Executive Summary of
Mathematical Opportunities in Digital Twins (MATH-DT) Workshop

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Synopsis

On December 11–13, 2023, the workshop "Mathematical Opportunities in Digital Twins" was held at George Mason University, Arlington, VA. The workshop was supported by NSF via grant DMS–2330895. The scientific organizing committee was Harbir Antil (GMU, local organization), Benjamin Seibold (Temple University), and Kathrin Smetana (Stevens Institute of Technology). The workshop featured 13 plenary talks by leading faculty in mathematics and numerous engineering and application fields, 2 applications panels with 6 panelists from industry and applications, a funding agencies panel, a poster and demo session (30 contributions, many of them from students and early-career researchers), and multiple discussion sessions in which participants formed teams and produced materials on the discussion outcomes on Digital Twins. Information about the workshop can be found at the workshop website[3] and in the detailed book of abstracts.[4]

The goals of the workshop were to determine the ways in which the discipline of mathematics can contribute to the research on Digital Twins (DTs), how DTs can open up new mathematical directions, as well as to identify connections, synergies, and organizational efforts, both within the mathematical community and with other disciplines. While researchers from different application fields work with different definitions of a DT, a unifying aspect is that there is always a real-world system and a digital copy of it. A difference across applications is how strong the feedback from the digital copy to the real-world system is (the terminology "digital shadow" was proposed if that feedback is weak or absent). Either way, it was a universal theme that DTs incur numerous critical challenges that require mathematical innovation and the involvement of researchers from the mathematics community.

Based on the talks and the discussion results, the following key questions and themes were identified:

- Funded research by mathematicians on DTs was identified as important for multiple reasons: (a) many applications encounter a concrete need of new methods and concepts incurred by the demands around DTs; (b) DT-related research inspires intrinsically new math; and (c) the involvement of mathematicians in cross-disciplinary research teams on DTs will generate a broader impact on the mathematics community.

- While mathematical models and simulations of real-world systems have existed for a long time, the coupling/interaction between a DT with its real-world system provides a completely new playing field, and many concepts in model development, efficient forward models and methods, optimization/control, UQ, software, HPC, and data must be fundamentally re-thought.

- DTs apply in a huge number of application fields (see "Mathematical Modeling" below), thus increased and new mathematical research on DTs carries a substantial potential for broader impacts and societal benefits. Moreover, the new mathematical challenges and opportunities that DTs impose will jump-start novel research directions within the mathematical discipline.

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[3]https://mathdt.science.gmu.edu

[4]https://mathdt.science.gmu.edu/wp-content/uploads/2023/12/Book_of_Abstracts_10.pdf

- Important examples for the role of mathematical research include: (i) to provide a rigorous foundation and framework for methods; (ii) the establishment of holistic methodologies to guarantee stability/robustness/convergence of coupled reality–DT systems; (iii) to combine all 6 blue boxes below (incl. mathematical software and HPC) within one discipline; and (iv) to serve as an information hub that connects different applications fields and exploits critical commonalities and cross-fertilization.
- There is a lot of ongoing effort labeled "Digital Twin", including in industry. It is therefore critical to establish appropriate research support structures now that enable the mathematical research community to effectively engage in productive research endeavours in the area.

Challenges and Opportunities

Throughout the workshop (in talks, discussions, and panels), challenges and opportunities within certain research areas have been highlighted. These are outlined in the boxes below. After the boxes we also emphasize overarching challenges and opportunities that keep reappearing or arise because Digital Twins (DTs) cut across many mathematical research areas and disciplines.

Mathematical Modeling

While the mathematics community has a fruitful record of developing principled models of many real-world processes, DTs impose a resurgent demand for the support of cross-disciplinary teams that develop novel models of real-world systems, which are compatible with a coupling between reality and its simulated twin. The engagement of mathematics researchers is critical in at least three aspects: (a) the advancement of fundamental methodologies for model development and learning, such as physics-informed learning, ODE-nets, etc., (b) the development of principled mathematical models (incl. PDE, dynamical systems) and their analysis, and (c) the engagement in cross-disciplinary teams of mathematicians and field scientists/engineers to ensure that the implicit needs/language of the application field are well captured. Talks, discussions, and panels at the workshop have showcased success stories of interdisciplinary work, involving mathematicians, on applications in traffic flow and autonomous vehicles, smart cities, medical and life science applications, industrial manufacturing, fusion energy, and more.

(Efficient) Forward Models and Methods

The vast majority of DTs rely on the real-time, reliable, and repeated solution of the forward model (e.g., for data assimilation, control, design and optimization) and can therefore not work without efficient or forward models or surrogate models, as standard numerical approximation methods are prohibitively expensive. Problems that are multi-physics, multi-component, transport-dominated, possess a high-dimensional parameter space, and/or involve moving or changing features (e.g., additive manufacturing), are challenging for state-of-the-art projection-based model order reduction methods relying on SVD-based compression or greedy algorithms. When localized and combined with multiscale methods, projection-based model order reduction methods are however well-suited to deal with challenging multiscale problems. The latter are difficult for current machine learning methods, which however seem to work well, e.g., for transport-dominated problems. Randomized methods represent another promising approach (which requires mathematical investigation) to construct efficient forward models and to detect structure in high-dimensional parameter spaces, as encountered in DTs, for instance, for creating surrogate models and/or with uncertain data functions.

Optimization, Control, and Inverse Problems

By definition, a DT continuously (i) assimilates data from the real-life object and updates the digital copy, and (ii) controls the real-life object using predictions from the digital copy. The former requires the calibration of the DT, i.e., the estimation of the (numerical) model parameters of the respective digital copy. This inverse problem can be formulated within the framework of Bayesian inference. The latter is a popular choice if, as for DTs, one wishes to quantify the uncertainties in the system. As a consequence of the uncertainties, the control objective and state constraints become random variables thus resulting in an optimization-under-uncertainty problem. Challenges include: (i) large or infinite-dimensional parameter spaces (e.g., spatio-temporal, additional hyperparameters), (ii) the need for informative priors within the Bayesian framework, and (iii) the method of adjoints (popular for solving the inverse problem or optimization under uncertainties) may not be applicable or may not perform satisfactorily, e.g., for legacy codes, non-smooth problems, and complex systems.

Prediction, Certification, Validation, and Uncertainty Quantification

In order to be able to trust the predictions made by the DT, and to be able to act on them, methodologies are imperative for the validation and certification (V&D) of the DT and the quantification of the involved uncertainties. Certification is already challenging for certain models that form part of the DT such as machine learning models; for the latter, explainability and interpretability are critical issues. In addition, when thinking of the full DT, completely new research questions and challenges arise in the context of V&D: (i) What is a good measure to determine the quality of a DT? (ii) For DTs based on different types of components, software, and models (statistical, physics-based, etc.), a complete certification framework only for the digital copy without the data updates is an important research theme. (iii) As the DT changes over time through updates triggered by incoming data, it is unclear whether and how these incoming data can also be used to validate the DT in some fashion. There was a consensus at the workshop that the development and maintenance of test or benchmark problems, which should ideally include the real-life object, appears to be an important route—which again represents a cross-disciplinary endeavour. Challenges that emerge in quantifying the uncertainties stemming for instance from the data or models include: (i) the selection of (efficient) forward models and their fidelity, (ii) the collection of data such that quantities of interest such as the mean can be estimated within a given budget, (iii) risk measures are often non-differentiable and require many samples to assess rare events, (iv) the proper choice of samples. Statistical analysis, which provides ideally non-asymptotic theoretical guarantees for uncertainty quantification, may provide a pathway to make DTs trustworthy.

Mathematical Software

Talks and discussions have highlighted that some of the existing challenges on mathematical software are likely intensified in DTs: (i) As software usage becomes increasingly modular and multi-faceted (a positive development in principle), there is an increasing disconnect of time scales: mathematical software requires development and user support for 10+ years; but external support operates on shorter and shorter time scales. (ii) How can the welcome trends towards open-source software and increased reproducibility be carried over to DTs which involve hardware, private data, or protected entities? (iii) How can mathematics students and young researchers be supported to produce excellent software, if DTs also require a mastery of a multitude of other components? (iv) The question how mathematical models, simulations, and data analysis can be cast into software that allows for an effective and intuitive interaction with human users was identified as a critical challenge that computational mathematicians need to be supported to engage in.

Data Acquisition, Processing, and Real-time Feedback

Incorporating data into models and algorithms is a critical task in science and engineering, and DTs are obviously no exception from this. In particular, the ongoing research on data science, randomized methods, machine learning, artificial intelligence, etc. will be crucial for many of the above aspects in DTs (e.g., randomized methods generate a compressed version of data which is critical for transferring, integrating, and analyzing data). However, the real-time feedback between a DT with its real-world system imposes the need for further dedicated research on stability, robustness, UQ, etc. in light of faulty data, missing data, cybersecurity (adversarial data), and other aspects. DTs also frequently involve the fusion of data from multiple sources, possibly with vastly different scales and accuracy; and new mathematical methods must be developed to reliably deal with that.

Cross-cutting challenges:

- Integration of methods from different boxes: As DTs tend to rely on methods from many or all of the boxes above, it is imperative to devote research efforts to methods that interplay well when combined. For instance, while classically surrogate models have been built and used (e.g., throughout an outer optimization loop), it has recently been found that novel, specifically adapted surrogate models are much more effective. Significant efforts must thus, for instance, be undertaken to create efficient forward models that are specifically designed to work within optimization, inverse problems, data assimilation, or uncertainty quantification. Another critical example is the needed quantification of uncertainties throughout the whole process, which will result in optimization problems that are non-smooth, non-convex, and large-scale and high-dimensional parameter spaces, thus requiring fundamentally new mathematical developments in those areas as well.
- Coupling of different models or components: The workshop has highlighted that DTs critically impose the need to couple different models (PDE-based, empirical, statistical, etc.), such that the full model/twin is explainable, interpretable, well-defined/-posed, and stable. Principled models (e.g., PDE models) in DTs already encounter the challenges of multiple scales, multi-physics, or high dimensionality. If one now, on top of that, couples structurally different types of models (such that data can effectively be incorporated to update the DT, that uncertainties within the whole system and process can be quantified, etc.), radically new methodologies must be developed and analyzed, which is a natural task for the mathematical research community.
- Even with the research in the boxes above conducted, and a successful integration and coupling ensured, the real-time application of DTs will in many situations require the invention of fundamentally novel frameworks to account for uncertainty, control, and data in a fully coupled real-time environment, in lieu of established, but too sluggish approaches. In addition, the workshop has highlighted that many real-world DTs may involve a human in the loop, and mathematical research must devote more attention to the behavior of such real-time interactive systems.
- Computational architectures available to DTs: Traditional research on efficient mathematical methods frequently assumes computer architectures employed for traditional high performance

computing. In contrast, many DTs will be run on very specialized architectures (e.g., board computer of cars), and the constraints and limitations of the system may require the development of completely different models, methods, algorithms, and data analysis techniques than what the boxes above individually would inspire/lead to.

Recommendations

The above synopsis and conclusions of the workshop give rise to the following recommendations:

- To optimally support the research needs around DTs, it must be ensured that mathematics researchers are supported in their roles of (a) providing foundational research (incl. frameworks and analysis of novel methodologies), (b) developing principled mathematical models (incl. PDE, dynamical systems, etc.) and their analysis, and (c) leading cross-disciplinary teams that leverage applied/computational expertise to advance DTs with application focus.
- The workshop has highlighted that the research needs imposed by DTs are widespread, cutting across many areas of mathematics, including fields not immediately associated with computing and simulation, as well as different disciplines such as engineering and the domain sciences. It is therefore important that funding is provided for projects that cut across different disciplines/programs, both within NSF DMS but also with other divisions or directorates. Attention must be given to the fact that important mathematical research related to DTs may not fall squarely within the existing DMS programs (e.g., the development of model hierarchies without a primary computational focus).
- Funding mechanisms that support bottom-up, "grassroots" research on ideas will be as important as support for already established teams. In particular, support must be ensured for small teams or single-PI research that targets specific aspects as well as for multi-PI cross-disciplinary teams in which mathematics researchers can play a lead role.
- Talks and discussions at the workshop emphasized the challenge of validating and certifying a DT. To ensure maximal impact of cutting edge mathematics research on DT, the explicit support of efforts towards establishing test and benchmark problems was identified as important. This includes the funding of (i) hardware, (ii) the instrumentation of real-life objects, and (iii) the associated maintenance, in research projects that mathematics researchers (co-)lead.
- We, the academic and research community, need to adapt how we train our students (and young researchers); and NSF's future structures/mechanisms must also account for that. This includes the need to more strongly appreciate/support young mathematicians engaging in truly cross-disciplinary research. Moreover, dedicated support of mathematicians should be considered to target future workforce development (e.g., the design of new educational materials, or curriculum development of graduate programs of interdisciplinary nature). The latter should be encouraged across all career stages (not just CAREER); and in turn, it should be ensured that proposals, particularly NSF CAREER projects, that truly cut across different programs within NSF DMS, or even across divisions or directorates, can be competitive.