Informationshanteringsystem - LIMS

1DL470, 5.0 credits

Spring 2011

Agenda for lectures, assignments and LIMS project

http://www.it.uu.se/edu/course/homepage/lims/vt11/

Kjell Orsborn
Uppsala Database Laboratory
Department of Information Technology, Uppsala University,
Uppsala, Sweden
Personell (LIMS project)

• Kjell Orsborn, lecturer, examiner:
  – email: kjell.orsborn@it.uu.se, phone: 471 1154, room: 1321, ITC building 1, floor 3

• Robert Kajic, course assistant:
  – email: robert.kajic@it.uu.se, phone: 471 7345, room 1306, ITC building 1, floor 3
Preliminary course contents

• Course introduction
  – agenda
  – overview of LIMS systems and web technology
• Lectures and invited lectures on suitable topics from the LIMS area and in web technology
• Assignment
  – introducing technology for project (NetBeans IDE, web server (Apache), database (MySQL), server-side scripting (PHP), client-side scripting (Javascript), etc.)
  – deployment of web application (on hold - possibly using Apache dept web server)
• Group project (forming groups, developing project idea, specification, design, development, testing, deployment)
  – i.e. to develop a multi-tiered LIMS web application
  – project documentation, reporting and demonstration
• Project examination - grades U, 3, 4 & 5.
Homework

• Prepare for your project by:

  – Choosing a group and emailing the names, ssn, emails and skills to the assistant Robert Kajic (cc: Kjell Orsborn) together with info on initial project leader

  – If you cannot find a group send your personal info, listed above, to assistant to get help forming a group

  – Discuss possible ideas for your project. Browsing the web might get you some ideas.

  – Discuss the business idea of your project in terms of possible advantages/disadvantages with your idea and how it can contribute support the business or how to earn money.

  – Go to assignment seminar

  – Do assignment

  – Go to project seminar

  – You are ready for project
Resources

• Course web site:
  – Main course page
  – Assignment page
  – Project page
  – You’ll also find
    • links to software required for the assignment
    • links to related material and interesting articles
  – Lecture notes
    • will be made available on the course web site

• Web resources (tools, tutorials, example code, open-source LIMS projects etc)

• Literature
  – Online material on the course web page
  – A book that introduces web technology: Ince (2002) Developing distributed and e-commerce applications, Addison-Wesley, 0-201-73046-4
    • a good overview of web-based systems (not just Java-based), but light on technology
Your LIMS project

• Develop a LIMS web application of your choice

• Suggested tools:
  – NetBeans IDE, MySQL, Apache, PHP, Javascript
  – … or possibly choose your own combination

• Important!!!
  – Academic honesty
  – Personal contribution
LIMS project milestones

• Week 3
  – Lecture - course introduction
  – Students should form groups and start to write Project plans
  – Lecture - intro to LIMS and web-based systems
  – Tutorial 1 (Netbeans, PHP, JavaScript, MySQL, TDD [1 h])
  – Tutorial 2 - intro to project
  – Assignment (Netbeans, PHP, JavaScript, MySQL, TDD [4 h])

• Week 4
  – Initial project meeting (each group + K + RK [30 min]).
    • Students should bring their Project plans to this meeting for discussion.
  – Assignment continued [4 h]

• Week 5
  – SCRUM meeting (each group + M [10 min])
    • During SCRUM meetings, we might detect the need of a more in-depth discussion of some aspects. The group should then agree on a time slot during Office Hours.

• Week 6
  – SCRUM meeting (each group + RK [10 min])
    Week 7
  – ......

• Week 8
  – mid term meeting (each group + K + RK [30 min])

• Week 9
  – Students are expected to continue SCRUM meetings without supervision. Students may request office hours.

• Week 10
  – ......

• Week 11
  – ......

• Week 12
  – final presentation/poster session (each group 30 min)
  – final meeting + final report (each group 30 min)
E-commerce project …

• Project idea and plan:
  – Description of the "LIMS case"
    • Motivation for your system?
    • Pros & cons
  – A system architecture
    • "How will it work?"
    • Must include: ER diagram, Use cases & Description of user interface
  – An implementation plan
  – Project time plan

• Mid term report:
  – to follow up on your progress

• Final presentation:
  – … of your project and demonstration of a working solution

• Final report:
  – The business case
  – A description of the system
Lecture topics

• My lectures
  – Intro to LIMS & web-based systems
  – Architectures and web servers (i)
  – Architectures and web servers (ii)
  – Web server frameworks
  – Security?
  – (ER modeling???)
  – (Databases, Relational model, SQL and DB API’s???)

• Invited lectures
  – LIMS within bioinformatics - Mikael Thollesson
  – LIMS within genom sequencing - Jan Andersson
  – To be announced.
  – To be announced.
Web based technologies ...

- Html, Xhtml, XML, CSS, Xslt
- JavaScript, Applets and client side programming
- SSI, CGI, SCGI, FastCGI
- JavaServer Pages (JSP), Java Servlets and server side programming
- ASP/ASP.NET
- Perl, PHP, Python, Ruby, Tcl
- JDBC and DB API’s
- Java DB (Derby)
- LAMP (Linux, Apache, MySQL and PHP)
- Apache & Tomcat
Web based technologies cont. …

- Semantic web, Web services, WSDL, SOAP, Document Object Model (DOM)
- Google web toolkit, JavaServer Faces, Struts, Tapestry
- Ruby on Rails, WebObjects, Catalyst, Django
- Web 2.0, Ajax Programming
- Semantic web, Web services, WSDL, SOAP, Document Object Model (DOM)
- NetBeans
- Data persistence, concurrency & transactions
- Architectures & case studies
- Java EE & Enterprise Java Beans, GlassFish, etc.
Preliminary grading of the course

- Assignment 10%
- Project 90%
  - forming group & providing project idea 5%
  - project plan 10%
  - mid term evaluation 10%
    - Report
    - presentation quality (story from 1st to last)
    - time (compare with plan)
    - Content
    - level of complexity
    - data model
    - use cases
    - test cases
  - final presentation 10%
    - presentation quality
    - technical content
    - effort made
  - final group discussion 10%
    - presentation quality
    - technical content
    - effort made
  - project 40%
    - Report
    - presentation quality (story from 1st to last)
    - time (compare with plan)
    - technical quality
    - technical content
    - level of complexity
    - data model
    - use cases
    - test cases
Mid-term project evaluation

For the half time evaluation we are going to ask about
1. Presentation of the idea
2. Overall design of the system
3. Data model
4. Use cases
5. Test cases
6. Working prototype
7. Present project status. Compare to project plan.
8. Plan for the rest of the project. Any changes of the initial plan?
9. Talk to us about how you divided the work between each other.

Note! similar questions will be asked for the final assessment. Hence, being active at the half time assessment is a good way of preparing for the final assessment.

• The technical project
  – project idea - business
  – technical quality (error handling, testing, etc)
  – project status

• The project work
  – communication
  – administration
  – group work
Final project presentation and evaluation

For the final presentation you should focus on:

1. Presentation of the idea
2. Overall design of the system
3. Data model
4. Use cases
5. Test cases
6. Working prototype
7. Present project status. Compare to project plan.
8. Plan for the rest of the project. Any changes of the initial plan?
9. Talk to us about how you divided the work between each other.
   Note! similar questions will be asked for the final assessment. Hence, being active at the half time assessment is a good way of preparing for the final assessment.
   • The technical project
     – project idea - business
     – technical quality (error handling, testing, etc)
     – project status
   • The project work
     – communication
     – administration
     – group work

For the final group discussion we are going to ask your group about issues like:

1. Overall design of the system
2. Data model
3. Use cases
4. Error handling
5. Test cases
6. Security
7. What is missing
8. The project work
9. Administration
10. Final report
11. Lessons learned …
Introduction to LIMS and Web-based systems

Darell Ince, ch 1

Kjell Orsborn

Department of Information Technology
Uppsala University, Uppsala, Sweden
• A Laboratory Information Management System (LIMS) is a software system used in laboratories for the integration of all laboratory softwares, instruments, and the management of samples, laboratory users, standards and other laboratory functions such as quality assurance and quality control (QA/QC), sample planning, invoicing, plate management, and workflow automation.
LIMS system environment

- Enterprise resource planning
- Laboratory Informatics
- PDES
- eHealth
- Medical Informatics
- LIMS
- Management information system
- Health informatics
- Biomedical informatics
- Product lifecycle management
LIMS industrial sectors

- Pharmaceutical Manufacturing
- Pharmaceutical Research and Development
- Petrochemical
- Chemical and Industrial
- Environmental
- Metals
- Mining
- Forensics
- Contract Services
- Tobacco
- Food and Beverage
- Public Health
- Healthcare
- Clinical Trials
- Biorepository
Common LIMS features

Requirements of a typical LIMS systems in an analytical testing laboratory can include the following:

– Sample login
– Sample tracking/barcode support/quoting
– Scheduling
– Chain of custody
– Instrument integration
– Result entry/audit trail
– QA/QC/specification checking
– Result reporting
– Web integration/links to enterprise software
– Chemical and reagent inventory
– Personnel training record tracking/instrument maintenance
– Archiving/data warehousing
Common LIMS features

A list of some LIMS functions at the analytical and managerial levels (note that not all of these features may be found on every system package).

Analytical level tasks:
• Automatic sample number generation.
• Bar code label generation.
• Sample log-in either manually or via bar-codes.
• Acknowledgement of sample receipt.
• Verification of data format entered into the computer.
• Worksheet generation.
• Construction and checking of calibrated curves.
• Direct data acquisition from chromatographs.
• Automatic data collection from analytical instruments.
• Entry of instrumental readings via RS232C or IEEE488.
• Manual results entry.
• Interpretation of calibrated curves and quality control samples.
• Interpretation and acceptance of sample data.
• Routine automatic calculations.
• Plotting routines for visualization of analytical data.

Managerial level tasks:
• Backlog investigation.
• Sample and status tracking.
• Database searches.
• Numbers of samples assayed.
• Tests utilized.
• Numbers of samples analysed per instrument.
• Cost per assay.
• Customer charges.
• Results collation and presentation.
• Report generation.
• Scheduling and rescheduling of work.
• Archival and retrieval of data.
• Workload status and the justification of equipment.
• Regulatory Agency Compliance:
• Audit trail for all database transactions.
• Security: Class or Hierarchy.
• Instrument records and calibration where appropriate.
Information flows within the laboratory
LIMS regulations and security

- ISO 9000 - ISO 9001:2008 Quality management systems — Requirements
- A laboratory might also have to operate in compliance with U.S. FDA and EU GLP and GCP regulations
LIMS Clinical Trial Features

- Protocol Design and Approval
- Clinical Trial Manager
- Kit Production & Distribution
- Kit Tracking
- Storage Management
- Visit Scheduling
- Query/Discrepancy Management
- Forms- Electronic Data Capture
- Trial Milestone Cost Management
- Subject Recruitment and Screening
- Complex Reflex testing and Delta checking rules
- Investigator notification
LIMS workflow example
## LIMS suppliers

<table>
<thead>
<tr>
<th>LIMS Vendor</th>
<th>Product</th>
<th>Underlying Database</th>
<th>Web Interface Supported</th>
<th>Web Address</th>
</tr>
</thead>
<tbody>
<tr>
<td>Accelerated Technology</td>
<td>Sample Master Pro</td>
<td>MS SQL Server, ORACLE, Access 2000</td>
<td>Yes</td>
<td><a href="http://www.atlab.com">www.atlab.com</a></td>
</tr>
<tr>
<td>Laboratories, Inc.</td>
<td>ScreenIT LIMS</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Applied Biosystems</td>
<td>SQL LIMS</td>
<td>Oracle</td>
<td>Yes</td>
<td><a href="http://www.appliedbiosystems.com">www.appliedbiosystems.com</a></td>
</tr>
<tr>
<td>Autoscribe Ltd.</td>
<td>Matrix Plus</td>
<td>Oracle, MS SQL Server, DB2</td>
<td>Yes</td>
<td><a href="http://www.autoscribe.co.uk">www.autoscribe.co.uk</a></td>
</tr>
<tr>
<td>Baytek International, Inc.</td>
<td>WinBLISS</td>
<td>Oracle</td>
<td>Yes</td>
<td><a href="http://www.baytekinternational.com">www.baytekinternational.com</a></td>
</tr>
<tr>
<td>Beckman Coulter, Inc.</td>
<td>LabManager iLIMS</td>
<td>Oracle</td>
<td>Yes</td>
<td><a href="http://www.beckmancoulter.com">www.beckmancoulter.com</a></td>
</tr>
<tr>
<td>Blaze Systems Corporation</td>
<td>BlazeLIMS</td>
<td>Oracle, MS SQL Server</td>
<td>Yes</td>
<td><a href="http://www.blazesystems.com">www.blazesystems.com</a></td>
</tr>
<tr>
<td>ChemWare</td>
<td>Horizon LIMS</td>
<td>Oracle</td>
<td>Yes</td>
<td><a href="http://www.chemware.com">www.chemware.com</a></td>
</tr>
<tr>
<td>Cogexel, Inc.</td>
<td>LabPlus</td>
<td>Oracle, MS SQL</td>
<td>Yes</td>
<td><a href="http://www.cogexel.com">www.cogexel.com</a></td>
</tr>
<tr>
<td>Creon Lab Control, Inc.</td>
<td>Q-DIS</td>
<td>Oracle, MS SQL</td>
<td>Yes</td>
<td><a href="http://www.creonlabcontrol.com">www.creonlabcontrol.com</a></td>
</tr>
<tr>
<td>LabVantage Solutions</td>
<td>QM-AQV-DM-R</td>
<td>Oracle, MS SQL Server</td>
<td>Yes</td>
<td></td>
</tr>
<tr>
<td></td>
<td>LV LIMS</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Sapphire Edition</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>LabWare Inc.</td>
<td>LabWare LIMS</td>
<td>Oracle, SQL Server, Sybase, Informix, DB2</td>
<td>Yes</td>
<td><a href="http://www.labware.com">www.labware.com</a></td>
</tr>
<tr>
<td>L.L.M.S. (USA), Inc.</td>
<td>StarLIMS</td>
<td>Oracle, MS SQL, SQL-based DBs, Sybase</td>
<td>Yes</td>
<td><a href="http://www.starlims.com">www.starlims.com</a></td>
</tr>
<tr>
<td>QSI Corp</td>
<td>WinLIMS &amp; WebLIMS</td>
<td>Oracle, MS SQL, SQL-based, Sybase</td>
<td>Yes</td>
<td><a href="http://www.qsius.com">www.qsius.com</a></td>
</tr>
<tr>
<td>RJ Lee Group</td>
<td>Lab Task</td>
<td>Btrieve/Pervasive SQL</td>
<td>Yes</td>
<td><a href="http://www.rjls.com">www.rjls.com</a></td>
</tr>
<tr>
<td>Thermo LabSystems, Inc.</td>
<td>Sample Manager, Nautilus</td>
<td></td>
<td>Yes</td>
<td><a href="http://www.thermolabsystems.com">www.thermolabsystems.com</a></td>
</tr>
<tr>
<td>Zumatrix Inc.</td>
<td>Matrix Plus</td>
<td>Oracle, MS SQL Server, DB2</td>
<td>Yes</td>
<td><a href="http://www.zumatrix.com">www.zumatrix.com</a></td>
</tr>
</tbody>
</table>
LIMS open source

- Bika LIMS by Bika Lab Systems, South Africa - Open Source LIMS based on Zope/Plone CMS
- SLIMS (Sample-Based Laboratory Information Management System) by Genapha
- WikiLIMS by Biotech Inc.
- Labmatica/FreeLIMS by LIMS at work GmbH
LabWare WebLIMS
LabWare LIMS

General LW Sample Login Template

Sample Type: POLYETHYLENE
Grade: Manufacturing Limits
Sampling Point: NONE
Description: Routine Sample
Customer Name: ACME
Charge Code: 93-83743
Priority: 2
Price List:
Project:

Sample Interface - GENERAL
The LabSoft LIMS Microbiology

<table>
<thead>
<tr>
<th>Facility</th>
<th>ACME</th>
</tr>
</thead>
<tbody>
<tr>
<td>Set Status</td>
<td>COMPLETE</td>
</tr>
<tr>
<td>Over Limit?</td>
<td>YES</td>
</tr>
<tr>
<td>Group</td>
<td>ENV/CONTACT</td>
</tr>
<tr>
<td>Program</td>
<td>ENV/CONTACT</td>
</tr>
<tr>
<td>Step</td>
<td>1</td>
</tr>
<tr>
<td>Sample Date</td>
<td>02/03/2004</td>
</tr>
<tr>
<td>Floor</td>
<td>206</td>
</tr>
<tr>
<td>Room</td>
<td>1003</td>
</tr>
<tr>
<td>Zone</td>
<td>ZONE 1</td>
</tr>
<tr>
<td>Line</td>
<td>0100</td>
</tr>
<tr>
<td>Product</td>
<td>LISTERIA</td>
</tr>
<tr>
<td>Classification Type</td>
<td>CLASSIFICATION</td>
</tr>
<tr>
<td>Test Positives</td>
<td>1</td>
</tr>
<tr>
<td>Total Sets</td>
<td>1</td>
</tr>
<tr>
<td>Total Positives</td>
<td>1</td>
</tr>
<tr>
<td>Samples Read</td>
<td>3</td>
</tr>
<tr>
<td>Samples Taken</td>
<td>3</td>
</tr>
<tr>
<td>Validation Code</td>
<td>NONE</td>
</tr>
<tr>
<td>Sample Date</td>
<td>02/03/2004</td>
</tr>
<tr>
<td>Sample No.</td>
<td>BOB</td>
</tr>
<tr>
<td>Window Start</td>
<td>2</td>
</tr>
<tr>
<td>Window End</td>
<td>4</td>
</tr>
<tr>
<td>Lab Request Document</td>
<td>Sample Set: 20040000005</td>
</tr>
</tbody>
</table>

**Sample Information Entry**

- **Facility**: ACME
- **Set Status**: SAMPLED
- **Program**: ENV/CONTACT
- **Step**: 1
- **Sample Date**: 02/21/2004
- **Zone**: ZONE 1
- **Line**: 0100
- **Product**: LISTERIA
- **Classification Type**: CLASSIFICATION
- **Action Date**: 07/12/2004
- **Action Type**: CORRECTIVE
- **Action Title**: SANITIZER CHECK
- **Action Description**: SANITIZER CONCENTRATION WAS LOW.

**Samples**

<table>
<thead>
<tr>
<th>Sample No.</th>
<th>Site ID</th>
<th>Operation</th>
<th>Sample Type</th>
<th>Sample Status</th>
<th>Sampled</th>
<th>Not Sampled</th>
<th>Sampled Time</th>
<th>Sample Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2004000065</td>
<td>SITE 001</td>
<td>0100 Floor Drain</td>
<td>FIXED</td>
<td>SAMPLLED</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>2004000066</td>
<td>SITE 009</td>
<td>0100 Waste Container</td>
<td>RANDOM</td>
<td>SAMPLED</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>2004000067</td>
<td>SITE 006</td>
<td>0100 Cart</td>
<td>RANDOM</td>
<td>SAMPLED</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>2004000068</td>
<td>SITE 007</td>
<td>0100 Control Panel</td>
<td>ALTERNATE</td>
<td>NOT SAMPLED</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
BIKA LIMS (open source)
SLIMS UML - diagram
Labmatica LIMS (open source)
Now – thinking out of the box!
http://www.google.org/flutrends/
http://www.gapminder.org/world/
http://www.who-umc.org/
Iphone AliveECG application
Iphone AliveECG application
Iphone snore monitor
Your LIMS project constraints
Your LIMS project constraints

Think Different!
A Quick 5-minute exercise

- Imagine having to build a large web site such as Amazon or eBay.
- Write down 5 major requirements of any such site.
A Quick 5-minute exercise

- Imagine having to build a large e-commerce site such as Amazon or eBay.
- Write down 5 major requirements of any such site.
  - secure purchase & secure site
  - robust & easy to use
  - fast (enough)
  - scaleable
  - customized experience
  - internationalization and localization (i18n & L10n)
Technical Issues for web-based system architects

- Security in all its forms
- Transactions & replication
- Coping with stateless HTTP protocol
  - User-tracking
- Dynamic pages
- Speed of development/change
- Division of labour:
  - graphics designers, programmers, business types
- Factoring the processes: tiers
- Support for data warehousing
A question

- Q: What distinguishes LIMS system from any other large system deployed on the web?
A question

• Q: What distinguishes an e-commerce system from any other large system deployed on the web?

• A: Not much.
  
  – Such sites must be secure, robust, scaleable, etc…
Enterprise computing

- Most of the aforementioned concerns apply to the architecture of any enterprise level solution
- Enterprise systems include those for e-commerce, but also denote
  - Internal, web-enabled, systems
  - Systems with no element of LIMS as it is usually understood
- Technologies discussed in this course applies to enterprise-level systems, not simply those involving e-commerce
What isn’t here

- Design
- Multimedia delivery
- Hosting
- Mobile internet
- Management
- Ethics, as e.g.
  - Is it a good thing that Hotmail has access to the personal messages of 100 million inhabitants of the globe?
  - Is it a good thing that Google have histories of browsing patterns?
  - Is it a good thing that Ebay have access to millions of trading details?