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Modeling, Analysis and Simulation Community

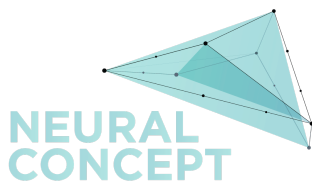
**Conference Abstracts**

# AI, Data Driven Models & Machine Learning:

## How Will Advanced Technologies Shape Future Simulation Processes

*April 28th - 29th, 2021 | Online*  
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## Day 1: Wednesday, 28 April

Title	Speaker	Company	Start Time (EDT)
<b>Welcome &amp; Introduction (Stage 1)</b>		NAFEMS Americas	<b>9:45</b>
AI for Simulation: Current Possibilities and Future Challenges	Peter Chow	Fujitsu Laboratories of Europe Limited	10:00
Challenges with Trustworthiness of Data-Driven and Machine Learning Approaches	Mahmood Tabaddor	UL LLC	10:30
<b>Case Studies (Parallel Presentations; Stages 1-2)</b>			
AI/ML/ROM-based Modelling, Prediction and Optimization for CAE Applications ( <i>Stage 1</i> )	Kambiz Kayvantash	CADLM	11:00
Machine Learning for Automation of Post-processing of Simulation Results and Extraction of 3D Digital CAE Reports ( <i>Stage 2</i> )	Mohan Varma	Visual Collaboration Technologies Inc	11:00
<b>Main Program; Stage 1</b>			
Efficient Multiscale Composite Modeling via an Embedded Long Short Term Memory Surrogate Microscale Model	Joshua Stuckner	NASA Glenn Research Center	11:30
<b>Case Studies (Parallel Presentations; Stages 1-2)</b>			
Combining Machine Learning and Physics-based Simulation for Product Development ( <i>Stage 1</i> )	Yangzhan Yang	Dassault Systemes SIMULIA	12:00
Best Practices for Data Driven Simulation Modeling ( <i>Stage 2</i> )	Danilo Di Stefano	Esteco SPA	12:00

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**Breakout Rooms (Parallel Discussions - Not Recorded; Rooms 1-4)**

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Differential Equations and Data Driven Models : Which one came first and which one is more reliable for engineering practices? ( <i>Room 1</i> ) <ul style="list-style-type: none"><li>- <i>The recognition of data science as a legitimate solution for solving engineering problems is in essence due to the arrival of data and advanced sensor technology. Contrary to classical model-based engineering, where models are numerical representations of partial differential equations (or are extracted from simple experimental setups such as material testing via equation fitting), data-driven engineering is based on direct observation and collection of data. Data mining, machine learning, and reduced-order modeling are the key accompanying technologies for AI/ML. How realistic and how important is this evolution for the future of engineering practices?</i></li></ul>	Kambiz Kayvantash	CADLM	12:30
Learn to Predict, or Learn to Simulate? Big Data, or Small Data? -- Reality in the Simulation World ( <i>Room 2</i> ) <ul style="list-style-type: none"><li>- When it comes to the application of machine learning in the simulation field, many researchers explore how machine learning could learn to predict - directly predict physical system responses without formulating physical laws explicitly, while others investigate how machine learning could learn to simulate – constructing the building blocks for a modeling and simulation framework. Some focus on adopting the power of big data for simulations while others struggle to extract enough structured data. In this panel discussion, we will discuss practical applications of machine learning in the simulation field, how machine learning could help capture both statistical data and physical rules, quality and forms of simulation data, and scalability/transferability of machine learned models, etc.</li></ul>	Zhenyuan Gao	Dassault Systemes SIMULIA	12:30
How to Trust ML/AI Algorithms? ( <i>Room 3</i> ) <ul style="list-style-type: none"><li>- <i>This session is meant to facilitate a conversation on the challenges and state of art on the topic of trustworthiness of AI/ML algorithms.</i></li></ul>	Mahmood Tabaddor	UL LLC	12:30
The Best AI is Invisible. Would you agree? ( <i>Room 4</i> ) <ul style="list-style-type: none"><li>- <i>Product engineers do not have to be computer scientists to benefit from computers, so why should they need to be data scientists to benefit from data? As software vendors, we should bring all these technologies – simulations, machine learning, and HPC to our customers so that they can benefit from them while working on their own challenges – designing high performing, robust, sustainable, pleasing, innovative designs.</i></li></ul>	Fatma Kocer	Altair Engineering	12:30
Open Discussions ( <i>Additional Rooms Available</i> )	N/A	N/A	12:30

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## Day 2: Thursday, 29 April

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Title	Speaker	Company	Start Time (EDT)
<b>Brief Welcome (Stage 1)</b>		NAFEMS Americas	<b>9:55</b>
Learning Simulation Using Graph Networks	Tobias Pfaff	DeepMind	10:00
Data Science Driving the Future of Engineering Simulation	Robin Tuluie	Physics X	10:30
<b>Case Studies (Parallel Presentations; Stages 1-2)</b>			
The New "AI" Wave: Does It Apply to Engineering? ( <i>Stage 1</i> )	Pierre Baqué	Neural Concept Ltd.	11:00
AI-Powered Product Design ( <i>Stage 2</i> )	Fatma Kocer	Altair Engineering	11:00
<b>Breakout Rooms (Parallel Discussions - Not Recorded; Rooms 1-5)</b>			
How will real-time simulations impact the products around us? ( <i>Room 1</i> ) - <i>The last decades have seen CAE grow from validation and analysis stages to simulation-driven design in Industry 4.0. Now, let us imagine another leap forward for CAE: simulation becoming pervasively real-time, thanks to ML. We invite you to a discussion to imagine the practical outcomes of such a scenario: the impact on industry processes, on final products and the way they are designed, the type of "users" (e.g. full democratization? no more "user" - just embedded simulation?) and the connection to product optimization. This speculative exercise can stimulate the discovery of new applications for ML, highlight actions to be taken on the way, and especially identify low-hanging fruits for the near future.</i>	Anthony Massobrio	Neural Concept Ltd.	11:30
What steps should I take to determine how my team might best utilize AI data driven models and the digital twin concept? ( <i>Room 2</i> ) - <i>There has been considerable hype recently about application of the advanced engineering data science topics of AI data driven models and digital twins in support of engineering simulation processes. Customarily, these processes have relied on physics-based mathematical models, logical models, and relevant data derived from physical model counterparts. This discussion session is aimed at addressing the steps that should be followed when the new techniques of using AI driven models and digital twins are to be considered in conjunction with engineering simulation processes. Several related terms are provided below.</i>	Rod Dreisbach	IEAC	11:30

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- *Data Driven Model (Ref: Internet): The relationship between input and output data of a process that is based on direct observation and collection of data, including the use of statistical and machine learning techniques.*
  - *Logical Model (Ref: Rod Dreisbach; NAFEMS Technical Fellow): A set of essential relevant characteristics and requirements that are not represented physically or mathematically but which are descriptive of a system and its components, what it does, and how it does it in its operational environment.*
  - *Digital Thread (Ref: JAMA Software on Internet): A data-driven architecture that links together information generated from across the product lifecycle and is envisioned to be the primary or authoritative data and communication platform for a company's products at any instance of time.*
  - *Digital Twin (Ref: Joint NAFEMS/INCOSE SMSWG): A digital surrogate that is a description of a physical asset such as one or more products, processes, systems, people, and devices that can be used for various purposes. It makes use of data to/from its real-world asset and may change in tandem throughout the lifecycle of the physical asset.*
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How is AI impacting the way we should train tomorrow's engineering simulation workforce? (Room 3)

Olivia Pinon  
Fischer

Aerospace  
Systems  
Design  
Laboratory

11:30

- As AI continues to transform engineering and the modeling & simulation industry by bringing increased capabilities and opportunities for humans to collaborate with intelligent machines and systems, it is expected that professional roles will shift and become more complex. Core competencies such as problem-solving, cross-functional collaboration, but also analysis and interpretation based on AI processing and outputs will likely become more important. In addition, new questions will have to be addressed such as the role that collaborative platforms and collective intelligence will have in how we develop and deploy expertise, or how to best allocate tasks between humans and machines. The use of simulation models which leverage ML/AI will also require that engineers understand how the algorithms work, and more broadly understand where and how AI benefits them and how to combine it with other forms of simulation (e.g. physics-based). Hence, as a result of the acceleration of AI, academic institutions and organizations will need to rethink how to prepare their workforces, from anticipating the skills needed, to identifying solutions to help people learn and develop new skills.

*(continued on next page)*

<p>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? (Room 4)</p> <ul style="list-style-type: none"> <li>- <i>Over the past few years we’ve seen the importance of ML/AI grow as it relates to its use in smart connected products. At the core of ML/AI algorithms is using data for these algorithms to learn and create insight. There has been increasing realization that simulation can provide insights, and as such, speed the learning process of ML/AI, thereby reducing the amount of other data required (i.e. “Small Data”). Therefore, the simulation community is likely to play a key role not only in the design of smart &amp; connected products, but also in optimizing the experiences and outcomes these devices provide its users.</i></li> </ul>	Juan Betts	Front End Analytics	11:30
<p>Autoencoders: Are they the future of ROM and generative design? (Room 5)</p> <ul style="list-style-type: none"> <li>- <i>Autoencoders have transformed the way we do image recognition and language translation. Now they have become popular for reduced-order modelling, principal component analysis and generative design. Various experts from Siemens to Stanford already recognise their powerful capabilities to retrieve information while ignoring complex noise. You may have seen chairs designed by autoencoders, but what are they actually capable of, and who is really using them?</i></li> </ul>	Marc Emmanuelli	Monolith AI	11:30
Open Discussions (Additional Rooms Available)	N/A	N/A	11:30
<b>Panel Discussion (Stage 1)</b>			
<p><b>State of Explainable AI/ML</b></p> <ul style="list-style-type: none"> <li>- <i>The panel will discuss the challenge of explainability for ML models and what the current state of art is in this area.</i></li> </ul> <p>Panelists will include:</p> <ul style="list-style-type: none"> <li>o <b>Mahmood Tabaddor, UL LLC (Panel Discussion Leader)</b></li> <li>o <i>Peter Chow, Fujitsu Laboratories of Europe Limited</i></li> <li>o <i>Ankit Patel, Rice University</i></li> <li>o <i>Olivia Pinon Fischer, Aerospace Systems Design Laboratory</i></li> <li>o <i>Robin Tuluie, Physics X</i></li> </ul>			12:30

**Presenter Name:** Peter Chow

**Presenter Company:** Fujitsu Laboratories of Europe Limited

**Presentation Title:** AI for Simulation: Current Possibilities and Future Challenges

**Location:** Stage 1

**Presentation Date & Time (EDT; New York):** 4/28/2021 @ 10:00

**Keywords:** Data-Driven AI, Digital Twin, AI for Simulation

**Abstract:**

If you have a smart phone then you have and using AI (data-driven artificial intelligence). A disruptive technology that is now ubiquitous in our daily life for work and play. Digital transformation, Industry 4.0, Society 5.0, digital twin, etc. are global topics driving a safe, sustainable and resilient society and businesses. AI and Simulation are key actors, individually and in combination. The latter is exciting, offers breakthroughs not possible before. For example, train a deep learning network model with existing physics-based simulation and metadata for AI to predict result to interact with users in real-time. With tacit and other knowledge learnt by the trained model, it further open up democratisation of simulation and usages. In this presentation, we look at the AI for Simulation journey so far – what is possible and challenges ahead. We will incorporate industrial use cases in CAD and CAE to demonstrate.

**Presenter Name:** Mahmood Tabaddor

**Presenter Company:** UL LLC

**Presentation Title:** Challenges with Trustworthiness of Data-Driven and Machine Learning Approaches

**Location:** Stage 1

**Presentation Date & Time (EDT; New York):** 4/28/2021 @ 10:30

**Keywords:**

**Abstract:**

The NAFEMS community is well aware of Verification & Validation (V&V), well developed guidelines meant to ensure that the predictions from computational engineering models can be credible and used with confidence to support decisions. AI techniques such as machine learning have become more prevalent, both within products, and as engineering tools. In this talk, we will cover the challenges associated with developing a similar set of V&V guidelines for data-driven, machine learning modeling approaches.



**Presenter Name:** Kambiz Kayvantash

**Presenter Company:** CADLM

**Presentation Title:** AI/ML/ROM Based Modelling, Prediction and Optimization for CAE Applications

**Location:** Stage 1

**Presentation Date & Time (EDT; New York):** 4/28/2021 @ 11:00

**Keywords:** ML/ROM, Real-Time CAE & OPTIMIZATION, CRASH, SAFETY, CFD, Multi-Physics

**Abstract:**

Machine learning and Reduced Order Modelling (ROM) techniques are interpolation methods exploiting data sets derived from existing virtual or experimental setup. They are essential to the concept of Digital Twins since they provide the missing link for both rapid re-design and operational evaluations in real-time. While the starting point is a DOE-type design with sufficient space filling properties, ML/ROM are different from response surface methods (RSM) where the approximation functions (surrogate model), often representing variations of a scalar entity within the design space, are imposed by the shape and nature of the fitting surface or a prescribed equation which also affects the number of runs required. ML/ROM techniques exploit the known physical behavior represented by the “modal” contents or similitudes expressed in terms of clusters of responses (ROM) in conjunction with various simple model prediction techniques (ML). In some cases, ML/ROM can be considered as algebraic solutions, exploiting decomposition techniques of special and temporal components, to reduce the volume of data set while preserving the most important parts of the information contained within that data set, which is necessary for retrieving all or the most essential part of the information when needed. Otherwise, we can also consider ML/ROM as implementation of clustering or other “lossy” data compression techniques, allowing for the reduction of the amount of data required for the reconstruction of the complete data set. Both such techniques allow for creating on-board and real-time applications based on voluminous experimental or simulation results (ex. Finite element). In this presentation, we shall provide state-of-the art robust and industrial solutions to typical applications in Crash & Safety, CFD, multi-physics and optimization. All have employed in one way or another.

**Presenter Name:** Mohan Varma

**Presenter Company:** Visual Collaboration Technologies Inc

**Presentation Title:** Machine Learning for Automation of Post-processing of Simulation Results and Extraction of 3D Digital CAE Reports

**Location:** Stage 2

**Presentation Date & Time (EDT; New York):** 4/28/2021 @ 11:00

**Keywords:**

**Abstract:**

In the product manufacturing industry, the significance of engineering simulations in the design and development of new products and product improvements has increased many fold over the past two decades. A typical engineering simulation workflow involves the CAE analysts pre-process and prepare models, run solvers to create simulations and finally post-process the simulation results and then document the insights and findings into CAE reports. These simulation insight reports play a major role in engineering decisions and design updates and are shared with the managers, designers & release engineers. Rapid advances in computing hardware and processing power increased the size and complexity of the problems that are being simulated and reduced the turnaround time that the solvers take to provide the simulation results. The improvements in meshing algorithms lead to more tolerance for dirty geometries, increased the automation and reduced the manual effort and time required to be spent by the engineers and analysts in the preprocessing step. However, post-processing of the simulation results to identify the simulation insights and documenting them into actionable reports still remained as a predominantly manual process. A typical analyst spends a considerable proportion of his effort and time in manual post-processing and documentation. This process is very inefficient and it involves a significant amount of repetitive usage patterns. The lack of mechanisms to identify the repetitive usage patterns and to create robust and repeatable processes to post-process the engineering simulation results and to automatically extract the high fidelity actionable simulation insights into Digital CAE Reports is hampering the manufacturing industry to realize the engineering simulations' full potential. We at, VCollab, have been working to create solutions that allow users to create repeatable and machine learnable processes for processing the simulation results and automatic generation of "3D Digital CAE Reports" with high fidelity insights. The software system that we are working on would come with a library of predefined set of templates and reports. When a new model/solution is introduced into its database, it first extracts critical model metadata and identifies suitable report templates from its template database, based on the user history and the model metadata. These templates will be used to generate high fidelity 3D "Digital CAE Reports" containing 3-D views, 2-D plots and all the required annotations. Analysts can visualize the generated reports, edit them, do further post-processing in the browser, add additional content and save the updated high fidelity "3D Digital CAE Report" back to its database. It avoids the pain of starting the post-processing from scratch for every new model/simulation and makes use of captured repetitive usage patterns. Machine learning algorithms will be used to update the classification/clustering mechanism based on the differences in the simulation metadata and the user changes to the reports, to identify suitable report templates that would be better for future model/solution files. This presentation provides additional details about the steps along with the use cases and demonstrations.

**Presenter Name:** Joshua Stuckner

**Presenter Company:** NASA Glenn Research Center

**Presentation Title:** Efficient Multiscale Composite Modeling via an Embedded Long Short Term Memory Surrogate Microscale Model

**Location:** Stage 1

**Presentation Date & Time (EDT; New York):** 4/28/2021 @ 11:30

**Keywords:**

**Abstract:**

A neural network was trained as a computationally efficient surrogate for a physics-based micromechanics model and embedded within classical lamination theory. The microscale model used generalized method of cells to predict the transversely isotropic homogenized stiffness of composite plies during loading as damage progressed. The surrogate model was able to learn a latent material damage representation to capture loading history and path dependence using long short-term memory layers in the neural network architecture. When the surrogate was embedded within a macroscale classical lamination theory model, the efficient model was able to make predictions with a 29 times speed increase compared to generalized method of cells and 145 times faster than high fidelity generalized method of cells. This speedup came without almost no loss in accuracy. The surrogate predicted almost identical laminate response as the physics-based multiscale model with a mean absolute error of 10.5 MPa and an R-squared of 0.98.

**Presenter Name:** Yangzhan Yang

**Presenter Company:** Dassault Systèmes SIMULIA Corp

**Presentation Title:** Combining Machine Learning and Physics-based Simulation for Product Development

**Location:** Stage 1

**Presentation Date & Time (EDT; New York):** 4/28/2021 @ 12:00

**Keywords:** Machine Learning, Physics-based Simulation, Finite Element Analysis, Product Development

**Abstract:**

Physics-based simulation and machine learning are both paradigms that build predictive models for engineering problems. Finite Element Analysis, as a physics-based approach, describe a physical system with differential equations and solve them numerically. Machine learning, as a data-driven approach, discovers underlying patterns using a large amount of data. With the rapid enhancement in algorithm and hardware, machine learning has become a disruptive technology in many industries, e.g., autonomous driving. In this presentation, we will discuss a few key areas how machine learning can be combined with physics-based simulations to accelerate product development, including design, engineering and manufacturing, life sciences and simulation technology. Realistic use cases will be presented from composites simulation, additive manufacturing to life sciences and data driven simulation technologies.

**Presenter Name:** Danilo Di Stefano

**Presenter Company:** Esteco SPA

**Presentation Title:** Best Practices for Data Driven Simulation Modeling

**Location:** Stage 2

**Presentation Date & Time (EDT; New York):** 4/28/2021 @ 12:00

**Keywords:**

**Abstract:**

The rapid growth of engineering data availability and the increasingly cheaper computational resources are elevating machine learning techniques as a safe and convenient tool used by engineers in their daily work. In particular, developments in machine learning algorithms and computational resources help boost engineering data analysis, decision making and design. However, this requires engineers to know the limitations and applicability of ML algorithms to specific engineering problems. In this presentation, we will highlight ESTECO best practices in applying ML methodologies to engineering data, with a special focus on how this can integrate and complement the knowledge coming from simulation.

**Presenter Name:** Tobias Pfaff

**Presenter Company:** DeepMind

**Presentation Title:** Learning Simulation Using Graph Networks

**Location:** Stage 1

**Presentation Date & Time (EDT; New York):** 4/29/2021 @ 10:00

**Keywords:** graph neural networks, simulation

**Abstract:**

While machine learning models promise to significantly speed up numerical simulations, they are often only accurate in a very narrow range around the training data. In practice, this requires running a large number of expensive reference simulations for each use case, negating the potential performance benefits of using learned methods. In this talk we will present our recent work on neural graph architectures for learning physical dynamics end-to-end. We believe these methods are the path forward in learned simulation; compared to the prevailing CNN architectures, they have much stronger generalization and stability properties, and even allow to simulate larger and more complex setups than seen during training. We will explain the core ideas behind our models, and demonstrate several examples of learned 2D and 3D mesh-based (FEM) and particle (SPH, MPM) simulations.

**Presenter Name:** Robin Tuluie

**Presenter Company:** Physics X

**Presentation Title:** Data Science Driving the Future of Engineering Simulation

**Location:** Stage 1

**Presentation Date & Time (EDT; New York):** 4/29/2021 @ 10:30

**Keywords:**

**Abstract:**

A fluid-fluid heat exchanger is optimized using CFD and Machine Deep Learning. A Geometrical Deep Learning model using Neural Concept Shape is integrated into a robust Geometry – CFD – NCS – Optimization loop and workflow. The AI designs, iterates and optimizes the heat exchanger. The heat exchanger performance is significantly improved.

**Presenter Name:** Pierre Baqué

**Presenter Company:** Neural Concept Ltd.

**Presentation Title:** The New "AI" Wave: Does It Apply to Engineering?

**Location:** Stage 1

**Presentation Date & Time (EDT; New York):** 4/29/2021 @ 11:00

**Keywords:**

**Abstract:**

With the striking progress of Deep Learning for physics simulations, industrial design is experiencing a breakthrough in several directions. In particular, multiple lines of approaches are now making simulations much faster and providing sensitivities of simulation results with respect to the geometries, either through automatic differentiation or through adjoint techniques. For instance, Geometric Convolutional Neural Networks can be trained to replace time-demanding physics-based simulations. Sensitivities (or gradients) are then obtained by back-propagation, which opens the door to a wide range of gradient-based optimization techniques. Neural Concept Shape (NCS) is a software platform that lets engineering teams, at all levels of expertise, implement this technology into their workflows. NCS is a platform dedicated to advanced or expert users who want to exploit all the possibilities of Deep Learning for one or several applications. NCS users are often having a centralizing role, working in support of multiple other teams, either as external consultants or internal experts. NCS makes is primarily built to create new models, train them, benchmark and improve their performances. It is dedicated to simulation engineers, data-scientists, optimization or methods engineers who want to fast-track their adoption of Deep-Learning methods and act in support to application-oriented users. The expert users benefit from the algorithmic infrastructure and the NCS library to start on a solid basis and focus on the specificities of his application. The NCS user is working in a fully managed environment, where everything has been thought to make his work, at the frontier between data-science and traditional engineering, as effective and efficient as possible.



**Presenter Name:** Fatma Kocer

**Presenter Company:** Altair Engineering, Inc.

**Presentation Title:** AI-Powered Product Design

**Location:** Stage 2

**Presentation Date & Time (*EDT; New York*):** 4/29/2021 @ 11:00

**Keywords:**

**Abstract:**

**Presenter Name:** Mahmood Tabaddor

**Presenter Company:** UL LLC

**Presentation Title:** State of Explainable AI/ML

**Location:** Stage 1

**Presentation Date & Time (EDT; New York):** 4/29/2021 @ 12:30

**Keywords:**

**Abstract:**

The panel will discuss the challenge of explainability for ML models and what the current state of art is in this area.