

Physical Science (Virtual) Research Spaces



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Talk

- Where do we do research?
- How and where do we find, access and interact with, research materials?
- How do we deposit research data (and what do we deposit)?
- The e-World



Smart Places & Things

We need Smart Labs and Smart Libraries



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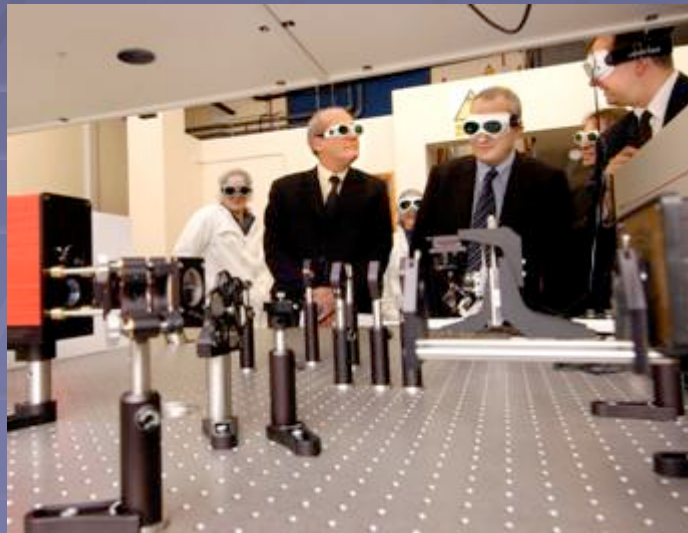
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UCB Guidelines

- Precise campus standards for space utilization are elusive, due to the enormous variety and complexity of research space: but precision is not the point. What UC Berkeley requires is a simple and objective, but flexible, set of guidelines to ensure space is responsibly used and equitably distributed.
- Research space is a more complex problem. Changes over the past decade have no doubt been even more profound for research space than office space: but those changes are unique to each discipline, and to identify and characterize them would be a significant project in itself, on the scale of the original CPEC study.
- However, the original CPEC taxonomy remains valid in terms of the basic types of research space. While specific factors may need to be recalibrated – for example, to reflect the increased use of simulation rather than field experiments – this may be done iteratively, as new program data become available from actual projects.



Specialized equipment may have
specific infrastructure
requirements

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Write-up space adjacent to the laboratory



Some information needed in the lab

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Virtual Organisation

- Virtual Research Collaborations
 - Much research is now global
 - Much research crosses academic industrial sectors
 - Concerns of how to find people
 - How to keep information flowing to keep the communities together



Wireless Technology

- Location independence? Is this always a good idea
- Library material can be brought to all places but knowledge & experience about the information available is more difficult
- Still have limitation on the speed, quantity and quality of access.



The changing face of
annotation....



Information is provided in new
ways, but ways that have the
potential for much great
automatic curation.



Research Students - are involved
in learning
Undergraduates - involved in
research
Staff - Continuing Education!

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But what
about the
laboratory
environment?



**"I just realized, Howard, that everything
in this apartment is more sophisticated
than we are"**

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From *The New Yorker Book of Technology Cartoons*.



Physical Space

- Need equipment! Not possible in just any room
- Use more reconfigurable systems but services (water, power, extract) make this much more of a problem
- The Network
 - Very high density of connections
 - Provides the ability to track people and functions
 - Monitoring but less useful feedback as yet



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Chemists escape labs via mobiles

By Jo Twist
BBC News science and technology reporter

A blend of mobile technology and award-winning software is letting scientists finally escape the lab.

The software, called "middleware", lets different computer systems talk to each other securely and instantaneously.

As part of a national e-Science project in the UK, it is being used to let Southampton University chemists monitor experiment conditions from mobiles.

Sensors in the lab pick up any changes in the environment so the system can alert chemists, wherever they are.

"It replaces the traditional notebook with some electronic

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r spectroscopy research
chem project, have been
t conferences - and in

im so that at a push of a
able to remotely change
down the temperature.

controlling home
1 seamlessly.



Chemists enjoy a drink at the bar while keeping an eye on the lab

IBM won the Royal Academy of Engineering's MacRobert prize which rewards technological and engineering innovation for the program in June last year.

Used by top global banks, the WebSphere MQ family is a decade old.

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Even run our labs from
home....or the arctic...

Increasing demand for
access to information
from remote places, even
from home or the train



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Space for model building.....



The tea room is the 'heart' of the department - plans to create a more interdisciplinary equivalent for the Life Science Interface

Until 10 years ago my Chemistry Department had a library but space charges put an end to this.

Few people have personal paper copies of journals - no space to hold them, with pdf etc we can hold a personal copy on the computer.



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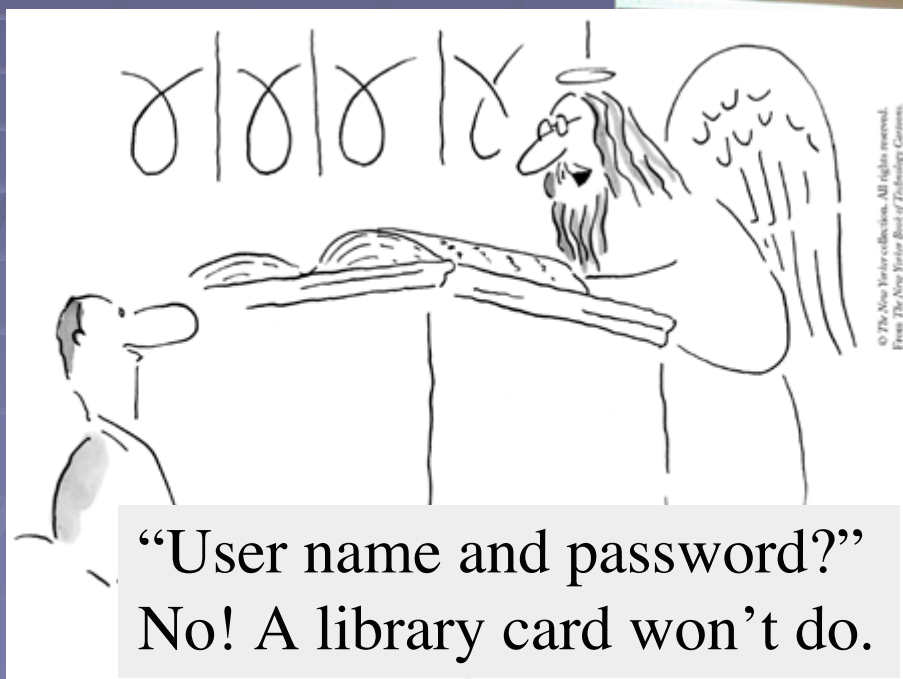
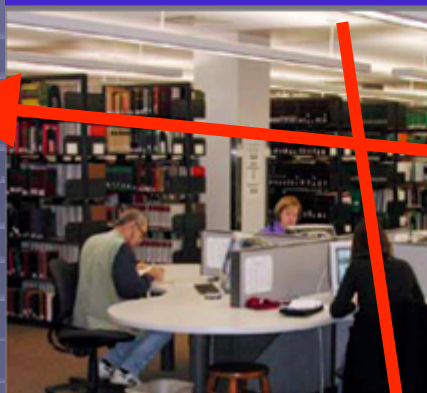
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Dartmouth College

Humanities and Social Sciences: "the Library is our laboratory"

Scientists deposit and retrieve information from libraries



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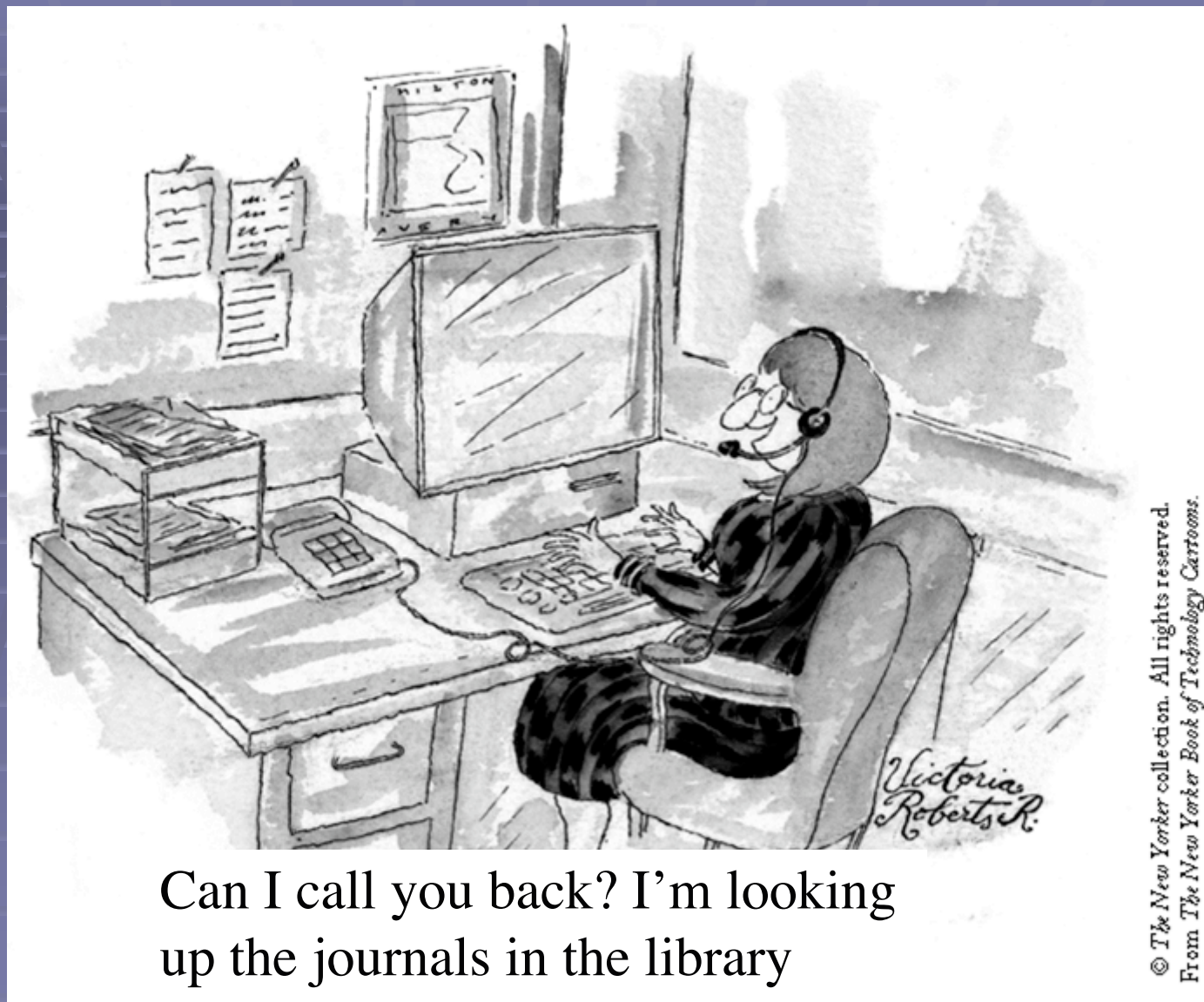
But access is changing

The Laboratory and the Office have become our routine access to the Library.....

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The *e*-
Library the
main
resource for
e-research?



Can I call you back? I'm looking
up the journals in the library



Publication

- No longer so clear what this means
- So no longer clear what we expect to “find” in a library
- Speed of access may be an issue



Access to Information

- More e-journals
- Improved automatics linking of citations
- Does bias information to the more recent publications
- The web has done this anyway
- Version control & archiving of web pages



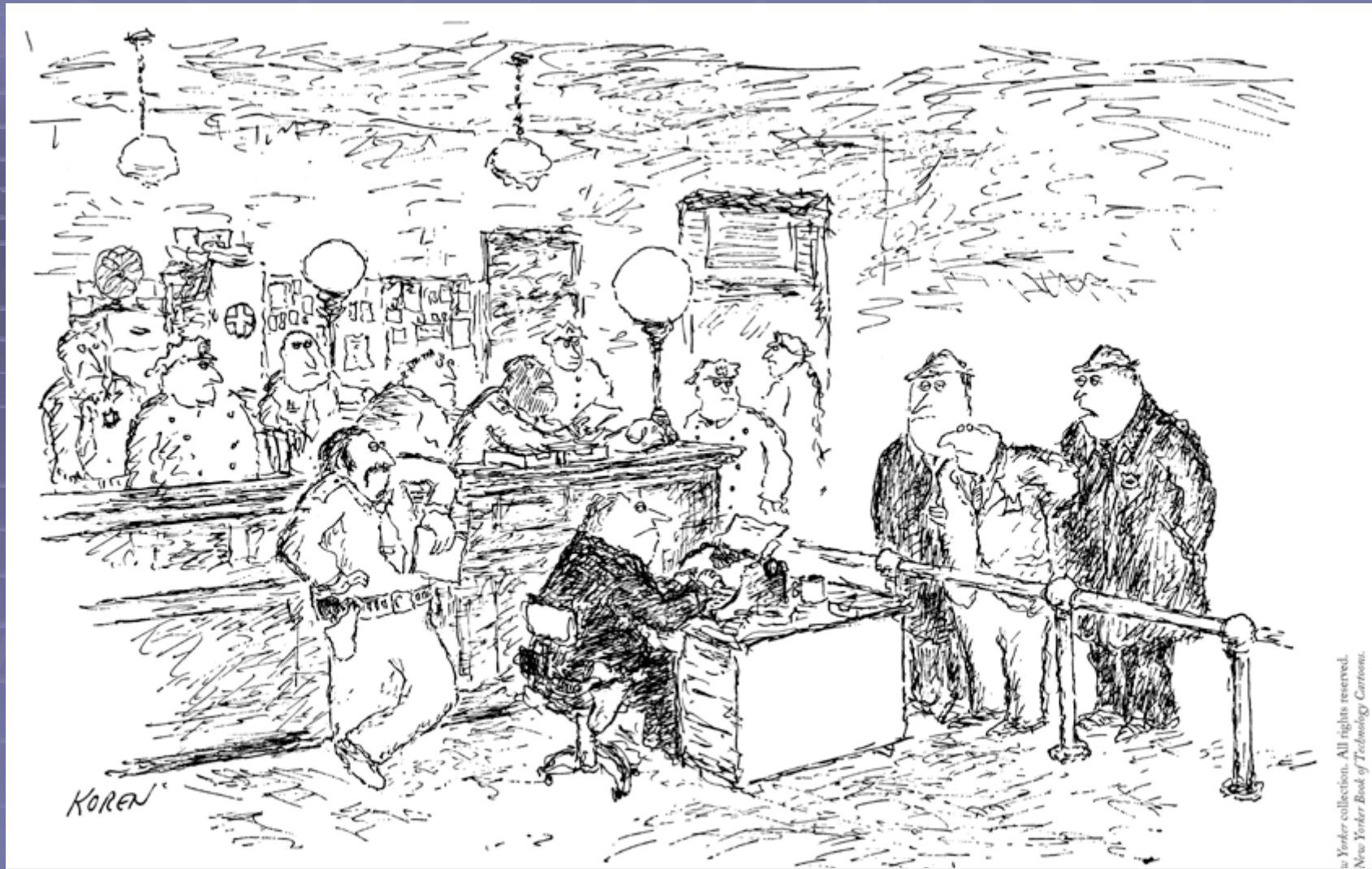
Need to make
the data
available

Need to be
able to find it

But how to
expose it?



First, they do an online search



He is charged with expressing contempt for meta-data



The Data!

- What is the issue here?
- The paper and the data (sets) are not the same thing
- Web removes space constraints (may be) and allows richer range of data resources to be disseminated publicly.
- Metadata, Attribution, Citation



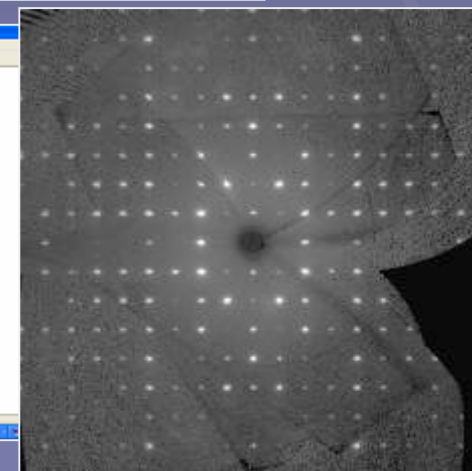
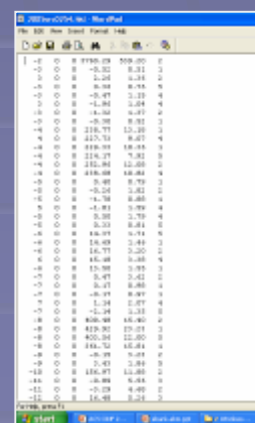
Structural investigations of phosphorus-nitrogen compounds. 4. Steric and electronic effects in dibenzylimino derivatives of hexachlorocyclotriphosphazatriene and 4,4,6,6-tetrachloro-2,2-diphenylcyclotriphosphazatriene¹

Seung Beek Kim, Suman B. Edeles,^{2a} David B. Dorcas,^{2b} Michael B. Hargreaves,^{2b} Aditya Kulkarni,^{2b} Thomas A. Mares,^{2b} Robert A. Shetter,^{2b} and Arvin C. Cole^{2a}

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Abstract: The steric and electronic effects of the substituents of the phosphorus-nitrogen compounds, 4,4,6,6-tetrachloro-2,2-diphenylcyclotriphosphazatriene (1) and 4,4,6,6-tetrachloro-2,2-diphenylcyclotriphosphazatriene (2), were investigated in order to determine whether steric or electronic effects played in the formation of dibenzylimino-substituted cyclophosphazenes. The influence of an electron-releasing group (i.e., phenyl) on the steric character and degree of substitution of the product was compared to the above two series. The difference in unsymmetrically substituted endocyclic P–N bond lengths, is used as a measure of the degree of the electronic contribution, in combination with steric constants, to quantify the degree of the electron-releasing capacity of the R group, in order to compare steric versus non-steric substitution, a dibenzylidene secondary amine was used to form the compound (P₃N₃Me₆Cl₄)(NMe₂) (7) (a catenylene-

[illegible][illegible]

[illegible]

The collage consists of three images:

- Top Image:** A screenshot of a software interface showing a list of reflection intensities (I-sigma). A red arrow points to a specific row in the list.
- Middle Image:** A screenshot of a 3D model of a protein structure. A red arrow points to a specific atom in the model.
- Bottom Image:** A screenshot of a summary report for a directory entry. The report includes unit cell parameters and a table of symmetry standard deviations.

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http://www.diamond.ac.uk/epsrc/national-crystallography-service/

EPSRC National Crystallography Service

Data Collection Summary

Summary report for Directory: diska/02sot082

Report generated: Sat 09, 2002, 10:13:51

Unit cell

17124 reflections with 2.91° theta (2θ max) (resolution between 7.00Å and 0.77Å) were used for unit cell refinement

Symmetry used in calculations	P21212
a (Angstroms)	9.3115 ± 0.0003
b (Angstroms)	9.8424 ± 0.0003
c (Angstroms)	18.4405 ± 0.0004
alpha (°)	90.000
beta (°)	90.000
gamma (°)	90.000
Volume (Å ³)	16415.69 ± 0.07
Mass (g)	0.743 ± 0.002

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Control of Access - not so simple in e-space



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Subversive
and furtive
sharing &
exploitation
of data in
virtual
space



PERPETRATOR OF A DARING DAYLIGHT ILLEGAL ELECTRONIC
TRANSFER OF FUNDS FLEEING THE SCENE OF THE CRIME

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Data

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“Knowledge Management”

- The importance of “Knowledge Management” is becoming more recognized
- Many disciplines are developing and “Informatics” arm.
- These have many aspects in common and need coordinating.

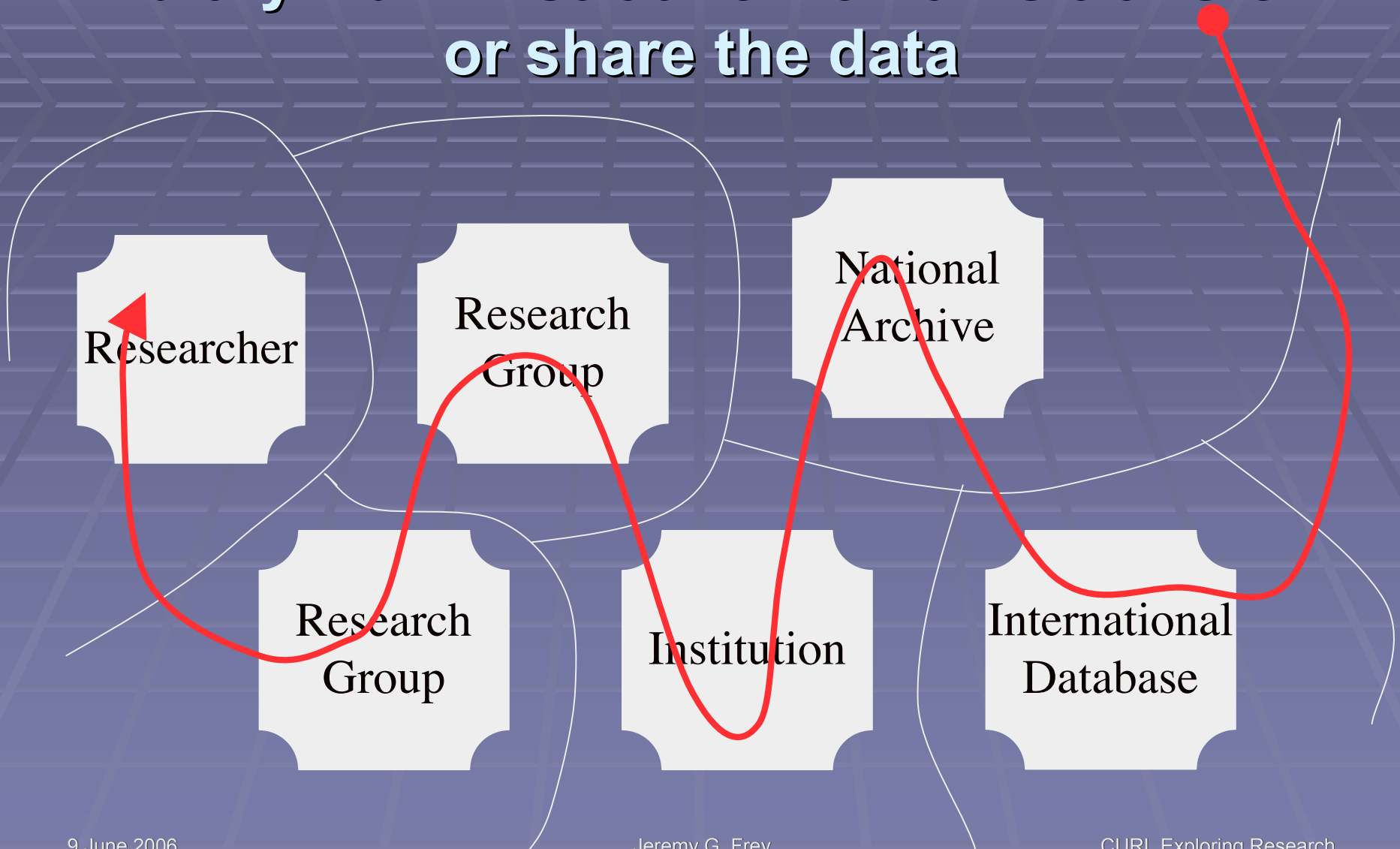


Recognition of Academic Output

- Citation of more varied information sources
- Repositories for “e-information” - not just papers, include the data
- Visibility of this information
- Curation and Archiving issues



Several groups making and analysing the library Administrative Domains transfer or share the data



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“Are we thinking here,
or is this just so much pointing and clicking”

Information
Providers

Information
Consumers

