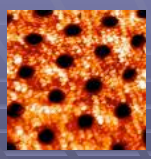
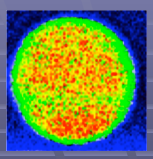
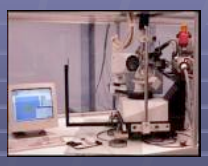





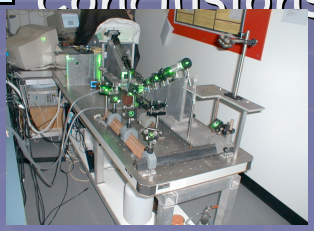
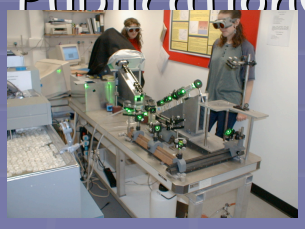

Semantic Support for Smart Laboratories

Jeremy Frey
School of Chemistry, University of Southampton UK.

CINF, ACS San Diego
17 March 2005

Talk: Workflow

- Introduction to e-Science & the Combechem Project
- Pub / Sub
- Semantics for Smart but not Dark Labs
- Conclusions: Publication@Source

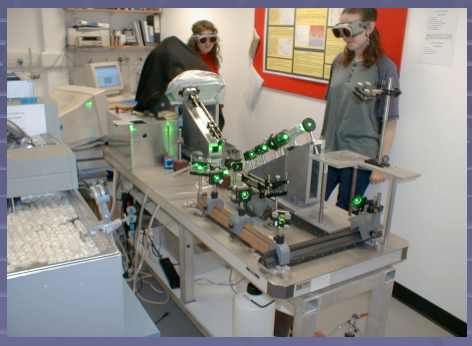



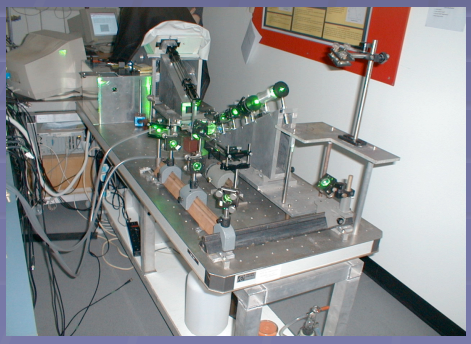

The CombeChem Project

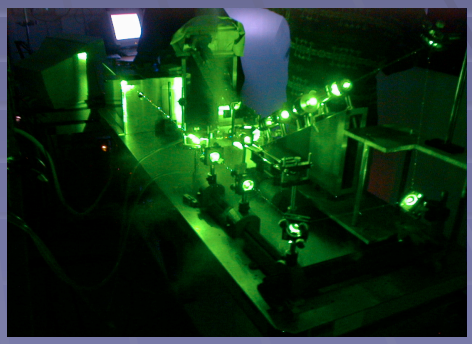
- Collect data with regard to how it could eventually be used
  - Make sure the metadata is of high quality
  - Record properly at source in Digital Form
- The Chemistry Lab
  - People & Machines working together
- End to End linking of data and information
  - Publication@Source
- But then.... "Who needs provenance?"
  - Bush, Blair The JIC, MI5, CIA & Hutton 2004

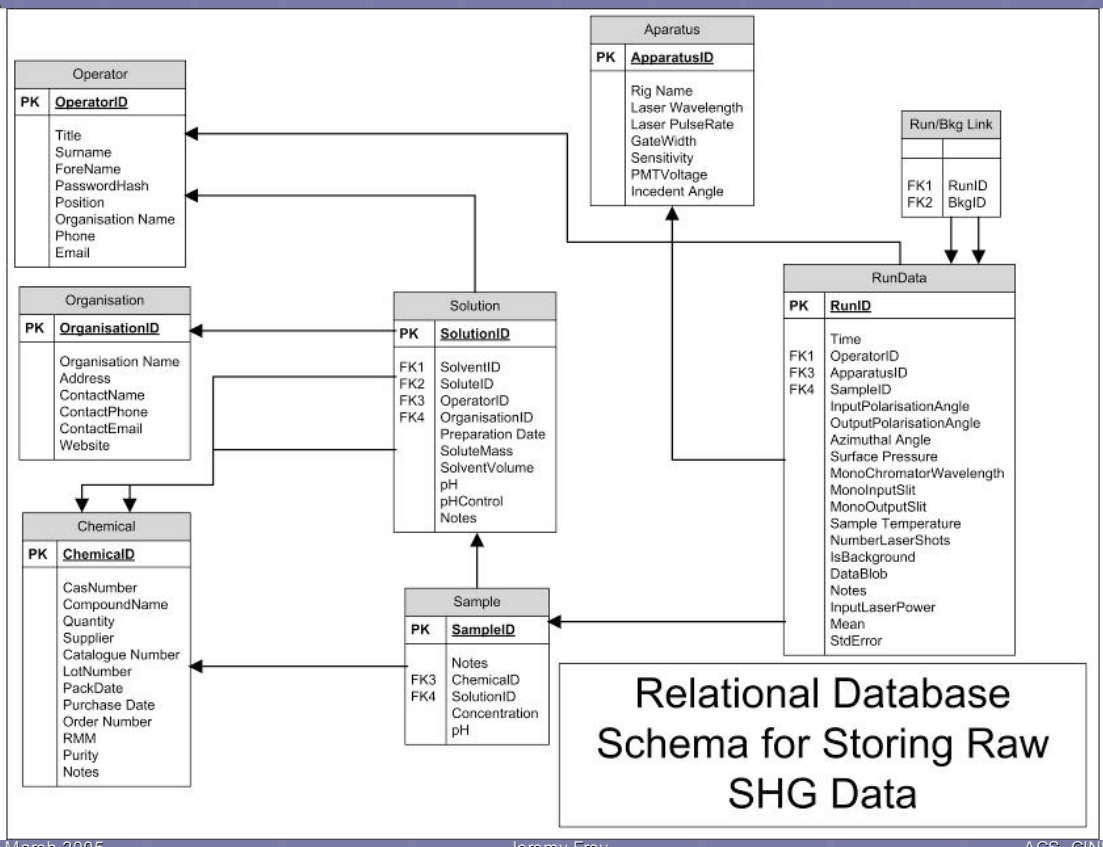
Adapt SHG lab

- Set out to store the data coming from our non-linear laser experiment
- Use a database!

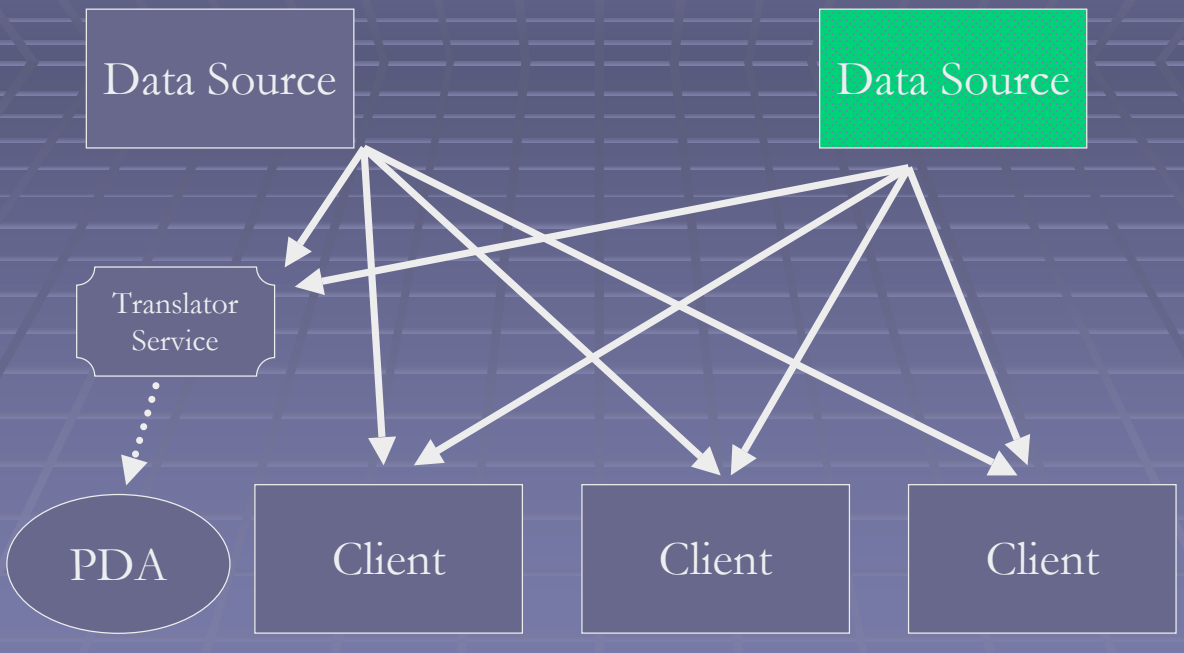




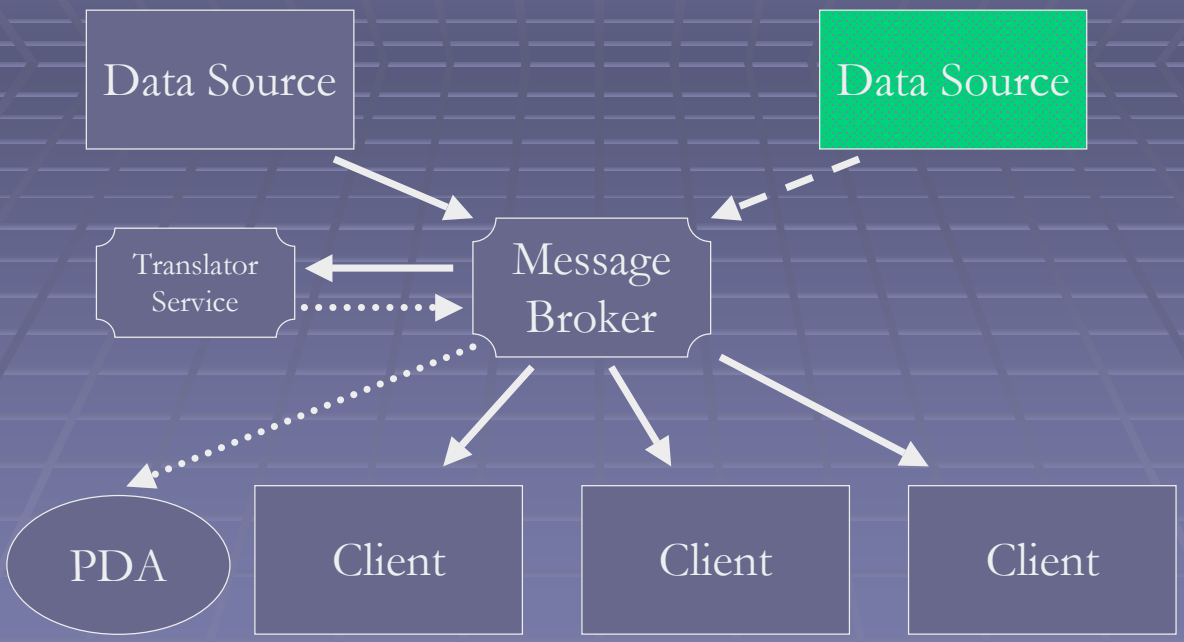




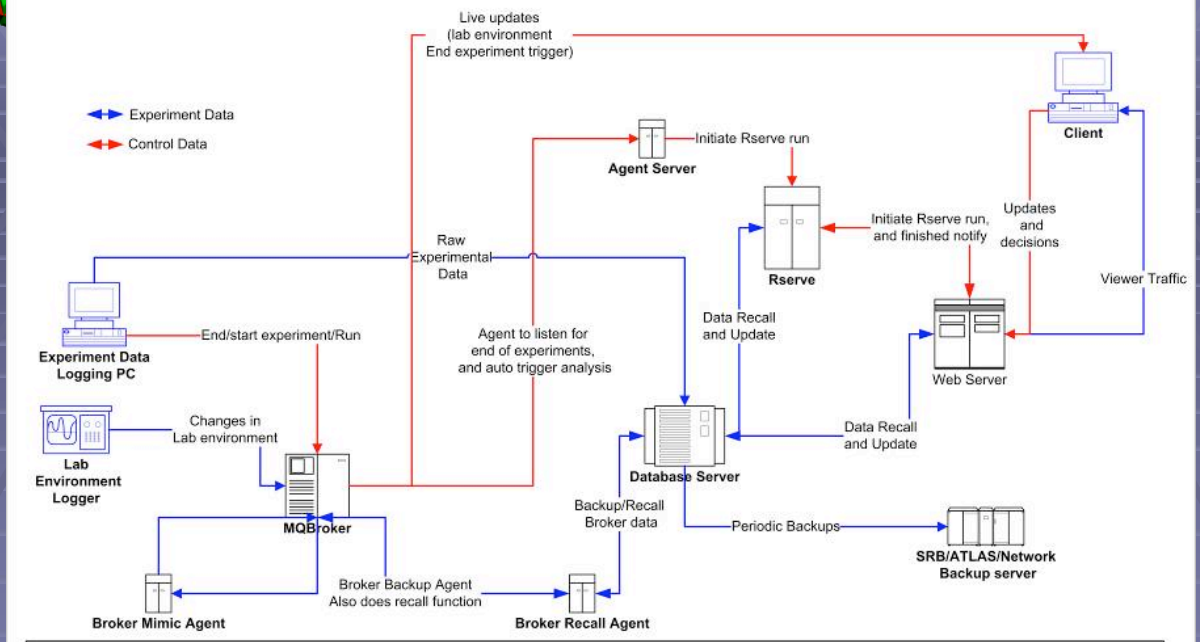
Monitor the semi-automated laboratory



Use IBM Web Sphere Technology (MQTT) - an asynchronous grid



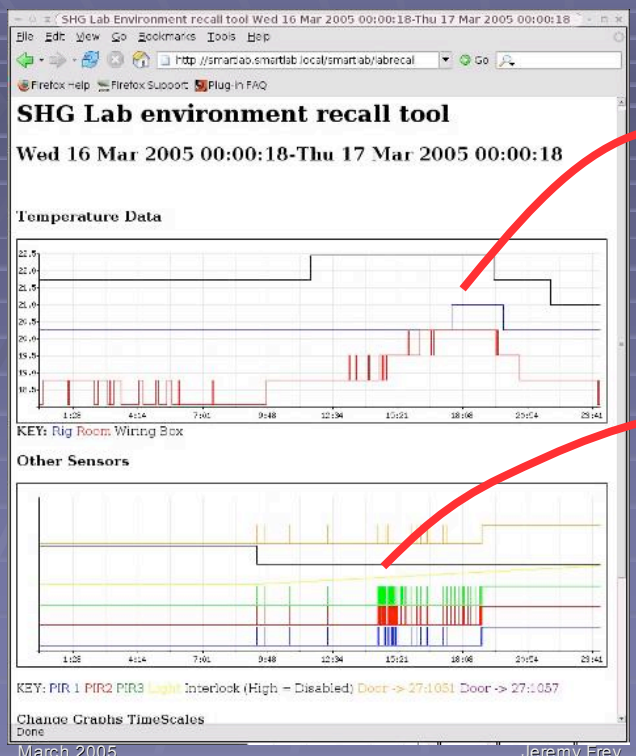
Pub - Sub for a Smart Lab



Smart(SHG)Lab Data Flow Processes

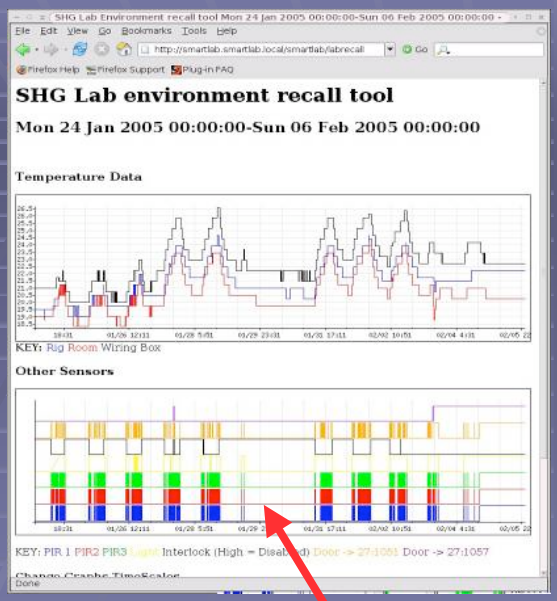
A "Smart-Lab" will require many interacting technologies.

Yesterday in the lab

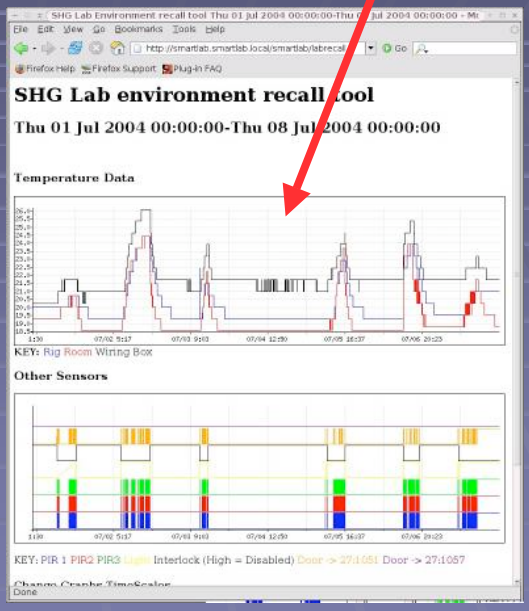


Temperature – room, laser

Door & interlock
Motion Sensors

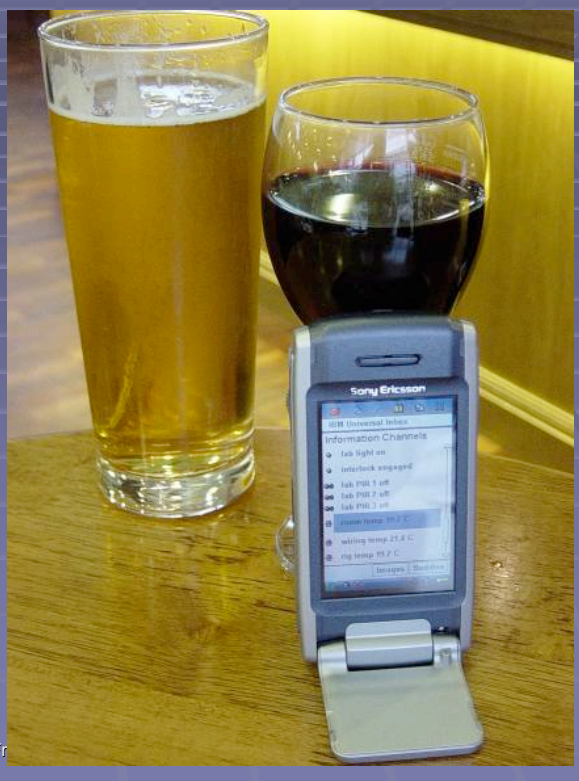


Student turned off a/c



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

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

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Last Updated: Friday, 4 February, 2005, 08:47 GMT

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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 system is not smart enough to actually buy a round yet

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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experiment in more detail.

PDAs everywhere

Members of Dr Frey's non-linear laser spectroscopy research group, working as part of the Combechem project, have been successfully trying out the system at conferences - and in the university bar.

The next step is to evolve the system so that at a push of a button on a mobile, scientists will be able to remotely change the conditions in the lab, like turning down the temperature.

It could also realise the promise of controlling home environments from phones easily and seamlessly.

But there are many other potential applications for the monitoring jobs done by the power industries, healthcare professions and other labs.

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.

It has transformed e-commerce because of its ability to allow data transfers across computer systems and different platforms without extra coding.

Combechem is a UK e-Science project funded by the

March 2005 Jeremy Frey ACS CINF

What are the people up to?

We can capture the environment
but need to capture the processes

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

There are privacy issues

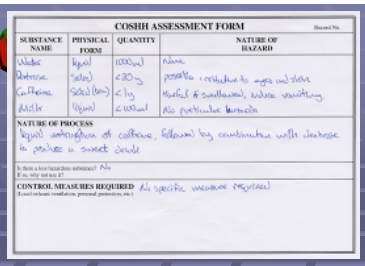
"When we implant your pacemaker, we can, for a modest additional fee, also implant your beeper."

- Like cash machine electronic notebooks have taken many forms – we want one that adapts to context, simple to use in the lab whilst doing actual bench chemistry but linked to more resources at the desk – the pervasive lab book grid

Smart Tea -

Keep the people involved!

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



COSHH ASSESSMENT FORM

SUBSTANCE NAME	PHYSICAL FORM	QUANTITY	NATURE OF HAZARD
Water	liquid	1000 ml	none
Caffeine	solid	< 30 g	possible irritation to eyes and skin
Caffeine	solid (dust)	< 1 g	Harmful if swallowed, irritate respiratory
Acetic	liquid	< 100 ml	No particular hazards

NATURE OF PROCESS: liquid extraction of caffeine, followed by crystallisation with sublimation to produce a sweet drink

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

CONTROL MEASURES REQUIRED: No specific measures required

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

Get chemists and computer scientists to understand each other

By Making Tea!

COSHH

leverage off things we already have to do

COSHH ASSESSMENT FORM Record No.

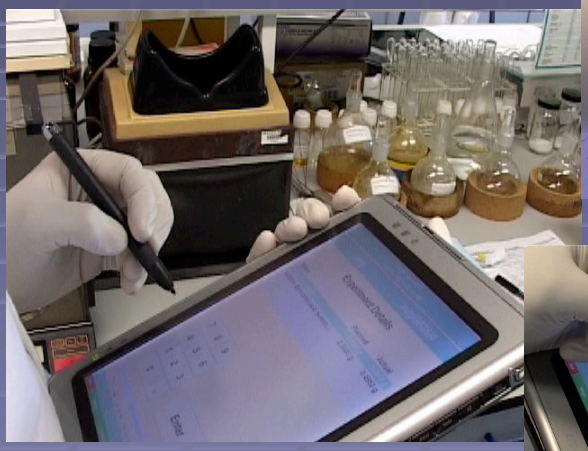
SUBSTANCE NAME	PHYSICAL FORM	QUANTITY	NATURE OF HAZARD
Water	liquid	1000ml	None
Dextrose	Solid	<20 g	possible irritation to eyes and skin
Caffeine	Solid (tea)	<1 g	Harmful if swallowed, induce vomiting.
Milk	liquid	<100ml	No particular hazards

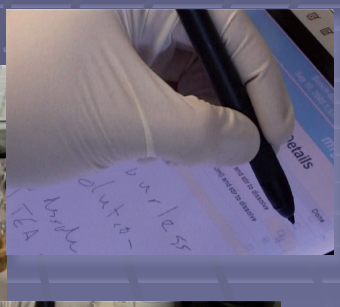
NATURE OF PROCESS
liquid extraction of caffeine, followed by combination with dextrose to produce a sweet drink

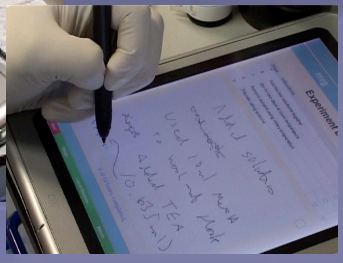
Is there a less hazardous substance? No
If so, why not use it?

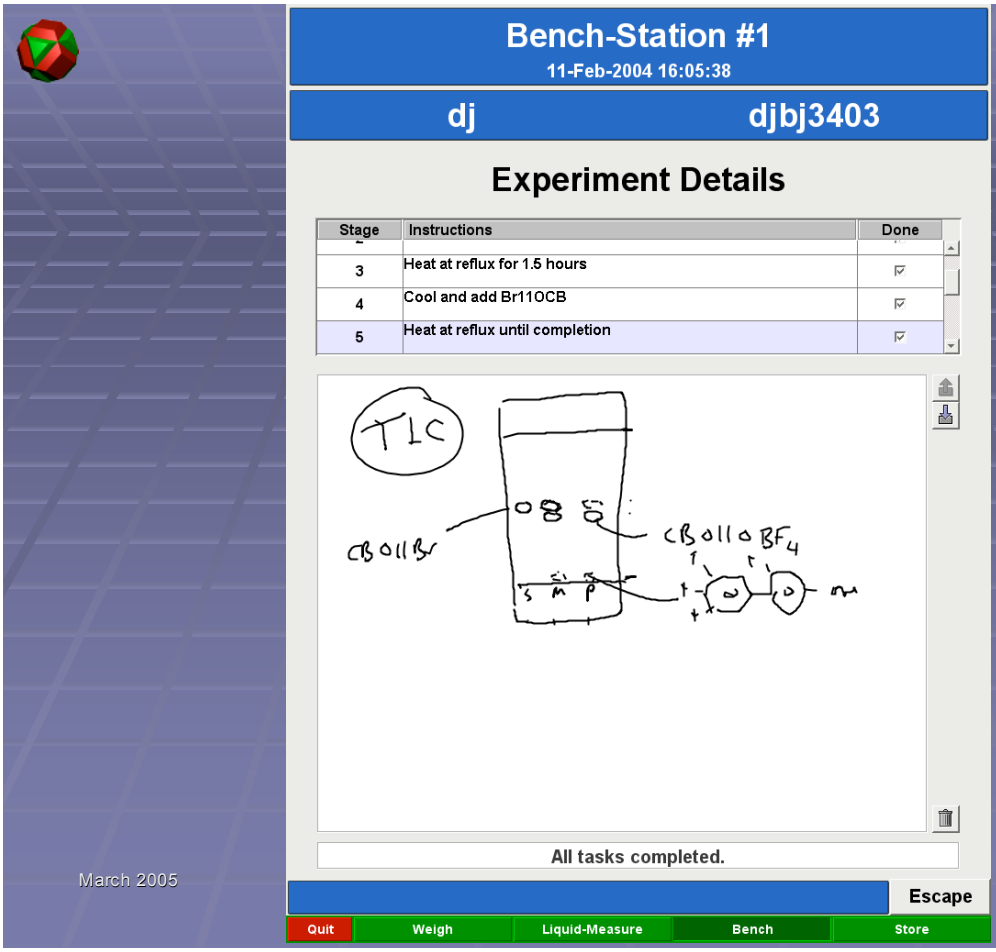
CONTROL MEASURES REQUIRED No specific measure required
(Local exhaust ventilation, personal protection, etc.)

Tablet version

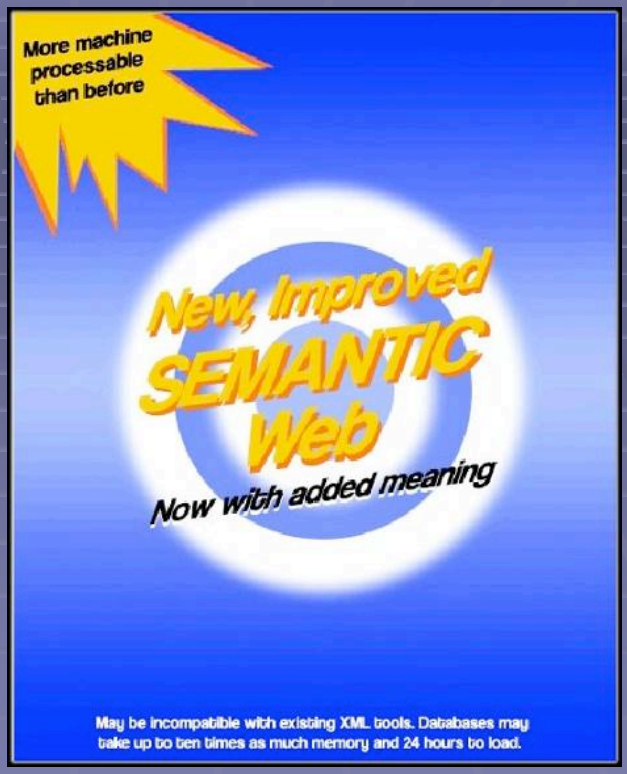


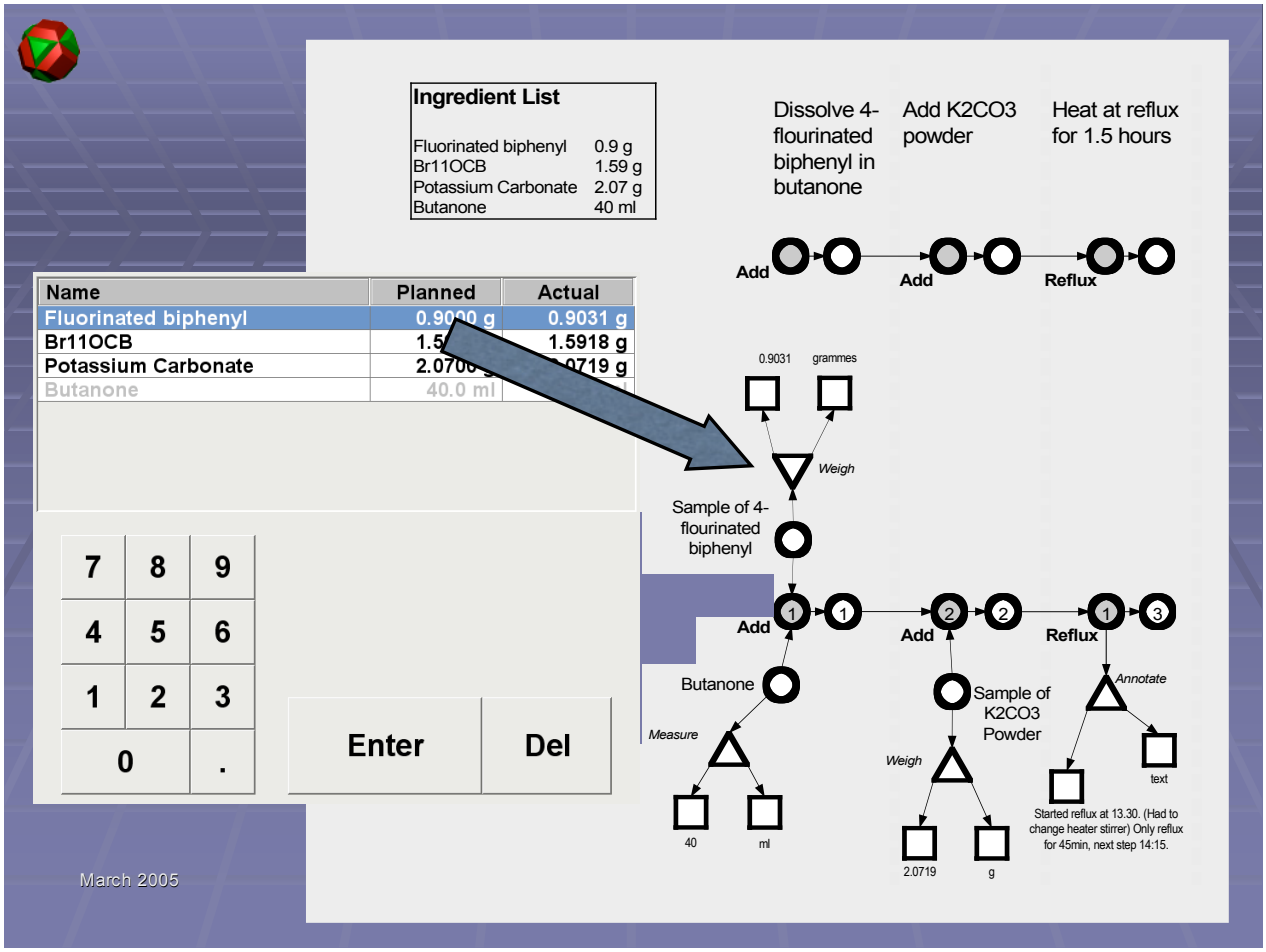


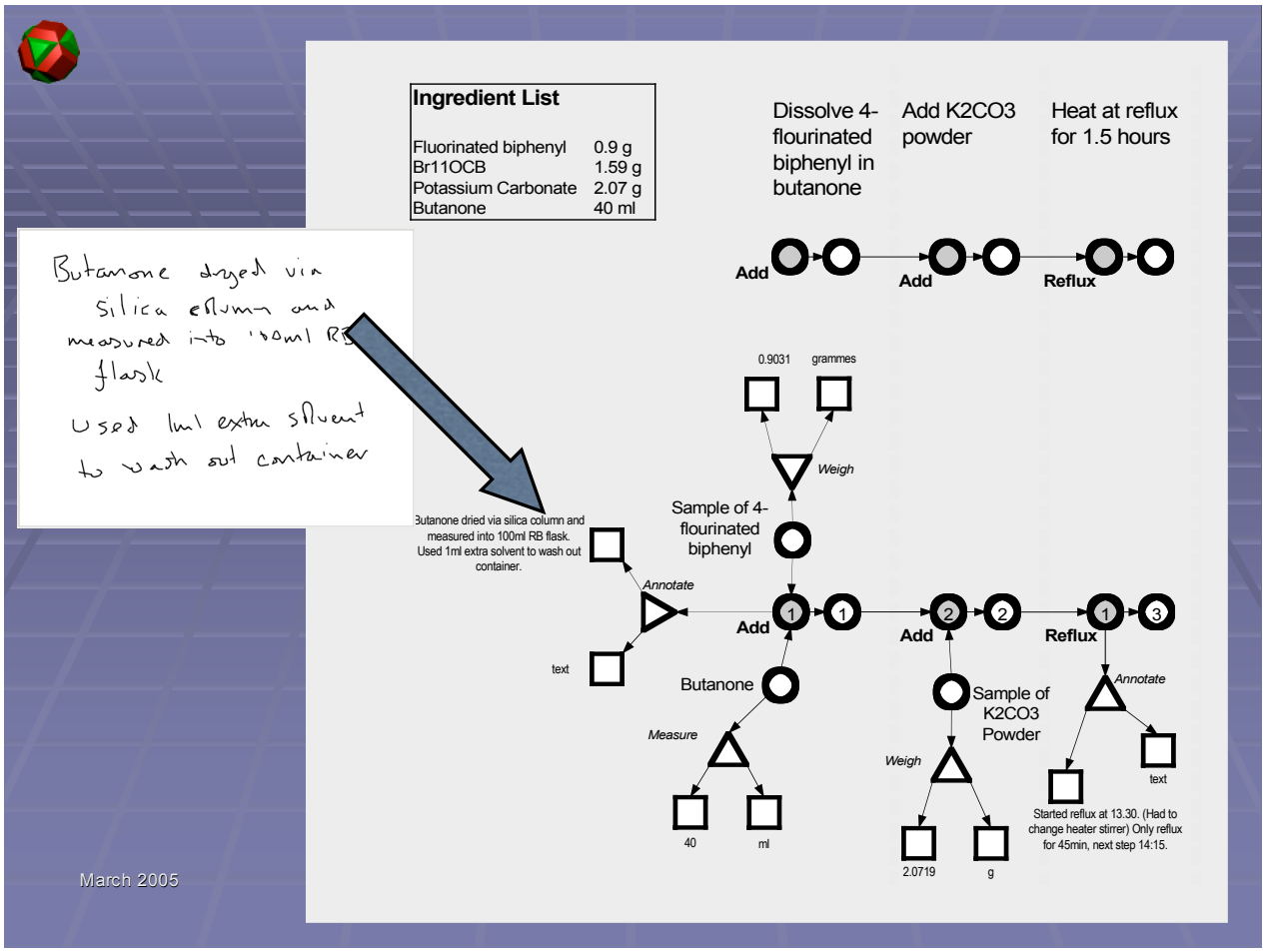




Use RDF for both data and processes




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
Name
Planned
Actual
Fluorinated biphenyl
0.9031 g
Br11OCB
1.5
1.5918 g
Potassium Carbonate
2.0700
0719 g
Butanone
40.0 ml
7 8 9
4 5 6
1 2 3
0 .
Enter
Del
0.9031
grammes
Weigh
Sample of 4-flourinated biphenyl
Butanone
Measure
40
ml
Sample of K2CO3 Powder
Weigh
2.0719
g
Annotate
text
Started reflux at 13.30. (Had to change heater stirrer) Only reflux for 45min, next step 14:15.
March 2005


Ingredient List
Fluorinated biphenyl 0.9 g
Br11OCB 1.59 g
Potassium Carbonate 2.07 g
Butanone 40 ml
Butanone dryed via silica column and measured into 100ml RB flask
Used 1ml extra sflvent to wash out container
Butanone dried via silica column and measured into 100ml RB flask. Used 1ml extra solvent to wash out container.
Dissolve 4-flourinated biphenyl in butanone
Add K2CO3 powder
Heat at reflux for 1.5 hours
Add
Add
Reflux
0.9031
grammes
Weigh
Sample of 4-flourinated biphenyl
Annotate
text
Butanone
Measure
40
ml
Sample of K2CO3 Powder
Weigh
2.0719
g
Annotate
text
Started reflux at 13.30. (Had to change heater stirrer) Only reflux for 45min, next step 14:15.
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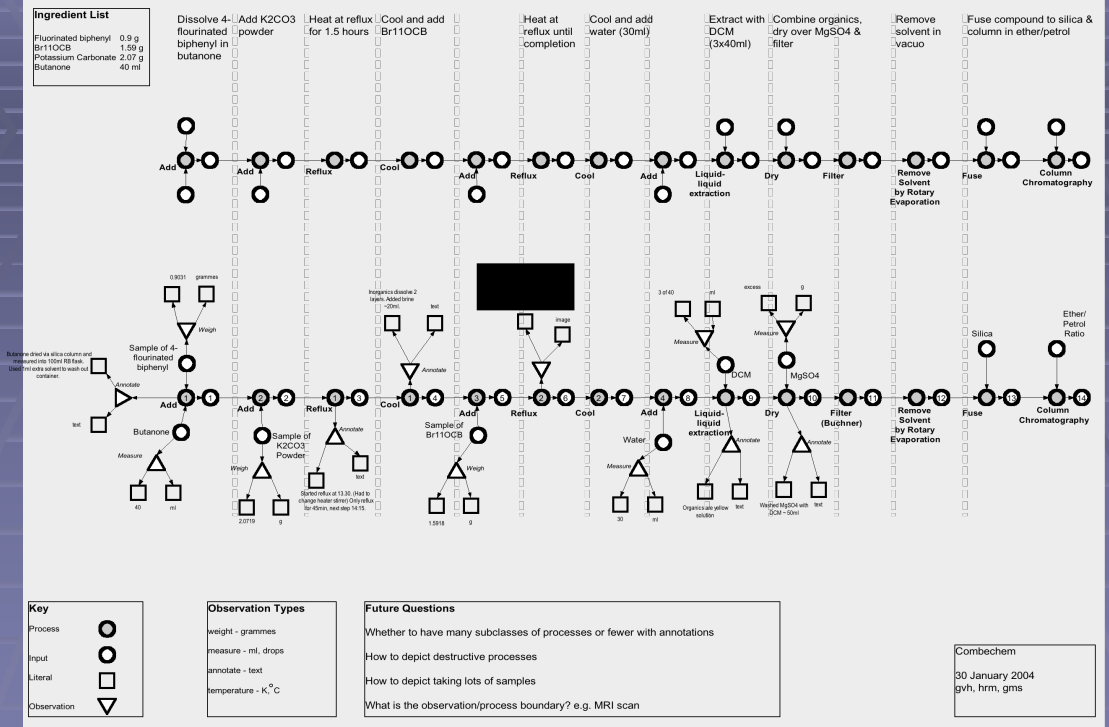
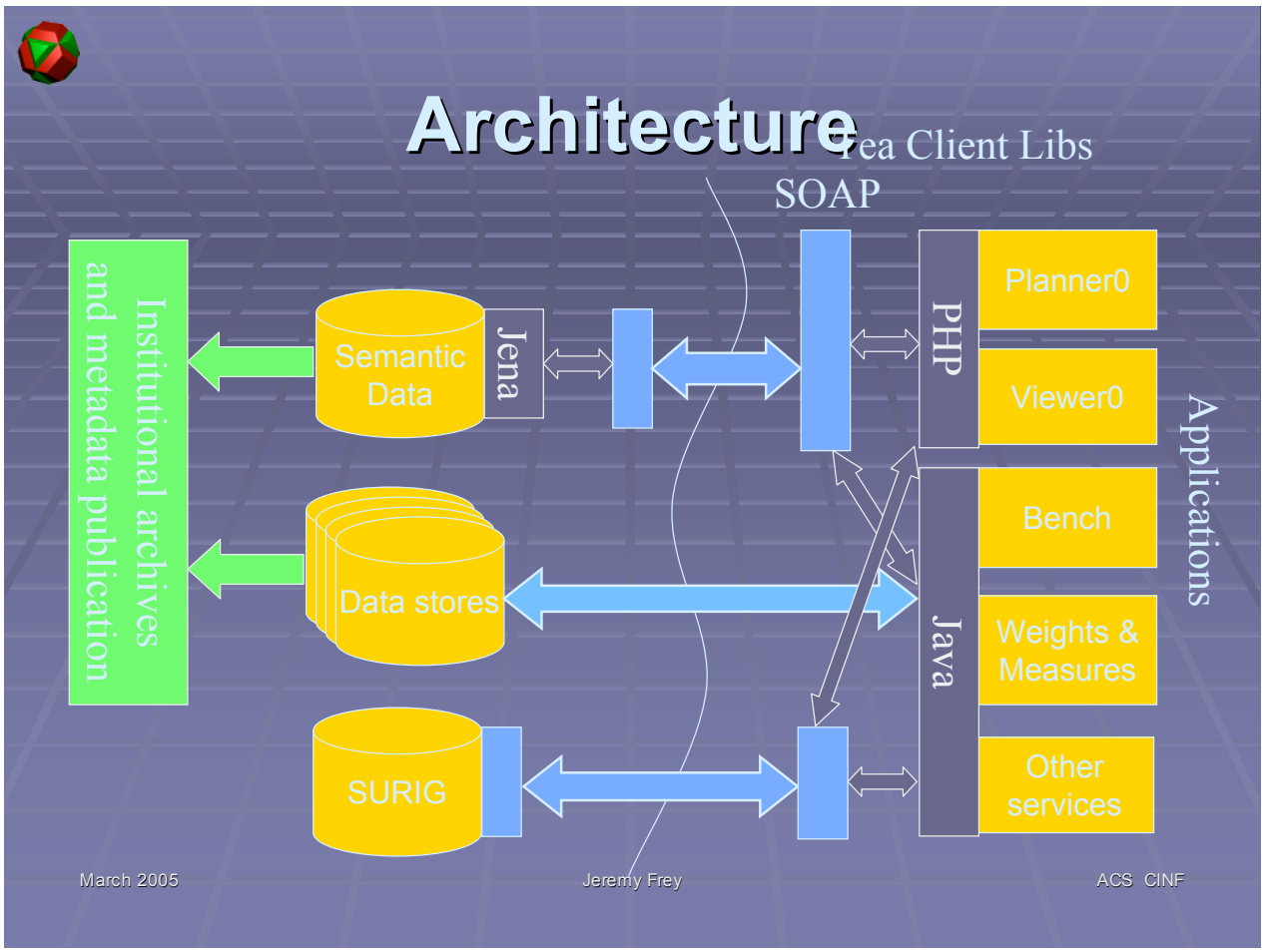
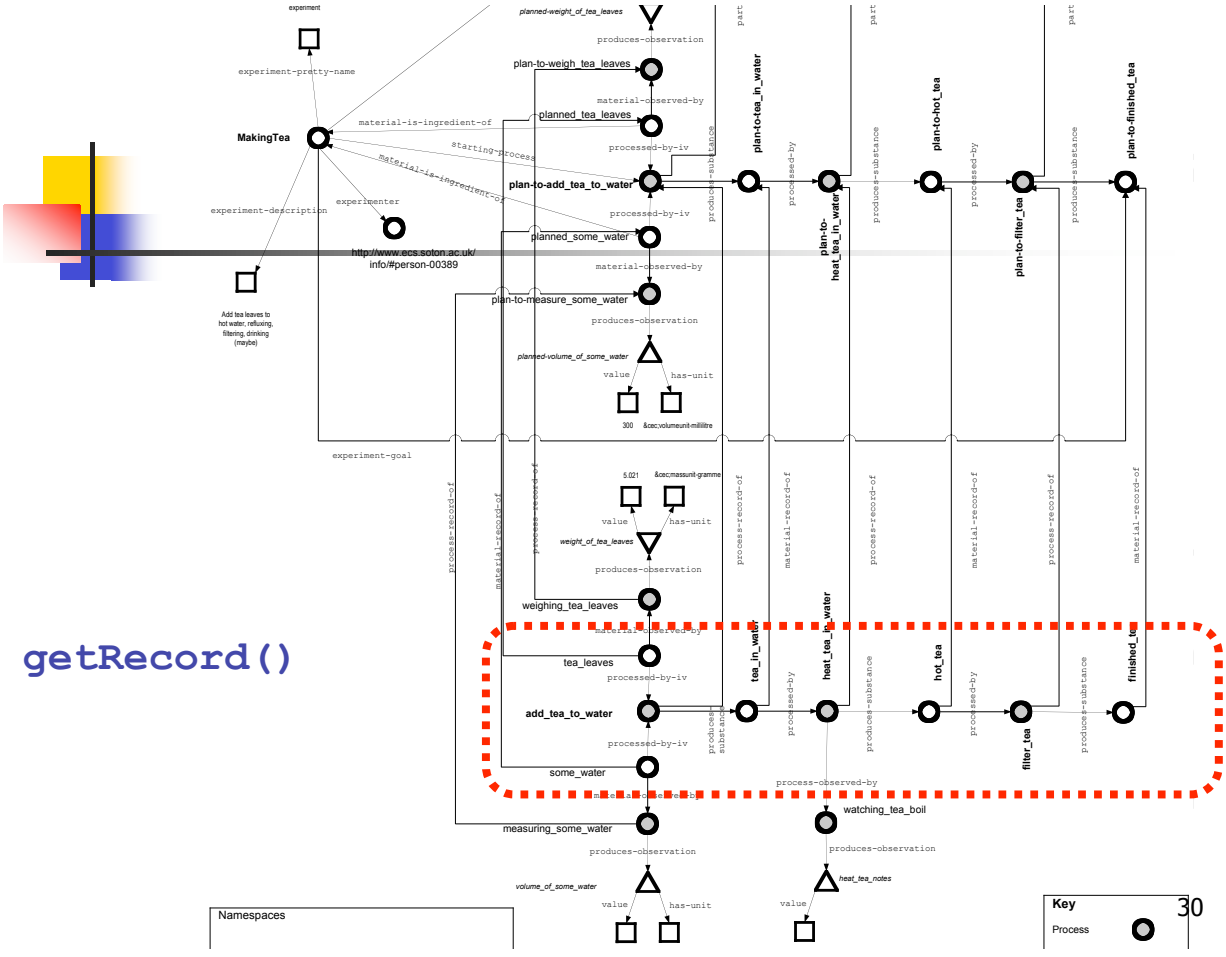
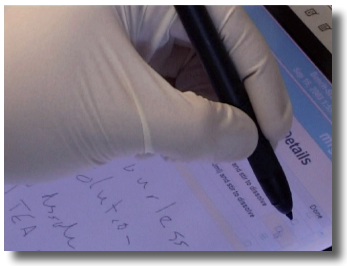


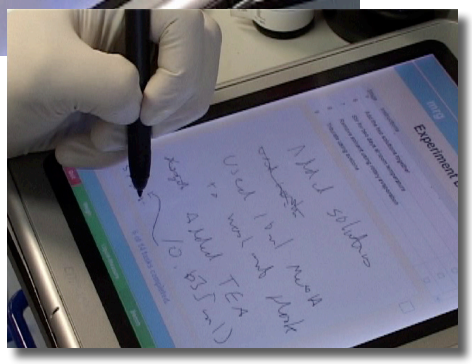
Lessons

- 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

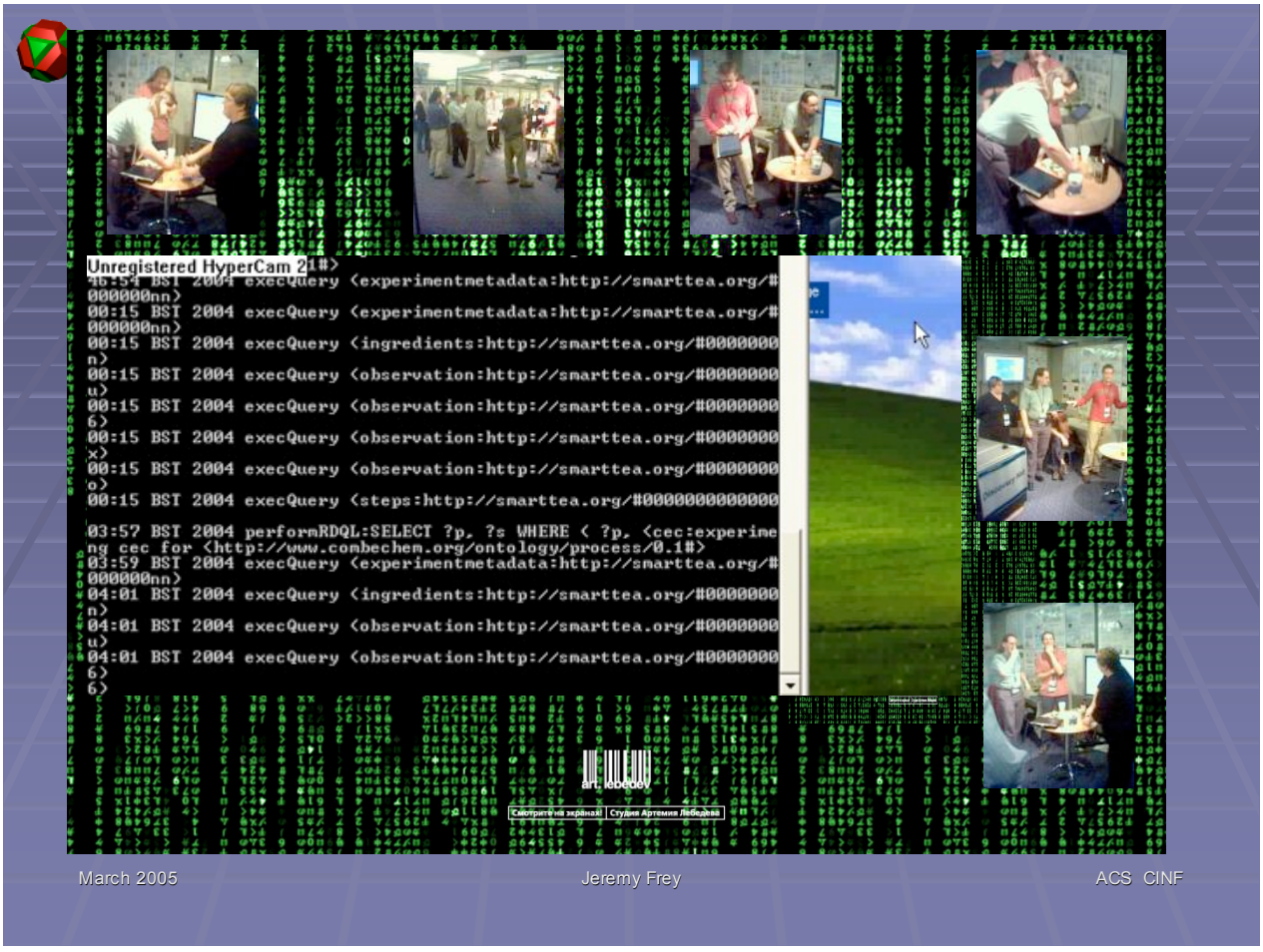

Architecture
Tea Client Libs
SOAP
Institutional archives and metadata publication
Semantic Data
Jena
Data stores
SURIG
PHP
Java
Planner0
Viewer0
Bench
Weights & Measures
Other services
Applications
March 2005
Jeremy Frey
ACS CINF


getRecord()
MakingTea
experiment-pretty-name
experiment-description
experimenter
http://www.ecs.soton.ac.uk/info/#person-00389
Add tea leaves to hot water, refluxing, filtering, drinking (maybe)
plan-to-weigh_tea_leaves
planned_tea_leaves
plan-to-add_tea_to_water
planned_some_water
plan-to-measure_some_water
planned-volume_of_some_water
300
&cec;volumeunit-millilitre
experiment-goal
5.021
&cec;massunit-gramme
weight_of_tea_leaves
weighing_tea_leaves
tea_leaves
add_tea_to_water
some_water
measuring_some_water
volume_of_some_water
plan-to-tea_in_water
plan-to-heat_tea_in_water
plan-to-hot_tea
plan-to-filter_tea
plan-to-finished_tea
watching_tea_boil
heat_tea_notes
Namespaces
Key
Process





A digital lab book replacement that chemists were able to use, and liked.



Design discussion

- Handling RDF both ends – tricky
- Structure to data:
  - good: clients can add what they want
    - Ontology extensions: Uncertainty to measurements
  - bad: clients can add what they want
    - Is the structure you're given navigable in the way you expect?
    - Use of libraries solves this to some degree

Design Discussion

- We have an ontology (shared understanding)
- But... experiment structure is a higher-level entity
  - Must be created and maintained by good programming, not simply by adherence to rules of the ontology

eBank publication

- Data sets stored for easy access via Web
- Metadata for experiment stored as RDF
- Representation of connections between data sets and concepts is RDF
- Domain specific structure

SmartLab system

- Data sets stored for easy access via Web
- Metadata for experiment stored as RDF
- Representation of connections between data sets and concepts is RDF
- Generic structure with domain-specific additions

Future…

- Understand the business process layer needed to keep the RDF under control

People

- Chemistry
  - Jamie Robinson, Sam Peppe, Hongchen Fu, Lefteris Danos, Kieron Taylor
- Electronics and Computer Science
  - Dave De Roure, Luck Moreau, Hugo Mills, Graham Smith, Simon Miles, Gareth Hughes, monica Schraefel
- IBM Hursley
  - Andy Stanford-Clark, Andrew Reynolds
- EPSRC for funding