Architecturally Significant Requirements - Architecture Proposal - SMART Lab

Due Date	25 Apr 2025
Status	WIP
Stakeholders	marie.goavec@syensqo.com, brian.bian@syensqo.com
Outcome	
Contributors	
Responsible	OLIVEIRA, Tiago

This page aims to translate the functional requirements into architecture tangible elements creating a engineering value perspective on the initiative - to assess business capabilities relevance versus architecture complexity.

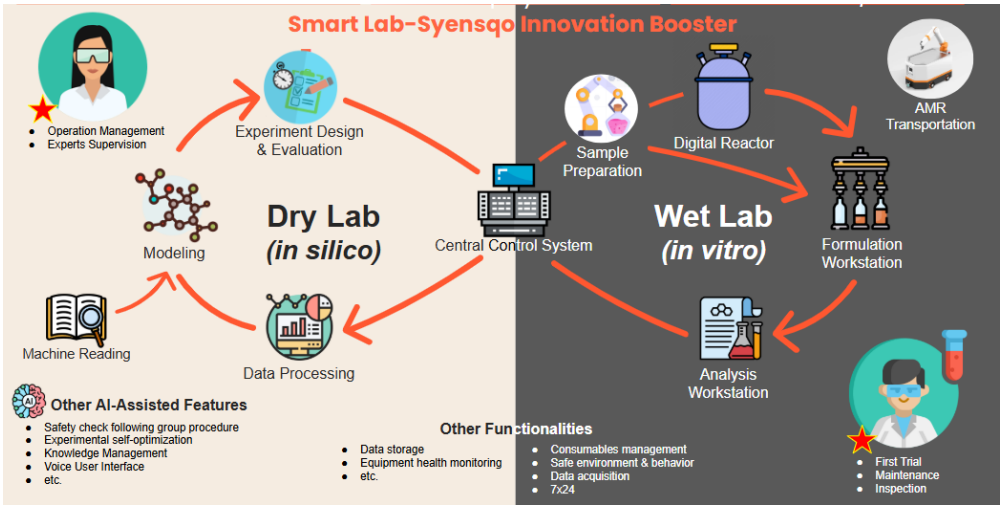
Architecture Requirements Assessment

Quality Attribute	Requirement - Architecture Concerns	Architectural Complexity	Business Criticality /Relevance	Business Requirement Item
Interoperability	How "AI system" gather info from public & internal sources for scientists real-time evaluation?	HIGH	HIGH	Understanding Experimental Requirements and Information Collection
Usability	How "AI system" filter and displays complex data structure and diagrams?	LOW	HIGH	Molecular Modeling and Simulation
Usability	How "AI system" supports/makes proposals to scientists on molecular modeling and simulation?	MEDIUM	HIGH	Molecular Modeling and Simulation
Usability	How "AI System" monitors digital reactor and formulation workstation processes to ensure accuracy/consistency of sample preparation?	HIGH	HIGH	Molecular Modeling and Simulation
Consistency	How "AI System" ensures accuracy/consistency of sample preparation?	MEDIUM	LOW	Execution of Experimental Plan
Usability	How "scientists" monitor progress of digital reactor and formulation process in real time?	LOW	LOW	Execution of Experimental Plan
Interoperability	How "Central Control System" capture instrument data and promote it to Data Analysis System?	MEDIUM	HIGH	Sample Analysis and Data Processing
Interoperability	How "Central Control System" onboard/integrate new instruments?	LOW	MEDIUM	Sample Analysis and Data Processing

Consistency	How can "AI System" make recommendations for the experimental scheme to the scientists based on historical data and current results?	HIGH	HIGH	Experimental Optimization and Iteration
Interoperability	What types of sensors "AI System" will connect and how it will monitor Environment and instrument parameters in real-time to schedule maintenance (to reduce downtime)?	MEDIUM	LOW	Intelligent Management and Maintenance
Safety	How "AI System" automatically checks existing group safety regulations/procedures and evaluates the safety of new instrument/processes/Management of Change to recommend additional safety monitoring parameters?	MEDIUM	HIGH	Safety and Compliance
Usability	How "AI System" allows scientists to access experiments database for evaluation?	LOW	LOW	Knowledge Management and Collaborative Work
Usability	How "Virtual Assistant" provides suggestions on best practices to scientists?	LOW	HIGH	Safety and Compliance
Usability	How "AI System" enhances team collaboration, allows sharing data and offers personalized collaboration tips (recommendations)?	LOW	LOW	Knowledge Management and Collaborative Work
Usability	How "Reporting - Visualization System" keeps track on the regular work-flow to create analysis?	LOW	MEDIUM	Automatic Report Generation and Environmental Control
Usability	How "AI System" automatically adjusts parameters based on experimental needs for optimal conditions?	MEDIUM	LOW	Intelligent Management and Maintenance
Usability	How "Reporting - Visualization System" allows multi-project management?	LOW	MEDIUM	Visualization System and Resource Scheduling
Interoperability	How "Voice User Interface (VUI)" allows personas in the lab to interact with Instruments and manage experiments?	HIGH	LOW	Voice User Interface

Reference:

Architectural Concerns



- Wet-Lab

a. The "Big Data Hub" should be compliant with CyberSec OT/IT constraints.
b. The solution must provide extensible and resilient interfaces mechanism for integrating with Syensqo LIMS, ELN and AI systems.
c. Foundational or Pre-trained AI/LLM models consumed by Edge or Regular computing must be validated from the Syensqo AI standpoint and CyberSec constraints (+AI Risk).
d. Local network capacity must be adequately dimensioned to support the throughput of the number of sensors and their potentially complex and large data types capturing.

- Dry-Lab

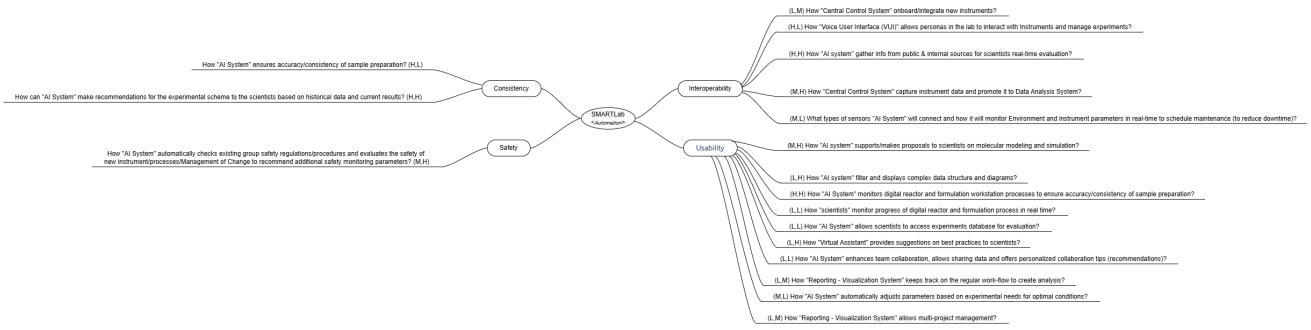
    a. *Interoperability between systems (Machine Learning, Modeling-Simulation and LIMS/ELN) becomes critical to achieve efficiently the target seamless workflow.*
    b. *Data integration should be taken into consideration to ensure the lineage and data consistency across different systems where users will perform their activities.*
    c. *Computer power is also critical for fine-tunning, training and real-time suggestions (here also low-latency network is a sensitive aspect to take into account).*

It is also a concern to consider that eventually the solution used for Shanghai may not be generalizable or reusable in other regions, outside of China, due to aspects related to:

1. Contract and legal for having the same vendors
2. Interoperability with Syensqo Application Platform for experiments (LIMS, ELN)
3. Data classification and data exchanges between regions

Utility Tree

The value engineering work on the user requirements allows to create such mind-map diagram so to visually capture the architectural significant requirement and its business criticality and complexity to be implementend.



(Arch degree complexity, Business critical relevancy**) Architecture Significant Requirement**

Personas - Profiles

- Syensqo Lab Expert
- AI System
- Scientists
- Researchers
- Lab Technicians
- Virtual Assistant
- Voice User Interface (VUI)

Environments

- Wet Lab:
- Dry Lab:
- OnPrem:
- Cloud Infra:

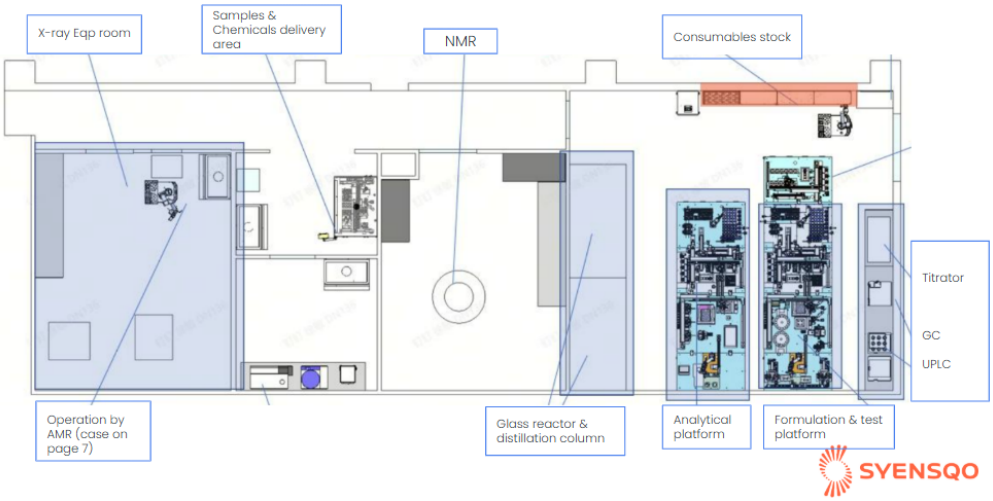
Components - Building Blocks

- AI System
- Digital Reactor
- Formulation Workstation
- Analytical Instruments
- Data Analysis System
- Central Control System
- Reporting - Visualization System
- Voice User Interface (VUI)

High Level Design Architecture

There are three different views to describe the laboratory environment and the application/infrastructure architecture to accomplish the business needs.

- **Shanghai Lab Setup**



- **High Level Design** (LabPC - application context)

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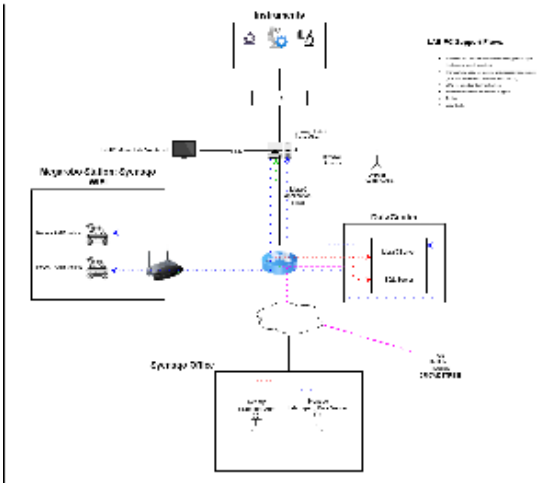
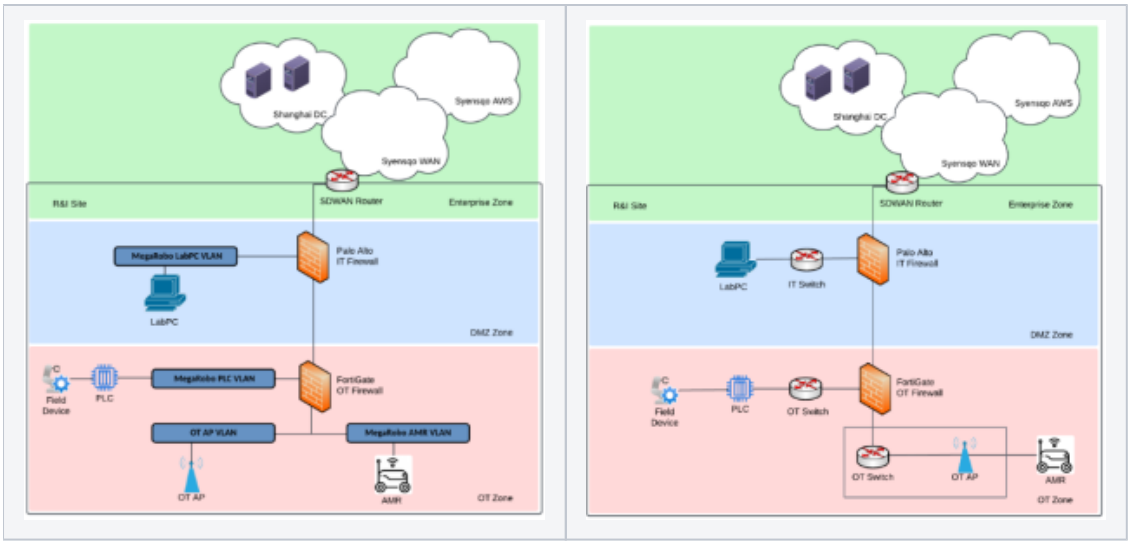
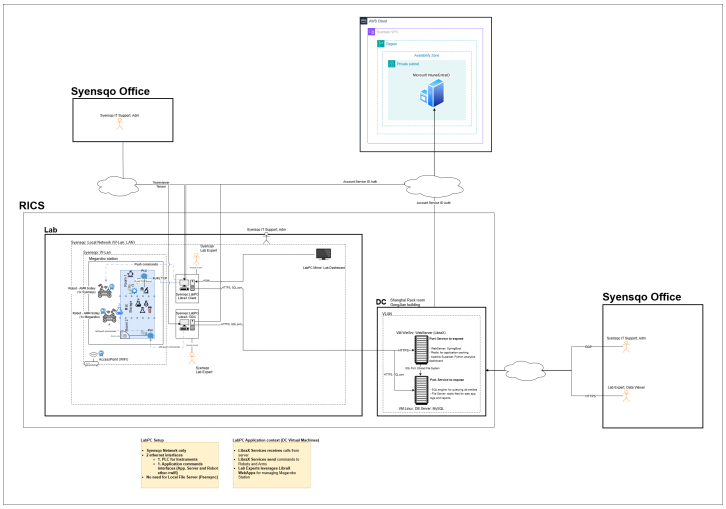


- **High Level Design** (application and OT-IT network architecture: *IEC 62443 - zones & conduits*)



- **High Level Design** (application, OT/IT + workflow context)



References

Functional Requirements

Smart Solution