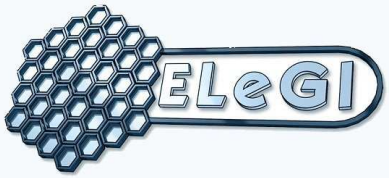


European Learning Grid Infrastructure

The European Learning Grid Infrastructure based on GRID technologies for supporting ubiquitous, collaborative, experiental-based, contextualised and personalised learning

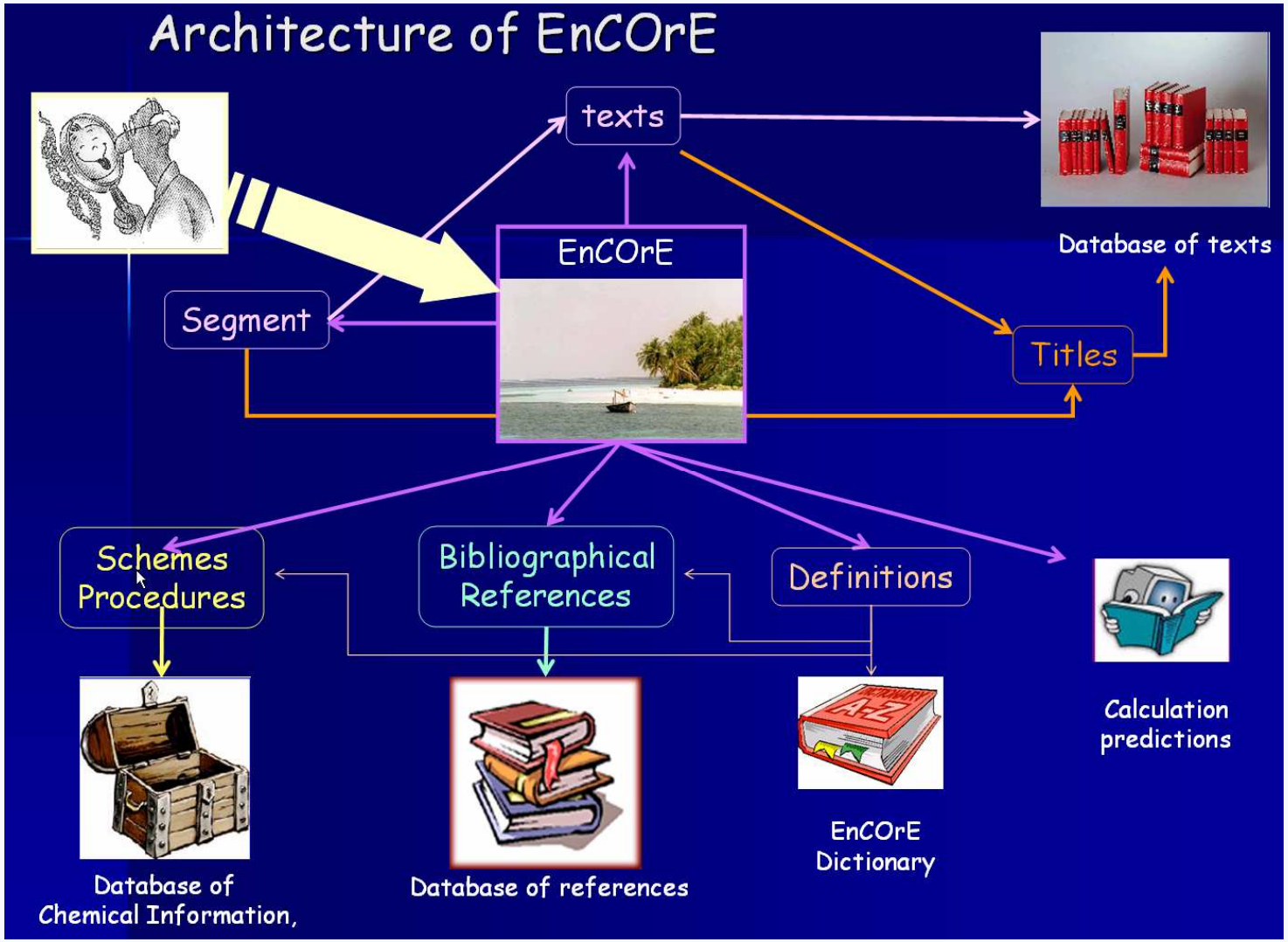
Protocols for building an Organic Chemical Ontology

"Research is what I'm doing when I don't know what I'm doing"

Wernher Von Braun

Technology-enhanced learning and access to cultural heritage

EnCOrE : Strategy & Practice

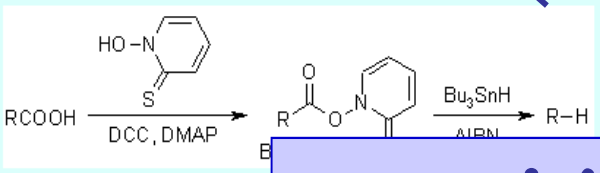


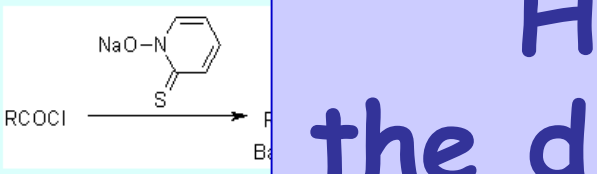
Organic Chemistry Portal

Name Reactions

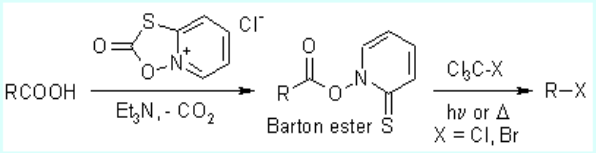
Barton Decarboxylation

The radical decarboxylation of a Barton ester proceeds to the corresponding alkane after treatment with tributyltin hydride or *t*-butylmercaptan:





An alternative possibility is the i… with a suitable radical trapping agent:



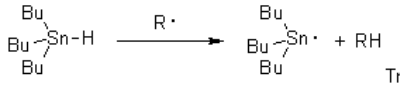
Mechanism

The initiation of the Barton Decarboxylation (Bu_3Sn-H -> Bu3Sn·) is effecte… Deoxygenation, the driving force for the reaction itself is the formation of the

Chemicals > Reducing Agents

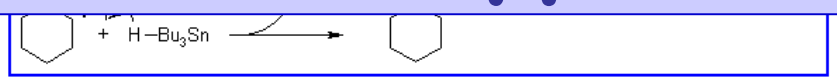
Tributyltin hydride (Tributylstannane) / Tin hydrides

Organotin hydrides are very good radical reducing agents due to the relatively weak, nonionic bond between tin and hydrogen (Bu_3SnH 74 kcal/mol) that can cleave homolytically.

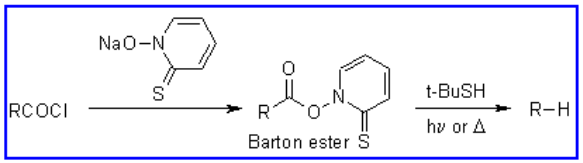


Tributyltin hydride

However, these compounds are plagued by their high toxicity and high fat solubility (lipophilicity). Therefore, with few exceptions, the use of tin hydrides should be avoided. The catalytic use of this reagents with a suitable second reducing



Barton-McCombie reaction

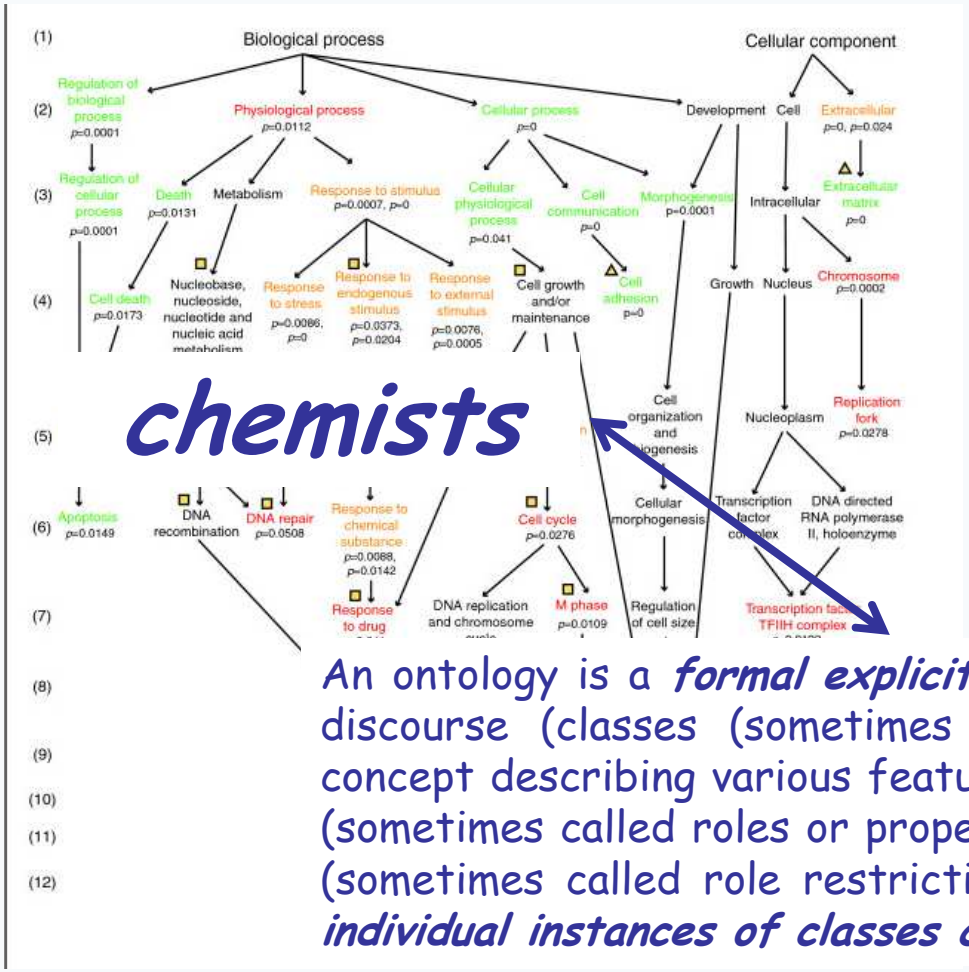


Barton decarboxylation

Additional interesting reactions that employ tin hydrides are dehalogenation and intramolecular radical cyclization.

How to imagine all the different hyperlinks ?

Ontology



chemists

What is an ontology?

Ontologists

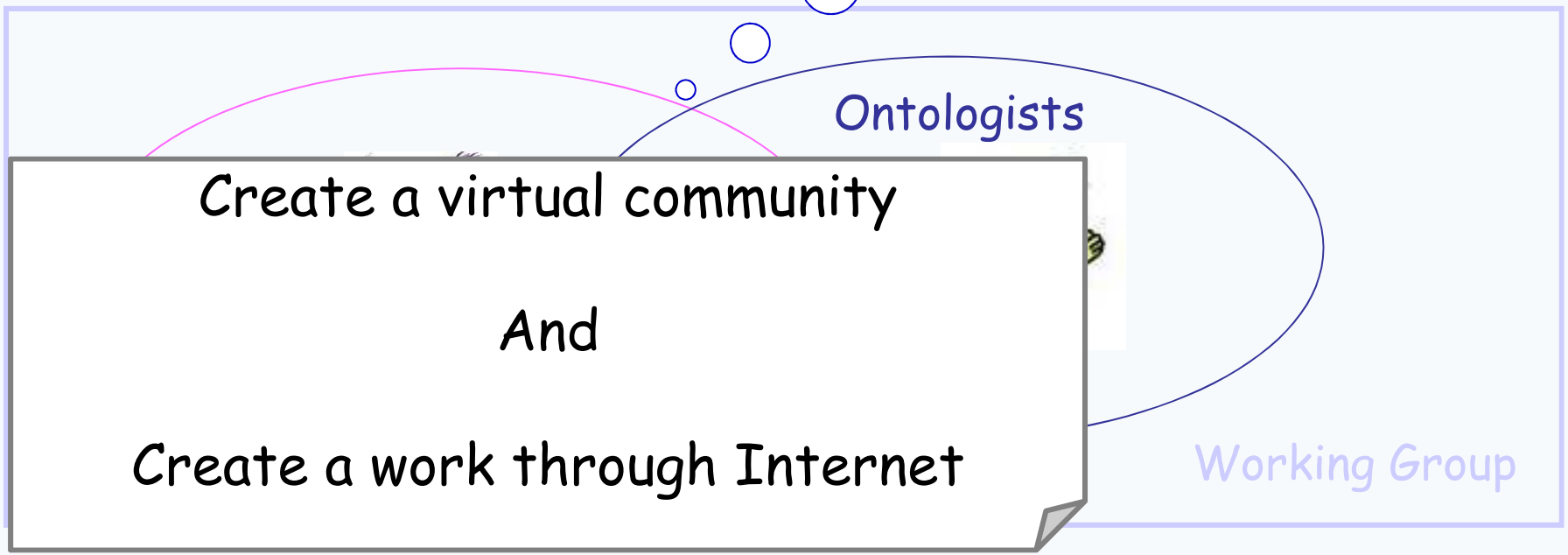
An ontology is a ***formal explicit description of concepts in a domain*** of discourse (classes (sometimes called concepts)), properties of each concept describing various features and attributes of the concept (slots (sometimes called roles or properties)), and restrictions on slots (facets (sometimes called role restrictions)). ***Ontology together with a set of individual instances of classes constitutes a knowledge base***.

Drafting a protocol: first step

Creation of a working group:

Gathering chemists of vari
technolog

How to gather so many persons?

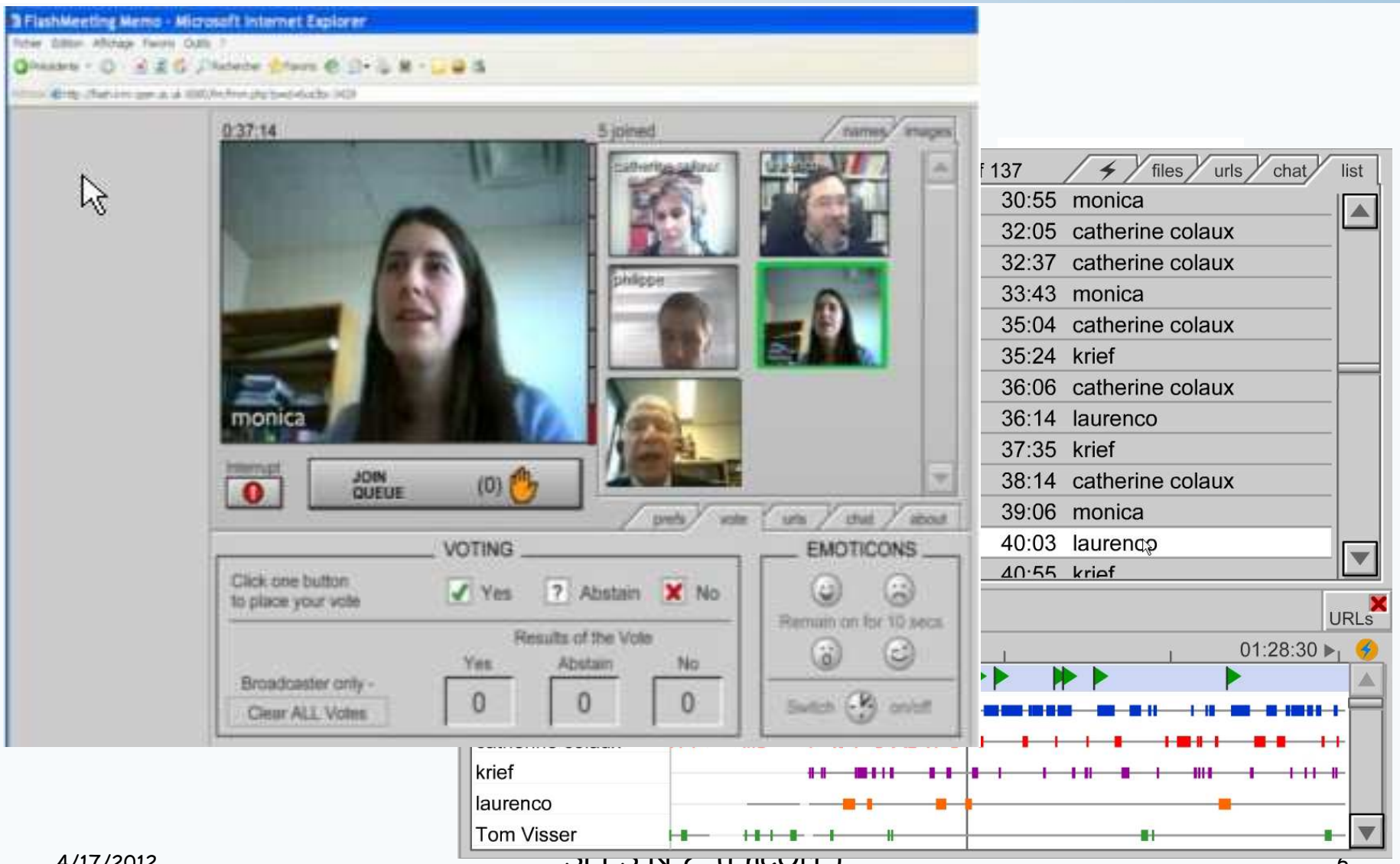


Create a virtual community

And

Create a work through Internet

Services needed for Conversation & Cooperation (C&C)



Drafting a protocol: distributing the tasks

- Discussion between chemists in presence of experts in Knowledge engineering (the "ontologist")

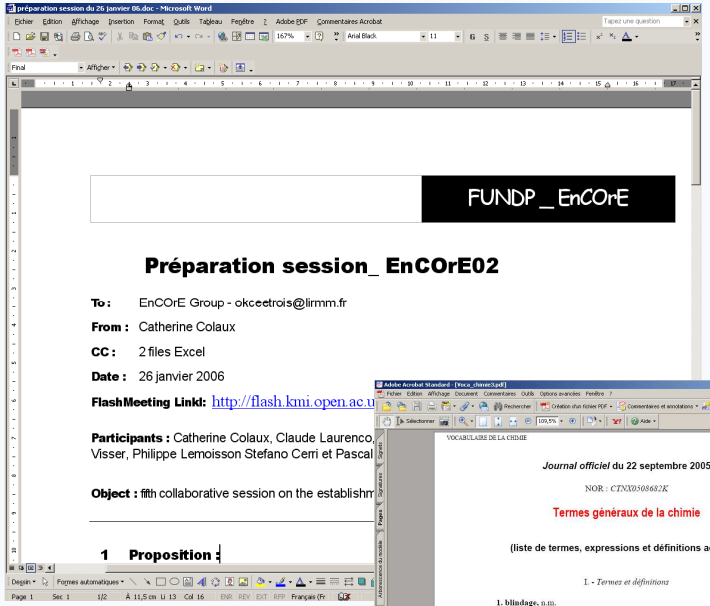
- Integration of the concepts in the ontology, by the "ontologist".

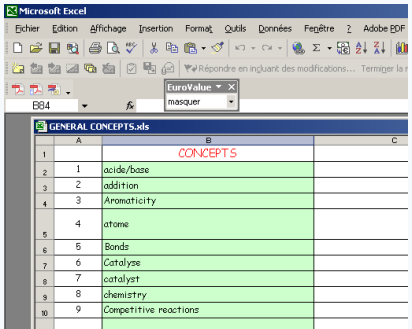
- Explanations of the "ontologist" on his choices and his manipulations in Protégé.

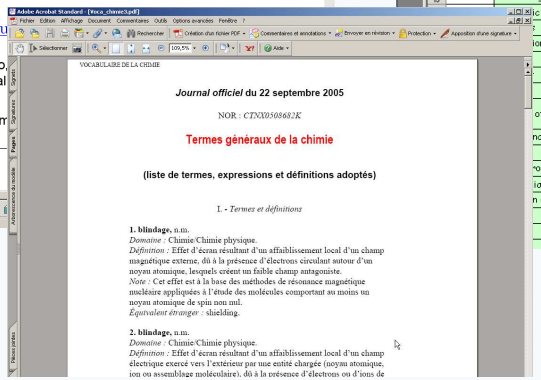
Drafting a protocol: preparation of a Collaboration Session (CS)

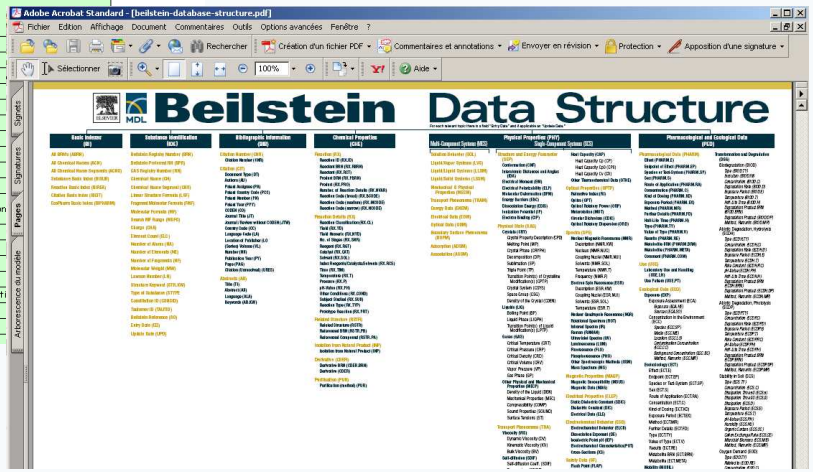
- Booking a weekly session of 1 H 30 with all the different participants

- Sending documents to the diffusion list in order to prepare the session and the agenda of the session



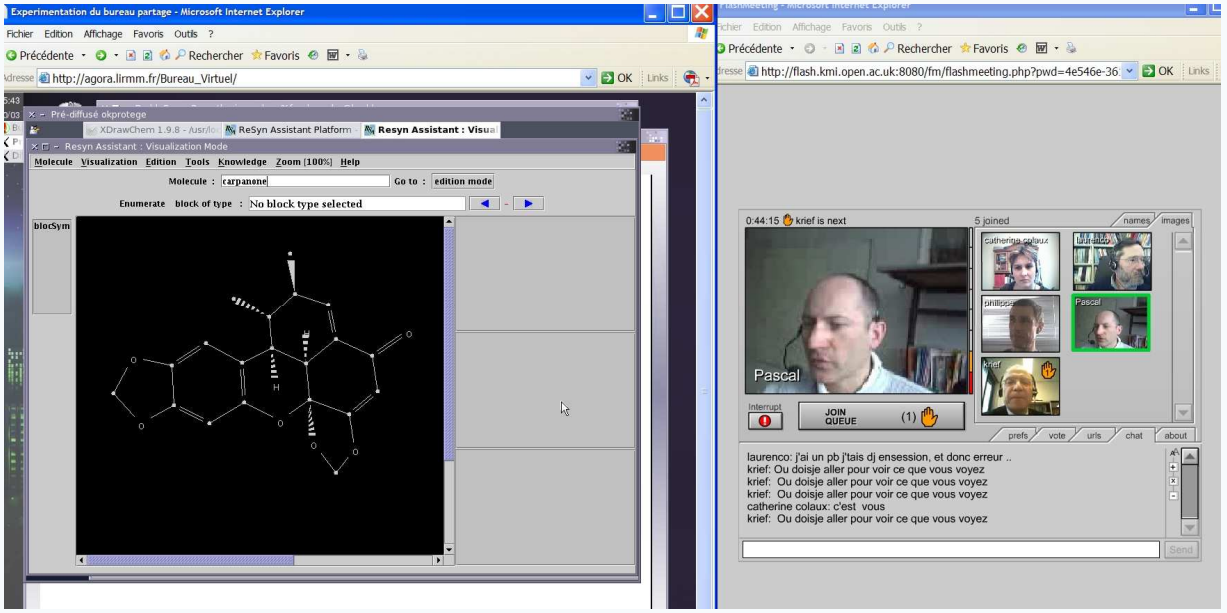






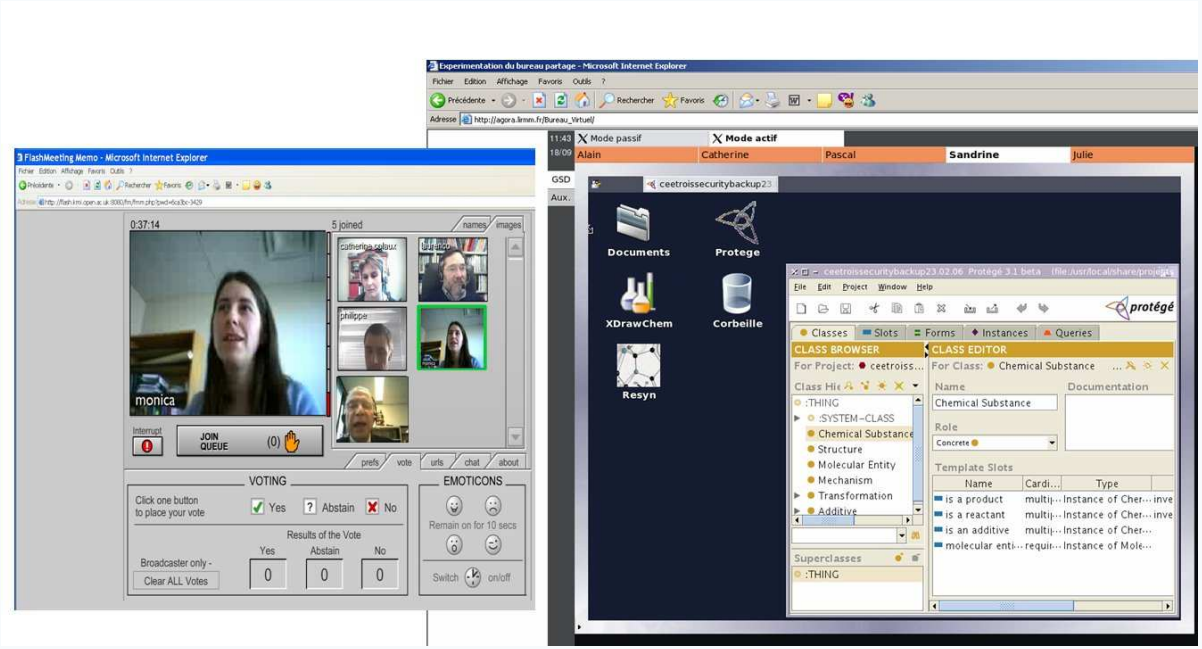
Drafting a protocol: the 'settings' for C&C

- Working through (GSD + FM) at the construction of the ontology
  - The chemists start the discussion, in the presence of ontology's expert, about the selected field, they **extract** from it the most adequate **terms and their relations**.



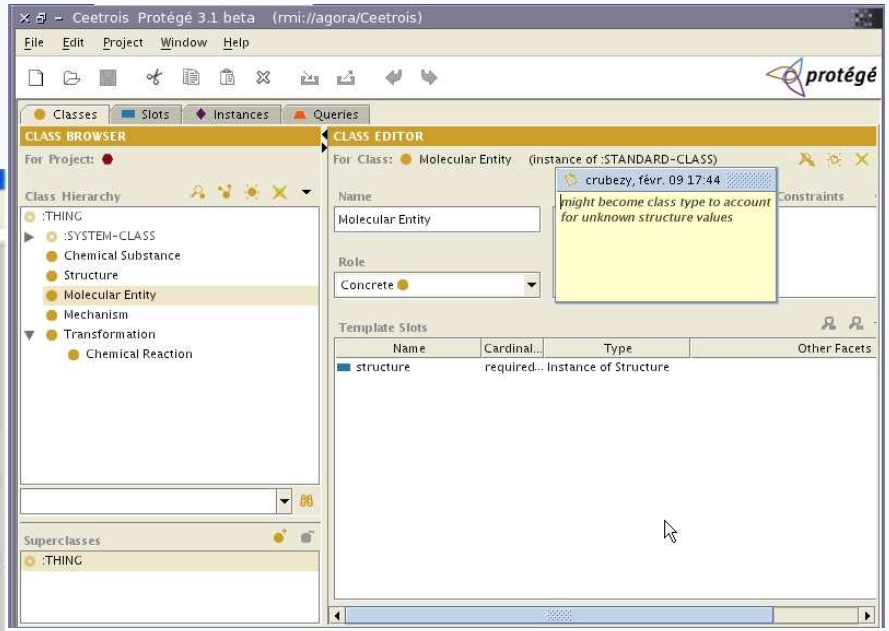
Drafting a protocol: a Common Virtual Environment

- Each time that a **concept is identified** and considered to be important by the chemists, the ontologist, on the spot, **integrates it in ontology**, in a synchronous way, by **using the shared desktop** and validates in the same time the relevance of the classes, properties or restrictions.



Drafting a protocol: conversations

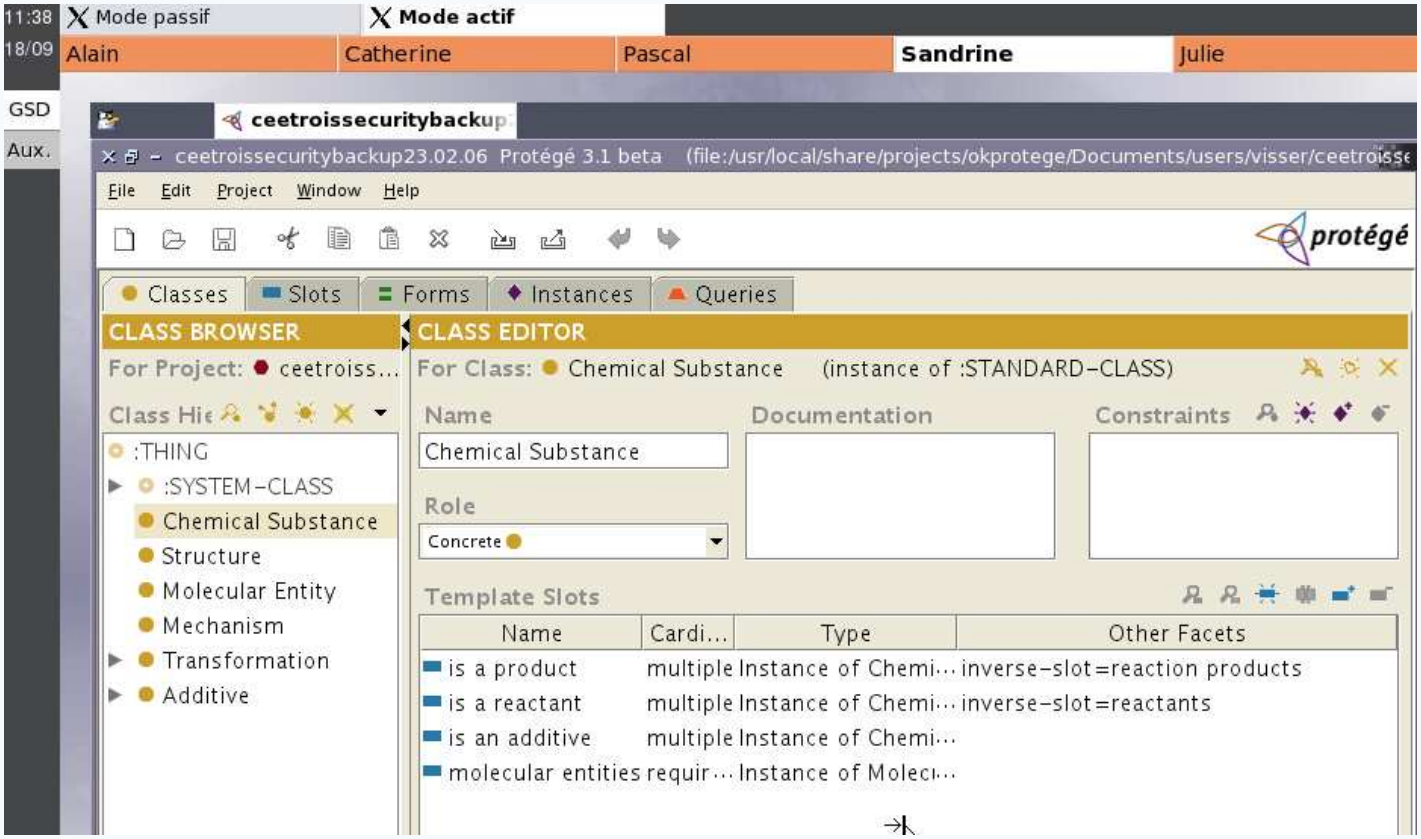
- The ontologist takes the time to explain to the chemist the reasons of his choices and how to implement it in Protégé. He also answers the questions and even in few cases revises his initial choice.



Drafting a protocol: keeping track of the collaboration

- ✓ Booking each week a session of 2h with the different participants
- ✓ Sending documents to the diffusion list in order to prepare the session
- ✓ Sending agenda of the session
- ✓ Working through (GSD + FM) at the construction of the ontology
- ✓ Writing a report about the session and planning future work
- ✓ Acceptation of the report by the group and working on the next session

Assessment of the first trial



The assessment of this set of experiments is quite weak… Why?

Assessment of the first trial

The facility to connect people through Internet induced us in error for gathering all these persons during the SAME MEETING

- No *precise determination of the g*
- No *definition of the terms and their l ations previously* to the session.
- Long discus hat ithout interest for Ontologist.

Working through Internet is not a simple transposition of the traditional way of working!!!!

- *or communication,*
- *Opportuni , the protocols of collaboration,*
- *Opportunity to analyze r errors.*

How to improve this first protocol?

- Thinking differently….
  - Taking advantage of the power and the facility offer by the GRID to the virtual community by
    - Cutting the work in different sessions
    - selecting the right person for the right session.
  - Selecting the tools in relation which each collaboration session.
  - Taking advantage of the recording for archiving and reporting

Selection of the specific field

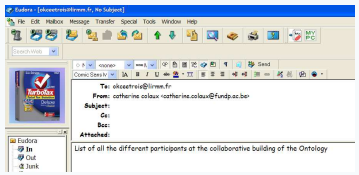
- Selection of a more technical field : The stirrer
- Goal? Answer to the following questions: "what is the more relevant equipment to use for an identified purpose?", "why this equipment is recommended for ?" or "where to buy it?"
- Integration of the "ontology of stirring laboratory equipment" to the "ontology of laboratory equipment" and the "ontology of organic reactions"

1. Study of the field to be treated

Implies Chemists

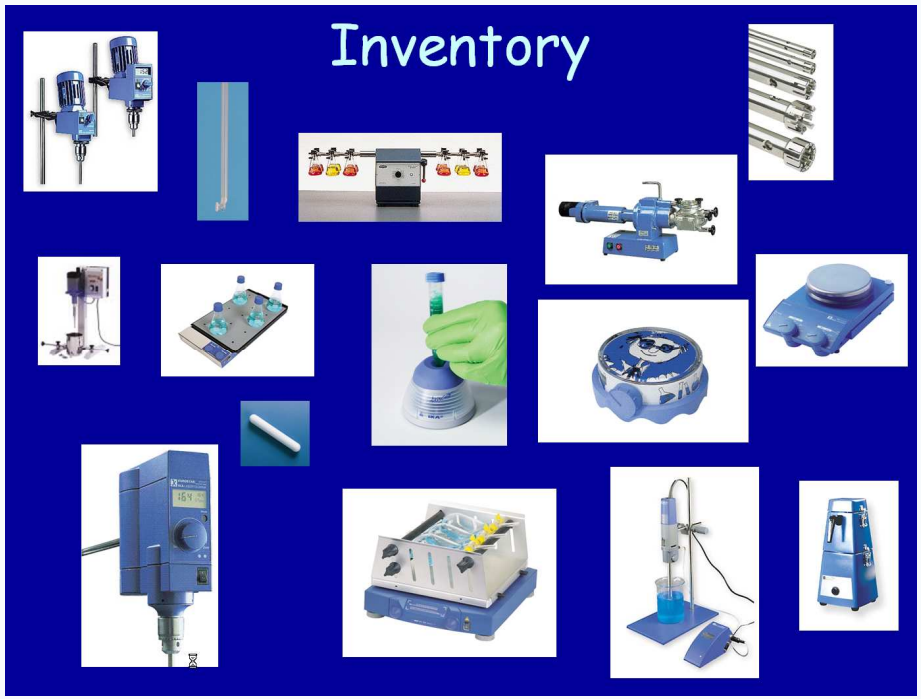
Listing of all the concepts and the terms of the delimited field to define them.

Tools



BuddySpace

FlashMeeting
The simple one-click video conference!
It works in a web browser running the Flash 7 plugin!



Asynchronous collaboration + Synchronous collaboration

2. First trail in the construction of the ontology

Construction of the first trial of the ontology by chemists who have learned protégé collaboratively with the ontologist

Tools

Implies Chemists skilled in ontology building with ontologists

BuddySpace

Protege

agora Laboratoire d'Informatique de Robotique et de Microélectronique de Montpellier LIRMM

The Grid Shared Desktop Experience (GSD Beta)

FlashMeeting

The simple one-click video conference!

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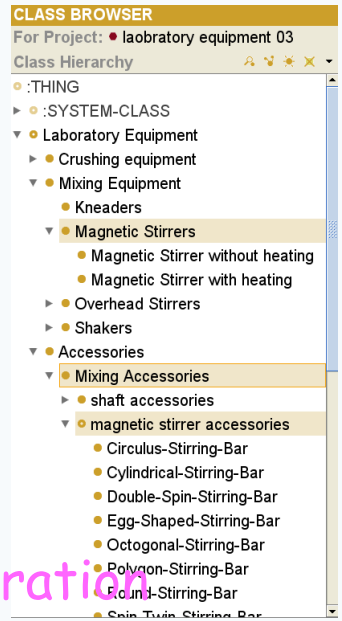


Asynchronous collaboration + Synchronous collaboration

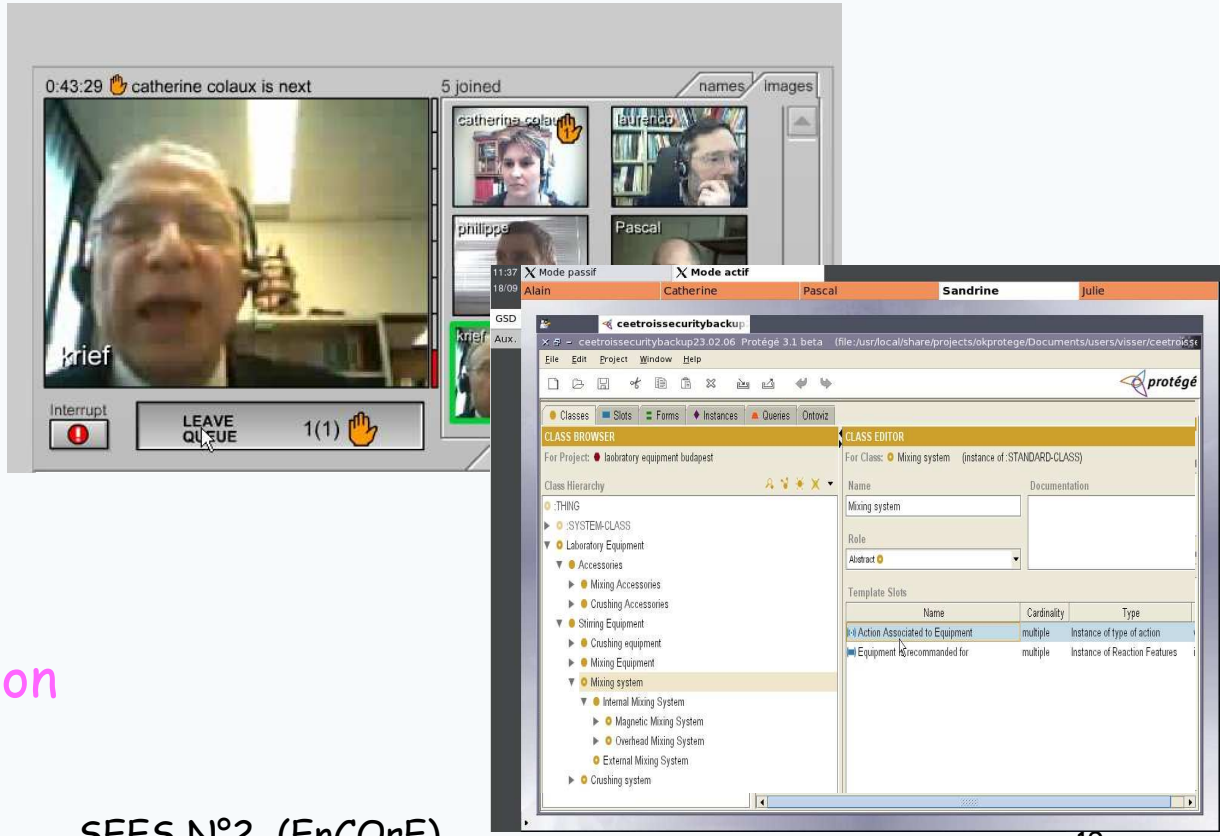
3. Testing period of the first outline

Presentation to chemists in a working session using the GSD in order to validate the organization of the concepts. Detection of missing concepts, inconsistencies…

Implies all the Chemists

Tools

agora
Laboratoire d'Informatique de Robotique et de Microélectronique de Montpellier
LIRMM
The Grid Shared Desktop Experience (GSD Beta)
GSD access
GSD demonstration
Audio-Video conference



FlashMeeting
The simple one-click video conference!
It works in a web browser running the Flash 7 plugin!

Synchronous collaboration

4. Evolution of the first version of the ontology

Integration of the remarks in the ontology.

Implies Chemists skilled in ontology building with ontologists

Tools

BuddySpace

Protege

agora — Laboratoire d'Informatique de Robotique et de Microélectronique de Montpellier — LIRMM

The Grid Shared Desktop Experience (GSD Beta)

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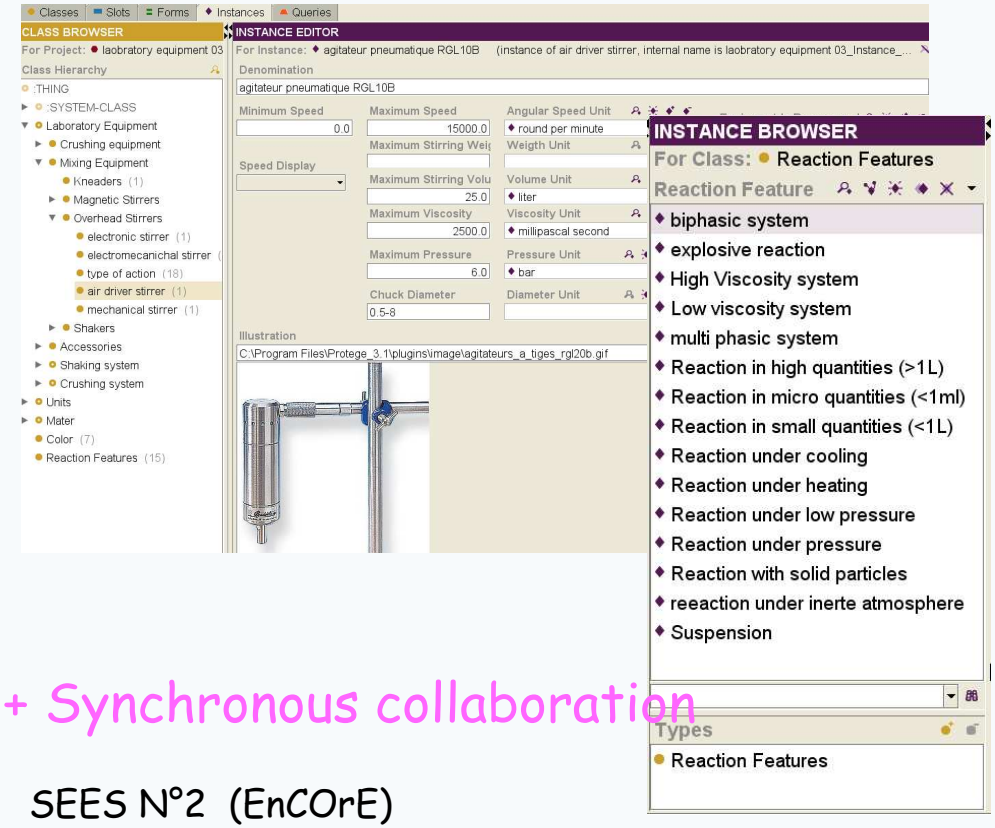


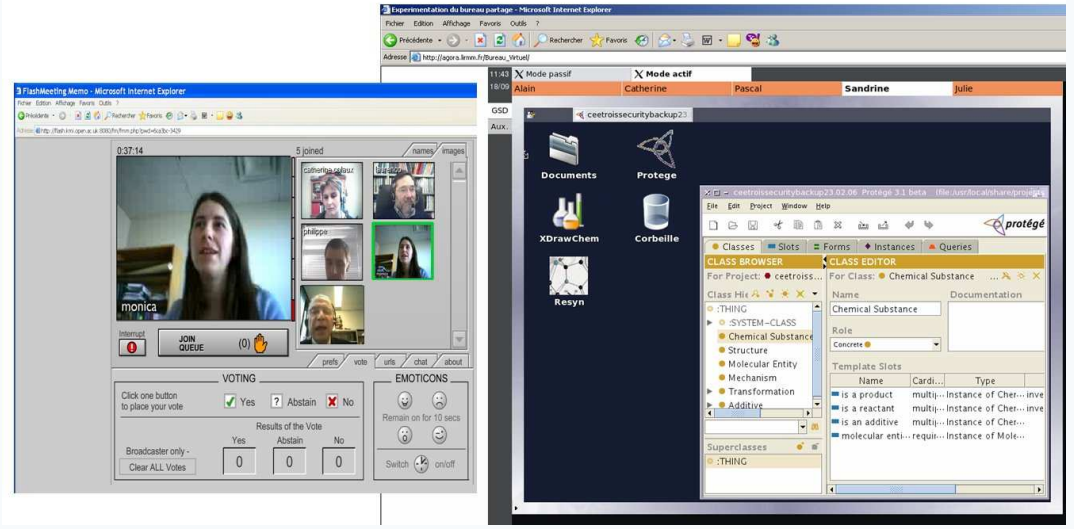
Asynchronous collaboration + Synchronous collaboration

5. Validation of the ontology by ontologists:

Validation by ontologists of the organization.

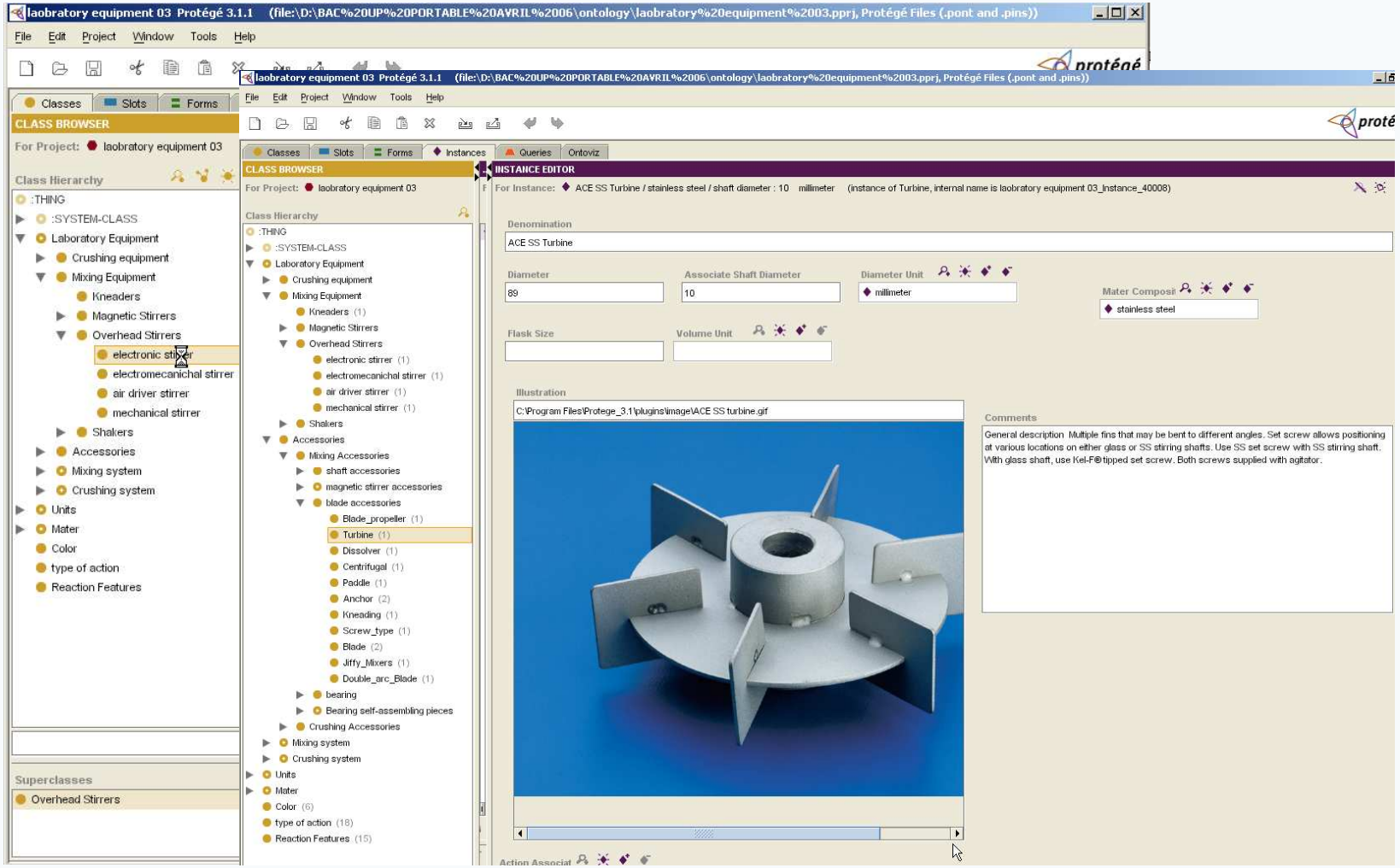
Tools

Implies Chemists skilled in ontology building with ontologists



Asynchronous collaboration + Synchronous collaboration

ontology of the stirring laboratory equipments



Conclusions before the update of the protocol

"Learning ontology building"

and

"building an ontology"

are

two distinct goals.

Which are the differences between a traditional working session and distant collaboration within a Virtual Community ?

Advantages :

- ☺ You can record the conversation and use it to archive the discussions, write a report,
- ☺ You can work with different persons from different countries at the same time without any problems linked to travels,
- ☺ In case of GRID architecture, you don't need to download software on your computer and therefore avoid all the problems linked to their management,
- ☺ You can easily benefit from a tailored tutorial,

Conclusions after the update of the protocol

Which are the differences between a traditional working session and distant collaboration within a Virtual Community ?

Disadvantages :

- No meeting could be initiated on the spot, you have to book the session to ensure that all the participants will be available at this time (taking into account the time difference between Europe and the rest of the world),
- It requires much more organization, more work before the meeting. You have to prepare the session by sending documents, etc. in order to be ready to discuss at the first seconds of the session… the value of the time is no more the same through Internet.
- You need a moderator to centre the discussion in "heterogeneous" collaboration session, make beneficial of the session.

Conclusions after the update of the protocol

Wishes :

- Opportunity to record the conversation simultaneously to the manipulation on the GSD.
- Possibility to invite someone to work on the GSD with least of constrain (only username and password….)

Impact on ELeGI

These requirements have been integrated into the design of a unified Common Virtual Environment:

- management of Users, Groups and Roles;
- single (and secure) sign-on for the whole C&C infrastructure;
- synchronized recording of the parallel conversational processes.