Getting started with an Electronic Laboratory Notebook

Second edition

John Trigg

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This guide, *Getting started with an Electronic Laboratory Notebook*, is written by John Trigg, and published jointly by *Scientific Computing World* magazine and phaseFour Informatics.

ABOUT *SCIENTIFIC COMPUTING WORLD*

Now in its 16th year of publication, *Scientific Computing World* is Europe's only publication dedicated to the computing and information technology needs of professionals working in science, technology, engineering, and medicine. Published in print and electronic media, it covers all aspects of computing, focusing particularly on laboratory informatics, and computing in engineering, chemistry, physics and life sciences.

Associated with the print magazine are: *SCNewsline*, a monthly emailed newsletter that keeps thousands of scientists and engineers in regular touch with breaking news in technology, research, and the business world as it affects scientific computing; the website, www.scientific-computing.com, which carries web-exclusive material, including reviews of scientific software and which is updated daily; and the annual *Laboratory Informatics Guide*, which provides a year-round reference tool for those involved in laboratory informatics, and in particular Laboratory Information Management Systems (LIMS) and Electronic Laboratory Notebooks (ELNs).

ABOUT PHASEFOUR

phaseFour Informatics Limited is an independent consulting practice, based in London, specialising in the ELN and knowledge management market. Its services are targeted at laboratories seeking to enhance performance by deploying strategic solutions to address technology, process and cultural requirements. Services include:

- Providing business justifications.
- Defining user requirements.
- Preparing and reviewing RFPs.
- Preparing a strategy for a successful deployment.
- Addressing cultural and behavioural practices.
- Running short courses, seminars and workshops.

ABOUT THE AUTHOR

John Trigg is director of phaseFour Informatics. Previously, he was the IT manager for the Kodak European Research Laboratories. He has more than 20 years' experience working in the field of R&D data, information and knowledge management, including 10 years' experience of the world's first enterprise level implementation of an ELN in the Eastman Kodak Company. John is author of a number of publications on ELNs and knowledge management in the laboratory, and has presented papers and run workshops at conferences in the UK, Ireland, Germany, USA and Australia. John is currently the chairman of the Automation and Analytical Management Group of the Royal Society of Chemistry. John was the recipient of the 2000 International LIMS Award.

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This short guide provides a brief background to Electronic Laboratory Notebooks with a specific focus on the factors that need to be taken into consideration when undertaking a project to transition from the bound paper laboratory notebook.

The guide does not go in to great detail, as this can be readily obtained through various on-line resources, conference presentations, vendors and consultants. Furthermore, in an era of constant change, the incorporation of too much detail could mean that the guide would rapidly become out of date.

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The 2nd edition contains updates to Chapter 3 – Industry Evolution, and Chapter 6 – Information Technology Considerations.

John Trigg
phaseFour Informatics

1. Introduction

Computers and information technology have penetrated almost every aspect of laboratory work over the past few decades, but even today, scientists still turn to the bound paper notebook, a pen, scissors and adhesive tape to fully document their experiments in a way that is compliant with legal and regulatory requirements, and that meets their corporate directives for intellectual property protection. However, the continued use of a reliable, convenient and trusted medium such as paper has its drawbacks too. In an age where the rapid dissemination of information is considered fundamental to collaboration and team-working, and where easy access to existing information is essential, the right information technology infrastructure, the right tools and the right processes are critical enablers to support the creation, sharing and re-use of an organisation's explicit knowledge.

Electronic Laboratory Notebooks (ELNs) have become a highly topical subject in laboratory environments over the past few years. On the one hand, it may seem surprising that at the start of the 21st century, the bound paper laboratory notebook is still the medium in which most experiments are documented, but on the other hand, there are some important reasons why the move away from paper has been treated with a good deal of caution. However, there is a growing trend towards implementing an electronic solution for documenting experiments, based on
(a) expected productivity gains and
(b) an enhanced approach to managing scientific knowledge.

The argument for an electronic solution is becoming increasingly powerful as one by one the objections to the transition from paper to electronic weaken. So what are the major objections? Basically they can be considered to fit into three different categories. Firstly, from a business perspective, there have been concerns about the admissibility of electronic records in support of patent interferences and patent infringements. There are concerns about the costs associated with an electronic solution, and in some instances there may be concerns regarding compliance issues. Secondly, from a technology perspective, there has been, and still exists, a certain amount of doubt about the available technologies that are able to preserve electronic records over the long term. And thirdly, from a user perspective, there is the worry about change management and the impact upon scientists of replacing an established and proven documentation process.

TRADITIONAL FUNCTIONS OF LAB NOTEBOOKS

- **Record ideas**
- **Inventions**
- **Experimentation records**
- **Observations**
- **Work details**

THE LABORATORY NOTEBOOK CAN HELP YOU PROVE:

- **Exact details and dates of conception**
- **Details and dates of reduction to practice**
- **Diligence in reducing your invention to practice**
- **Details regarding the structure and operation of your invention**
- **Experimentation observations and results**
- **A chronological record of your work**
- **Other work details**

2. What is an ELN?

In its simplest form, an ELN can be considered to be a direct replacement for the paper lab notebook. In this instance, it can provide the generic functionality to support 'broad' documentation processes that apply to all scientists, such as patent evidence creation, cross discipline collaboration and general record keeping. However, the integration capabilities that we readily associate with information technology raise the possibility of a tighter coupling of other laboratory systems into the ELN. In other words, can the information that is currently printed from other laboratory systems, cut out and pasted into the paper lab notebook be electronically entered or linked into the ELN? For example, systems that provide chemical structure drawing, structure and sub-structure searching, compound registration, etc. are an integral part of the chemistry laboratory's process, and therefore would be expected to become part of an electronic solution. Similarly, other scientific disciplines will have specific requirements consistent with their particular laboratory processes. Figure 1 illustrates the relationship between 'broad' (generic) and 'deep' (specific) systems. Another way of looking at this is to define an information structure (see Figure 2) that identifies how different systems fit into the laboratory architecture. The triangle represents the different layers of abstraction that exist in R&D information flows. These are almost always handled by different systems. Above the experimental layer is a management context that is handled by traditional IT tools that are used elsewhere in the enterprise. Cross discipline collaboration tends to happen around the experiment layer. Below the experiment level there is an increasing specialisation of data types and tools, and only a few systems are comfortably deployed across workgroups.

From a patent perspective, the experimental layer is crucial as it captures what the scientist is thinking and doing, and therefore will provide the evidence of conception and reduction to practice of the 'invention'. In broader Intellectual Property (IP) terms, it is the experiment layer that constitutes a record of the laboratory's work and as such contributes to the scientific knowledge repository. While this repository resides on paper, the ability to access, collaborate and share scientific knowledge is constrained. The implementation of an ELN therefore offers a significant opportunity to bring about greater efficiencies in these processes.

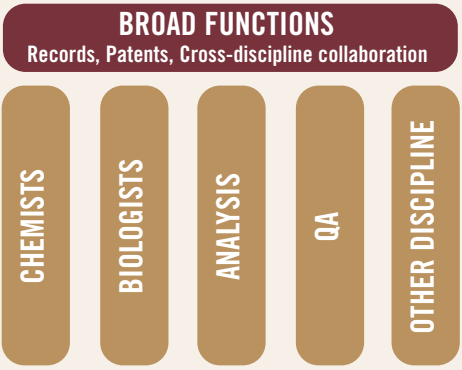

FIGURE 1
Broad vs. Deep

The generic function of an electronic laboratory notebook supports the 'experimentation' layer, and contains abstractions from the lower data levels. So in terms of 'what is an ELN?', the CENSA[1] definition, *'a system to create, store, retrieve, and share fully electronic records in ways that meet all legal, regulatory, technical and scientific requirements'* is all encompassing, and can therefore mean different things to different scientists. For this reason, a clearly defined understanding of the role that the ELN is going to play in a given organisation is absolutely essential at the start of an ELN project.

An ELN can therefore serve the organisation in two ways: firstly, it can take advantage of the capabilities of IT to improve the ability to acquire, manipulate, share and store data (productivity). Secondly, it can provide a scientific knowledge repository that can be easily accessed to recover records of the laboratory's work (content/knowledge management).

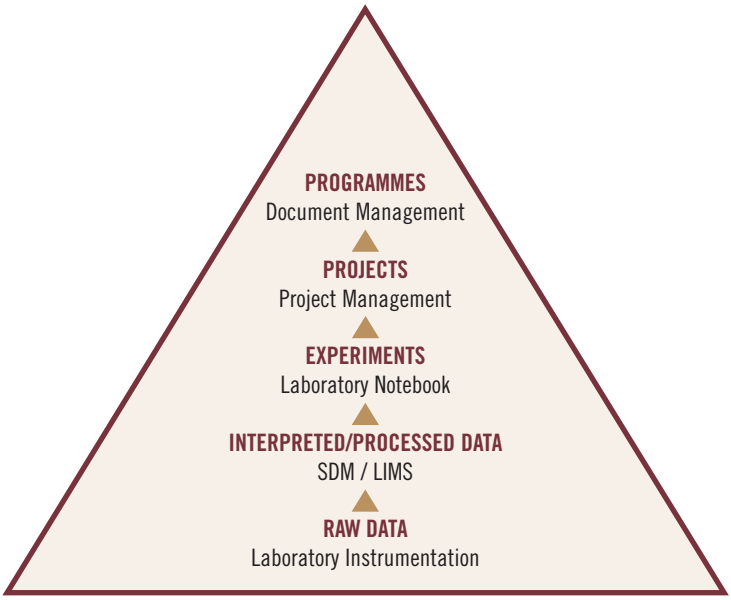

FIGURE 2 Information Structure

AN ELN SYSTEM (LIKE THE BOUND LABORATORY NOTEBOOK) HAS A NUMBER OF POTENTIAL ROLES:

- **A place to do science – a working environment**
- **A place to write up the experimental work**
- **A record of the work**
- **A long-term preservation mechanism**

It is important to separate out these roles because:

- **One solution is unlikely to do it all**
- **Most companies will already have a significant investment in specific tools.**