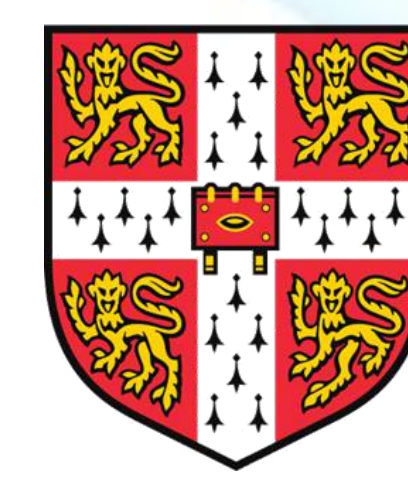


# Connected digital twin for holistic lab automation

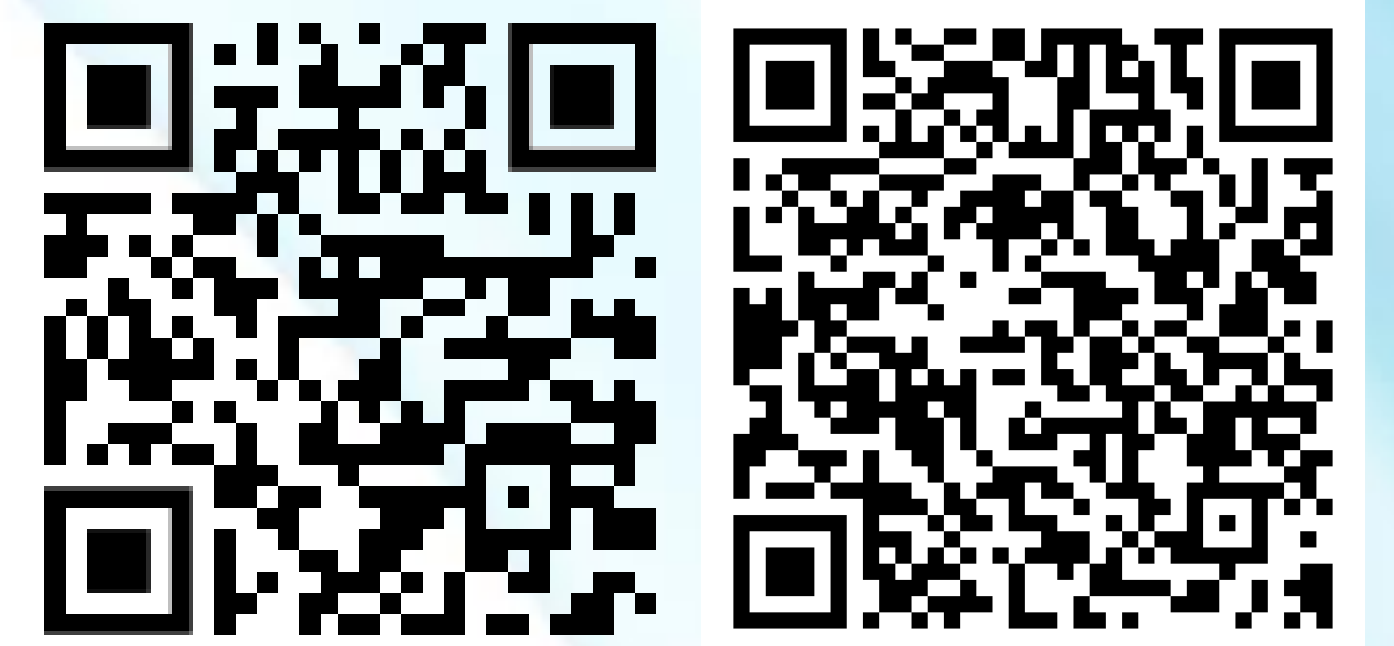


UNIVERSITY OF CAMBRIDGE

Jiaru Bai<sup>1</sup>, Simon Rihm<sup>1,2</sup>, Markus Kraft<sup>1,2,3,4,5\*</sup>

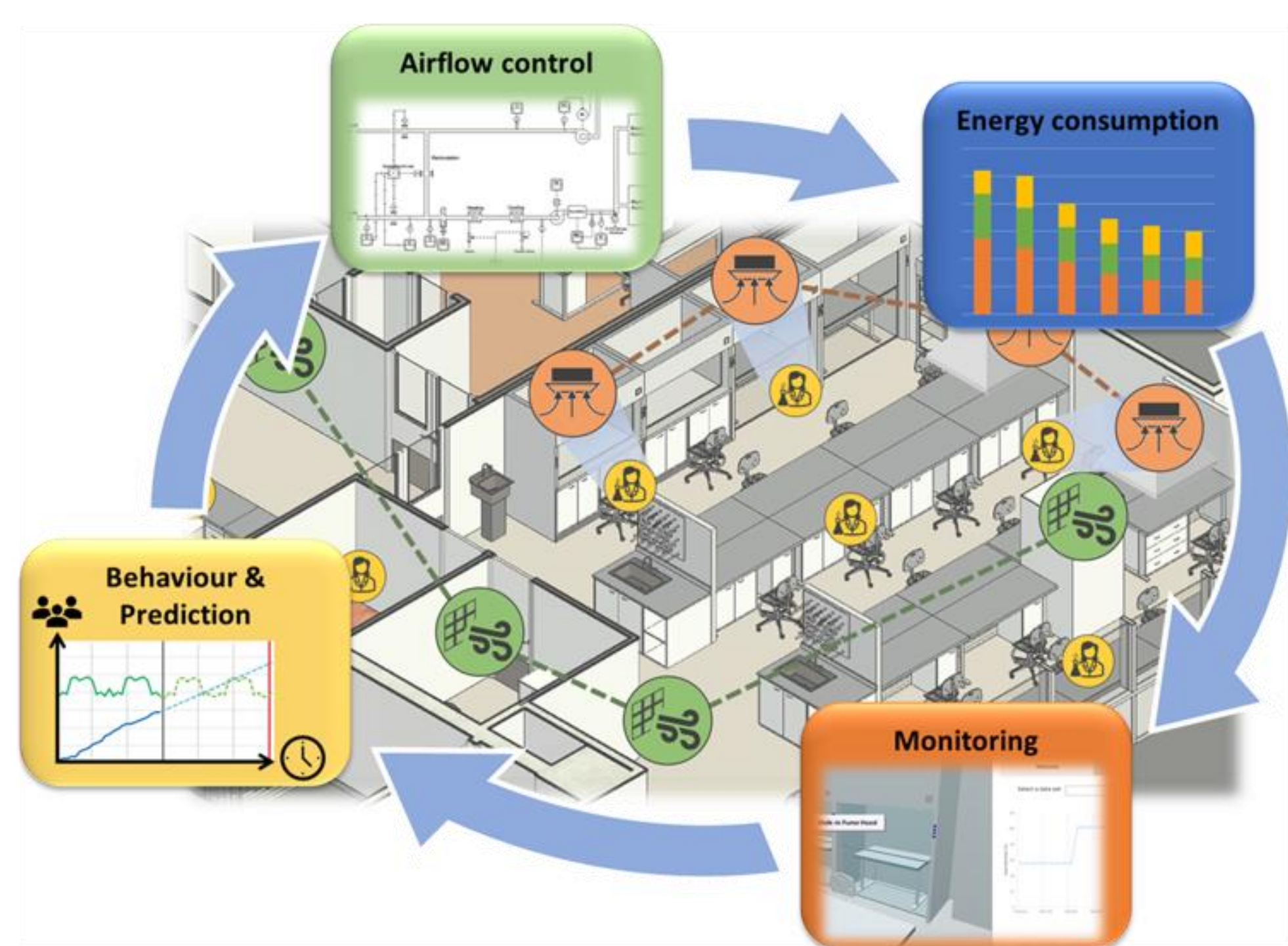
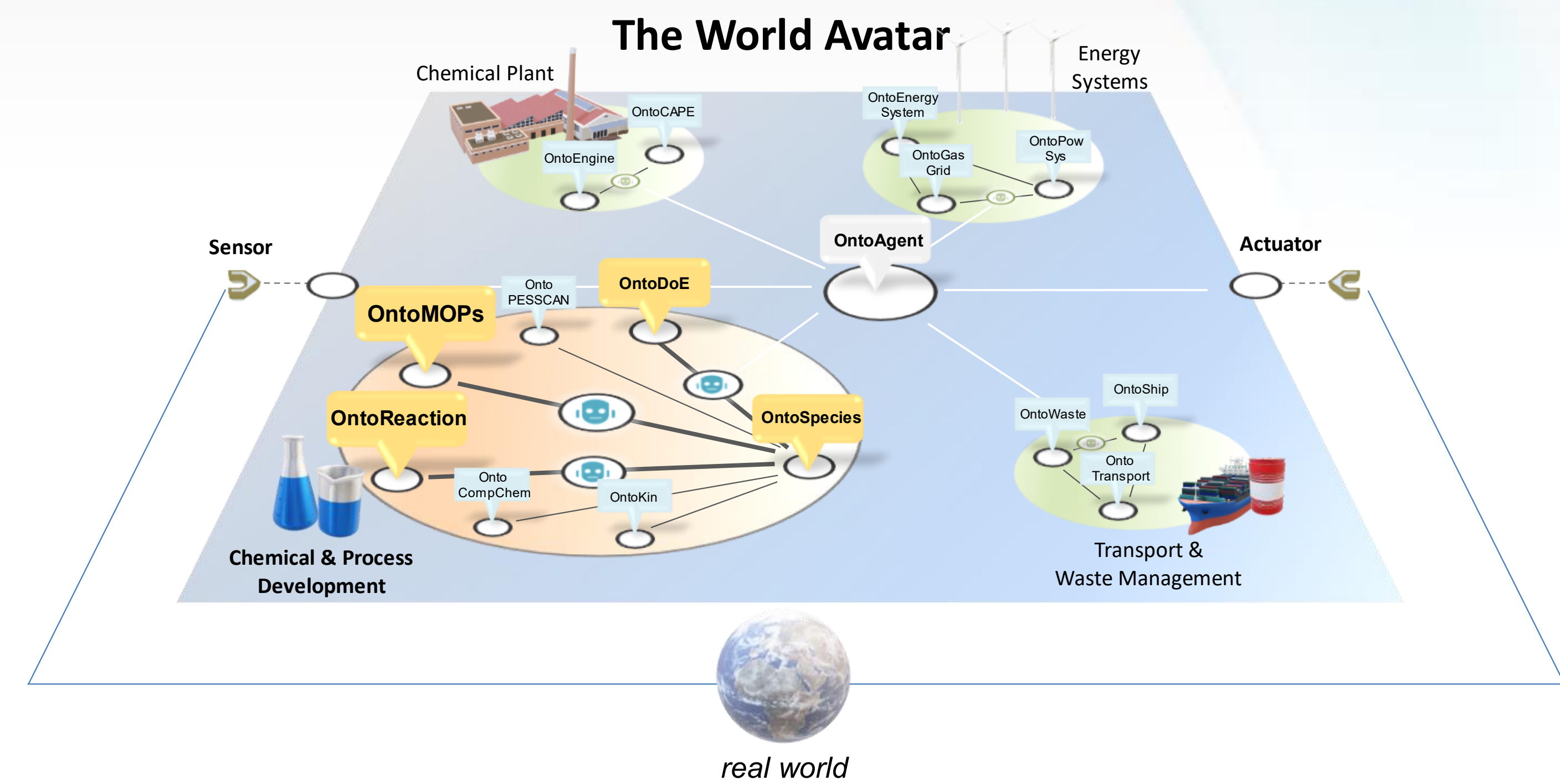
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## THE WORLD AVATAR (TWA)

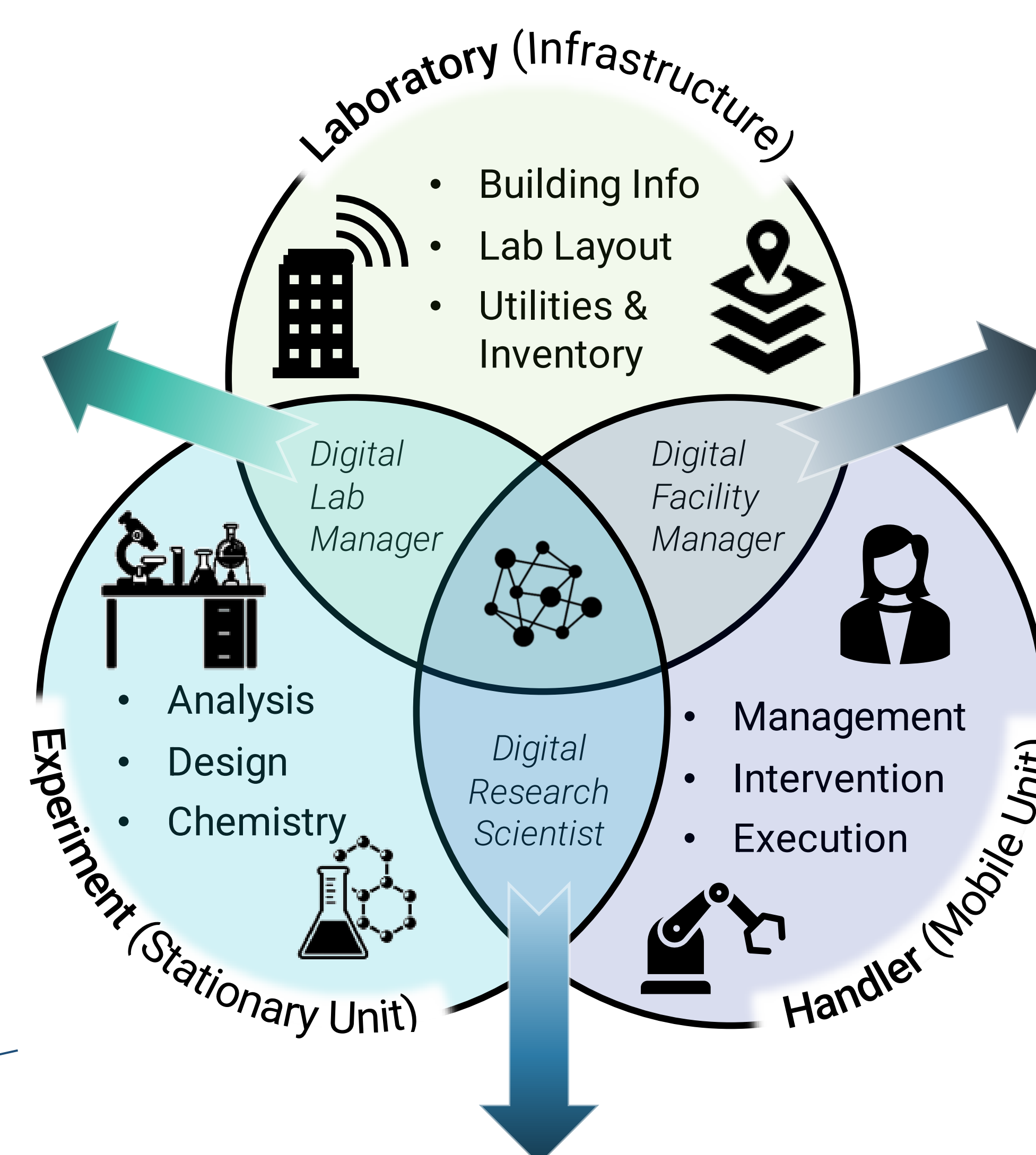
The **World Avatar** aims to represent an all-encompassing **world model** that can consistently capture anything that can be conceptualised. It uses a **dynamic knowledge graph** that semantically describes relationships between concepts and instances. The World Avatar is **modular** and **scalable** by design, and new concepts and relationships can be added continuously while maintaining connection to everything existing. It allows **decentralisation** and enables **interoperability** across heterogeneous data sources and software. The intelligent agents that are part of the World Avatar act as **executable knowledge component**, keeping the system current and self-evolving.



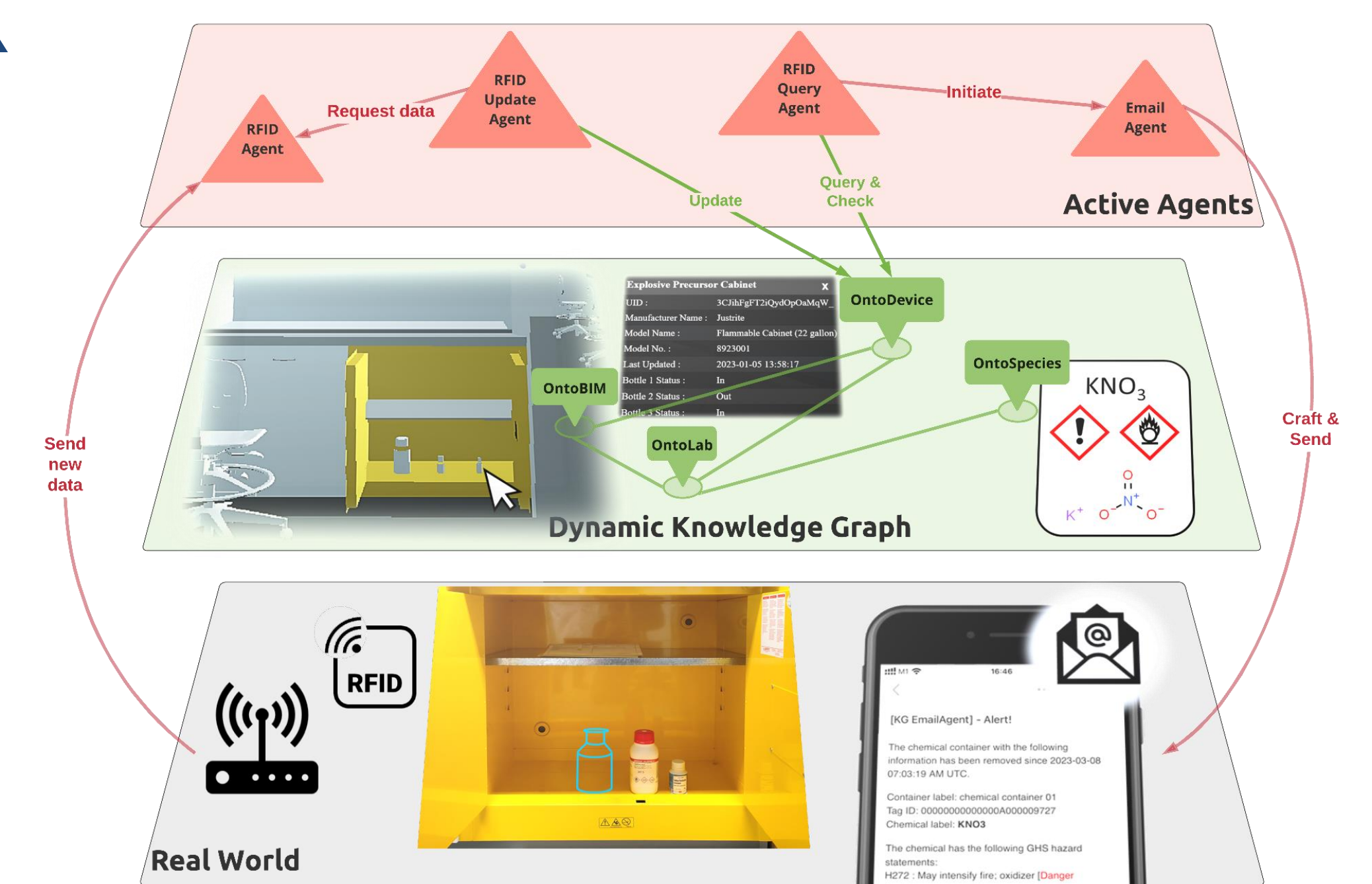
e.g., **Lab Energy Analyst...**

- Integration of BIM and BMS
- Monitoring of energy consumption
- Resource allocation based on cost effectiveness next to scientific merit

## DIGITAL LAB FRAMEWORK



e.g., **Distributed Self-Driving Labs...**

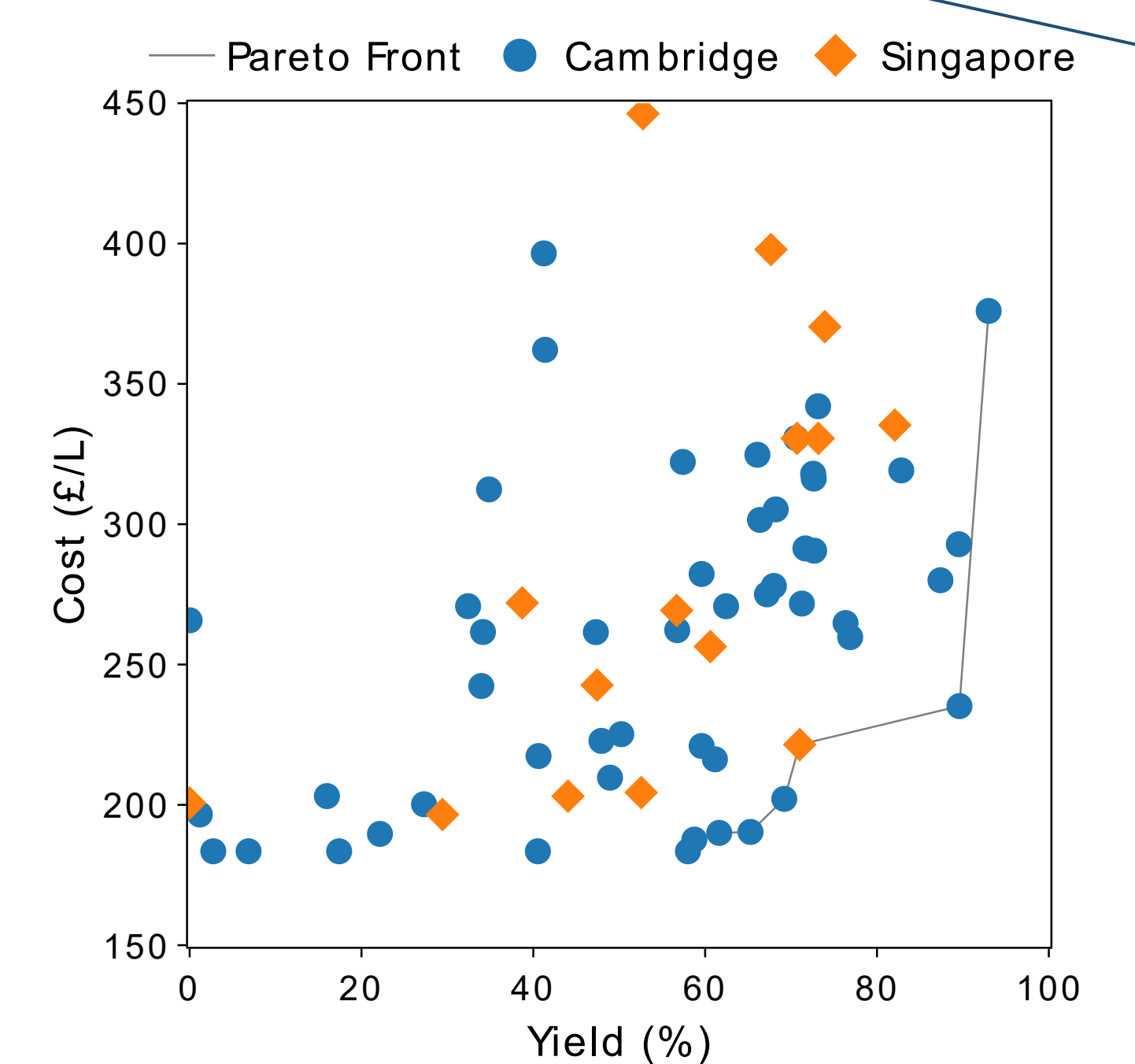
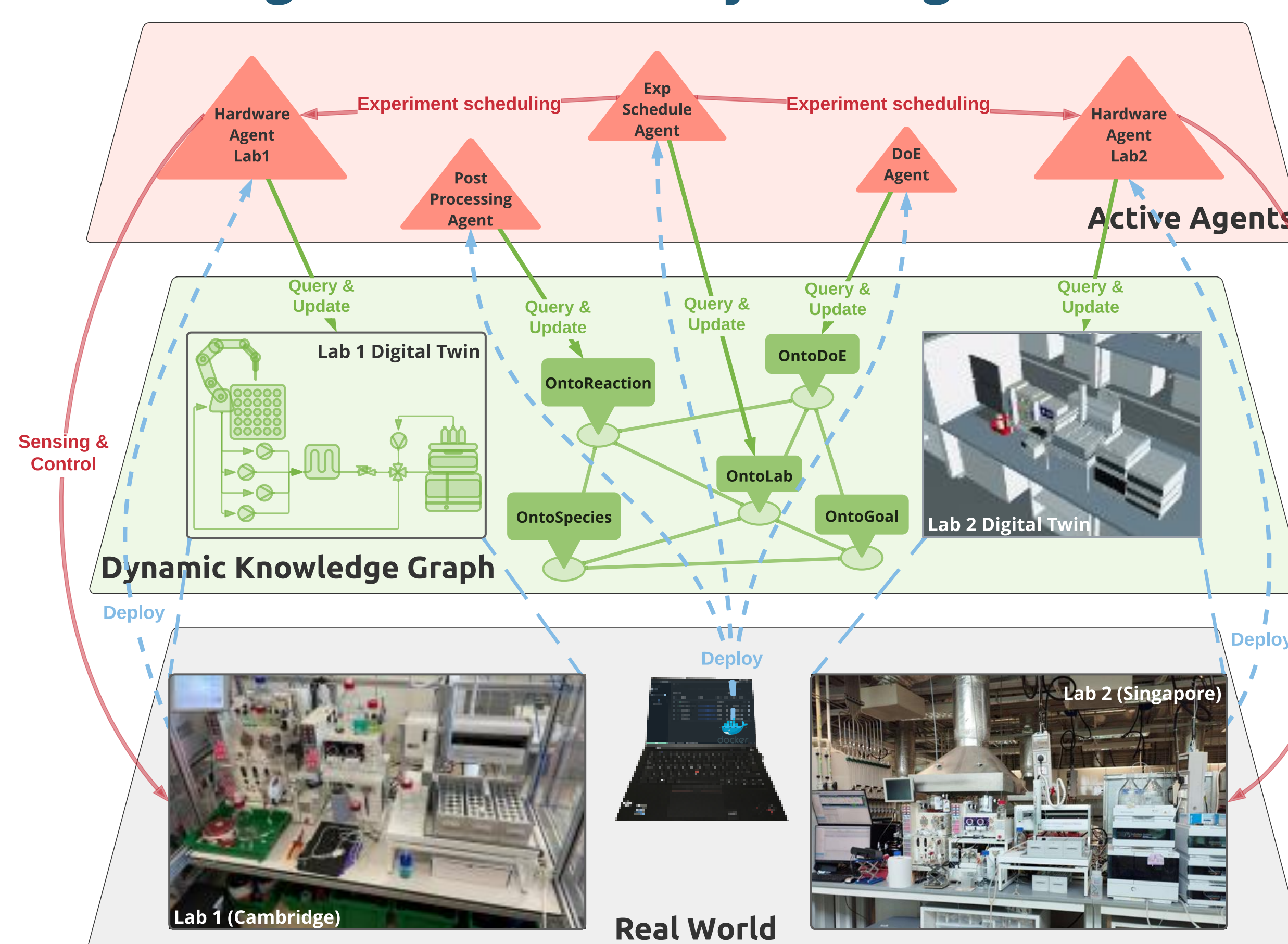


e.g., **Explosive Precursor Tracker...**

- RFID-based inventory tracking
- Utilisation of chemistry knowledge to identify safety-critical substances
- Communication with humans via app and email



- Closed-loop optimisation
- Goal-oriented derivation
- FAIR data provenance



- 10,800 km real-time collab
- 3 days continued operation
- 65 experiment runs

## CONCLUSION

- Top-down approach enables goal-driven automation of all aspects of a chemical research laboratory
- Holistic view of lab activities towards 'AI scientist'
- Demo for a globally collaborative research network
- AI infrastructure for open science

## REFERENCES

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2. J. Bai, L. Cao, S. Mosbach, J. Akroyd, A. A. Lapkin, and M. Kraft. From Platform to Knowledge Graph: Evolution of Laboratory Automation. *JACS Au* **2022** 2, 292–309.
3. S. D. Rihm, J. Bai, A. Kondinski, S. Mosbach, J. Akroyd, and M. Kraft. A Comprehensive Laboratory Digital Twin: Top-Down Automation of a Chemical Research Laboratory. *In Preparation*.
4. J. Bai, S. Mosbach, C.J. Taylor, D. Karan, K.F. Lee, S.D. Rihm, J. Akroyd, A.A. Lapkin, and M. Kraft. From Platform to Knowledge Graph: Distributed Self-Driving Laboratories. *In Preparation*.