Three Pillars for Digital Twins: Experiments, Simulation, and Artificial Intelligence

Alireza Hashemi¹, Pavel Ryzhakov^{1,2}, Angela Ares¹

¹ Centre Internacional de Mètodes Numérics en Enginyeria (CIMNE), C/Gran Capitán s/n, Campus Nord UPC, 08034, Barcelona, Spain

e-mail: ahashemi@cimne.upc.edu, web page: https://droplets.cimne.com/

² Universitat Politècnica de Catalunya - BarcelonaTech (UPC), Escola Tècnica Superior d'Enginyers de Camins, Canals i Ports, C/Jordi Girona 1, Campus Nord UPC, 08034, Barcelona, Spain e-mail: pavel.ryzhakov@upc.edu, web page: <u>https://www.upc.edu</u>

1. Introduction: Digital Twins

This presentation aims to highlight the synergy between experimental studies, Computational Fluid Dynamics (CFD) simulations, and Artificial Intelligence (AI) in developing high-fidelity, real-time digital twins that optimize and enhance the precision and performance of microfluidic systems. Digital twins are virtual replicas of physical systems that enable improved decision-making and performance optimization. These systems are particularly useful in complex scenarios where physical testing is costly or impractical. Digital twins allow for the exploration of 'what-if' scenarios and the prediction of outcomes under varying conditions, thus offering a comprehensive tool for modern engineering challenges. The impacts of effective digital twins are substantial, ranging from cost reduction and quality improvement to faster time-to-market, product differentiation, and enhanced product reliability.

Ideal properties of digital twins include real-time operation, automation, ease of use, integration with CAD systems, multiphysics capabilities, flexibility, and bidirectional communication. A digital twin is not just a customized simulator, which consists only of a "digital model" (mirror) of the original physical product. There should be a mechanism to dynamically update the digital model based on the feedback received from the physical product. By providing this unidirectional connection between the model and its physical counterpart, we obtain a "digital shadow" of the real product. To achieve a true "digital twin", there must be a bidirectional connection between the model and the physical product. This means the model not only receives feedback from the physical product but also provides optimized configurations that are automatically applied to enhance the product's performance (Fig. 1).

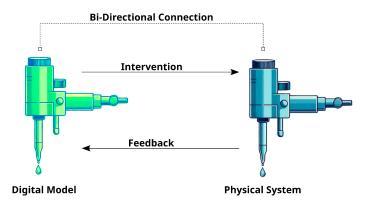


Figure 1: Schematic diagram illustrating the bidirectional connection between the digital model and the physical product in Digital Twins.

2. Digital Twins for microfluidics applications

Microfluidics, the study of fluid behavior at the microscale, has numerous applications across diverse fields [1-3]. In biomedical engineering, microfluidics is used in DNA arrays, cell printing, drug delivery systems, and lab-on-a-chip devices. In electronics, microfluidic technologies contribute to the development of microchips, MEMS, and integrated optics. Optical technologies benefit from microfluidic devices such as tunable lenses and photonic devices. Furthermore, microfluidics plays a critical role in fundamental physics research by enabling the study of fluid dynamics at the microscale. The versatility and precision of microfluidic applications underscore the importance of digital twins in this field.

Historically, the first attempts at creating digital twins for microfluidic products were based on employing CFD simulations. CFD simulations enhance the understanding of fluid dynamics at the microscale, enabling precise predictions and optimizations. Several efforts have been made to enhance CFD capability for microfluidic applications, including considerations of surface tension, wettability of surfaces, and effectively capturing complex interfacial dynamics[4-8]. However, CFD simulations still face significant challenges, such as high computational costs, difficulties in capturing all multi-physical intricacies, ink rheology, and issues related to interface tracking, interfacial dynamics, and multiscale problems [9]. Considering these challenges, pure CFD is not an efficient tool for producing real-time, flexible, and bidirectional digital twins.

Additionally, experimental data can support data-driven approaches, such as Reduced Order Modeling (ROM) and optimization methods, helping to enhance and speed up CFD simulations [10,11]. Additionally, experimental data can train machine learning models to directly predict the outcomes of complex processes that CFD simulations struggle to perform. For instance, organizing a CFD model for an inkjet printhead that includes the propagation of pressure fluctuations due to the oscillation of piezoelectric elements inside the ink chamber, meniscus dynamics, contact-angle dynamics at the nozzle plate, surface tension, and Marangoni flows, and droplet pinch-off is not feasible.

3. A proposal for a Digital Twin for inkjet printing

At the Droplet Dynamics Group (DDG) at CIMNE, we used experimental data from our in-house experimental setup to train a neural network that accurately predicts the intricate geometry of the ejected droplet from the dispenser, only by receiving the parameters of the dispenser's input signal (Fig. 2) [12].



Figure 1: Neural network prediction for droplet geometry

In recent years, reinforcement learning methods have made real-time bidirectional digital twins for microfluidic systems feasible. Reinforcement learning provides the capability to optimize operational input parameters to minimize the deviation of the system's output from the desired state. At DDG, we have designed a closed-loop high-level digital twin for inkjet printheads that can dynamically optimize the operational configuration of the input signal to maintain the system's quality in the desired state. The structure of this digital twin consists of a Real-Time Sensing Unit (RTSU), a ROM Unit (ROMU), a Quality Deviation Detection Algorithm (QDDA), and an Artificial Intelligence Unit (AIU) (Fig. 3).

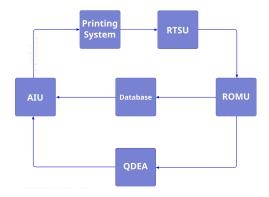


Figure 1: Schematic flow graph of the designed digital twin for inkjet printing systems

The integration of these elements enables the creation of a robust, efficient digital twin system that leverages the strengths of experiments, CFD, and AI to push the boundaries of microfluidic technology, ensuring that the advancements in digital twins continue to meet the evolving demands of various high-precision fields.

REFERENCES

[1] C. Narváez-Muñoz, A.R. Hashemi, M.R. Hashemi, Luis Javier Segura, P.B. Ryzhakov, "Computational ElectroHydroDynamics in microsystems: A review of Challenges and Applications", Archives of Computational Methods in Engineering, 1-35, (2024), https://doi.org/10.1007/s11831-024-10147-x.

- [2] C. Narváez-Muñoz, P. Ryzhakov, J. Pons, "Determination of the operational parameters for the manufacturing of spherical PVP particles via electrospray", Polymers, 13(4), 529, (2021), https://doi.org/10.3390/polym13040529.
- [3] C. Narváez-Muñoz, M.R. Hashemi, P.B. Ryzhakov, J. Pons-Prats, "Towards electrohydrodynamic cone-jet regime simulation in planar films for microfluidic-based manufacturing", ECCOMAS Coupled Problems, 1-4 June 2023, Crete, Greece.
- [4] A.R. Hashemi, M.R. Hashemi, P.B. Ryzhakov, R. Rossi, "Optimization-based level-set re-initialization: A robust interface preserving approach in multiphase problems", Computer Methods in Applied Mechanics and Engineering, 420, 116699, (2024), https://doi.org/10.1016/j.cma.2023.116699.
- [5] P.B. Ryzhakov, J. Marti, M.R. Hashemi, "Advances in Numerical Modeling of Coupled CFD Problems", Journal of Marine Science and Engineering, 11 (5), 978, (2023).
- [6] C. Narváez-Muñoz, M.R. Hashemi, P.B. Ryzhakov and J. Pons-Prats, "An enriched finite element/level-set model for two-phase electrohydrodynamic simulations", Physics of Fluids, 35, 012004, (2023), https://doi.org/10.1063/5.0127274.
- [7] M.R. Hashemi, P.B. Ryzhakov and R. Rossi, "Three Dimensional Modeling of Liquid Droplet Spreading on Solid Surface: an Enriched Finite Element/Level-set Approach", Journal of Computational Physics, Open access: https://doi.org/10.1016/j.jcp.2021.110480.
- [8] A. Jarauta, P.B. Ryzhakov, M. Secanell, P. Waghmare, J. Pons-Prats, "Numerical study of droplet dynamics in a polymer electrolyte fuel cell gas channel using an embedded Eulerian-Lagrangian approach", Journal of Power Sources, 323, 201-212, (2016), https://doi.org/10.1016/j.jpowsour.2016.05.030.
- [9] A.R. Hashemi, P.B. Ryzhakov, M.R. Hashemi, R. Rossi, N. Dialami and R. Zorrilla, "Challenges in modeling inkjet printing: physical and numerical aspects", 2nd Spanish Fluid Mechanics Conference, 2-5 July 2023, Barcelona, Spain.
- [10] P.B. Ryzhakov, M. Nuñez, M.R. Hashemi, R. Rossi, O. Antonova, "Data-driven approaches as a possible means for modeling water transport in gas diffusion layer of fuel cells", 8th European Congress on Computational Methods in Applied Sciences and Engineering, 5-9 June 2022, Oslo, Norway.
- [11] A. Hajisharifi, F. Romanò, M. Girfoglio, A. Beccari, D. Bonanni, G. Rozza, "A non-intrusive data-driven reduced order model for parametrized CFD-DEM numerical simulations", Journal of Computational Physics, 491, 112355, (2023).
- [12] A.M. Ares de Parga, A.R. Hashemi, N. Sibuet, R. Rossi and P.B. Ryzhakov, "Droplet Characterization through Neural Network Geometric Analysis and Classification for Drop-on-Demand Inkjet Systems", 9th European Congress on Computational Methods in Applied Sciences and Engineering ECCOMAS 2024, Lisboa, Portugal, (2024).