Digital Twins in the Life Sciences: Turning Raw Data into Dynamic Models

Report of Contributions

https://events.hifis.net/e/dt2025

Contribution ID: **9** Type: **not specified**

Digital Twins in the life sciences —from an engaged ecosystem to an incipient infrastructure

Thursday 24 April 2025 14:00 (1h 30m)

The past decade has produced overwhelming evidence that changes in the health status of individuals, measured by well-defined quantitative clinical endpoints, can be predicted by computer models. This has opened the door to several applications for computer modeling and simulation technologies. The modeling approach depends on the technologies used and the quality and strength of the data and knowledge. When models are built using available scientific knowledge in biophysics, biochemistry, and physiology of the human body, both in healthy and diseased states, we refer to them as knowledge-driven/mechanistic models. When they are developed directly from data, without making any causal assumption, we refer to them as data-driven models. This talk will provide an introduction to and a general overview of digital twins, from digital twins to digital cohorts, focusing on eventually developing integrated virtual human twins. This talk will also discuss several non-technical elements that are essential to the successful translation and uptake of digital twins in the life sciences, starting with an engaged ecosystem and including regulatory, ethical, legal and social sciences advances.

Presenter: GERIS, Liesbet (University of Liege, KU Leuven, Executive Director of VPH Institute)

Session Classification: Lecture Series

Contribution ID: **11** Type: **not specified**

Mechanistic models

Thursday 15 May 2025 14:00 (1h 30m)

Even though machine learning and data-driven models acquire more and more momentum, traditional mechanistic models are still very useful in different fields. Mechanistic models can be thought of as virtual mimics of real systems with some simplifications if necessary. Such models are very useful when the amount of data is limited, or we need to understand the causation of the made observations in detail. In this lecture, we will describe how such models can be built, and show several examples, including realistic modeling of blood flow and of cell-mimicking active systems. These models help us better understand the underlying physical mechanisms and their effect on the behavior of real systems of interest.

Presenter: FEDOSOV, Dmitry (Institute of Advanced Simulation (FZJ))

Session Classification: Lecture Series

Contribution ID: **12** Type: **not specified**

Building Trust in Medical Digital Twins: Bridging the Gap Between Research Models and Patient Outcomes

Thursday 5 June 2025 14:00 (1h 30m)

This lecture explores the integration of medical digital twins in patient care, focusing on the personalised modelling of individual patients. We will discuss the necessary data sources for highly parametrised models, exemplified by the scarcity of measurements associated with personal harm to the patient and the potential role of machine learning in this problem. Practical examples of regulatory-approved models, particularly in the cardiac domain, will be presented. Clinical challenges such as limited computational resources, unstructured data, and strict legal boundaries (MDR, AI Act, GDPR) will be addressed. The need for multidisciplinary collaboration will be emphasised to build trust in model outputs within the medical and patient community, as well as to tailor them to clinically meaningful endpoints.

Presenter: NIKLAS, Christian (Heidelberg University Hospital)

Session Classification: Lecture Series

Contribution ID: **14** Type: **not specified**

Uncertainty Quantification in Machine Learning

Thursday 26 June 2025 14:00 (1h 30m)

In this lecture, we will motivate why the successful application of machine learning models in the real world (in the context of Digital Twins or otherwise) requires a careful quantification of predictive uncertainty. We will review different fundamental approaches to uncertainty estimation, such as frequentist and Bayesian ones. We will give an overview of several practical methods for uncertainty quantification with different machine learning models, traversing the tradeoff between fidelity and computational cost.

Presenter: FORTUIN, Vincent (Helmholtz AI, TU Munich)

Session Classification: Lecture Series

Contribution ID: **16** Type: **not specified**

Acquisition, processing and provision of data in the domain of chemistry - and beyond

Thursday 8 May 2025 14:00 (1h 30m)

This lecture will give an overview about basic mechanisms and workflows that can be used to collect and prepare data for different re-use cases in the domain of chemistry. It will emphasize the importance of standardized processes and data conversion routines and will describe the role of open data for the development of new AI-based scientific methods in the long run.

Presenter: JUNG, Nicole (Karlsruhe Institute of Technology (KIT))

Session Classification: Lecture Series

Contribution ID: **21** Type: **not specified**

Data-driven models

Thursday 22 May 2025 14:00 (1h 30m)

In this lecture, we will discuss approaches to learning predictable models directly from data. We will start with the fundamentals of statistical learning theory, statistical inference, and machine learning. We will then cover the basics of deep learning, a few network architectures, and current applications in biology and medicine.

Presenter: RULANDS, Steffen (Ludwig-Maximilians-Universität München)

Session Classification: Lecture Series

Contribution ID: **22** Type: **not specified**

Next-Generation Surgery: AI-Driven Digital Twins for Personalized and Predictive Healthcare

Thursday 31 July 2025 14:00 (1h 30m)

Advanced surgical technologies, like digital ORs and robotics, generate vast data for enhancing patient care. However, leveraging this data efficiently during surgery, a complex and time-sensitive process, remains heavily reliant on surgical staff experience.
This lecture introduces digital twins for AI-powered robotic surgery with a particular focus on analysis of intraoperative data. By making surgical expertise accessible to machines, digital twins help democratize skills and optimize patient-specific treatment. Real-world examples illustrate their impact on decision-making and therapy. Finally, we discuss key challenges and strategies for integrating digital twins into surgical practice.

Presenter: SPEIDEL, Stefanie (National Center for Tumor Diseases, Dresden)

Session Classification: Lecture Series

Contribution ID: **23** Type: **not specified**

Building Digital Twins of Development and Disease

Thursday 10 July 2025 14:00 (1h 30m)

Computational simulations have long been used to study emergent phenomena in biology. Data-driven in silico models of tissue behaviour in development and disease now enable the creation of Digital Twins—virtual counterparts with applications in bioengineering and precision medicine. I will present our simulation frameworks for high-resolution tissue modelling and parameter inference from imaging and experimental data. Finally, I will discuss our progress in constructing Digital Twins for epithelial tissues, morphogenesis, and medical treatments.

Presenter: IBER, Dagmar (ETH Zürich)

Session Classification: Lecture Series

Contribution ID: **24** Type: **not specified**

Towards a Virtual Cell - the Need for Actionable Perturbation Models

Thursday 17 July 2025 13:30 (1h 30m)

Single-cell genomics has enabled the construction of detailed organ atlases, offering unprecedented insights into cellular states and their perturbations by signaling, drugs, or disease. A key challenge is moving to actionable models that can predict and steer cellular responses. Therefore, we need generative models that not only organize single-cell data in meaningful manifolds but also learn how cells respond to perturbations. These models may be useful early instances of a multimodal model (or digital twin) of cellular transitions.

I will introduce representation learning approaches for identifying gene expression manifolds and modeling perturbation-induced changes, and will discuss recent extensions incorporating optimal transport and flow matching. If time permits, I will compare these methods to prior-based modeling approaches for constructing a Virtual Cell capable of predicting, simulating, and guiding cellular behavior.

Presenter: THEIS, Fabian J. (Helmholtz Munich)

Session Classification: Lecture Series

Contribution ID: **25** Type: **not specified**

Bayesian Optimization for Digital Twins

Thursday 24 July 2025 14:00 (1h 30m)

Many scientific questions, both experimental and computational, require us to solve optimisation problems. In order to achieve an optimal outcome, we need to choose values for free variables in our (computational) experiments. This can range from experimental conditions in chemical synthesis over parameters in a digital twin all the way to the selection of hyperparameters when training a neural network. In many cases, (computational) experiments are too time-consuming and expensive to fully explore the potentially high-dimensional parameter space in order to find ideal parameter values. In this lecture, we will discuss Bayesian optimisation as a data-efficient method to tackle optimisation problems that have multiple free variables and strong limitations on the total number of experiments that can be performed.

Presenter: FRIEDERICH, Pascal (KIT)

Session Classification: Lecture Series

Contribution ID: **26** Type: **not specified**

The Virtual Humans Factory: Modelling and simulation for healthcare industries

Thursday 7 August 2025 14:00 (1h 30m)

Computational modeling and digital twins have become state-of-the-art methodologies in all industries to analyze, monitor, and assess the possible outcomes of a system under different conditions. Specifically, in the healthcare sector, the full exploitation of computational models is on the rise. ELEM Biotech is a spinoff of the Barcelona Supercomputing Center that commercially exploits Alya, a high-performance-computing finite-element code, for applications in the healthcare domain. In this lecture, applications for cardiac resynchronization therapy, cardiac valve modeling, digital twins of human cardiac cohorts, and cardiac safety drug testing will be discussed. Furthermore, the V.HEART-SAFETY platform will be presented, which provides ELEM clients with the ability to fully deploy cardiac in-silico trials and compare them to human clinical trials.

Presenter: AGUADO-SIERRA, Jazmin (ELEM Biotech)

Session Classification: Lecture Series