NTK
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Národní technická knihovna
National Library of Technology

"Reverse Design" for Developing e-Research Support Offerings

Using Research Findings to Inform Creation of Tailored Services for PhD Students, Post-Doctoral Researchers, and Professors

S. Krueger, Prague, 11.2015

Overview

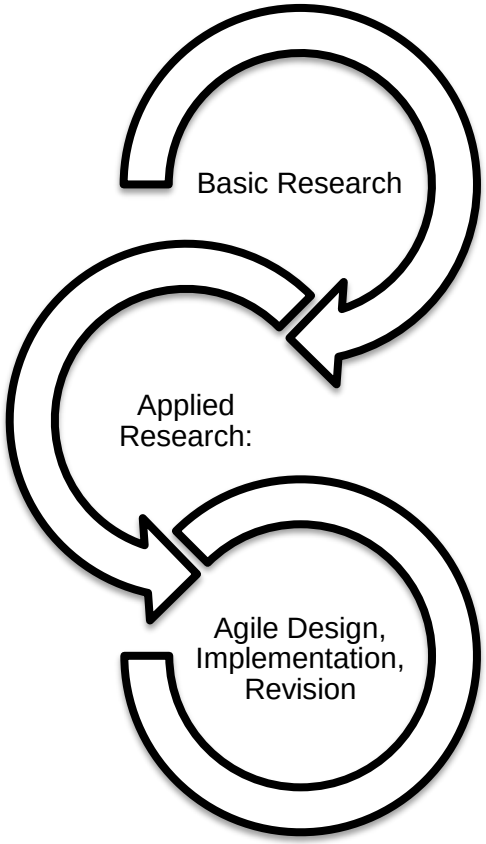
Basic Research: Actual Behaviors of Six Scientists

- Before Creating a Service
- Background: Ethnographic Methods in HCI, IS
- Research Design
- Participants
- Research Data Description
- Results and their relation to e-Research tool design

Bonus (not today, read at your leisure) Applied Research: Testing Observations with Agile Solutions

- Backward Instructional Design for e-Research Support: Pilot One, Pilot Two
- HCI in Action: Examples
- Future Research: Basic and Applied

Before Embarking on e-Research Support Services: Basic Research into Real Behavior Patterns First



Ethnographic Methods in Human-Computer Interaction (HCI) & Information Science (IS)

Ethnography & HCI

- "Long" (1980s+) tradition, with applied aspects in commercial sector
  - Likely used by your favorite software or even online academic resource; see Dourish for history and reference list
- Unfortunately, not encountered as often in academic settings
  - Library websites, repositories, online instructional modules

Ethnography & IS

- Scattered projects with varying levels of quality; some recent work with scientists and engineers, combined with quantitative network studies
  - Pepe, Velden
- Instruction/online library services: most research to date has been with undergraduate populations (i.e., Foster and Gibbons, Pukkila and Freeman); work with PhD/researcher/professor populations in STM is scarce
  - It is very difficult to achieve engagement in a long-term project. These are busy people with many demands.

Research Design

Qualitative, using multi-sited ethnographic strategies

- How do scientists really work with information (broadly defined) today?
- Do the patterns of observed information-related behaviors differ—not only in terms of research discipline, but also in terms of other factors (language, type of institution, gender, etc.)?
- Do our assumptions about e-Research needs match the real ways in which scientists conduct their work?

Multi-sited ethnographic research enables us to begin answering such questions, by comparing data gathered across field sites, including the “virtual field”

- Assumption: Global networked academic environment requires inclusion of virtual fieldwork

Research Design: Duality

Virtual

Global

Physical

Local

Extremely interesting area when considering e-Research support services

Deleuze and Guattari (1987, p. 40) come to mind; phenomena manifest themselves as pairs (“the Lobster, or a double pincer, a double bind”), with content and expression intermingling, multiplying, and dividing “ad infinitum” (p. 44).

Multi-sited ethnographic research must examine intertwined dualities: within the GNAE, the work of scientists is both local/global, physical/virtual—these double articulations combine and complement each other.

The necessary virtual field complements the conventional setting, and vice versa.

Image: "Lobster NSRW". Licensed under Public Domain via Commons - https://commons.wikimedia.org/wiki/File:Lobster_NSRW.jpg#/media/File:Lobster_NSRW.jpg

Research Design: Summary

- Six participants / two countries / four institutions
- Three languages (US English, Czech, Ukrainian)
- Humboldt Institutional Research Board (IRB) approved
- Over three years (2012 to 2015); PhD Thesis 2016
- “Traditional” fieldwork: Original transcripts, coded
  - In-person and virtual interviews
  - Observation
  - Analysis of supplementary materials and information resources
- Virtual fieldwork
  - Screenshots taken by participants
  - Originally conceived as video screencaptures

Formal Participants (n=6)

Participant	Subject	(State or City), Country	Native Language	Connection	Gender	Role During Study	Institution	Age Range
1 (key informant)	Theoretical Physics	New York, US	US English	Friend of Friend US	F	Assistant Professor	Large Private Research University	40-50
2 (key informant)	**Condensed Matter Physics (experimentalist)**	Prague, Czech Republic (CZ)	Ukranian	Random CZ	F	PostDoc	Large Public Research University	20-30
3	**Condensed Matter Physics (experimentalist)**	Prague, Czech Republic	Czech	Colleague of Participant CZ	F	PostDoc	Large Public Research University	20-30
4 (key informant)	**Cheminformatics (theorist AND in silico experimentalist)**	Prague, Czech Republic	Czech	Colleague Recommendation CZ	M	PhD Student	Large Public Research University	20-30
5 (key informant)	**Cheminformatics (theorist AND in silico experimentalist)**	Prague, Czech Republic	Czech	Colleague Recommendation CZ	M	PhD Student	Large Public Research University	20-30
6	**Immunology & Infectious Diseases (experimentalist)**	Montana, US	US English	Friend of Fellow Doctoral Student US	F	Associate Professor	Large Public Research University	40-50

Fieldwork Artifacts

Participant	In-Person Observation	In-Person Interview or Discussion	Emails	Skype Discussion	Total Coded Interactions
1	One month (informal); scratchnotes captured in coded fieldnotes	One hour captured in coded fieldnotes	Sixteen substantive interactions coded in fieldnotes	Two hours captured in coded fieldnotes	20
2	Two hours; scratchnotes captured in coded fieldnotes	Two hours; scratchnotes in email form read and commented by participant	Eight; coded in fieldnotes	None (in Prague)	12
3	None	One hour; scratchnotes in email form read and commented by participant	Three	None (in Prague)	4
4	Half hour; scratchnotes captured in coded fieldnotes	7.5 hours; scratchnotes captured in coded fieldnotes	Thirteen	None (in Prague)	22
5	Half hour; scratchnotes captured in coded fieldnotes	7.5 hours; scratchnotes captured in coded fieldnotes	Two	None (in Prague)	10
6	None (in US)	None (all interaction by email to date)	Three	None to date	5
Total All Participants	**One month (informal) plus three hours**	**19 hours**	**47**	**Two hours**	**73**

Questions about e-Research activities:

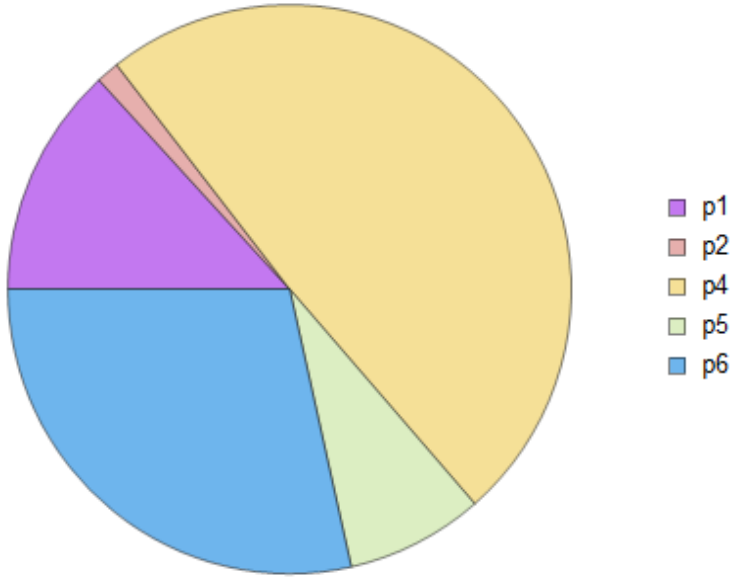
What information resources do you use in your research or to keep aware of publication trends?

What software tools do you commonly use to collaborate with other researchers (e.g., Skype, Dropbox, GoogleDrive, other)?

What software tools do you commonly use in your research (e.g., Surface Evolver, etc.)?

Screenshot Artifacts

Participant	Total Screenshots
1	30
2	3
3	None
4	112
5	18
6	65
Total All Participants	229



Purposefully Open Instructions/No "Pre-Determined" Definition of Information:
Please provide me with screenshots over a two week period of your work with information.

Coding Data: Samples

Screenshot data

97. Filename or other: 11.3.2014.1
Format: png GDrive folder
Participant: p4
Storage Location: GDrive, local copy
Theme: Cocrystal
Emic: I wasn't sure what 'cocrystal' is, so I spent some time on wikipedia repairing this hole in my education. It probably came up in the context of protein--ligand interaction modelling.
Analytic Commentary/CODES:
WIKI EN
NON-COMM
NON-LIB
VIEW ARTICLE
FORM
NON-AUTH

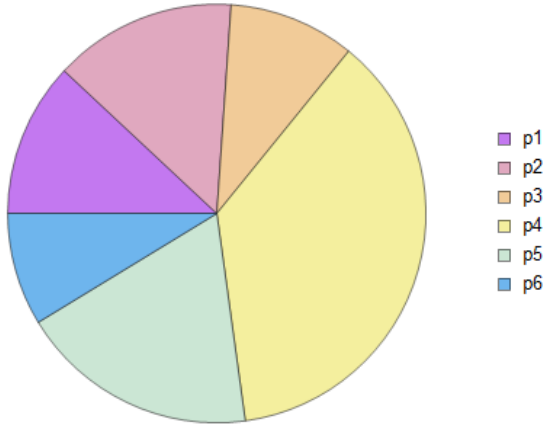
Fieldwork data

4. Format: Email and questionnaire and observation final review
Participant: p3
Date: 3 Nov 2013
Storage Location: Gmail
Theme: Questionnaire and observation review, editing
Excerpt (text or image):
Time-constraints: "I am a bit more busy and and [sic] answers may be delayed, howere [sic], I am interested in this project.
"showed me a typical day, which begins by opening up ArXiv in the morning in order to check news and the landscape of what's happening in the field."
LIBRARY SERVICES: "doesn't go to faculty/departmental library but requests articles and have these sent to them." Library catalog "doesn't often find it useful and sometimes ends up purchasing books themselves." Reference Manager and BibTeX (for LaTeX). "does not have a library subject specialist; typically, a more senior researcher will show students how to use research tools, how to read articles, and how to find. In the beginning this process is more difficult so the supervisor/mentor recommends and shows junior scholars what to look for. It is difficult for the research participant to imagine how a librarian might assist this process because the subject areas are so specific." Does use older books for example Solid State Physics (Ashcrost and Mermin 1976) and Introduction to Solid State Physics [Kittel; latest edition 2005, original edition 1953] because they are well-written and the basics don't change.
Occasional collaboration with Skype and email
Analytic Commentary/CODES:
ArXiv
American Physical Society Physics Portal (Physics APS): at least once a month
Nature: at least once a month
Science: at least once a month
Google (?version): important source of finding articles and tracking citations
Web of Knowledge: important source of finding articles and tracking citations. Sometimes delays and things might be several months behind.
Reference Manager
BibTeX (for LaTeX)
Review of Modern Physics, APS: "most impact factor"
Google Scholar: "doesn't often use"/"too many irrelevant results"

Data Description & Analysis

Information Resources Mentioned: Fieldwork Data

p1	p2	p3	p4	p5	p6	TOTAL
11	13	9	34	17	8	92



No participants mentioned library websites during fieldwork

No information resource mentioned by all six participants, because I broke **Google** into components:

- Google Scholar (five participants)
- Google Patent (two participants)
- Google Czech version (Google CZ, two participants)
- Google (likely Google CZ but not confirmed, one participant)
- Google Drive (one participant)
- Google Hangout (one participant)

Most commonly-mentioned resources were:

- **arXiv.org** (four participants), **English Wikipedia** (four participants), and **Web of Science** (formerly Web of Knowledge; three participants).
- Participants 4 and 5 both mentioned the following resources: **BitBucket, Google Patent, RDKit, Skype, and StackOverflow**
- Participants 1 and 5 both indicated they use **Python**

Data Description & Analysis

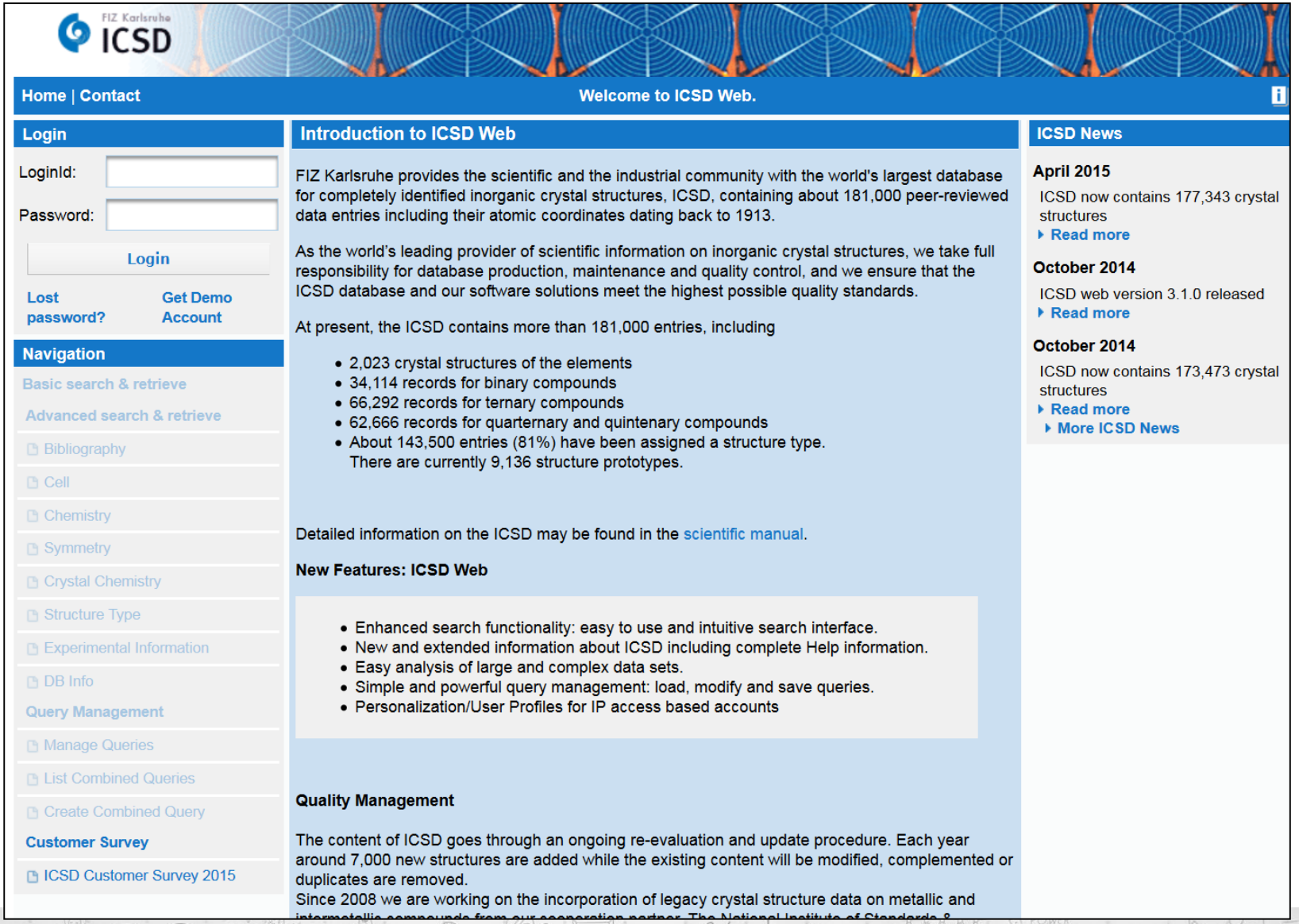
Fieldwork Data:

Relevance for e-Research support services is the **wide variety of tools and platforms utilized, particularly specialized tools** created by scientific communities for their peers or by commercial entities

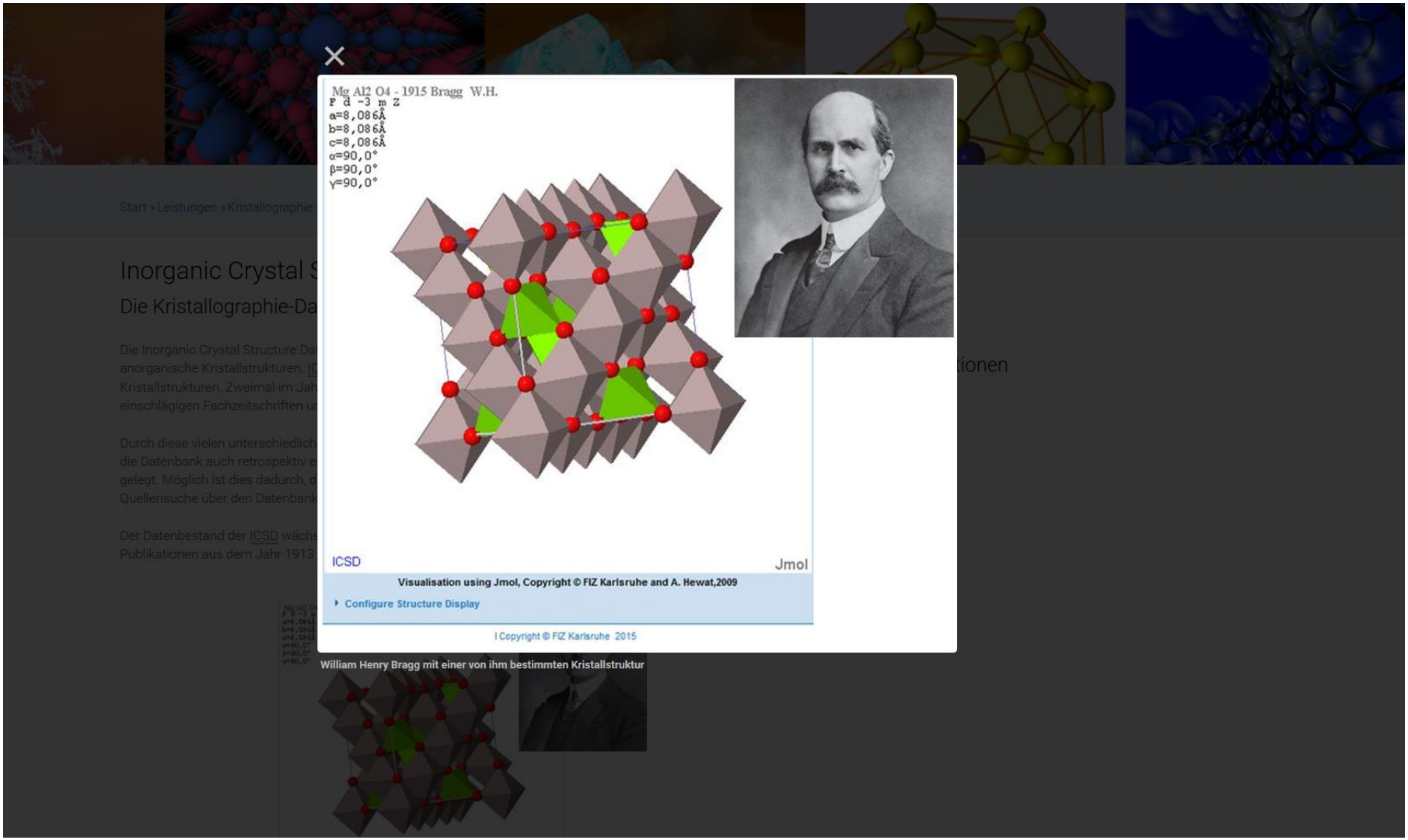
Only selected examples here.

Information Type	Description	Example, where applicable
Team code management	Tool or platform for teams creating code together	BitBucket
Filesharing	Tool for sharing files in the cloud	Dropbox
Facebook RSS	RSS provided by publisher directly via Facebook	Environmental Health Perspectives on FB alerts
FDA RSS	One-off code; United States Food and Drug Administration provides RSS directly; no library intermediation	
Patents	Patent database or search tool	Google Patents
Code simulating x-ray spectroscopes	Specialized code; one-off descriptive code	FDMNES
Crystallographic programs	Tools to view crystal structures developed for Rietveld analysis of neutrons, nuclear, and magnetic or X-ray powder diffraction	FullProf Suite
Database inorganic crystal structures	Peer-reviewed completely identified structures since 1913; one-off descriptive code	FindIt
Cheminformatics software platform	Visualization and drawing tools for chem- and bioinformatics	ChemAxon
Data analysis/graphing	Tool for manipulating and understanding data	Open Babel (chemistry-specific)

FindIt (FIZ Karlsruhe)

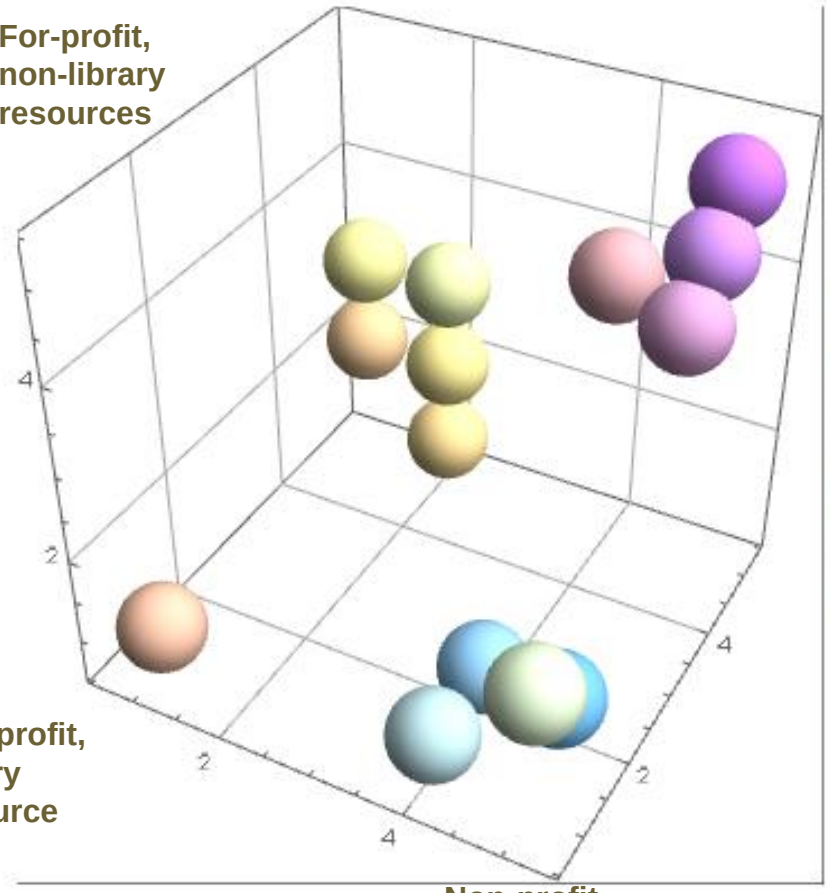


FindIt (FIZ Karlsruhe)



Data Description & Analysis

Resources Common to Both Datasets (Fieldwork & Screenshot Data)

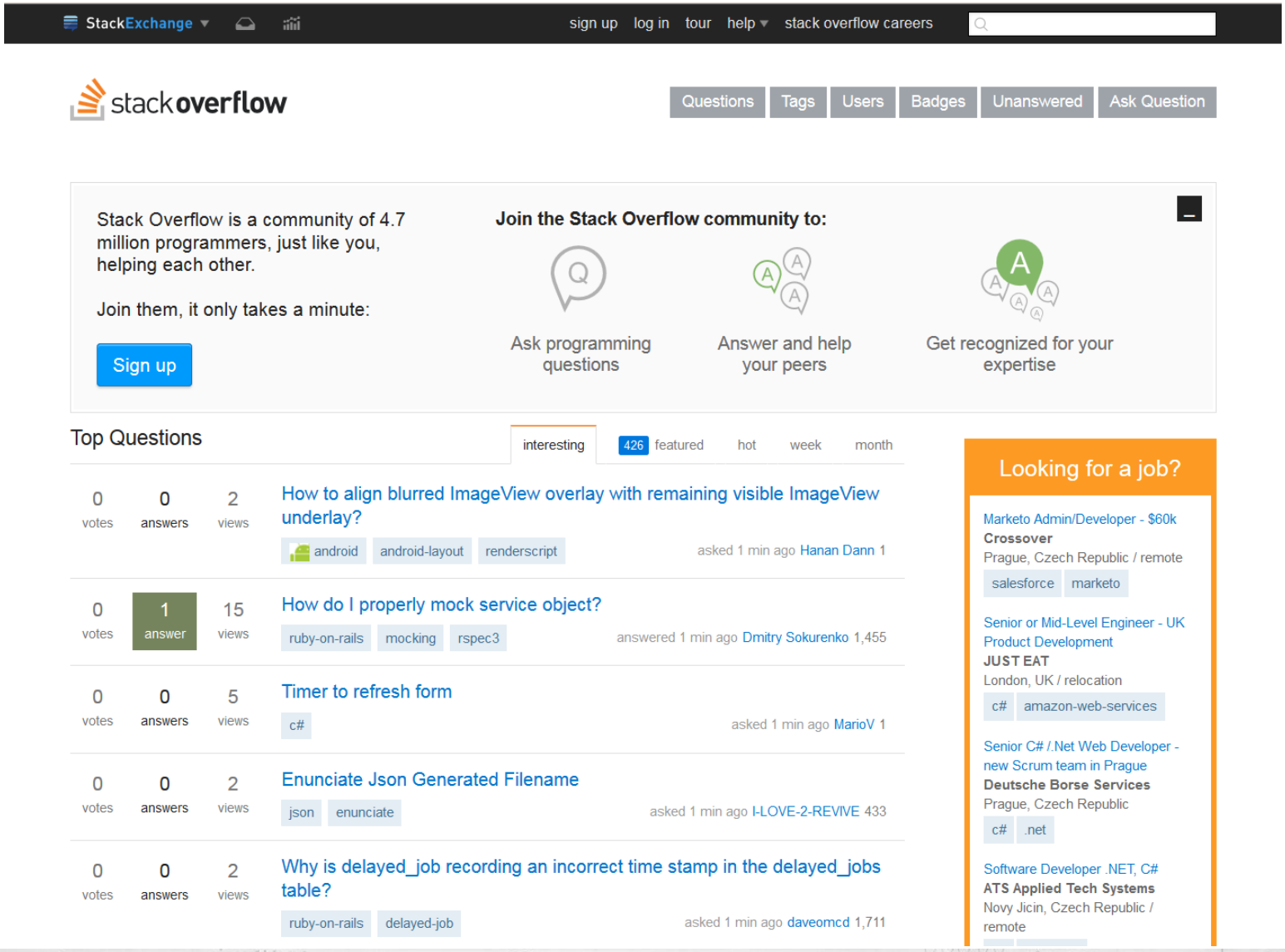


For-profit, library resources

- Web of Science
- Reaxys
- Nature
- Science Direct
- arXiv
- Google Patents
- Google Scholar
- StackOverflow
- Google CZ
- Journal of Cheminformatics
- Wikipedia EN
- PubMed
- RDKit
- MetaCentrum

e-Research tools beyond library infrastructures

Stack Overflow/Programmer Forum



MetaCentrum

9. 3. 2015: **Big data - Hadoop in MetaCentrum**
METACentrum has commissioned a dedicated Hadoop cluster for big data processing...

From October 8 to 9 the Pilsen's /storage/plzen1/ will be unavailable due to moving on a new hardware...

Welcome to the MetaCentrum Virtual Organization portal!

MetaCentrum VO is catch-all virtual organization of the Czech National Grid Organization **MetaCentrum NGI**. MetaCentrum operates and manages distributed computing infrastructure consisting of **computing and storage resources** owned by CESNET as well as resources of co-operative academic centres within the Czech Republic. Users registered in MetaCentrum get access to a wide range of **application software** and utilities free of charge, for example Matlab, Maple, or Gaussian.

To become a MetaCentrum VO member, complete our **application form**, please. MetaCentrum membership is free for researchers and students of academic institutions in the Czech Republic, the members of the **CESNET** association.

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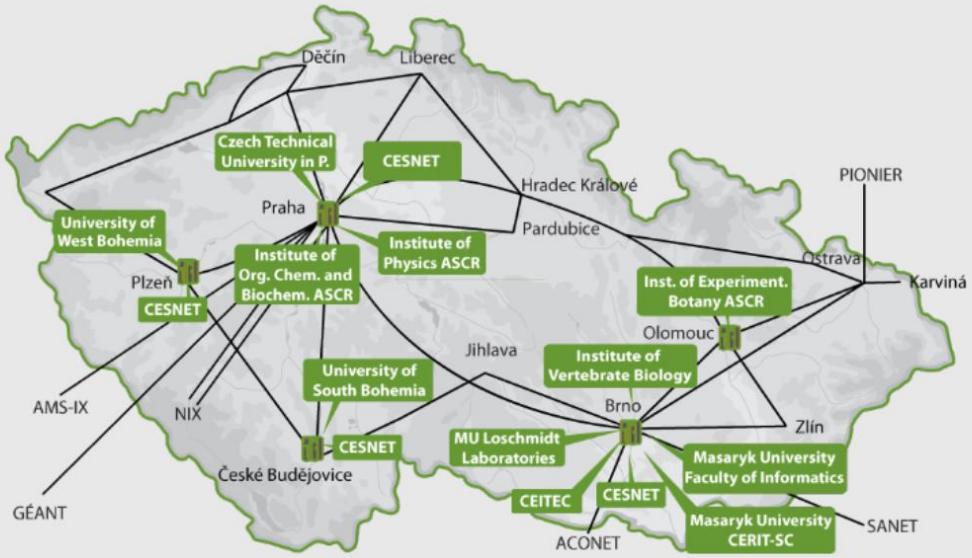
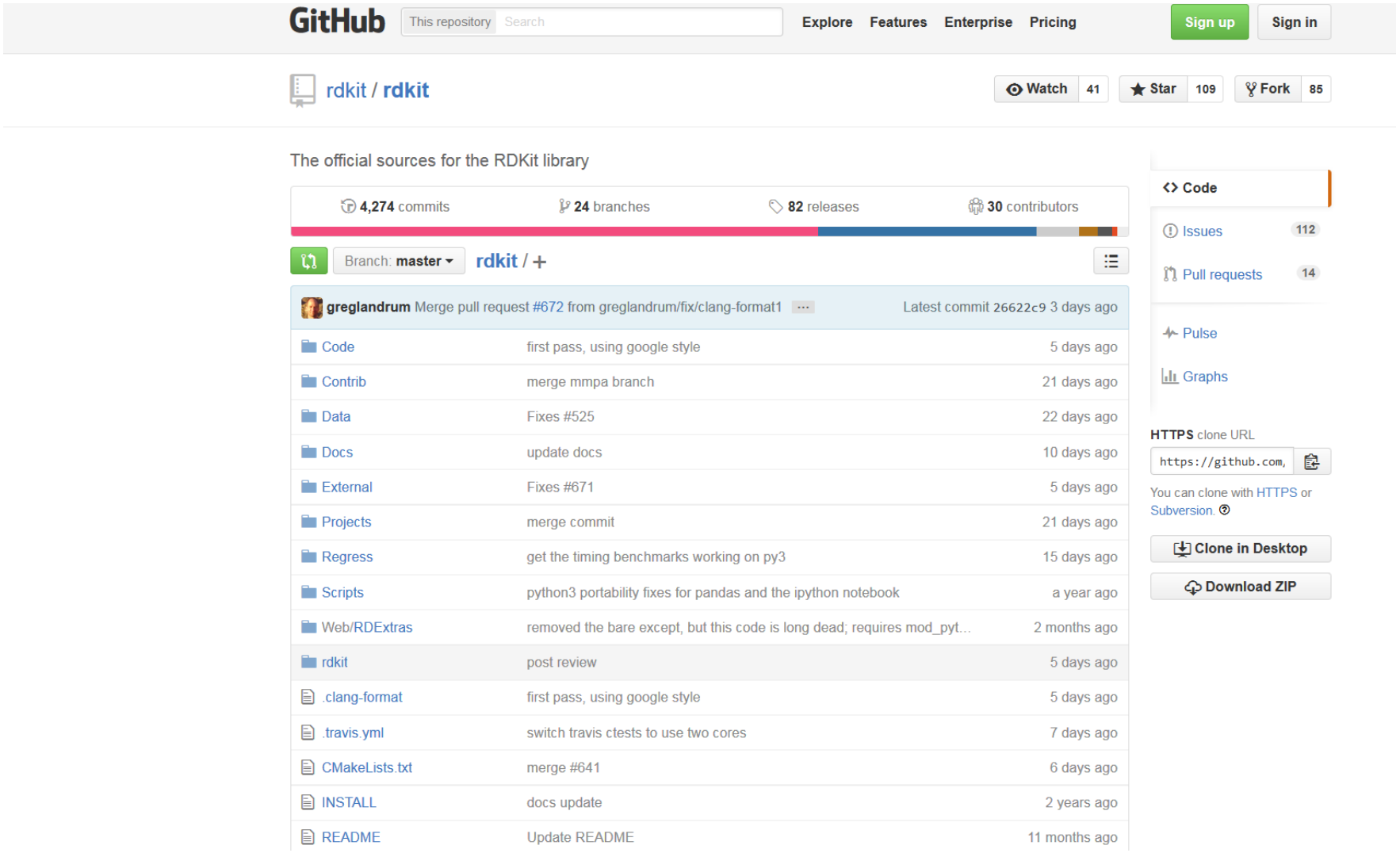


Projects:

At present the MetaCentrum sites are: Masaryk University in Brno (**Center CERIT-SC** and Faculty of Science), **UOCHB**, University of West Bohemia in Pilsen (**Faculty of Applied Sciences**), University of South Bohemia (**Faculty of Science's cluster**), Academy of Sciences (FZU), **Departement of Telecommunication Engineering FEL ČVUT**, and **CESNET z.s.p.o.**.

RDKit, Cheminformatics



GitHub This repository Search Explore Features Enterprise Pricing Sign up Sign in

rdkit / rdkit Watch 41 Star 109 Fork 85

The official sources for the RDKit library

4,274 commits 24 branches 82 releases 30 contributors

Branch: master rdkit / +

greglandrum Merge pull request #672 from greglandrum/fix/clang-format1 ··· Latest commit 26622c9 3 days ago

Code	first pass, using google style	5 days ago
Contrib	merge mmpa branch	21 days ago
Data	Fixes #525	22 days ago
Docs	update docs	10 days ago
External	Fixes #671	5 days ago
Projects	merge commit	21 days ago
Regress	get the timing benchmarks working on py3	15 days ago
Scripts	python3 portability fixes for pandas and the ipython notebook	a year ago
Web/RDExtras	removed the bare except, but this code is long dead; requires mod_pyt...	2 months ago
rdkit	post review	5 days ago
.clang-format	first pass, using google style	5 days ago
.travis.yml	switch travis ctests to use two cores	7 days ago
CMakeLists.txt	merge #641	6 days ago
INSTALL	docs update	2 years ago
README	Update README	11 months ago

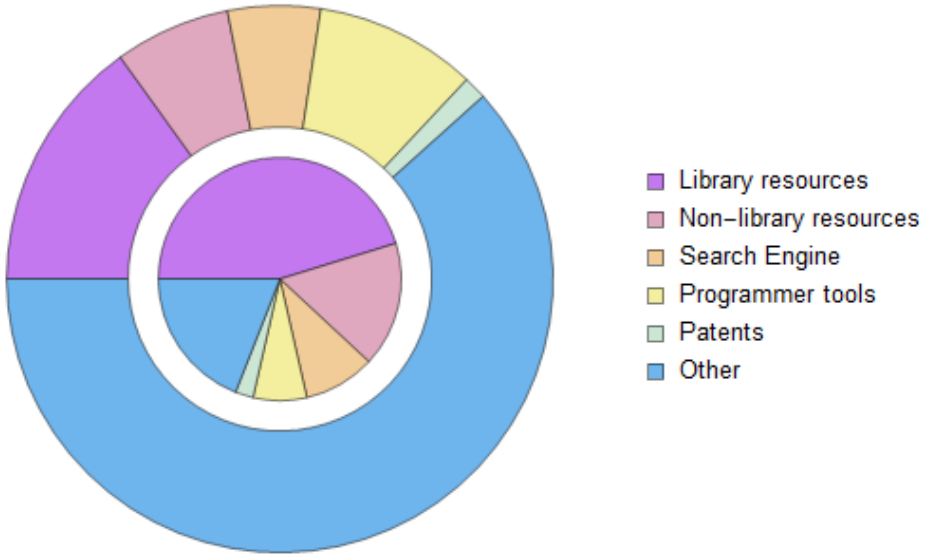
Code
Issues 112
Pull requests 14
Pulse
Graphs

HTTPS clone URL
https://github.com,
You can clone with HTTPS or Subversion.
Clone in Desktop
Download ZIP

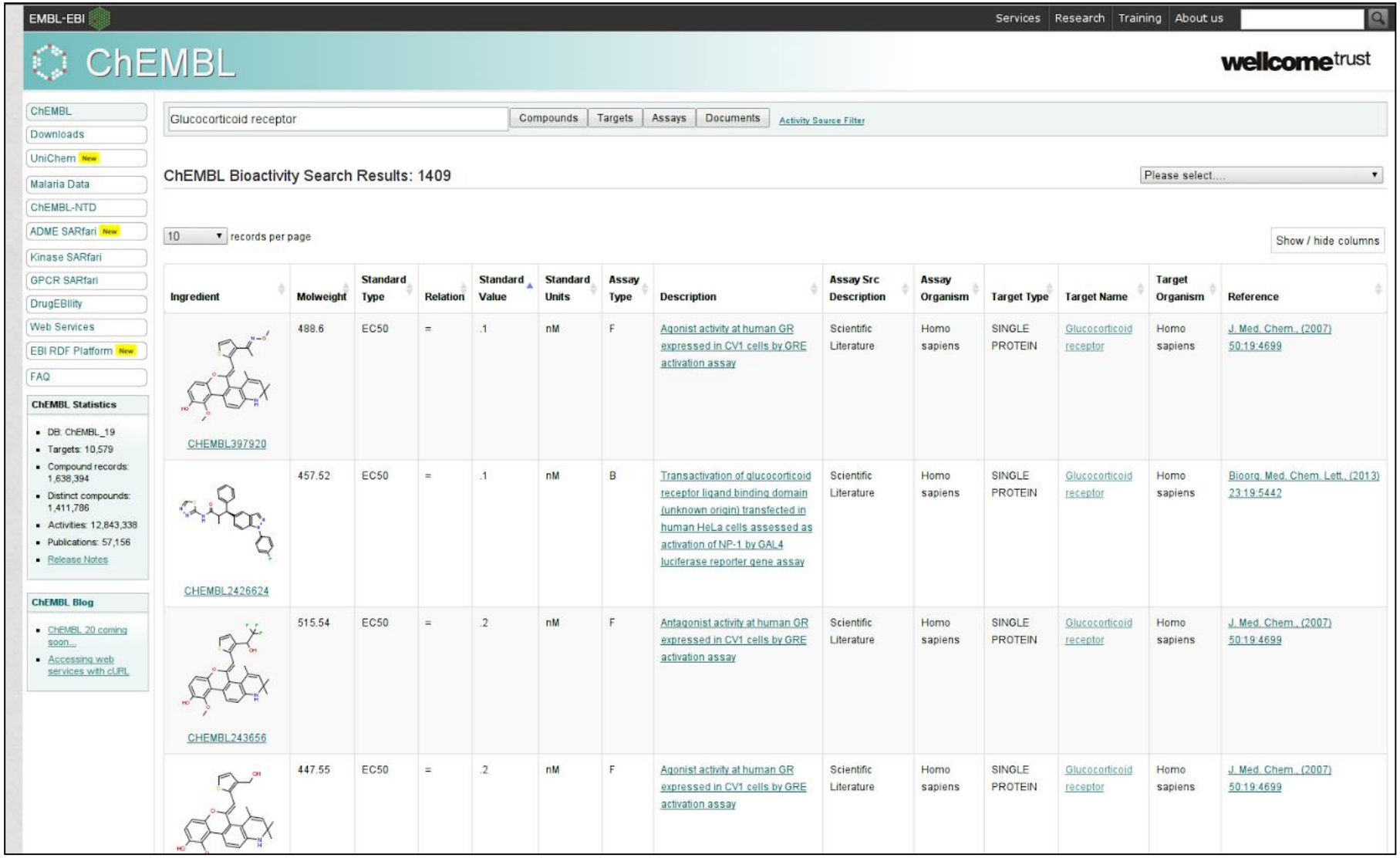
Data Description & Analysis

Resources By Type (Fieldwork & Screenshot [inner pie] Data Comparison)

Type	Number (Screenshots)	Number (Fieldwork)
Traditional library journals or platforms	20	11
Non-library science resources or platforms	6	5
Search Engine	4	4
Programmer Tools	3	7
Patents	1	1
Other	8	45
TOTAL	**42**	**73**



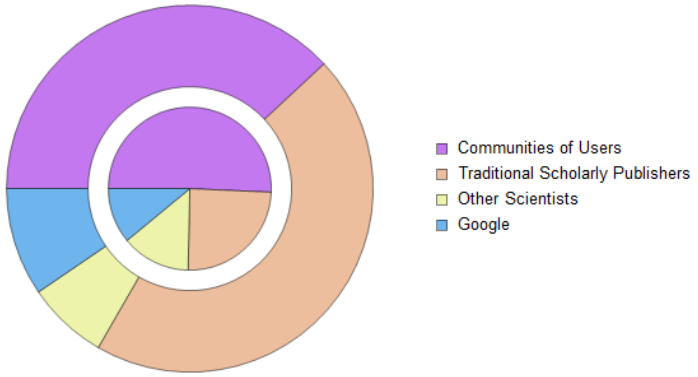
“Other”: ChEMBL



Data Description & Analysis

Resources By Mode of Production (Fieldwork & Screenshot [outer pie] Data Comparison)

Type	Number (screenshots)	Number (fieldwork)
Traditional Scholarly Publishers	19 (arXiv coded as Communities of Users because of its global review board)	18 (higher than "library" resource code because of open access journals which have traditional mechanisms but do not require library intermediation)
Communities of Users	16	37
Google	4	10
Other (research groups, conferences)	3	8
TOTAL	**42**	**73**



“Other”: Raymond Research Group

Raymond Group Research

Home | Research | Members | Photos | Ken Raymond | Publications | Links

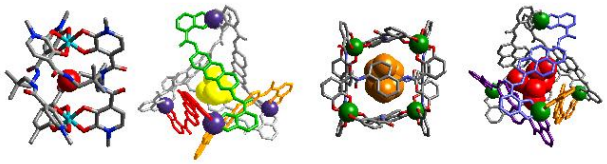
Supramolecular Coordination Chemistry

Introduction

The Raymond group has developed a predictive design strategy resulting in the synthesis of various high-symmetry coordination clusters, including M_2L_3 helicates and mesocates; M_4L_6 and M_4L_4 tetrahedra; M_6L_6 and M_8L_8 cylinders; and M_8L_6 octahedra. These examples all focus on the coordination of three bidentate chelators to a tri- or tetravalent metal ion in a pseudo-octahedral fashion at the apices of the clusters to generate local three-fold symmetry at these metal centers. These chelators are contained in rigid, symmetric multi(bidentate)-ligands which supply the other symmetry elements of the cluster (2-fold, 3-fold, or mirror plane). By simultaneously fulfilling the symmetry requirements of both the ligand and metal centers, discrete high-symmetry clusters are generated under thermodynamic control. We are exploring the self-assembly of new clusters, thermodynamics and kinetics of cluster formation and host-guest interactions, electrochemistry, luminescence, ligand exchange, and chiral resolution and isomerization in the context of these supramolecular clusters.

Cluster Design and Synthesis

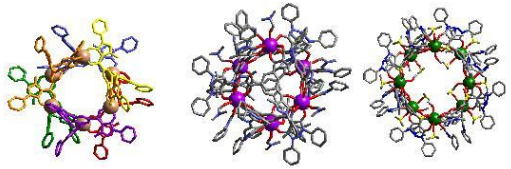
Our design strategy has already allowed us to generate many different cluster architectures, as mentioned above. Self-assembly of helicate complexes of the formula $[M_2L_3]^{6-}$ and tetrahedral complexes with the formula $[M_4L_6]^{12-}$ can be achieved via the self-assembly of an octahedrally coordinating, trivalent metal ion (e.g., Fe^{3+} or Ga^{3+}) with an appropriate bis-bidentate ligand, L. The use of diamagnetic Ga^{3+} in the synthesis of these clusters has enabled study of these novel molecules by NMR spectroscopy, as these highly symmetric molecules have a distinctly simple spectrum, shifted from that of the free ligand.



1 2 3 4

Three-fold symmetric tris-bidentate ligands have been used to synthesize clusters with triangular faces, such as M_4L_4 tetrahedra, M_6L_6 and M_8L_8 rings, and M_6L_8 octahedra. Again a labile tri- or tetra-valent metal ions is used as the vertex of the given topology, but the ligand comprises a face of the cluster, rather than an edge as in the earlier example.

A continuing pursuit in our laboratories focuses on the synthesis of new cluster topologies, as well as generating larger versions of the clusters we already have in hand. For example, the use of a five-fold symmetric ligand may allow for formation of a cluster with icosahedral symmetry, whereas using "expanded" versions of our new ligands, we hope to synthesize clusters with larger cavities.



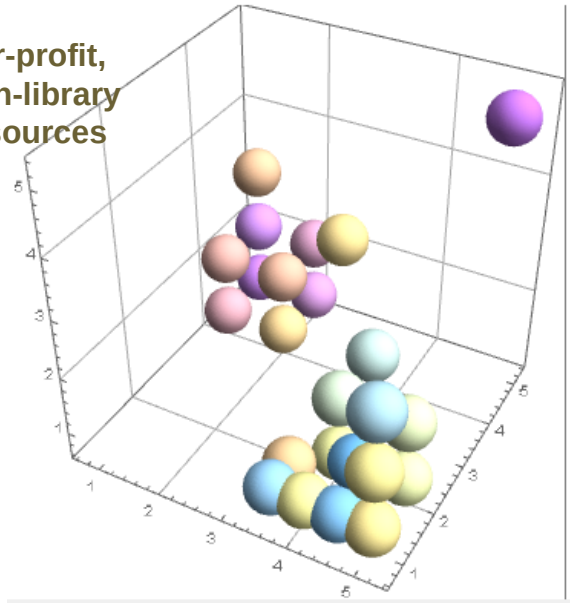
5 6 7

Data Description & Analysis

Sample Visualizations, Participant “Kurt”: Fieldwork (L) & Screenshot Data (R)

For-profit, non-library resources

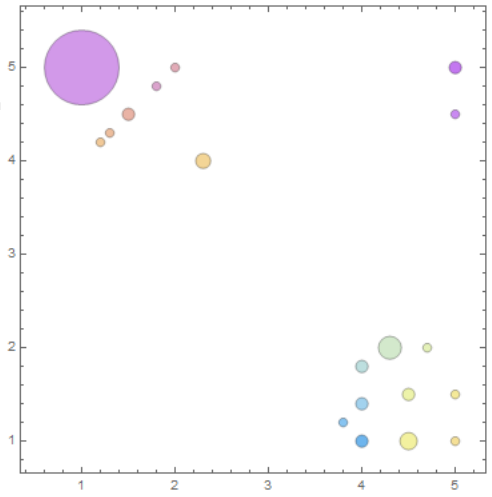
For-profit, library resource



- Web of Science
- eBooks and docs
- Google Patents
- Google Scholar
- StackOverflow
- Gtalk
- BitBucket
- GitHub
- Google CZ
- Journal of Cheminformatics
- RSS Nature News
- RSS Nature Reviews
- Espacenet
- Wikipedia EN
- PubMed
- RDKit
- SciPy
- Open Babel
- KNIME
- Zinc–fans
- RDKit discuss 1
- RDKit discuss 2
- Cheminformatique
- UDOCK

Non-profit, non-library resources

For-profit, non-library resources



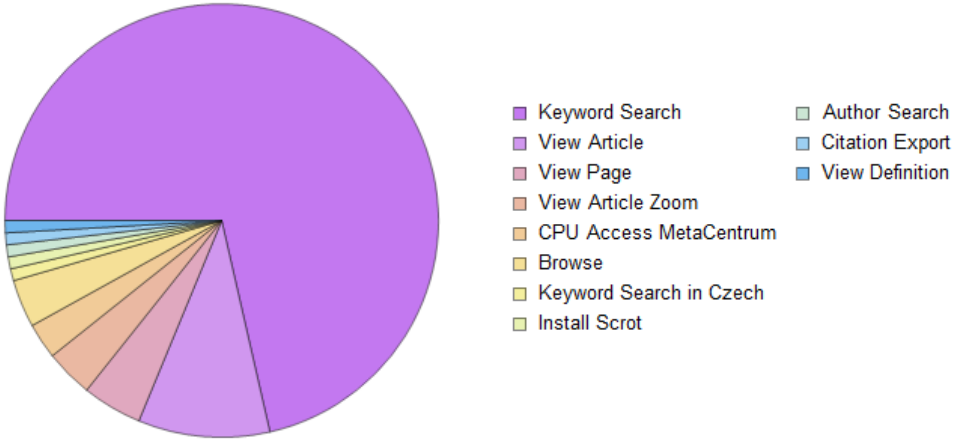
For-profit, non-library resources

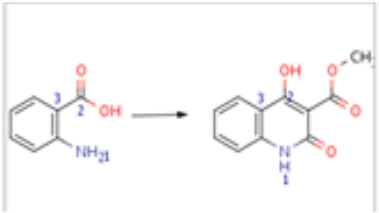
- Reaxys
- J. of Invest. Derm.
- Google CZ
- Google Scholar
- Google Patents
- J. of Cheminformatics
- All Things Metathesis
- StackOverflow
- Sigma–Aldrich
- Unix Interface
- Linux Doc. Man. Page
- MetaCentrum
- SIS
- ChEMBL
- Wikipedia English
- RDKit
- PubMed
- J. of Med. Chemistry
- PostgreSQL Support

Non-profit, non-library resources

Data Description & Analysis

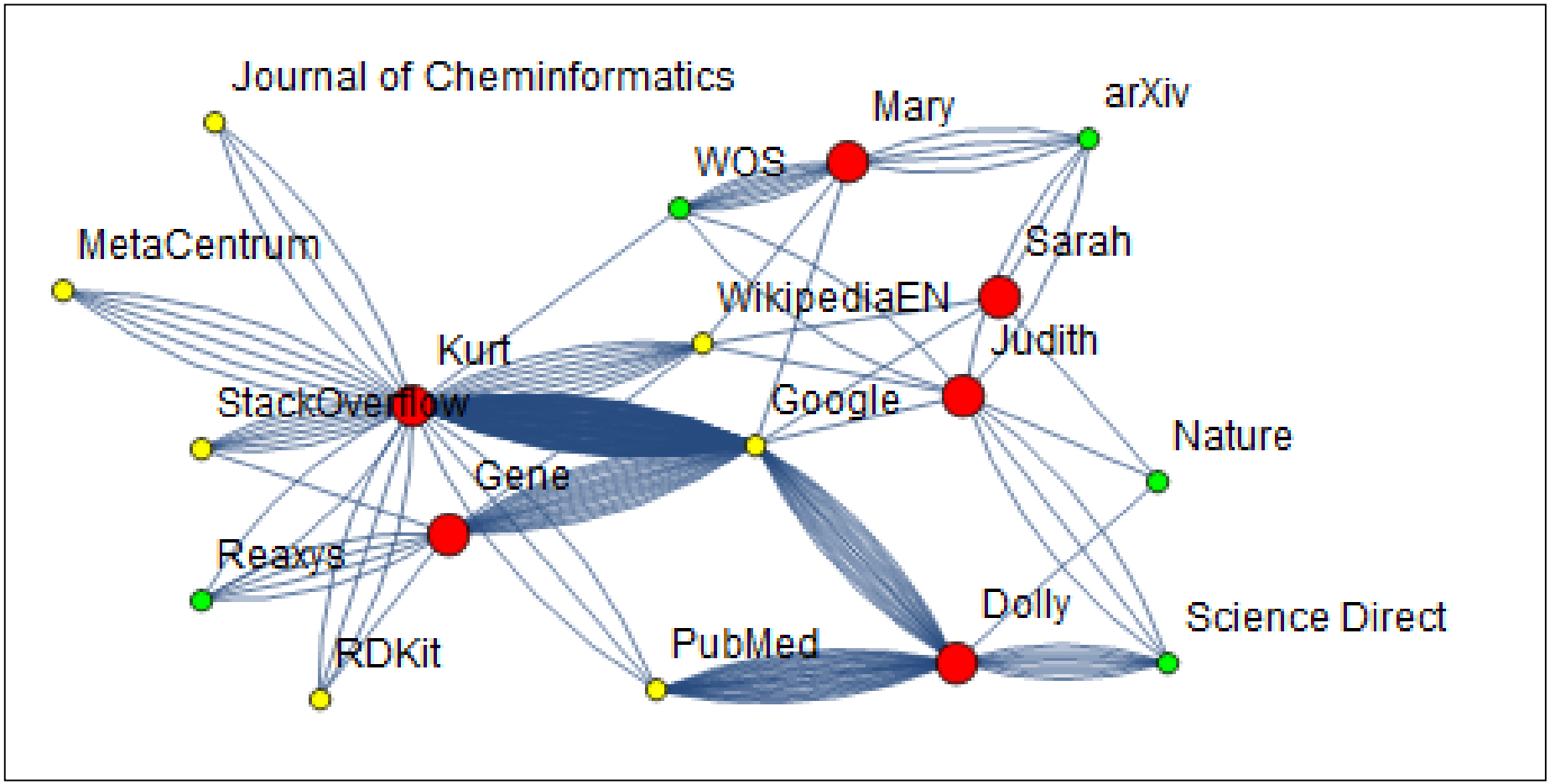
Screenshot Behavior (L; “Kurt”) & Sample of Detail (R; “Gene”/2 behaviors)



Activity	Occurrence	Source(s)	Examples
Keyword search	16	Google CZ	sql select random rows brufen wiki
Search on Structure Drawing	2	Reaxys	

Data Description & Analysis

Network Visualization of Screenshot Data and Top Resources Used by Participants



Selected Findings/Thoughts

All participants in this study utilized **data manipulation/analysis tools**. However, no one tool was preferred. The cheminformaticians used open source KNIME.

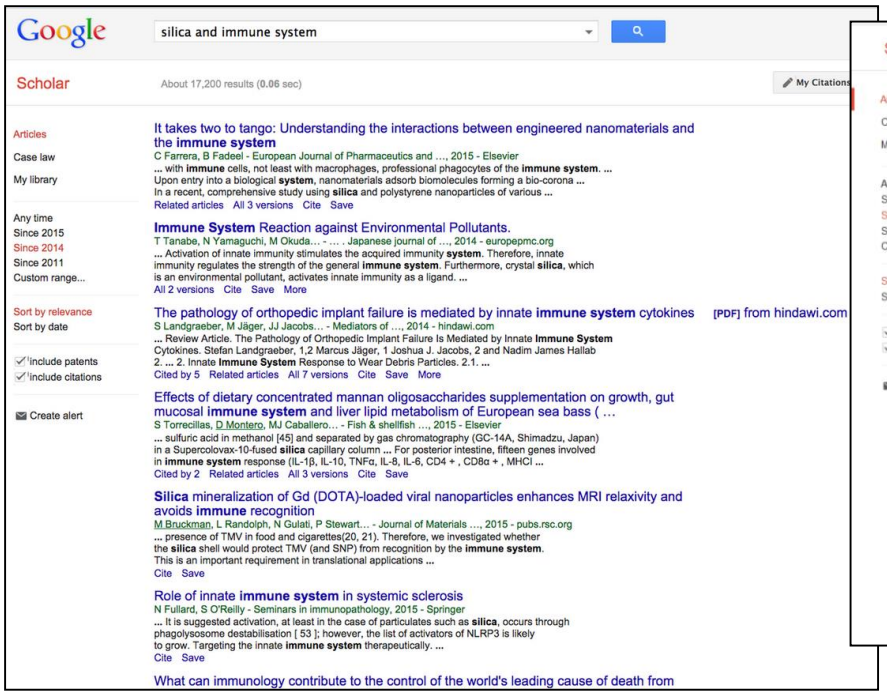
Even those participants who had had information literacy/library resource training created **simple search queries** and did not use library websites. What does this mean in terms of instructional and library web design? We must do better.

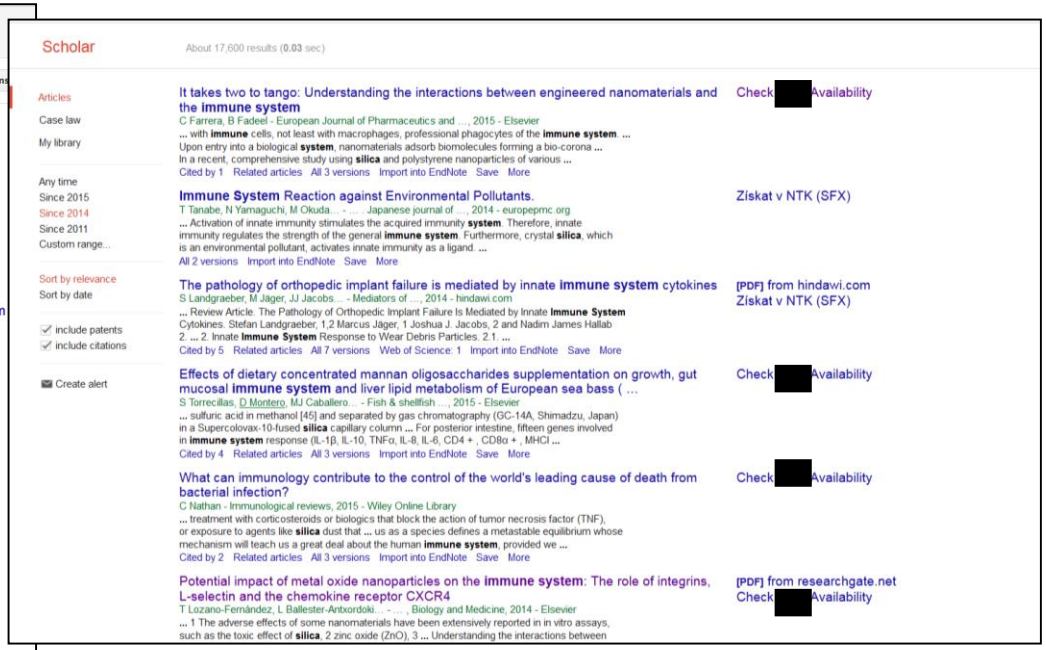
Four participants used Google (Google CZ, Google US, or Google Scholar) as a discovery tool. **No participants in this study used library discovery tools**. What does this mean over the long-term horizon? Should we give up on our discovery tools and use Google?

The one participant who had library links in Google Scholar theoretically enabled **did not notice** they were not working properly (this was the highest-ranked professor in this study). We must ensure students and scholars are aware of library links in Google Scholar...and perhaps even approach Google Scholar as a community to have influence on its functionality (?).

The cheminformaticians **cannot do their research** without their national computing infrastructure and open datasets in their field. But large open datasets have curation challenges; e.g., ChEMBL (Papadatos et al. 2015)

Data Example: Most Advanced Scholar in Study Underutilized/Underestimated Library Resources





DG: "[My] library is connected to my google scholar searches and brings up availability automatically."

…but this was note the case, according to screenshot data (L); ideal (R), black squares (library name hidden to ensure participant anonymity)

Implications for e-Research Support and Service Design

Libraries will likely be increasingly disintermediated from e-Research generally unless they integrate themselves more into **real scientific workflows**.

This is extremely difficult, because each discipline and each user have unique needs and demands—if the findings from this study hold true in future studies over larger populations and across disciplines.

Though research findings from such a study cannot be generalized, using interim research findings can **positively inform agile, user-centered e-Research support and service development** in the classroom and online (two examples in next slides).

How do we as a community collaborate better in terms of e-Research support? The information universe is extremely fragmented, particularly in terms of open data and tools, and is **confusing to even experienced researchers**.

The six scientists in my study had no concept of something which might be considered "**data literacy**"; they assigned trust to providing institutions to data and information which had not been "authenticated" in a traditional scholarly publishing sense but relied on other indicators of quality (i.e., trust in a particularly community of peer researchers, institutional provider, etc.).

Instructional Example, Design Informed with Data

- 30 minutes only; four-part cycle developed with civil engineering professors
- Based directly on research data analysis (i.e., ethnographic data harvested before Autumn 2014)

1. Beyond Google: QuickStart to Effectively Using Information Resources
2. The Scholarly Publishing/Research Universe: What You Might Not Know Yet & Tools to Help You
3. Professional Scientific Writing for Civil Engineers: Useful Resources and Tips
4. Evaluating Citation Metrics, Journal Impact Factor, and the World of the Scientific Author

HCI Example: Library Web Design Based on Data First

- Minimize clicks to content
  - (i.e., wherever possible, try to make useful content accessible within one click)
- Replicate shopping site functionality
  - Easy login that tells the user he or she is authenticated to the library, even from home
  - Include online payment options
- Create parallel design in English—not all pages have to be there, but overall architecture should match that of the original language pages
  - This addresses the “striving” nature of the surrounding technology universities, enabling scholars to practice their English
  - Provides a welcoming environment to the increasing numbers of international students on campus

Contact Information

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Czech National Library of Technology

Head, Office for Specialized Academic Services

stephanie.krueger@techlib.cz

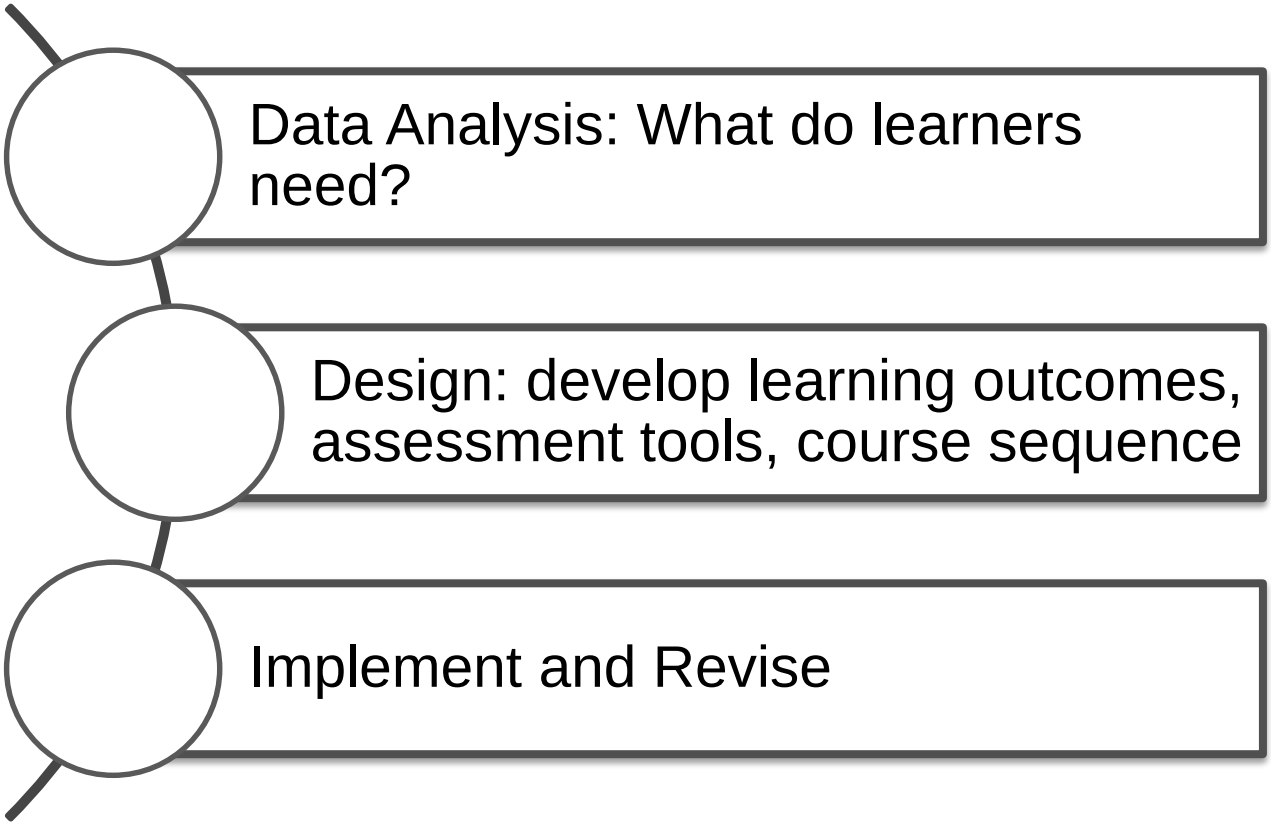
Full dissertation referenced here to be publishing openly with data, if it is possible; otherwise, I will provide codebooks, data gathered, and advice upon request

- Title: *Beyond the Paywall: A Multi-Sited Ethnographic Examination of the Information-Related Behaviors of Six Scientists*
- Planned for publication by Spring/Summer 2016 at: http://edoc.hu-berlin.de/

Extra Slides

Related to original abstract; for those interested.

Backward Design for Instruction

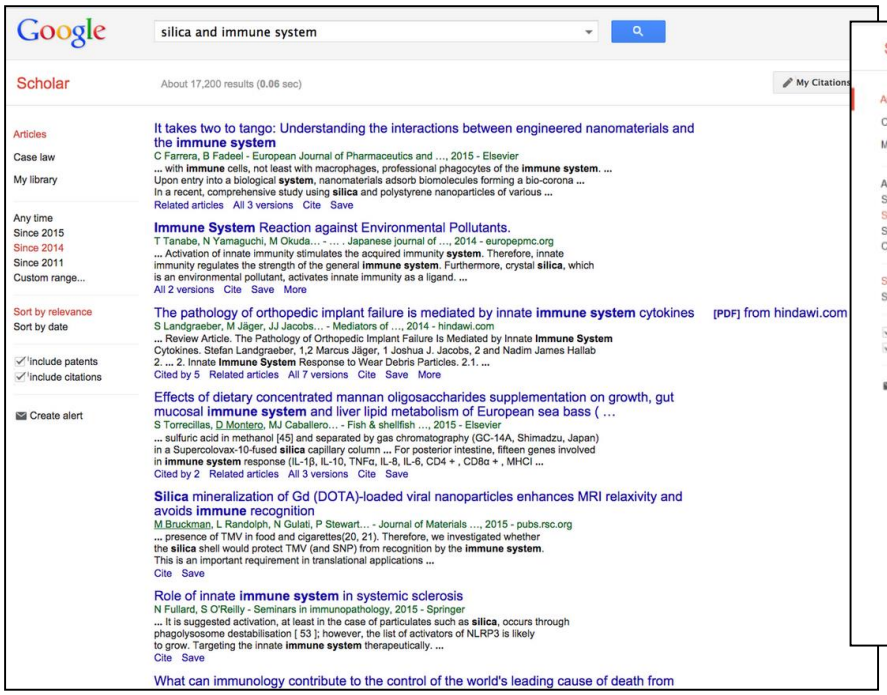


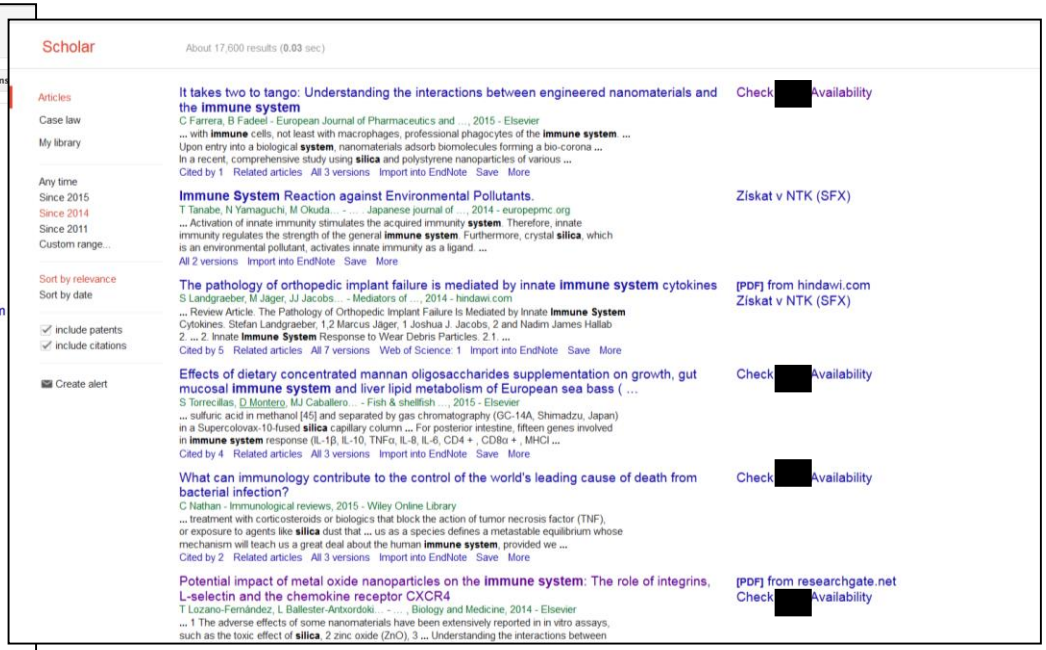
Instructional Topics, Pilot One

- 30 minutes only; four-part cycle developed with civil engineering professors
- Based on research data analysis as of Autumn 2014

- Beyond Google: QuickStart to Effectively Using Information Resources
- The Scholarly Publishing/Research Universe: What You Might Not Know Yet & Tools to Help You
- Professional Scientific Writing for Civil Engineers: Useful Resources and Tips
- Evaluating Citation Metrics, Journal Impact Factor, and the World of the Scientific Author

Data Example: Two Most Advanced Scholars in Study Underutilized/Underestimate Library Resources





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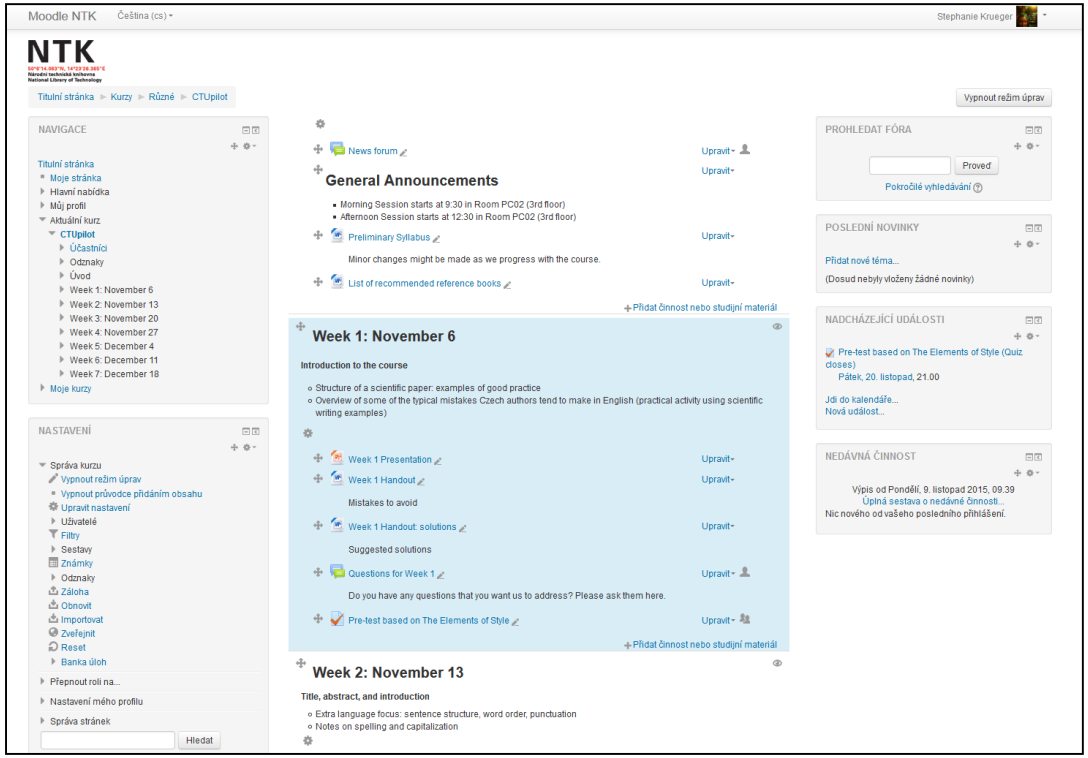
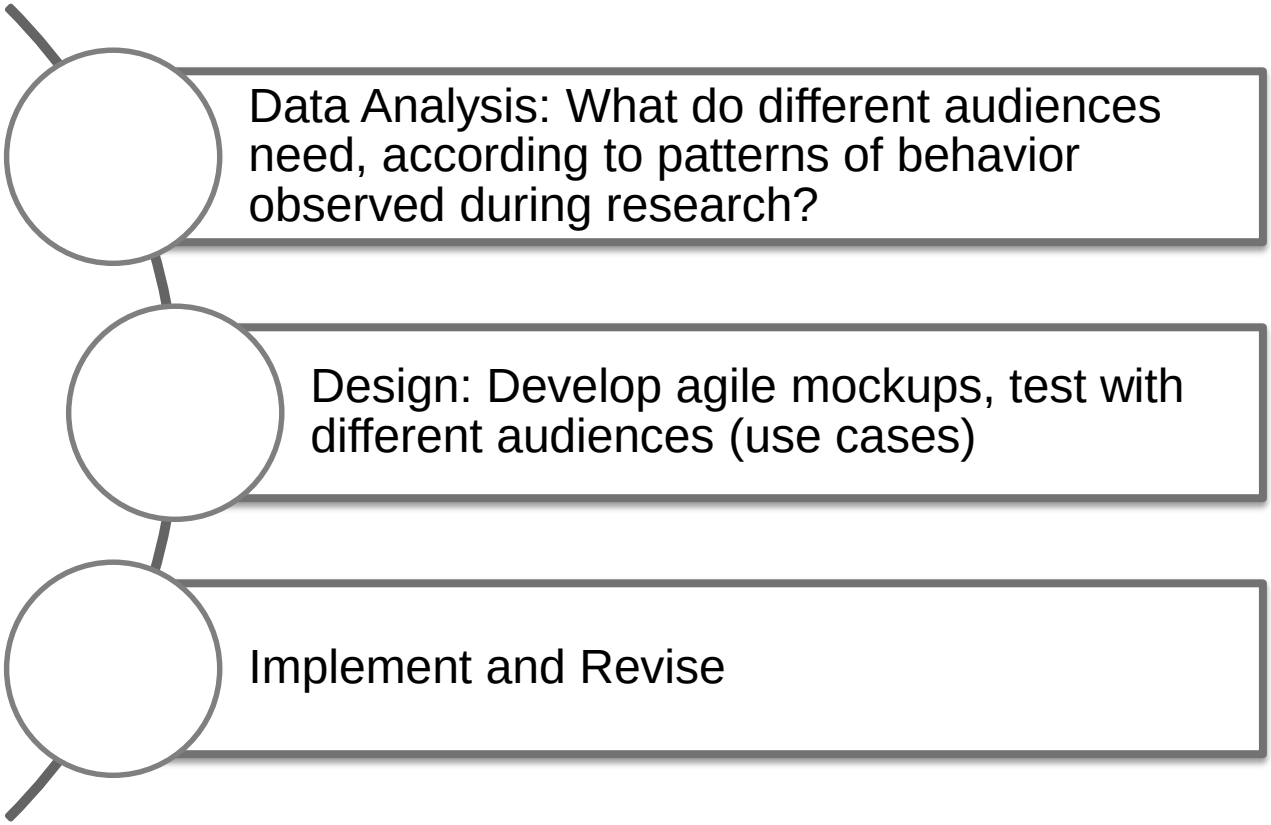
Pilot Two: More Writing, Critical Thinking

- 1.5 hours; seven sessions; currently in process
- Focused even more on scientific writing, promotion, publishing
- Library:
  1. Hosts sessions
  2. Hosts/manages course on Moodle, but
  3. Is team leader/project manager and integrated into one session only, using practical examples focused on scientific writing, publication, promotion



HCI Context: User-Centered Design



HCI Example: Improving Online Experience

- Minimize clicks to content
  - (i.e., wherever possible, try to make useful content accessible within one click)
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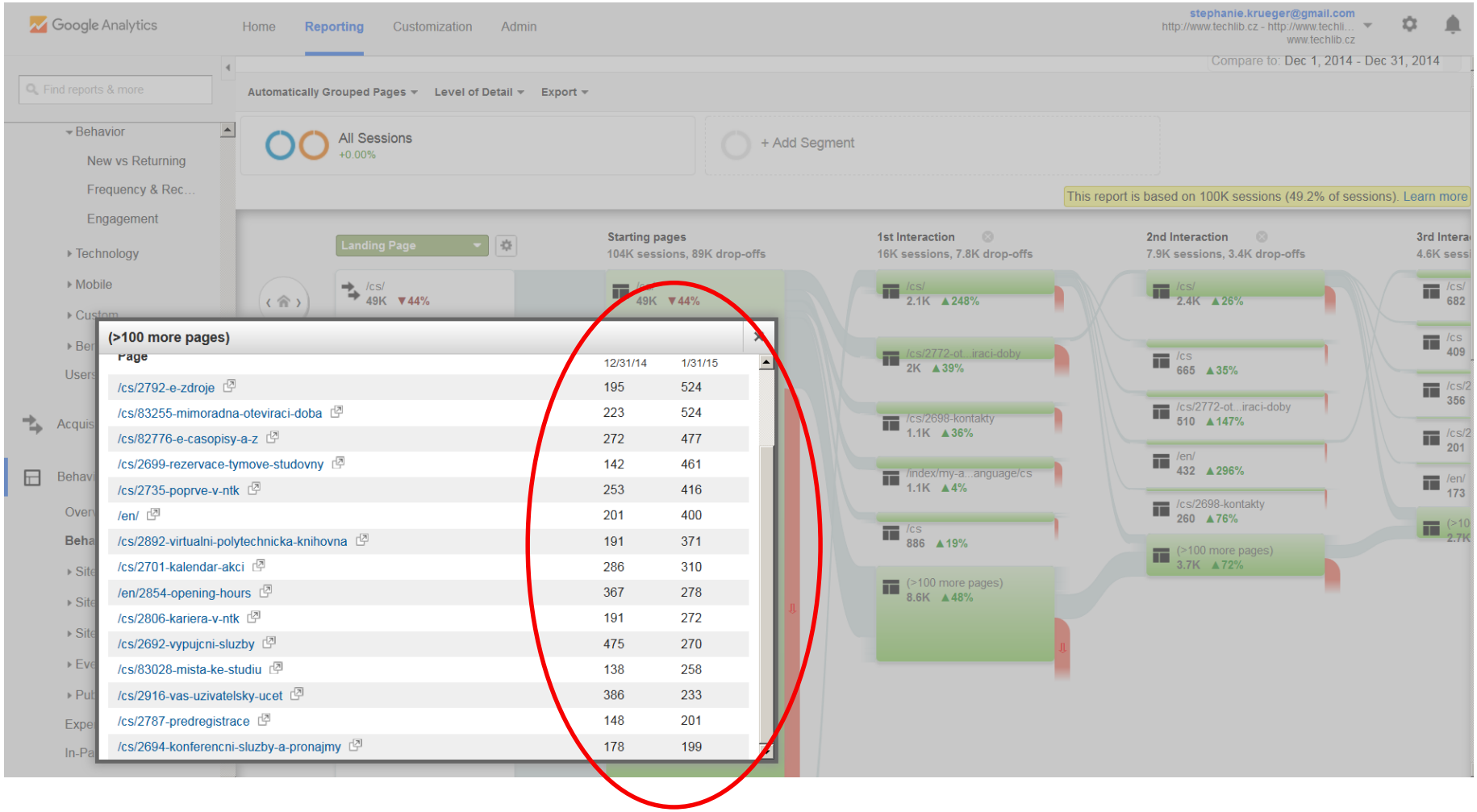
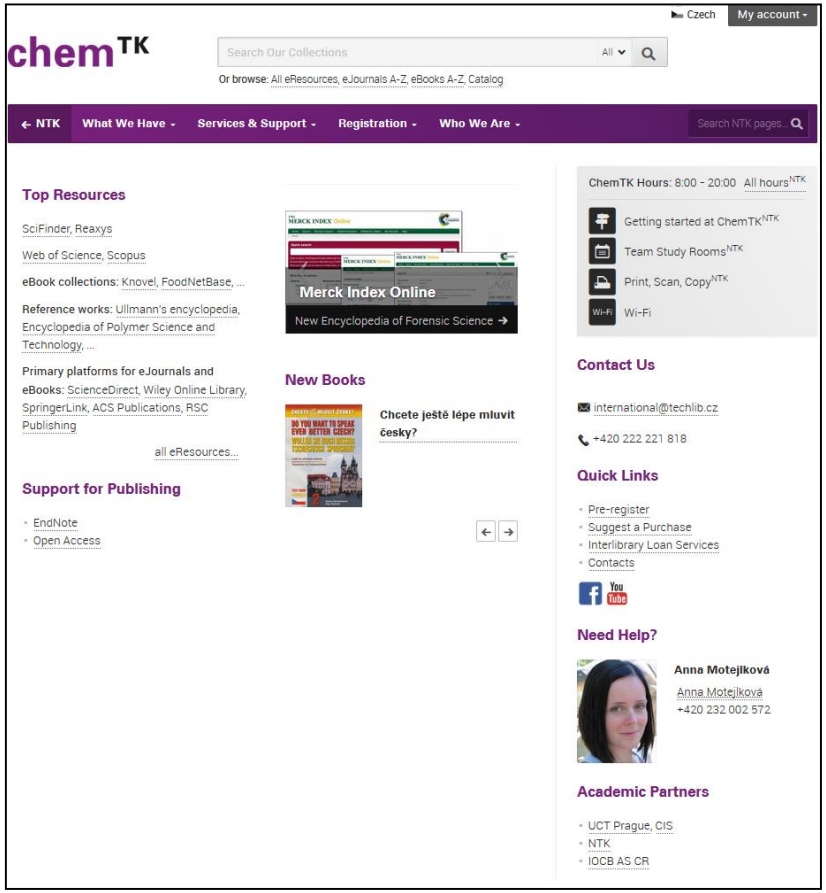
  - Provides a welcoming environment to the increasing numbers of international students on campus

HCI Example: Monitoring Implementation



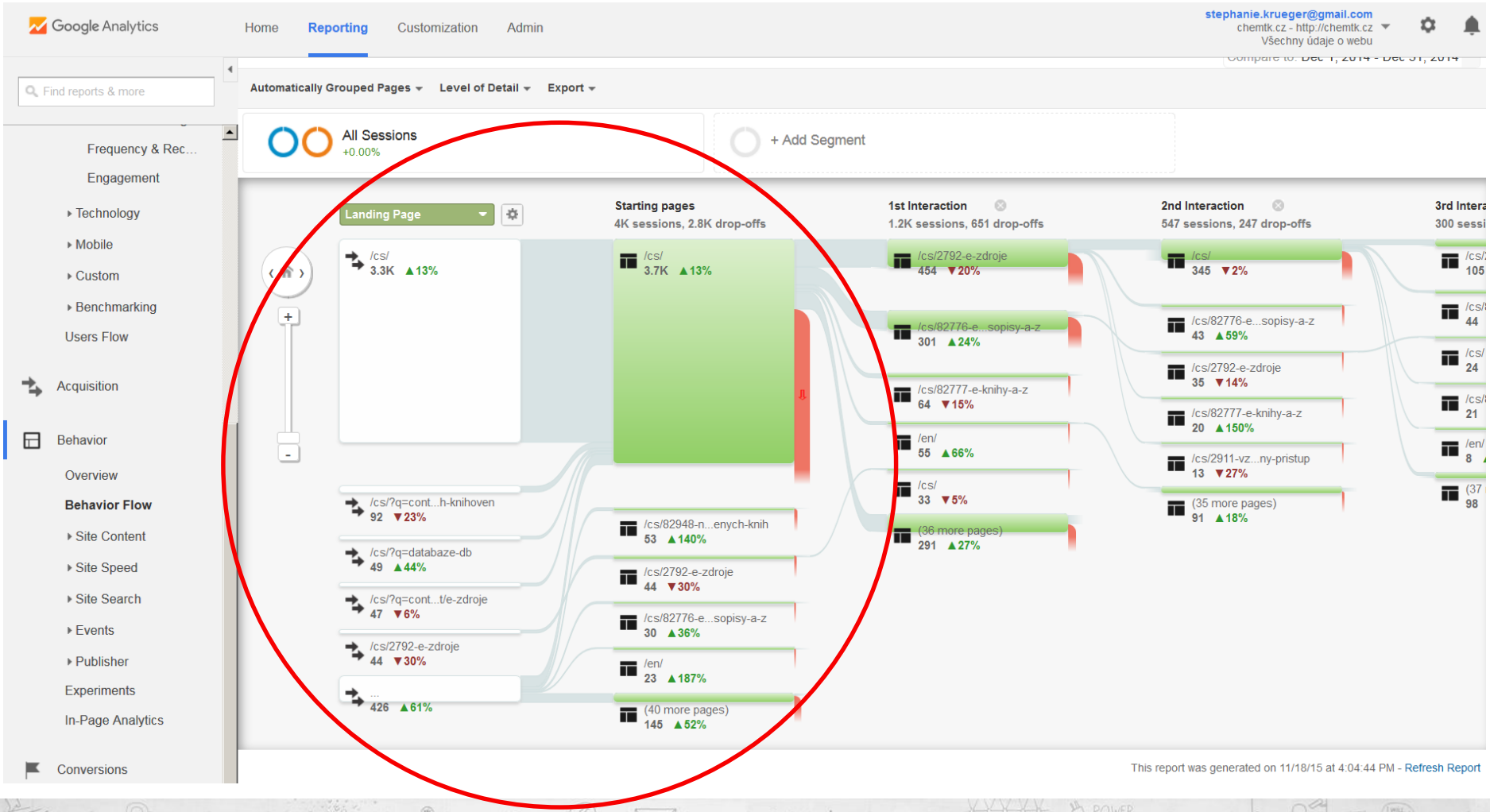
Page	12/31/14	1/31/15
/cs/2792-e-zdroje	195	524
/cs/83255-mimoradna-oteviraci-doba	223	524
/cs/82776-e-casopisy-a-z	272	477
/cs/2699-rezervace-tymove-studovny	142	461
/cs/2735-poprve-v-ntk	253	416
/en/	201	400
/cs/2892-virtualni-polytechnicka-knihovna	191	371
/cs/2701-kalendar-akci	286	310
/en/2854-opening-hours	367	278
/cs/2806-kariera-v-ntk	191	272
/cs/2692-vypujcni-sluzby	475	270
/cs/83028-mista-ke-studiu	138	258
/cs/2916-vas-uzivatelsky-ucet	386	233
/cs/2787-predregistrace	148	201
/cs/2694-konferencni-sluzby-a-pronajmy	178	199

HCI Example: Improving Online Experience



- Version of main entry page modified by particular stakeholder community for their own purposes
- Focus on:
  - Community-specific subscription databases
  - Support for publishing

HCI Example: Monitoring Implementation



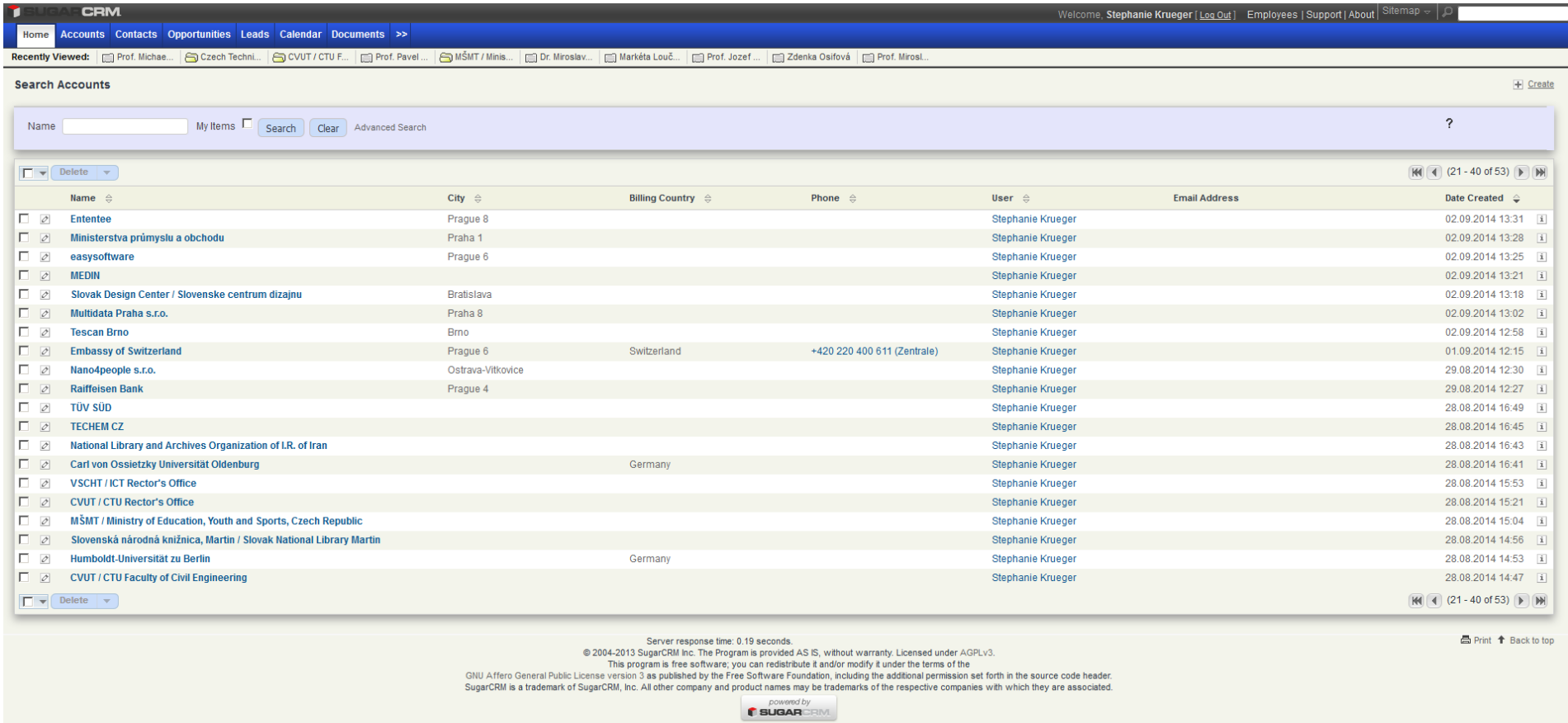
Future Research Plans: Basic and Applied

Basic (ideal; can be done without funding, but takes time and commitment of the IS community for less “patchy” research agendas):

- Apply sample research method to new groups of scientists
- Compare results against first set
- Repeat

Applied:

- After pilots, acquire funding for ongoing courses, with **credit** for students (a new concept in the Czech context)
- Google Scholar library links: how to approach Google to have some kind of library advisory board? How might we as a community have any influence over our links?
- Monitor behavior patterns for ALL online library usage paths (including: discovery, various eResources, etc.) and improve these, making more demands on vendors to respond to us

Future Plans: CRM (Sugar Open)

NTK
50°6'14.083"N, 14°23'26.365"E
Národní technická knihovna
National Library of Technology