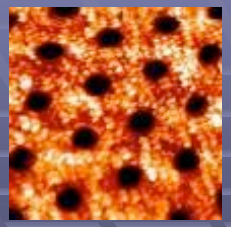
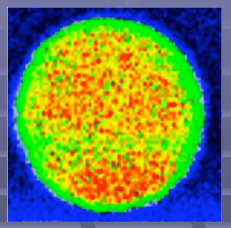
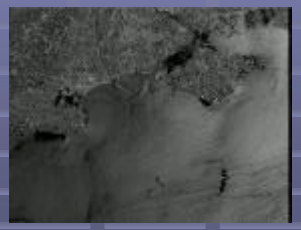
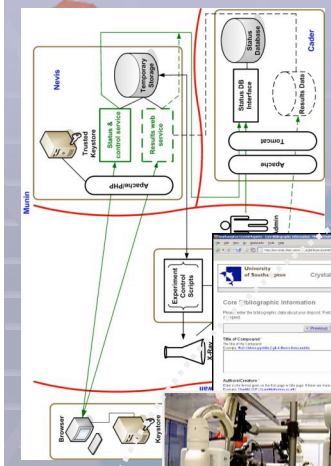
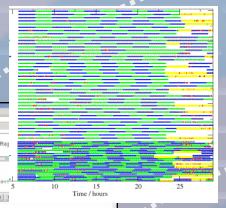
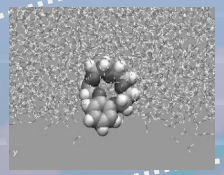
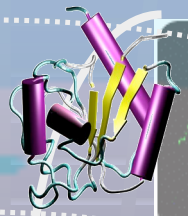
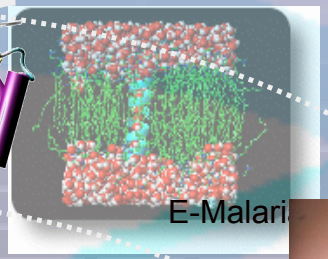
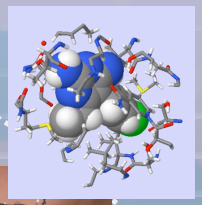
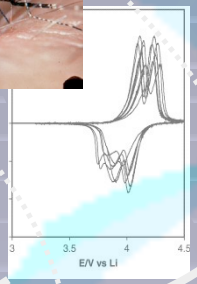
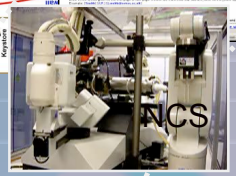
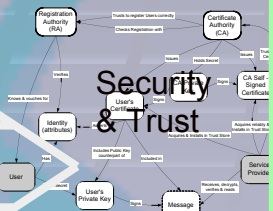
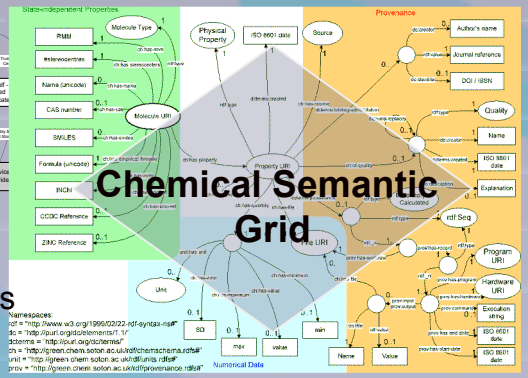
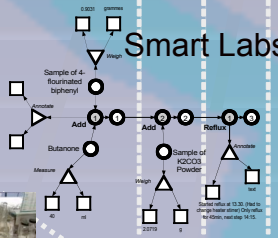
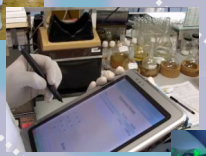




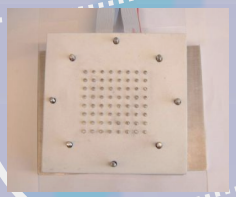
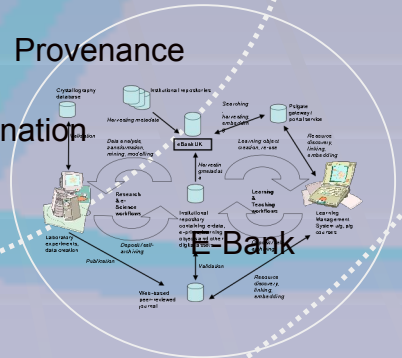
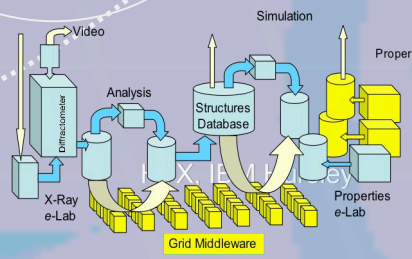
# Future Lab - "Smart Not Dark"

Jeremy G.Frey
School of Chemistry, University of Southampton, UK

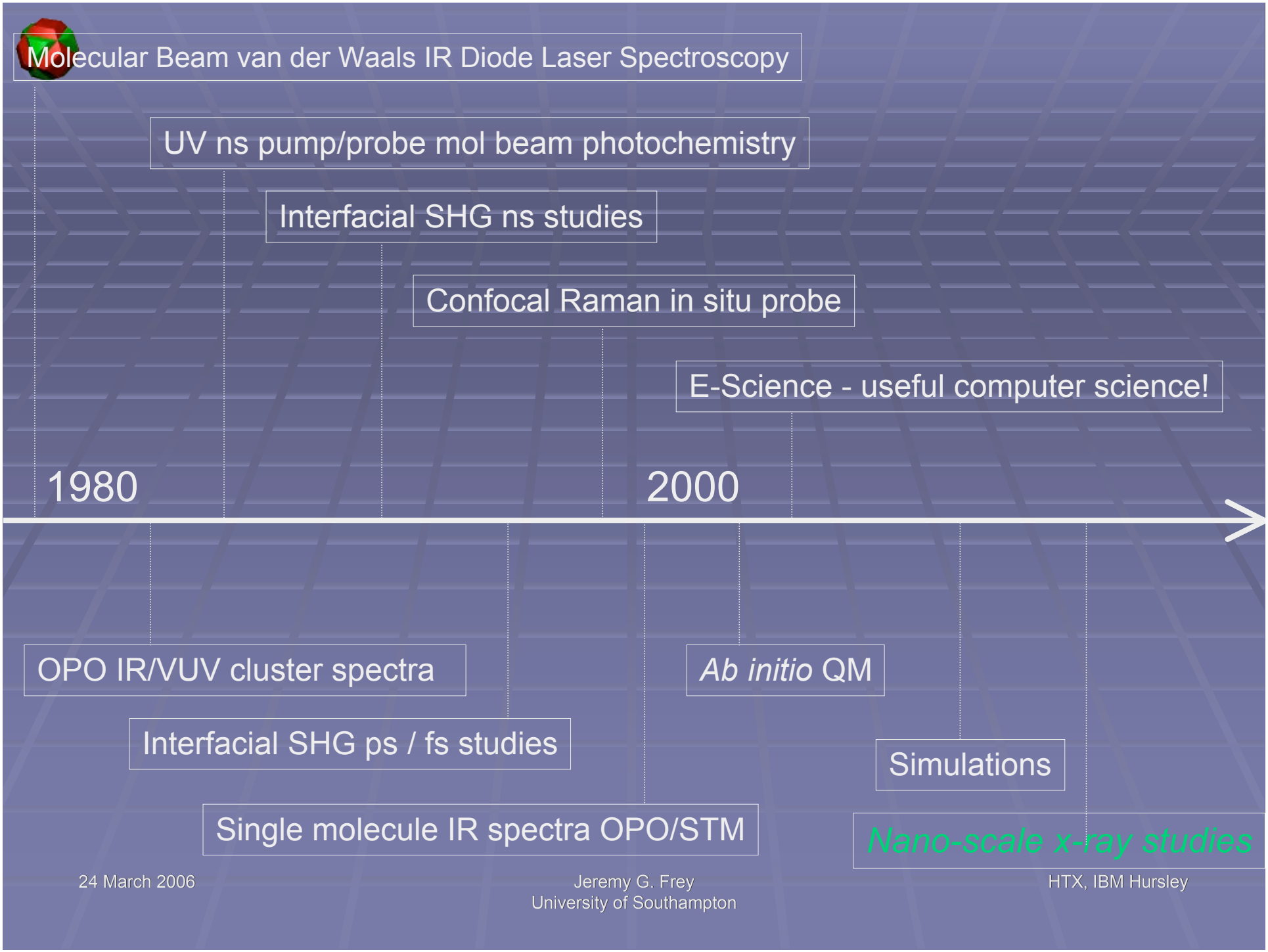








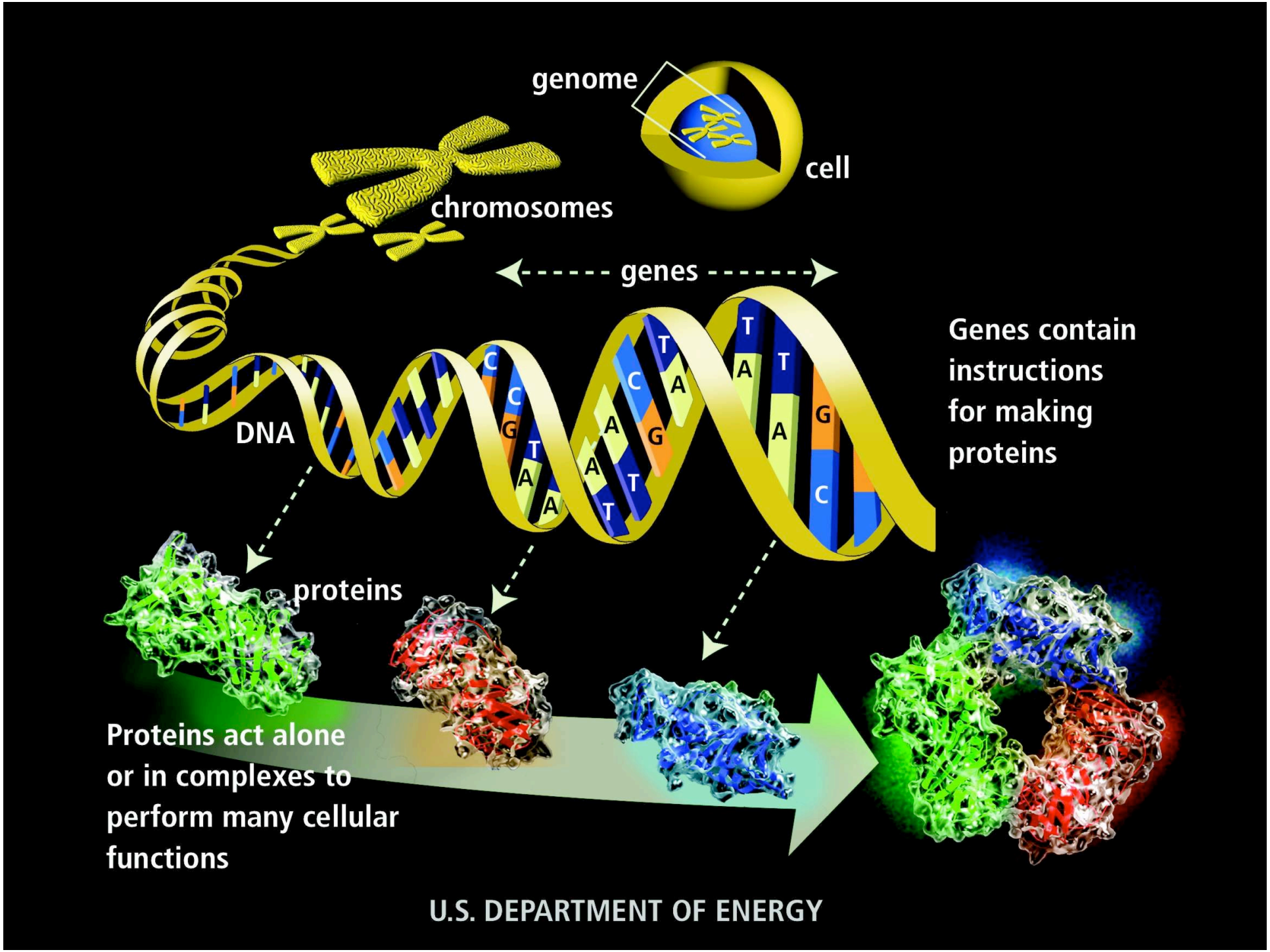



Jeremy G. Frey
University of Southampton

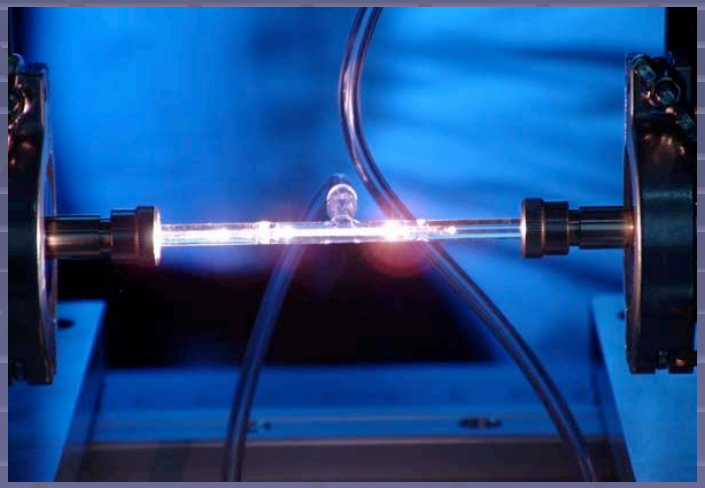


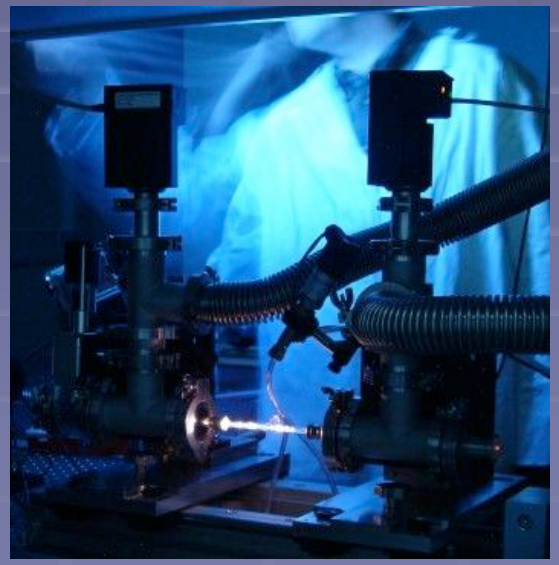



Jeremy G. Frey
University of Southampton

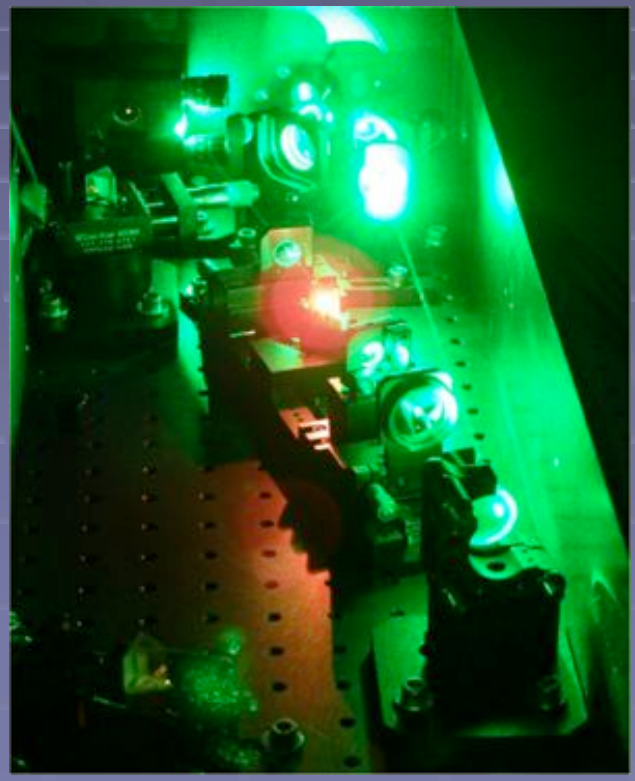

genome
cell
chromosomes
genes
DNA
Genes contain instructions for making proteins
proteins
Proteins act alone or in complexes to perform many cellular functions
U.S. DEPARTMENT OF ENERGY

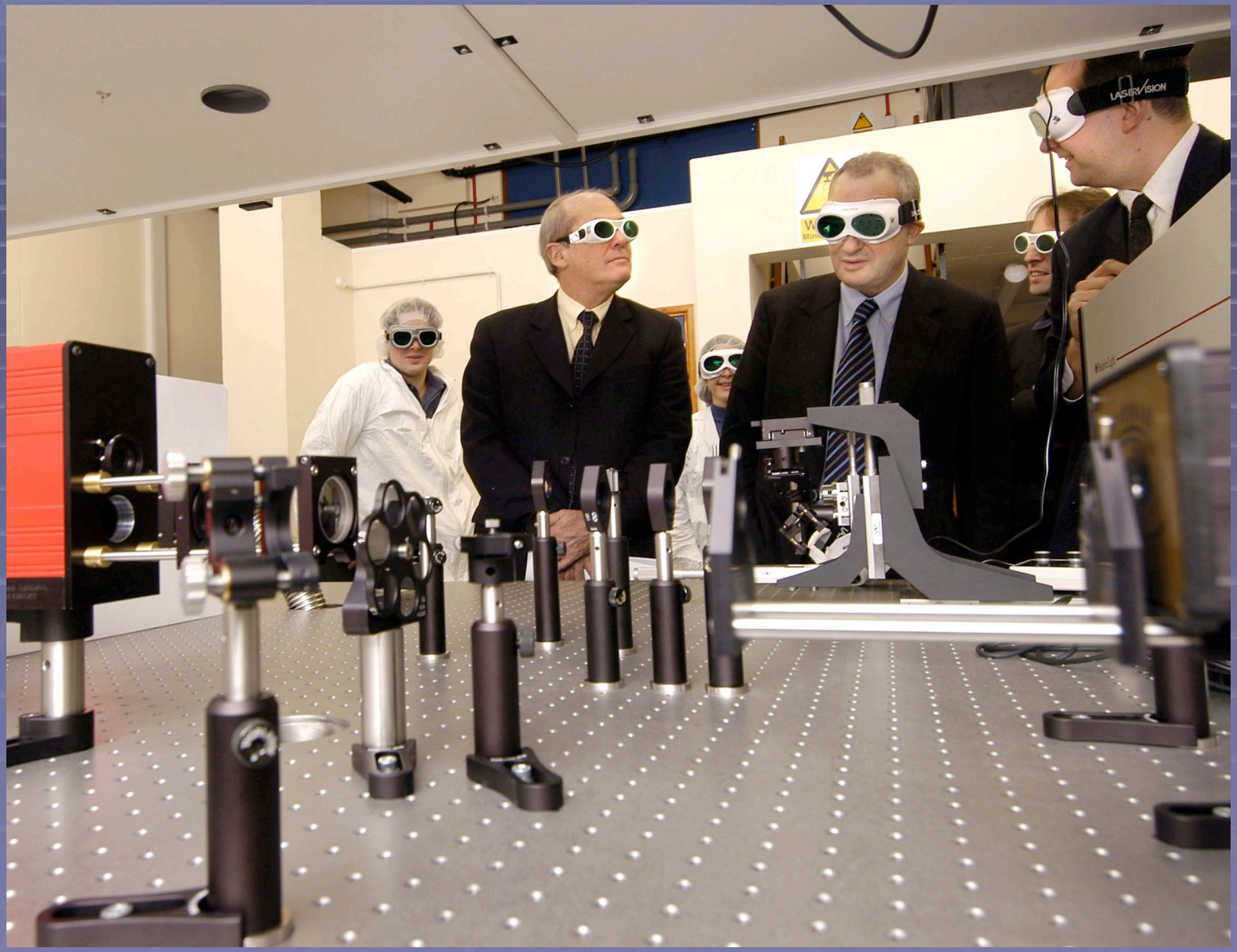
# Laser X-ray generation





- Need **very high** laser powers:
  - Peak intensity ~$10^{15}$ W/cm$^2$
  - Peak E-field ~100 GV/m

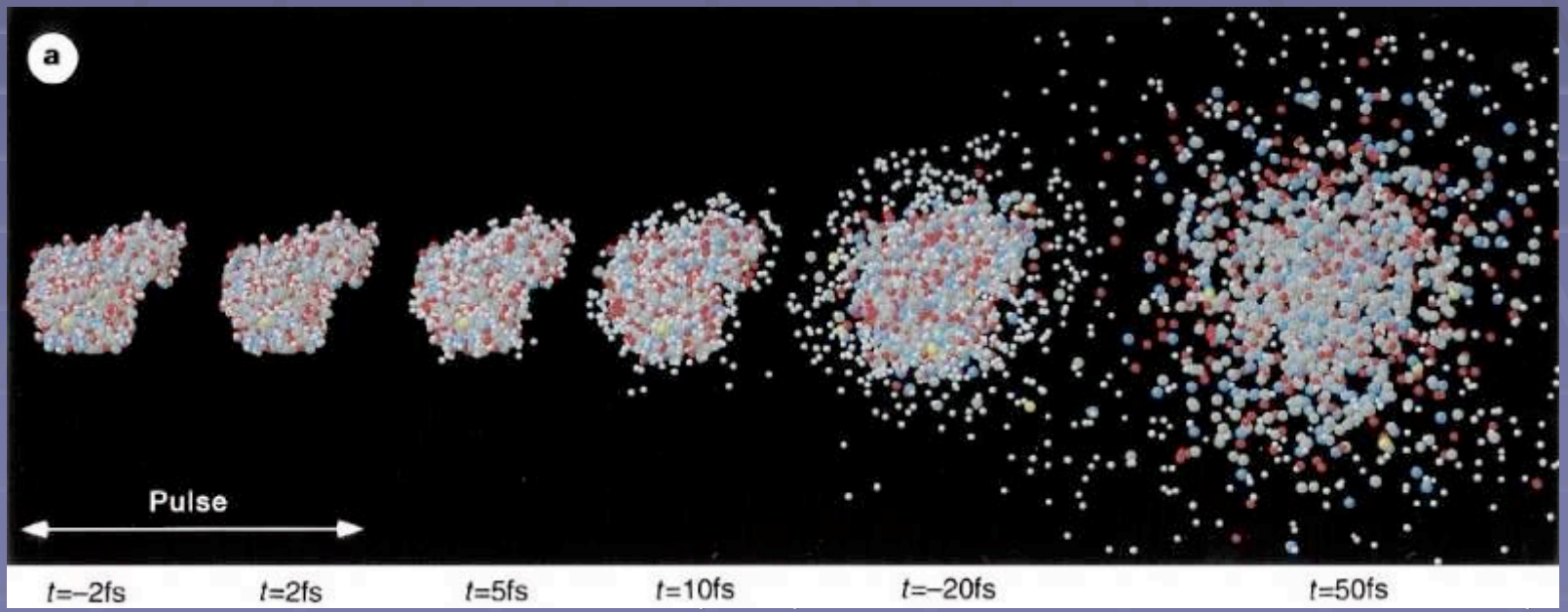



LASERVISION

# Damage limitation

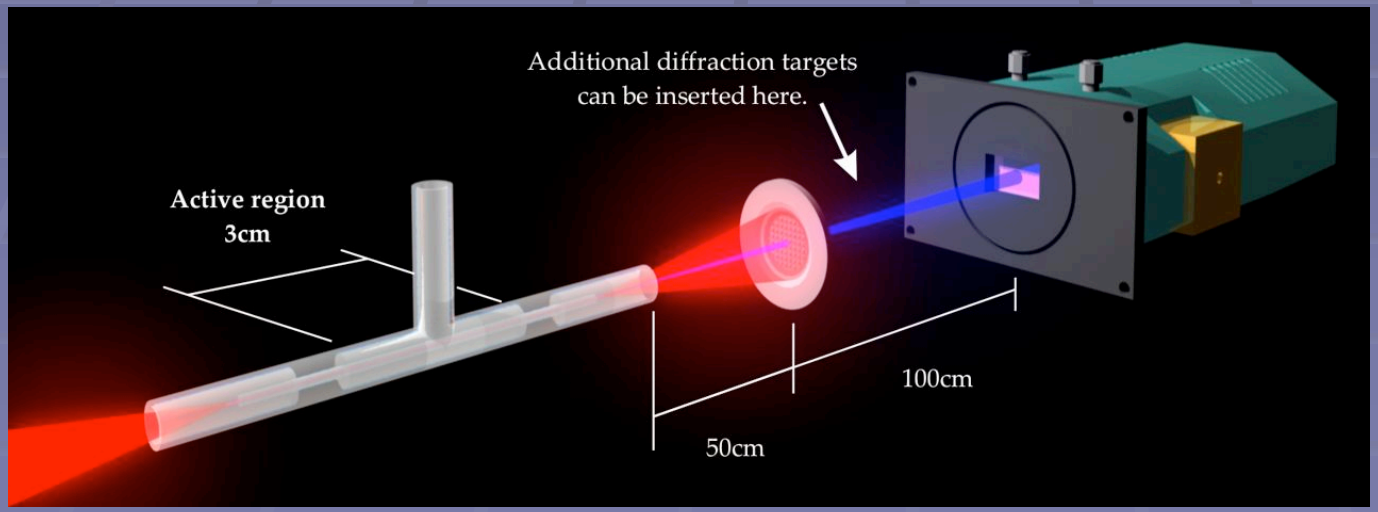
- Conventional damage threshold: 200 ph/Å$^2$ Damage process
  - inelastic scattering of electrons out of molecule
  - Coulomb repulsion of remainder
- Timescale? fs

Neutze *et al.*, Nature (2000) **406**, 752

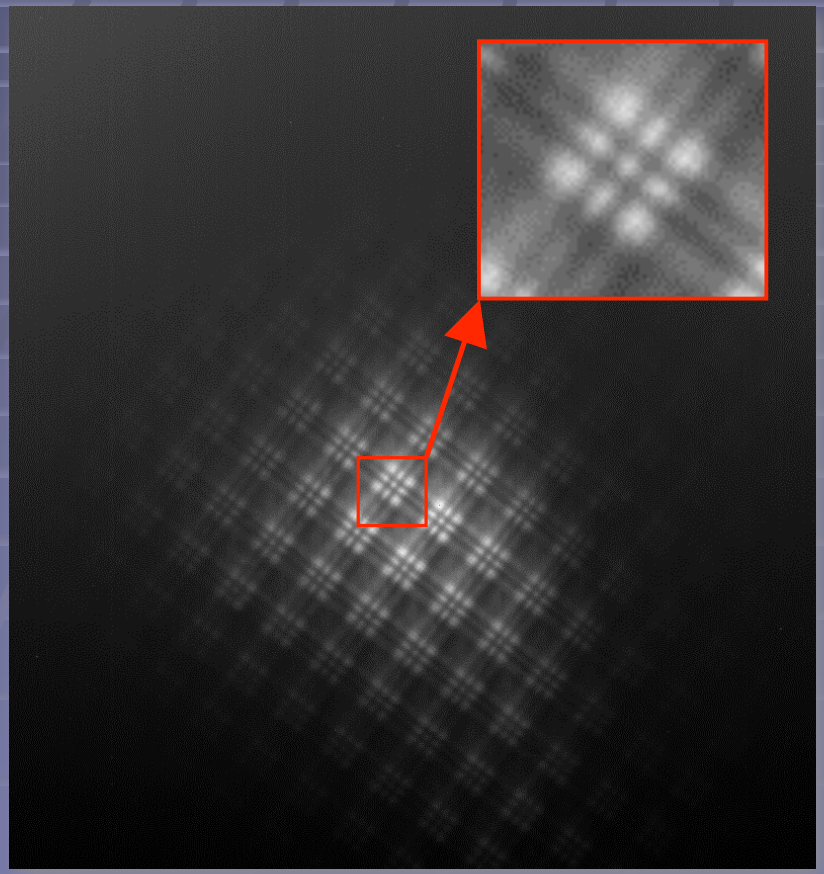


# Square Grid Diffraction

- Record x-ray diffraction by filter support grid.
- 340μm square apertures, 18μm bars.
- 50cm source to grid, 100cm grid to camera.
- Observe spatial variation of diffraction patterns.
- We can extract the x-ray spectrum.



# Fresnel diffraction of EUV beam



- Wire mesh: 18μm bars, 340μm spacing (Al filter support)
- Experiment and theory agree.
- Incoherent sum of all harmonics.

# Chemical Grids

- Start in the laboratory – pervasive physical grid (Smart Tea)
- Computational chemistry very significant source – *in silico* grid (*Chem* MyTea)
- Used by chemists so must be simple to support & maintain - *simple, stable, secure, & autonomic*

# What are the people up to?

Who is doing what?

Where are they doing it?

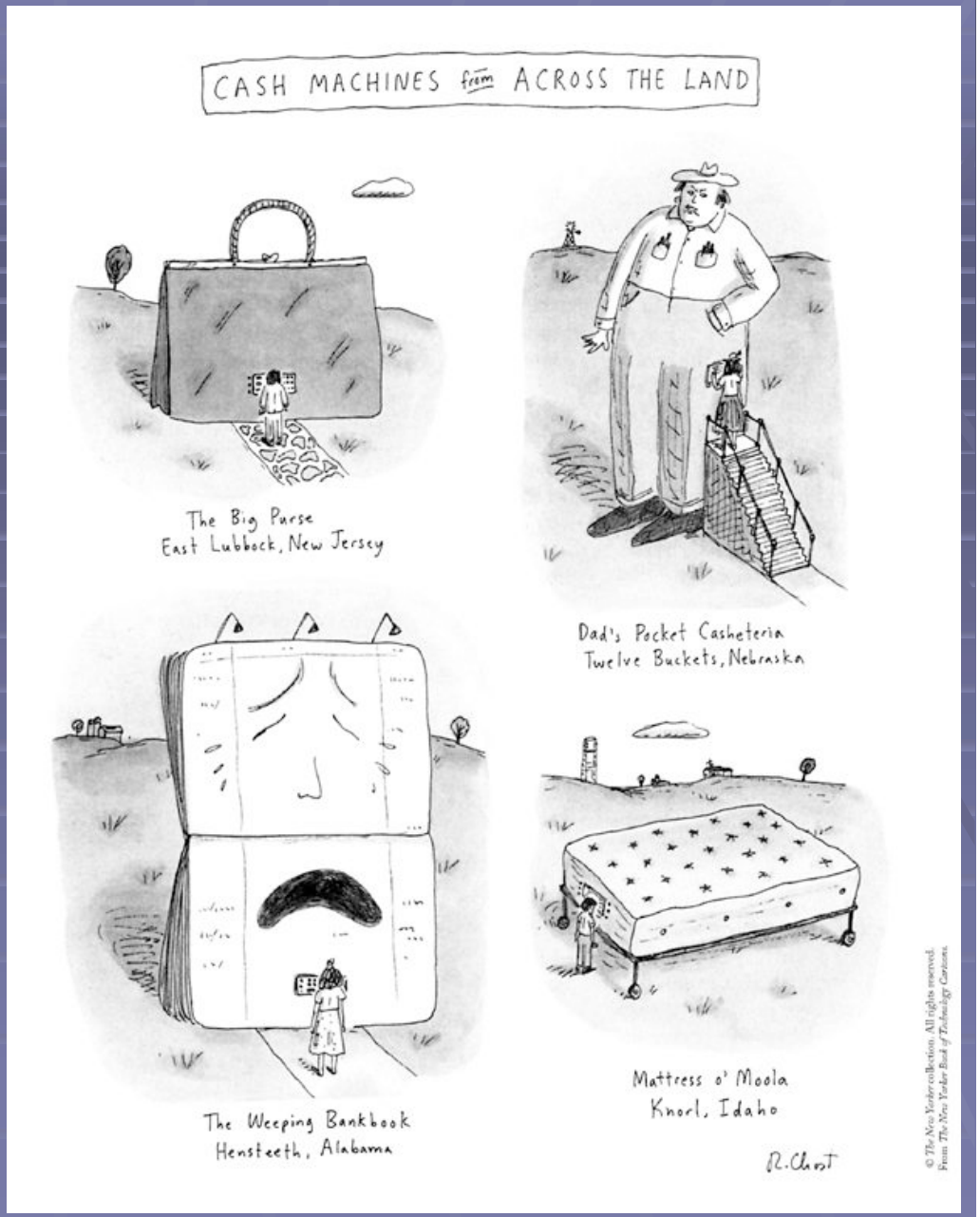
What is the environment like?

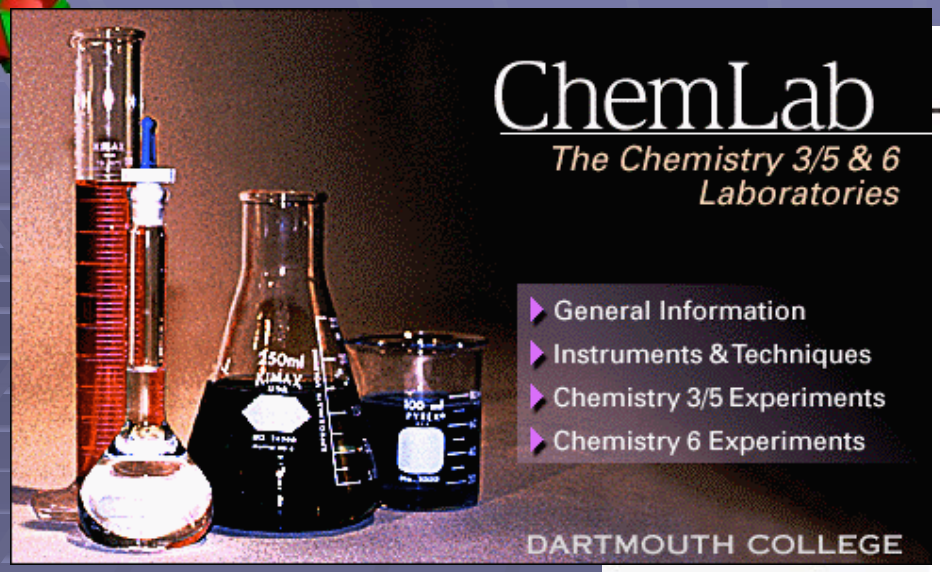

The laboratory notebook has been the way scientific research has been recorded for over 200 years

Can we do better now?

How about an electronic notebook?

Like cash machine electronic notebooks have taken many forms we want one that is simple to use in the lab whilst doing actual bench chemistry






Permanent, primary record ***Observations***

Write down what you see

24 March 2006

**Safety**
General Rules
Safety Equipment
Safety Hazards
[illegible] Procedures

**Resources**
Applets
General FAQ
Uncertainty

ChemLab Home

Info | Techniques | Chem 3/5 | Chem 6

**How to Keep a Notebook**

One of the most useful skills you will acquire in the laboratory is the proper use of a laboratory notebook. Notebooks, or other formally kept records, are an essential tool in many careers, ranging from that of the research scientist to that of the practicing physician. The effort invested in developing good habits of notebook use will be amply repaid for students who pursue a future in the basic or applied sciences. Experience has indicated that skillful notebook use is developed by most students only through continued special effort--it does not come naturally. Some of the main principles of sound notebook use are outlined below.

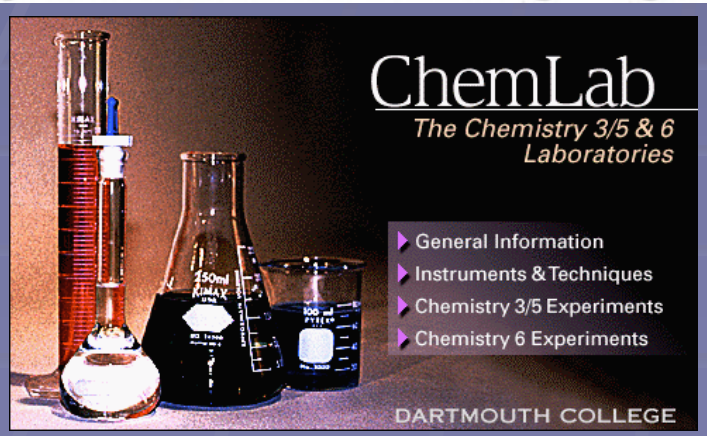
The laboratory notebook is a permanent, documented, and primary record of laboratory observations. Therefore, your notebook will be a bound journal with pages that should be numbered in advance and never torn out. A notebook will be supplied to you before the first laboratory period. Write your name, the name of your TA, and your lab section on the cover of your notebook. All notebook entries must be in ink and clearly dated. No entry is ever erased or obliterated by pen or "white out". Changes are made by drawing a single line through an entry in such a way that it can still be read and placing the new entry nearby. If it is a primary datum that is changed, a brief explanation of the change should be entered (e.g. "balance drifted" or "reading error"). No explanation is necessary if a calculation or discussion is changed; the section to be deleted is simply removed by drawing a neat "x" through it.

necessary if a calculation or discussion is changed; the section to be deleted is simply removed by drawing a neat "x" through it.

In view of the fact that a notebook is a primary record, data are not copied into it from other sources (such as this manual or a lab partner's notebook, in a joint experiment) without clear acknowledgment of the source. Observations are never collected on note pads, filter paper, or other temporary paper for later transfer into a notebook. If you are caught using the "scrap of paper" technique, your improperly recorded data may be confiscated by your TA or instructor at any time. It is important to develop a standard approach to using a notebook routinely as the primary receptacle of observations.

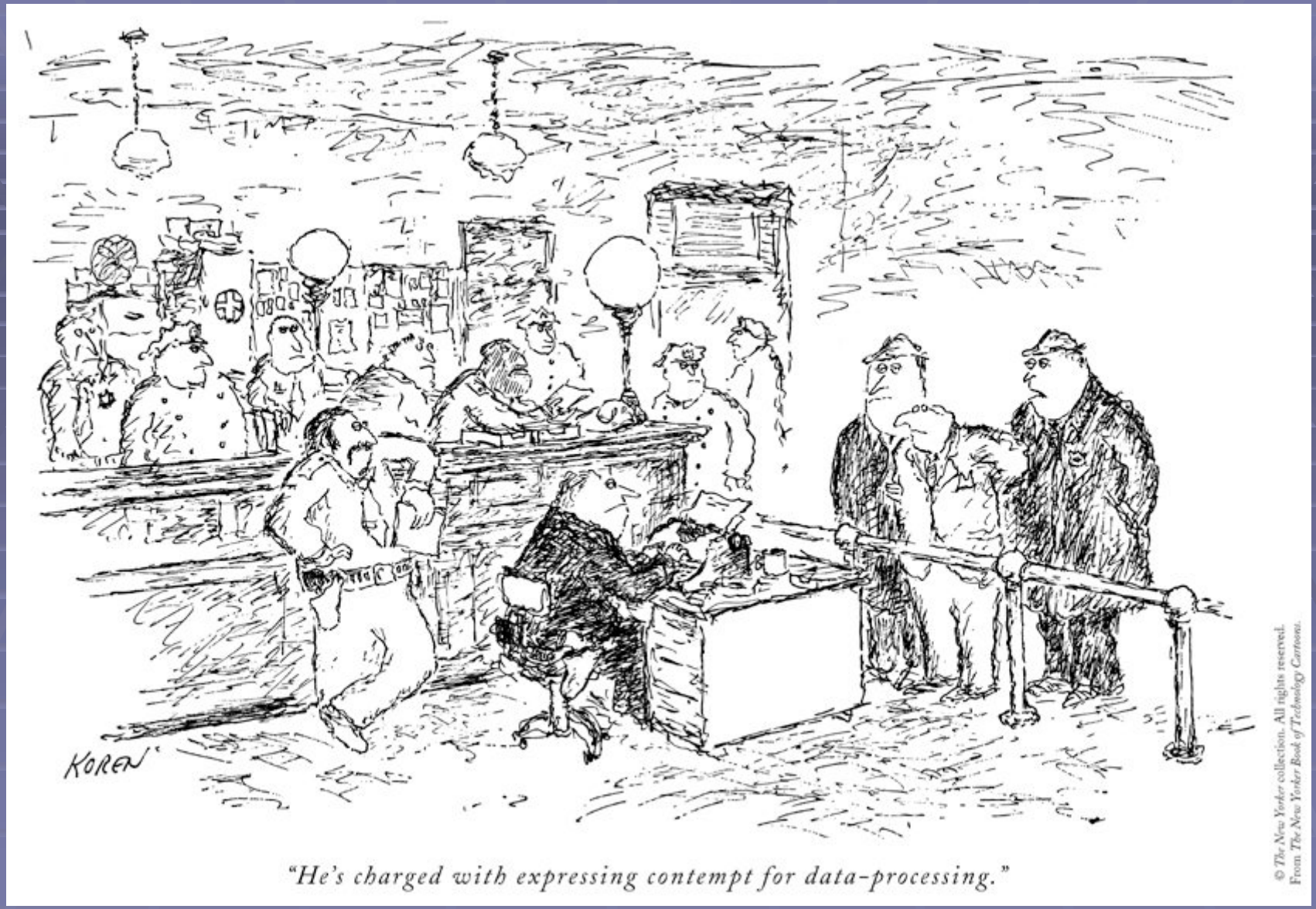
Each week at the beginning of lab lecture, you will turn in your prelab problems from the manual for grading. [illegible] problems not turned in at the beginning of lab lecture [illegible] be

Observations are never collected on bits of paper to be written up later on!




If you are caught using the "scrap of paper" technique, your improperly recorded data may be confiscated by your teacher!

Jeremy G. [illegible] Hursley
University of Southamp[illegible]




# He is charged with expressing contempt for meta-data

24 March 2006

Jeremy G. Frey
University of Southampton

HTX, IBM Hursley

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the New Yorker Book of Technology Cartoons.

Digital record at source don't try to add metadata after the fact

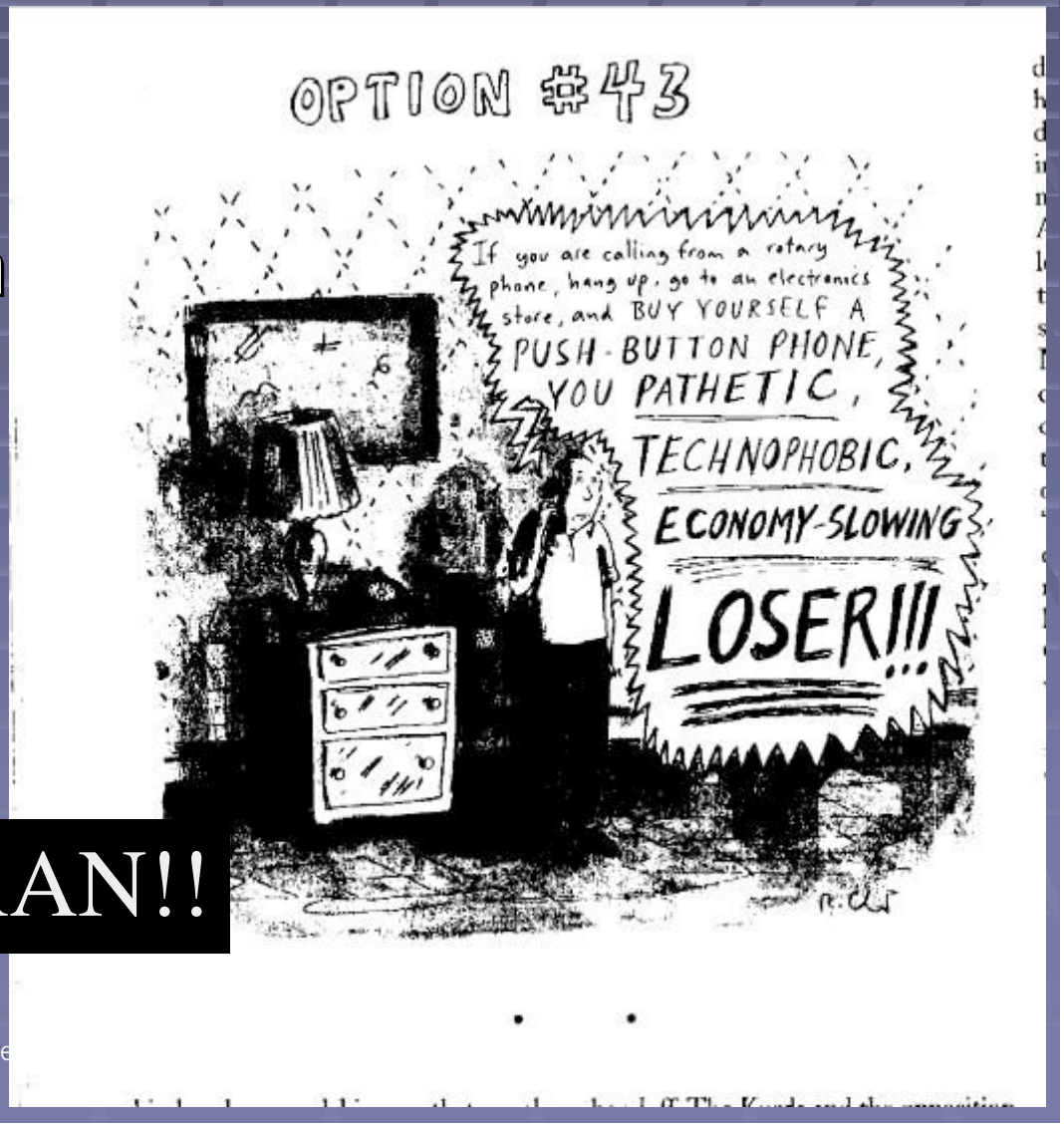
*"We can pause, Stu—we can even try fast-forwarding—but we can never rewind."*




# Different labs

# Chemists and programming

- Many Chemists think that they can program
- So leave the systems to the Chemists




You still use FORTRAN!!

# *e*-Workflow

Some Chemists can and leaving it to the computer scientists can give you a perfect system for a problem you didn't know you had!

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From *The New Yorker Book of Technology Cartoons.*

What about that! His brain uses formal logic! No wonder it took so long to get a result

# COSHH

## leverage off things we already have to do

**COSHH ASSESSMENT FORM** Record No.

| SUBSTANCE NAME | PHYSICAL FORM | QUANTITY | NATURE OF HAZARD |
|---|---|---|---|
| Water | liquid | 1000ml | None |
| Dextrose | Solid | <20 g | possible irritation to eyes and skin |
| Caffeine | Solid (tea) | <1g | Harmful if swallowed, induce vomiting. |
| Milk | liquid | <100ml | No particular hazards |

**NATURE OF PROCESS**
liquid extraction of caffeine, followed by combination with dextrose to produce a sweet drink

Is there a less hazardous substance? No
If so, why not use it?

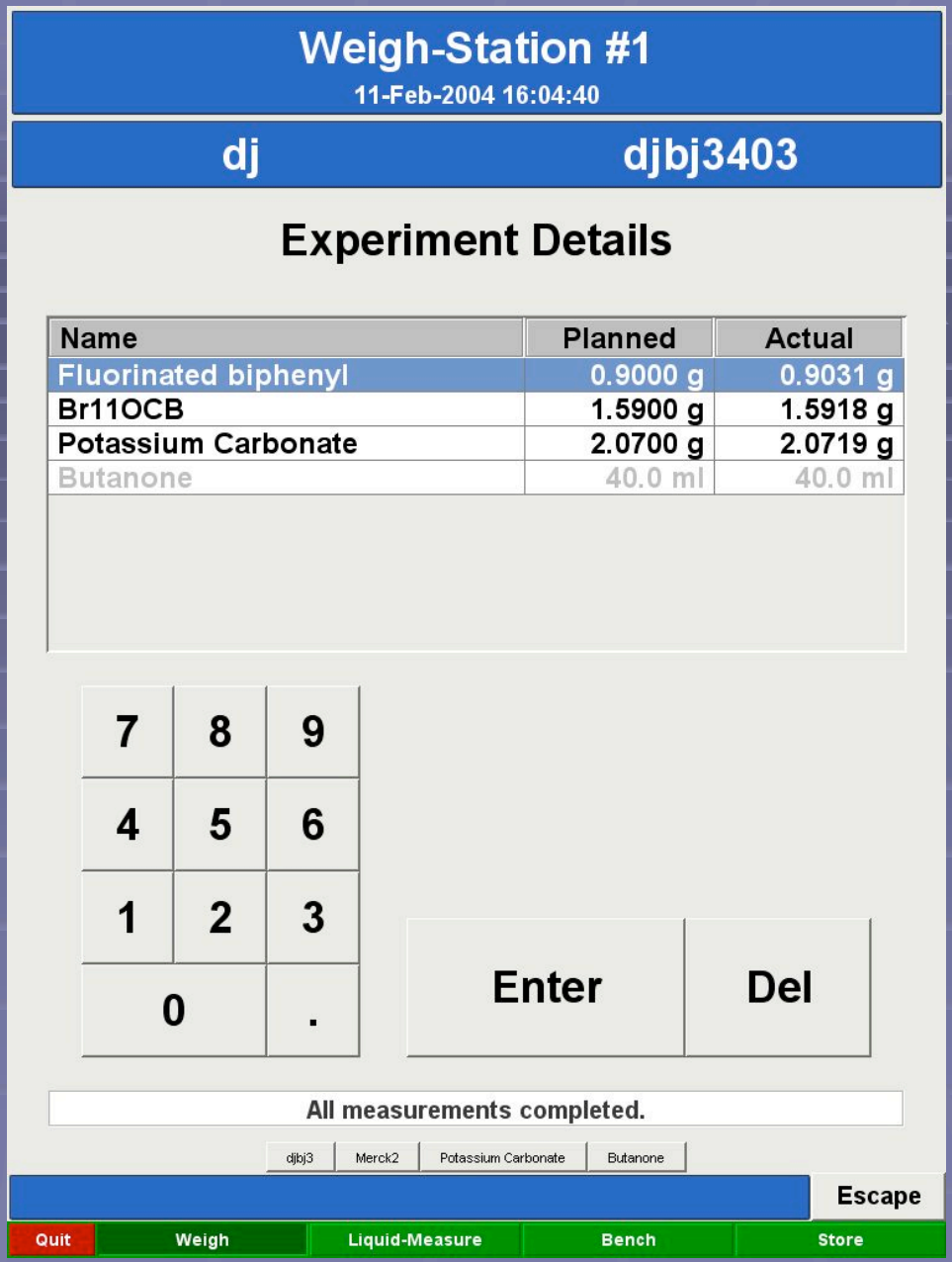
**CONTROL MEASURES REQUIRED** No specific measure required
(Local exhaust ventilation, personal protection, etc.)

But How to get chemists and computer scientists to understand each other

***By Making Tea!***


Weigh-Station #1
glh/4205/practice45d
Arthur Dent
Experiment Details
Del

Result of extensive collaborative HCI research between Computer Scientists and Chemists over Tea






Jeremy G. Frey
University of Southampton


# The underlying digital world - The Matrix!



Jeremy G. Frey
University of Southampton

Back to Safety issues

Incompatible Chemicals

http://ptcl.chem.ox.ac.uk/MSDS/incompatibles.html

chemical safety phrases

Apple (147) ▾ Amazon eBay Yahoo! News (834) ▾

# Incompatible Chemicals

A wide variety of chemicals react dangerously when mixed with certain other materials. Some of the more widely-used incompatible chemicals are given below, but the absence of a chemical from this list should not be taken to indicate that it is safe to mix it with any other chemical!

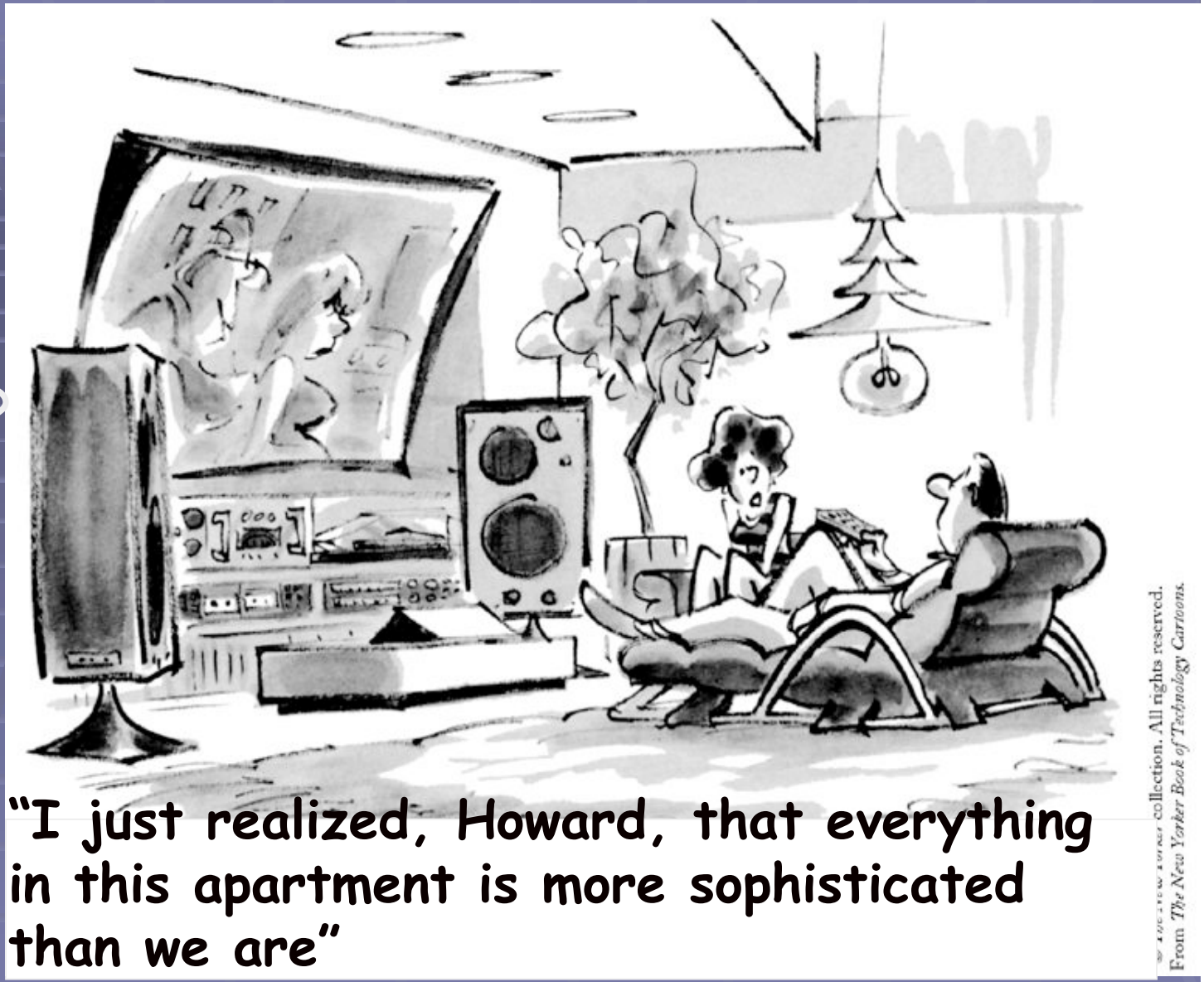
I'm adding links to MSDS data for these chemicals, but if there is no link from this page to MSDS data for a chemical in which you are interested, try the main page on this web site. through which you can access MSDS data for a large number of chemicals. Click here to get to the Safety web pages of the Physical and Theoretical Chemistry Laboratory, Oxford University.

- acetic acid:
  chromic acid, ethylene glycol, nitric acid, hydroxyl compounds, perchloric acid, peroxides, permanganates
- acetone:
  concentrated sulphuric and nitric acid mixtures
- acetylene:
  chlorine, bromine, copper, fluorine, silver, mercury
- alkali and alkaline earth metals:
  water, chlorinated hydrocarbons, carbon dioxide, halogens, alcohols, aldehydes, ketones, acids
- aluminium (powdered):
  chlorinated hydrocarbons, halogens, carbon dioxide, organic acids.
- anhydrous ammonia:
  mercury, chlorine, calcium hypochlorite, iodine, bromine, hydrofluoric acid
- ammonium nitrate:
  acids, metal powders, flammable liquids, chlorates, nitrites, sulphur, finely divided organic combustible materials

aniline:
  nitric acid, hydrogen peroxide

- arsenic compounds:
  reducing agents
- azides:
  acids

# But what about the laboratory envionement?



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

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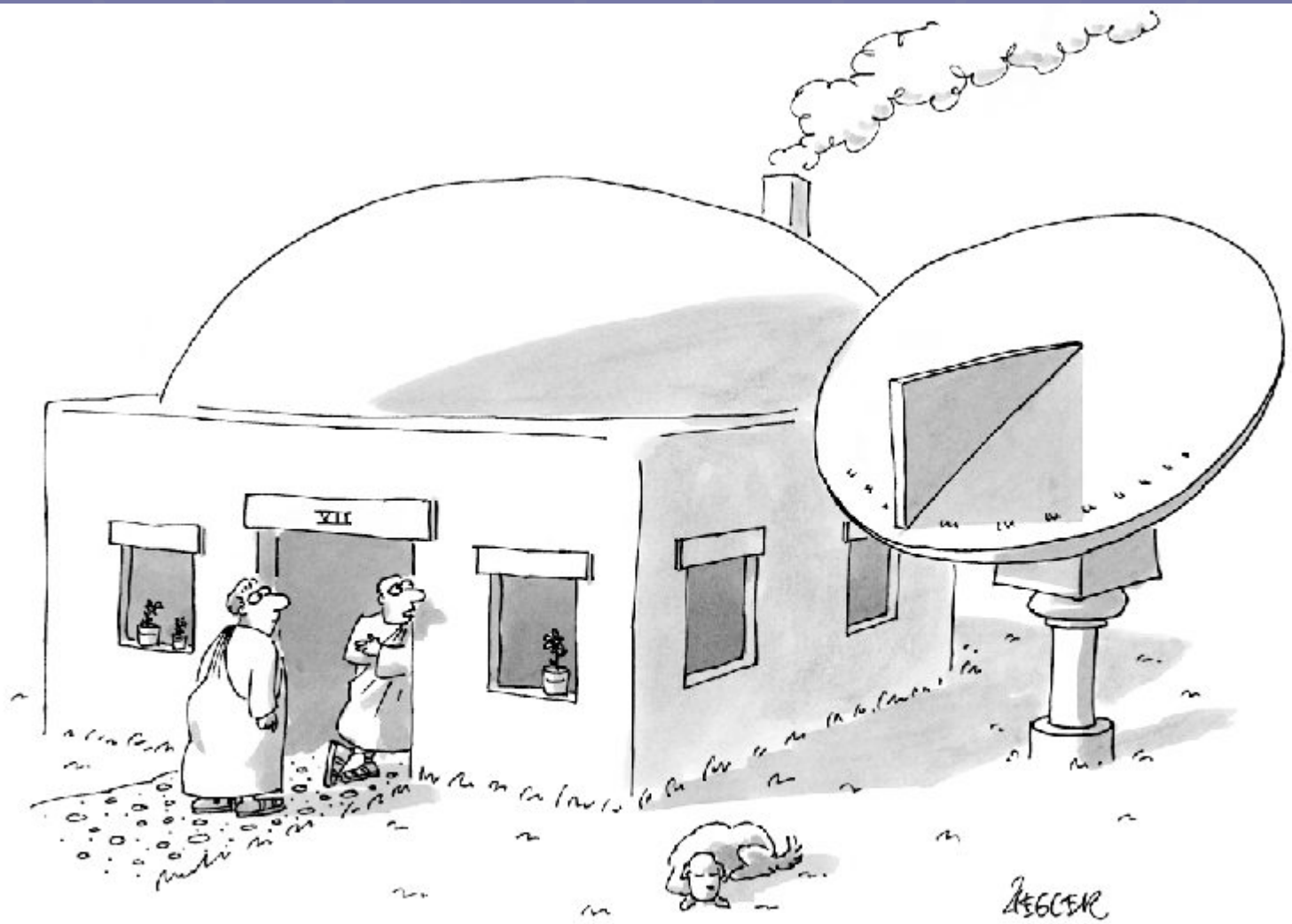
From *The New Yorker Book of Technology Cartoons.*

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From The New Yorker Book of Technology Cartoons.

*"Sure, it's an eyesore, but we get better time than anyone else in the neighborhood."*

# Will the technology scale?

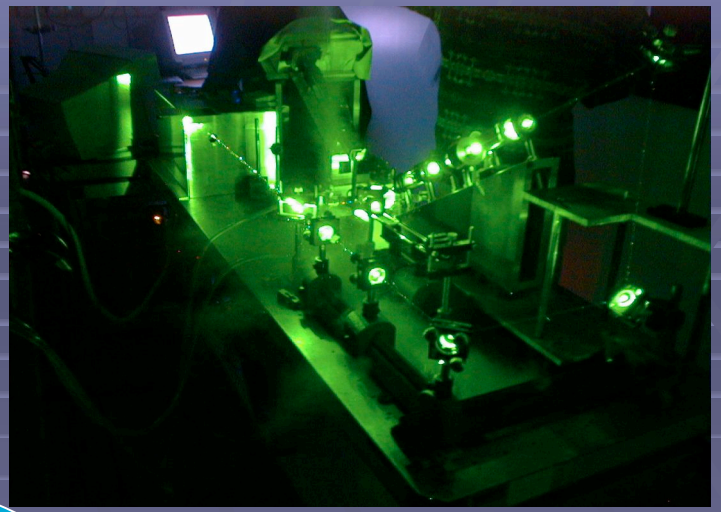
# Smart Places & Things


We need Smart Labs!



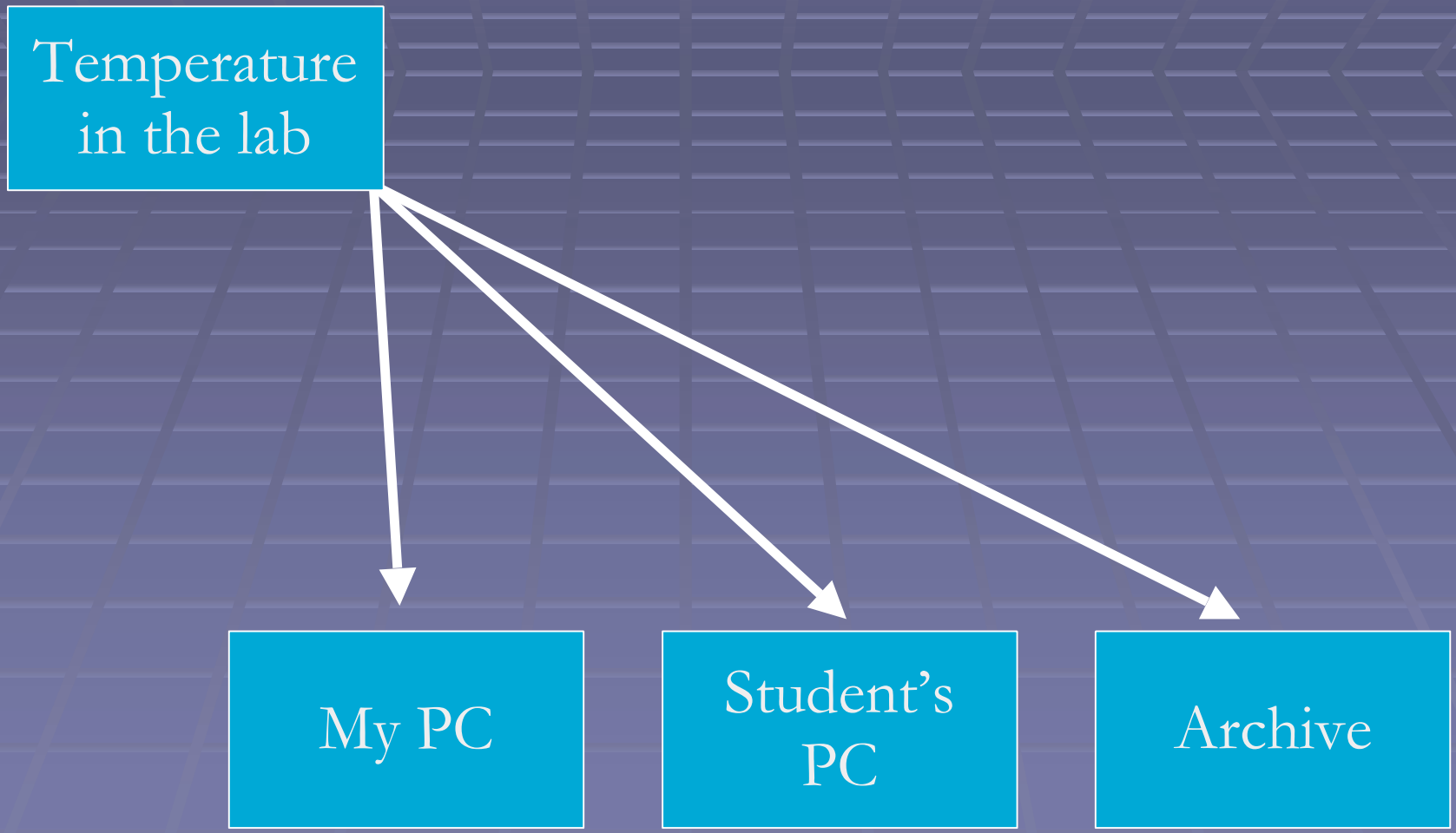
Jeremy G. Frey
University of Southampton

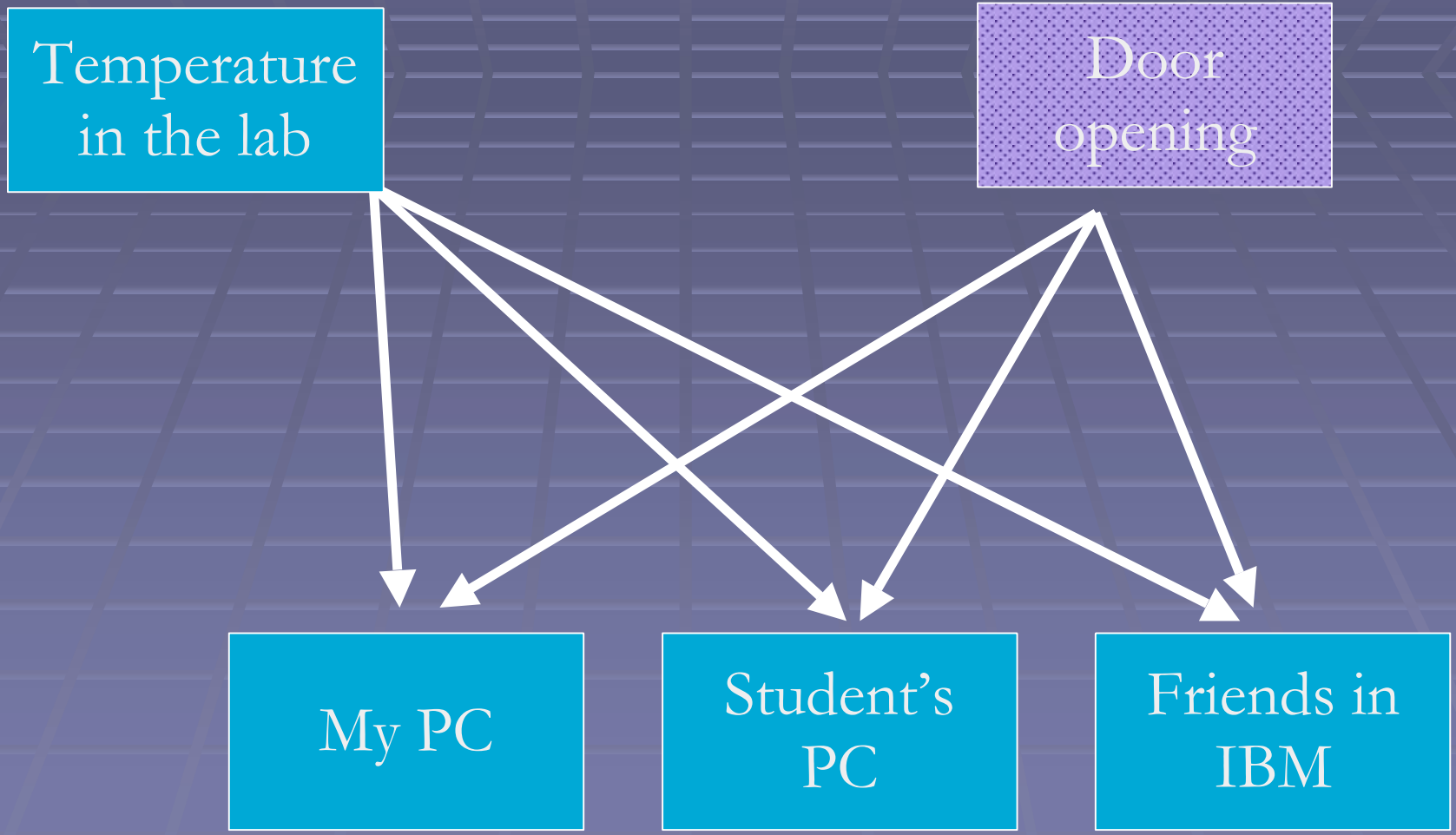
Temperature in the lab

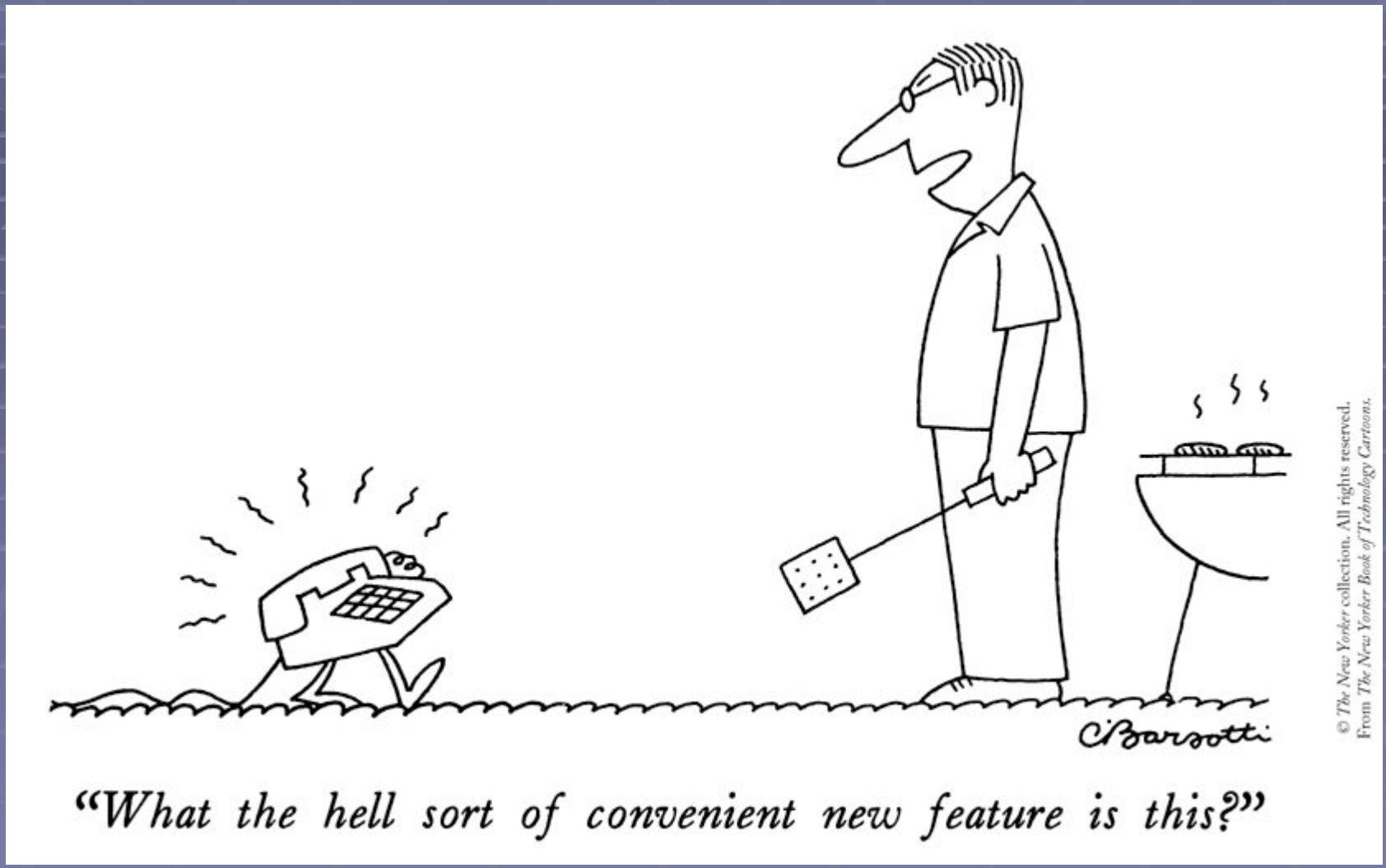


Distribute

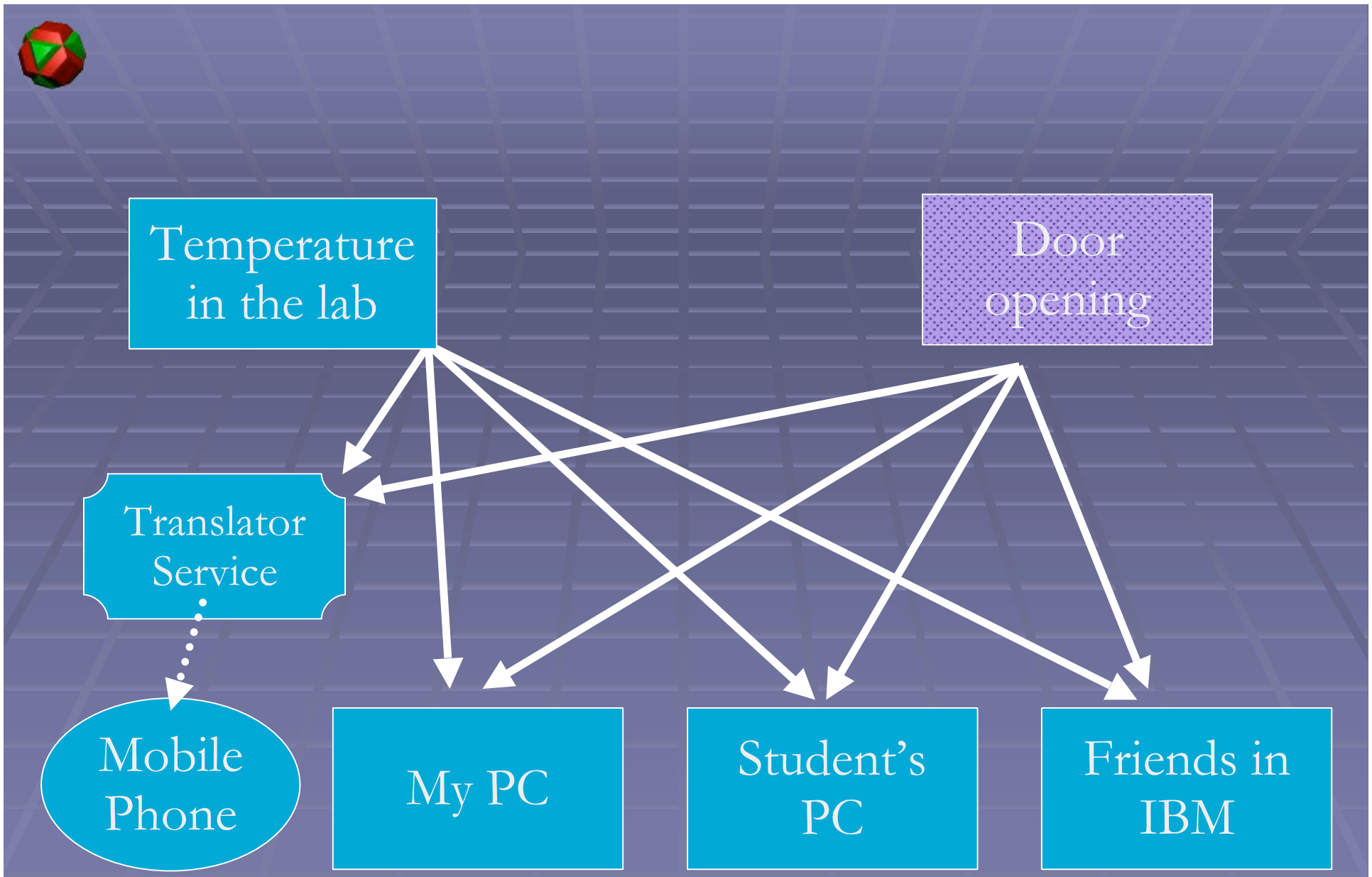
My PC

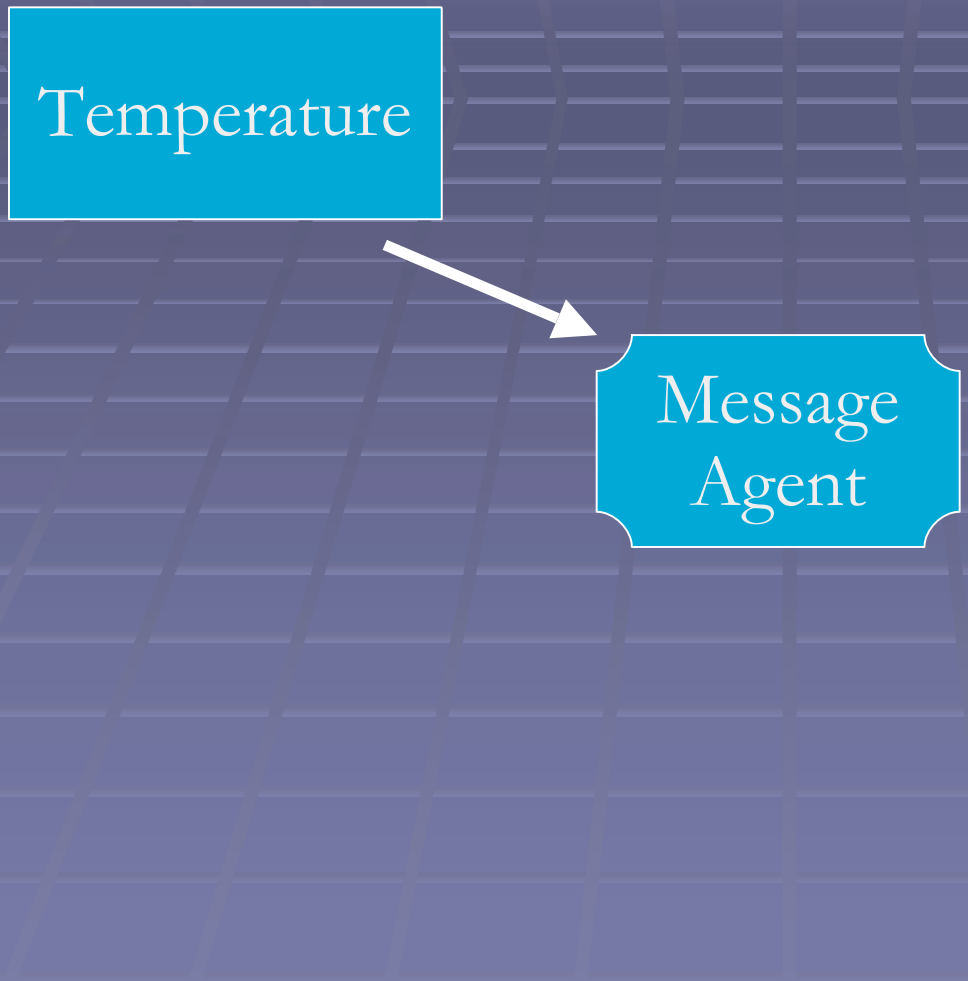

Temperature in the lab
My PC
Student's PC
Archive

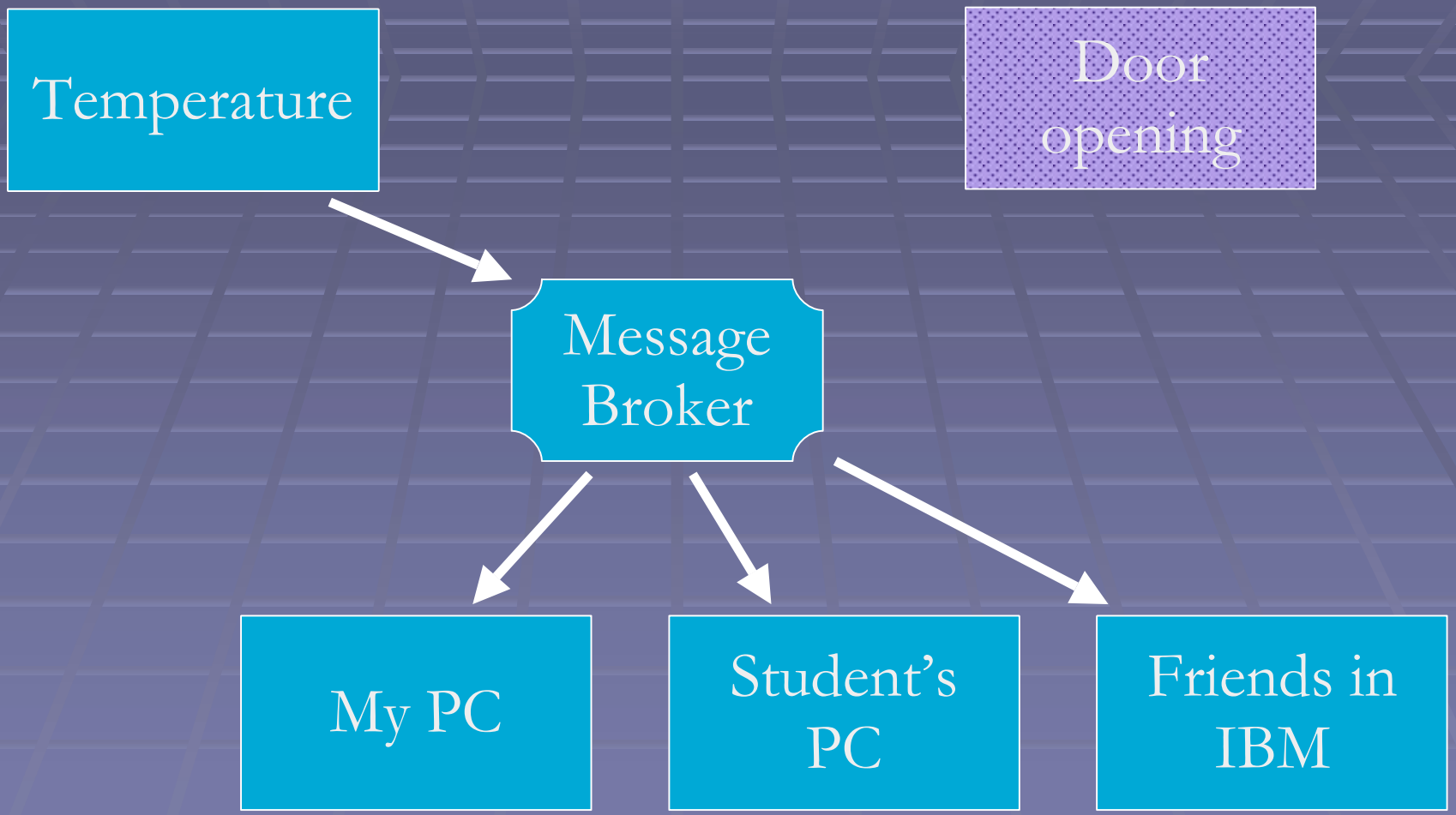

Temperature in the lab
Door opening
My PC
Student's PC
Friends in IBM

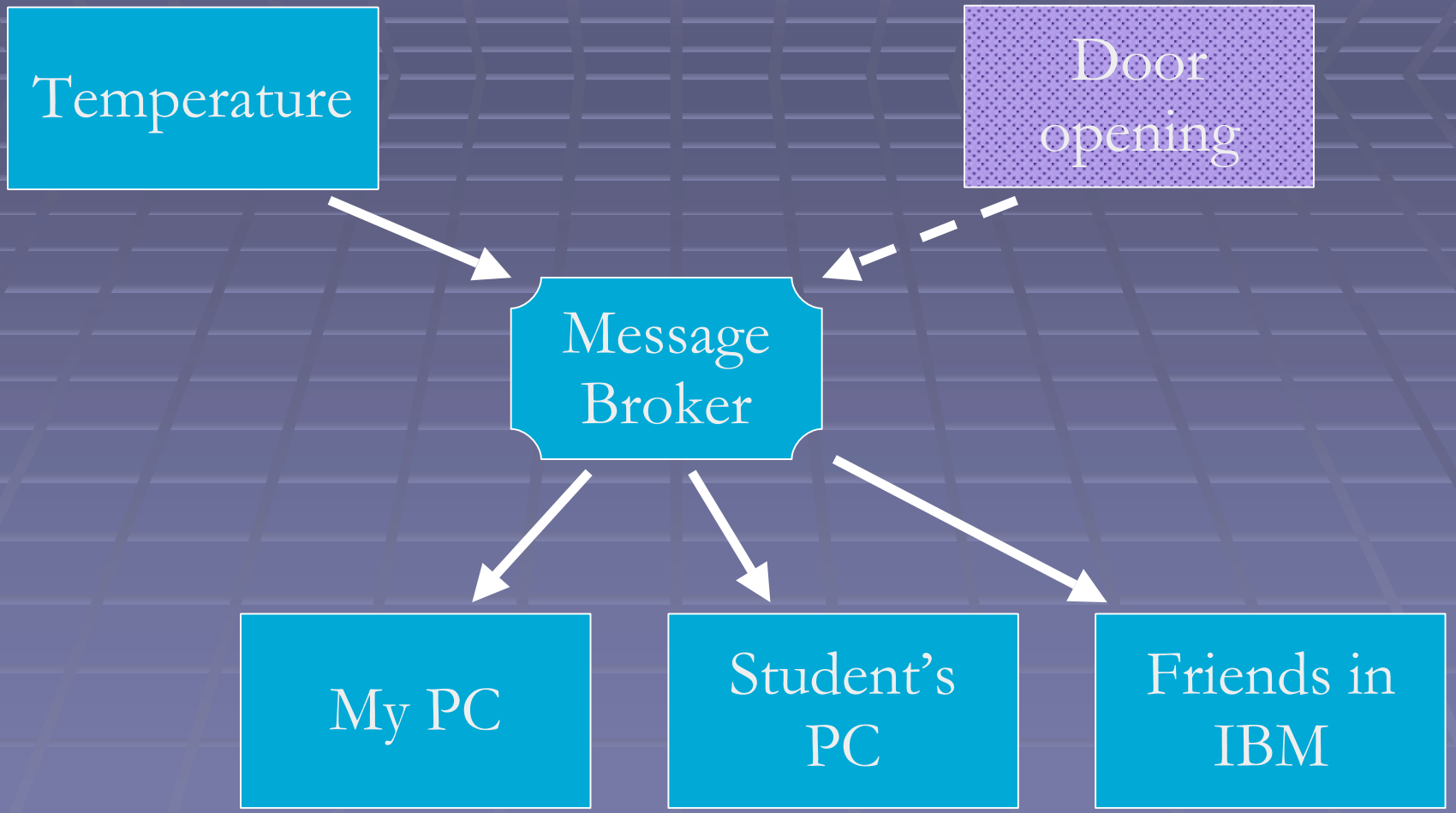


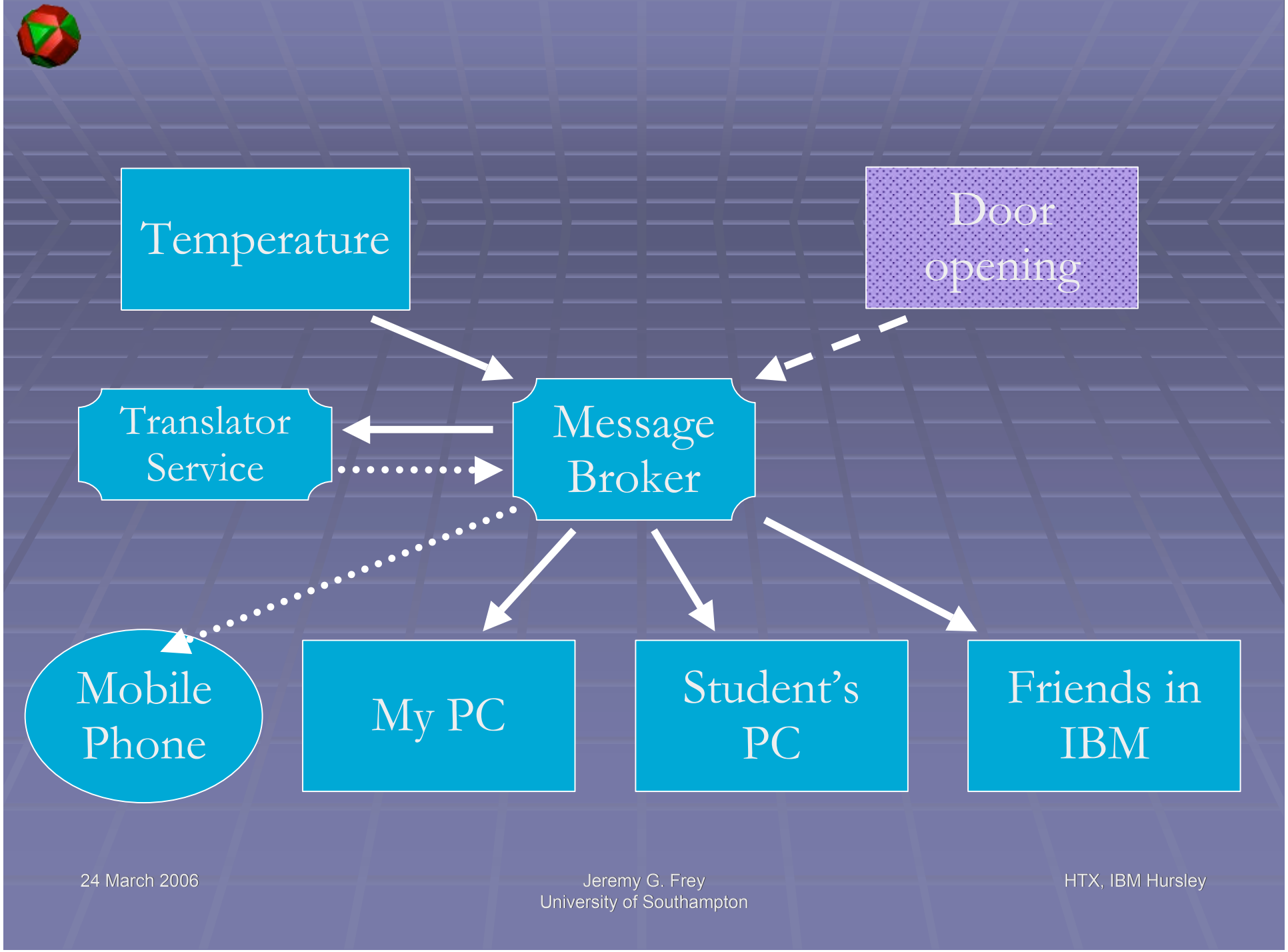

"What the hell sort of convenient new feature is this?"


Temperature in the lab
Door opening
Translator Service
Mobile Phone
My PC
Student's PC
Friends in IBM


Temperature
Message Agent
My PC


Temperature
Door opening
Message Broker
My PC
Student's PC
Friends in IBM


Temperature
Door opening
Message Broker
My PC
Student's PC
Friends in IBM


Temperature
Door opening
Translator Service
Message Broker
Mobile Phone
My PC
Student's PC
Friends in IBM

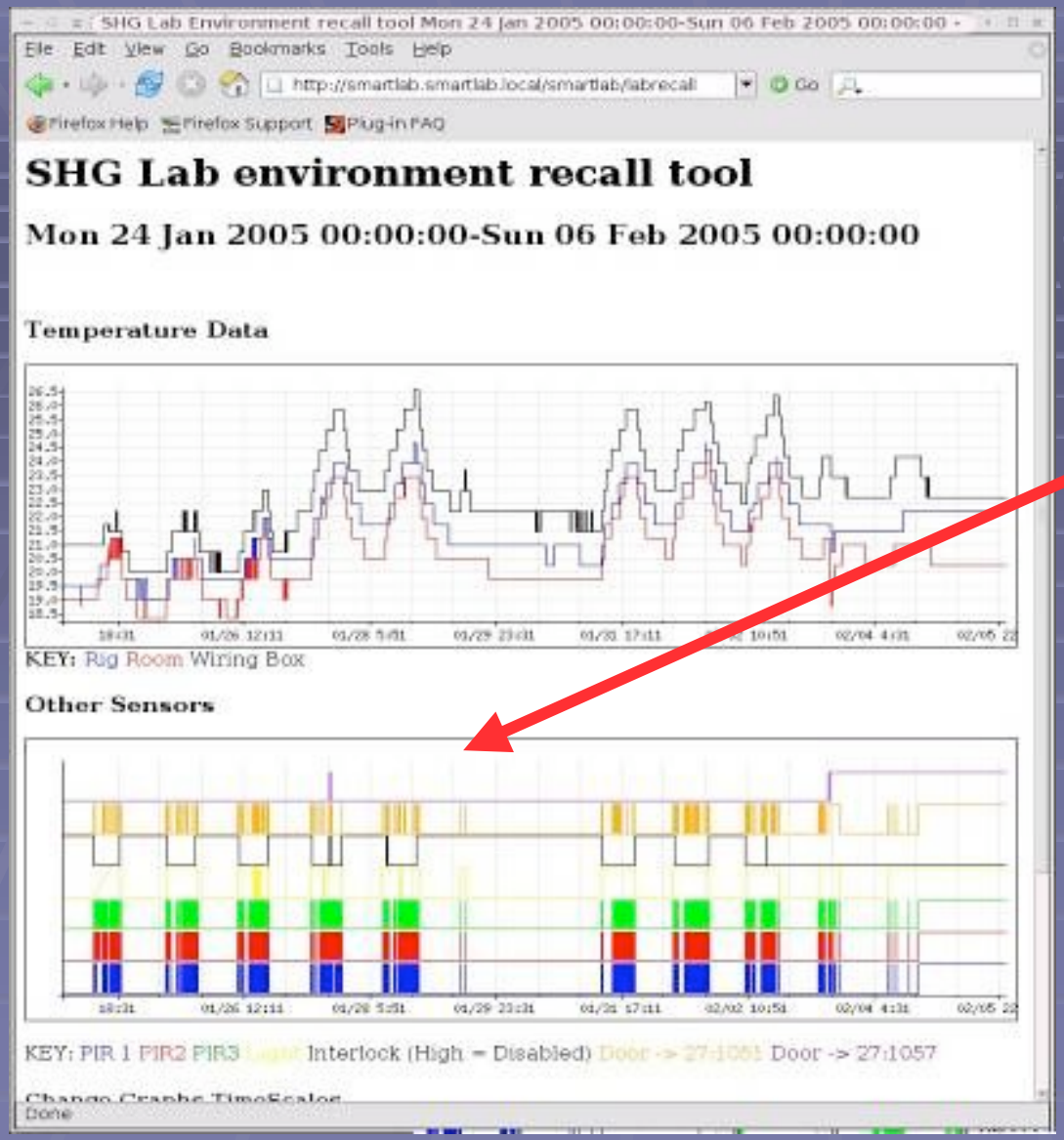
# Monitoring by Phone




# "I love the convenience, but the roaming charges are killing me"



Jeremy G. Frey
University of Southampton




Air Conditioning failed

# What you have to do to get on to the BBC web site


Pub/Sub for Laboratory data using a broker and ultimately delivered over GPRS



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BBC NEWS | Science/Nature | Chemists escape labs via mobiles - Microsoft Internet Explorer

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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

The system is not smart enough to actually buy a round yet

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obiles - Microsoft Internet Explorer

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

m so that at a push of a
able to remotely change
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seamlessly.

Chemists enjoy a drink at the bar while keeping and 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.


"Not tonight, hon. It'll just wreak havoc with the motion sensors again."

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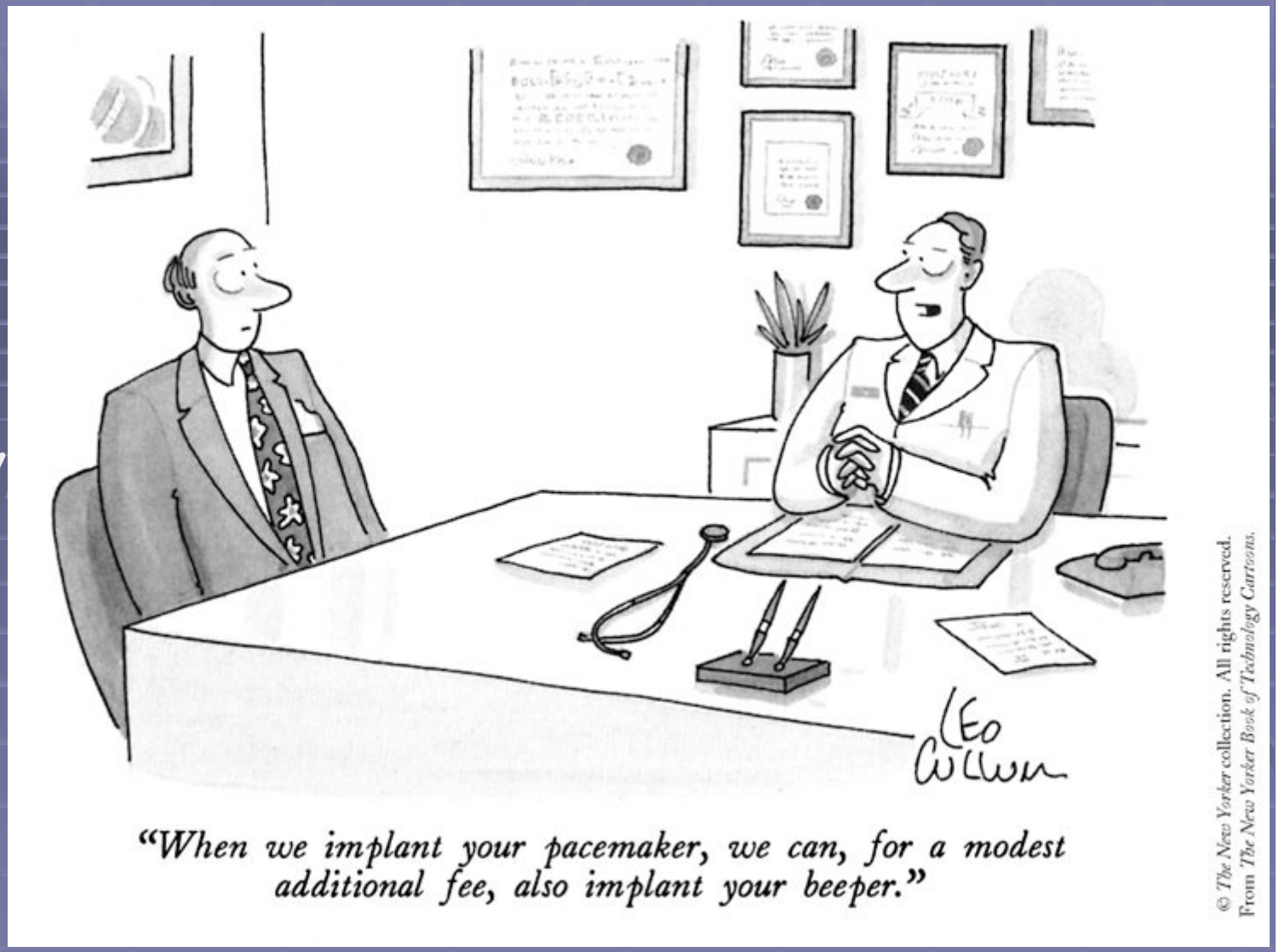
We don't want to take this technology too far.

There are privacy issues




*"When we implant your pacemaker, we can, for a modest additional fee, also implant your beeper."*

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"When we implant your pacemaker, we can, for a modest additional fee, also implant your beeper."



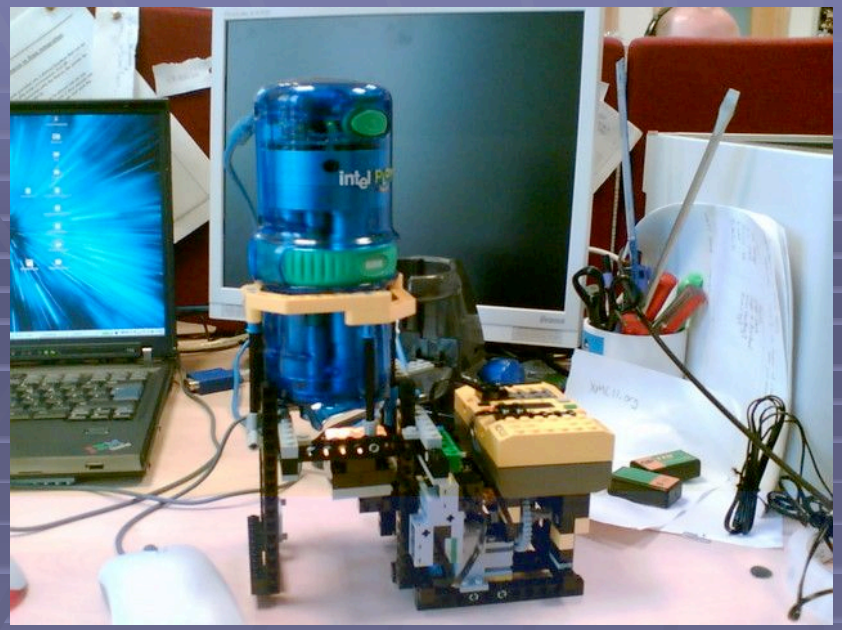
Jeremy G. Frey
University of Southampton

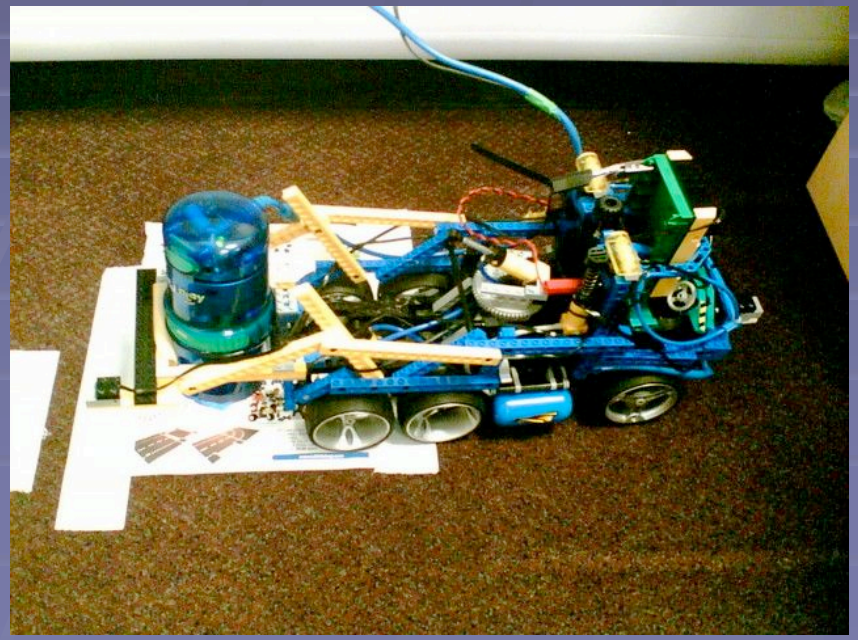

# Remote control?


Jeremy G. Frey
University of Southampton

# Security and trust for experiments and data


*"On the Internet, nobody knows you're a dog."*





Need to make the data available

Need to be able to find it

But how to expose it?

"First, they do an on-line search."

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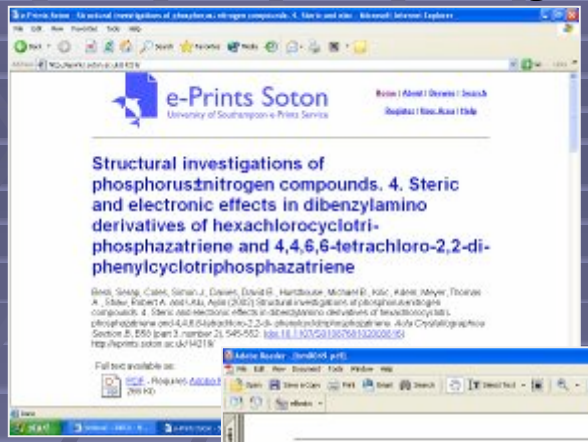
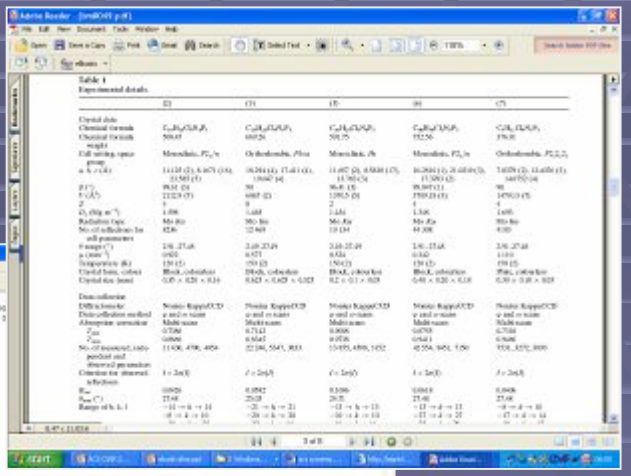
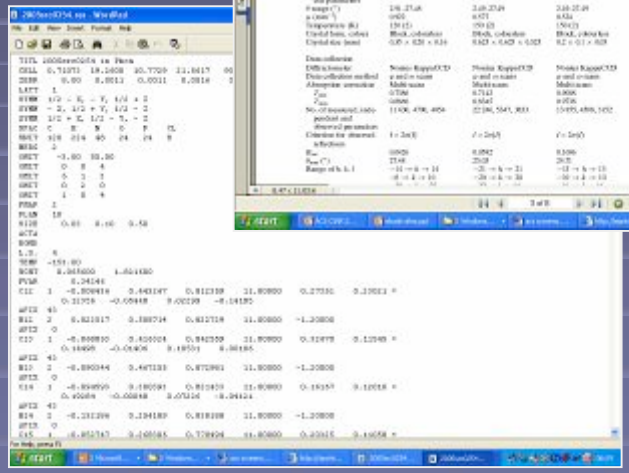
# First, they do an online search

# Separating Data from Interpretations: A crystallography example

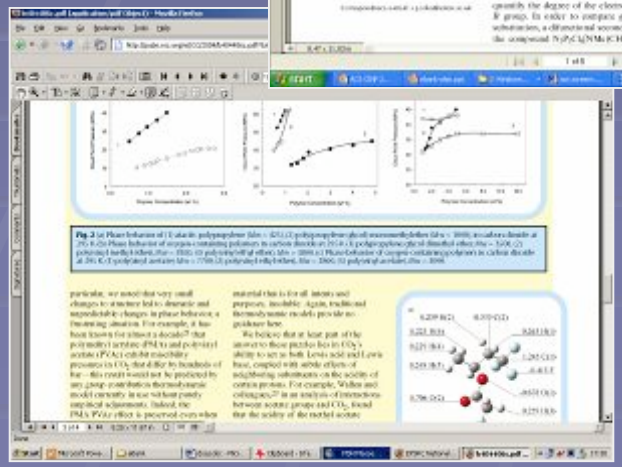




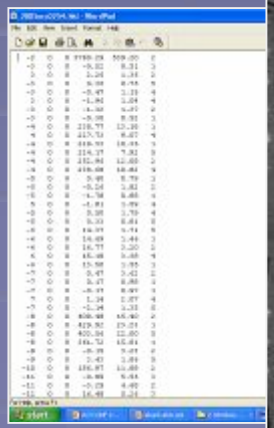


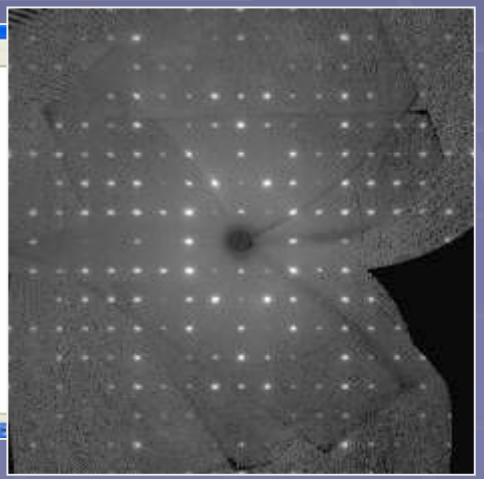


Underlying data



Intellect & Interpretation





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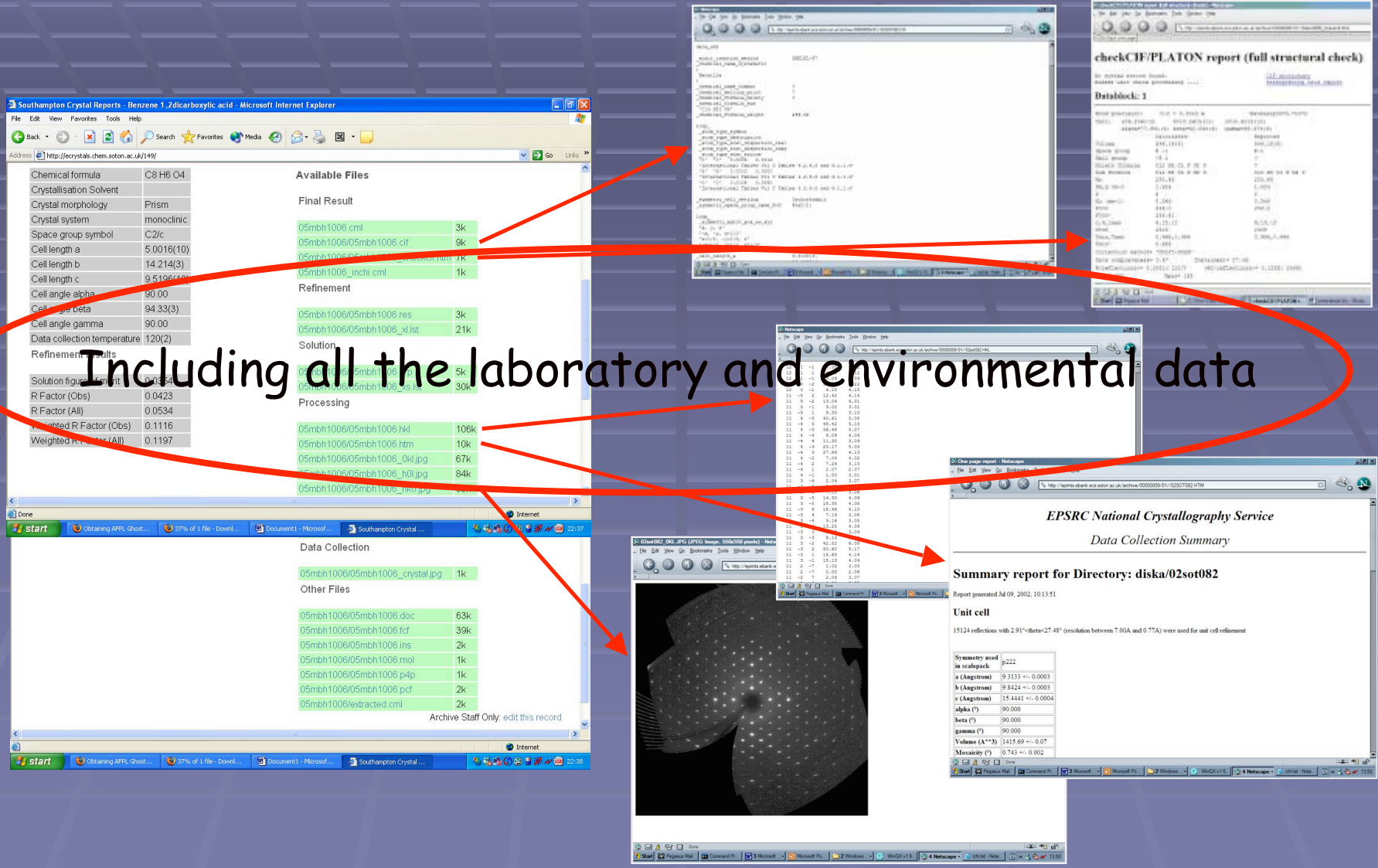
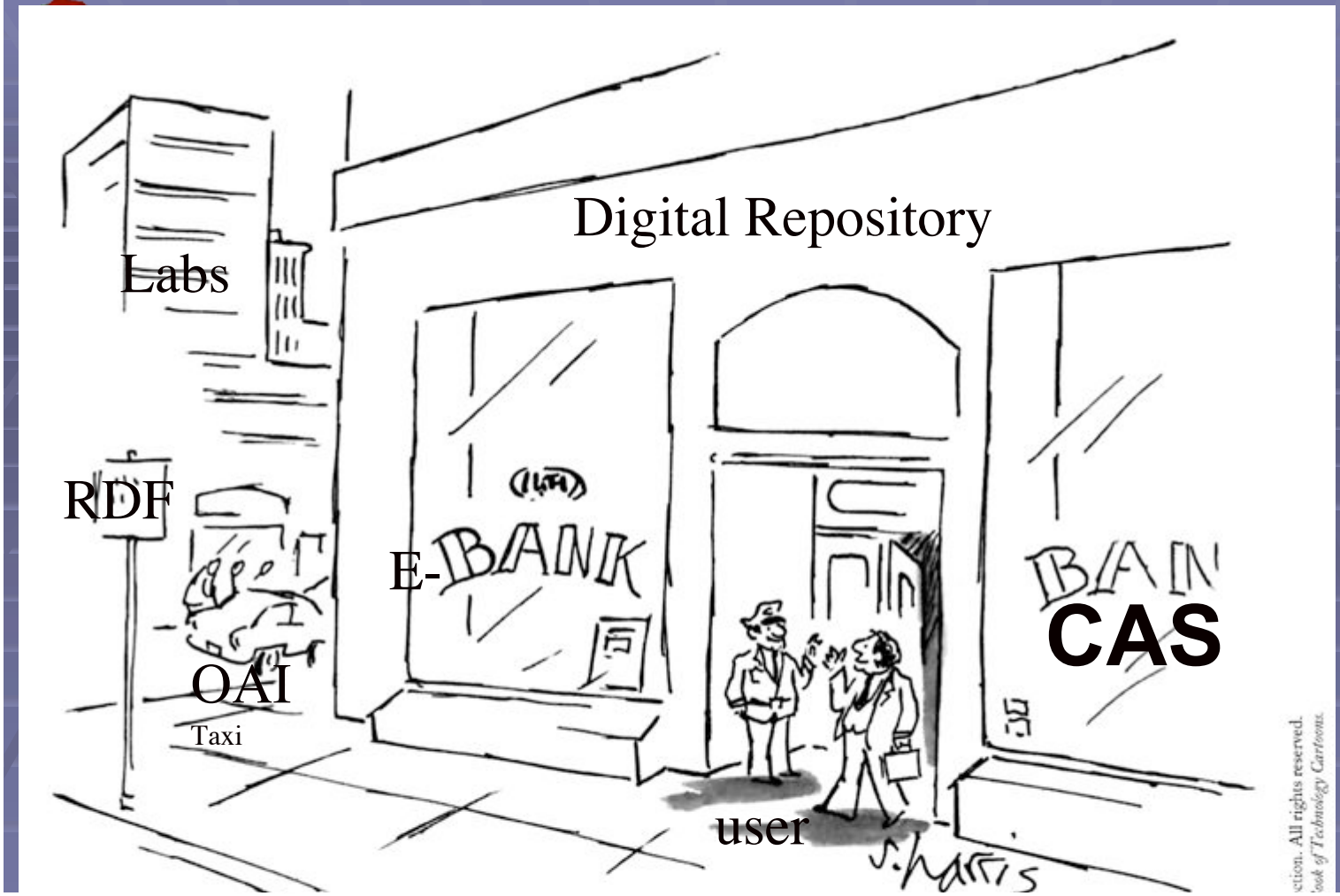
# Access to ALL underlying data






Subversive and furtive sharing & exploitation of data

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

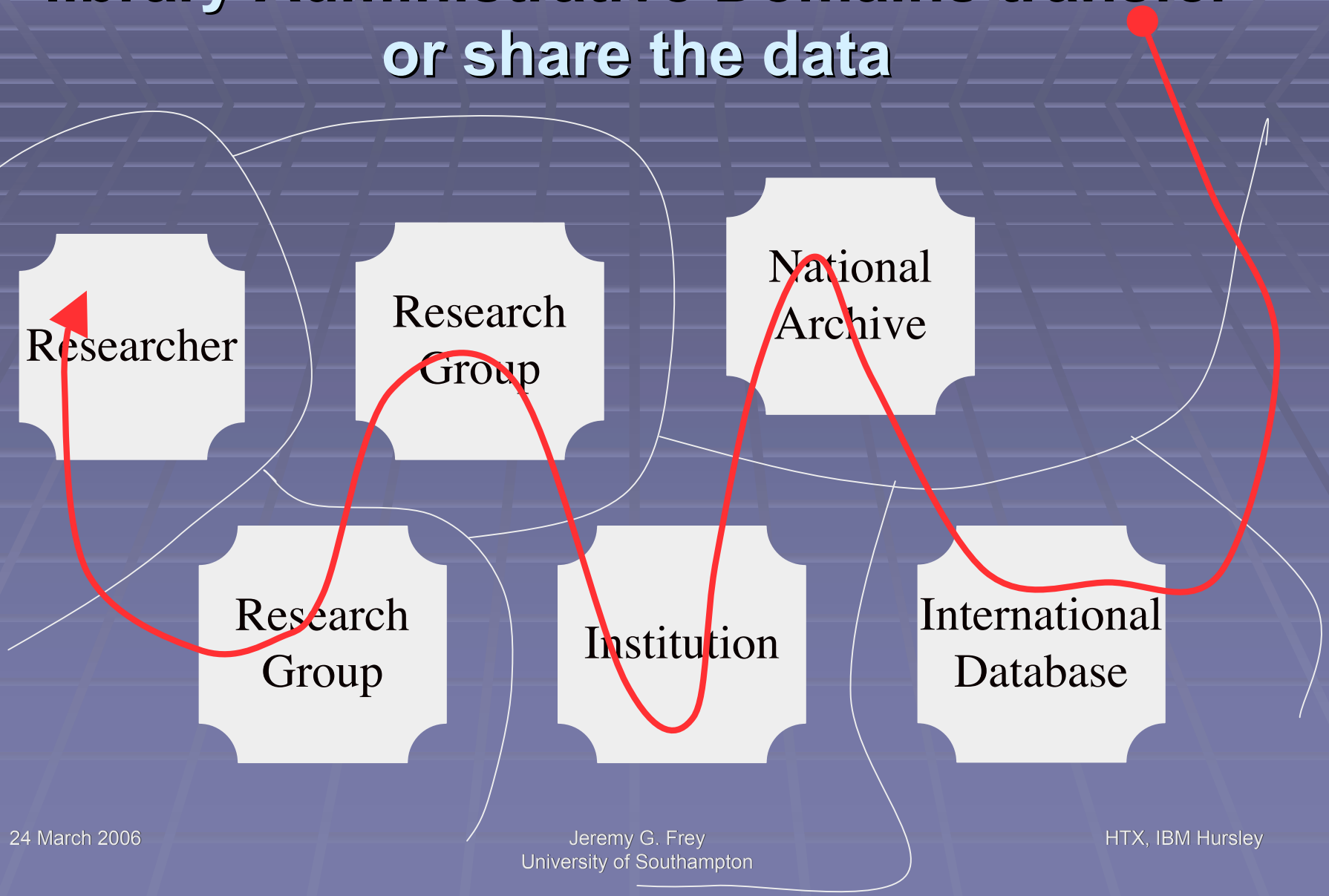
**Data**

# Chemistry Data

private or public,

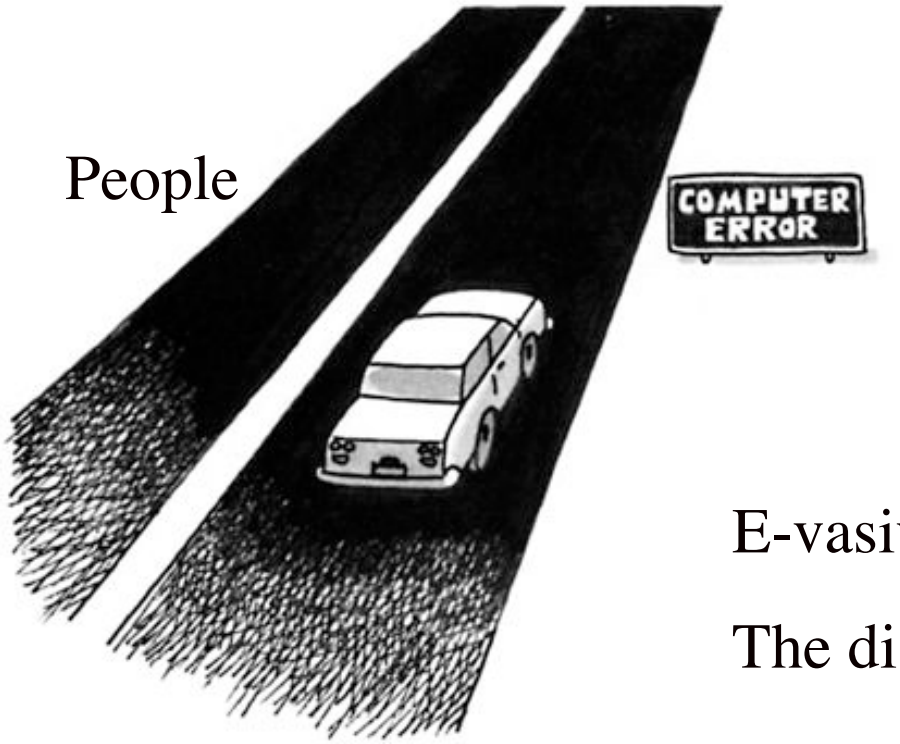
open or controlled access

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



Technology

People

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E-vasive Computing

The disappearing human

ZIEGLER