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Preface

Dear Participants,

Confronted with the ever-increasing complexity of technical processes and the growing demands on their efficiency, security and flexibility, the scientific world needs to establish new methods of engineering design and new methods of systems operation. The factors likely to affect the design of the smart systems of the future will doubtless include the following:

- As computational costs decrease, it will be possible to apply more complex algorithms, even in real time. These algorithms will take into account system nonlinearities or provide online optimisation of the system's performance.
- New fields of application will be addressed. Interest is now being expressed, beyond that in "classical" technical systems and processes, in environmental systems or medical and bioengineering applications.
- The boundaries between software and hardware design are being eroded. New design methods will include co-design of software and hardware and even of sensor and actuator components.
- Automation will not only replace human operators but will assist, support and supervise humans so that their work is safe and even more effective.
- Networked systems or swarms will be crucial, requiring improvement of the communication within them and study of how their behaviour can be made globally consistent.
- The issues of security and safety, not only during the operation of systems but also in the course of their design, will continue to increase in importance.

The title "Computer Science meets Automation", borne by the 52nd International Scientific Colloquium (IWK) at the Technische Universität Ilmenau, Germany, expresses the desire of scientists and engineers to rise to these challenges, cooperating closely on innovative methods in the two disciplines of computer science and automation.

The IWK has a long tradition going back as far as 1953. In the years before 1989, a major function of the colloquium was to bring together scientists from both sides of the Iron Curtain. Naturally, bonds were also deepened between the countries from the East. Today, the objective of the colloquium is still to bring researchers together. They come from the eastern and western member states of the European Union, and, indeed, from all over the world. All who wish to share their ideas on the points where "Computer Science meets Automation" are addressed by this colloquium at the Technische Universität Ilmenau.

All the University's Faculties have joined forces to ensure that nothing is left out. Control engineering, information science, cybernetics, communication technology and systems engineering – for all of these and their applications (ranging from biological systems to heavy engineering), the issues are being covered.

Together with all the organizers I should like to thank you for your contributions to the conference, ensuring, as they do, a most interesting colloquium programme of an interdisciplinary nature.
I am looking forward to an inspiring colloquium. It promises to be a fine platform for you to present your research, to address new concepts and to meet colleagues in Ilmenau.

Professor Peter Scharff
Rector, TU Ilmenau

Professor Christoph Ament
Head of Organisation

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Data Management for Automated Life Science Applications

Laboratory information management systems (LIMS) have been established for supporting project management, process planning, evaluation, and long-term management of the results in life science laboratories. The conventional function of a LIMS is the database-supported management of all business process information which results from laboratory operations [1-3]. The complete system integration of a LIMS covers recent topics of automated, bidirectional data communication with an alterable process control layer in laboratories, embedded high-parallel High Throughput Screening (HTS) / High Content Screening (HCS) process tracking, secure e-business, as well as embedded or off-line post processing, data mining or ERP and quality management.

The stream of data is continuously growing as a result of increasing laboratory automation, high throughput experiments, and modern analysis methods. Therefore, the central, user-friendly management of these data is of crucial importance for quality assurance and information availability.

Current challenges for information management solutions of life science automation focus on:

- Demand-oriented, arbitrarily hierarchical flexible process mappings of interdisciplinary applications in changing automation environments
- Guarantee of a cost-efficient, complete horizontal and vertical operating automation
- Support of the global e-business in compliance with quality standards, legal regulations, as well as data security
- Accomplishment of the automatically generated data flood of high-parallel laboratory processes (HTS, HCS), inclusive support of analysis of experiments and information discovery

LIMS and electronic laboratory notebooks (ELN) are both used for mapping especially parts of sequential workflows of laboratories. For issues of data consistency, dedicated solutions of LIMS and ELN have to be coupled by using reliable synchronization algorithms. Our approach consequently assumes LIMS and ELN as integrated.

Flexible prozess hierarchie mapped different laboratory workflows completely

The presented LIMS supports the interdisciplinary character of experiments in life sciences by a free mapping of laboratory processes and parameter definitions. This is a demand from a R&D

LIMS particularly in fast changing automation environments. A hierarchical process mapping which flexibly adapts to manual and automated process structures, working tasks and workflow phases based on an open system and parameter concept. Thereby, freely definable parameters with arbitrary data structure secure adjustment flexibility and application independence of the LIMS for flexible laboratory automation.

Important structuring elements are a variable project classification hierarchy in any number of discretionary steps, parallel sequences oriented on laboratory reservoirs, processes, process steps, process parameters, structured process parameters, as well as parameter sequences based on structured process parameters for the coverage of asynchronous and synchronous records. Expectations to ELN can be considered by an extension of the parameter system with multimedia data types and adapted user interfaces sufficiently in the LIMS.

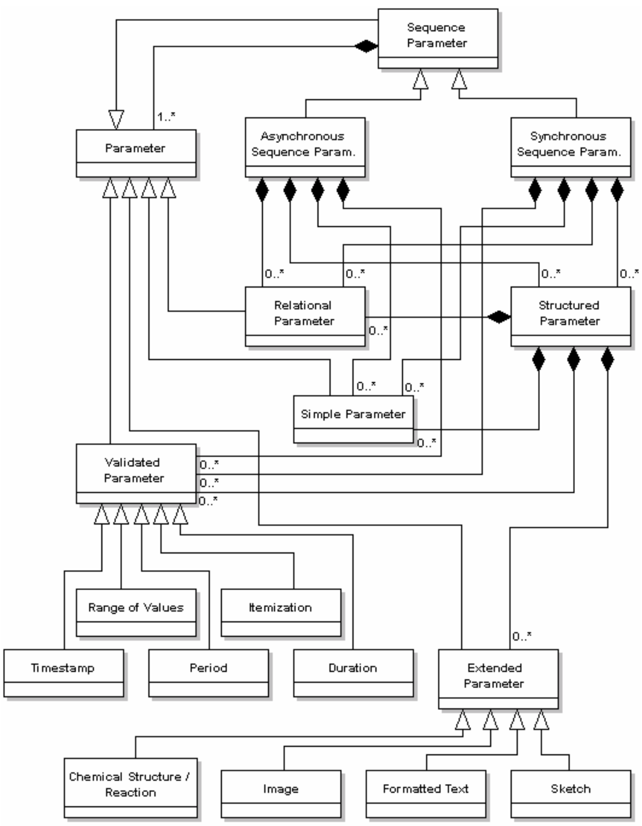

Figure 1 Parameter model of the presented LIMS

Figure 1 shows the class model of process parameters used in sequential and parallel activity structures to meet the requirements of comprehensive system integration within LIMS. Structured parameters can summarize for example multi-parameter data for individual measuring points (wells on microtiter plate or the like) or process variables and their meta-data (e.g., parameters of image acquisition, surroundings conditions, and process notes). Time series can be formed synchronously or asynchronously from any number of several parameters. Special data types offer particular user interfaces within LIMS: image browser for photos, integrated appropriate editors for the generation of sketches or formatted texts, tools for processing and search for specialized information like chemical structures, etc.

Automated communication between LIMS and laboratory instruments

The secure and efficient control of immense data amounts generated by drug discovery requires a bi-directional automated communication between LIMS and laboratory instruments (e.g., sensors, analytical devices, robot process control systems, cell handling systems). Therefore, a framework concept with lose coupling process mappings based on configurable fast process database coupling and XML communications for horizontal and vertical system integration of

LIMS is observed. The developed LIMS interfacing to laboratory processes is based on a configurable converter for syntax and semantic adaptation of an open process hierarchy for project master data up to structured multimedia-based measurement parameters [4].

Complete experiment documentation with integrated ELN

The complete documentation of the laboratory workflow combines all process parameter, measured values and results of the laboratory process supplemented to notes, documents, literature, etc. for a complex and consistent documentation, evaluation, as well as decision making. Figure 2 presents several user interfaces and information relations using an example of HTS experiments based on processes of plate positions.

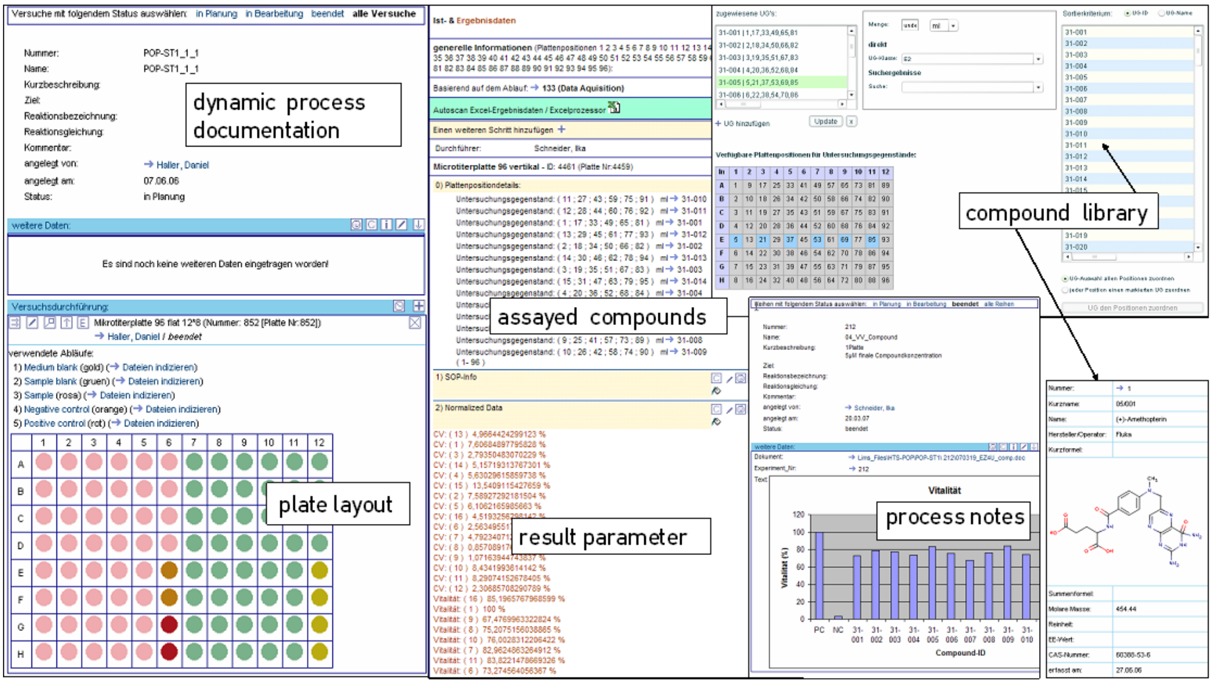

Figure 2 Complex experiment documentation within LIMS

Attached barcodes allow a complete sample tracking. Compounds from compound libraries, which are also managed in LIMS, can be used in the biological experiment. Therefore, these experiments are related to additional information like chemical attributes and chemical structures. The management of compound libraries is supported by integrating special applications for drawing, showing, and searching of chemical structures.

The integrated ELN functionalities (text and graphic editor, including pen computing) allow the storage of unstructured data at any point within the hierarchical documentation as done in usual paper based laboratory notebooks. The electronic documentation of the development including motivations for methods and parameters is available for other team members and secures long-term reproducibility.

These functionalities are complemented by a flexible data processing option for operative using of mathematical and logical algorithms between workflow parameters and process variables based on a spreadsheet oriented processor. Free programmable calculation templates link inputs from LIMS or laboratory instruments in terms of a complex instruction of mathematical and logical instructions to outputs which are new data sets within LIMS. This concept creates a self-consistent calculation process which can be automatically executed by a task manager of compatible operating systems on the server side.

Data reduction by selection

Keeping the overview and the detailed analysis of these immense, miscellaneous data amounts can become the bottleneck. The diversity and complexity of mapped process data can result in losing clarity of process documentation. Therefore, another main focus is the supply of far-reaching possibilities for data selection, data verification, and information visualization, as well as information supply by using standardized interfaces.

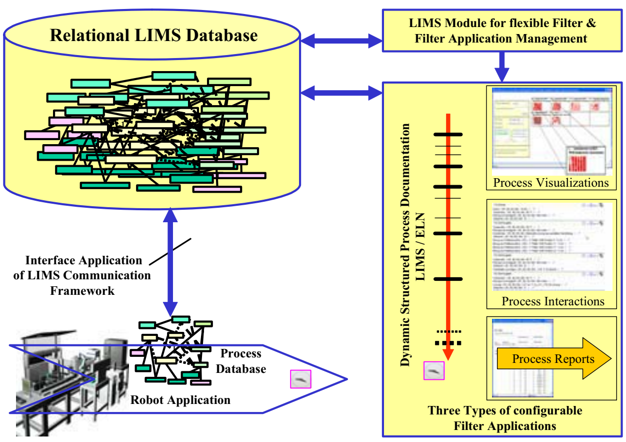

Figure 3 Architecture of a filter- and filter application management

An adaptive filter concept (figure 3) allows a user-defined selection of process parameters in the flexible process documentation and a combination with different applications for visualization and reporting. The applied LIMS generates user interfaces or output routines depended of filter definitions within the process hierarchy. Important configurable types of filter application are embedded process visualizations, interactive user interfaces of process documentation, and reporting tools.

Visualizations, reports and interfaces

The direct communication with the laboratory devices allows ad hoc generated process visualizations for fast process tracking as well as automated import of primary and calculated data from the devices. Embedded interactive visualizations with abstraction degrees can offer optimal support to extract all relevant information from the primary data for further decisions as soon as possible [5]. Topics of visual analysis method can be the exploration of process data, the comparison of process values, correlation, identification of hits or errors as well as keeping the overview. Manifold visualization techniques for nominal valued (plate layout down right in figure 4) and numerical data are integrated in the concept of user configurable filter application. The quality of experiment results can be conceived fast and supports time near decisions on following experiments (e.g., identification of hits of luminescence in primary screening data for secondary screening experiments, as shown in the middle of figure 4). Figure 4 presents also the visualization of several process variables (here luminescence and incubation times). One up to six parameters per well of a microtiter plate (MTP) or a virtual MTP can be displayed in this manner for a comparing or uncovering correlations.

Another well-known visualization technique of process data are trend curves for time series. Further methods can expand this concept [6], in particular HCS analyses are assisted with configurable image browser.

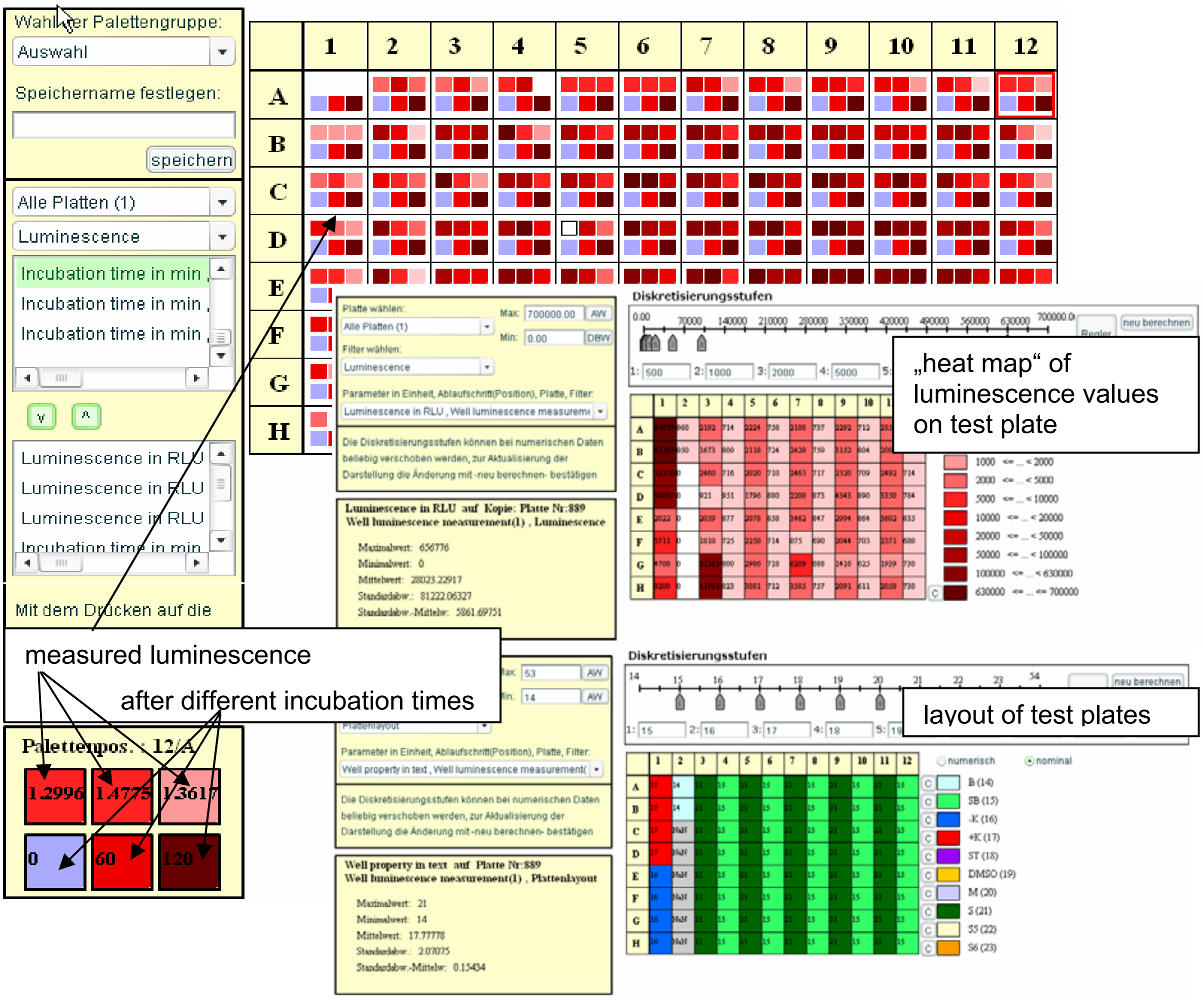

Figure 4 Visualization of experiment results based on microtiter plate format for overview and comparison

Process reports accumulating for post processing examined data records are a further example for system integration. These reports are made available by LIMS via standardized interfaces (XML, data bases, text, or csv file format), including automated communication for external processing to facilitate detailed analysis or presentations.

Conclusion

Complex and flexible laboratory automation requires adaptive laboratory information management systems and an according LIMS system integration. Therefore, the direct, automated, and bi-directional communication between LIMS and laboratory components is key to secure and efficient control of generated data.

Fast process tracking embedded in LIMS creates a new integration level for process control systems. Process data filters and modern scientific data visualizations are components in a flexible concept for the integration of diverse applications.

The achieved scalable and flexible process mapping in a web-based LIMS ensures the performance of arbitrarily challenging obligations to documentation and evidence as well as a high system availability in cooperation networks which also includes modern mobile computing.

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