



HUBzero™ Roadmap

and Community Feedback

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HUBzero Consortium

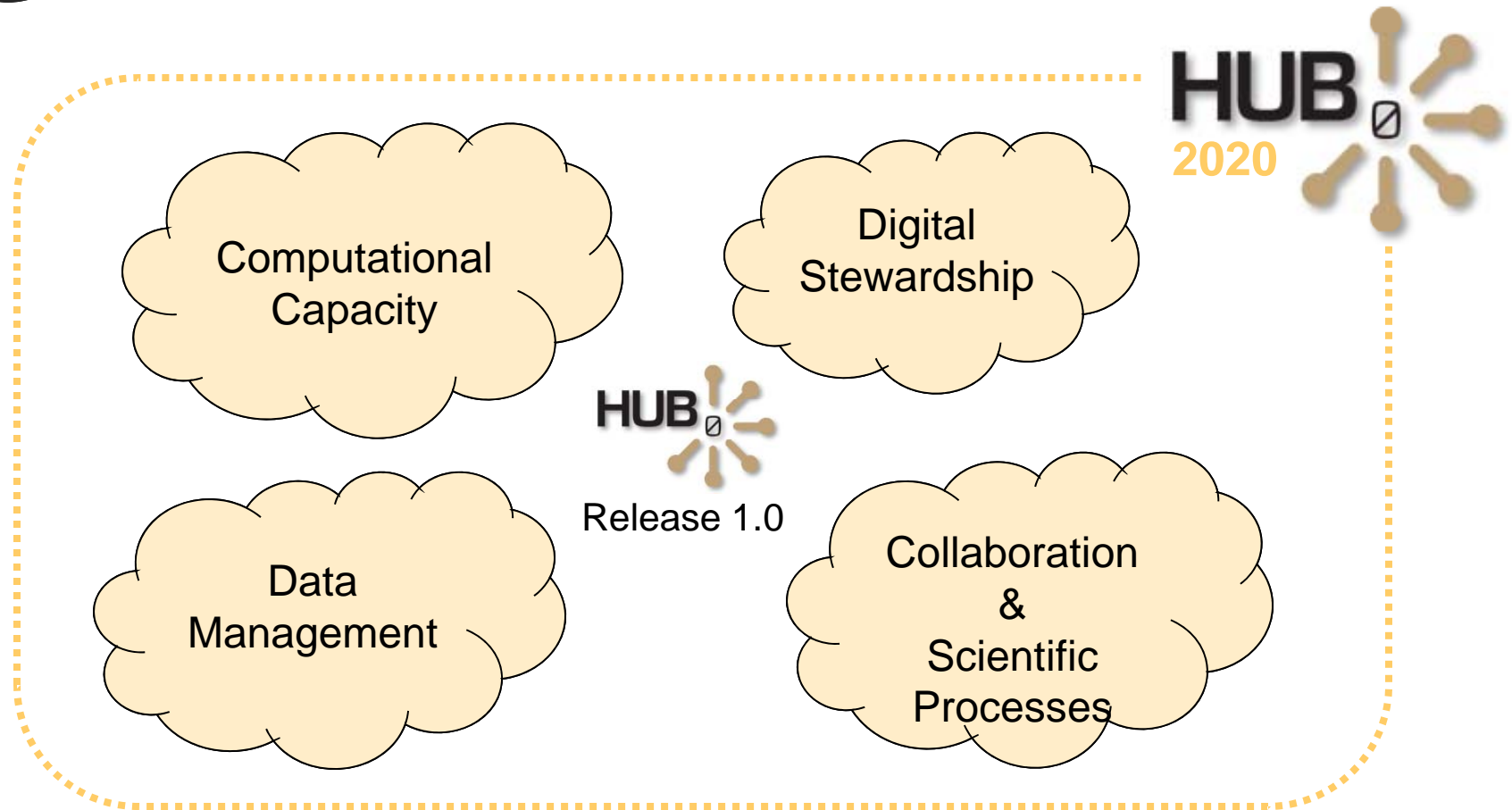
Challenges: Dealing with large data sets, usability, visualization

Feedback from our survey

Federated access to the hub so I can integrate a variety of web resources and so my users can seamlessly access resources in multiple security domains.

Creating the tools to enable community authoring of content to share between teachers, as well as enabling and enforcing the proper relationships and data privacy for teacher/student and teacher/class relationships.

Elevate computing and software development to the same level of reproducibility and peer review as traditional publishing.



The best way to predict the future is to invent it.
Alan Kay

Resonant Tunneling Diode Simulator
About this tool | Questions? | Cite this tool

Want results faster? [here's how](#)

Overview

Enter simulation

Example runs

- 2-barrier device
- 3-barrier device
- 6-barrier device
- [more...](#)

Recent runs

- 7/13/2009 - 2-barrier device
- 7/13/2009 - 2-barrier device
- 6/30/2009 - 3-barrier device
- [more...](#)

Check simulation

0 jobs running

View simulation

Recent runs

- 7/13/2009 - 2-barrier device
- 7/13/2009 - 2-barrier device
- 6/30/2009 - 3-barrier device
- [more...](#)

Input Parameters

Structure: Carbon Nanotube

Simulation Method: Pz o

Tube configuration

Chirality (n,m) = (7

Model parameters

Tight Binding Energy

Carbon-c

- Single v
- Sweep
- From
- With
- Using
- Multiple
- Optimiz

Progress

Currently running 3 jobs:

- T=25C (launched today, 10 minutes ago)
- T=300K (launched today, 8 minutes ago)
- T=4.2K (launched today, 6 minutes ago)
- T=1.3K (launched today, 3 minutes ago)
- T=77K (launched today, 1 minutes ago)

30% Solving...

Electrode	Voltage (Volts)	Electron Current (Amps)	Hole Current (Amps)
1	0.0000	-8.81672E-10	0.00000E+00
2	0.0500	8.81675E-10	0.00000E+00
3	0.0000	0.00000E+00	0.00000E+00
4	0.0000	-2.68857E-17	0.00000E+00

Electrode	Flux (Coul)	Displacement Current (Amps)
1	-7.61641E-17	0.00000E+00
2	-6.8	

nanoHUB.org Middleware

- \$1.35M NSF SDCI award, Michael McLennan (PI)
- Redesign Rapture for sweeps/optimizations
- Release HUBzero as Open Source

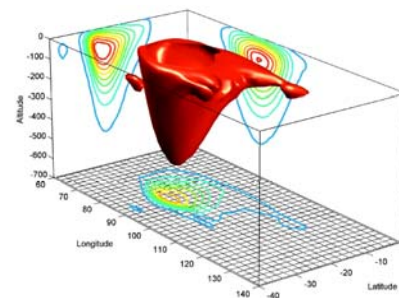


Instant-On Computing for nanoHUB.org

- \$1.4M NSF ARRA award, Gerhard Klimeck (PI)
- Execute jobs without waiting in a queue
- Make TeraGrid “wide” and “open”
- Partner: UT / Oak Ridge National Lab

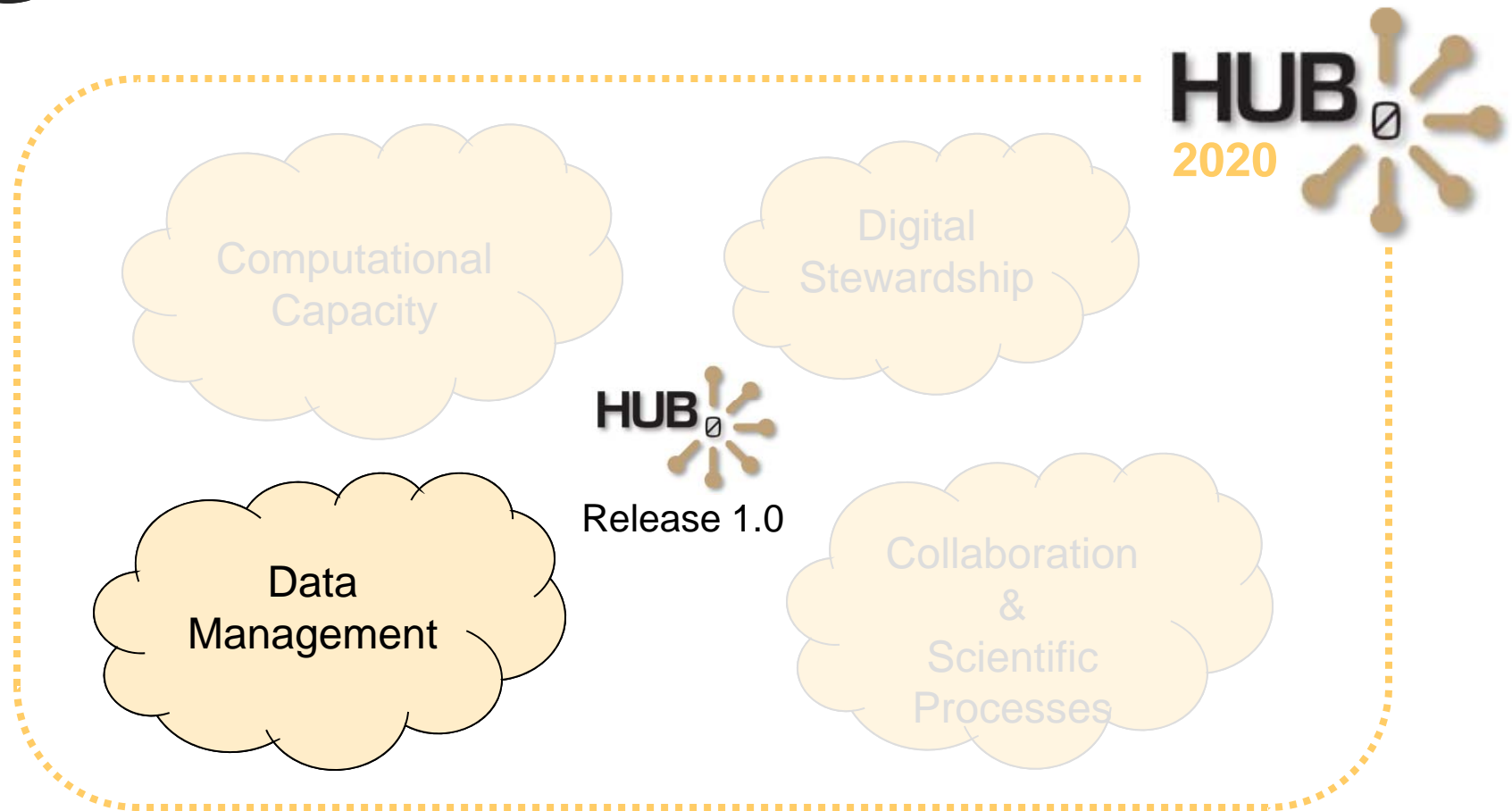
Cornell MATLAB Cluster

- \$660K NSF ARRA award, David Lifka (PI)
- Send nanoHUB.org MATLAB jobs to Cornell cluster

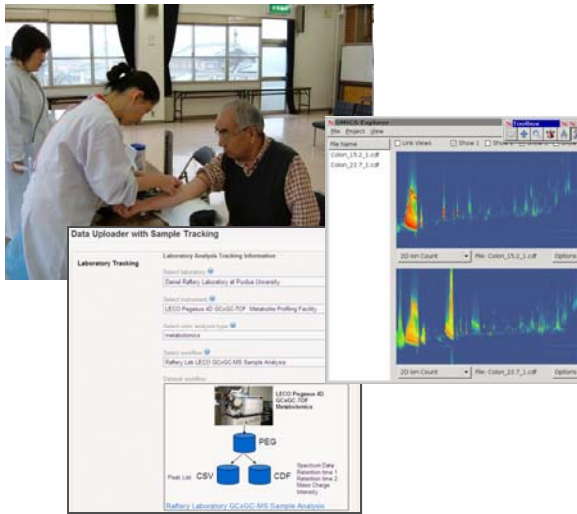


Pharmaceutical Engineering Pipeline

- \$1.9M NSF CDI award, Rex Reklaitis (PI)
- Build a workflow system for Rapture-based models
- Study pharmaceutical performance in diverse patient populations



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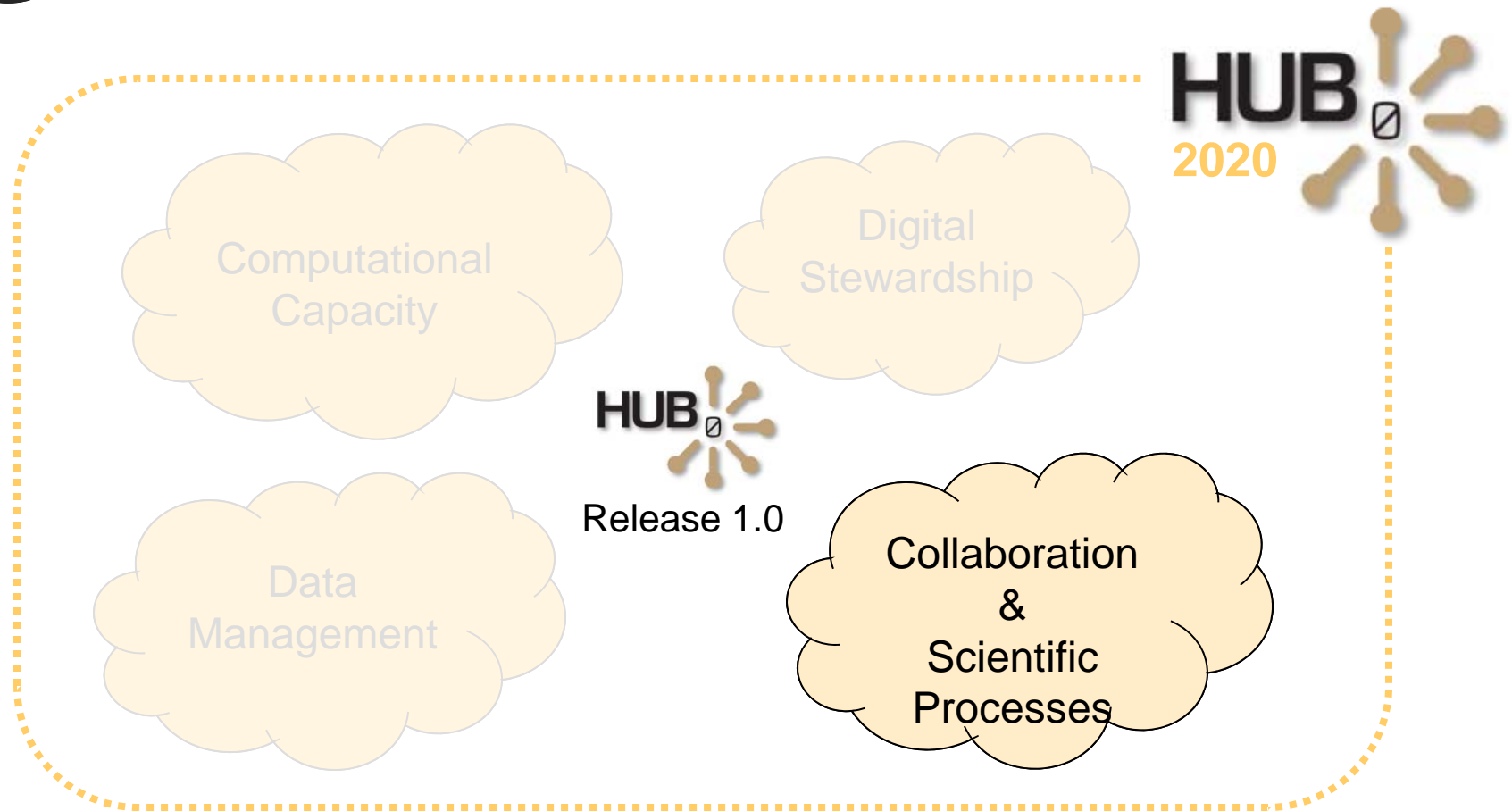
Cancer Care Engineering - cceHUB.org

- Led by Ann Christine Catlin
- Built a Rappture-like spec for databases
- Collective blood samples
- Building an analysis pipeline

Network for Earthquake Engineering Simulation (NEES)

- \$105M NSF project across 14 institutions
- Share/analyze experimental data

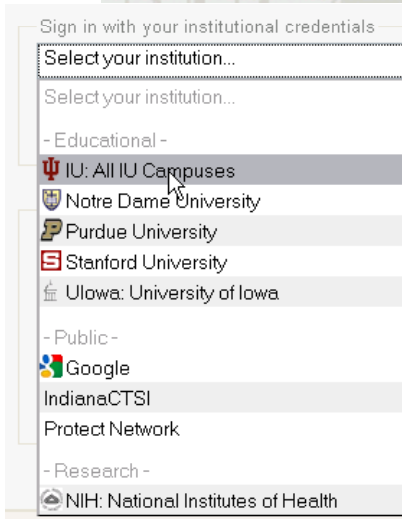




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Single Sign-on for researchers from multiple institutions

- Uses institutional credentials
- Login is transparent with little additional overhead
- Logins managed institutionally so there is confidence in the real identities
- Authentication credentials can be carried to multiple resources with one login
- As new staff/faculty come on board, they are automatically authenticated



Indiana University - IndianaCTSI.org

- Bill Barnett, Director of Advanced IT Core, IUSM
- Indiana is the first CTSA org to accept InCommon
- NIH is pushing InCommon and uses it on their sites (eg., CTSAWeb.org)
- NSF moving toward InCommon

Based on Open Journal System – PKP (pkp.sfu.ca)

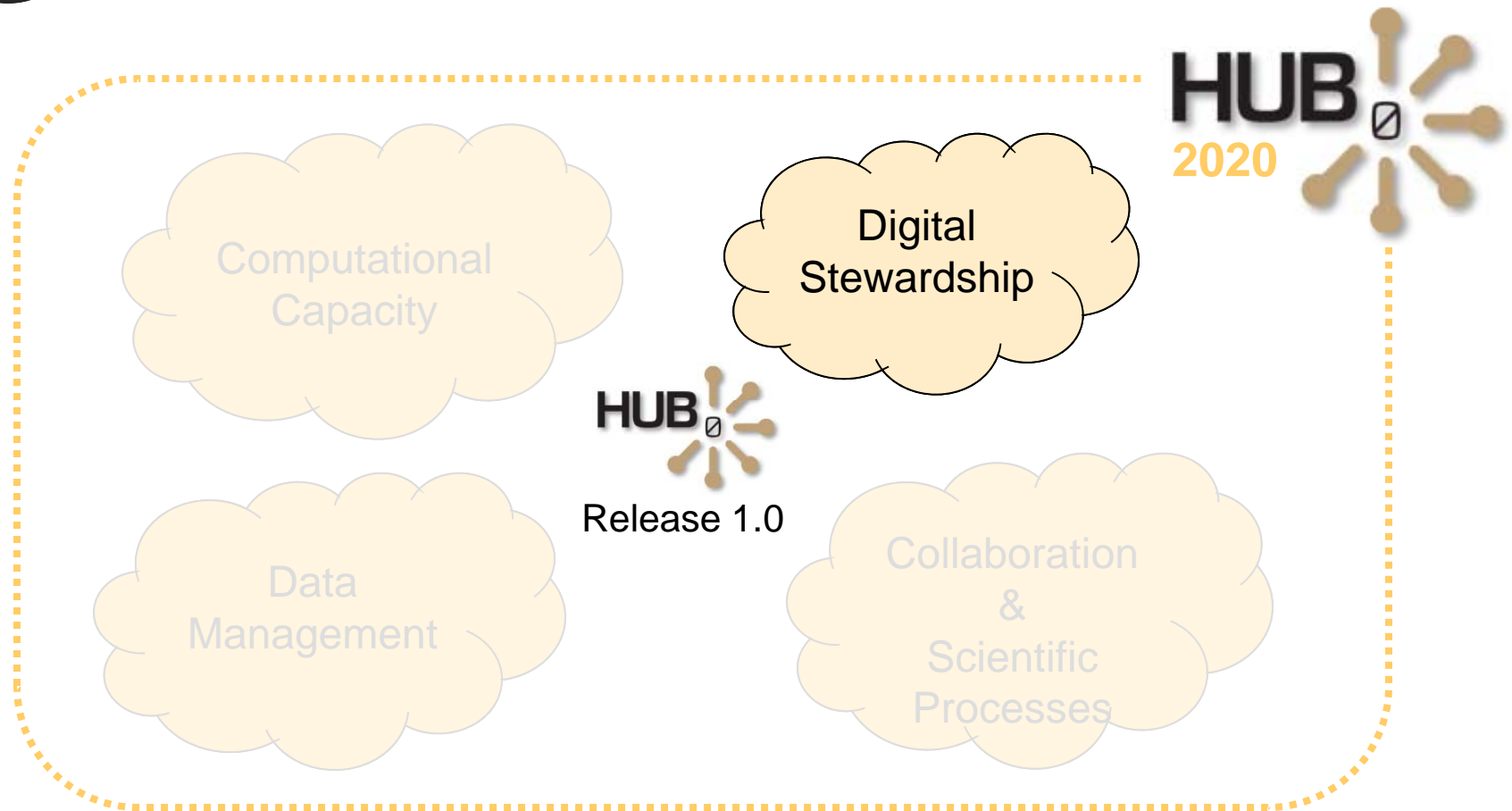
- Originally designed for review of journal article submission for online journals
- Currently used for over 5000 titles
- Supports online advertisement, submission, reviewer selection, reviews, and notification including email-based notification and submission

PKP | PUBLIC KNOWLEDGE PROJECT

Adopted for Indiana CTSI HUB

- Used for internal grant competitions
- Used for Project Development teams to assess and advise on new translational science projects
- Provides automated usage metrics
- Being modified to support online forums for reviewers, scoring, and other features

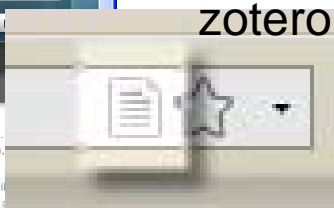




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Band Structure Lab
 By Abhijeet Paul¹, Mathieu Luisier¹, Neophytos Neophytou², raseong kim¹, Michael McLennan¹, Mark Lundstrom¹, Gerhard Klimeck¹
 1. Purdue University, West Lafayette; 2. Technical University of Vienna;
 Computes the electronic structure of various materials in the spatial configuration of bulk (infinitely periodic), quantum wells (confined in



Connections to literature:

- Citation instructions
- COinS for Zotero



Seed Project: *RDF triples for tools and other resources on nanoHUB.org*

- Michael Witt, Assistant Prof of Library Science
- Explore the utility of Linked Data within the hubs

CNTbands

By Younki Yoon¹, James K. Fodor², Jing Guo³, Akira Matsubara³, Diego Kizito⁴, Gangchao Liang⁴, Gerhard Hämel⁴, Mark Lundstrom⁵

1. University of California - Berkeley; 2. University of Florida; 3. University of Illinois at Urbana Champaign; 4. Purdue University, West Lafayette; 5. Purdue University - West Lafayette

This tool simulates E-k and DOS of CNTs and graphene nanoribbons.

Launch Tool

Version 2.2 - published on 10 Dec 2009
DOI: 10.254/nanohub-r1030-5 cite this
Open source license (download)

[First-Time User Guide](#)
[View All Supporting Documents](#)

Description: CNTbands can simulate electronic band structure and density-of-states for carbon nanotubes (CNT) and simulate graphene nanoribbons (GNR). It also computes some basic parameters, such as nanotube diameter, number of hexagons in the unit cell, and band gap. Users may select the GNR structure to be simulated by selecting a starting point and components for a chiral vector. CNTs are simulated either with a simple P2 orbital model or Extended Huckel theory. The Extended Huckel model can deliver more accurate simulation results, especially for small-diameter CNTs.

Tool versions

- Version 2.2 introduces numerical DOS calculation, to complement the numerical E-k calculation.

Please see the carbon nanotube and graphene nanoribbon topics page for more related nanoHUB

RECOMMENDATIONS

- [Introduction to CNTbands](#)
- [CNTbands](#)
- [CNTbands: First Time User Guide](#)
- [CNTbands Download](#)
- [NanoTCAD VIDES](#)

Powered by ...

Seed Project: Recommendation engine for nanoHUB.org

- Luo Si, Assistant Prof in Computer Science, Statistics
- Suggest resources based on similarity and access patterns

Digital objects archive

New visualization modalities: Paraview, VISIT, GIS

Free online web meeting capability

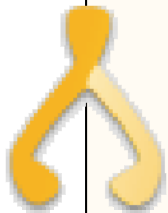
Integration with Facebook, LinkedIn, Skype

Group calendar

Blogs on the member profile page

...

Discussion time: ***What do you want?***



Make a “wish”

<http://hubzero.org/wishlist>