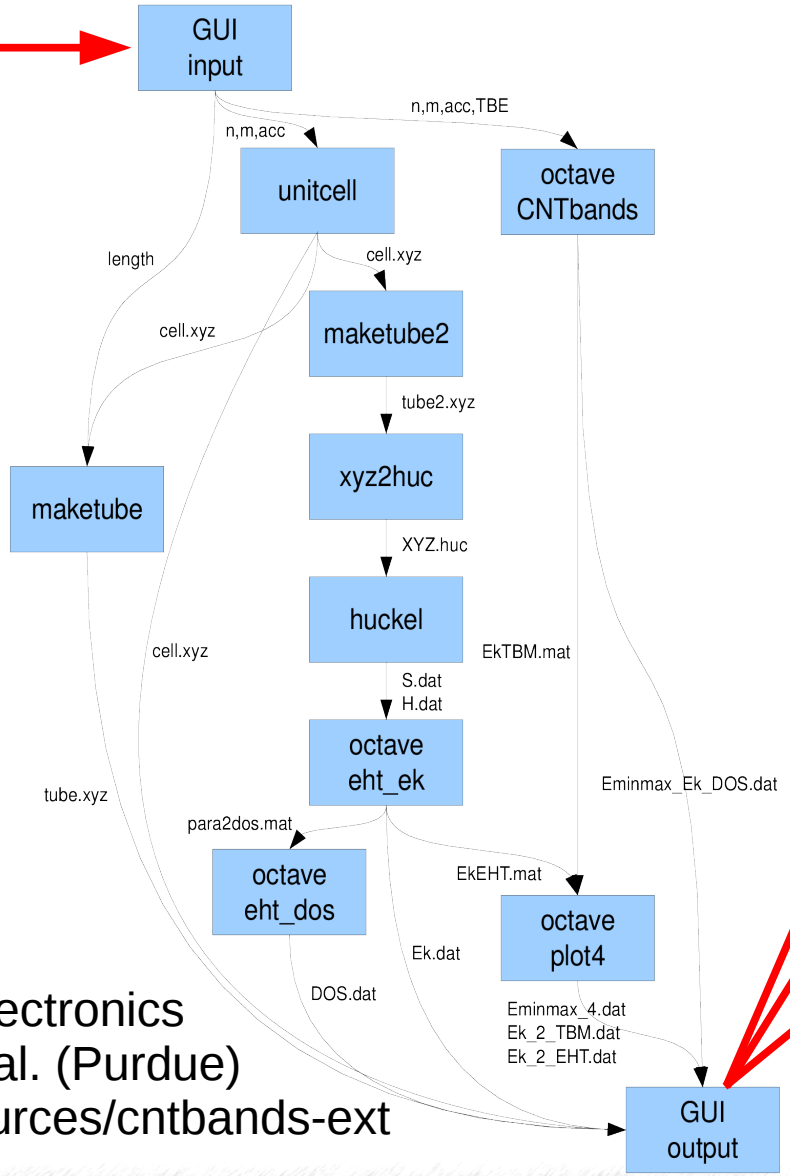
CNTbands

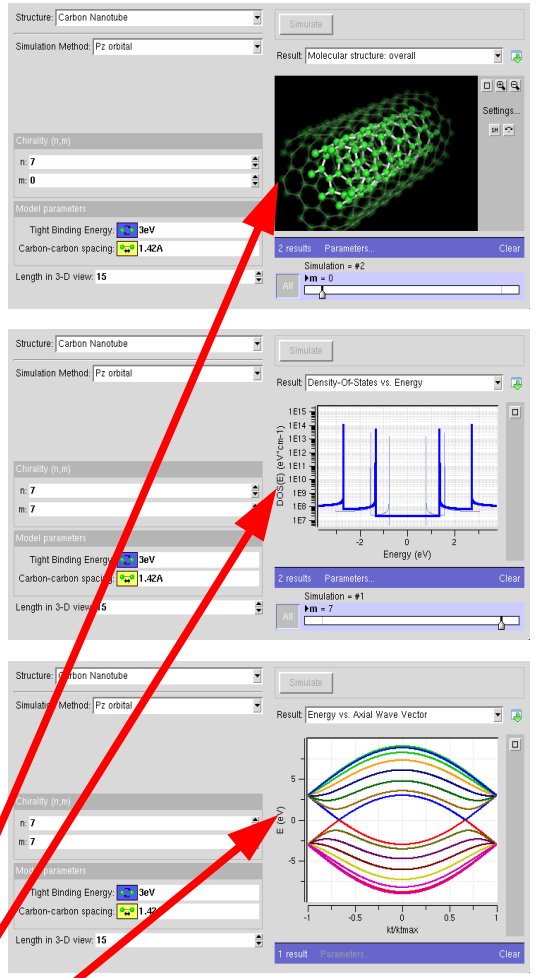


CNTbands
Science Domain: Nanoelectronics
Scientists: Lundstrom et al. (Purdue)
https://nanohub.org/resources/cntbands-ext

Many Pieces by Different Developers







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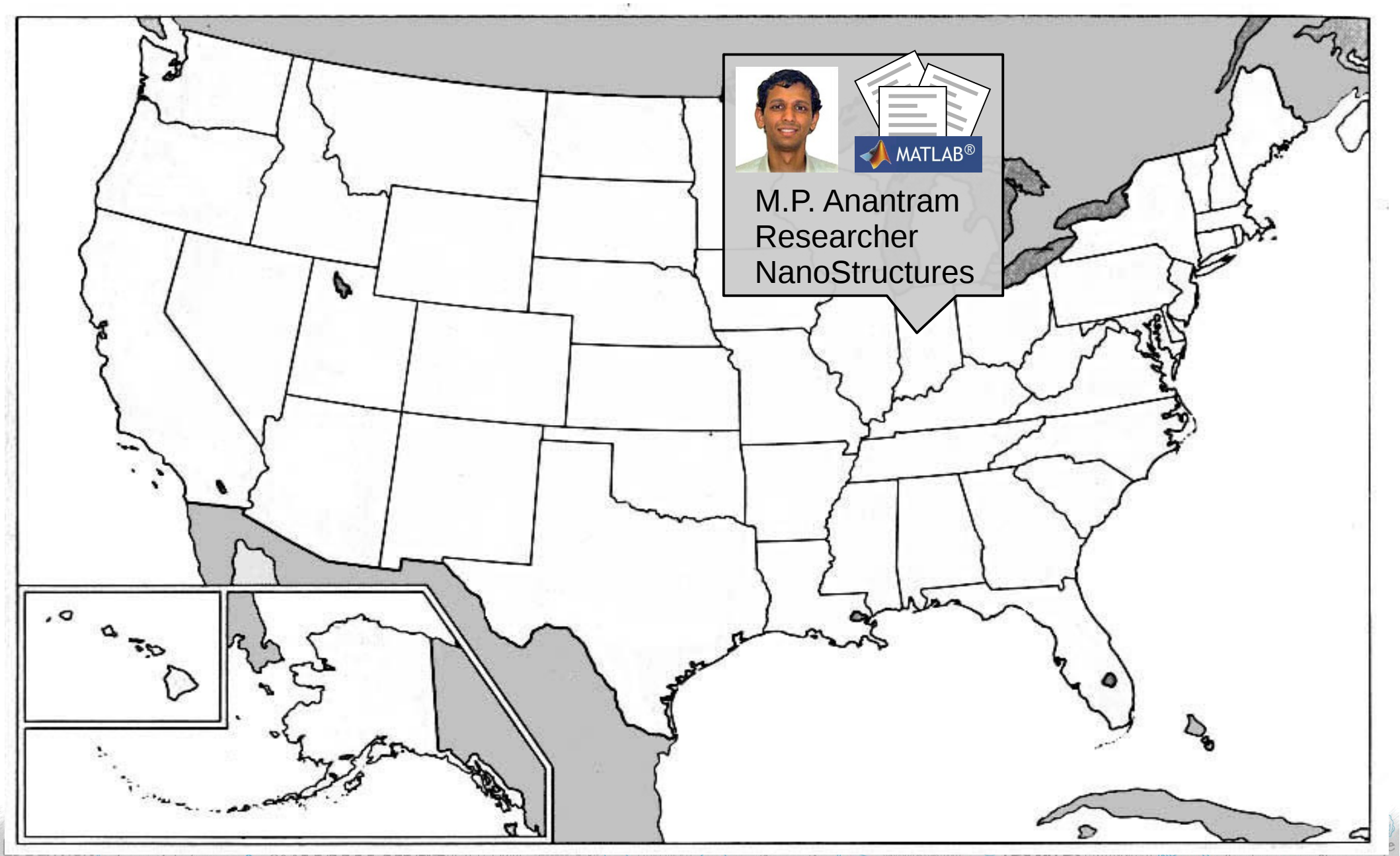
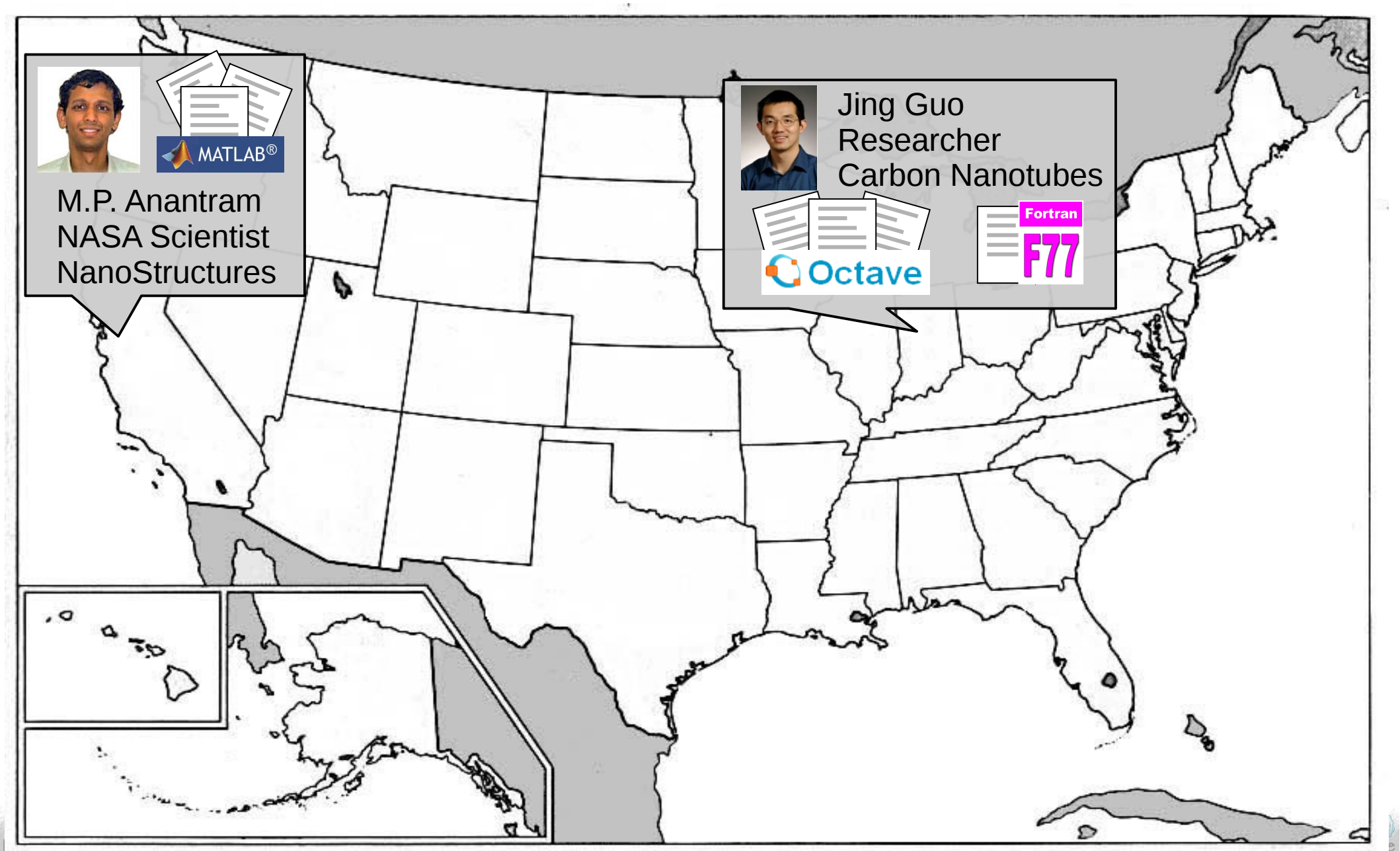
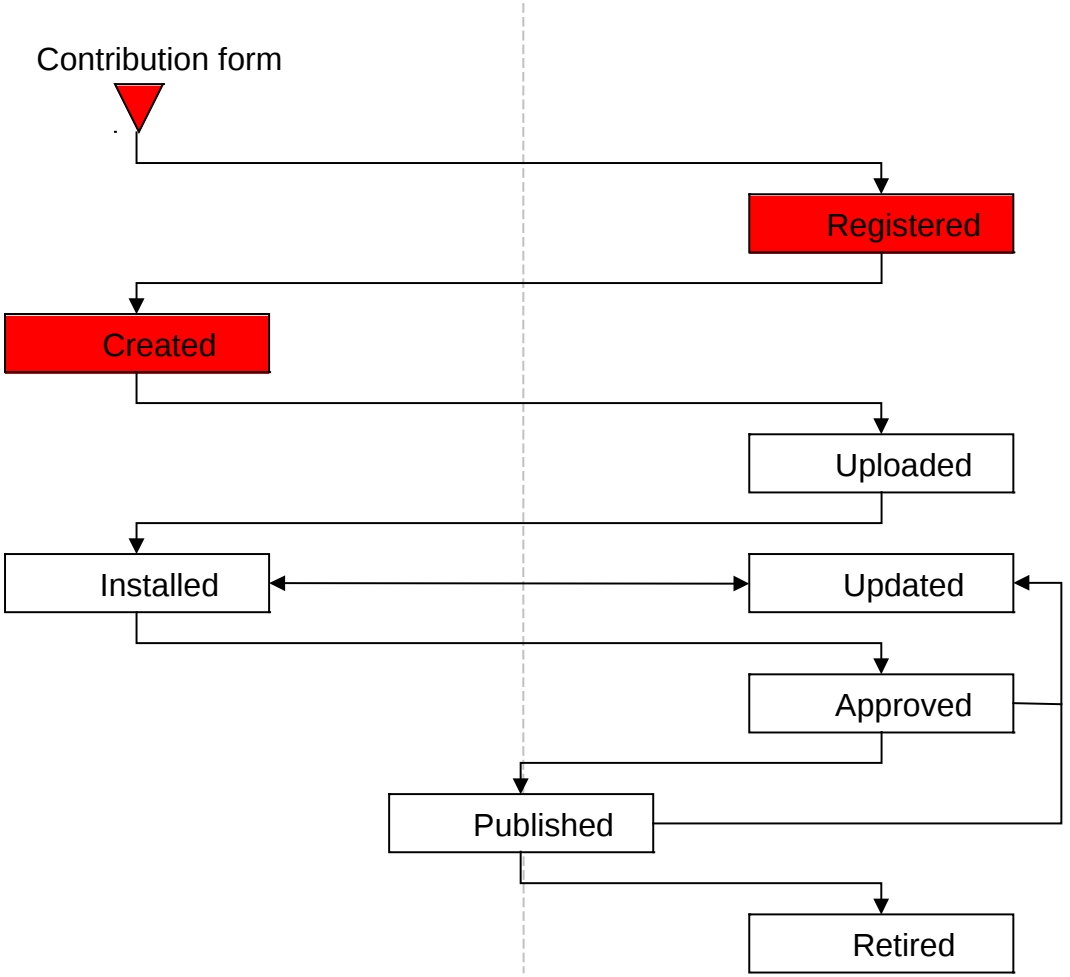
1990s – Initial Algorithms



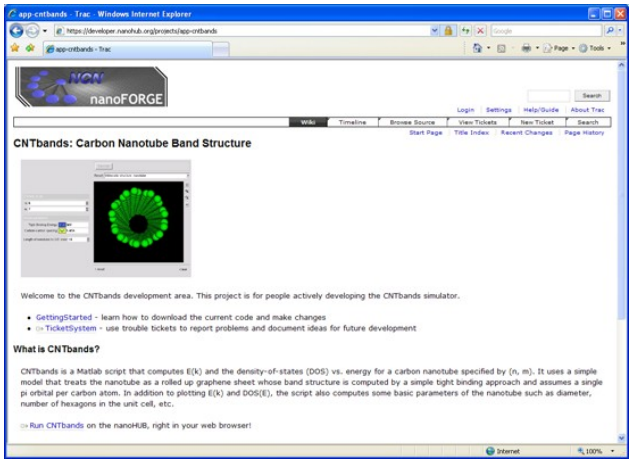
2002 – Idea for a Tool



Tool Registered



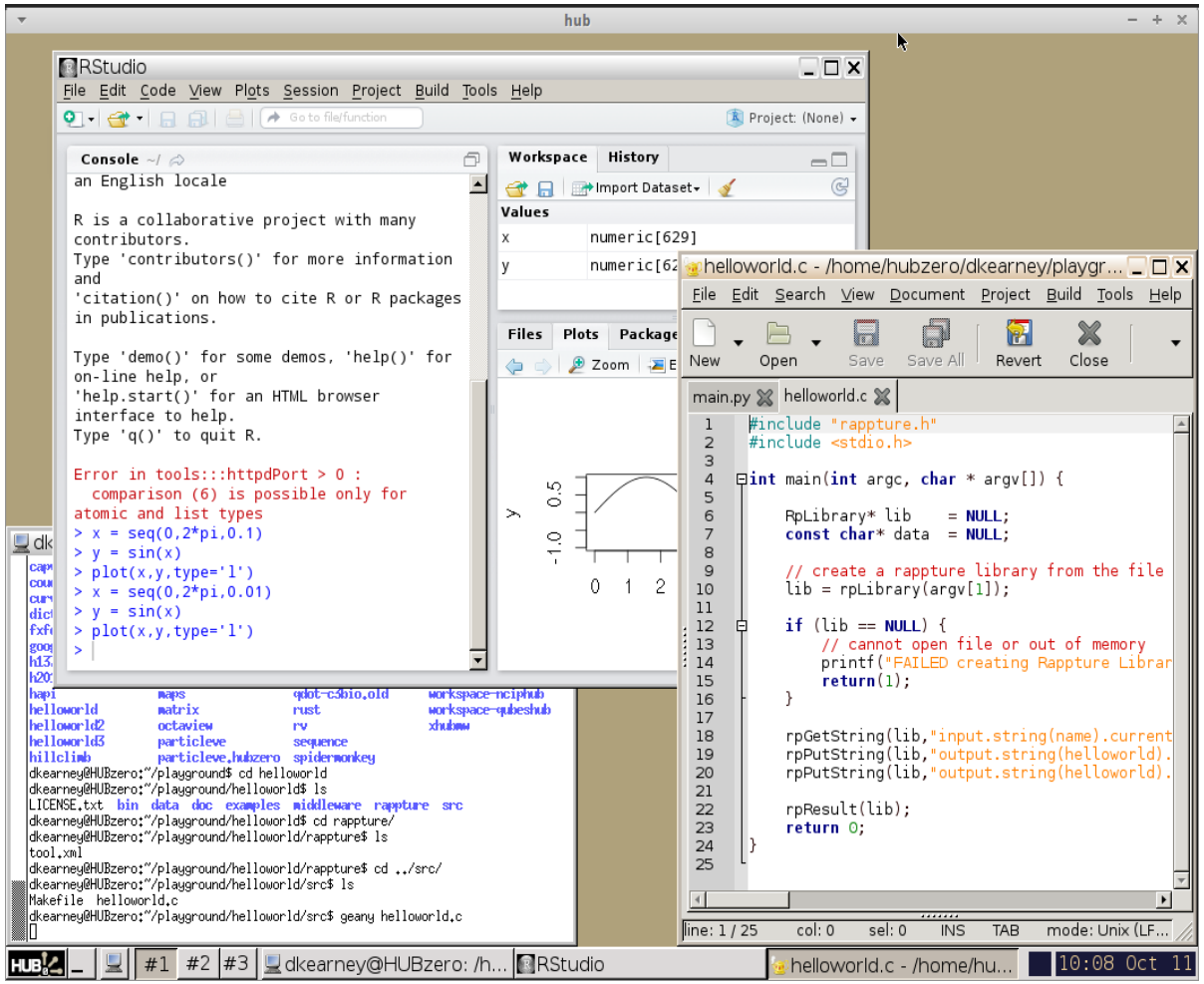
https://yourhub.org/tools



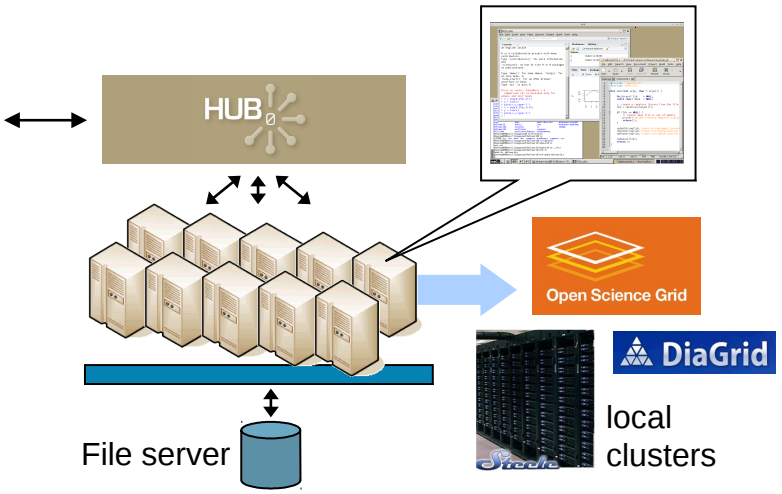
Provides:

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

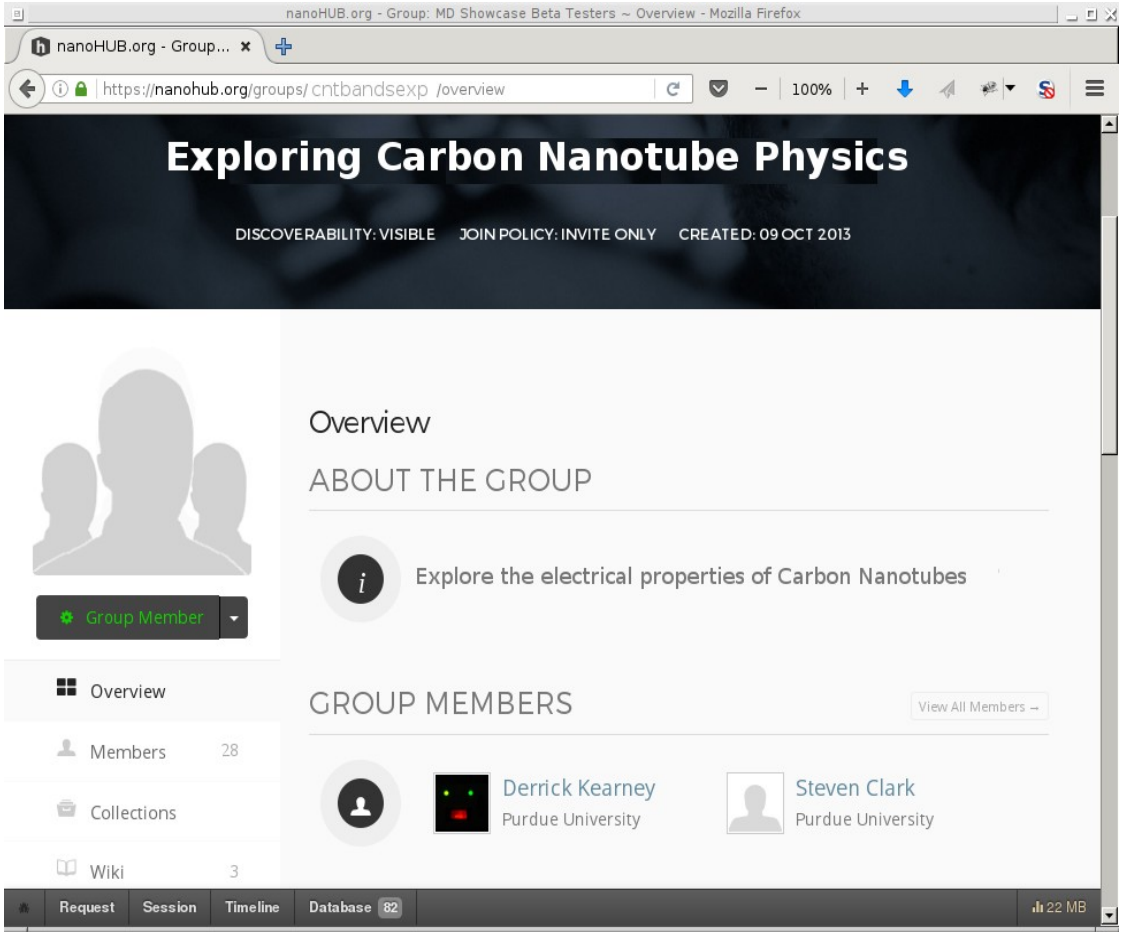
What is a Workspace?



- 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

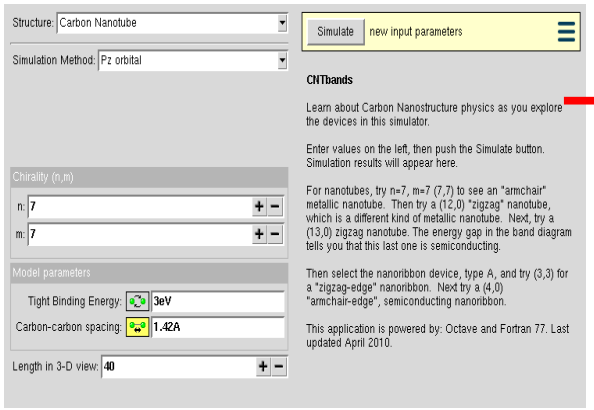


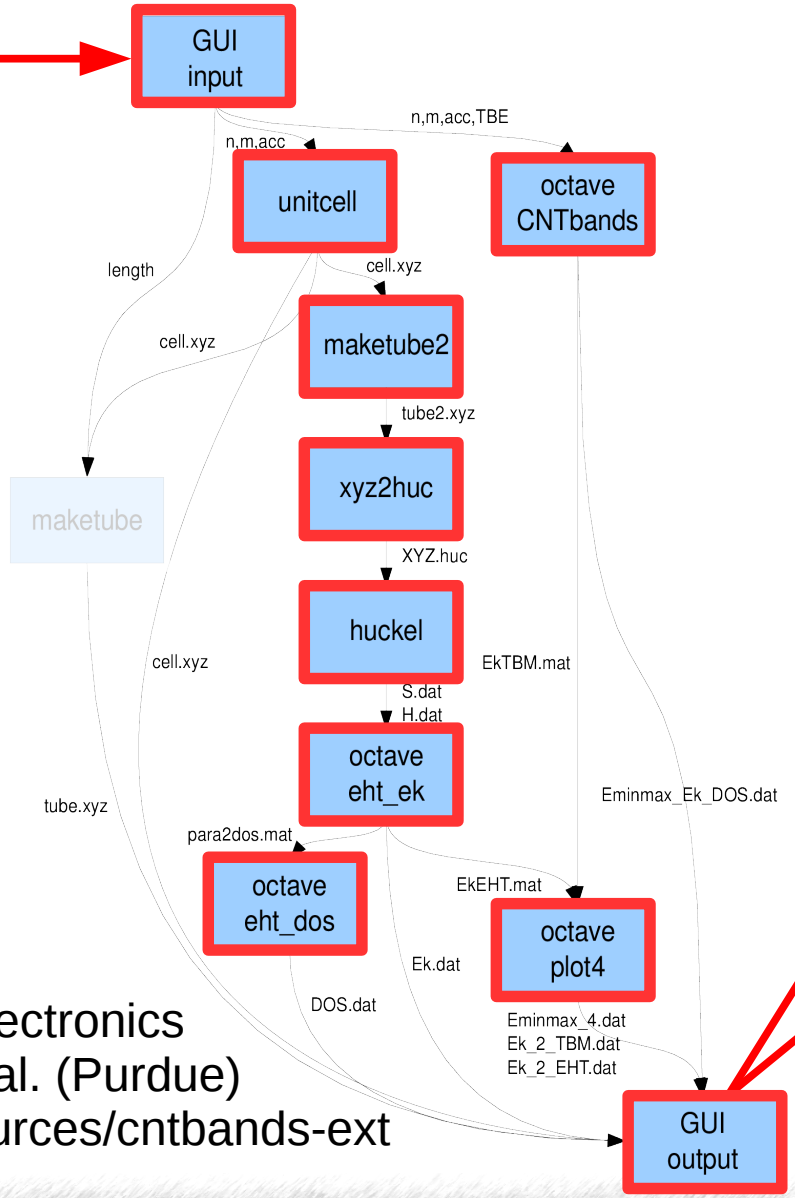
Collaborate within a Group

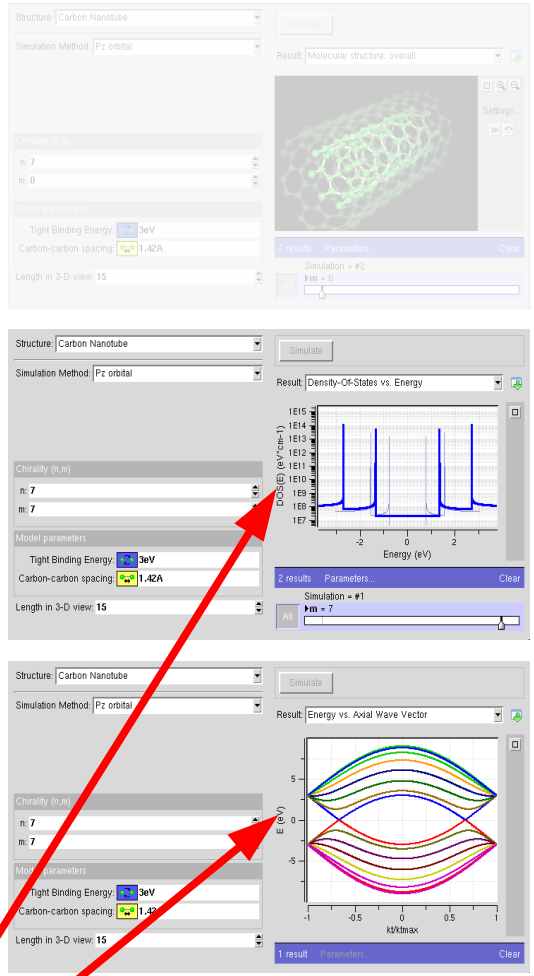


- Build a community around your research
- Share links, papers, and data
- Forums encourage discussion
- Create how-tos with wiki pages
- Keep everyone informed with Announcements

CNTbands







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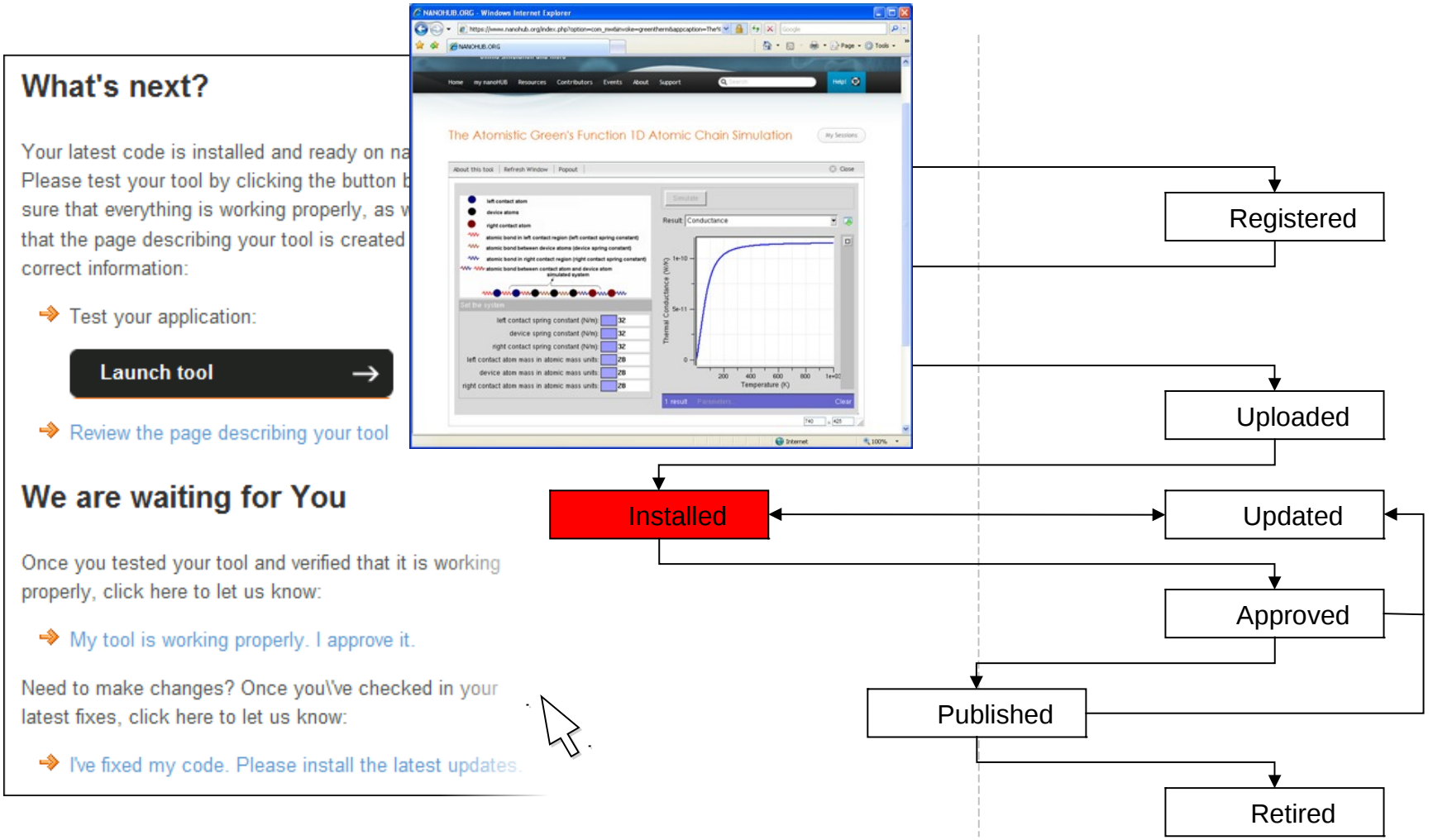
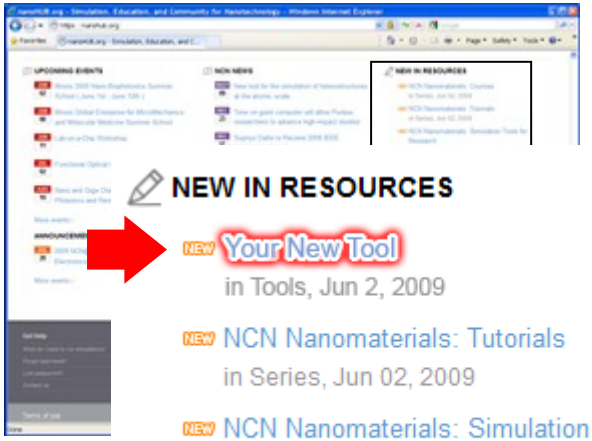
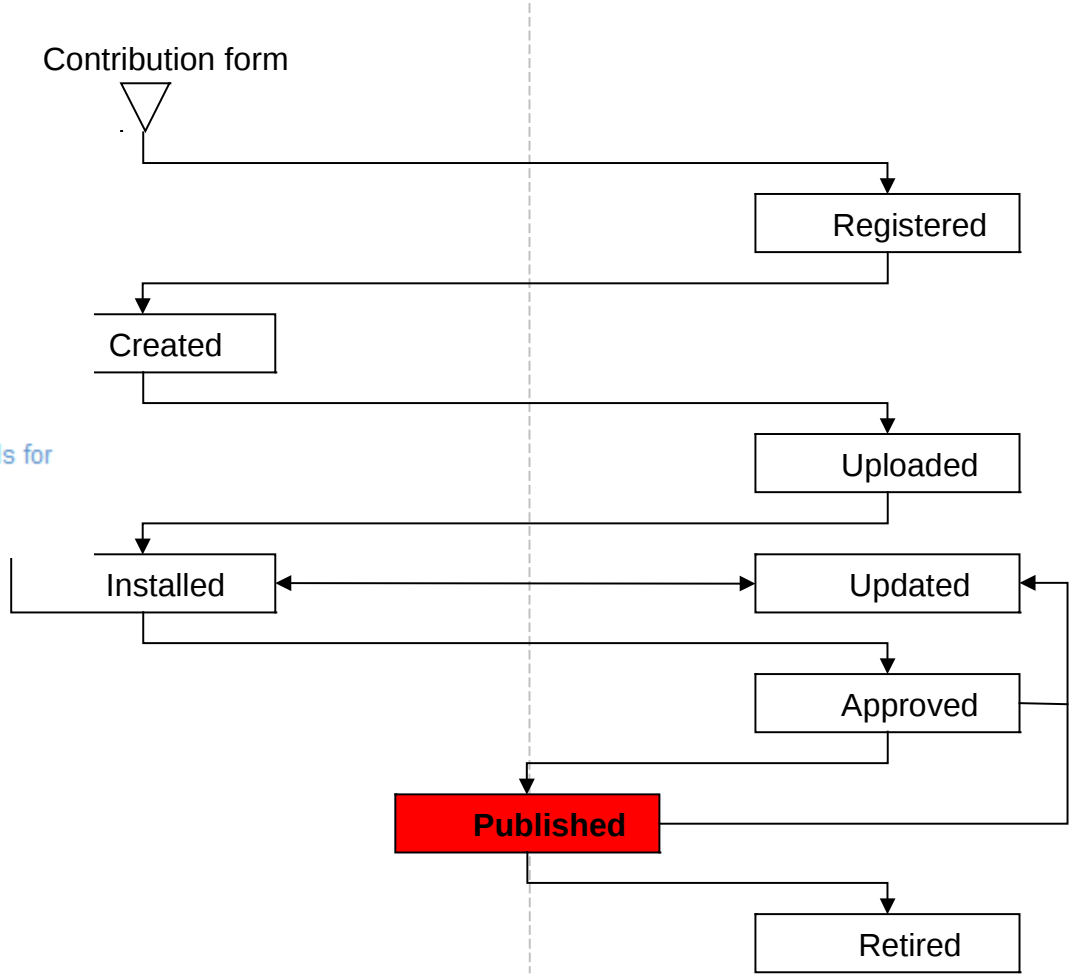
Installing Applications



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:

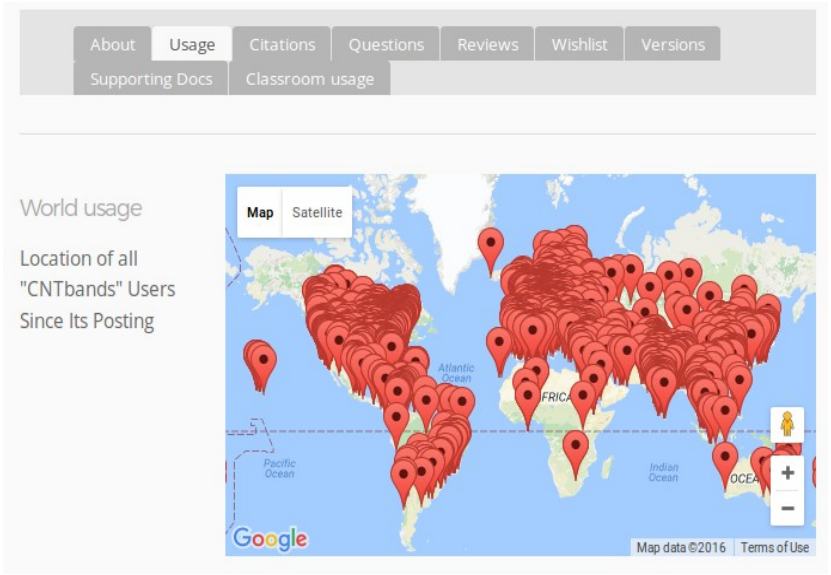
About | Usage | Citations | Questions | Reviews | Wishlist | Versions | Supporting Docs | Classroom usage

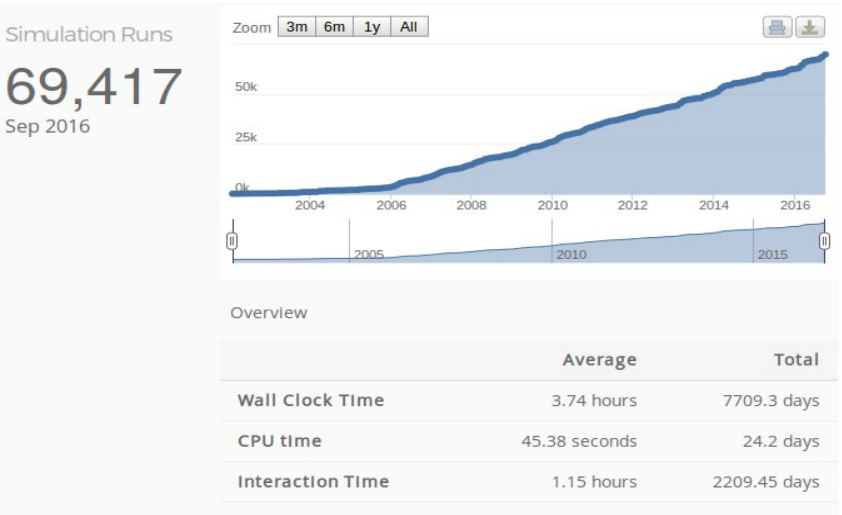
See also

Part of: NCN Nanoelectronics: Simulation Tools for Education

Part of: NCN Nanoelectronics:

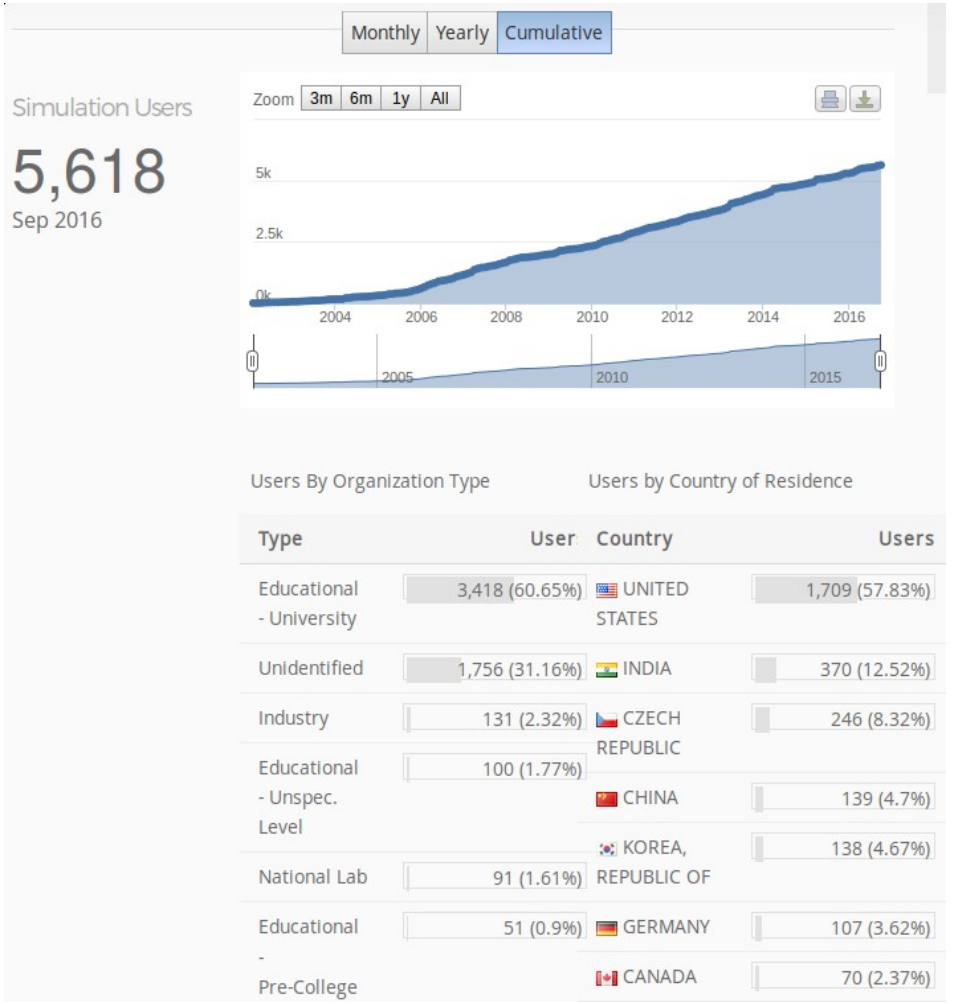
Track Usage Metrics





Overview

	Average	Total
Wall Clock Time	3.74 hours	7709.3 days
CPU time	45.38 seconds	24.2 days
Interaction Time	1.15 hours	2209.45 days



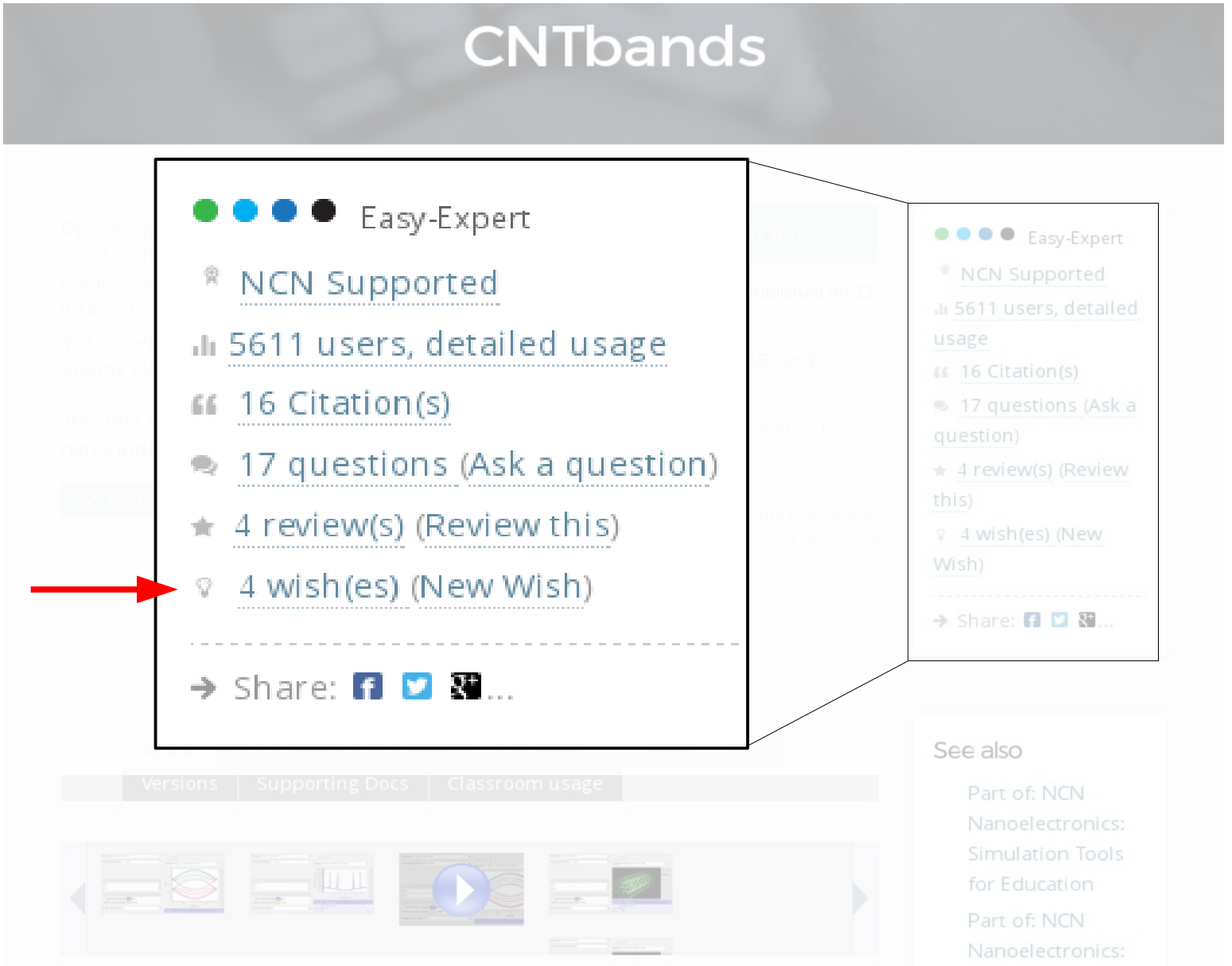
Users By Organization Type

Type	User
Educational - University	3,418 (60.65%)
Unidentified	1,756 (31.16%)
Industry	131 (2.32%)
Educational - Unspec. Level	100 (1.77%)
National Lab	91 (1.61%)
Educational - Pre-College	51 (0.9%)

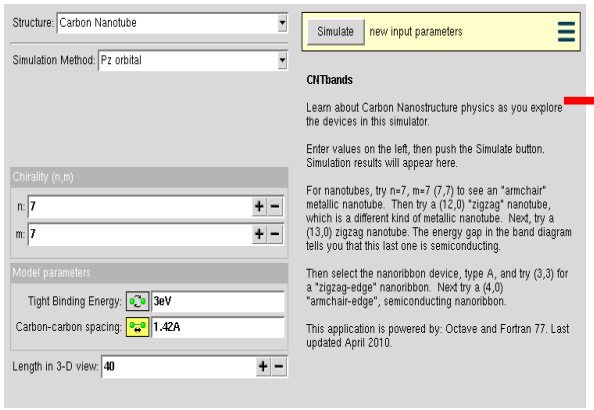
Users by Country of Residence

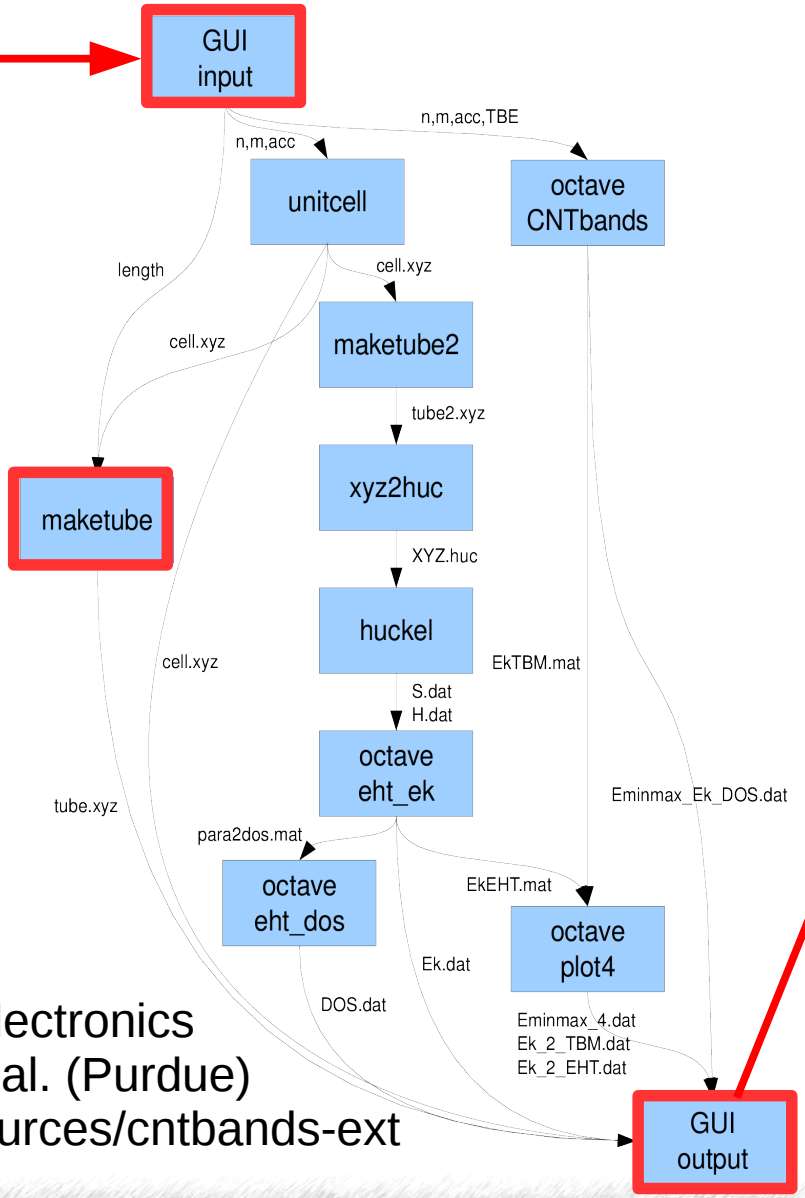
Country	Users
UNITED STATES	1,709 (57.83%)
INDIA	370 (12.52%)
CZECH REPUBLIC	246 (8.32%)
CHINA	139 (4.7%)
KOREA, REPUBLIC OF	138 (4.67%)
GERMANY	107 (3.62%)
CANADA	70 (2.37%)

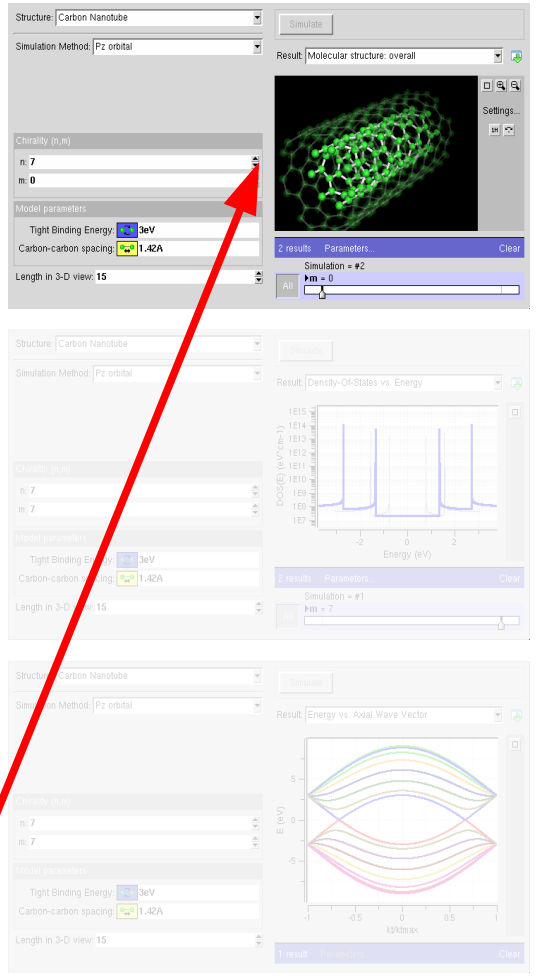
Communicate With Users



Adding New Features







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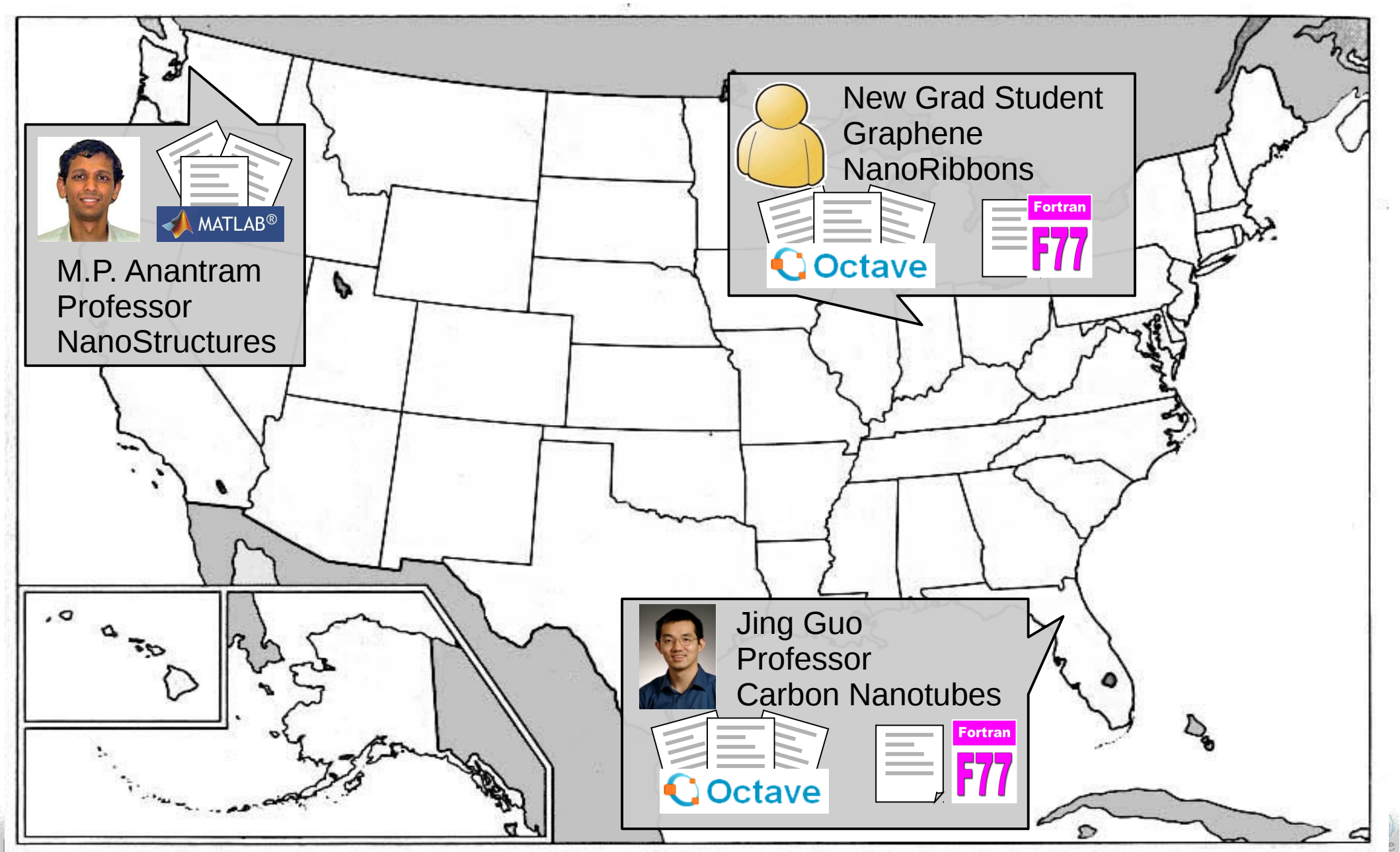
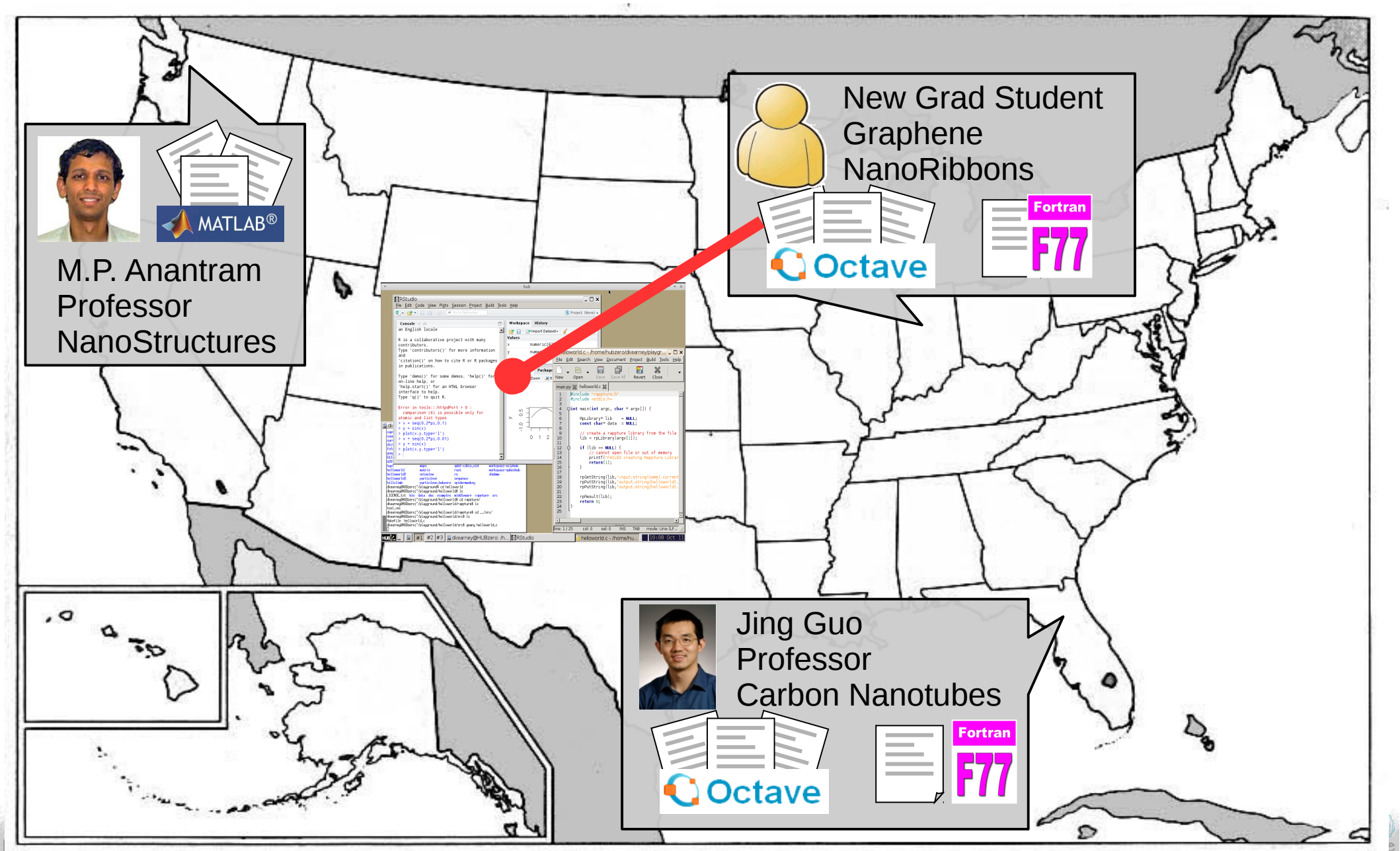
2010 – Introducing New Researchers



Collaborate in the Workspace



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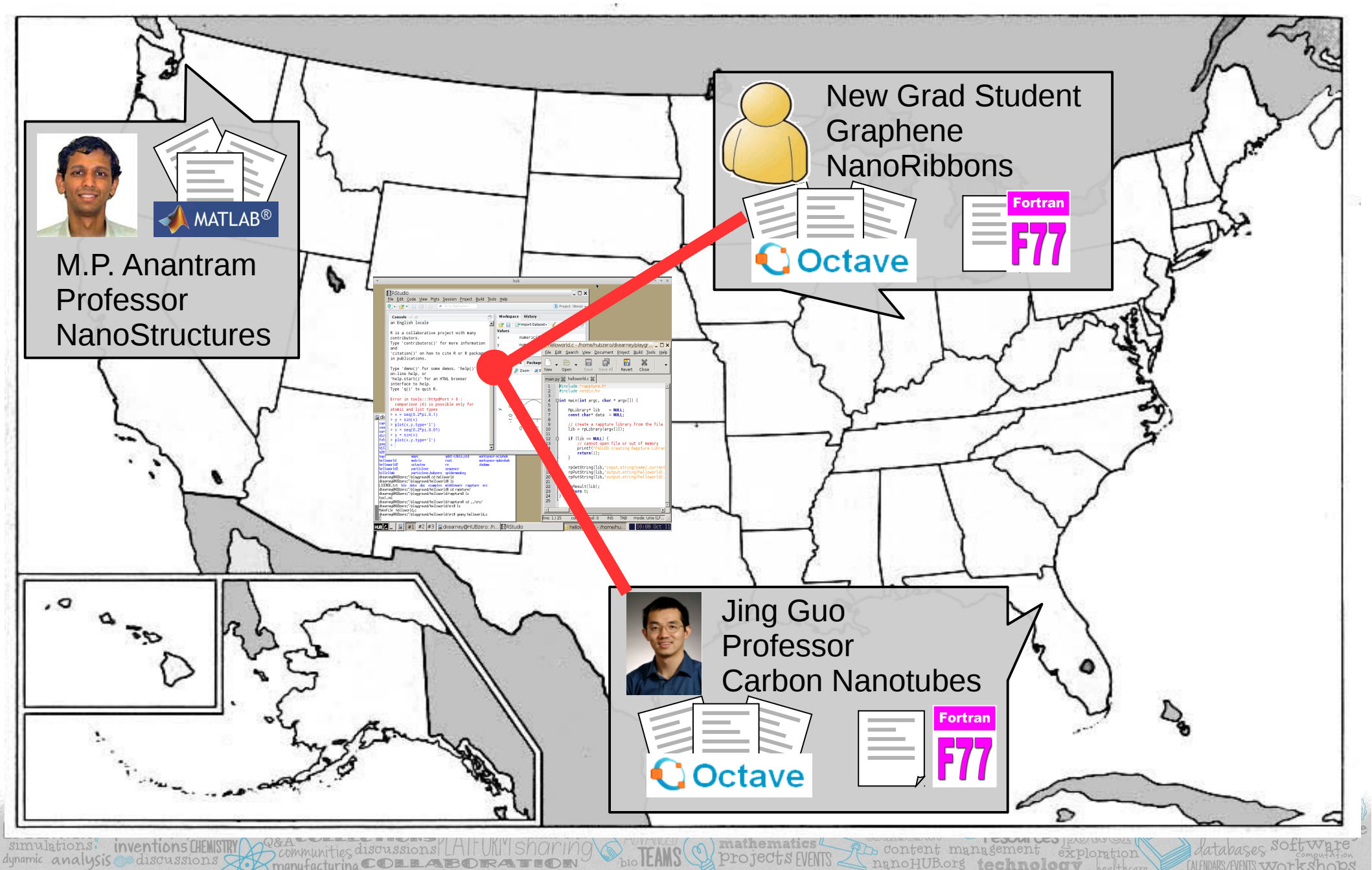
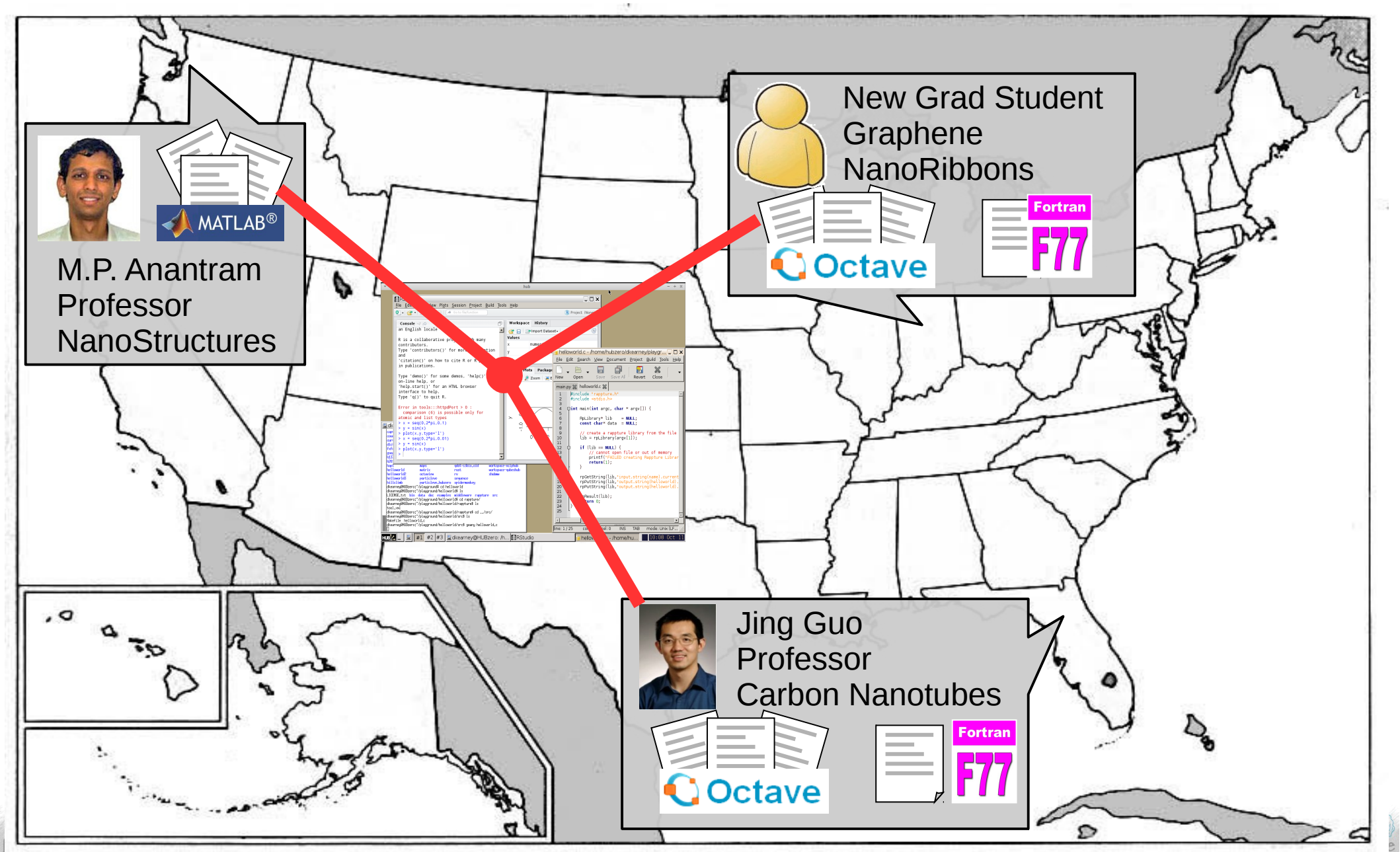
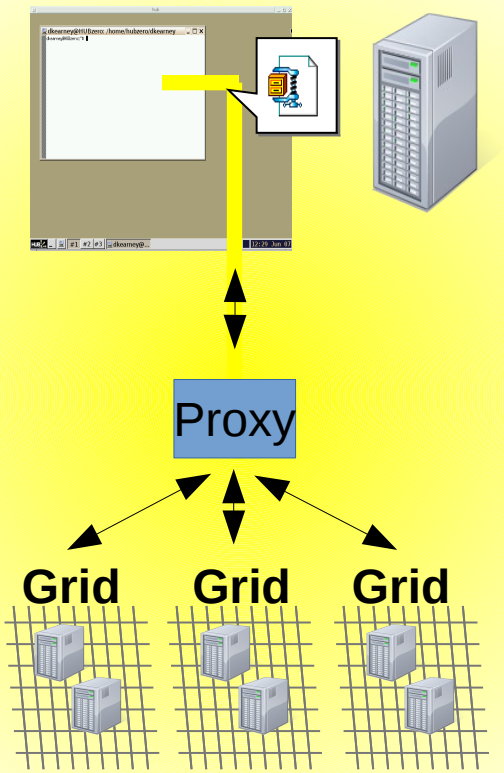


Collaborate in the Workspace

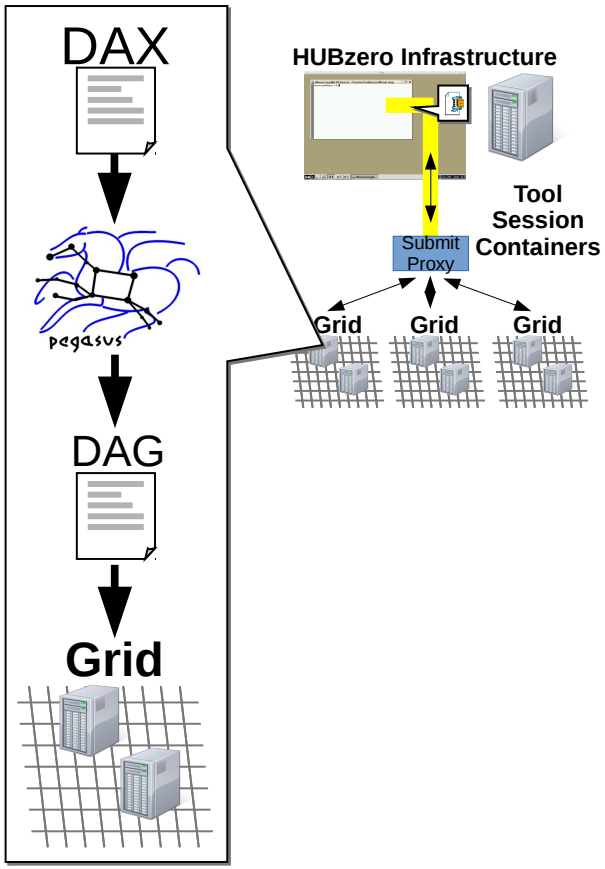


Productivity in the Workspace

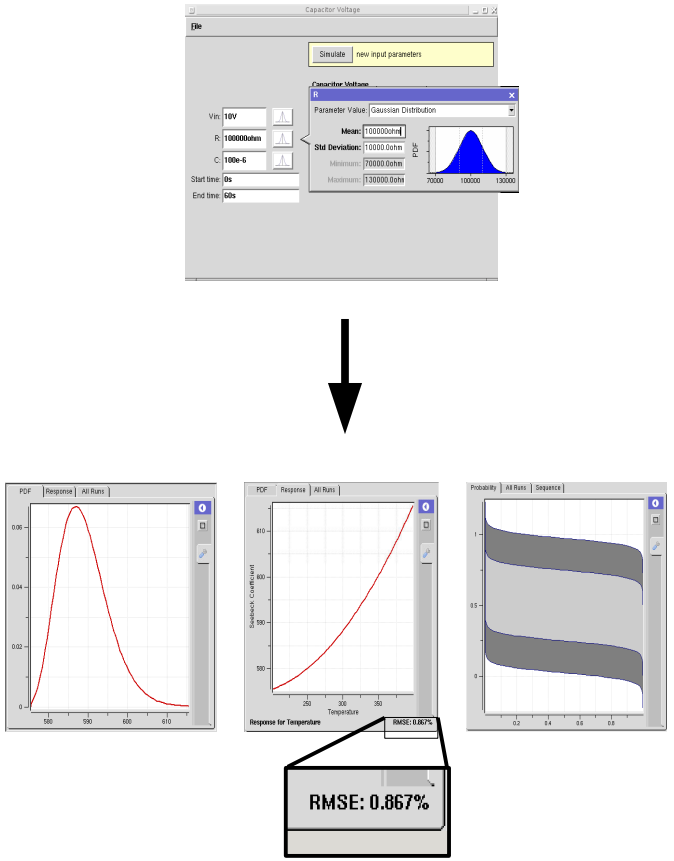
Submit



Pegasus Workflows



Uncertainty Quantification

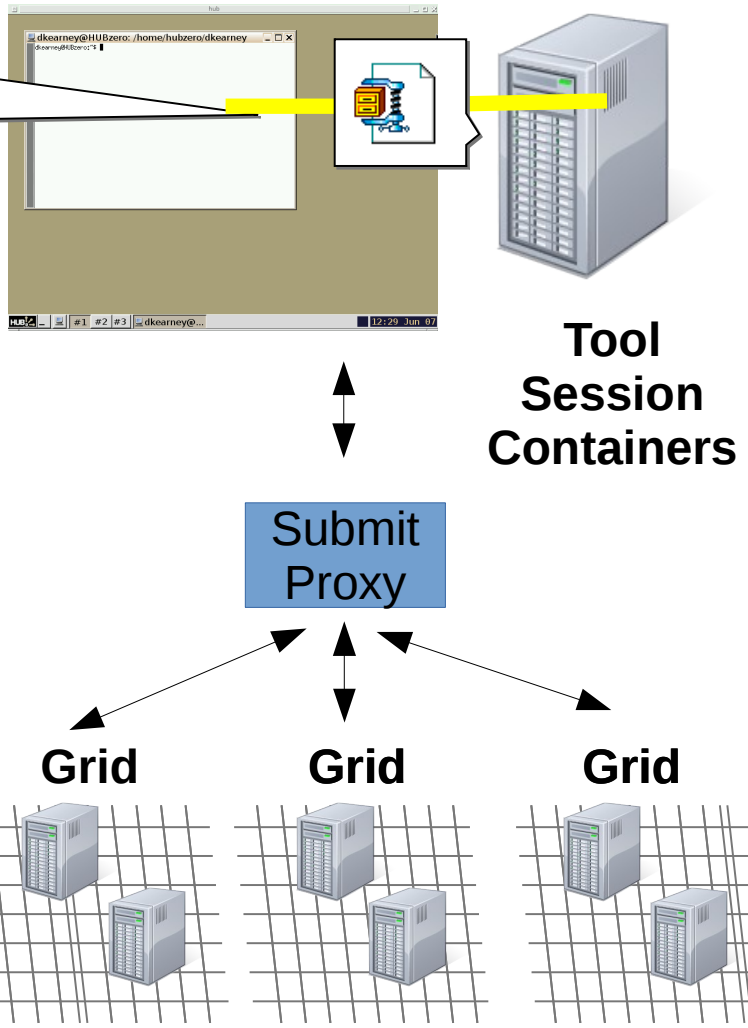


Run tools locally in Workspace

User's Workspace Terminal

```
$ echo hi
hi
$
```

HUBzero Infrastructure

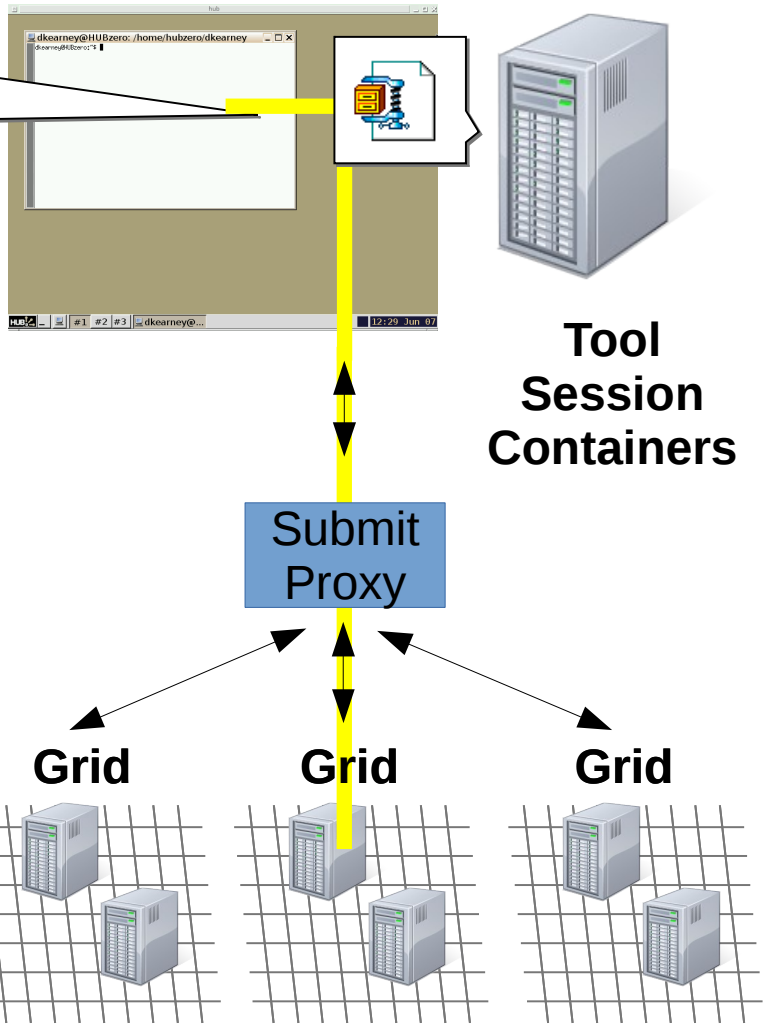


Submit Jobs to Grid

User's Workspace Terminal

$ submit echo hi

HUBzero Infrastructure

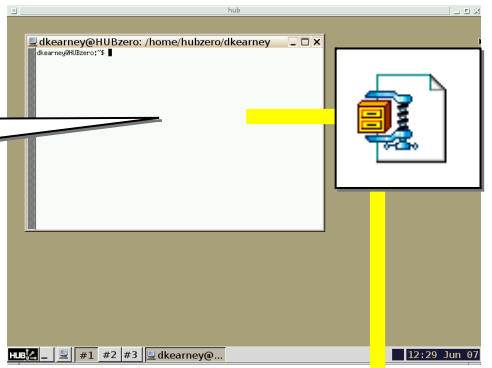


Let Submit create a workflow ...

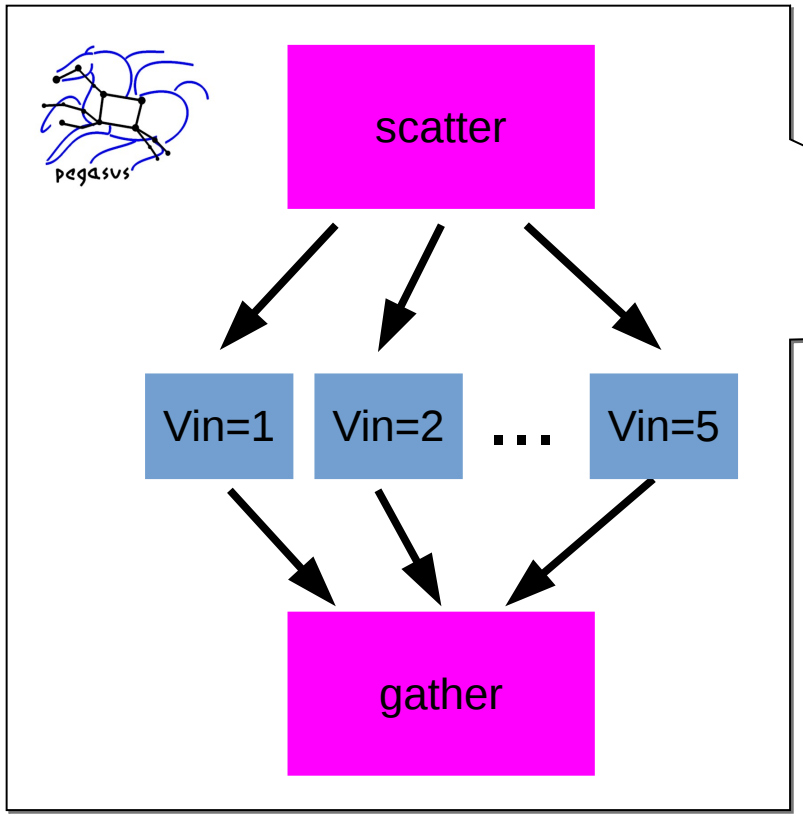
User's Workspace Terminal

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

HUBzero Infrastructure

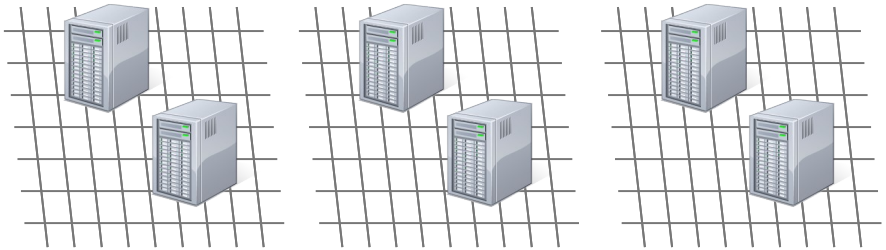


Tool Session Containers

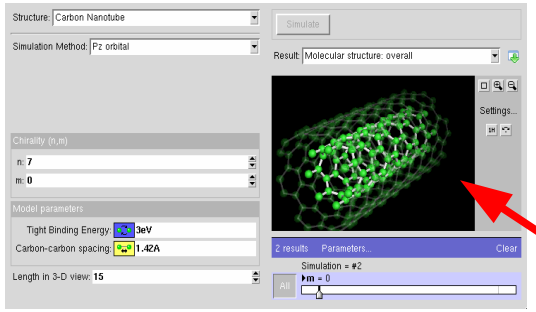


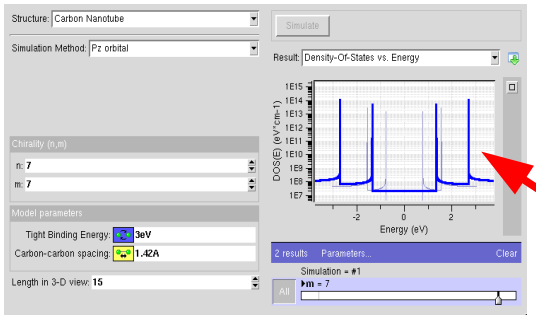
Submit Proxy

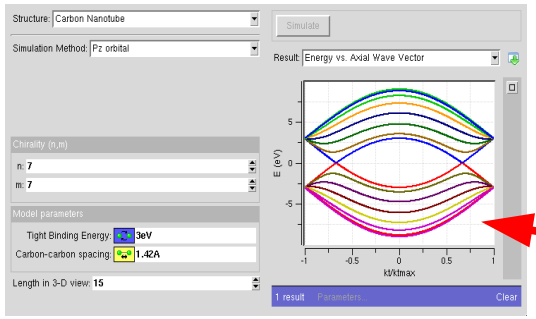
Grid **Grid** **Grid**

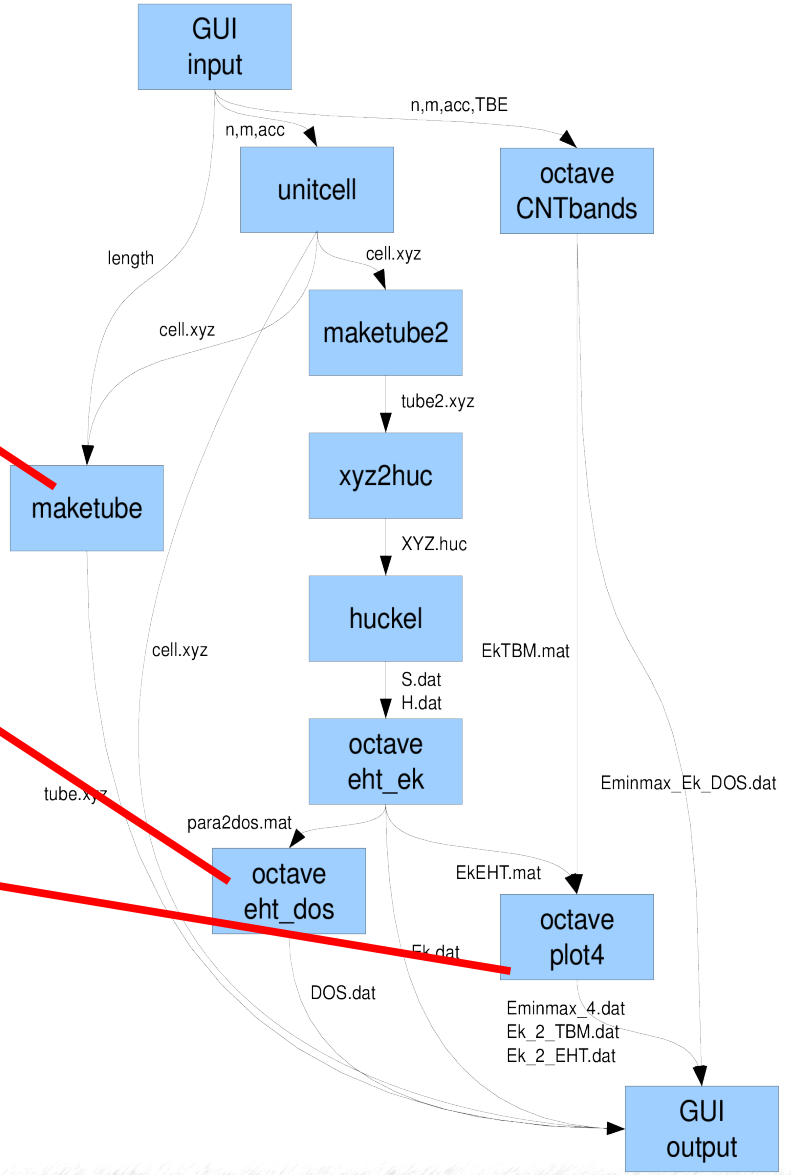


… or write your own workflow









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Productivity in the Workspace

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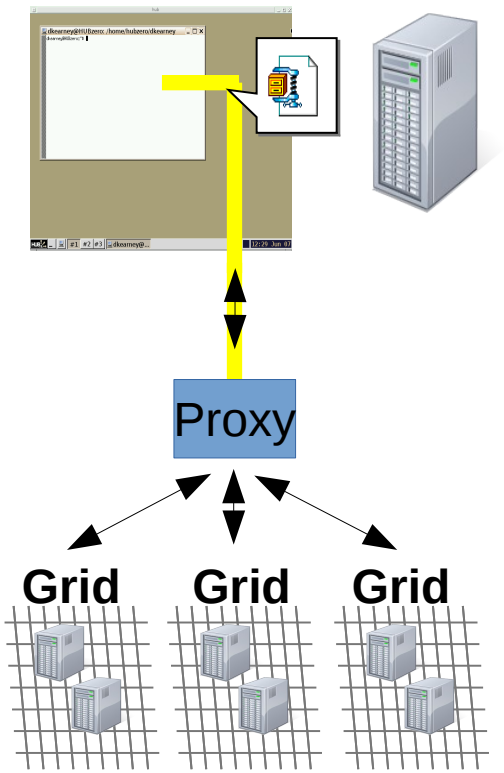
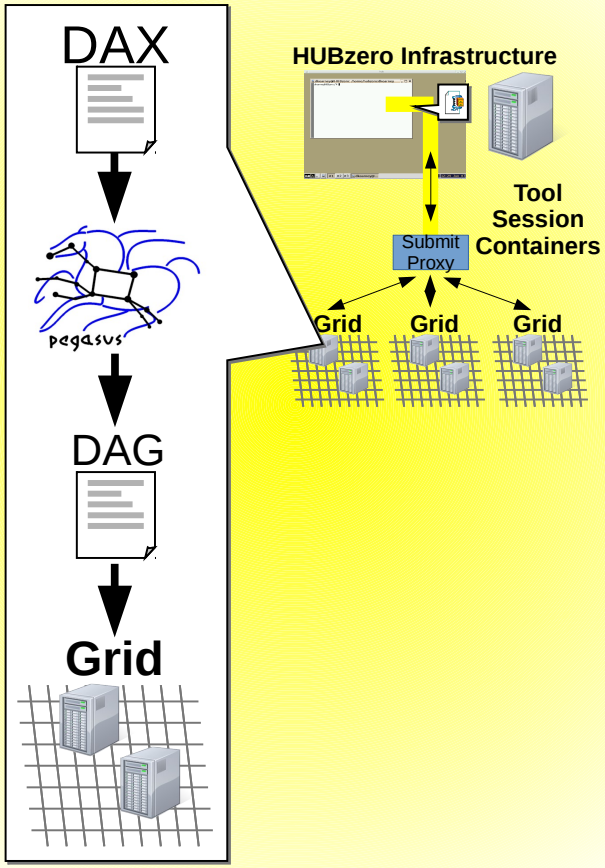
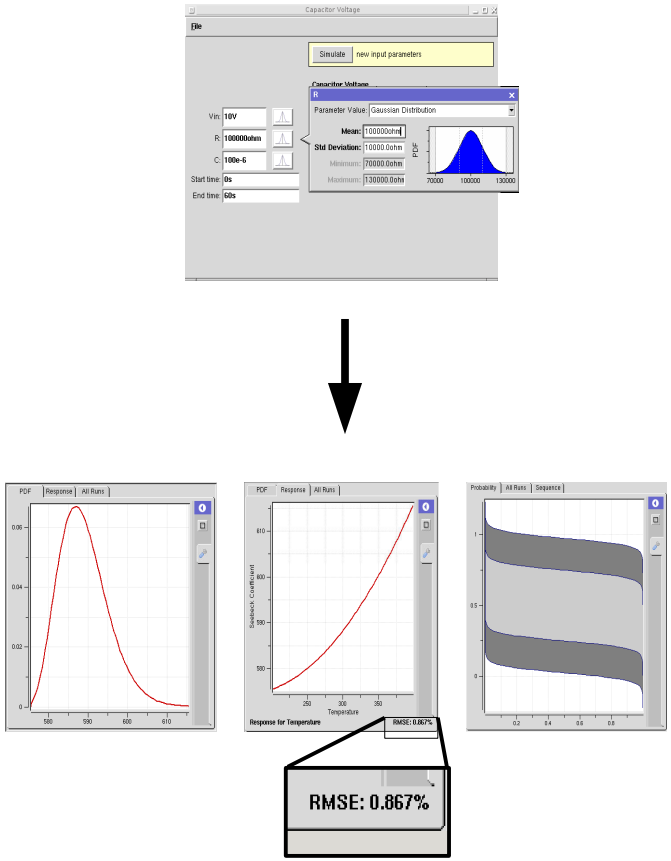


Pegasus Workflows

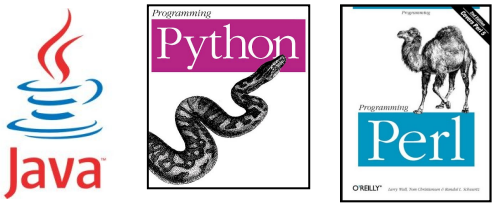


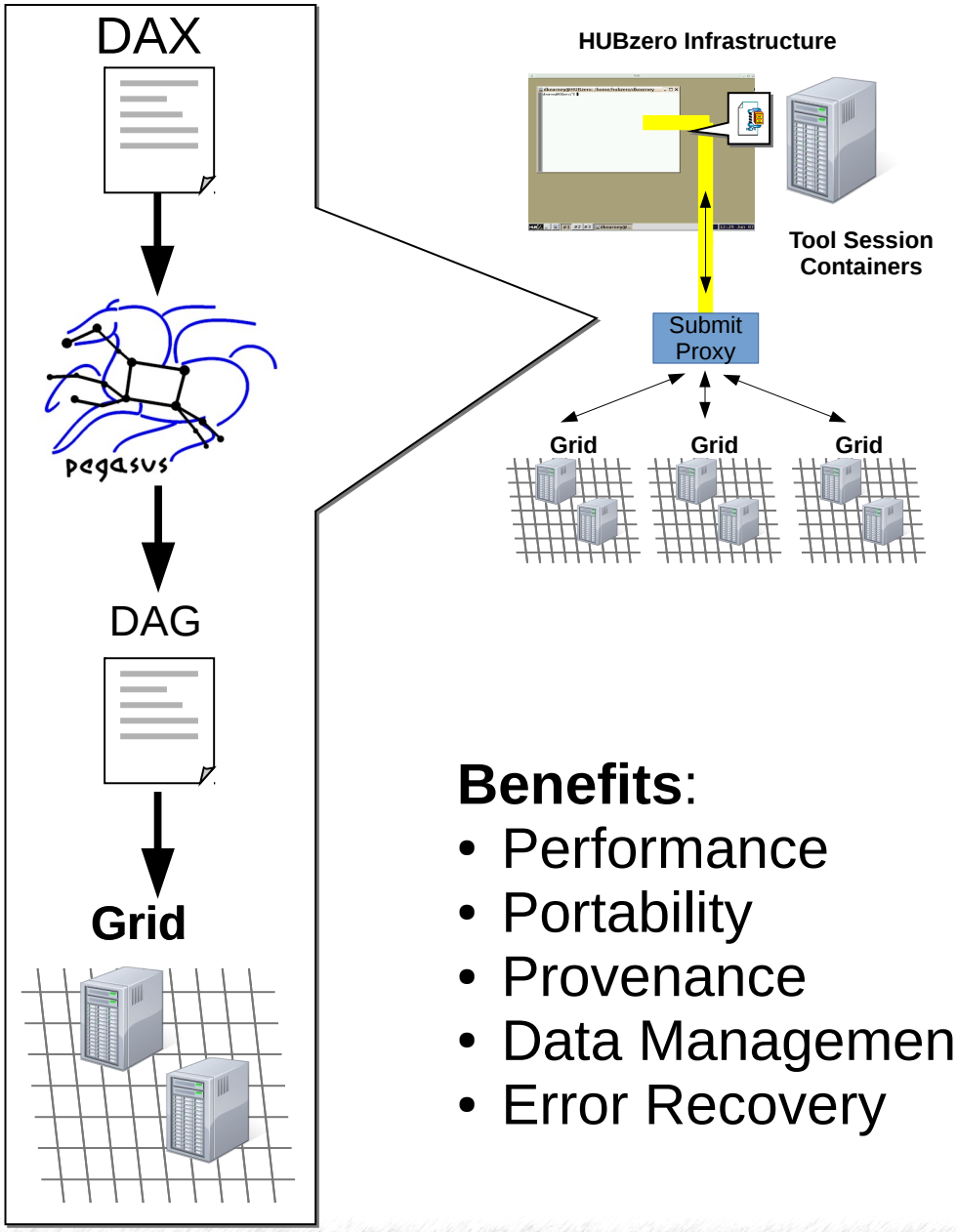
Uncertainty Quantification



Pegasus Workflow Management

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



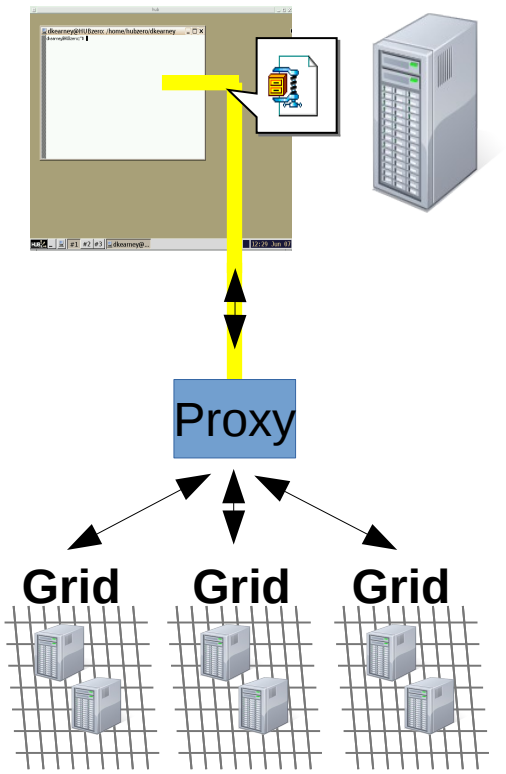


Benefits:

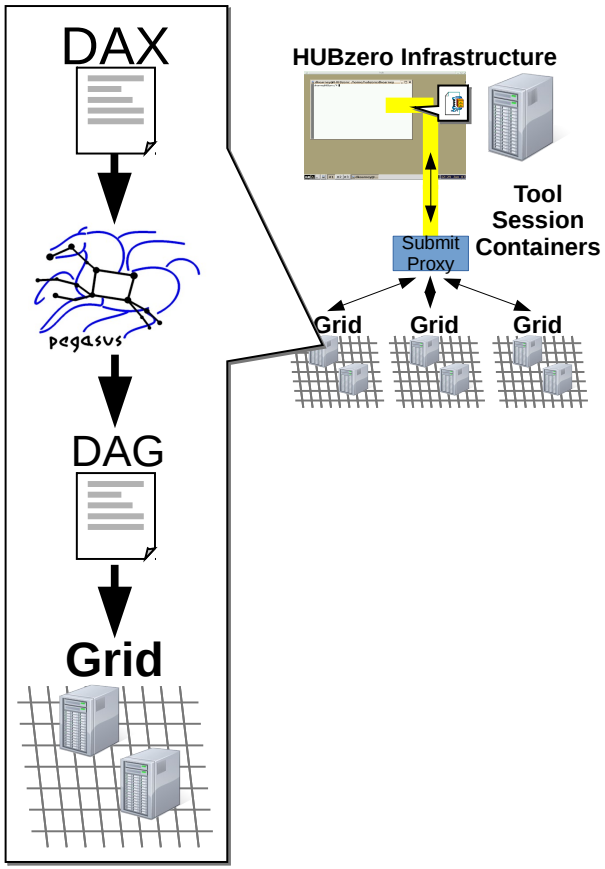
- Performance
- Portability
- Provenance
- Data Management
- Error Recovery

Productivity in the Workspace

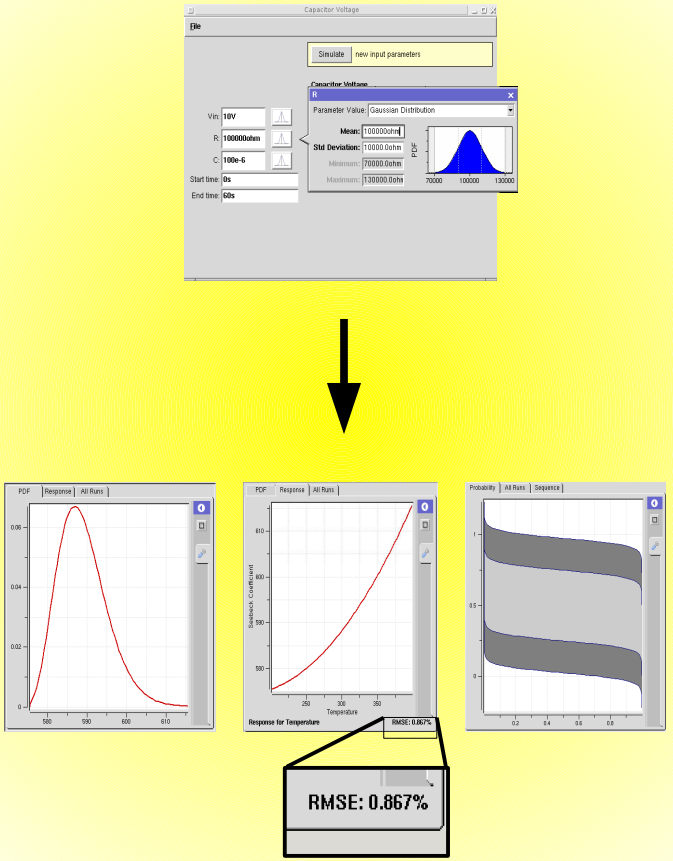
Submit



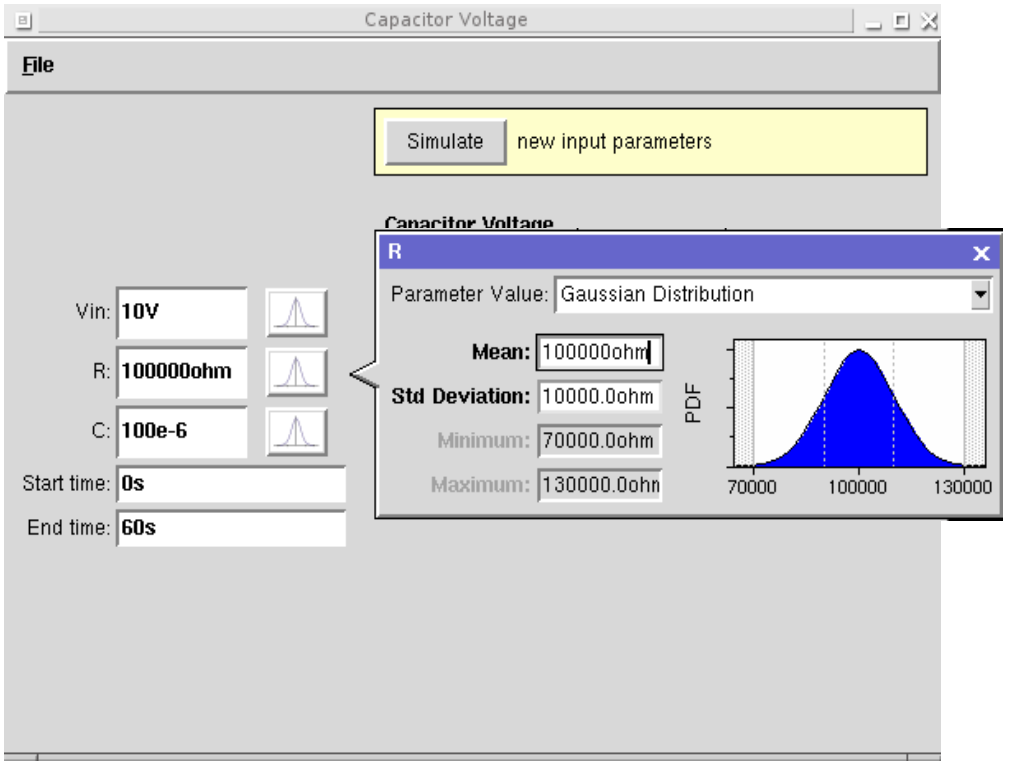
Pegasus Workflows

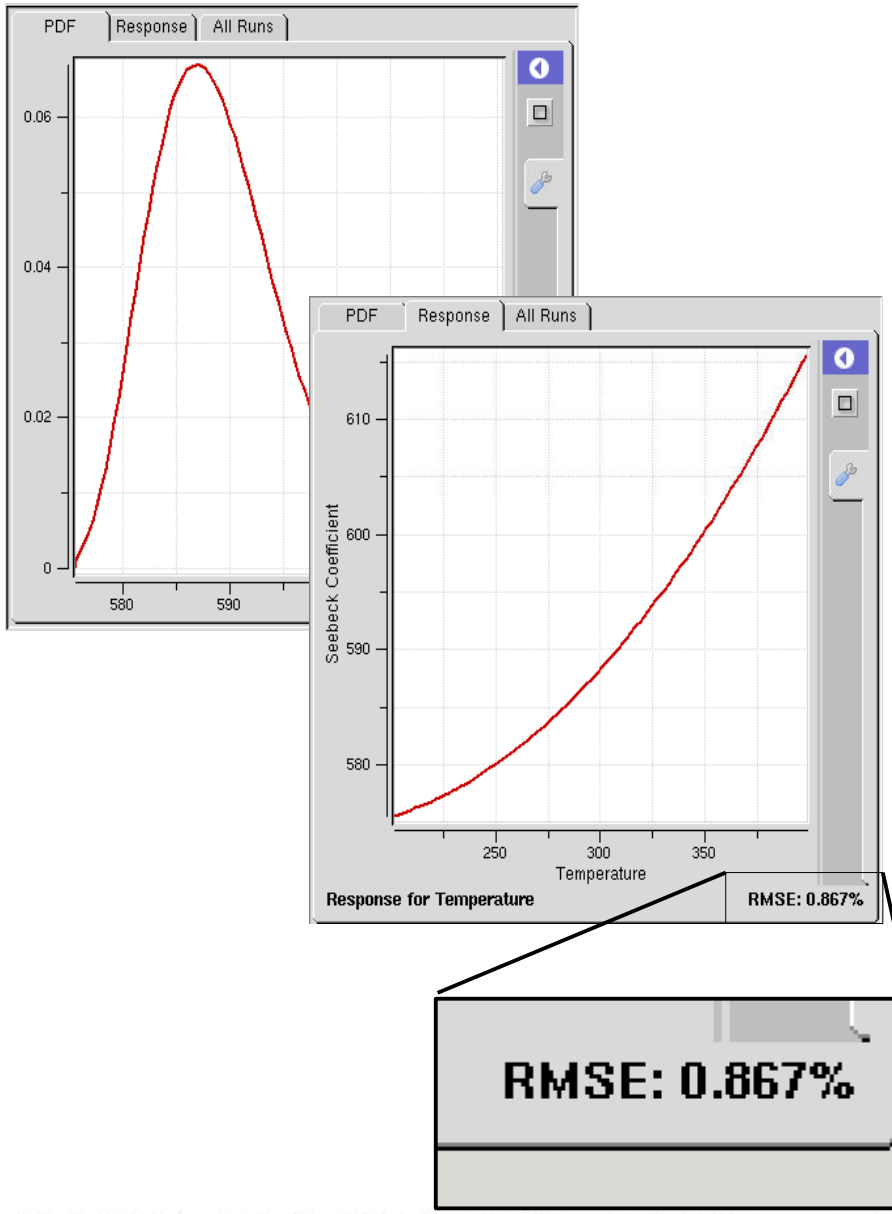


Uncertainty Quantification



Inputs and Outputs as Distributions



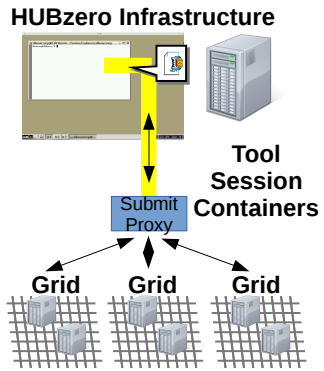


27 FTEs
18 Developers
5 Support/Training

10+ Years
Supporting Research
And Collaboration

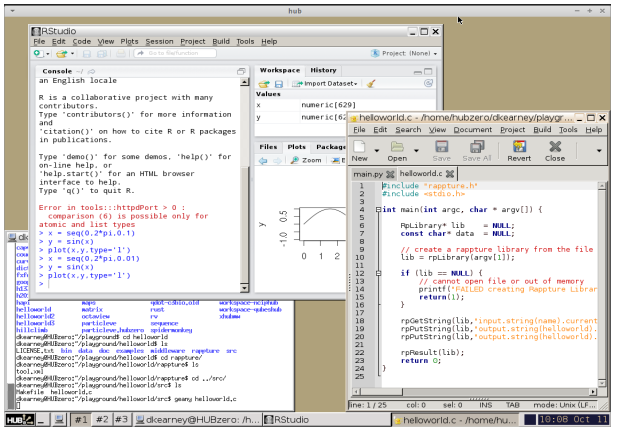
2+M
Visits

hubzero



XSEDE
Extreme Science and Engineering Discovery Environment

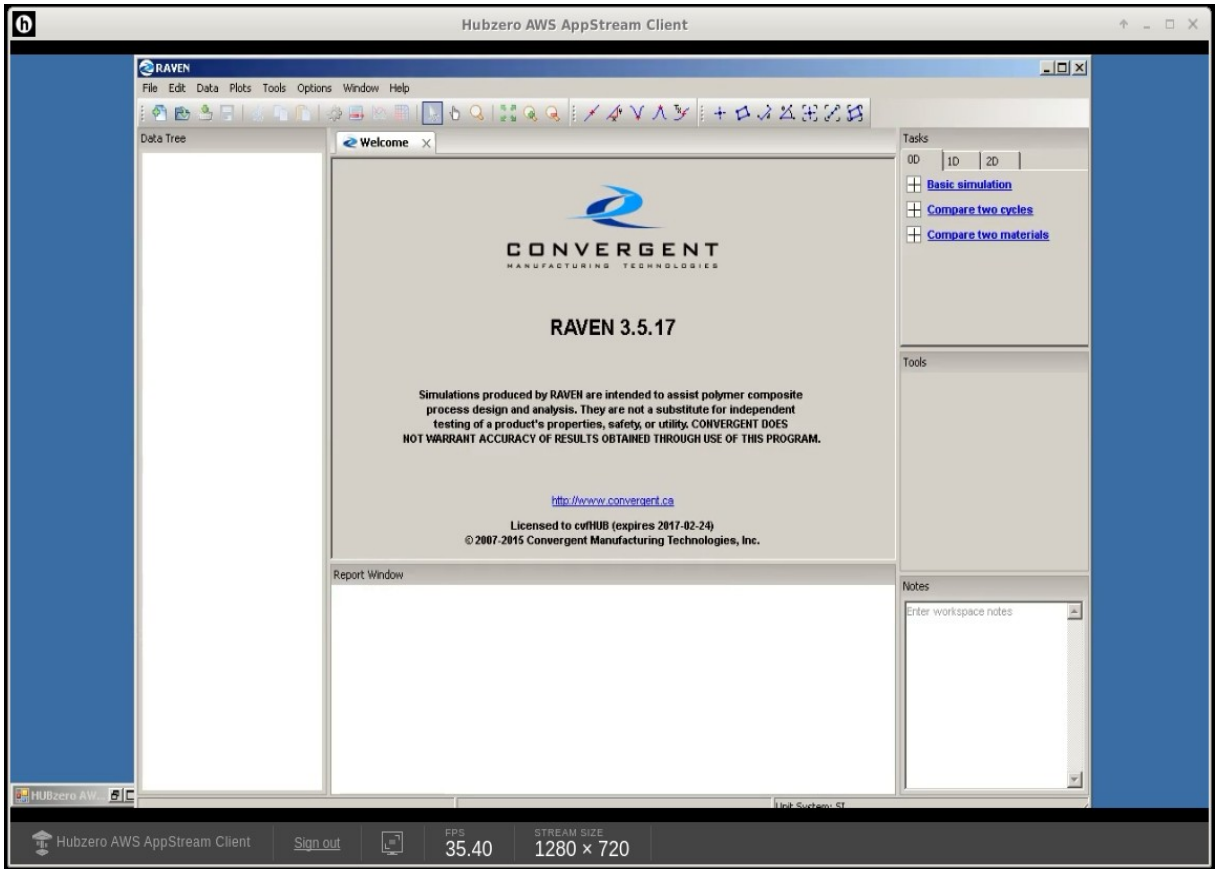
Open Science Grid



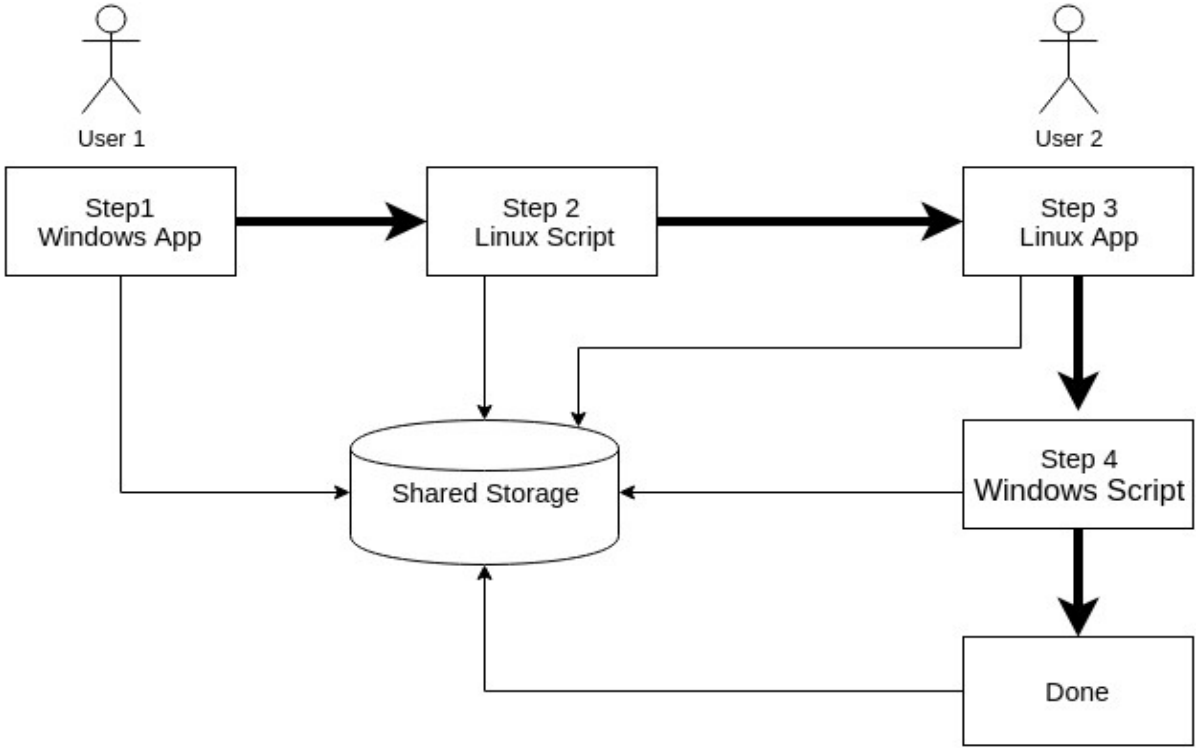
Secure, Scalable, Sharable
Dev Environments

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