Making Tea

A human centred approach to designing a pervasive smart lab "notebook"

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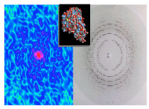
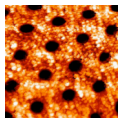
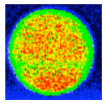






Talk

- The UK *e*-Science Programme
- The Comb-*e*-Chem Project
- Smart Tea or How to introduce Computer Scientists to the Lab
- Smart Labs - data streams & inference
- Relational databases in science?
- The Ontological Imperative
- The future's bright the future's….

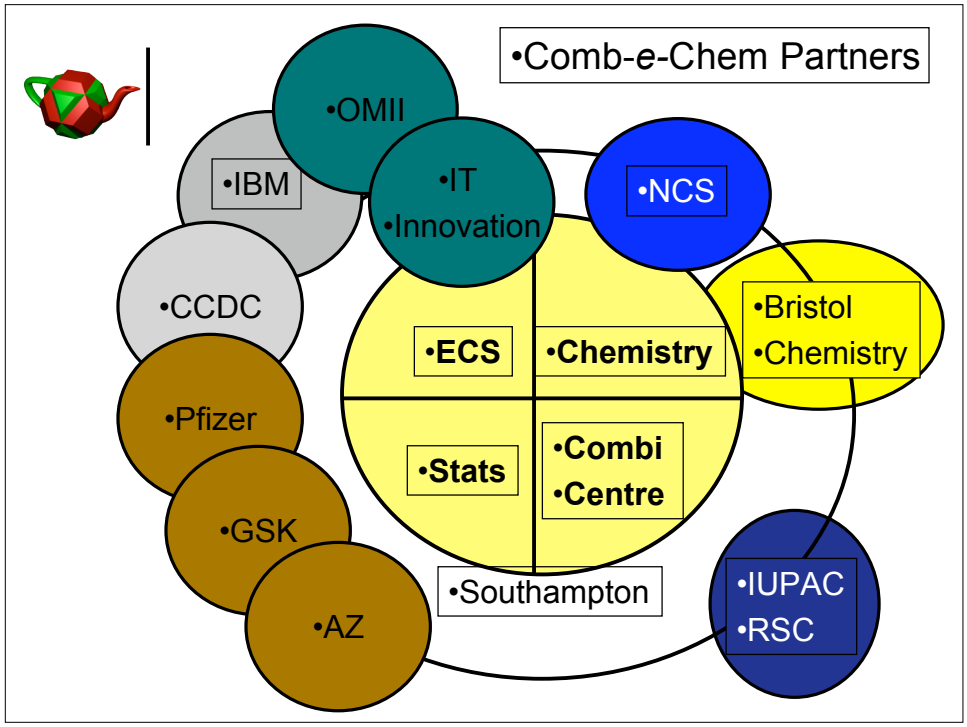
e-Science

- **'e-Science is about global collaboration in key areas of science, and the next generation of infrastructure that will enable it.'**
- **'e-Science will change the dynamic of the way science is undertaken.'**

  John Taylor, DG of UK OST
- **'[The Grid] intends to make access to computing power, scientific data repositories and experimental facilities as easy as the Web makes access to information'** Tony Blair, 2002

The Comb-*e*-Chem Project

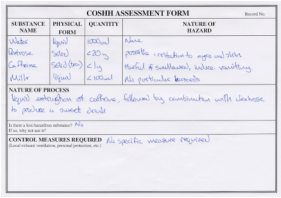
- The exponential world of Combinatorial Synthesis and High throughput analysis meets the exponentially growing power of computing
- **Funding**
  EPSRC, JISC, IBM, GSK, AZ, Southampton



Smart Tea People

- **Electronics and Computer Science**
  - Gareth Hughes, Hugo Mills, Graham Smith, monica Schraefel, Luck Moreau, Terry Payne, Dave De Roure
- **Chemistry**
  - Martin Grossel & research group
  - Jamie Robinson, Hongchen Fu, Sam Peppe

Laboratory Context

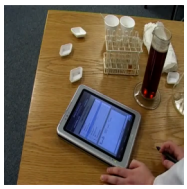


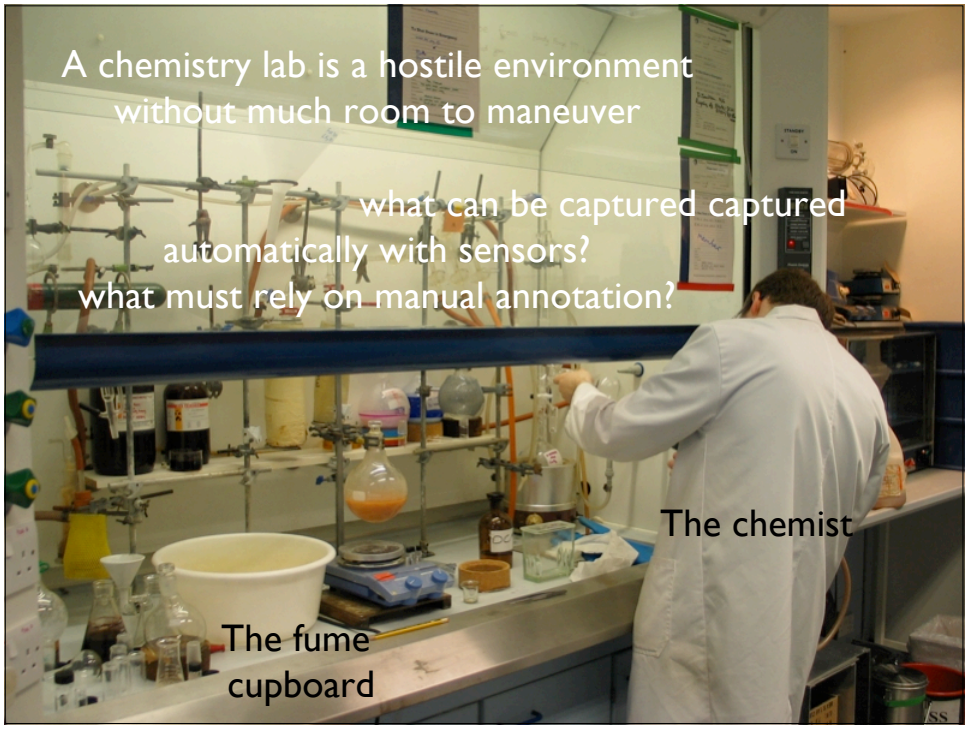
COSHH → Plan → Record

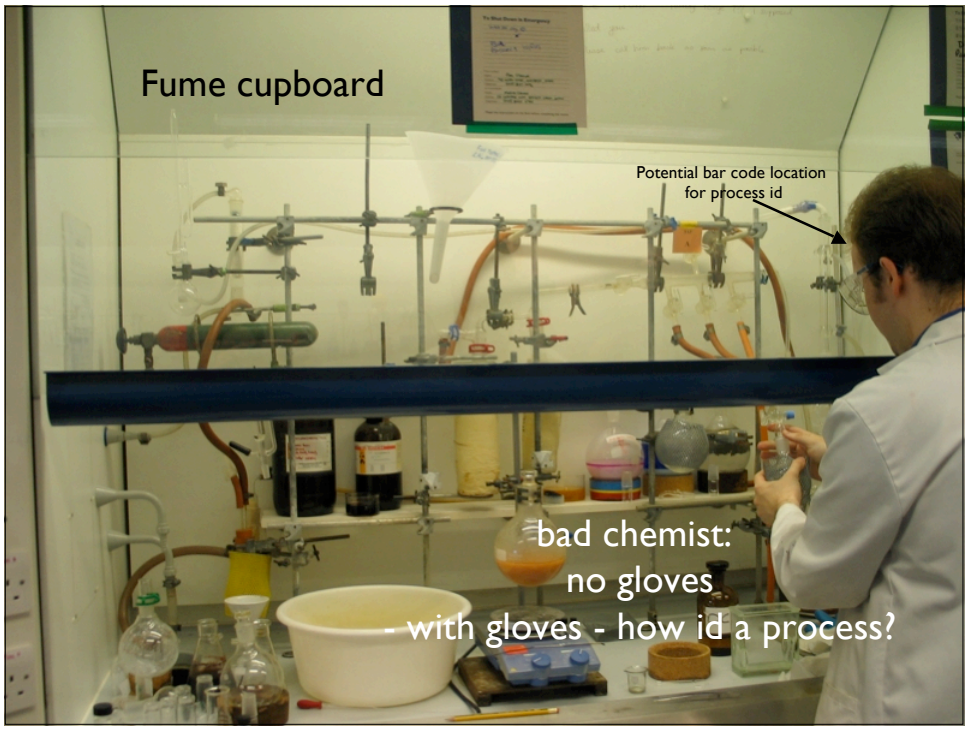
Annotation

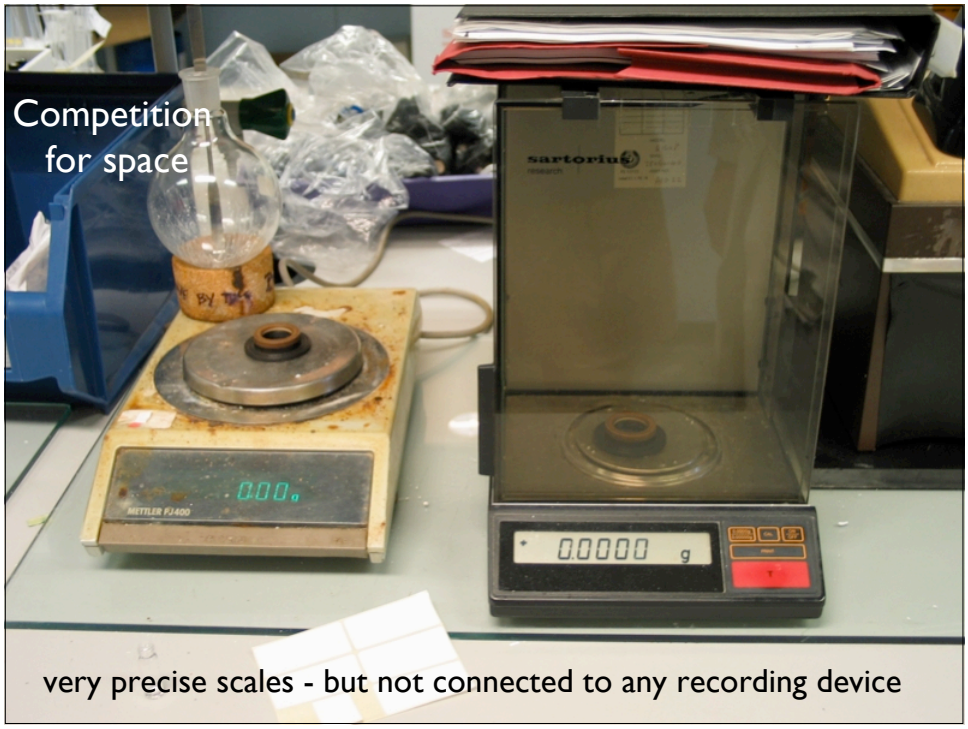
Guide → Digital Context

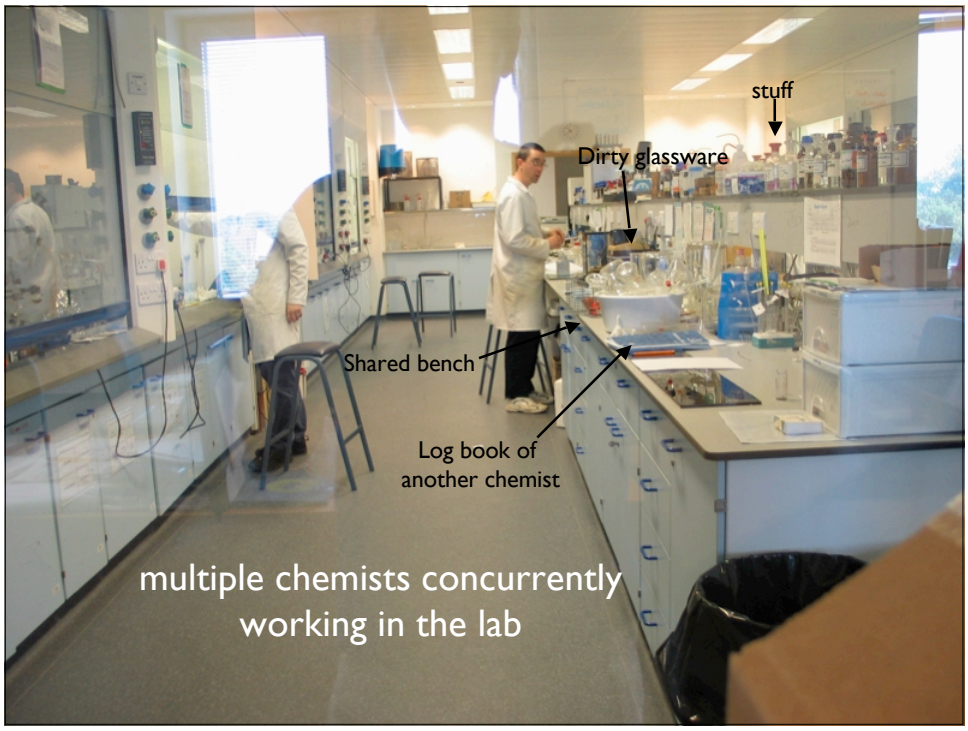
Experimenters

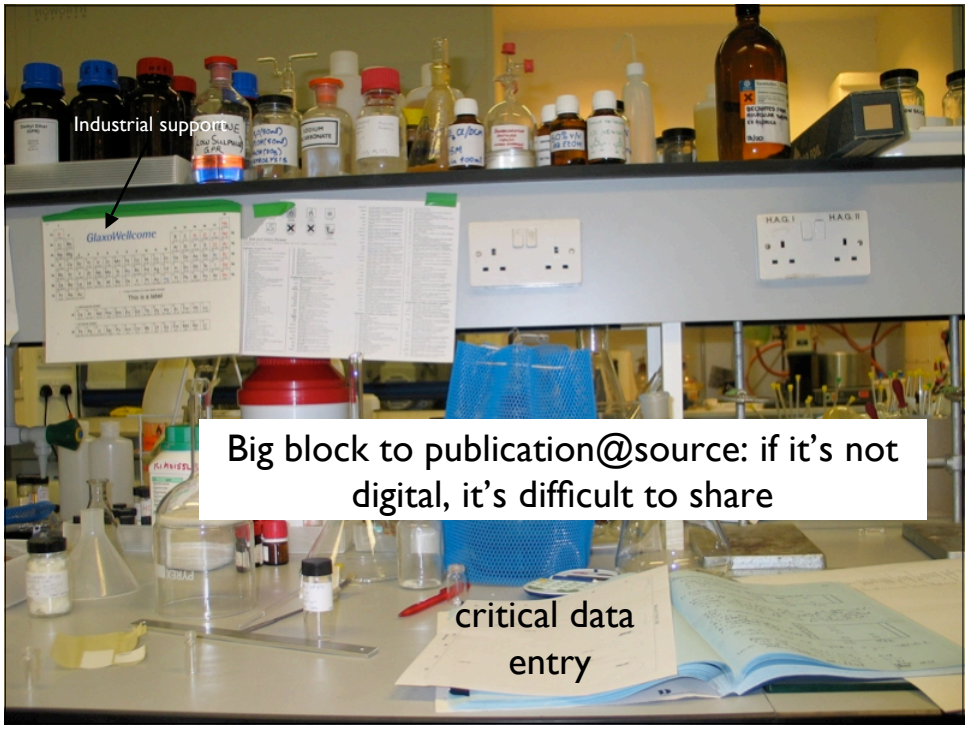





Fume cupboard
Potential bar code location
for process id
bad chemist:
no gloves
- with gloves - how id a process?


Competition
for space
sartorius
0.0000 g
very precise scales - but not connected to any recording device


stuff
Dirty glassware
Shared bench
Log book of another chemist
multiple chemists concurrently working in the lab


Industrial support
GlaxoWellcome
Big block to publication@source: if it's not digital, it's difficult to share
critical data entry

The Lab book II

no dedicated location

vulnerability of data captured

access to data by others is limited

privilege (IP) • rights

uniqueness

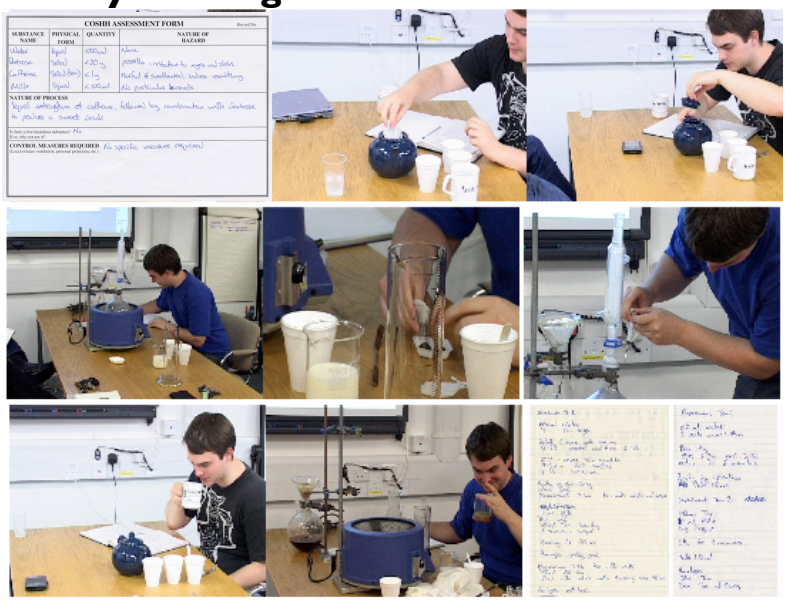
history

Many Lab book Replacements have been tried.

Currently Southampton Chemists don't use one
So…..

How would we succeed?

By Making Tea!



Getting not just the what and how, but the *why*

Problem: why make tea?

- We wanted to build a digital lab book replacement and the services to support that system.
- Even after the observations and interviews, they knew about the environment (good)
- But they didn't know beyond a general sense
  - what chemists did,
  - how they did it or
  - the role the lab book played in their doings.

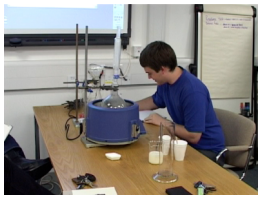
Background: available approaches and problems in ucd

- Observation of an Experiment
- Expert and artefact walk throughs
- Apprenticeship and Prototyping
- Cultural Probes
- Task Analysis
- Deconstruction/Reconstruction

What we needed

- A way to compress time
- A faithful, not overly simplified process
- A way to engage the process
  - A language we (chemists and designers) could all understand to interogate the process (the experiment)
- Enter Analogy

Making Tea: design elicitation through analogy



- Developed and validated the analogy with chemists
- Gave us a way to ask questions that would not otherwise have been possible
- Let us maximize observation
- Gave us repeatability
- Derived rudiments of a process model, too
- Provided lingua franca with chemists

Review over Tea

me

- We ran through our lo-fi prototypes with chemists by running the tea experiment
  - They knew what was going on and could comment on veracity, features, process

Cup of tea demo

Recording takes place throughout an experiment.
In this clip
- a reagent is measured out
- the weight is entered by fast keypad input
- a step is selected and ticked off when completed
- the compound is tested
- that action is annotated

- Digital Tea II
- We join our heroes after having completed Exp 1, Making Tea, and are now into Exp 2 Making a cup of Tea with Milk and Sugar
- Design based on what chemists

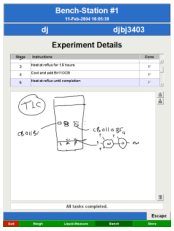
The recording of steps is part of the COSSH requirement
We leverage this in our system

Getting real

- Functional prototype for in-lab, real use testing

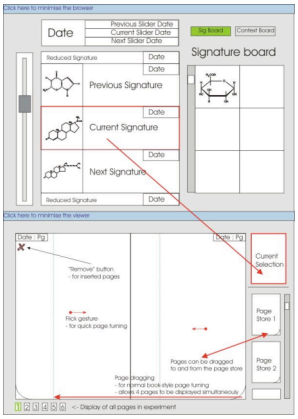
Results

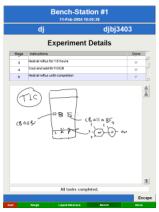
"I can go anywhere and its, like, this is me and my data. It's all there! Bang!"



- In real use, chemists were able to record their experiments
- After about ten minutes of use, they forgot about it as a new thing, and just used it

Extensions: 3rd Yr UG Projects





- Ray Cooke
  - Scrolling through lab books
- Will Davies
  - Automating TLC plate capture for record and annotation

Models

- Making Tea gave us:
  - A new design elicitation method for loosely structured, high expertise domain processes
    - From this, a way to model the interaction
  - A functional interaction prototype to evaluate approach
    - No clearly defined architecture or model
    - No plan entry or data retrieval interfaces

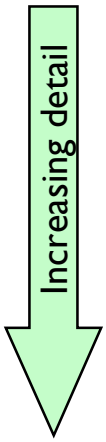
(hope you don't need your notes, guys)

  - But…

More Models

- But Tea
  - Not only valuable for understanding interaction but also for developing a process model
  - Making Tea as an experiment formed the basis of our initial discussions for describing experimental process for provenance modelling

Data model



Plan

Intended actions:
guide to chemist,
or [later] workflow

Process record

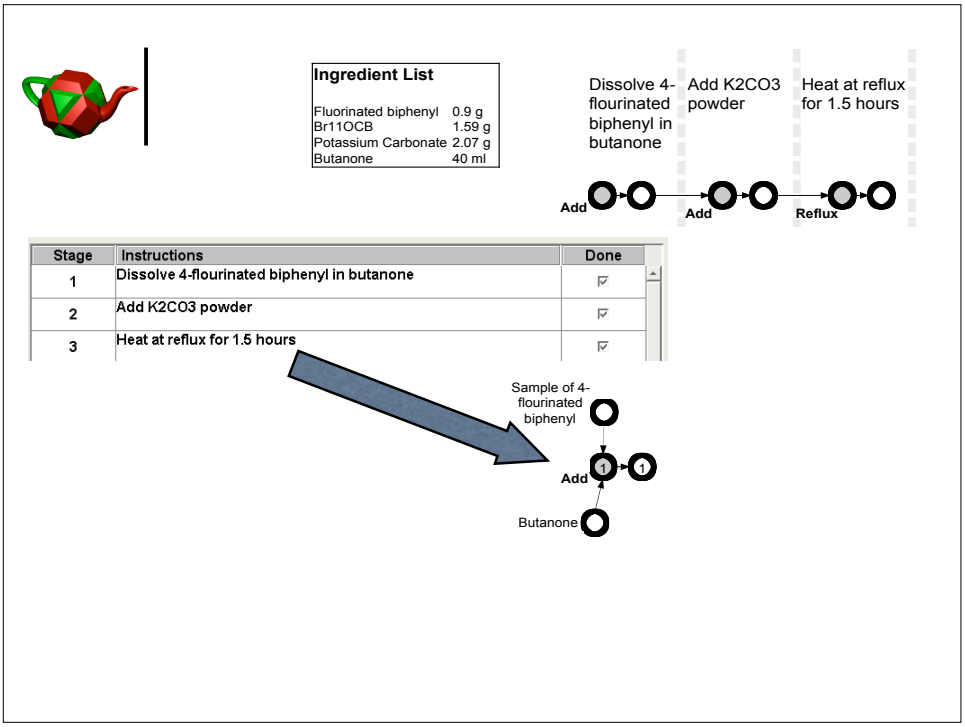
Measurements
Processes
Annotations

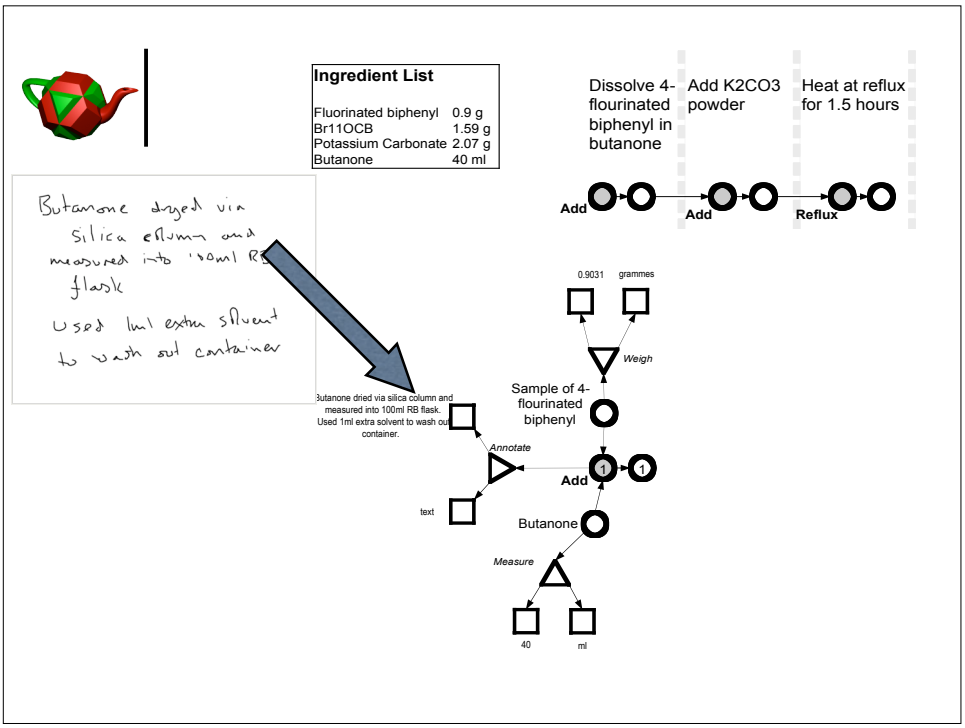
Provenance record

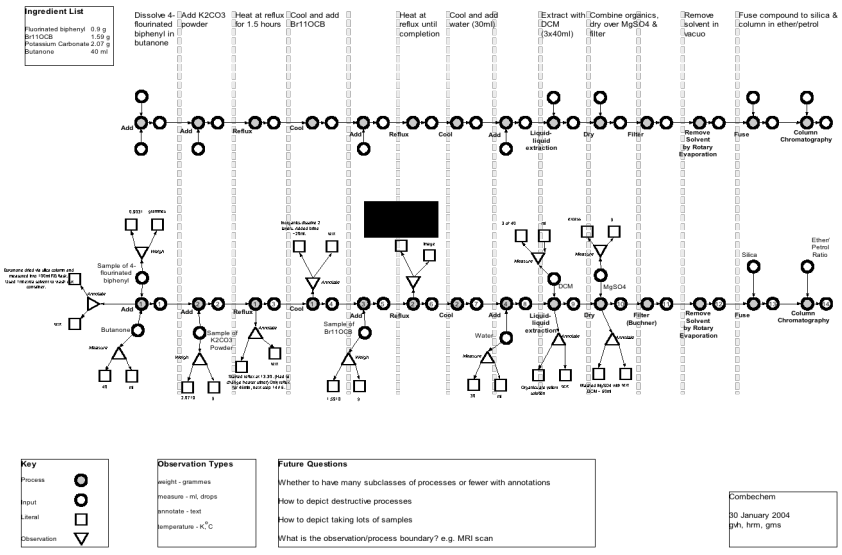
Service invocations
Secure time-stamps
etc…

Process record notation

- Analyse a real experiment
  - What information do chemists record?
  - What should they record?
  - What do they want to record?
  - How does this differ from their experiment plan?
- Evolved our own graph of plan and record
  - *Initially, this was to be modelled on tea, but we tested it on one of the actual experiments a chemist ran with the tea tablet*


Ingredient List
Fluorinated biphenyl 0.9 g
Br11OCB 1.59 g
Potassium Carbonate 2.07 g
Butanone 40 ml
Dissolve 4-flourinated biphenyl in butanone
Add K2CO3 powder
Heat at reflux for 1.5 hours
Add
Add
Reflux
Stage
Instructions
Done
1
Dissolve 4-flourinated biphenyl in butanone
2
Add K2CO3 powder
3
Heat at reflux for 1.5 hours
Sample of 4-flourinated biphenyl
Add
Butanone


Ingredient List
Fluorinated biphenyl 0.9 g
Br11OCB 1.59 g
Potassium Carbonate 2.07 g
Butanone 40 ml
Dissolve 4-flourinated biphenyl in butanone
Add K2CO3 powder
Heat at reflux for 1.5 hours
Add
Add
Reflux
Butanone dryed via silica column and measured into 100ml RB flask.
Used 1ml extra solvent to wash out container
0.9031
grammes
Weigh
Sample of 4-flourinated biphenyl
Annotate
text
Add
Butanone
Measure
40
ml



Lessons

- That we need two related ontologies
  - Plan – that are going to be done
  - Record – what was done
- Not necessarily the same thing
  - Steps are added/repeated during the experiment
  - Different annotations required for each

Semantic Grid?

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From The New Yorker Book of Technology Cartoons.

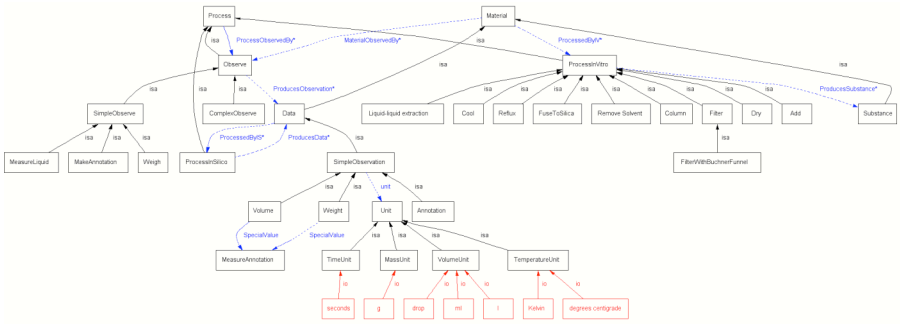
~~Grid~~ C. Barsotti

"Oh, like you know something the Internet doesn't know."

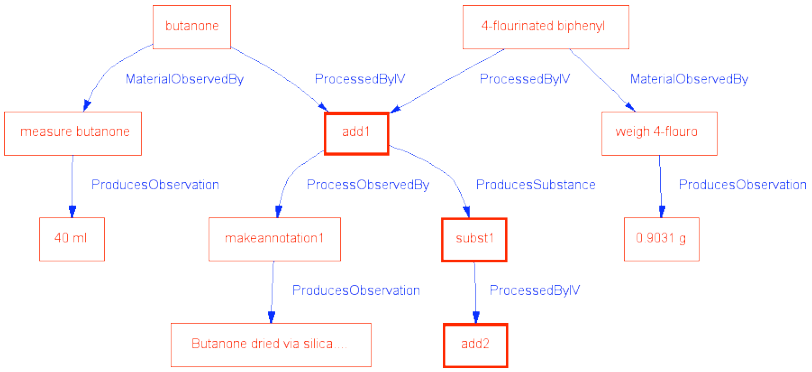
The Ontological Imperative

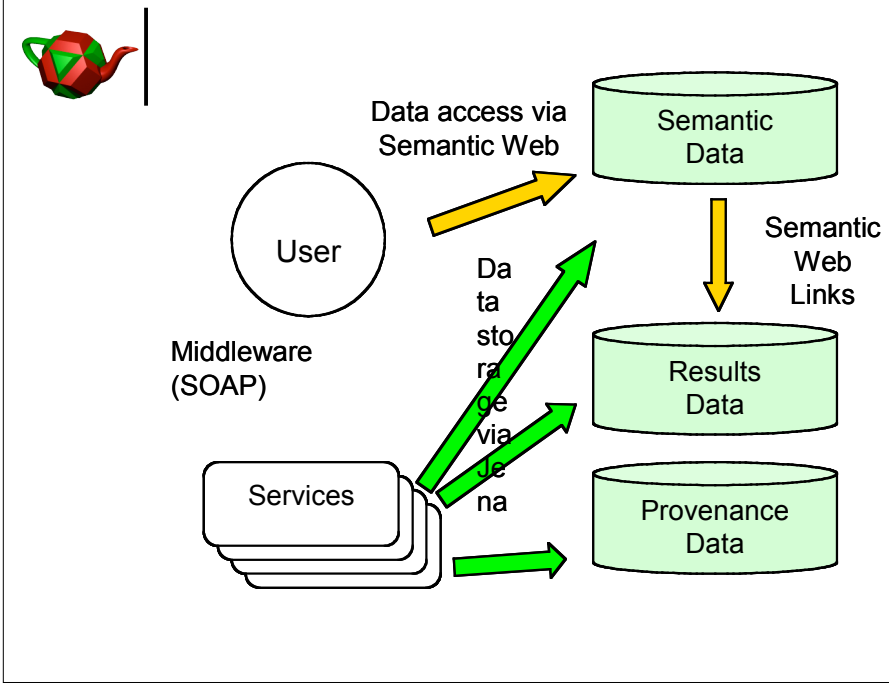
Is this categorical?

Process Record Ontology

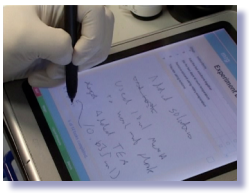


Example Record Instances



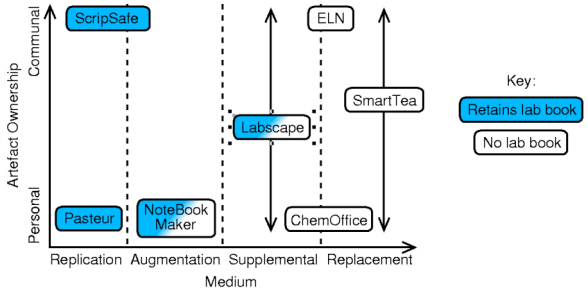


Questions – Plan Viewer



A personal tablet or distributed terminals?

A pervasive issue

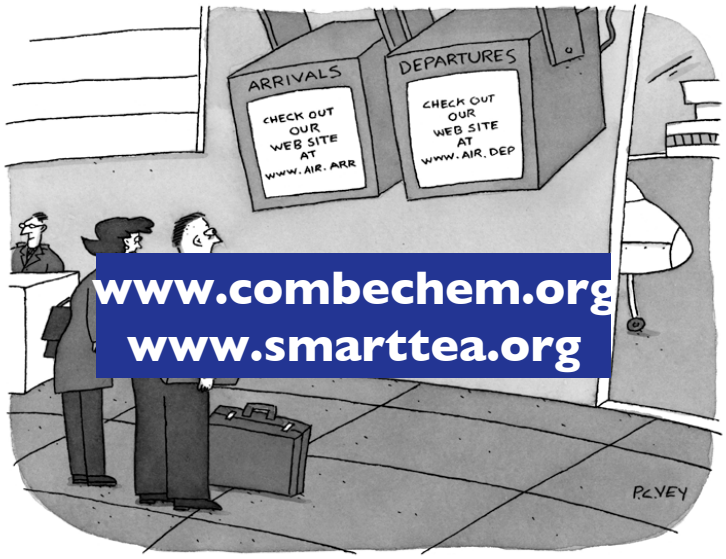


Pervasive Semantic Grid?

Grid

"Oh, like you know something the Internet doesn't know."

Web sites?



The Semiotic Web
Are semantics sufficient?

- Chemists use signs and symbols as much as, if not more than words
- Icons have a great significance – The Periodic Table
- People & Computers need to communicate with each other as well as themselves
- Need a more powerful (general) concept than the semantic web & grid.