A summary of the Breakout Discussions that took place at the 2021 virtual event.

AI, Data Driven Models & Machine Learning:

How Will Advanced Technologies Shape Future Simulation Processes?

Learn to Predict, or Learn to Simulate? Big Data, or Small Data? – Reality in the Simulation World.

Zhenyuan Gao | Dassault Systemes SIMULIA

From the presentations/case studies of the day, we started out talking about the current applications of machine learning (ML) to simulation. It was summarized that the two main categories of applications nowadays were: 1. directly using ML as a black box for surrogate models (low hanging fruit); 2. discovering new areas by extracting physics using ML method. As we saw more of the first category in a lot of case studies, the next question was on what's stopping people from going with the second category. The second category was also directly tied in with the data extraction problem. It was concluded data in reality came from many different sources (sensors, simulations, etc.), which a lot of times had discrepancies among them. This made getting consistent physics from the data very hard, but we should still try to combine them at the same level, without separating them into labels like "experimental data" and "simulation data". From here, we could have two separate directions to go. One was to make a physics-informed ML model, implementing physics directly, which had already been done in a lot of studies.

The other was to add engineering expertise as another set of data, which was a new direction. It was shared with us that some had already been doing similar explorations in this regard. It was summarized that a lot of engineering expertise could be concluded as data that said "yes" or "no", and easy to implement into models. We agreed that if more engineering expertise could be quantified, it should be considered as important data for building tools that learn to simulate. Finally, we discussed whether the currently developed applications were going to change the simulation field since we thought a lot of CAD engineers will not be willing to change their ways of solving problems. In those cases, tools that implement engineering expertise will be more applicable. With so many different methods that interpret data in different ways, we thought a standardization process would be necessary for us to build consistent ML tools.

Autoencoders: Are they the future of ROM and generative design?

Marc Emmanuelli | Monolith AI

During this discussion, we explored how Autoencoders can learn design DNA from historic CAD data. They can automatically scan unstructured polygon meshes to extract the distinct geometric features which characterises each design.

The two main benefits of Autoencoders for 3D CAD are:

1. To compress an existing design into a set ofgeometric parameters, in order to predict its performance.
2. To generate new, performance-optimised 3D designs which satisfy target goals and constraints.

What steps should I take to determine how my team might best utilize AI data driven models and the digital twin concept?

Rod Dreisbach | IEAC

The team recommended initial steps that included an assessment of the skills needed to address the new technologies of advanced engineering data science topics and digital twins. A precursor to digital twins is the understanding and scope that should be addressed by developing and implementing the required digital threads. The preferred approach would be to define a small, focused team to address these topics; however, cultural issues such as instilling a sense of ownership by all the associated management and technical personnel is a prerequisite (i.e., an appropriate set of Governance Policies and Procedures is required). Proposals for considering the adoption of such new technologies must address the business drivers for their pursuit such as what and how they will contribute to the company's profitability and competitive position in the marketplace. For the sake of end-user companies in addressing their independent needs for data interoperability between disconnected systems, the ongoing challenge that should be addressed in a broad sense is to achieve better alignment of the CAE vendor proprietary capabilities and their individual company's focus on business profitability. Conversely, the focus by vendors maybe should be on supporting international standards and procedures that address openness and interoperability issues which, in turn, would enable their customers to develop more value for themselves.

Neural networks are a key element of deep learning and artificial intelligence, which today are capable of some hugely impressive feats. Yet too few really understand how neural networks actually work. An initial reading on this topic is provided by a guide that takes you on a fun and unhurried journey, starting from very simple ideas, and gradually building up an understanding of how neural networks work, namely the 2016 book entitled "Make Your Own Neural Network" by Tariq Rashid.

An introduction to a broad range of topics in deep learning, covering mathematical and conceptual background, deep learning techniques used in industry, and research perspectives is provided by the 2016 textbook entitled "Deep Learning" by Ian Goodfellow, Yoshua Bengio and Aaron Courville.

How will real-time simulations impact the products around us?

Anthony Massobrio | Neural Concept Ltd.

Interestingly, some participants stated that almost at the end of the NAFEMS conference they felt convinced about the positive effects of real-time, Machine Learning (ML)- based engineering simulation.

The discussion steered towards what could be the functionalities needed today in ML and, looking into the future, what would be the evolution in the organization and life of engineering design departments.

In terms of functionality, we reviewed the importance of deploying confidence indices associated with inference by Deep Learning (see [1]) and the importance of having a well-represented sample. There was a discussion on how some CAE teams are still operating withdrawn from real CAD and work on an idealized CAD. ML with realistic "CAD-read" and "CAD-write" capabilities (i.e., inference and generative design) would create a reconsideration of some jobs in engineering. For instance, ML will zero all the time spent doing meshes and other preprocessing activities. The impact of ML could even reach other departments working on CAD data, even with implications on who is going to control this corporate-wise ML.

The topic of CAD assemblies (vs. parts) was introduced. Objects such as a complete car cannot be conceived as parametrically representable, today or midterm. This is where non-parametric solutions stemming from computer vision can come to help engineers to deal with seemingly untractable topics and unlock the potential of ML for realistic engineering design.

[1] "Masksembles for Uncertainty Estimation", Nikita Durasov, Timur Bagautdinov, Pierre Baque, Pascal Fua; https://arxiv.org/abs/2012.08334

Is physics based knowledge the future of ML/AI? What is "Small Data" and are we at the cusp of a revolution in ML/AI?

Juan Betts | Front End Analytics

We had a very interesting group from industry, academia, and one software vendor. There was discussion on the relative validity/credibility of lab/field vs. simulation data and how this intertwined in physics informed machine learning approaches. There was a discussion on how or whether these approaches could extrapolate outside the training set as opposed to interpolate. There was discussion on the importance of explain-ability of ML/AI. Credibility of models was a recurring theme during this session. There was also a discussion on how ML/AI applied to simulation felt like the beginnings of FEA/CFD and how this "revolution" was also different. In the FEA/CFD revolution the major driver was product validation as opposed to AI where the forces are more transformational (IoT, Autonomy, etc.).

The Best AI is Invisible. Would you agree?

Fatma Kocer | Altair Engineering

During the breakout session, we discussed the following:

- Synthetic data creation using DOEs
- Data driven reduced order models
- How we can increase productivity by using ML for building CAE models

How is AI impacting the way we should train tomorrow's engineering simulation workforce?

Olivia Pinon Fischer | Aerospace Systems Design Laboratory

We talked about how the AI landscape is developing within small companies and the fear that AI may be replacing jobs and people. We also discussed the difference in mindsets between engineers and scientists, how, depending on their expertise and experience, people tend to approach problems, validate results and solve problems altogether very differently. There was a pretty strong consensus that to be able to apply AI properly, one needs to understand statistics and the science behind AI. However, it is not clear which field of AI one needs to train himself/herself in. Finally, we briefly talked about the challenges associated with properly evaluating models.

We also had a side discussion on the development of Digital Twins in the Design phase, instrumentation approaches, etc.