Considerations for the digital laboratory

Connecting your scientific ecosystem

Automation, robotics and digital technologies are transforming laboratory processes in life sciences, R&D and manufacturing, and driving a new era in data-focused disease and drug discovery. While the lab sector is still on an evolutionary road to the fully automated lab-of-the-future, or Laboratory 4.0, digital transformation is accelerating the move away from analog processes, and so reducing the need for paper-based and manual processes and human intervention.

A shift towards more flexible, secure cloud computing and service-based software platforms supports investment in and deployment of transformative technologies such as artificial intelligence (AI), machine learning (ML), automation and voice recognition, as well as enabling safe, secure collaboration and supporting regulatory compliance.

We can envisage that the tools and informatics systems on which Laboratory 4.0 are built will converge in secure cloud-hosted, open platforms for connectivity, and utilize common data standards that will aid data curation, contextualization and sharing. At the most basic level, robotic systems, process automation, smart software and intuitive connectivity across and between labs are dramatically reducing the need for manual tasks and data input, capture, handling and transfer. And this will, of course, reduce errors that almost inevitably accompany manual processes, and so prevent accidental data loss or manipulation. Integration is also supporting the stepwise creation of a wider networked environment that extends beyond the laboratory to other areas of the in-house operation, and to external collaborators and partners.

However, implementing, maintaining and supporting digital transformation requires organizations to look at their existing capabilities and create a structured plan to advance their laboratory operations. This must include a strategy to help navigate IT challenges that a laboratory or organization must overcome on the path to a connected scientific ecosystem. In order for these scientific organizations to manage this transition, they must have a good understanding of the potential challenges they face, which include deployment strategy, integration considerations, cybersecurity and data storage and management.

Deployment of modern laboratory systems that are suitable for digital transformation initiatives need to make use of the cloud in order to facilitate the necessary data sharing, but this also provides the backbone for other services. Cloud provides the platform for data sharing, instrument connectivity and security of laboratory informatics data. Cloud is often a key element on the journey to digital transformation.

Integration is also essential to modern lab operations. Connectivity is an instrumental piece of any digital strategy as this enables scientists to reduce manual data entry. This is also a prerequisite for automation as instruments and data systems need to be able to communicate effectively. Connecting instruments and data storage systems also helps to facilitate collaboration, not only through enabling data sharing, but also by making it easier to generate reports and get access to data that may previously have been siloed and hard to reach.

The challenge for many organizations that have already invested in several point solutions is often how to connect what they already have and to make use of those investments by bringing data together to deliver actionable information. Where scientists need to use multiple systems to complete a workflow, the actions spanning those systems could be automated to drive users logically through the process, and share data at relevant points.

Integration and automation offer enormous potential for laboratories to reduce their reliance on manual processes. The convergence of cloud computing intelligent software and digital systems support data integrity by reducing the chance for transcription errors, while streamlining information retrieval and sharing.

Laboratory connectivity is critical to remove barriers associated with digital lab technologies. This is true in the case of sharing data with collaborative partners, but also in connecting disparate digital systems, software frameworks and data storage. Lab connectivity facilitates the flow of information and the implementation of a laboratory orchestration platform can further integrate workflows, data and systems.

Orchestration platforms can help labs to integrate the flow of tasks, personnel, inventory, consumables, instruments and experimental data, to streamline processes, and improve efficiency and quality. Laboratory orchestration helps scientific organizations realize the full potential of digital transformation to improve quality, efficiency and the user experience. These software platforms can be used to automate workflows and experiments from design to execution, enabling tasks, such as instrument maintenance, to be scheduled automatically - helping an organization to maximize productivity and efficiency.

Data storage and management considerations include proper standardization, and the ability to move data across departments or to share data with other organizations. Metadata is key, but there are additional factors such as multiple data types, conversion of data to standard formats and access to data, that can then be used for secondary-use cases such as AI, ML or other advanced analytics.

Of course, all of this new data must be accessible and shareable with third parties, but it must also be tightly controlled where necessary with the correct parameters to ensure data security.

DISPARATE... **User experiences**
Data silos
Compliance levels

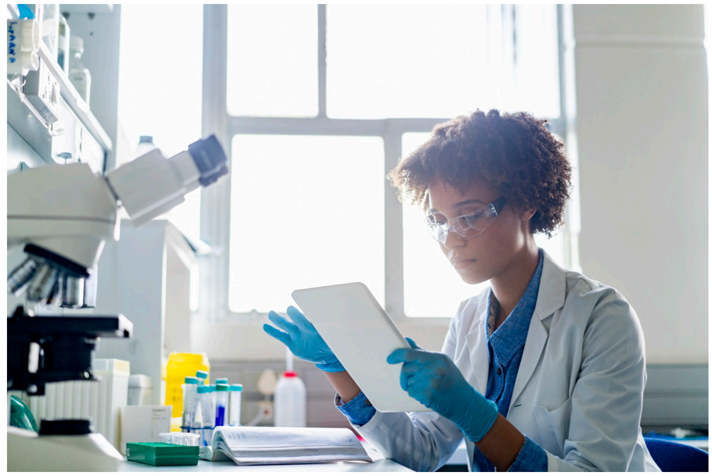
HARMONIZED... **User experience**
Data repository
Security and compliance

Moving digital functionality into the cloud is unlocking opportunities to exploit the internet of laboratory things, (IoLT) – effectively the integration of smart devices with the internet. The power of cloud computing and the adoption of cloud-based software as a service (SaaS) is opening the pathway to exploit massive in-house and public datasets – think both data volume and diversity – that can be used to train networks for modeling, analysis and simulation. The ability to store and utilize huge volumes of standardized clean, curated, and contextual datasets in easily mined and interrogated data lakes is, at the clinical level, already helping scientists better understand disease processes, design more accurate, insightful diagnostics, and develop new approaches to personalized medicine. In specialty chemical production, organizations are also mining their historic data to generate new understandings of chemical properties, and previously untapped avenues of research to deliver novel compounds faster.

In parallel, adopting standards for digital communication between hardware and software platforms will be central to enabling systems to talk to and understand each other, and provide a foundation not just for automating workflows, but for automating instrument calibration and servicing, and linking in with inventory, so that labs can achieve optimum use out of the capital investment. Acquiring and reporting data in standardized formats makes it possible to curate data from disparate sources, which can then be food for machine learning tools and AI. Datasets from large-scale genomic and proteomics research, imaging studies and high-throughput screens, for example, are generating new insights into disease processes, informing ongoing R&D and decision making, and accelerating drug discovery.

In the R&D sector, labs can exploit automation and AI to help identify and test new molecules, and evaluate data from high throughput and content-rich in vitro cell and tissue-based experiments for in vitro modeling, and to reduce the need for animal experimentation.

The digital lab will also be better equipped to meet environmental and sustainability goals, through the design of processes that use less toxic reagents, for example, or that reduce waste and emissions. Using smart software to maintain real-time oversight of inventory, instrument calibration and validation further supports lean, just-in-time manufacturing models, which further reduces costs associated with over-ordering, unnecessary storage and management, and waste.



Challenges to digital transformation

There are, of course, challenges to digital transformation, not least being the change required in operational culture, as well as in IT infrastructure. Progressing to a Laboratory 4.0 operating model isn't just a case of applying and integrating hardware and software, but will require attaining digital maturity, and extending this culturally to all personnel, from the bench scientists and lab technicians, to key stakeholders and IT departments.

A typical lab today will operate some digital platforms, robotics and automation systems, but integrating disparate platforms from different vendors is still problematic. It's likely that workflows will be punctuated by manual processes – for example, transferring data that is uploaded onto USB drives, typing in readings from weighing scales or pH meters, or recording experiments in paper notebooks, and manually creating spreadsheets and other 'flat' files.

Labs may also have to maintain proprietary software for legacy systems that are too good to retire, but which don't fit in with the evolving, connected lab. And maintaining vendor-specific software can restrict labs from investing in new digital systems that fit in with this existing lab setup, rather than selecting systems that best carry out the required tasks and align with organizational strategy and progress. The advantages to users of a vendor-agnostic lab setup are driving developers of hardware and software to support standard communication and data formats.

Storing and reporting R&D data in files – think PDFs, spreadsheets and Word files – that don't include metadata or any experimental context reduces the intelligence contained in those files. Existing data silos may effectively act as graveyards for data that can't be mined or searched intuitively, while a lack of standard terminology and ontologies can make it hard to find historical data, or compare like for like.

For Laboratory 4.0, then, data will be acquired and maintained in human-readable, standardized formats that can be linked with experimental and process metadata that is also acquired directly from hardware and automation software. Contextualized data housed in data lakes can be searched, visualized and analyzed, but also shared and understood both within an enterprise, and with collaborators, partners and service providers. Having data available in standard formats, in real-time, and with this added context of metadata, will accelerate and drive more successful R&D, and also help to secure leaner, more efficient and less error-prone manufacturing environments.

The digitally transformed lab infrastructure will naturally support FAIR guiding principles for data management, which are founded on the findability, accessibility, interoperability, and reusability of data. As the Go Fair initiative states, these principles highlight machine-actionability, described as "the capacity of computational systems to find, access, interoperate, and reuse data with none or minimal human intervention". And our reliance on computational support to deal with data is, at least in part, a result of the increase in volume, complexity and creation speed of data.

The need to ensure security and traceability of data and of processes is inherent in any manufacturing or R&D setting. The imperative is to ensure that data cannot be entered, manipulated, accessed or passed on without appropriate authorization. While this may historically have been a key concern, digital signatures are today just the most basic layer in a hierarchy of security that is built into digital processes to effectively track and allow, or deny, access to un/authorized or un/trained personnel, and data manipulation or transfer, improving transparency and facilitating compliance.

Digitalization supports data integrity, and so helps to smooth the process of regulatory audit both for the lab, and for the regulator. Hands-off workflows, data management, and the traceability afforded by digital processes make it easier for regulators to track and audit data, and reduce the likelihood that data might have been inadvertently altered, or lost.

Thermo Fisher Scientific is investing in digital capabilities and technologies that support labs of today and of the future. As laboratory-based organizations decide to adopt digital transformation, Thermo Fisher Scientific can provide the building blocks and support to help them overcome the challenges of developing and maintaining the necessary infrastructure. The aim is to enable the connection of disparate software systems and laboratory instruments and to generate an automated, intelligent engine for laboratory processes. Customers will have the ability to automate workflows, store contextual data, visualize, analyze and share data securely, and measure and monitor experiments in real-time, remotely and through mobile channels, from anywhere in the world.

Scientists will have more time to focus on the complex tasks that really need their expertise, rather than transcribe data, write reports, or waste time searching for data that is buried in silos. And a truly digitally enabled environment offers up the potential for generating new revenue streams, and enabling leaner, more intelligent business models.

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