

# Design and Testing of Laboratory Instruction Management System (LIMS)



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Laboratory Integration Management Solution (LIMS) is a software/hardware system which is used in industrial laboratories for the integration of all laboratory software and instruments, training laboratory users, QA and QC. LIMS may also support data mining, data analysis, and decision making. In this project, we propose to introduce Laboratory Instruction Management System thus redefining the acronym LIMS.

In chemistry educational laboratories, paper based laboratory notebooks and paper reports create an obvious bottleneck. They take hours of student's time; they also overload the instructor with enormous amount of reading (40 - 60 pages of a notebook with multiple attachments plus over 100 pages of reports per student per semester). Purchasing paper notebooks and printing supplies dramatically increases the education costs. All these expenses, both time-related and financial, can be eliminated or at least dramatically reduced by implementation of LIMS. Electronic notebook was designed to replace traditional, paper-based methods of documentation. Students plan and document all aspects of an experiment from execution to results; laboratory instructions will be incorporated into a template and adjusted at time of preparation for a new lab experiment. Report preparation can be simplified by integrating with existing data acquisition system to reduce clerical errors and provide the ability to search on previous experimental results.

The obvious challenge is the necessity of incorporating numerous instruments controlled by various types of microprocessors and devices running different operating systems (various versions of Windows, Linux, Android, and iOS) with wired and wireless connection. Concurrently, the user interface must be simple and easy to learn in order to direct student attention towards studying the subject (in our case - various chemistry disciplines) and not spending extra time on learning software. Special challenge is coming from use of non-electronic devices, e.g. traditional glass burets and pipets. We study and discuss the ways to overcome this obstacle. A number of data acquisition software options were employed: NI Labview, Vernier LoggerPro, home-made macros for Excel, as well as proprietary programs from instrumentation manufacturer. In addition to professional cameras, several types of smart phones and tablets were tested for image and video recording. The resulting report format was a PDF file with appropriate link to data analysis files and raw data in electronic notebook.

The system was tested with participation of students from Analytical Chemistry and General Chemistry classes in 2012 - 2013.

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M.S.Goodman, K.F.Jonmaire, and A.Y.Nazarenko. Contemporary Undergraduate Qualitative Analysis: Use of CCD-Based Raman, Atomic Emission, and Reflectance Spectrometers. Spectroscopy Letters 40, 253-463(2007)

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## Digital manual (lab instructions, images, video)

4. Start data collection (Click on "Collect" icon) and observe the falling temperature of the molten solvent. Gently stir the liquid with the probe during the period of cooling. The temperature should level off as the solvent begins to crystallize. Record this freezing-point temperature ( $\pm 0.1^\circ\text{C}$ ) for your data. Note that you may have some jump of the temperature because of supercooling.

5. In the window data, click at "Store latest run".

6. Repeat steps 3-5. Calculate an average freezing-point temperature ( $\pm 0.1^\circ\text{C}$ ) and an average deviation ( $\pm 0.1^\circ\text{C}$ ) for your data. Do not forget to click on "Store latest run" before the next run.

Na Sodium atoms emit light at 589 nm coloring the flame to yellow. Use a clamp to hold the fiberoptic light input in place, make sure that it is pointing directly at the flame. Dip a wire into the Sodium solution and hold it above the burner. The Sodium should immediately begin burning. Remember to save the resulting spectrum. Your spectrum should look something like this:

is the indication of  $\text{Co}^{2+}$ :  
 $\text{Co}(\text{NCS})_2$

Attention: the  $\text{Fe}^{3+}$  ions need to be masked by NaF while  $\text{Cu}^{2+}$  ions.

**NI.** A very selective reaction for Ni(II) determination is known for the complex compound:

$$2 \text{Ni}^{2+} + 4 \text{OH}^- + 2 \text{C}_6\text{H}_8\text{N}_2\text{O}_2 \rightarrow \text{Ni}_2(\text{C}_6\text{H}_8\text{N}_2\text{O}_2)_2 + 2 \text{H}_2\text{O}$$

$\text{Ni}^{2+}$ : To several drops of unknown, add some tartaric acid, dimethylglyoxime aqueous ammonia. Drops of ammonia solution must go by the wall of the glyoximate appears.

## Digital notebook template (e.g., Excel or PDF form)

Worksheet for exercise on measurement uncertainty in pipetting

Fill the table with your data

Sample No.	Volume (mL)	Mass (g)	Density (g/mL)
1	10.00	10.00	1.000
2	10.00	10.00	1.000
3	10.00	10.00	1.000
4	10.00	10.00	1.000
5	10.00	10.00	1.000
6	10.00	10.00	1.000
7	10.00	10.00	1.000
8	10.00	10.00	1.000
9	10.00	10.00	1.000
10	10.00	10.00	1.000
11	10.00	10.00	1.000
12	10.00	10.00	1.000
13	10.00	10.00	1.000
14	10.00	10.00	1.000
15	10.00	10.00	1.000
16	10.00	10.00	1.000
17	10.00	10.00	1.000
18	10.00	10.00	1.000
19	10.00	10.00	1.000
20	10.00	10.00	1.000
21	10.00	10.00	1.000
22	10.00	10.00	1.000
23	10.00	10.00	1.000
24	10.00	10.00	1.000
25	10.00	10.00	1.000
26	10.00	10.00	1.000
27	10.00	10.00	1.000
28	10.00	10.00	1.000
29	10.00	10.00	1.000
30	10.00	10.00	1.000

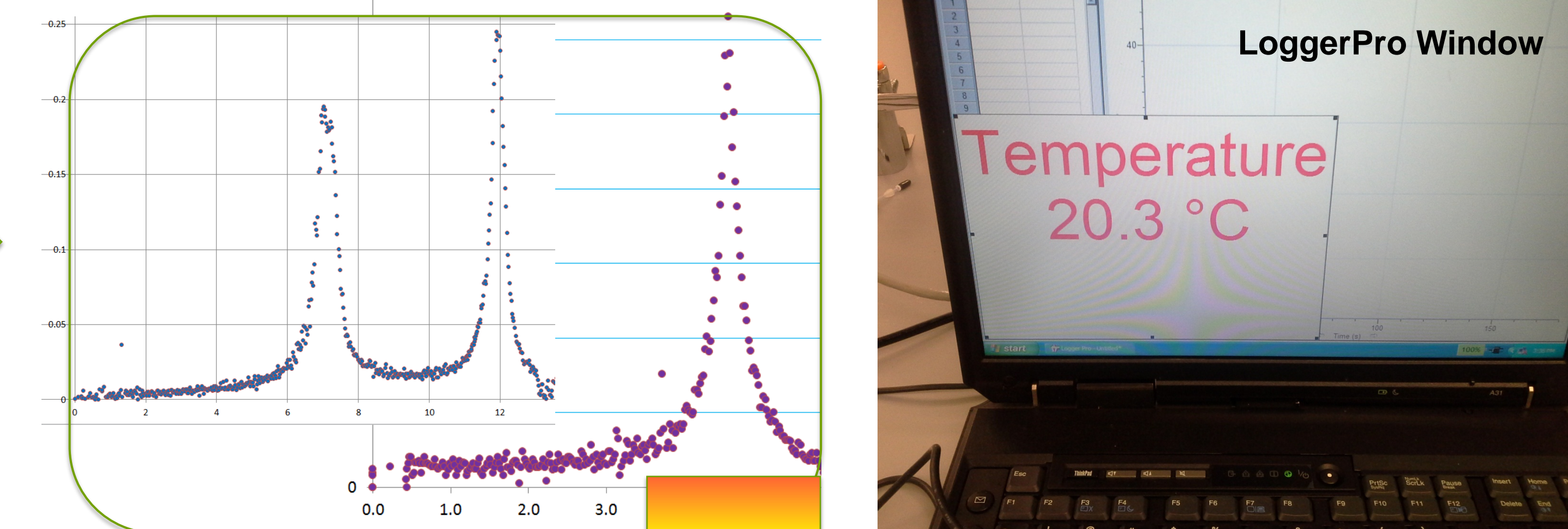
Worksheet for exercise on measurement uncertainty in pipetting

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7	10.00	10.00	1.000
8	10.00	10.00	1.000
9	10.00	10.00	1.000
10	10.00	10.00	1.000
11	10.00	10.00	1.000
12	10.00	10.00	1.000
13	10.00	10.00	1.000
14	10.00	10.00	1.000
15	10.00	10.00	1.000
16	10.00	10.00	1.000
17	10.00	10.00	1.000
18	10.00	10.00	1.000
19	10.00	10.00	1.000
20	10.00	10.00	1.000
21	10.00	10.00	1.000
22	10.00	10.00	1.000
23	10.00	10.00	1.000
24	10.00	10.00	1.000
25	10.00	10.00	1.000
26	10.00	10.00	1.000
27	10.00	10.00	1.000
28	10.00	10.00	1.000
29	10.00	10.00	1.000
30	10.00	10.00	1.000

## Instructor Input and Corrections

## Digital Collection and Processing (e.g., LabView, LoggerPro, Collect6.1)



## Automatic Report Creation (e.g., PDF)



Chromatography/Mass Spectrometry with network data transfer instead of manual separations



Electronic balances with RS-232 or USB instead of manual read

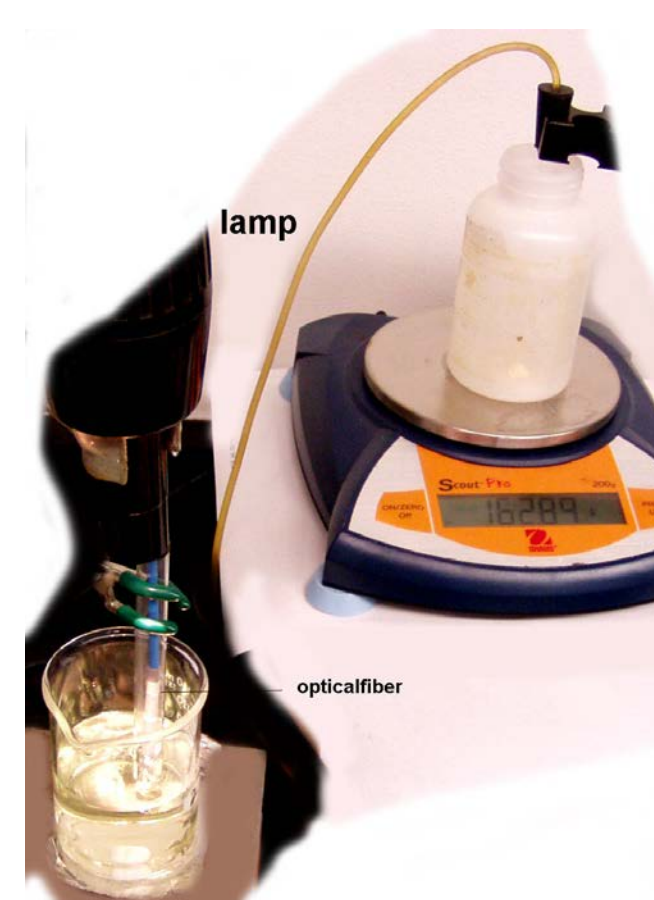


Electronic titrators with RS-232 or USB instead of glass buret



Thermogravimetric Analysis with RS-232 instead of manual gravimetry

Home-made automatic electronic titrators with RS-232 or USB instead of glass buret



THANKS:

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