

# QTreds: a flexible LIMS for omics laboratories

**NETTAB 2012**

16th November, 2012

Piergiorgio Palla

CRS4 – DS3 Program  
email: [pg@crs4.it](mailto:pg@crs4.it)

- ◆ CRS4 founded in 1990 by C.Rubbia and P.Zanella
- ◆ Sardinian Technology Park

- Focus Areas:
  - Data Fusion
  - Information Society (ICT)
  - Energy and Environment
  - **Biomedicine**



- ◆ Introduction
- ◆ Motivation
- ◆ Core Modules
- ◆ Conclusions
- ◆ Future perspectives

# Motivation

- ◆ High-throughput technologies and data explosion
- ◆ The development of complex lab procedures
- ◆ A LIMS to efficiently handle these issues
- ◆ What is a Lims?

What is it



**QTreds** is a LIMS



What is it



QTreds is a LIMS



# QTreds for:

- ◆ Tracking and monitoring lab activities
- ◆ Quality control and error tracking
- ◆ Access control policy
- ◆ Sample handling



# Our approach

## An anthropological approach



Bronislaw Malinowski

“to grasp the native’s point of view, his relation to life, to realize his vision of his world”  
(Argonauts of the Western Pacific, 1961)



# Building new habits

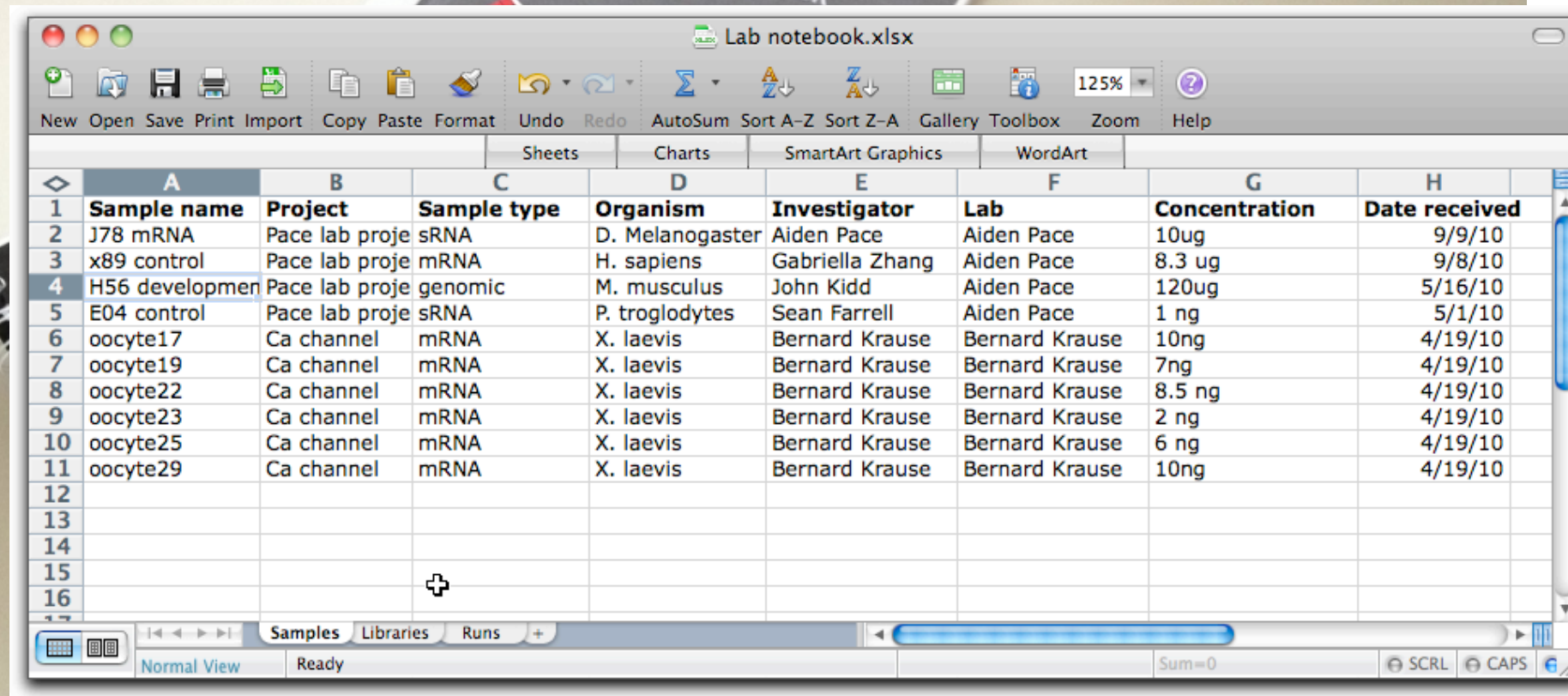


# Building new habits





# Building new habits



Lab notebook.xlsx

New Open Save Print Import Copy Paste Format Undo Redo AutoSum Sort A-Z Sort Z-A Gallery Toolbox Zoom Help

	A	B	C	D	E	F	G	H
	Sample name	Project	Sample type	Organism	Investigator	Lab	Concentration	Date received
1	J78 mRNA	Pace lab proje	sRNA	D. Melanogaster	Aiden Pace	Aiden Pace	10ug	9/9/10
2	x89 control	Pace lab proje	mRNA	H. sapiens	Gabriella Zhang	Aiden Pace	8.3 ug	9/8/10
3	H56 developmen	Pace lab proje	genomic	M. musculus	John Kidd	Aiden Pace	120ug	5/16/10
4	E04 control	Pace lab proje	sRNA	P. troglodytes	Sean Farrell	Aiden Pace	1 ng	5/1/10
5	oocyte17	Ca channel	mRNA	X. laevis	Bernard Krause	Bernard Krause	10ng	4/19/10
6	oocyte19	Ca channel	mRNA	X. laevis	Bernard Krause	Bernard Krause	7ng	4/19/10
7	oocyte22	Ca channel	mRNA	X. laevis	Bernard Krause	Bernard Krause	8.5 ng	4/19/10
8	oocyte23	Ca channel	mRNA	X. laevis	Bernard Krause	Bernard Krause	2 ng	4/19/10
9	oocyte25	Ca channel	mRNA	X. laevis	Bernard Krause	Bernard Krause	6 ng	4/19/10
10	oocyte29	Ca channel	mRNA	X. laevis	Bernard Krause	Bernard Krause	10ng	4/19/10
11								
12								
13								
14								
15								
16								

Normal View Ready Sum=0 SCRL CAPS

# Related issues

- ◆ Data Sharing
- ◆ Scalability
- ◆ Access Control
- ◆ Data Integrity Loss
- ◆ Data Redudancy





# Managing complex protocols

## DNA Library Preparation Exome Enrichment



# From this

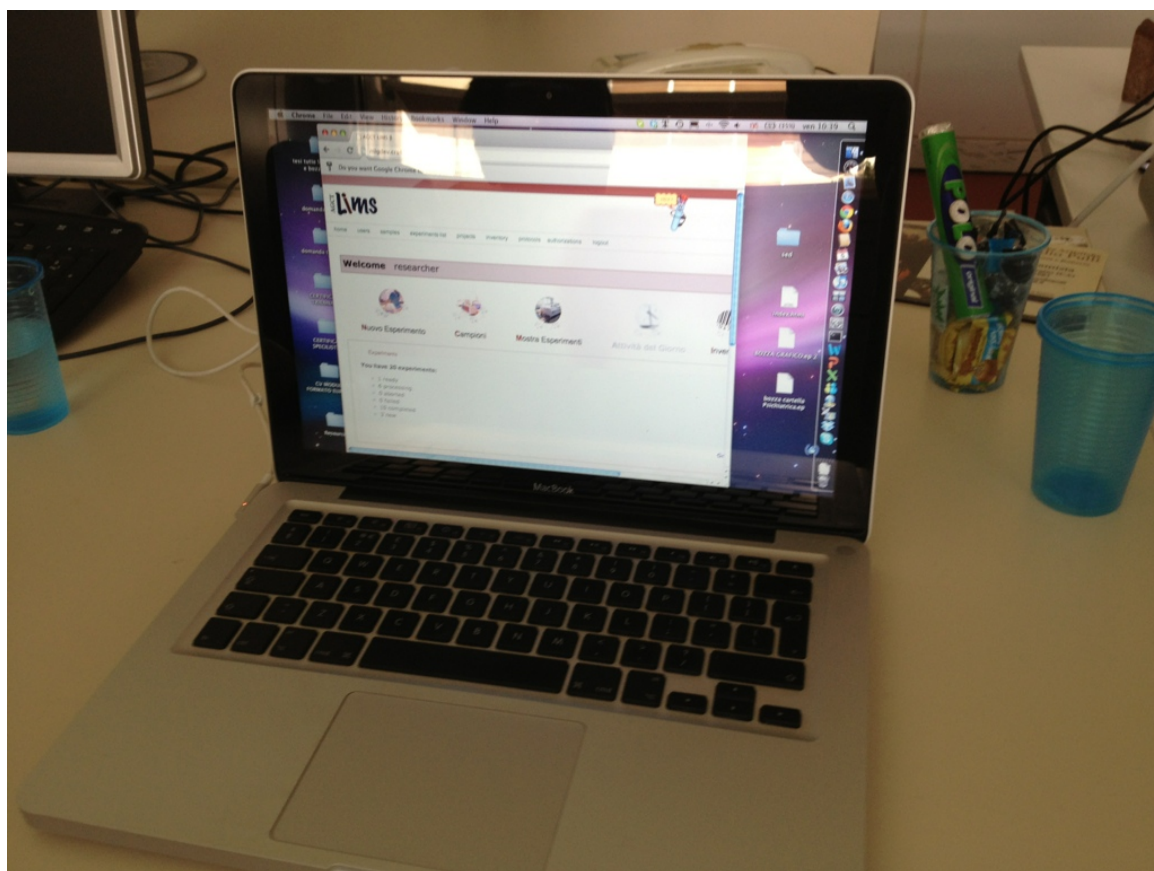
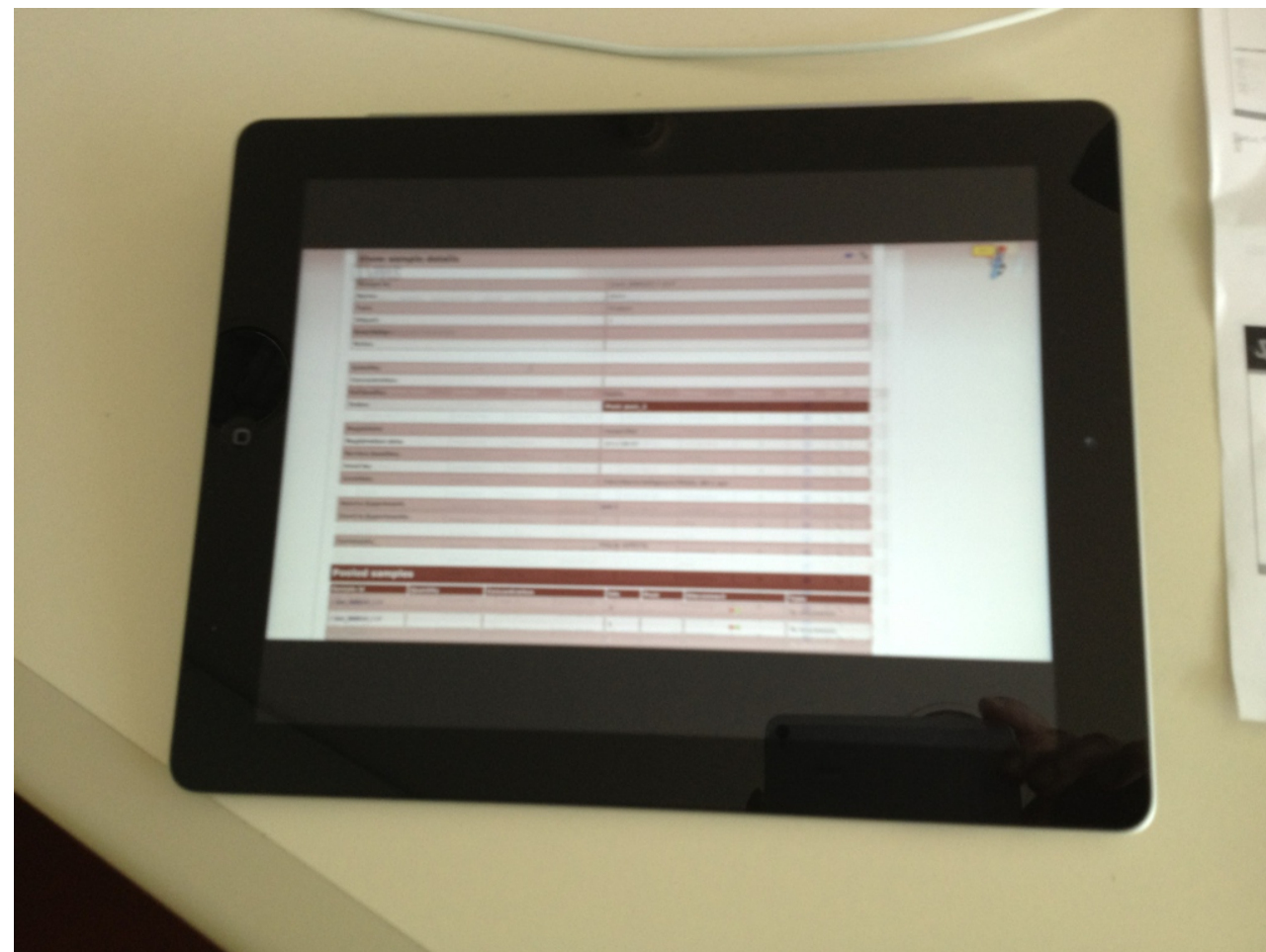
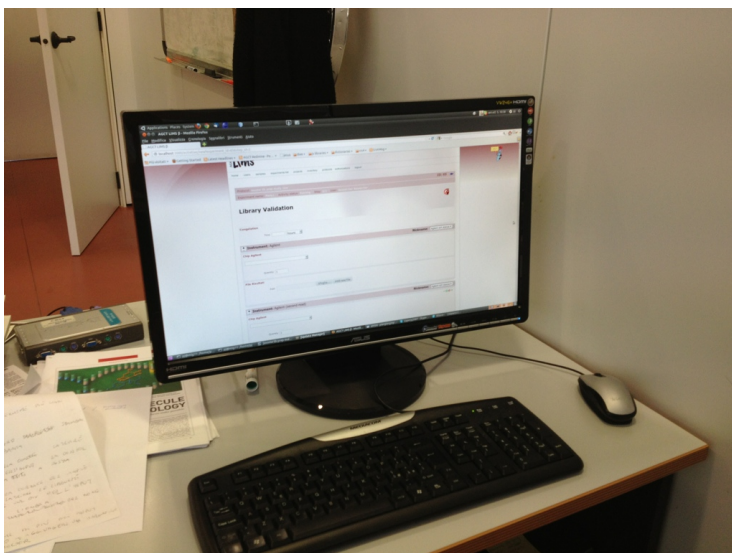


# From this

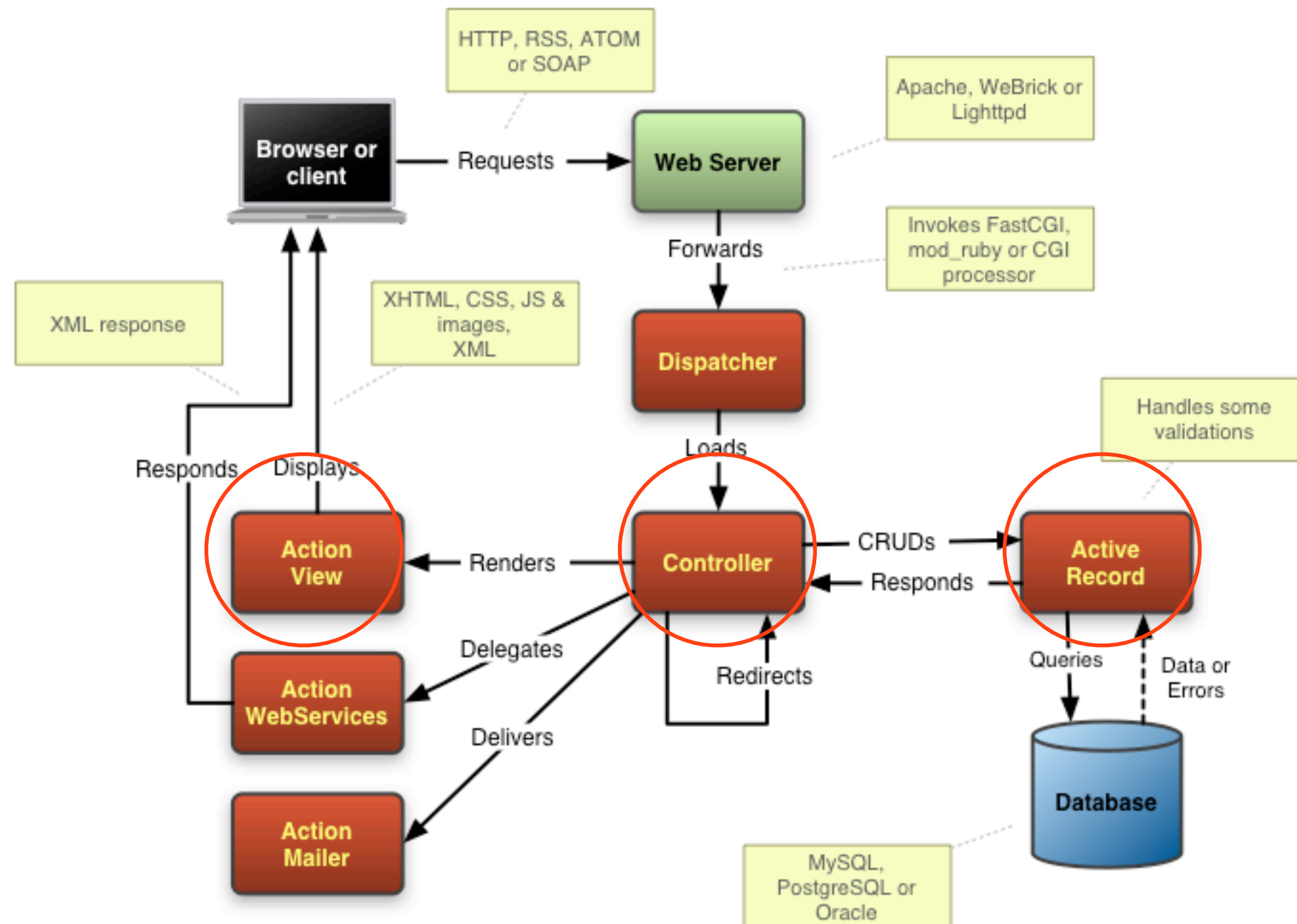




to this

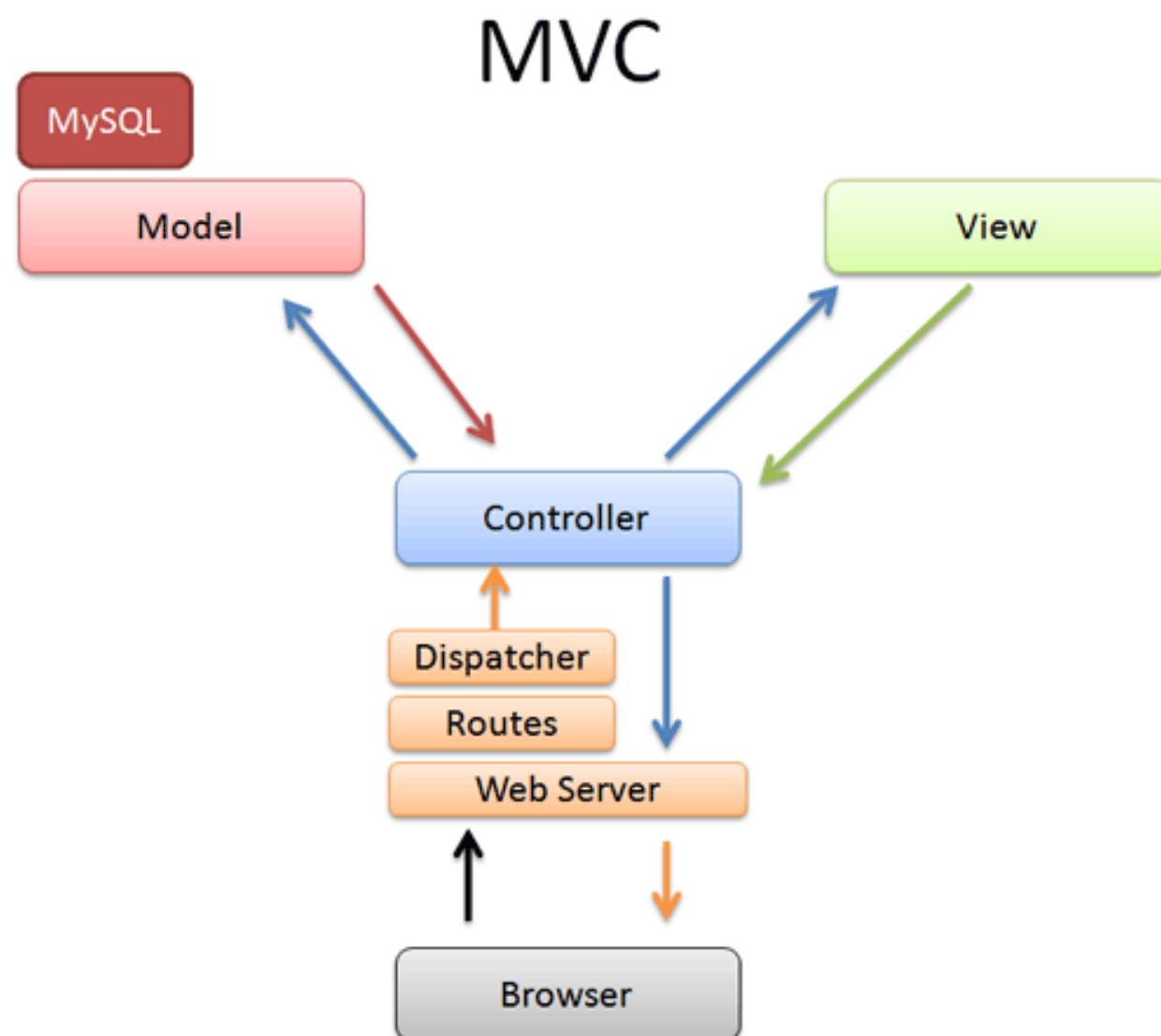


# QTreds overview





# MVC pattern



**MVC** divides the work of the application into **three** separate but closely cooperative subsystems

- Web-based application
- The Ruby programming language
- The Rails framework



# QTreds functional blocks

**Workflow Generator**

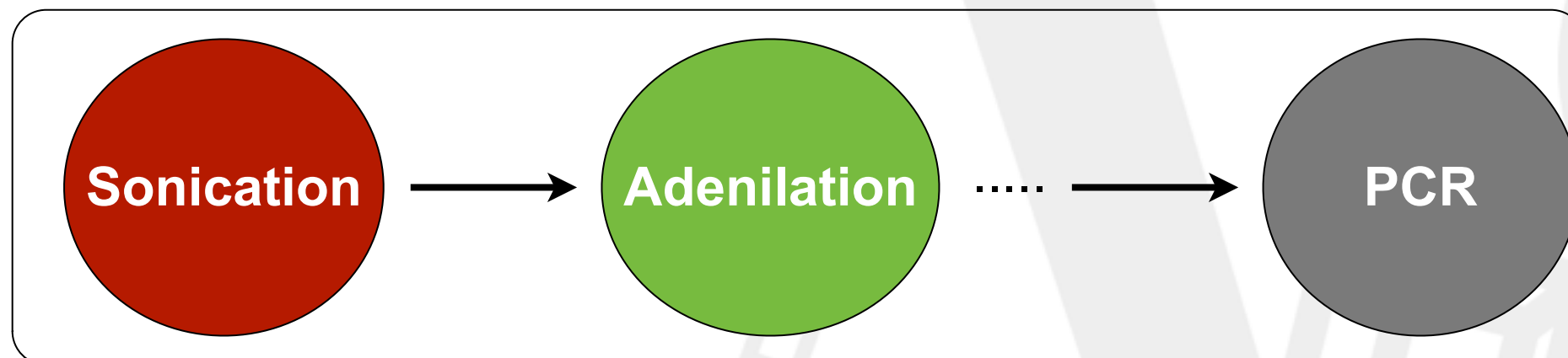
**Sample Handler**

**Inventory Management  
System**

**User Management  
System**

- Key point: Protocol definition
- Protocol: the sequence of steps of an experiment

## Workflow



- Each experimental protocol is defined as XML document
  - XSD to define:
    - structure
    - elements
    - attributes
    - constraints
- syntax



# Long and boring task

```
<protocol name='Exome Library Preparation' xmlns:xsi='http://www.w3.org/2001/XMLSchema-instance'
xsi:noNamespaceSchemaLocation='/LimsDemo/db/migrate/dev_data/protocols.xsd' locksources='no,yes' output='P,S'
version='1' input='U'>
  <activities>
    <activity name='Sonication' id='1'>

      <instrument name='Covaris S-Series' required='true' category='sonicator' default='Covaris -1p' id='1.1'>
        <input name='Device parameters' id='1.1'>
          <attribute type='decimal' key='duty cycle'>8</attribute>
          <attribute type='decimal' key='intensity'>3</attribute>
          <attribute type='decimal' key='cycles per burst'>200</attribute>
          <attribute type='decimal' key='second frequency sweeping'>60</attribute>
          <attribute type='decimal' key='number of cycles'>2</attribute>
        </input>
      </instrument>

      <input name='Note' id='1.2'>
        <attribute type='textarea' key='note' />
      </input>

      <comment title='Alternative procedure' />
    </activity>

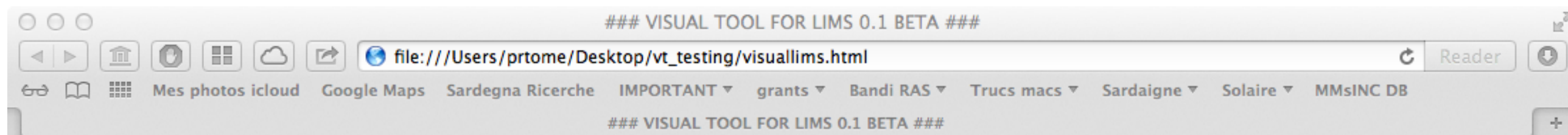
    <activity name='End repair' id='2'>

      <input name='Schema Multiwell-Samples' id='2.1'>
        <attribute type='file' key='Path' />
      </input>
    </activity>
  </activities>
</protocol>
```

## List of:

- activities
- instruments
- reagents
- items ...

# Visual Tool



THIS IS THE WORKBENCH

[x] Activity element1\_activity

[x] Input element2\_input

[x] Label element4\_label

X=958 Y=471



activity



instrument



input



dose




attribute

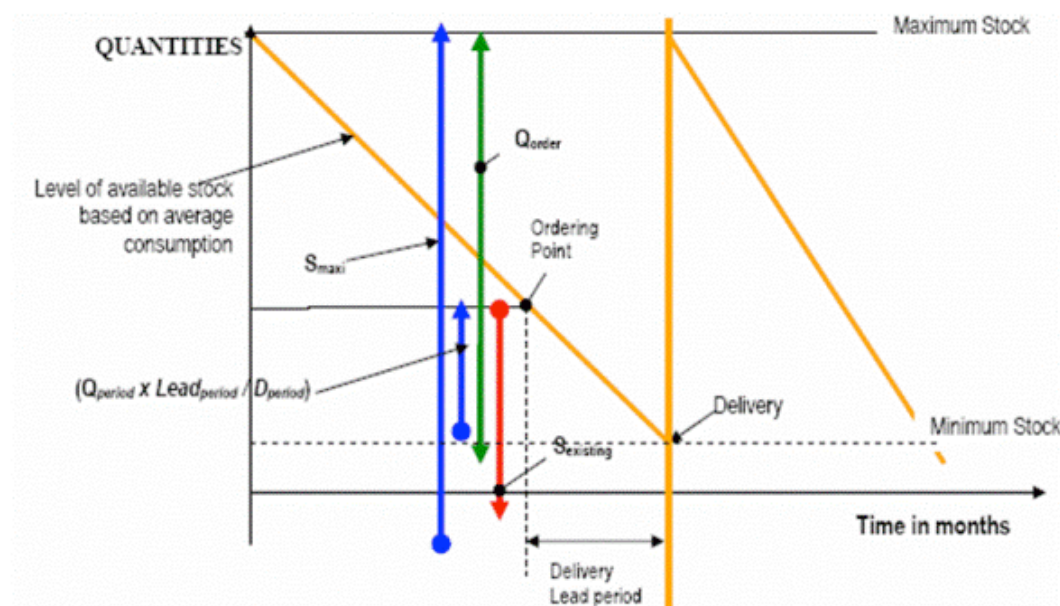


label

# Sample handling

- **Qtreds** records:
  - the path of each sample – chain of custody
- **Storage Location Management**
- allows to handle:
  - One sample at a time
  - Multiple samples
- Multiple samples can be combined into one entity (**Pooling**)

- Reagents, lab glassware and consumables easily added through their **barcodes** 
- **Minimum stock levels** can be handled to avoid shortages of essential products





# Inventory Modules



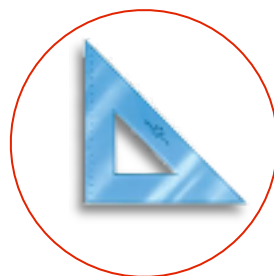
# Inventory Modules

**Catalog** where all categories of items have to be inserted



**Stock** to register all consumables in the lab





**Topology** a virtual representation of the lab to keep track of the locations



# Inventory Modules



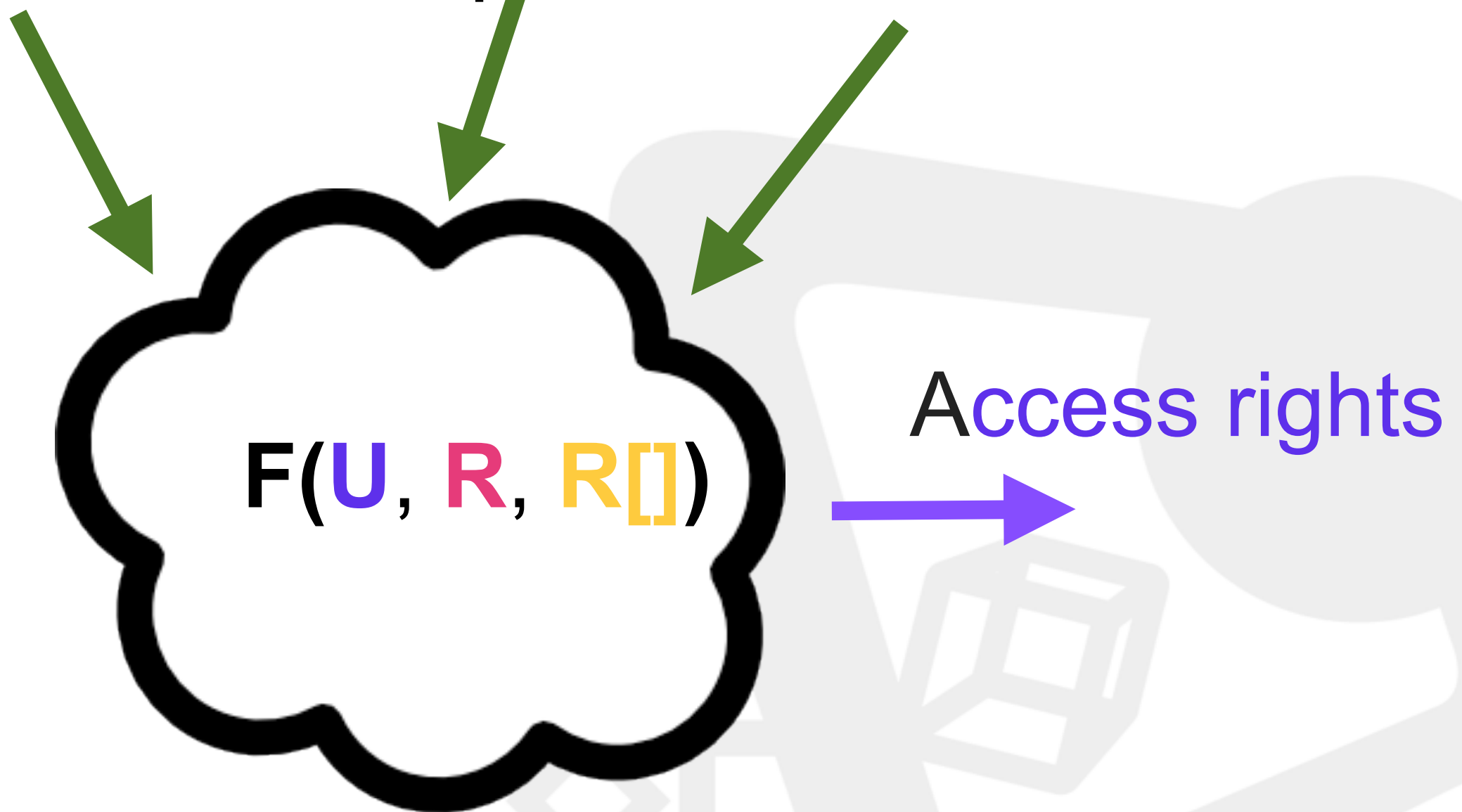
Personal  
Stock a sort  
of “shopping  
cart”

## Centralized Authorization Function

User

Request

Role



# Multiple roles




# Multiple roles

- ◆ Admin
- ◆ Supervisor
- ◆ Inventory manager
- ◆ User
- ◆ Analyzer



# Multiple roles

- ◆ Admin
- ◆ Supervisor
- ◆ Inventory manager
- ◆ User
- ◆ Analyzer



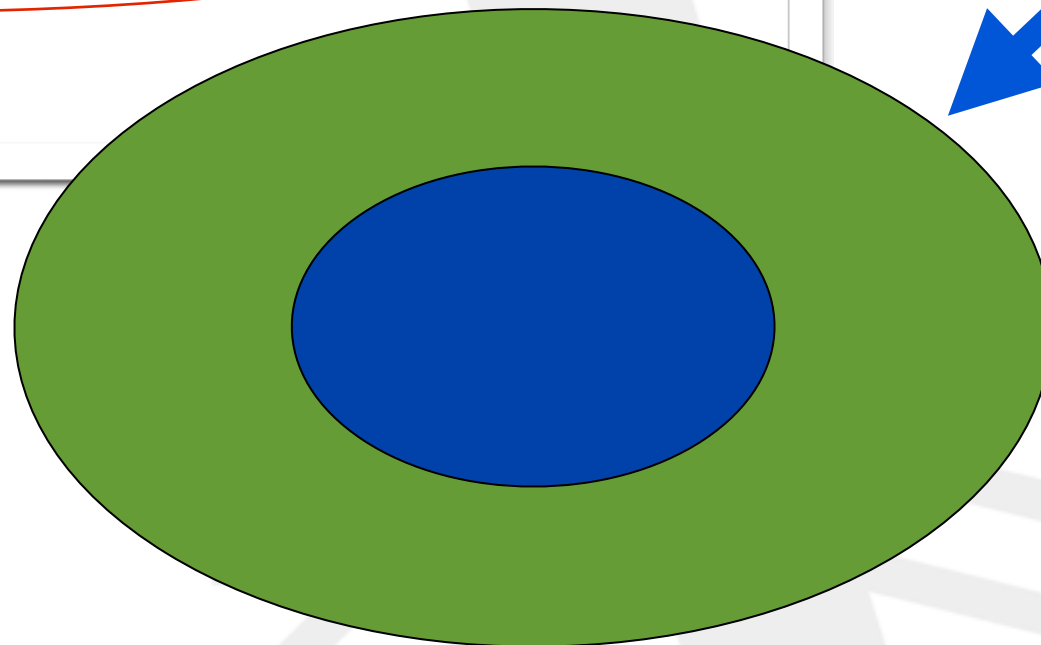
A user can  
have different  
roles

# Multiple roles

- ◆ Admin
- ◆ Supervisor
- ◆ Inventory manager
- ◆ User
- ◆ Analyzer

A user can have different roles

$F(\text{U}, \text{R}, \text{R}[])$



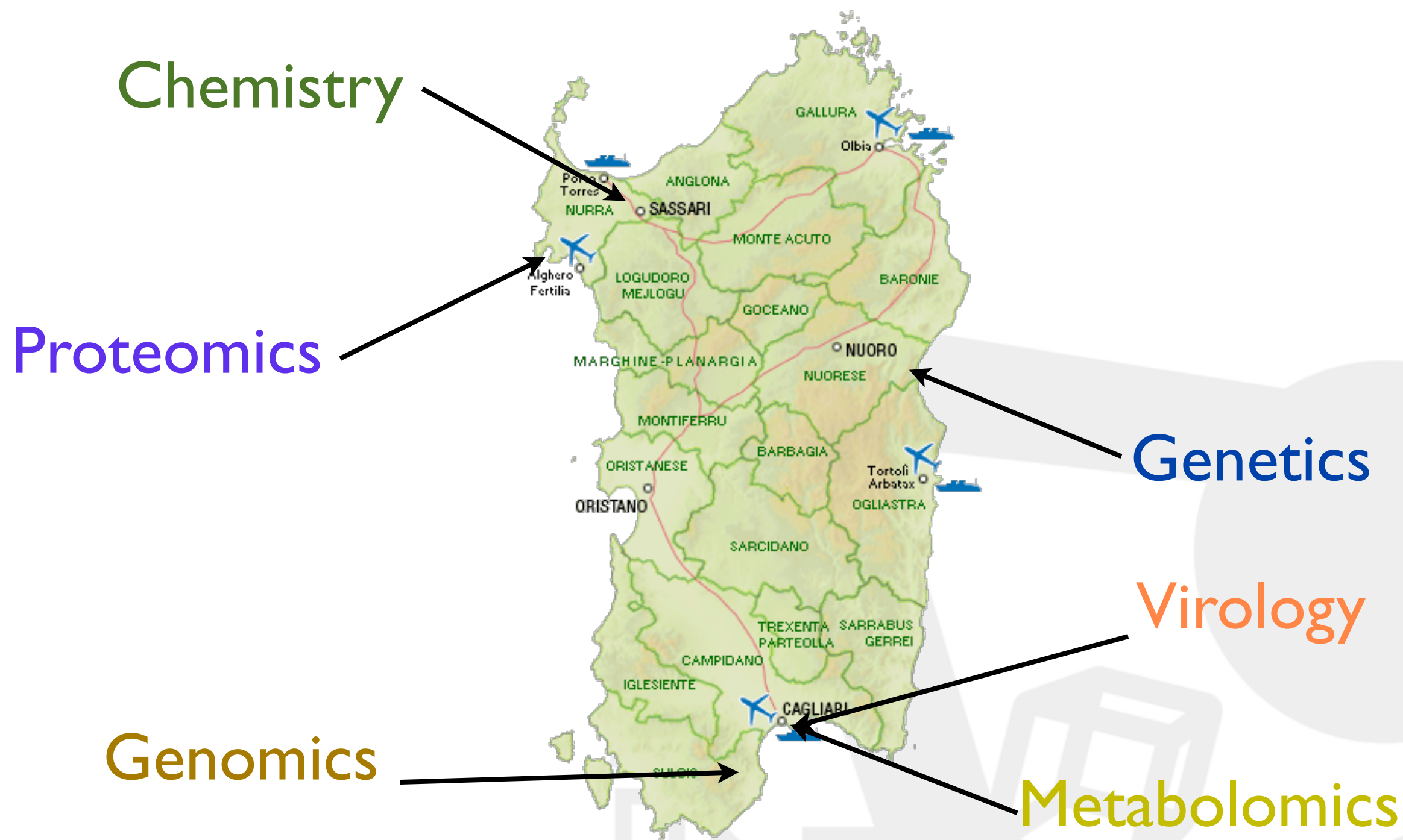
# Other features

- ◆ **Internal Messaging System** a collaborative tool to allow users to interact with each other
- ◆ **REST API** to allow an automated access to information

- ◆ QTreds and the CRS4 Sequencing and Genotyping Platform (CSGP)
- ◆ Different kinds of experiments:
  - DNA Library Preparation
  - Exome Enrichment
  - Sequencing



# Collaborations



- ◆ **New version** early 2013
- ◆ **New features:**
  - **Plugin system** to directly interface instruments to QTreds
  - **Ad-hoc reporting** visual tool to create your own reports
  - **"Calendarization" system** to schedule the activities and the workload balancing

# DS3 group

	<b>Personnel</b>	<b>Expertise</b>
	Patricia Rodriguez-Tomé	Bioinformatics, Seismology (HEAD)
	Giuliana Brunetti	Biology, Science dissemination
	Gianfranco Frau	Computer Engineering
	Elisabetta Marras	Statistics
	Piergiorgio Palla	Computer Engineering
	Luana Vargiu	Biology

# The End



# The End

Thanks for your attention!





# The End

Thanks for your attention!

<http://qtreds.crs4.it/demo>

user: labuser

psswd: qtreds