A Software Engineering Approach to the Design and Application of Digital Twins in Industrial Chemical Processes

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Digital Twin technology is seen as transformative in many industries, as they enable new methods of control, optimisation, scheduling, and design [Walmsley et al., 2024]. The increase in efficiency they promise is particularly attractive in the energy sector, where it can reduce both emissions and cost.

Some key technologies underpining digital twins include:

- Traditional Process Simulation techniques, where mathematical physics-based models are used to simulate the behaviour of a system [Lee et al., 2021].
- Data Collection and Processing techniques, such as SCADA systems or Industrial IoT systems, which enable observability and control [Udugama et al., 2020],
- Physics-Informed Machine Learning, where machine learning models are combined with traditional physics-based models to improve accuracy and generalisation [Karniadakis et al., 2021].

There is a growing body of research into new machine learning techniques that can be used to accurately model complex systems. New fields of machine learning, such as Operator Networks, are particularly promising as they offer the ability to predict the solution to Ordinary Differential Equations (ODEs) and Partial Differential Equations (PDEs)[Lu et al., 2019], which are commonly used in physics-based models.

These techniques exist as research concepts, but Software Engineering principles have not been applied to implement them in a live industrial environment. This project aims to explore the development of a framework for implementing Digital Twins, with industrial chemical processes providing a case study.

Research Questions

This project aims to answer the following research questions:

How does the level of abstraction impact the effort required to design and implement a Digital Twin for an industrial chemical process? To what extent does it enable wider applicability of Digital Twin tools and techniques?

A Digital Twin platform must implement functionality from many different types of models, in a way that is suitable for real-time systems [Cao et al., 2021]. Thus each Digital Twin is unique and application-specific. A high level of abstraction is a barrier to customising Digital Twins, but a low level of abstraction reduces reusability. This research question will apply Software Engineering principles to determine where abstraction is beneficial in the design and implementation of a Digital Twin.

How effective are Operator Networks at surrogate modelling dynamic chemical processes in an online setting?

Operator networks are a new machine learning technology that have the potential to model dynamic systems more accurately than traditional machine learning techniques. This research question aims to adapt existing operator networks to support online learning, and to test their effectiveness in a live industrial environment.

What are the real-world performance benefits associated with implementing Digital Twin Techniques?

Recent work has outlined a conceptual framework for implementing Digital Twin Technologies [Örs et al., 2020], but there is little research into how they perform in a real-world setting. This research question aims to deploy the Ahuora platform in a live industrial environment, and to measure the performance benefits that these techniques provide. This will provide evidence to industrial partners that these techniques are effective.

What software engineering principles, practices, and frameworks help build more maintainable Digital Twin systems?

The development of the Ahuora platform will provide a case study in building Digital Twin Systems, and the effectiveness of Software Engineering principles and practices. As a suitable architecture is developed, this can be generalised into a software model for building Digital Twins.

Proposed Methodology

Literature and technology from the fields of Software Engineering, Data Science, and Chemical Engineering will be reviewed in context of the other fields. Development will be conducted using Software Engineering principles. Small-scale experiments, case studies, and prototypes will be used to test the effectiveness of different modelling techniques, and their suitability for a live industrial environment. This research will extend the Ahuora Platform to support dynamic modelling, surrogate modelling, data-driven modelling, optimisation, and control tooling.

Expected Outcome

This research will enable Digital Twin technologies, Operator Networks, and multi-fidelity modelling to be used in conjunction with one another, outside of their core research communities.

By the end of this project, the Ahuora Digital Twin Platform will support each of these modelling techniques. The Ahuora will be deployed in New Zealand industries, providing real-world performance benefits. This will provide evidence to industrial partners that these techniques are viable, feasible, and desirable, enhancing their uptake by the Industrial Process sector.

Additionally, this research will provide a case study for how Software Engineering principles can be applied to the development of Digital Twins, and a framework for implementing Digital Twins in other industries.

References

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