Informationshanteringsystem - LIMS

1DL470, 5.0 credits

Spring 2013

Agenda for lectures, assignments and LIMS project

http://www.it.uu.se/edu/course/homepage/lims/vt13/

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Personell (LIMS project)

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• Minpeng Zhu, course assistant:
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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 Minpeng Zhu and me (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 4**
  - Lecture - course introduction
  - Students should form groups and start to write Project plans
  - Initial project discussions (each group + KO [30 min]).
  - Lecture - intro to LIMS and web-based systems (KO)
  - Tutorial 1 (Netbeans, PHP, JavaScript, MySQL, TDD [1 h]) (MZ)

- **Week 5**
  - Tutorial 2 - intro to project (MZ)
  - Assignment (Netbeans, PHP, JavaScript, MySQL, TDD [4 h]) (MZ)
  - Initial project meeting (each group + KO [30 min]).
    - Students should bring their Project plans to this meeting for discussion.
  - Assignment continued [4 h] (MZ)

- **Week 6**
  - SCRUM meeting (each group + KO [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 7**
  - SCRUM meeting (each group + KO [10 min])

- **Week 8**
  - mid term meeting (each group + KO + MZ [30 min])

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

- **Week 10**
  - SCRUM meeting (each group)

- **Week 11**
  - SCRUM meeting (each group)

- **Week 12**
  - final presentation/poster session (each group 30 min) (KO + MZ?)
  - final meeting + final report (each group 30 min) (KO + MZ?)
LIMS 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?
  – Web services?
  – (ER modeling???)
  – (Databases, Relational model, SQL and DB API’s???)

• Invited lectures
  – LIMS within bioinformatics - Mikael Thollesson
  – To be announced – N.N.
  – To be announced – N.N.
  – To be announced – N.N.
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
    - user interface
  - 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
    - user interface
Mid-term project evaluation

- In the midterm evaluation you will present your project and the current status and future plans for finalizing your project. We might ask questions about various topics such as:

1. Presentation of the idea and LIMS case
2. Overall design of the system
3. Data model
4. Use cases
5. Test cases
6. Working prototype
7. User interface
8. Present project status. Compare to project plan.
9. Plan for the rest of the project. Any changes of the initial plan?
10. Talk to us about how you divided the work between each other, how project communication, administration and group work is progressing.
11. Additional technical aspects such as security, error handling, code management and revision control, bug control, etc.
12. Encountered problems?

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.
For the final presentation you should focus on:

1. Presentation of the idea and LIMS case
2. Overall design of the system
3. Data model
4. Use cases
5. Test cases
6. Working prototype
7. User interface
8. Talk to us about how you divided the work between each other, how project communication, administration and group work is progressing.
9. Additional technical aspects such as security, error handling, code management and revision control, bug control, etc.
10. Encountered problems?
11. Present project status - compare to project plan.

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. User interface
8. Code management and revision control, bug control, etc.
9. What is missing
10. The project work
11. Administration
12. Final report
13. Lessons learned …
Final LIMS project report

• In the final evaluation you should hand in a project report.

• It should be a normal technical project report. A possible report structure that I took from this book: http://www.amazon.co.uk/Thesis-Projects-Students-Computer-Information/dp/1848000081/ref=sr_1_3?ie=UTF8&qid=1306270835&sr=8-3.

• The suggested structure cover:
  • Title page
  • Abstract
  • Ch 1: Introduction
  • Ch 2: Background
  • Ch 3: Problem description and statement
  • Ch 4-6: The core of the report (in this case e.g. requirements specification, design, implementation, results, evaluation.
  • Ch 7: Related work
  • Ch 8: Conclusion
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 (process development and execution system)

eHealth

Medical Informatics

Health informatics

Management information system

Product lifecycle management

Biomedical informatics
LIMS software

• Common for several of the those software’s, including LIMS software, is the aim to increase:
  – traceability,
  – productivity, and
  – quality
• of the delivered result.
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 in 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 analyzed 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

Management Information

- Budget Projection
- Resource Planning
- Productivity Assessment
- Financial Assessment

Sample labelling
Acknowledgement of Sample receipt
Worksheet Generation
Status of samples
Sample Location
Assay progress
Standard operating procedures
Backlog of samples
Instrument service and calibration records

Comparison of results
Word Processing
Archival/Retrieval

Sample → Preparation → Test → Validation → Result

Analytical Information
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

Diagram:
- User name and password protection
- Limit access via permissions
- Prevent data modification
- Security
- Integrity
- Change control
- Version control
- Link raw data to results
- Audit Trail / full Chain of Custody
  - Who did what, when and why?
  - Record of previous entries (Must not be deleted or able to delete)
  - Date and time stamp
  - Security
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>
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<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>
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<tr>
<td>Laboratories, Inc.</td>
<td>ScreenIT LIMS</td>
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<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>
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<tr>
<td>Autoscribe Ltd.</td>
<td>Matrix Plus</td>
<td>Oracle, MS SQL Server, DB2</td>
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<tr>
<td>Baytek International, Inc.</td>
<td>WinBLISS</td>
<td>Oracle</td>
<td>Yes</td>
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<tr>
<td>Beckman Coulter, Inc.</td>
<td>LabManager iLIMS</td>
<td>Oracle</td>
<td>Yes</td>
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<tr>
<td>Blaze Systems Corporation</td>
<td>BlazeLIMS</td>
<td>Oracle, MS SQL Server</td>
<td>Yes</td>
<td><a href="http://www.blazessystems.com">www.blazessystems.com</a></td>
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<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>
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<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>
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<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>
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<tr>
<td>LabVantage Solutions</td>
<td>LV LIMS, Sapphire Edition</td>
<td>Oracle, MS SQL Server</td>
<td>Yes</td>
<td><a href="http://www.labvantage.com">www.labvantage.com</a></td>
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<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>
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<td>L.I.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>
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<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>
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<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>
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<tr>
<td>Thermo LabSystems, Inc.</td>
<td>Sample Manager, Nautilus</td>
<td>Oracle</td>
<td>Yes</td>
<td><a href="http://www.thermolabsystems.com">www.thermolabsystems.com</a></td>
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<tr>
<td>Zumatix Inc.</td>
<td>Matrix Plus</td>
<td>Oracle, MS SQL Server, DB2</td>
<td>Yes</td>
<td><a href="http://www.zumatix.com">www.zumatix.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

http://localhost:8080/lims?lims=true [Laboratory Analyst] LIMS DemoV6: LabWare LIMS - Windows Internet Explorer

General LW Sample Login Template

- Num. Samples: 1
- Edit Tests: ✓

Enter Results: □
Attendance: □
Label: □

Sample Type: POLYETHYLENE
Grade: Manufacturing Limits
Sampling Point: NONE
Description: Routine Sample

Customer Name: ACME
Charge Code: 93-83743
Priority: 2
Price List: □
Project: □
The LabSoft LIMS Microbiology
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/
Welcome to the UMC

The Uppsala Monitoring Centre (the UMC) is the field-name of the WHO Collaborating Centre for International Drug Monitoring. The UMC is responsible for the management of the WHO Programme for International Drug Monitoring. An independent centre of scientific excellence, the UMC offers a range of products and services, derived from the WHO Global Individual Case Safety Report (ICSR) database, from healthcare providers and patients in member countries of the WHO Programme. There is no other official body with as independent and global perspective on drug safety as the WHO and its Collaborating Centres, the UMC.

We provide essential resources for regulatory agencies, health professionals, researchers, the pharmaceutical industry.

Activities of the UMC include:

- co-ordinating the WHO Programme for International Drug Monitoring
- collecting, assessing and communicating information from member countries about the benefits, harms, effectiveness and risks of drugs
- collaborating with member countries in the development and practice of pharmacovigilance (Click for WHO definition of pharmacovigilance)
- alerting regulatory authorities of member countries about potential drug safety problems via the WHO signal process

We welcome contact from those involved or interested in drug safety and public health in academia, government, NGOs and the pharmaceutical industry.

Message from the Director

Click here for the latest quarterly message from Marie Lindquist.
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 a LIMS system from any other large system deployed on the web?
A question

- Q: What distinguishes a LIMS 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 LIMS, 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 LIMS activities
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?