HUBzero™ Roadmap
and Community Feedback

George Adams and Michael McLennan

HUBzero Consortium
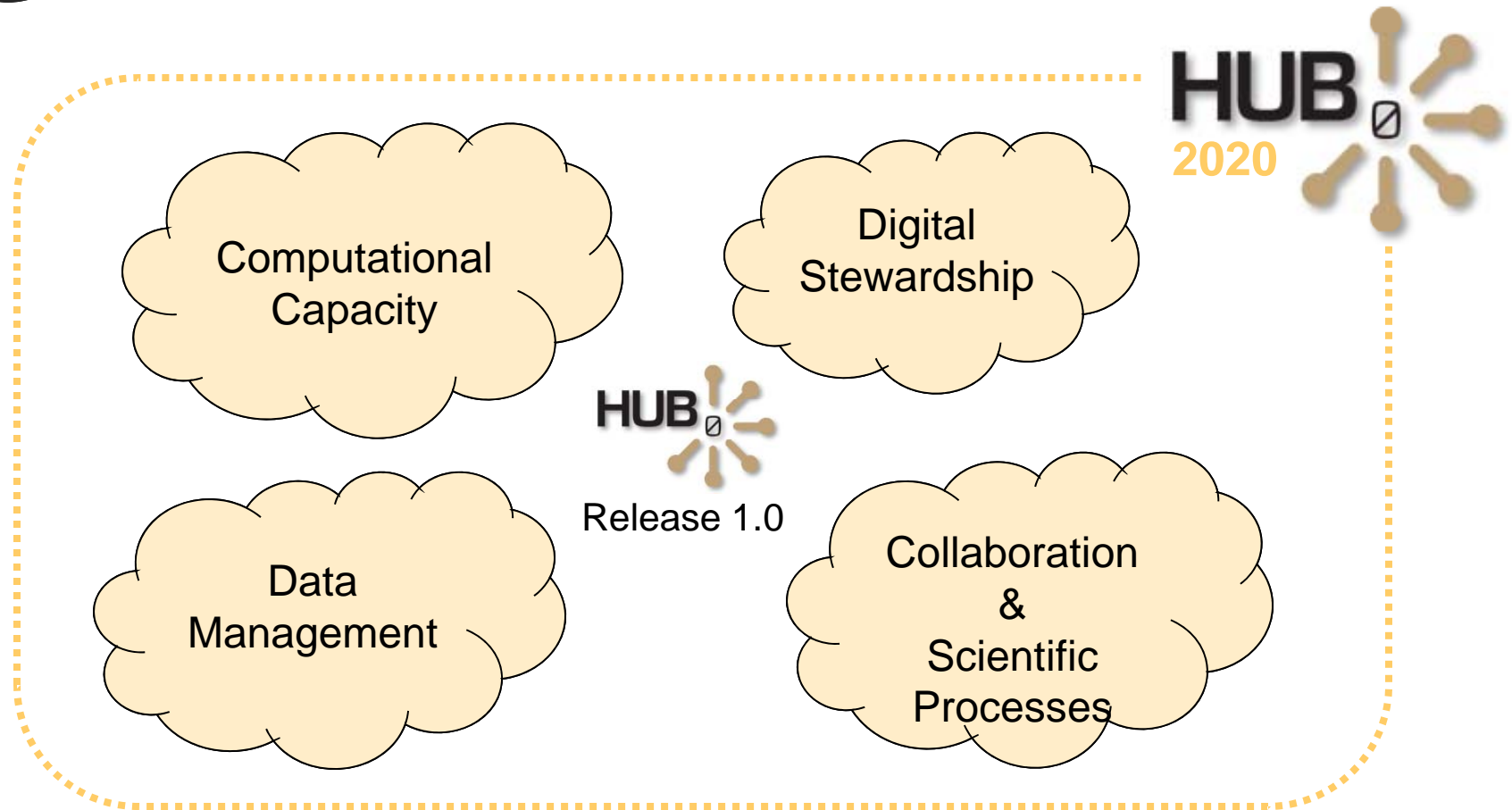
Feedback from our survey

Challenges: Dealing with large data sets, usability, visualization

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.

Computational Capacity

Digital Stewardship

HUB 2020

Release 1.0

Data Management

Collaboration & Scientific Processes

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

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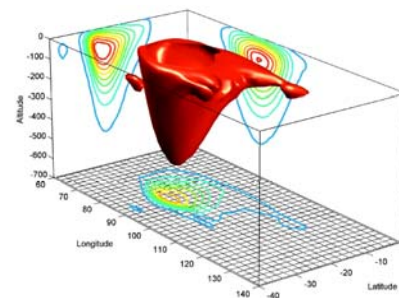- Redesign Rapture for sweeps/optimizations
- Release HUBzero as Open Source

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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"
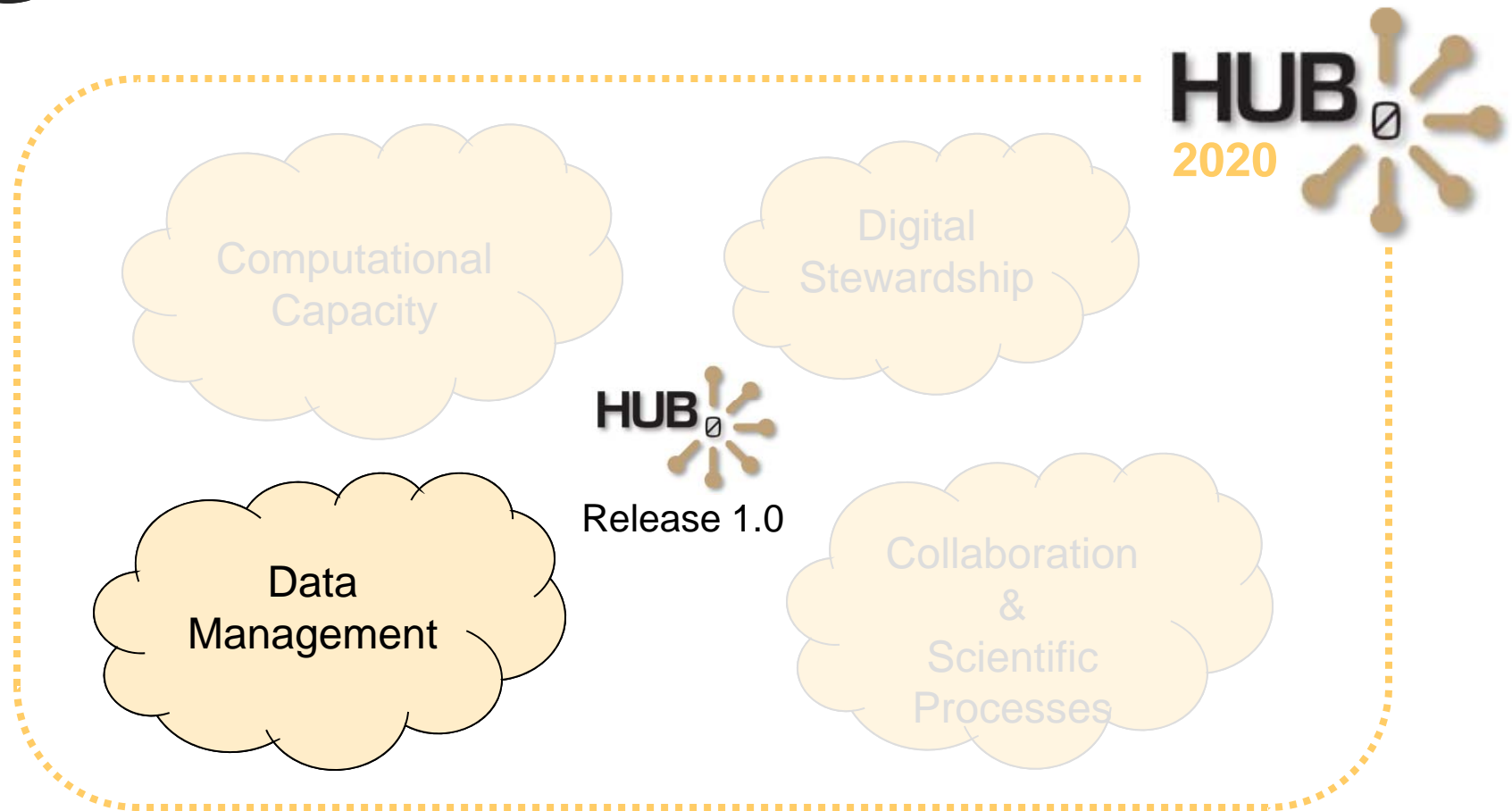- Partner: UT / Oak Ridge National Lab

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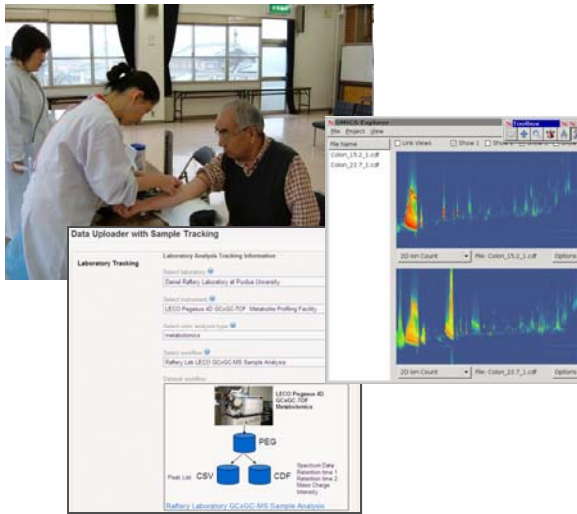- Send nanoHUB.org MATLAB jobs to Cornell cluster

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

HUB **2020**

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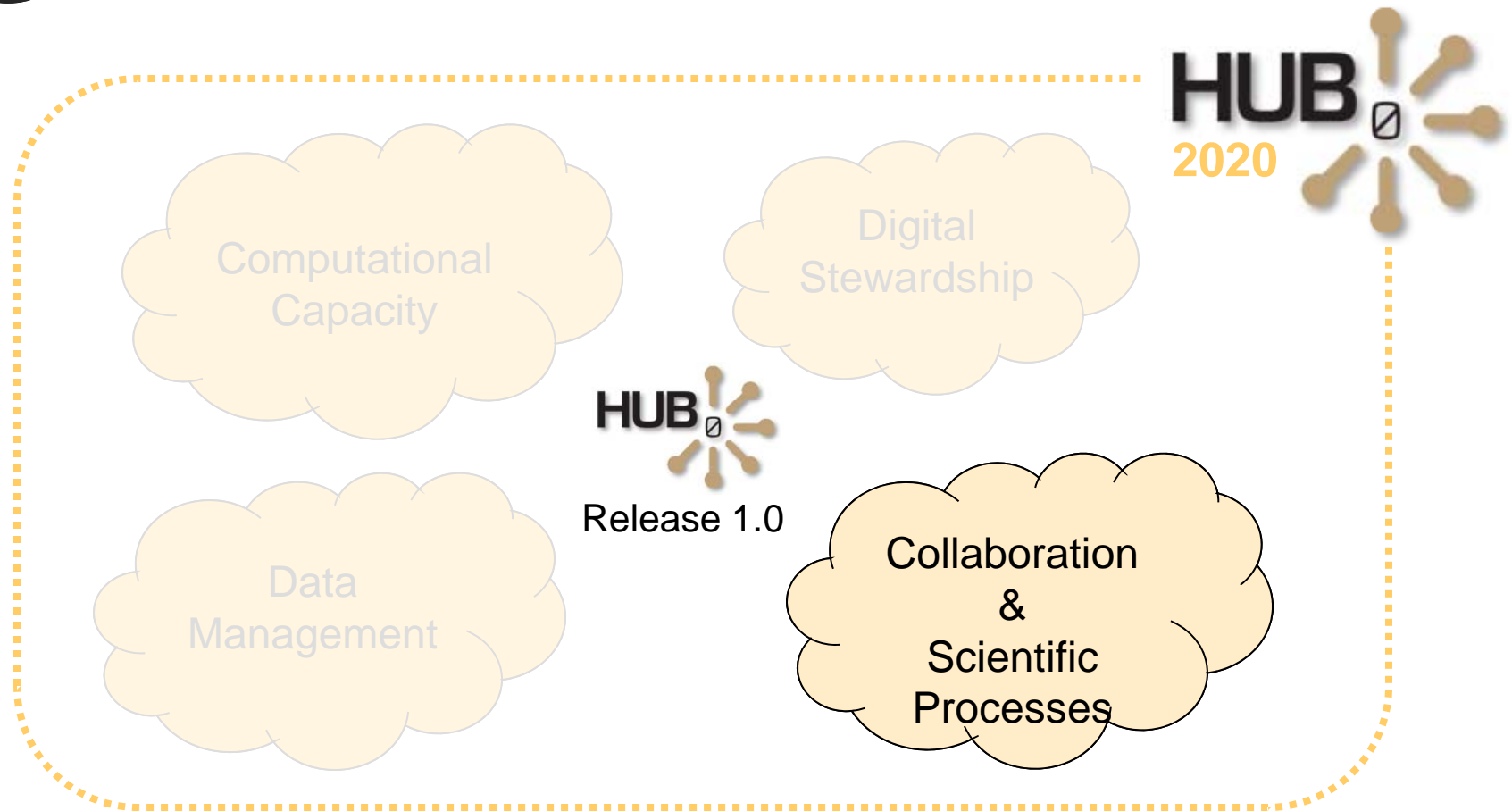
Alan Kay

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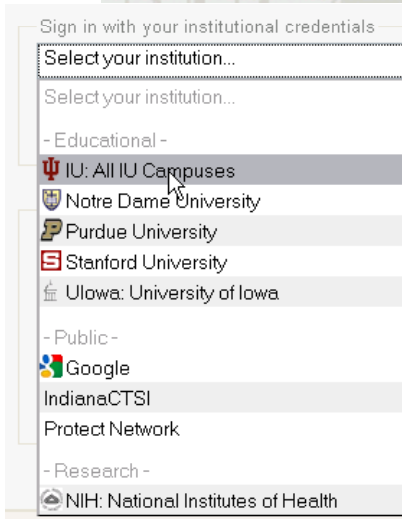- $105M NSF project across 14 institutions
- Share/analyze experimental data

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Alan Kay

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

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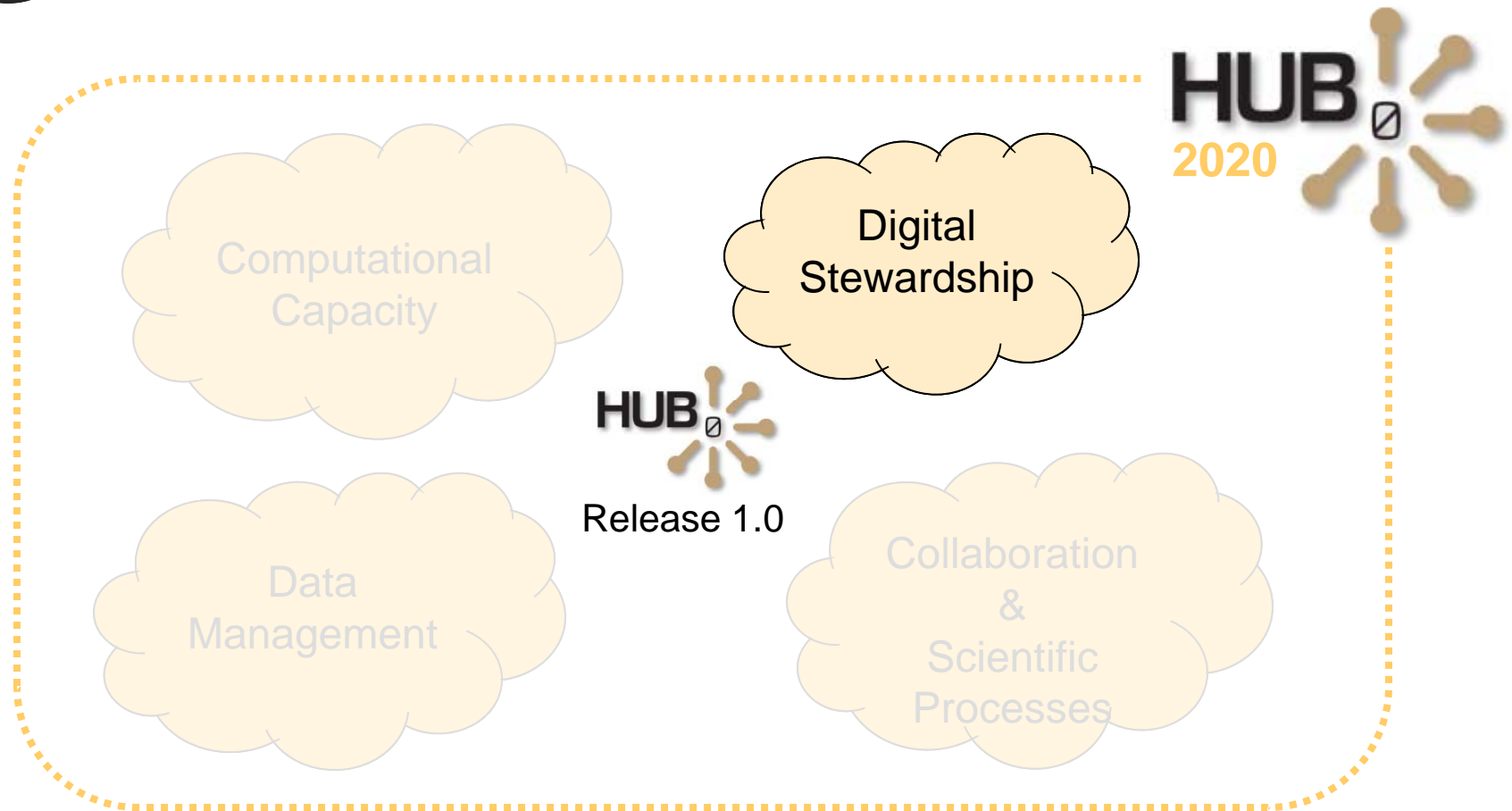***Based on Open Journal System – PKP (pkp.sfu.ca)***
- Originally designed for review of journal article submission for online journals
- Currently used for over 5000 titles
- Supports online advertisement, submission, reviewer selection, reviews, and notification including email-based notification and submission

PKP | PUBLIC KNOWLEDGE PROJECT

IndianaCTSI

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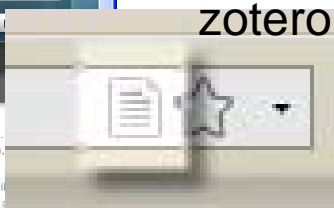
The best way to predict the future is to invent it.

Alan Kay

zotero

Connections to literature:
- Citation instructions
- COinS for Zotero

Band Structure Lab

By Abhijeet Paul[1], Mathieu Luisier[1], Neophytos Neophytou[2], raseong kim[1], Michael McLennan[1], Mark Lundstrom[1], Gerhard Klimeck[1]

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

Launch Tool

Version **2.0.8** - published on 26 Jan 2010

DOI: 10254/nanohub-r1308.12 cite this

This tool is closed source.

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

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

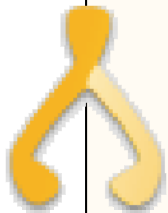Free online web meeting capability

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