Making Tea

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

Jeremy Frey
School of Chemistry
University of Southampton, UK

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
A chemistry lab is a hostile environment without much room to maneuver. What can be captured automatically with sensors? What must rely on manual annotation?
Fume cupboard

- bad chemist: no gloves
  - with gloves - how id a process?

Potential bar code location for process id

very precise scales - but not connected to any recording device

Competition for space
multiple chemists concurrently working in the lab

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?
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 interrogate 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

- 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

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

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

This recording of steps is part of the COSHH 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*
Sample of 4-flourinated biphenyl
Add Reflux Butanone

Sample of K2CO3 Powder
Weigh 0.9031 g
Measure 40 ml
Add

Butanone dried via silica column and measured into 100 ml RB flask. Used 1 ml extra solvent to wash out container.

Dissolve 4-flourinated biphenyl in butanone
Add K2CO3 powder
Heat at reflux for 1.5 hours

 Ingredient List
Flourinated biphenyl 0.9 g
Br11OCB 1.59 g
Potassium Carbonate 2.07 g
Butanone 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?

The Ontological Imperative

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

Is this categorical?

Process Record Ontology
Example Record Instances
Questions – Plan Viewer

A personal tablet or distributed terminals?

A pervasive issue

Pervasive Semantic 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.