The Evolution of LIMS, ISO 1578 and the Future of Laboratory Informatics

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Instrument Data

Field Data Capture

ELN

ISO E1578

LIMS

TNI Requirements

AI

Cloud Computing

SDMS

Document Control

Software Compatibility

Databases

Machine Learning

TNI Requirements

4.1.5, 4.13.3 and

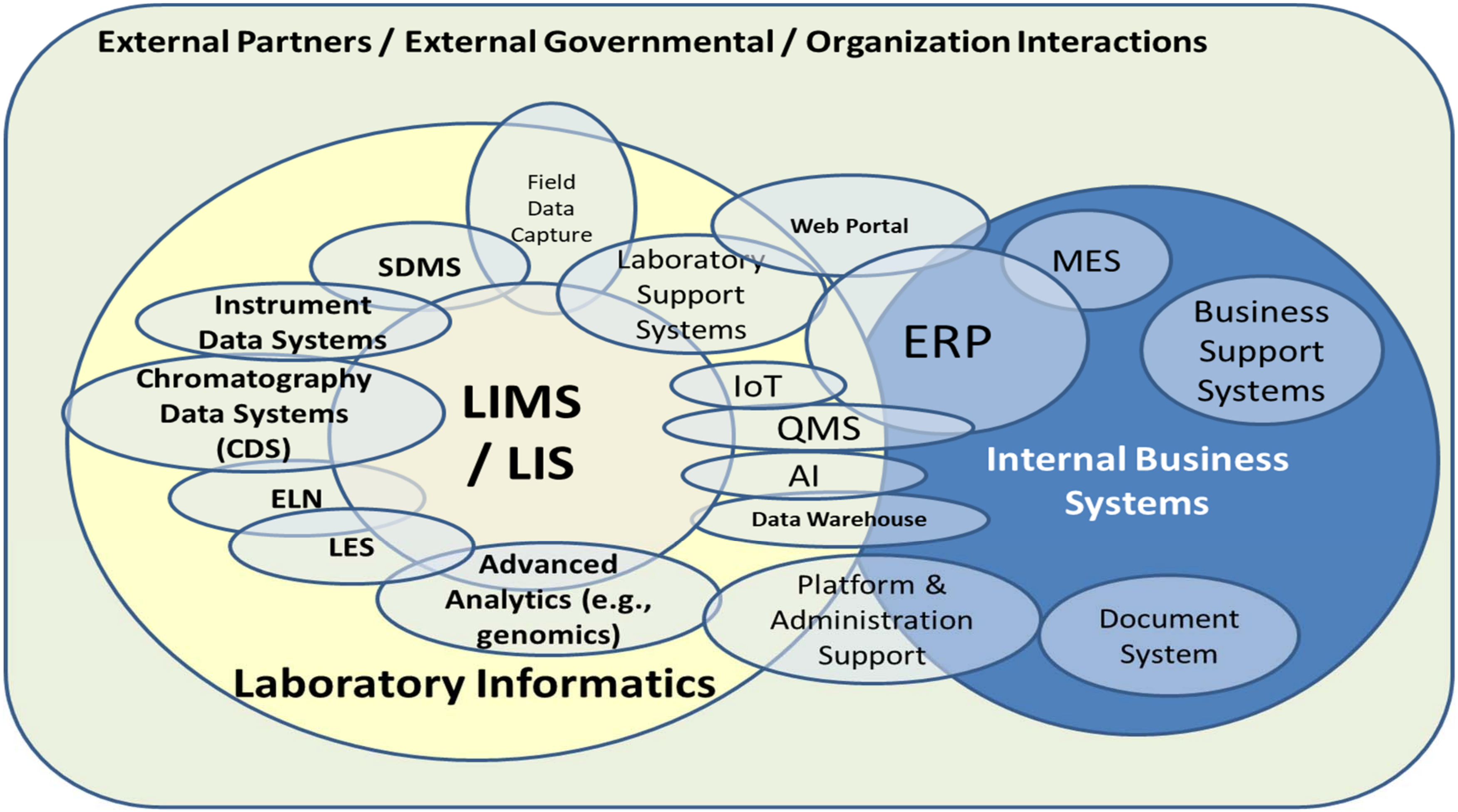
5.4.7 Control of Data *(ISO/IEC 17025:2005, Clause 5.4.7)*

5.8.2, 5.8.5, and 5.8.7.3

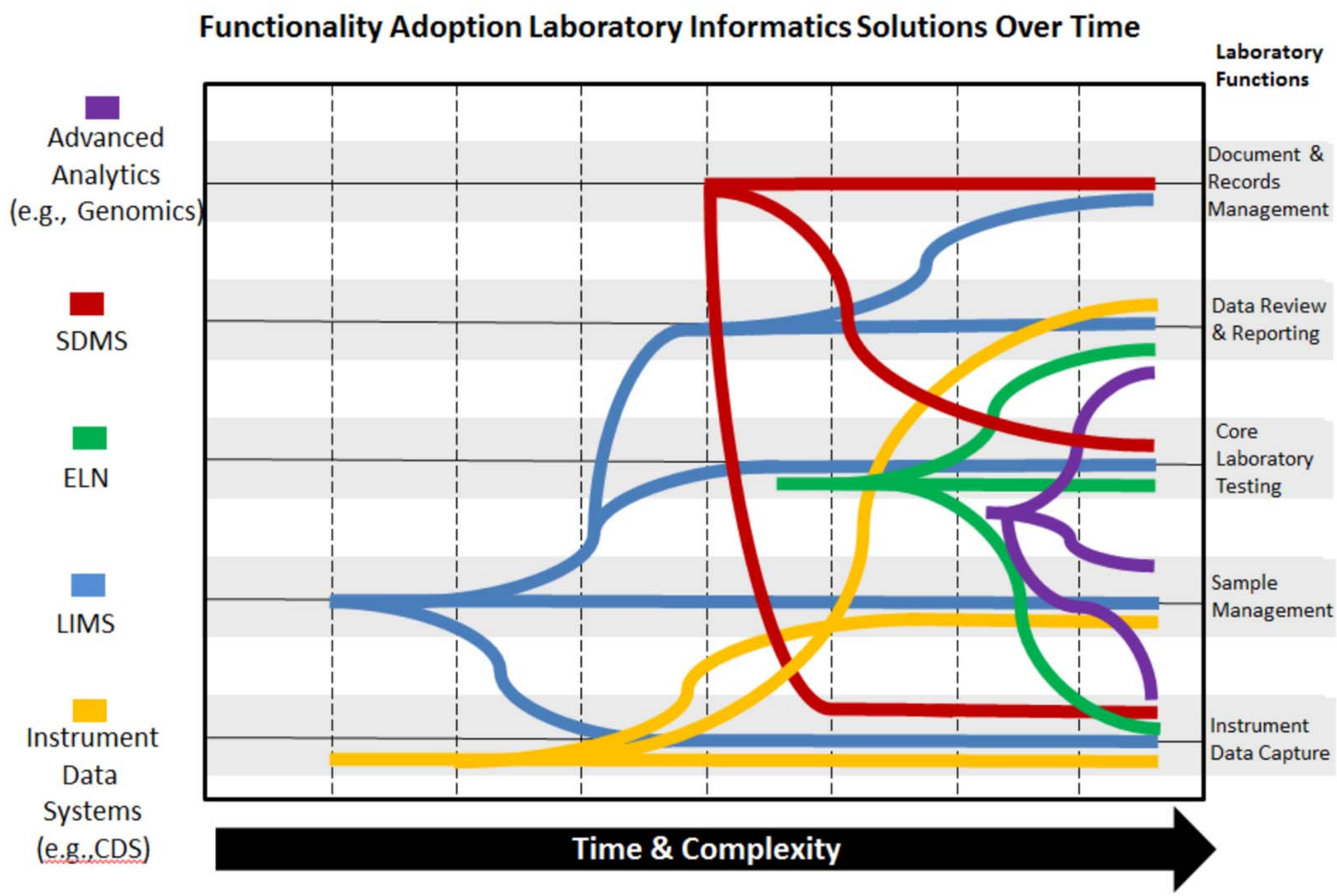
ISO E1578 – 13 Laboratory Informatics

1. Scope

1.1 This guide helps describe the laboratory informatics landscape and covers issues commonly encountered at all stages in the life cycle of laboratory informatics from inception to retirement. It explains the evolution of laboratory informatics tools used in today's laboratories such as laboratory information management systems (LIMS), laboratory execution systems (LES), laboratory information systems (LIS), electronic laboratory notebooks (ELN), scientific data management systems (SDMS), and chromatography data systems (CDS). It also covers the relationships (interactions) between these tools and the external systems in a given organization. The guide discusses supporting laboratory informatics tools and a wide variety of the issues commonly encountered at different stages in the life cycle. The sub-sections that follow describe the scope of this document in specific areas.



External Partners / External Governmental / Organization Interactions
Field Data Capture
Web Portal
SDMS
Laboratory Support Systems
MES
Instrument Data Systems
ERP
Business Support Systems
Chromatography Data Systems (CDS)
LIMS / LIS
IoT
QMS
Internal Business Systems
AI
ELN
Data Warehouse
LES
Advanced Analytics (e.g., genomics)
Platform & Administration Support
Document System
Laboratory Informatics



Functionality Adoption Laboratory Informatics Solutions Over Time
Laboratory Functions
Advanced Analytics (e.g., Genomics)
SDMS
ELN
LIMS
Instrument Data Systems (e.g.,CDS)
Document & Records Management
Data Review & Reporting
Core Laboratory Testing
Sample Management
Instrument Data Capture
Time & Complexity

Additional Functions Required by Laboratory Types		**Laboratory Functional Area**					
		Sample / Experiment Management	**Lab Testing**	**Review, Verification Approval**	**System Integration**	**Reporting and Trending**	**Other Functions**
Laboratory Type	**General Laboratories**	Chain of custody	Batch Processing of Samples including QA		ELN, SDMS, instrument integration	Electronic Reporting of QC Results	
	Environmental	Container management, Chain of custody, regulatory compliance - significant auxiliary data	Batch Processing of Samples including QA	Multiple levels of review and approval	GIS integration	Electronic Reporting of QC Results by batch	Method QA/QC, Calculation validation, electronic data delivery
	Public Health Sector- (clinical microbiology and chemical)	Chain of custody, electronic test ordering, Emergency response, public health surveillance	Batch Processing of Samples including QA, agent regulations	Multiple levels of review and approval, CLIA certification	Emphasis on surveillance at multiple state and federal levels	Electronic Reporting multiple data formats, vocabulary, and secure transport	Clinical and non-clinical, sample centric and patient centric
	Life Sciences	Controlled substances Stability samples	Uniformity Calculations Product Specifications	Multiple levels of review and approval	ERP integration	SPC and Process variability analysis	Instrument maintenance and calibration tracking
	Food and Beverage	Lot geneology	Product Specifications		MES and ERP integration	SPC and Process variability analysis	Exception Reporting
	Heavy Industry	Automatic scheduling, Lot Management	Product Specifications		Process Control / PM integration	SPC and Process variability analysis	
	R&D	Experiment sharing	Method versioning		ELN, SDMS, instrument integration	Experiment Conclusions, Technical Reports	Expanded Search capability
	Medical Laboratory	Embedded LIS Standalone LIS Niche LIS Patient centric			interface engines to external systems	Unique functions Diagnostic and Surveillance	electronic medical records; direct clinician access, billing modules

Specific to Environmental

Increasing use of ELNs
Importation of more field data/GIS
Improved integration with other software platforms like SDMS
Web portals becoming commonplace
Instrument data/imports
One-offs & data points that do not fit – explanations or non-conformance required

IoT (Internet of Things)?

Increase in automation - QA/QC
- Artificial Intelligence

What about machine learning?

IoT by definition is:

3.2.14 *Internet of things, IoT, n*—a system of objects—computing devices, machines, objects, people, animals, etc.—that can connect to a network and communicate among themselves, often without human intervention. An *IoT device* is an object operating within that system.

Artificial Intelligence by definition is:

3.2.1 *artificial intelligence, AI, n*—a behavior by machines or computers versus the natural intelligence of humans and animals.

3.2.2.1 *Discussion*—In the computer science arena, any device that perceives its environment and takes action to maximize success in achieving a goal is exhibiting AI...

Examples

Total Nitrogen – total kjeldahl nitrogen (ammonia, organic and reduced nitrogen) plus nitrate-nitrite
- checks to make sure parts are not greater than total

ICP-OES interference – B/Fe, As/Cd; programmed checks/flags at various concentrations

Specific Queries – Method 245.1 before Method 1631

GC-MS interferences – generally drug related testing/false positives and negatives

Application of user notifications to move forward before finalizing data

Application of flags in an automated fashion

Temperature adjustments

Machine Learning:

Machine learning is an application of artificial intelligence that provides systems the ability to automatically learn and improve from experience without being explicitly programmed. (ISO E1578)

Machine learning (**ML**) is the scientific study of algorithms and statistical models that computer systems use in order to perform a specific task effectively without using explicit instructions, relying on patterns and inference instead. It is seen as a subset of artificial intelligence. Machine learning algorithms build a mathematical model based on sample data, known as "training data", in order to make predictions or decisions without being explicitly programmed to perform the task. (Wikipedia)

- Data mining is a field of study within machine learning.

Linked Software

SDMS
Sampling Software
Reporting Packages (Level IV, etc.)
Instrument Software
ELNs
Excel/Any Spreadsheet Program
Compliance Tracking and Industrial Pretreatment Software
Automated Backup Software (SQL or Oracle)
Confident Cannabis
Accounting Packages
Freezer/Incubator Software
Etc...

“Other” software package questions

Instrument Software – should the instrument software do the calculation and then provide the LIMS finalized data or should the LIMS handle the calculations? Always import or give the analyst a chance to override?

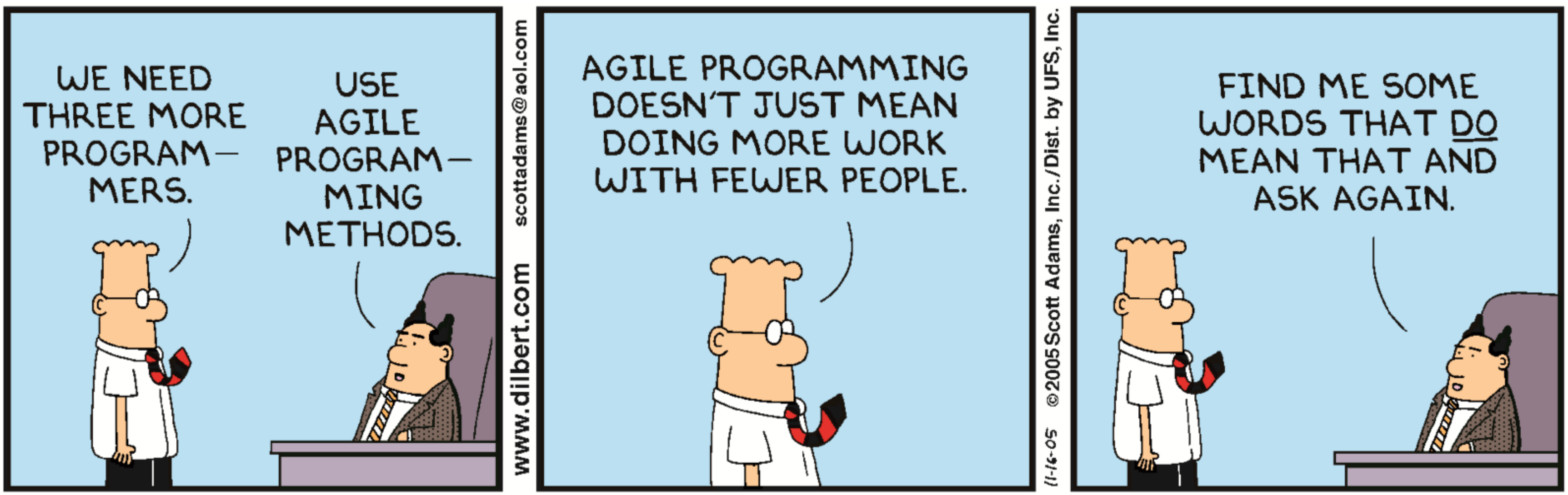
SDMS – should the quality control be within the LIMS itself or handled by the SDMS before importing into a LIMS? Case by case?

Sampling Software – what data should the LIMS bring in and record? What is really required versus possibly desired? Should sample tracking just be handed to the LIMS?

Should backend data (raw data) from the LIMS be available for calculations and manipulation outside of the LIMS itself in Excel or other statistical programs?

What may need to be customized (i.e. programmed) and what can be customized to fit a LIMS?

Keep in mind, in every Informatics company everywhere... Everything has a cost...



Changing of the guards!

Younger generations are more computer savvy.

Younger generations less inhibited by the “old ways”.

Internet access to our retirement accounts is expected but lab data is protected?

Sometimes, the old ways are best. Age guards against mistakes.

Where does validated, good data blend perfectly with lab informatics and where do things get fuzzy?

So…

LIMS and other lab informatics do a LOT!

LIMS and other informatics could do more and will do more.

So, pretending $$$ was not a limiting factor, then...What else do we want our lab informatics to do?

So Then…

At what point do we, as chemist/analyst and managers want to LIMIT what LIMS and lab informatics can do?

Can AI & machine learning go too far? At what point is it appropriate to limit this functionality and assume more mistakes will happen based upon using AI/machine learning than mistakes in human hands?

Where is it all going now?

Open Discussion – Panel Answers

A lab geek turned auditor – Matt Sica

An EPA chemist pulled into the ring – Michelle Kerr

A chemist turned programmer – Bin Yu

A geologist turned CEO in a tech startup – Russell Schindler

And

A biologist turned LIMS salesperson – Robert Benz

We may not all be brilliant but we do offer a wide breadth of experience in lots of different areas!

What's next?

Where do we go from here?

Embrace AI?

What's too far?

Trust the human?

Updates

IT Security

IT

VS

Chemist

Standalone pieces or complete integration?