Scientific ML in the Context of the Digital Twin

CWI Amsterdam

December 8th, 2023

SIEMENS

F. Schnös

F. Sievers

S. Gavranovic

B. Peherstorfer

M. Schulz

E. Uy

G. Jouan

D. Berger

C. Lessing

Q. Zhuang

T. Richter

F. Dietrich

H. Van der Auweraer

B. Obst

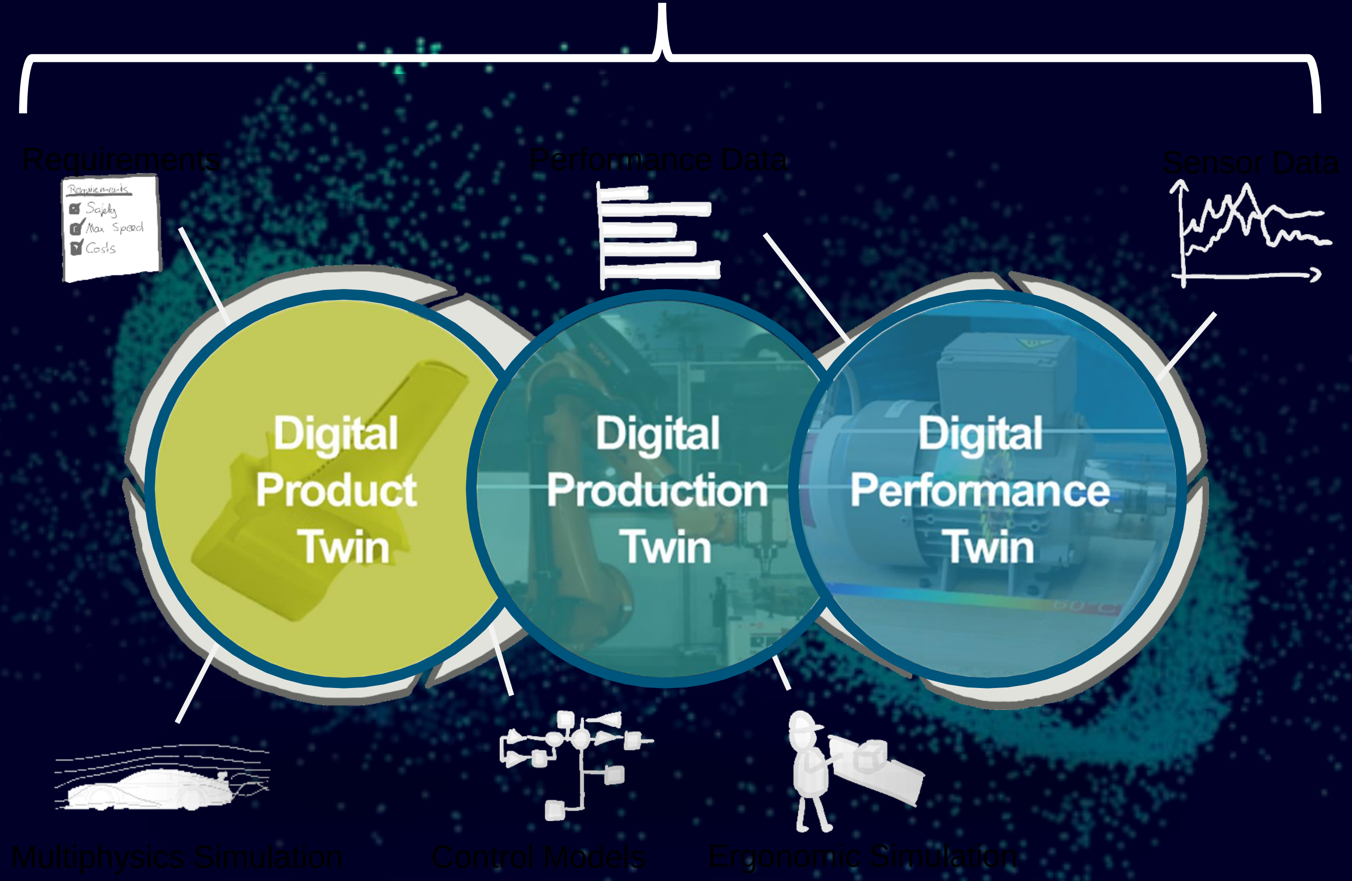
?

> We are able to combine the real and digital worlds like no other company!

Dr. Roland Busch,
President and CEO of Siemens AG

The comprehensive Digital Twin

Digital world



Real world

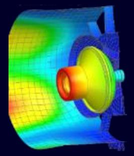
SIEMENS

1

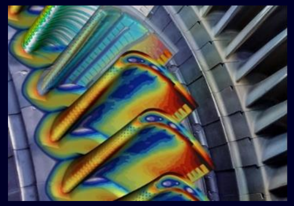
Digital Twin

Digital Twin - *An old story!*

Model Pioneers



CAx Sunrise



R&D Pervasion

~1985

~2000

- Geometry
- Single-Physics

- Computer-Aided Tools in R&D
- Multi-Physics

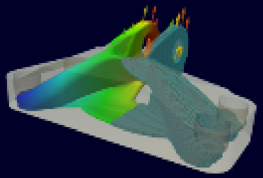
- Collaborative
- Model-based Engineering

CAx: Computer Aided Design, Engineering, & Manufacturing

SIEMENS

Why now? Enablers & Drivers

"Moore's Law" – More than Moore - Cloud: Exploding computing capacity beyond scaling of chip performance and cloud power, e.g. GPUs, Reconfigurable Computing, …



Algorithmic improvements: Creating breakthroughs will contribute significantly to efficiency of engineering process as well as open new ways of working and business propositions

Integrating Heterogeneous Models: different physics, different formulations, different scales: Multiphysics simulation – Co-simulation – FMI/FMU - Model Order Reduction - …

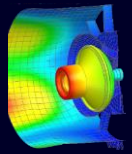
Internet of Things: performance data everywhere and readily accessible
Data analytics – Data driven performance monitoring and modeling

Challenged by increasingly complex systems and system requirements:
Mechanics – electronics – control – software… get tightly interconnected.
Performance demands become increasingly complex

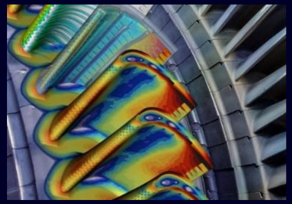
SIEMENS

Digital Twin - *A new age of computational paradigms*

Model Pioneers



CAx Sunrise



R&D Pervasion

Digital Twin Era

~1985 **~2000** **~2015**

- Geometry
- Single-Physics

- Computer-Aided Tools in R&D
- Multi-Physics

- Collaborative
- Model-based Engineering

- Democratization
- Model-based Operations
- X-as-a-service

CAx: Computer Aided Design, Engineering, & Manufacturing

SIEMENS

The Digital Twin Paradigm

"A comprehensive set of digital models accepted as full substitutes for reality to understand, predict, and optimize the physical counterpart's performance characteristics for specific purposes.

Dirk Hartmann (2023)

The Digital Doppelgaenger

"

Have you ever had a dream, Neo, that you were so sure was real? … How would you know the difference between the dream world and the real world?

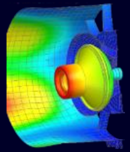
Morpheus,
The Matrix (1999)

Source: https://commons.m.wikimedia.org/wiki/File:Digital_rain_animation_medium_letters_shine.gif

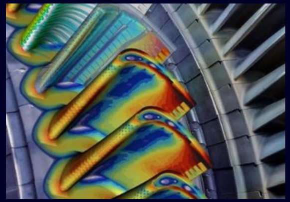
SIEMENS

Digital Twin - *A new age of computational paradigms*

Model Pioneers



CAx Sunrise



R&D Pervasion

Digital Twin Era

Industrial Metaverse

~1985 **~2000** **~2015** **~2022** **TODAY**

- Geometry
- Single-Physics

- Computer-Aided Tools in R&D
- Multi-Physics

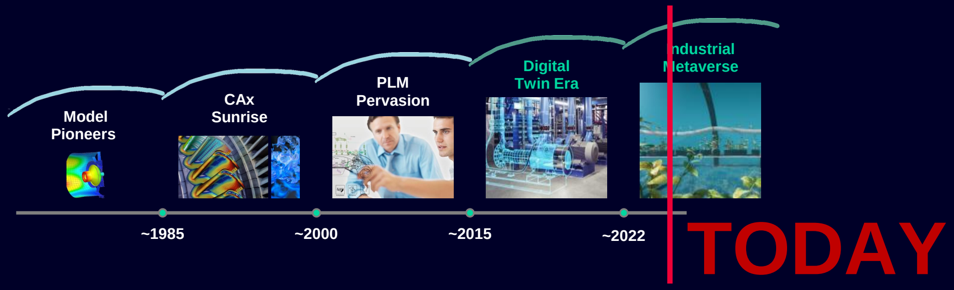
- Collaborative
- Model-based Engineering

- Model-based Operations
- X-as-a-service

- Democratization
- Realtime++ Predictions

CAx: Computer Aided Design, Engineering, & Manufacturing

Digital Twin – *State of Industrial Adoption Today*



The Digital Twin market **grows** with annual **CAGRs of 40-60%** in maintenance, business optimization, performance monitoring, …

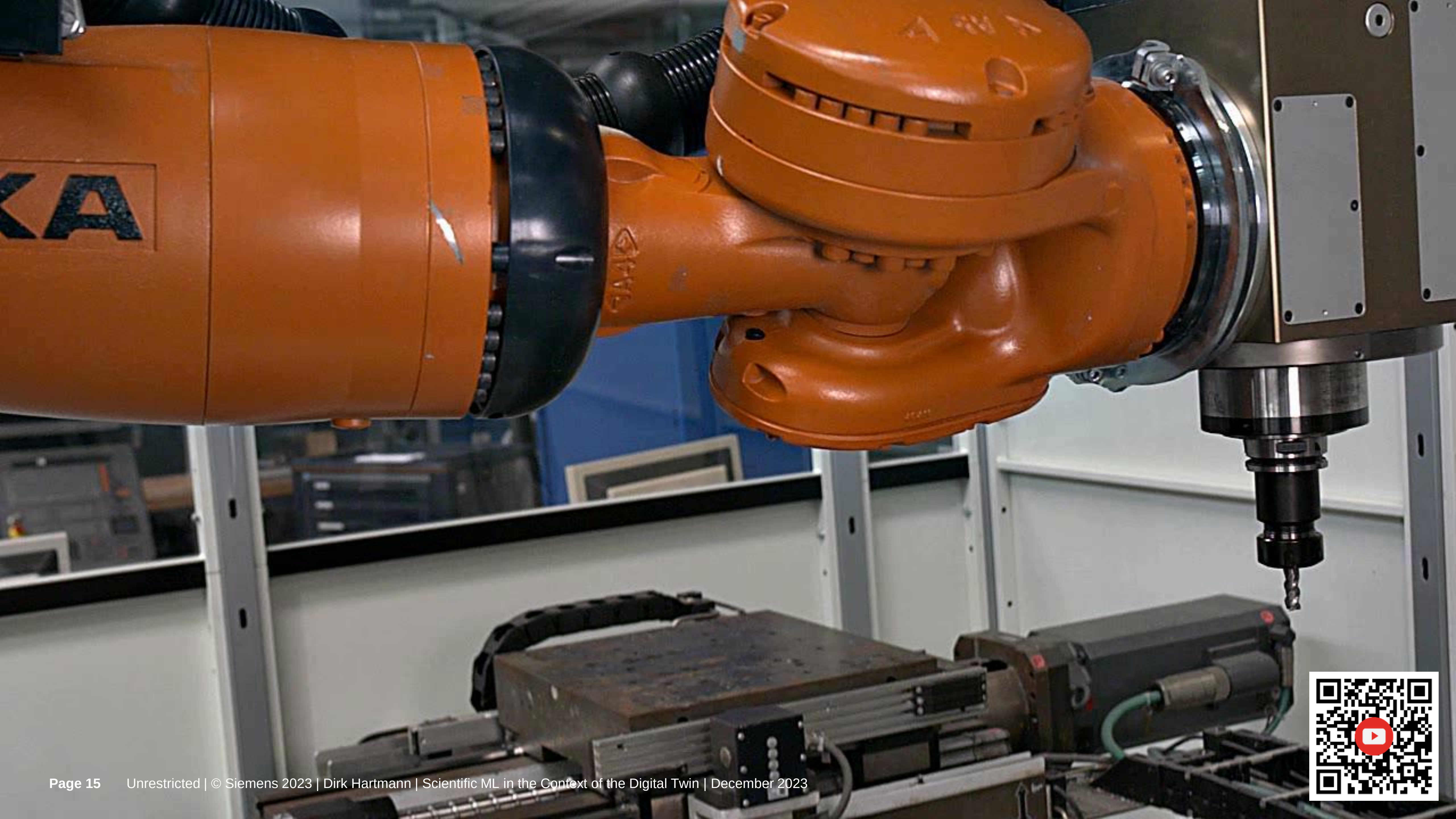
Many companies struggle to implement Digital Twins: “Digital Twins are slow and bespoke!”

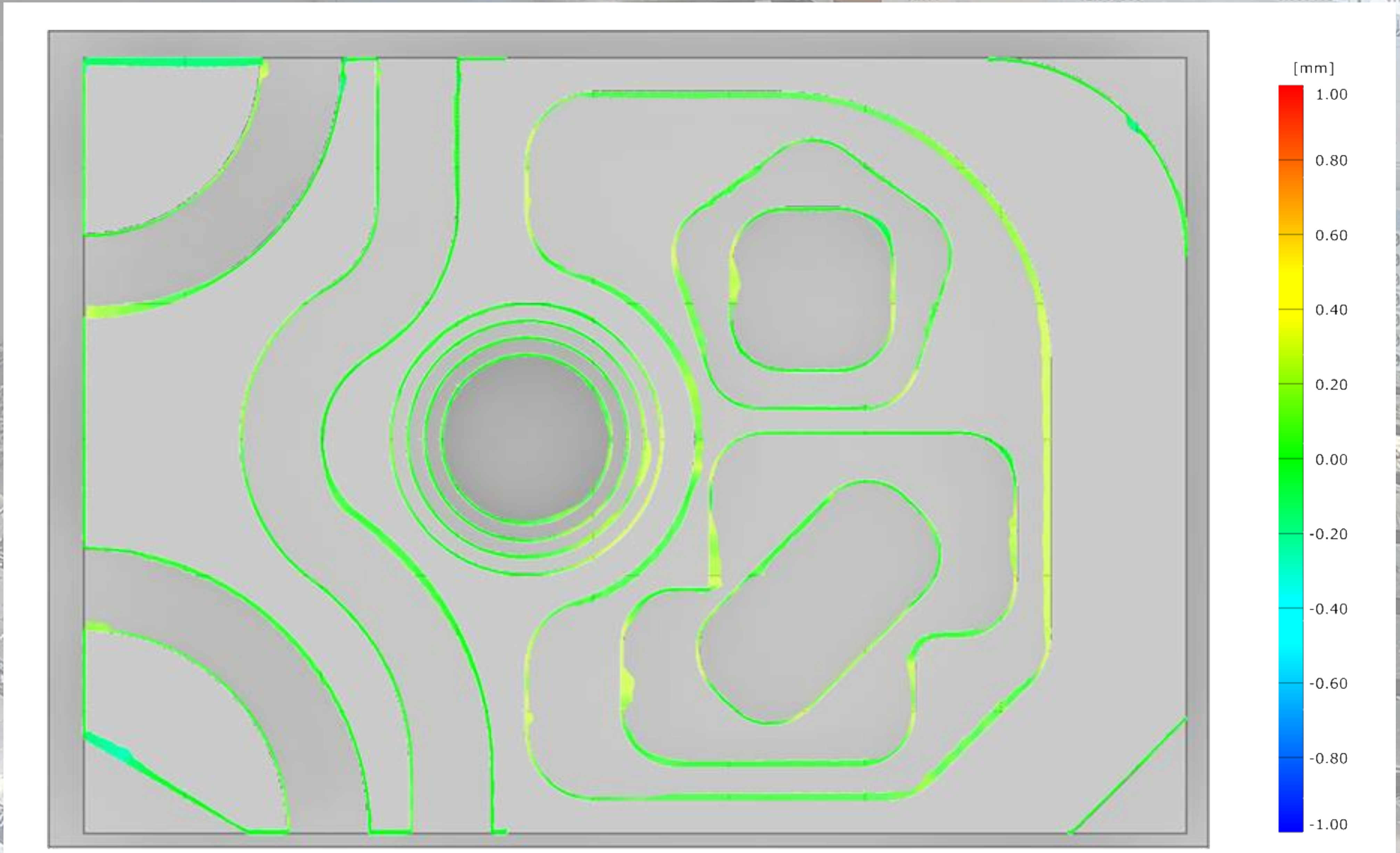
Road-blocks include company organizations change of business and processes, IT, …

Sources: Digital Twin Market by Technology, Type, Application, Industry, and Geography – Global Forecast to 2026, Markets and Markets
Implementation Model in the Context of Use of Digital Twins, Digital Twin Readiness Assessment
Major Challenges in Digital Twin based Operations, LinkedIn Survey

2

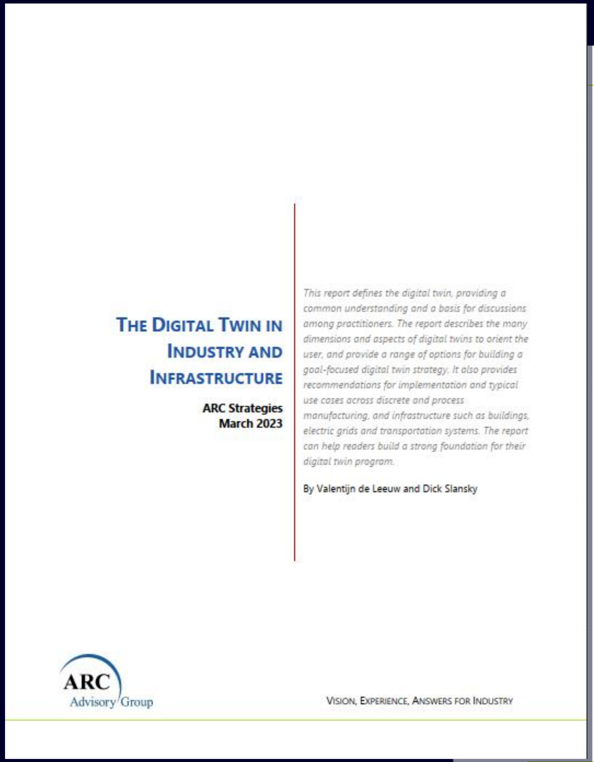
Scientific ML enabled Digital Twins




[mm]
1.00
0.80
0.60
0.40
0.20
0.00
-0.20
-0.40
-0.60
-0.80
-1.00


e impossible
on combined with
Augmented Monitoring
in real time during

The "first" math paper quoted in an Industry Analyst paper


THE DIGITAL TWIN IN INDUSTRY AND INFRASTRUCTURE

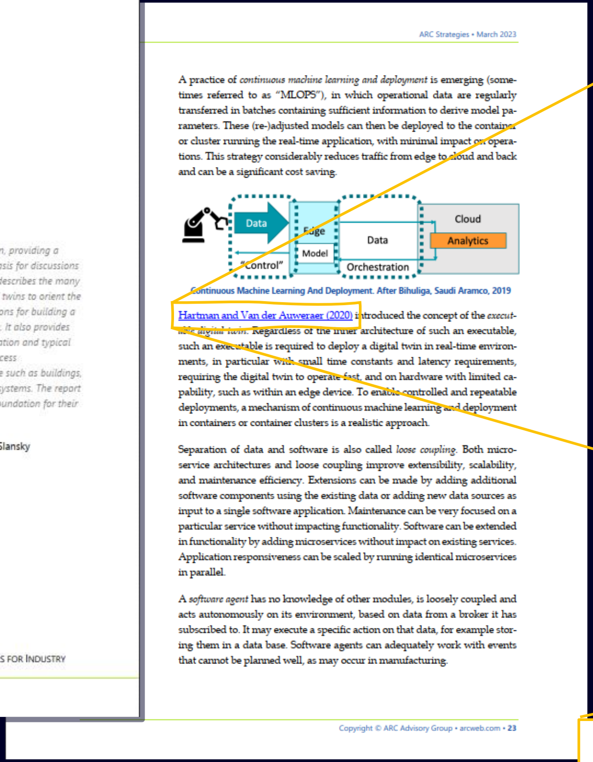
ARC Strategies
March 2023

This report defines the digital twin, providing a common understanding and a basis for discussions among practitioners. The report describes the many dimensions and aspects of digital twins to orient the user, and provide a range of options for building a goal-focused digital twin strategy. It also provides recommendations for implementation and typical use cases across discrete and process manufacturing, and infrastructure such as buildings, electric grids and transportation systems. The report can help readers build a strong foundation for their digital twin program.

By Valentijn de Leeuw and Dick Slansky

ARC Advisory Group

VISION, EXPERIENCE, ANSWERS FOR INDUSTRY


ARC Strategies • March 2023

A practice of *continuous machine learning and deployment* is emerging (sometimes referred to as "MLOPS"), in which operational data are regularly transferred in batches containing sufficient information to derive model parameters. These (re-)adjusted models can then be deployed to the container or cluster running the real-time application, with minimal impact on operations. This strategy considerably reduces traffic from edge to cloud and back and can be a significant cost saving.

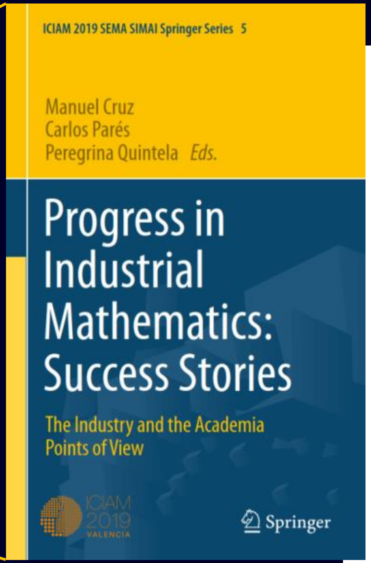
Continuous Machine Learning And Deployment. After Bihuliga, Saudi Aramco, 2019

Hartman and Van der Auweraer (2020) introduced the concept of the *executable digital twin*. Regardless of the inner architecture of such an executable, such an executable is required to deploy a digital twin in real-time environments, in particular with small time constants and latency requirements, requiring the digital twin to operate fast, and on hardware with limited capability, such as within an edge device. To enable controlled and repeatable deployments, a mechanism of continuous machine learning and deployment in containers or container clusters is a realistic approach.

Separation of data and software is also called *loose coupling*. Both microservice architectures and loose coupling improve extensibility, scalability, and maintenance efficiency. Extensions can be made by adding additional software components using the existing data or adding new data sources as input to a single software application. Maintenance can be very focused on a particular service without impacting functionality. Software can be extended in functionality by adding microservices without impact on existing services. Application responsiveness can be scaled by running identical microservices in parallel.

A *software agent* has no knowledge of other modules, is loosely coupled and acts autonomously on its environment, based on data from a broker it has subscribed to. It may execute a specific action on that data, for example storing them in a data base. Software agents can adequately work with events that cannot be planned well, as may occur in manufacturing.

Copyright © ARC Advisory Group • arcweb.com • 23


ICIAM 2019 SEMA SIMAI Springer Series 5

Manuel Cruz
Carlos Parés
Peregrina Quintela *Eds.*

Progress in Industrial Mathematics: Success Stories

The Industry and the Academia Points of View

ICIAM 2019 VALENCIA

Springer


Digital Twins 13

Fig. 6 Mixed reality setup allowing to measure spatial temperature distributions parallel to operations by means of online simulations. Reproduced with permission. Copyright © Siemens AG

a tremendous achievement [27]. At the same time using model order reduction technologies [28] the concept can be built directly on top of engineering models allowing to achieve the benefits with only little additional efforts. Mathematics enables quasi thermal X-rays for electrical motors allowing to monitor temperature distributions in real time (Fig. 6).[10]

5 The Next Wave—Executable Digital Twins

Albeit the previous section has shown four great examples of Digital Twins, a major limiting factor today is the manual work required to realize a Digital Twin, i.e. transfer of the corresponding models between different domains or life cycle phases. Most applications require to provide the models in the right execution environments with the right online capability in particular during the operations phase.

We therefore introduce the concept of an Executable Digital Twin, which will be from our point of view a key aspect in any future Digital Twin driven application.

Definition (Executable Digital Twin) An Executable Digital Twin is a specific encapsulated realization of a Digital Twin with its execution engines.[11] As such they enable the reuse of simulation models outside R&D. In order to do so, the

[10] Virtual X-ray for large motors https://youtu.be/86vkjykbHRM.
[11] Typically models today are distributed separately from their execution/simulation tools.

Definition (Executable Digital Twin) An Executable Digital Twin is a specific encapsulated realization of a Digital Twin with its execution engines.[11] As such they enable the reuse of simulation models outside R&D. In order to do so, the …

Sources: V. De Leeuw, D. Slansky (2023): The Digital Twin in Industry and Infrastructure, ARC Advisory Group Industry Report
D. Hartmann, H. van der Auweraer (2020); Digital Twins, Progress in Industrial Mathematics: Success Stories

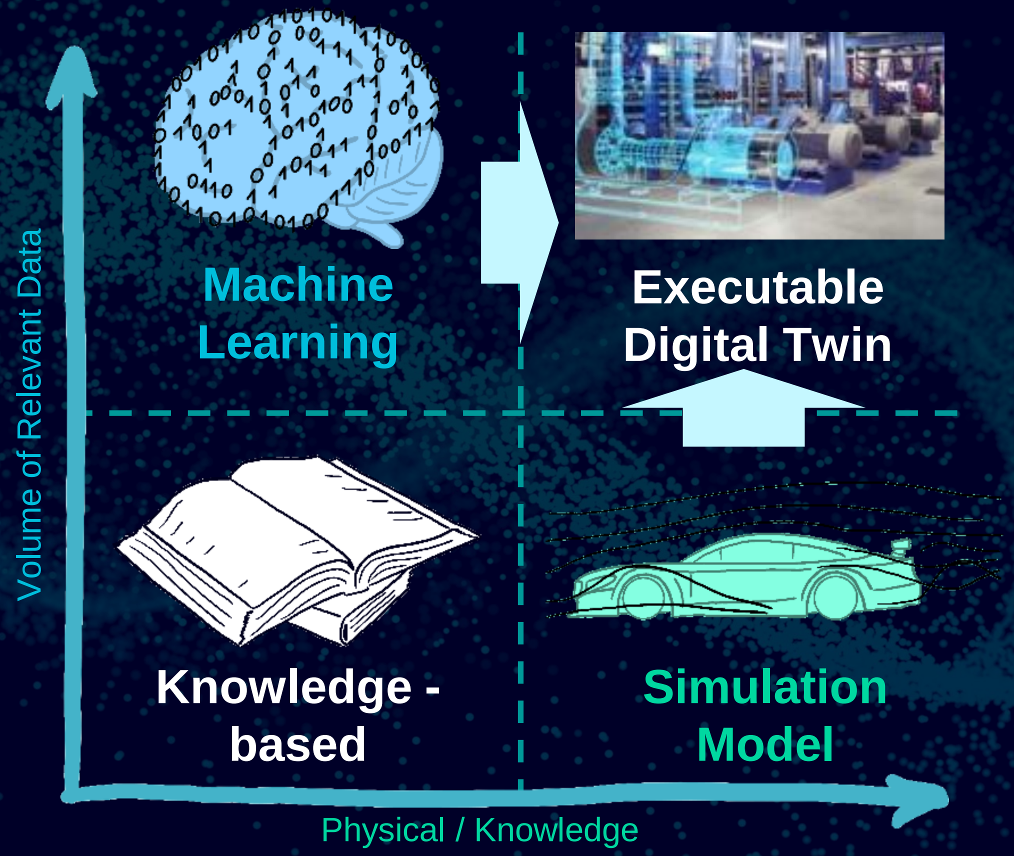
SIEMENS

3

Math Deep Dive

SIEMENS

ML combined with Simulation enable the Executable Digital Twins at scale

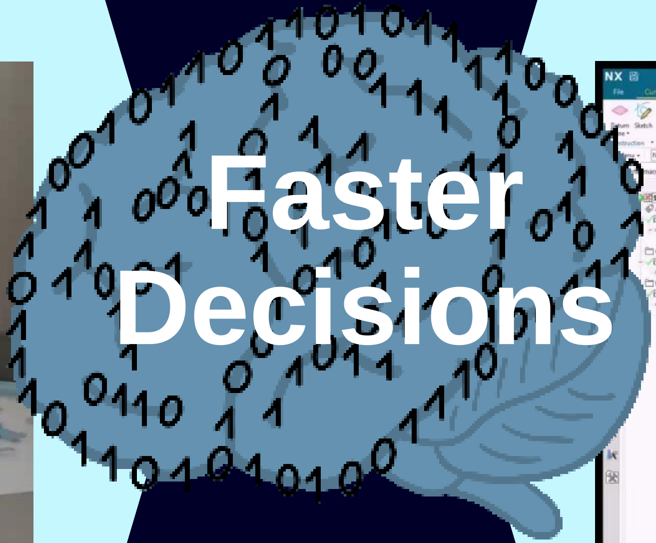


Courtesy to L. Horesh (2016): Should you derive? Or let the data derive - Towards a first-principles data-driven symbiosis

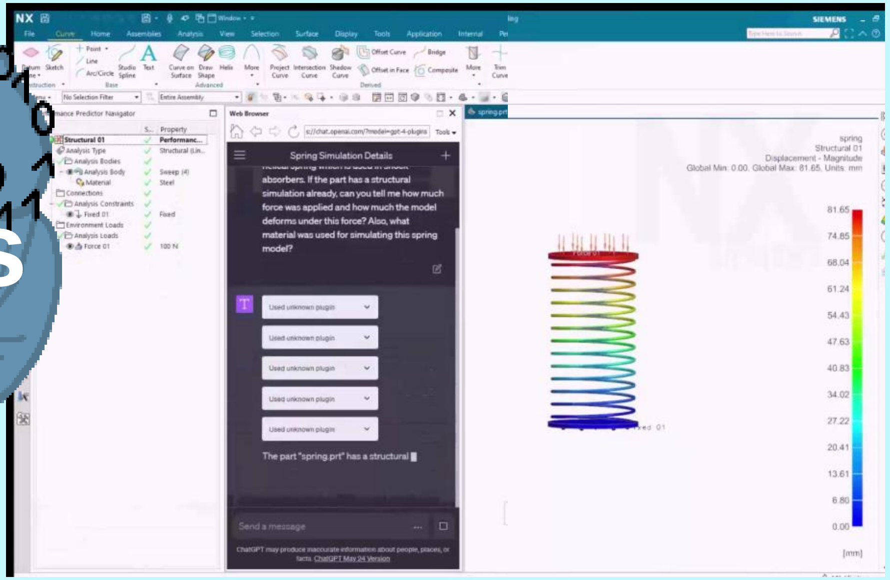
AI and ML boost Decisions in Engineering and Operation

Accelerate Predictions

High End CFD simulation of a car



Improve User Efficiency



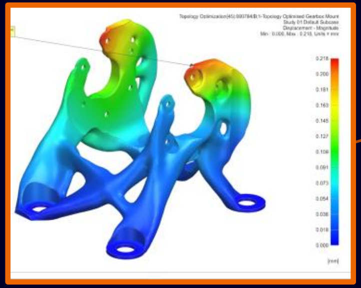
PoC

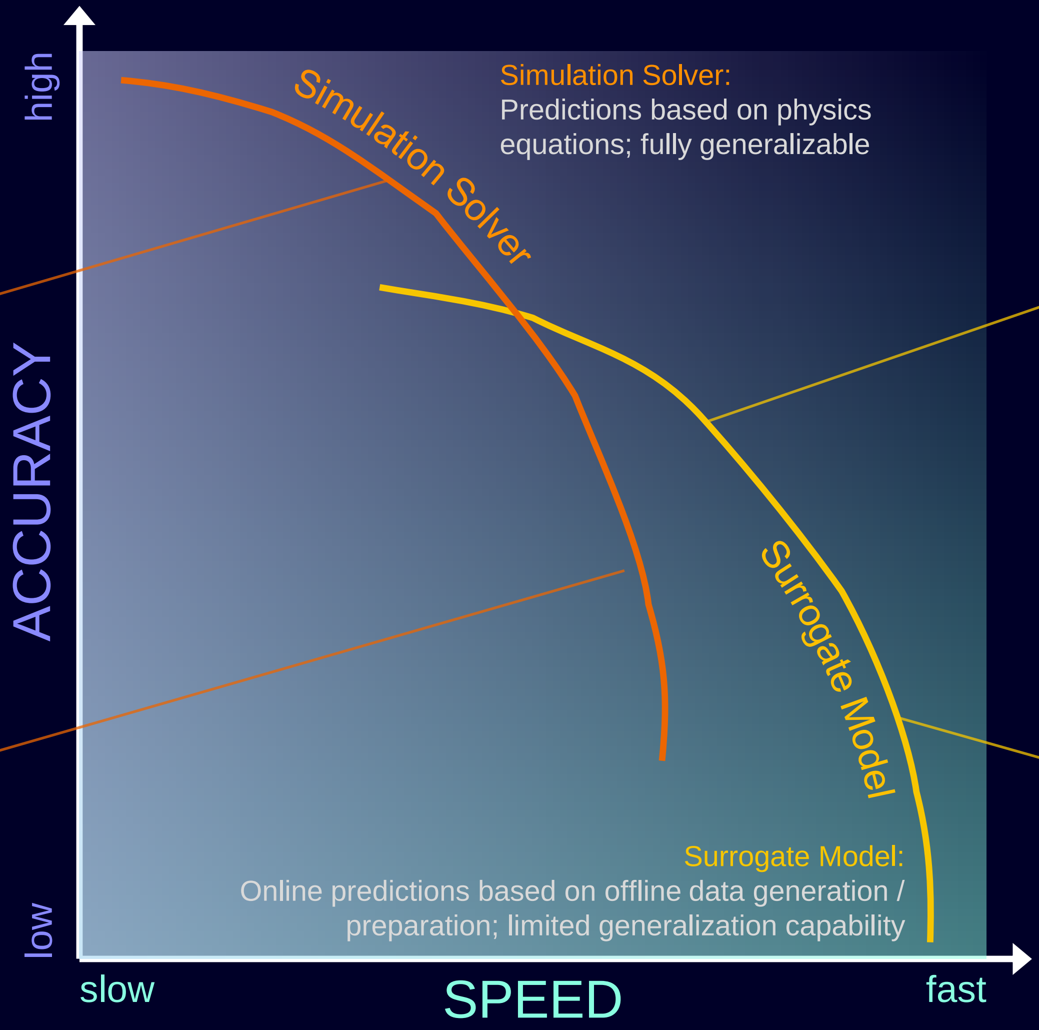
SIEMENS

ML-accelerated Prediction Use Cases

High End CFD simulation

Design integrated simulations



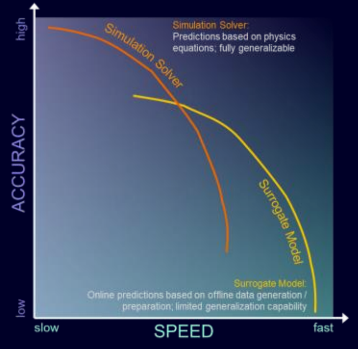


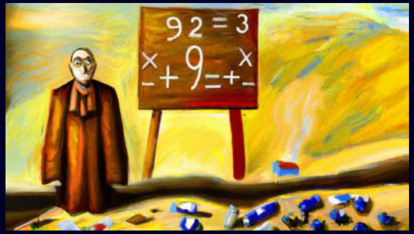
Product Configurator

ROM building

SIEMENS

ML-accelerated Prediction Use Cases





The Good

Acceleration of classical solvers

The Bad

Regression-based Model Order Reduction

The Ugly

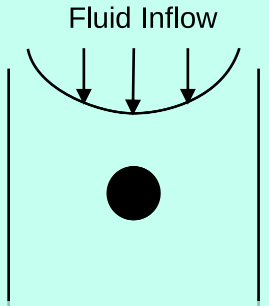
Sampling strategies for industrial MOR workflows

The Good

Acceleration of classical solvers

ML augmented CFD solver

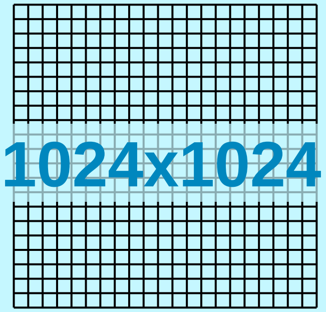
Simulation Task

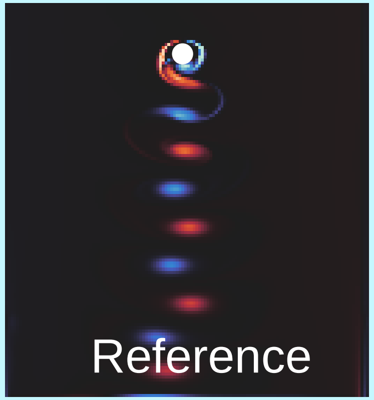


$$\rho \frac{D\vec{V}}{Dt} = -\nabla p + \mu \Delta \vec{V}$$

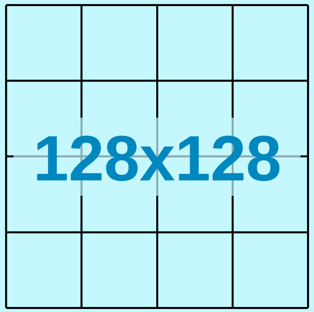
$$\nabla \cdot \vec{V} = 0$$

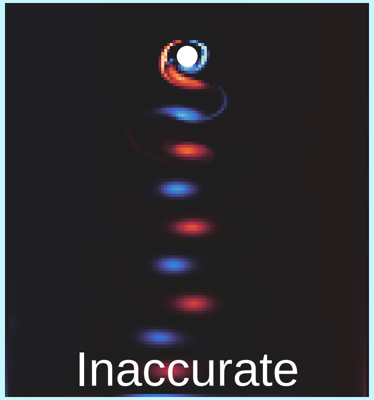
HiFi Simulation





LoFi Simulation

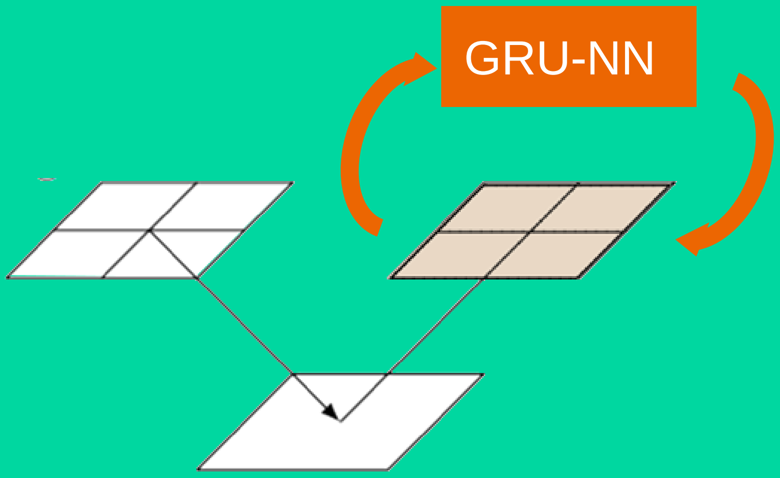




Using a coarser mesh allows a significant acceleration

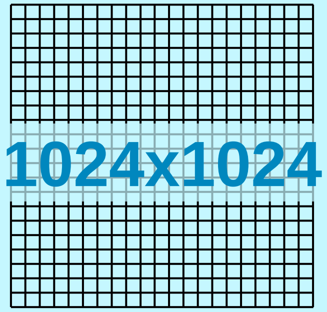
ML augmented CFD solver

NN-based Multigrid

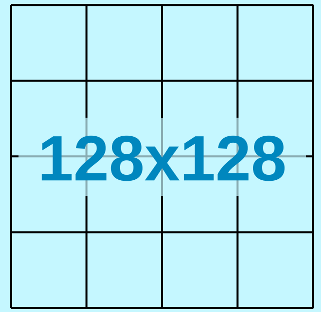


- Geometric multi-grid method
- NN-based smoother

HiFi Simulation



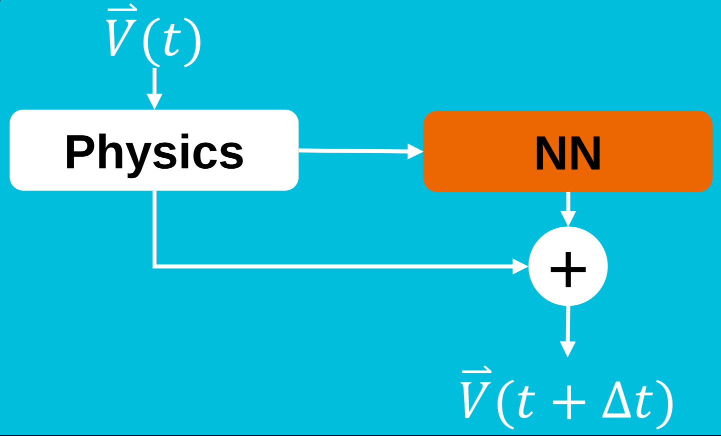
LoFi Simulation



ML-based Hybrid Modelling

$$\rho \frac{D\vec{V}}{Dt} = -\nabla p + \mu \Delta \vec{V} \quad + NN(\vec{V}, \omega_i)$$

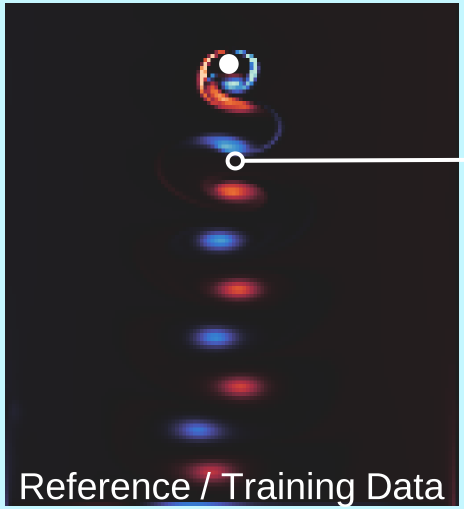
$$\nabla \cdot \vec{V} = 0$$



Source: N Margenberg, D Hartmann, C Lessig, T Richter (2020): A neural network multigrid solver for the Navier-Stokes equations; J. Comp. Phys.
D Kochkov, JA Smith, A Alieva, S Hoyer (2021): Machine learning–accelerated computational fluid dynamics. PNAS

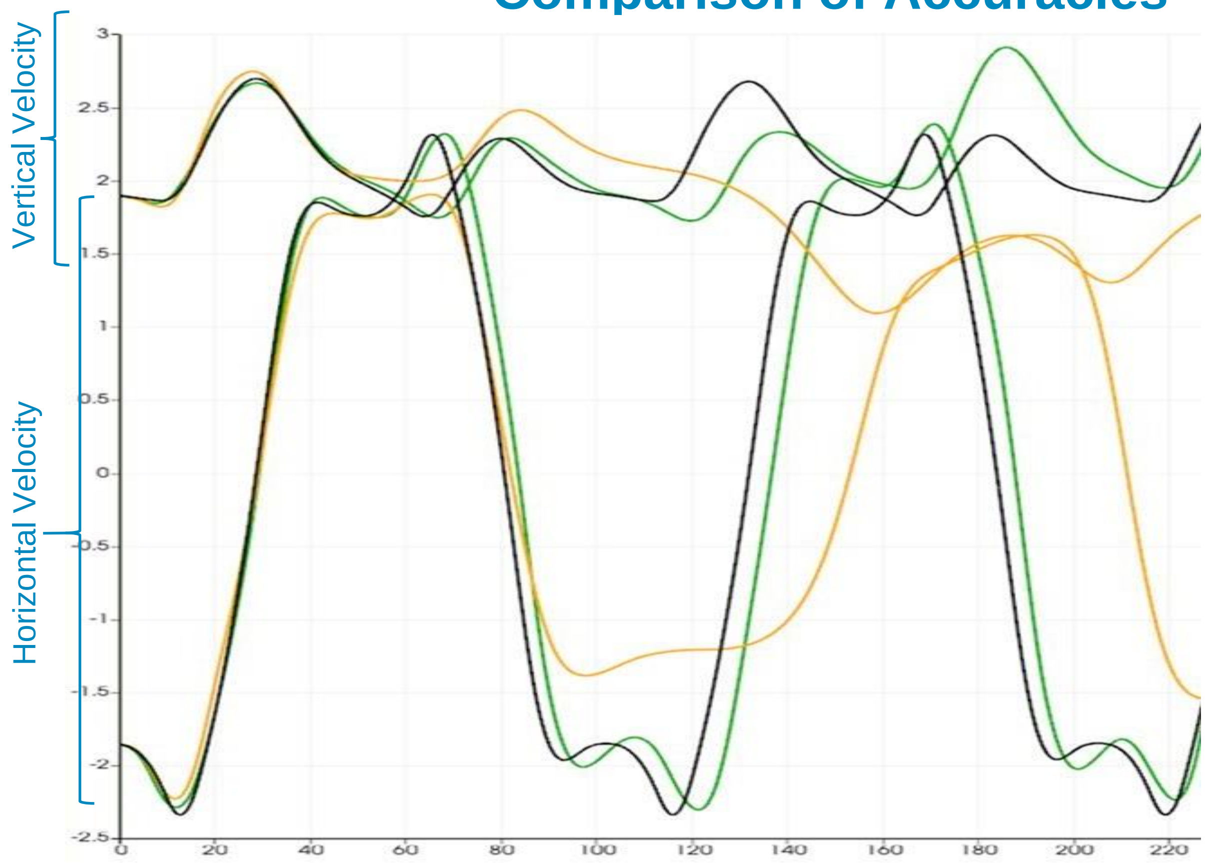
ML-based hybrid Modelling - Accuracy

HiFi Simulation



Grid: 1024 x 1024
Solver: Industry-grade solver

Comparison of Accuracies



HiFi Simulation:
Reference & Training Data

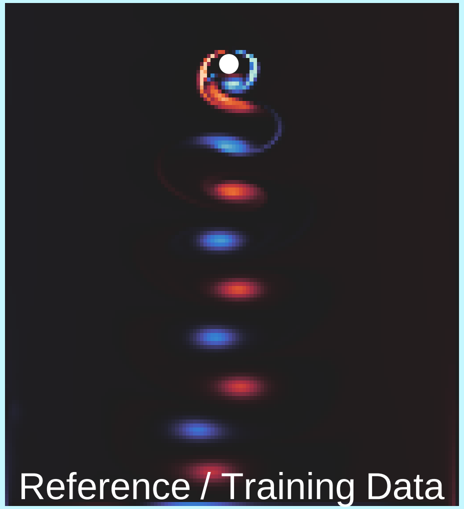
LoFi Simulation:
128 x 128 grid
40x speedup

ML-augmented Simulation:
128 x 128 grid
+ NN augmentation
18x speedup

SIEMENS

ML-based hybrid Modelling - Generalization

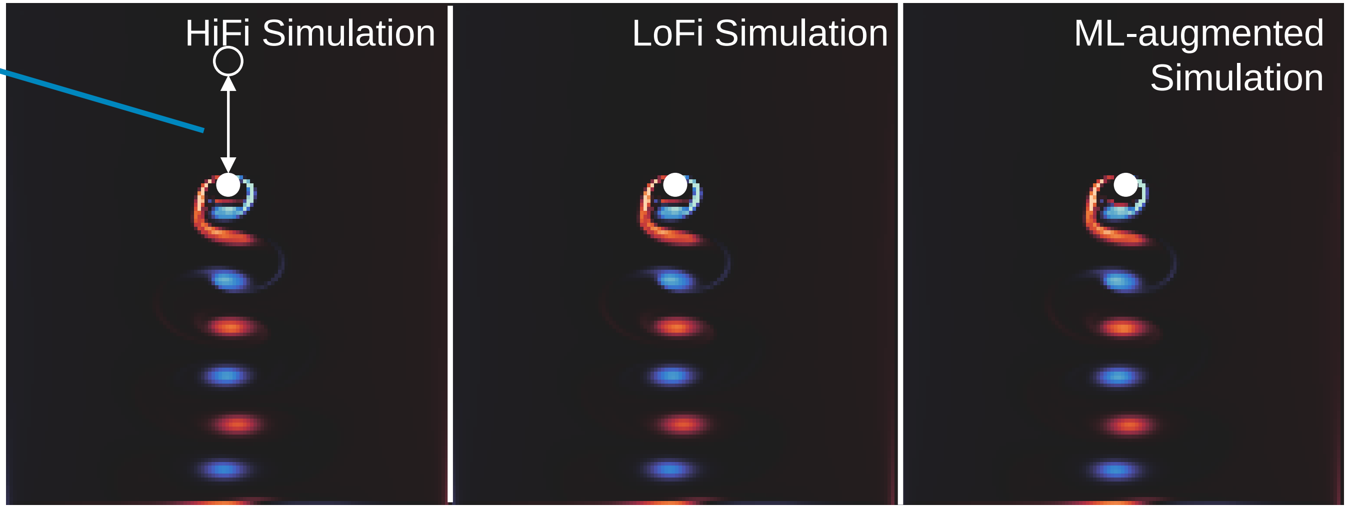
HiFi Simulation



Grid: 1024 x 1024
Solver: Industry-grade solver

Exploration of Generalization Accuracies

Cylinder moved compared to Training Data

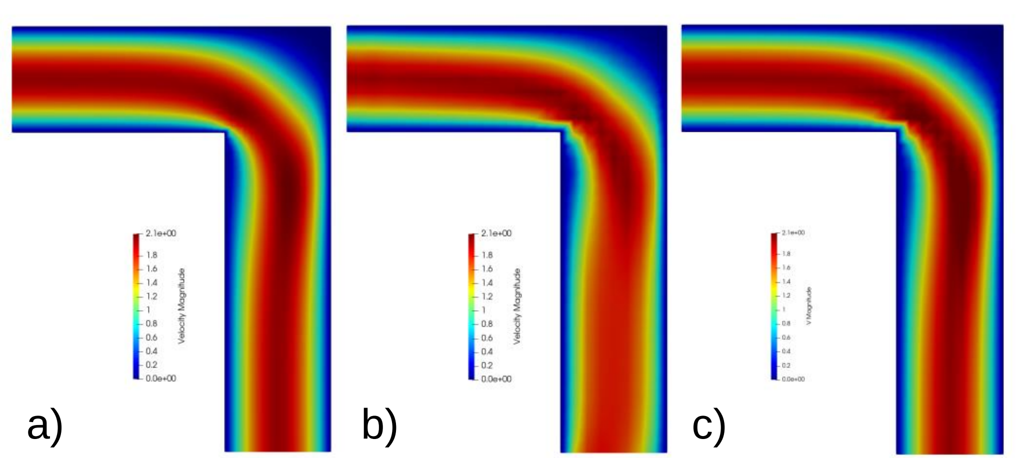


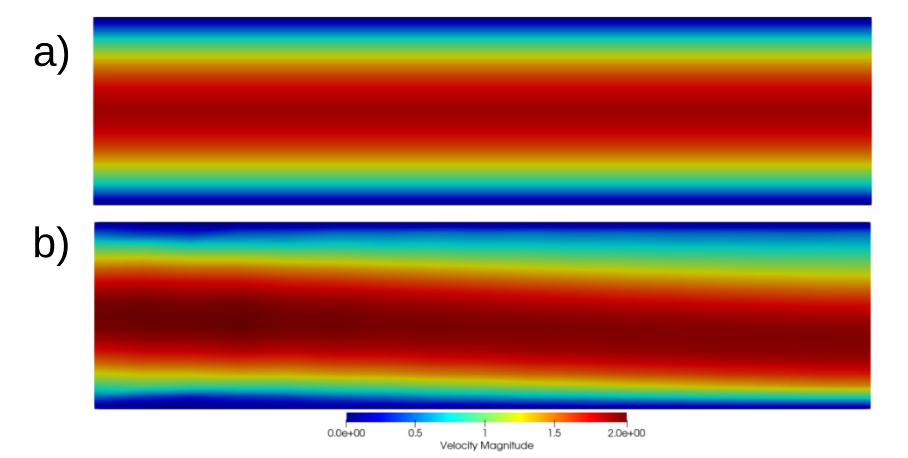
Grid: 1024 x 1024 | Grid: 128 x 128 | Grid: 128 x 128

The model **extrapolates well into scenarios not seen in the training data**, something where classical ML methods fail

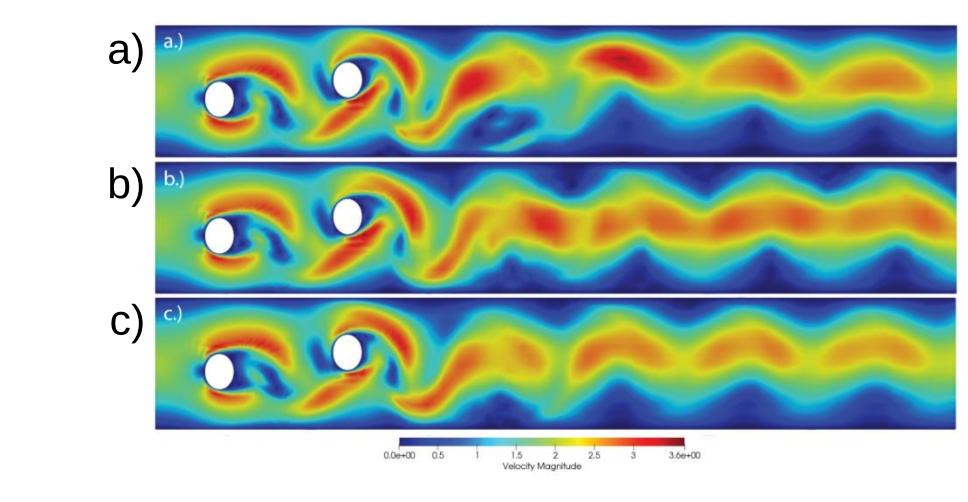
SIEMENS

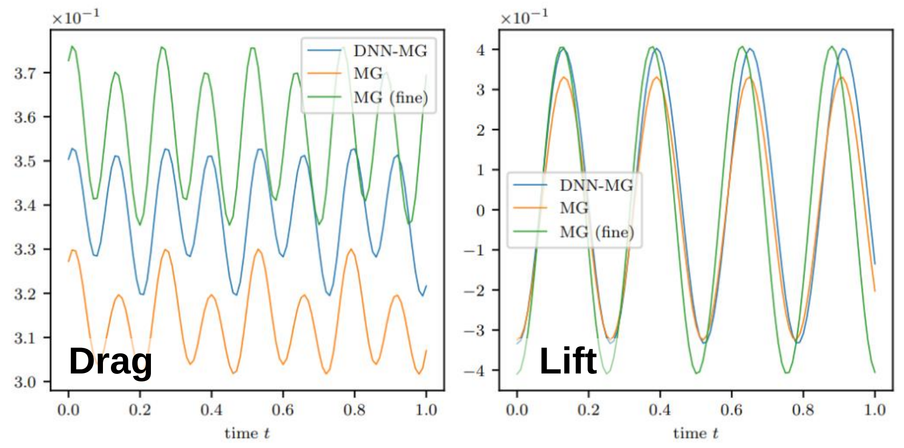
NN-based Multigrid Method - Generalization





a) $\mathrm{MG}\ (L+1)$
b) $\mathrm{DNN\text{-}MG}\ (L+1)$
c) $\mathrm{MG}\ (L)$

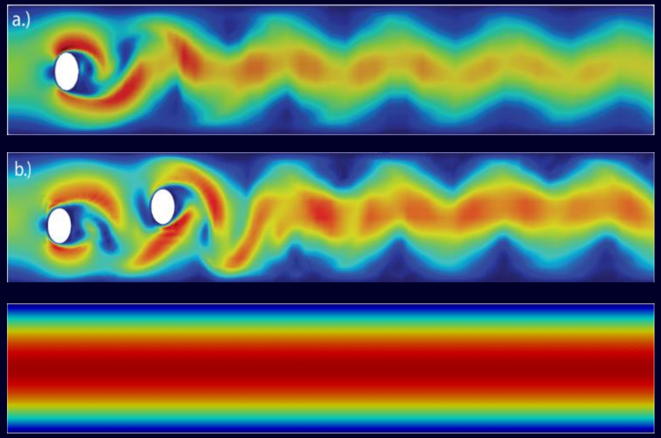




Source: N Margenberg, D Hartmann, C Lessig, T Richter (2020): A neural network multigrid solver for the Navier-Stokes equations; J. Comp. Phys.

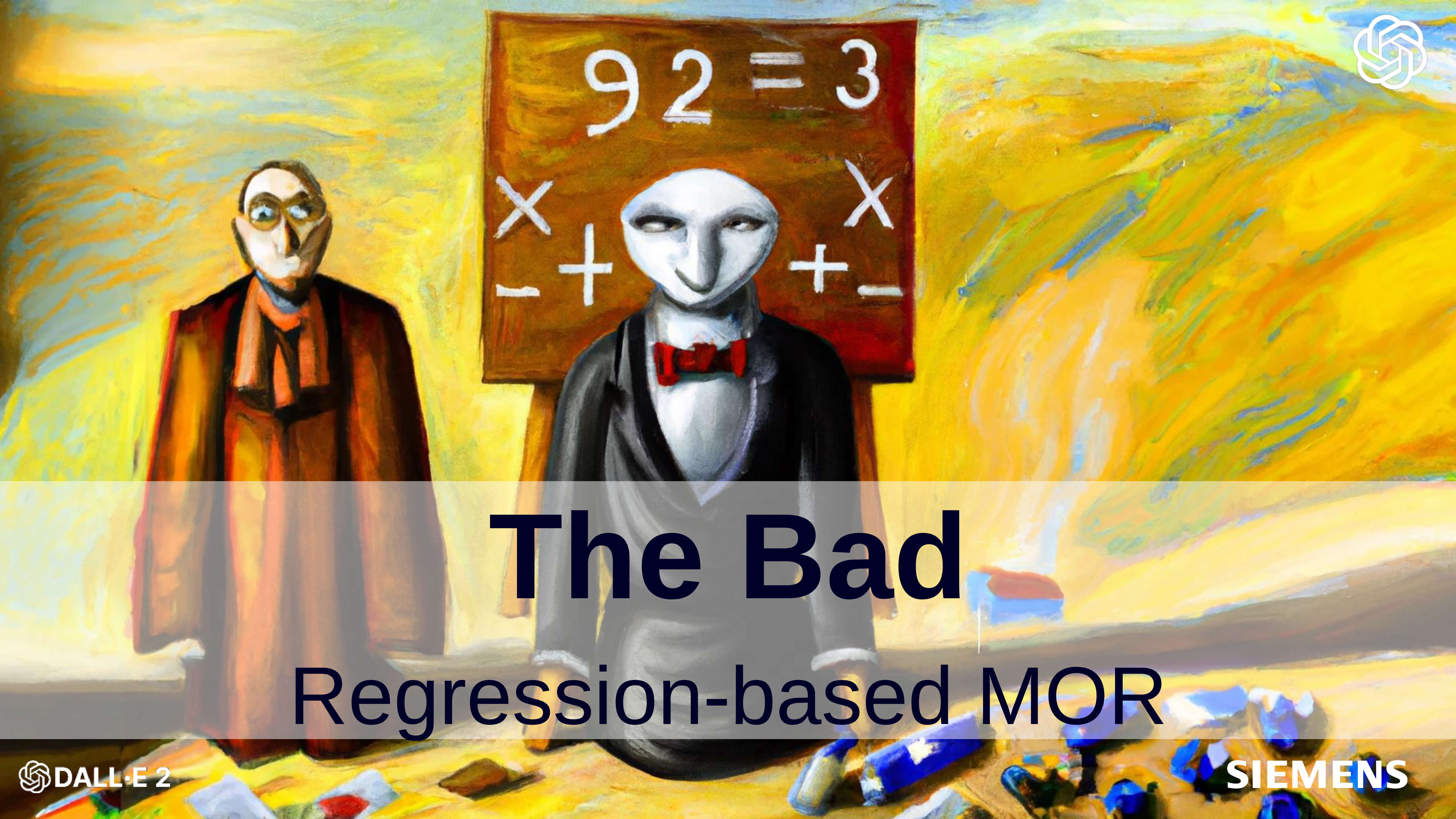
SIEMENS

Intrusive Solver Acceleration



- ✓ Local super-resolution approach (with the Model or Solver) ensure accessibility to training data
- ✓ Local structure provides impressive generalization capabilities
- ✓ Allows to build / extend classical well proven solver technology
- ? Further research and development required

SIEMENS

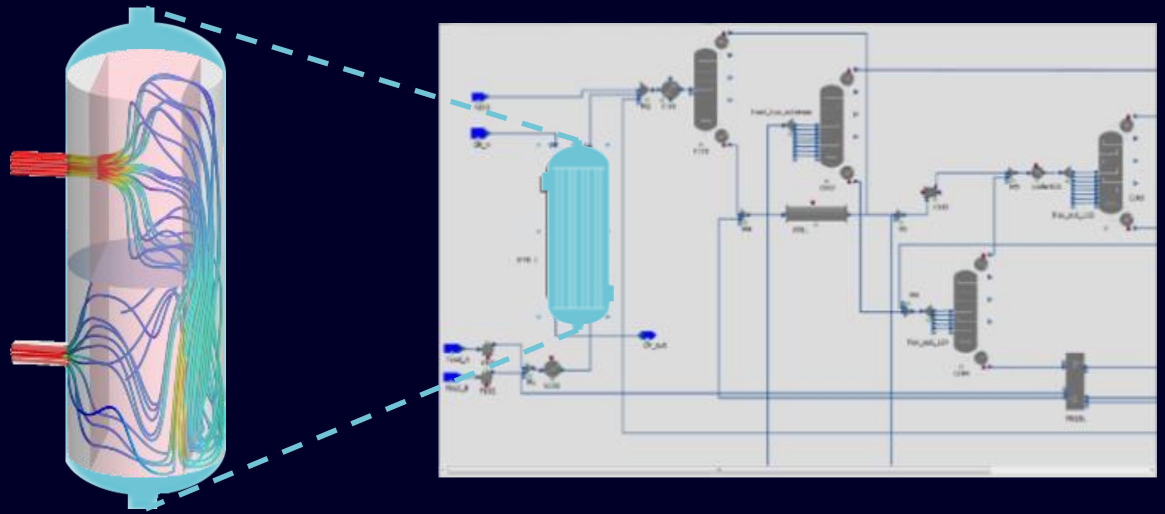


The Bad

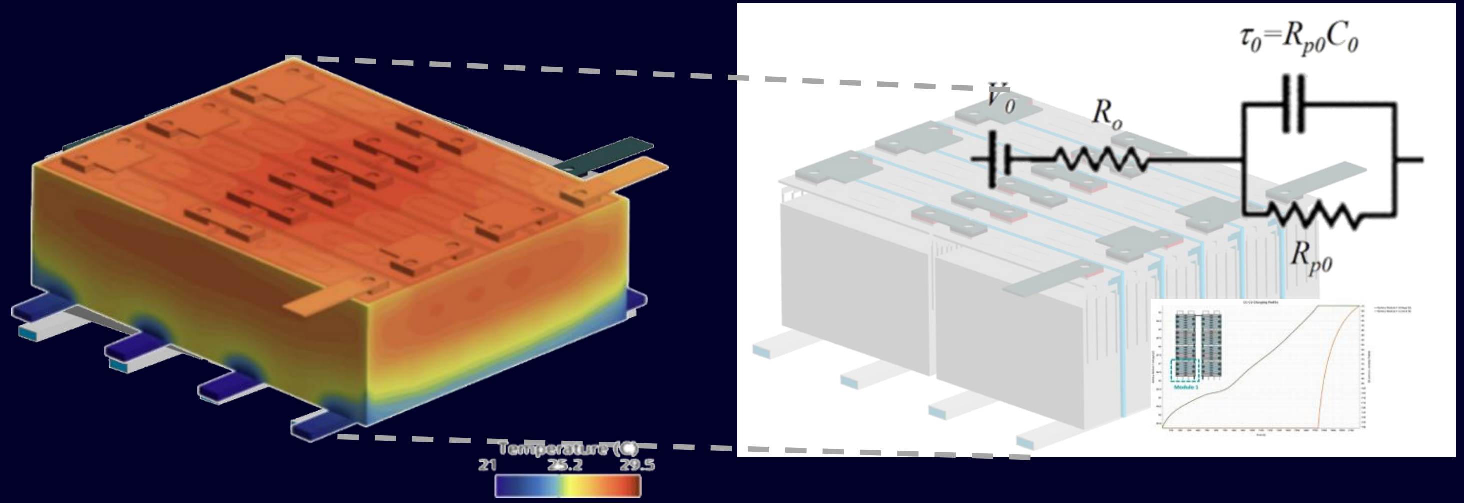
Regression-based MOR

Real-time capable model – a building block of future industrial solutions

Use Case A:
Detailed resolution of flows in Process Engineering



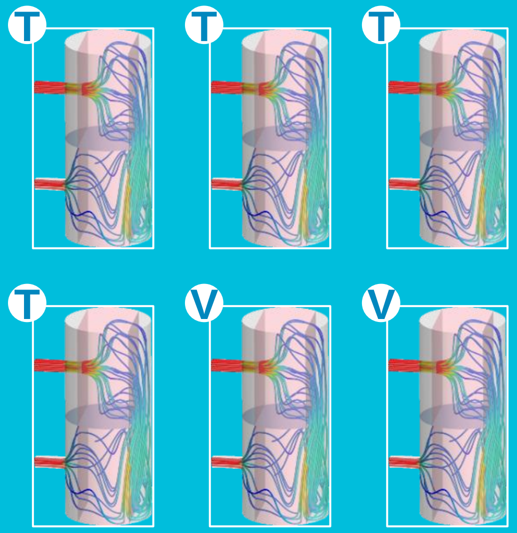
Use Case B:
Accurate prediction of Thermal management in Electrification



SIEMENS

Model Order Reduction in a nut-shell

Full Model Snapshots

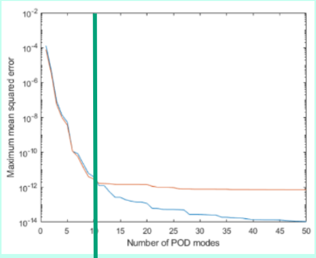


$x \in \mathbb{R}^n$

n is very large, typically $n \gg 10^6$

Latent Dimension Identification

- Autoencoder
- Diffusion Maps
- Dynamic Mode Decomposition
- Proper Orthogonal Decomposition



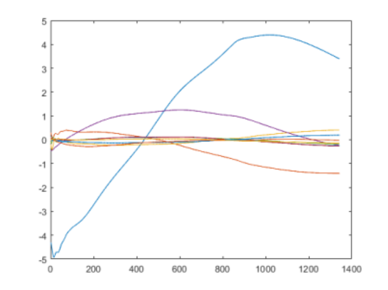
$\hat{x} \in \mathbb{R}^m$

with $m \sim 10 - 100$

Reduced Model Operator Discovery

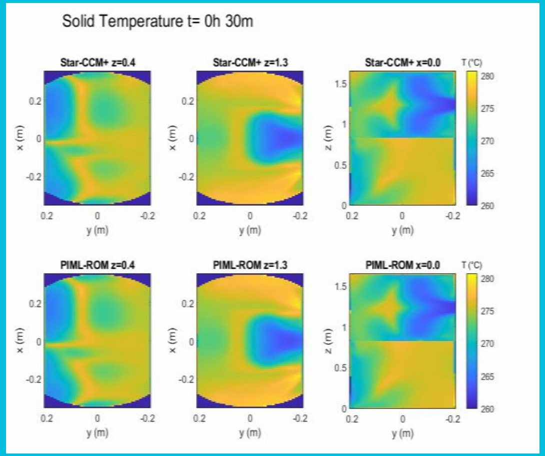
$$\partial_t \hat{x} = \hat{f}(\hat{x}, \mu)$$

- Discrete Empirical Interpolation
- Neural Networks
- Operator Inference



Reduced Coordinate trajectories

Reduced Model



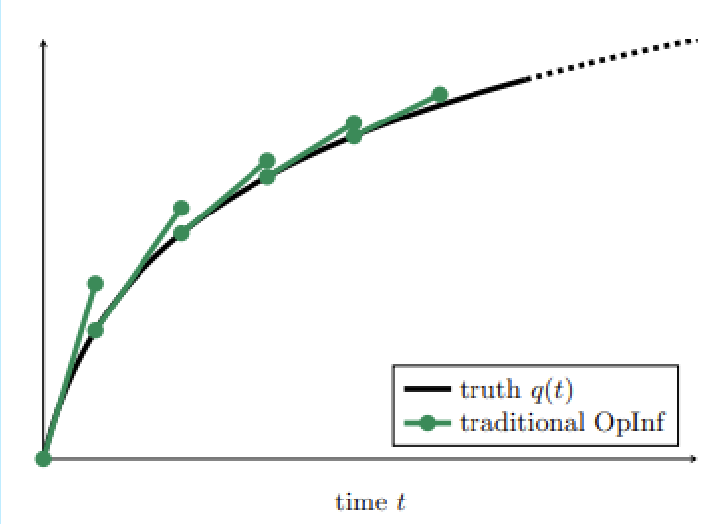
Real-time capable model, predicting the full field

Source: D. Hartmann, L. Failer (2021): A Differentiable Solver Approach to Operator Inference; arXiv
Q Zhuang, JM Lorenzi, HJ Bungartz, D Hartmann (2021): Model order reduction based on Runge–Kutta neural networks; Data-centric Eng
W Uy, D Hartmann, B Peherstorfer(2023): Operator inference with roll outs for learning reduced models from scarce and low-quality data; Comput. Math. Appl..

SIEMENS

Solver-in-the-loop Model Order Reduction

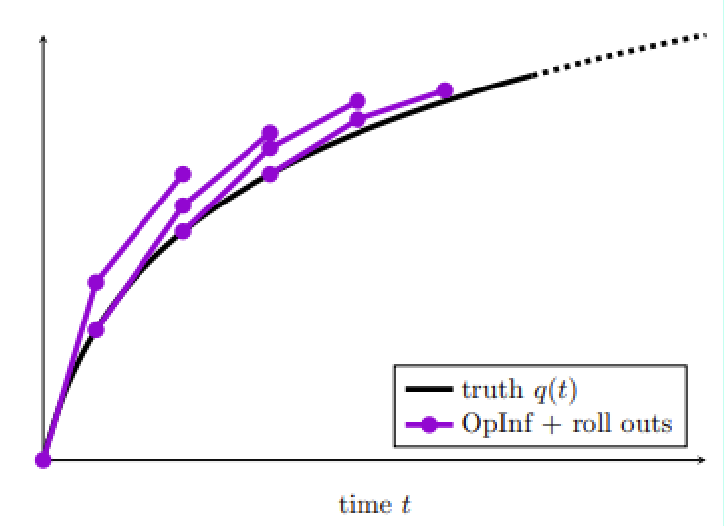
Classic Operator Inference



Least-Square Optimization Problem:

$$\arg\min_A \sum_i (\partial_t x_i - A x_i)^2 + \lambda\, x_i^2$$

Solver-in-the-loop Operator Inference



Constraint Optimization Problem:

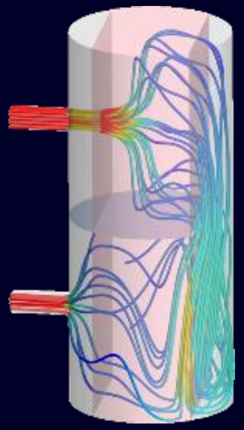
$$\arg\min_A \sum_i (x_i - \tilde{x}_i)^2$$

such that $\partial_t \tilde{x} = A\tilde{x}$

Source: D. Hartmann, L. Failer (2021): A Differentiable Solver Approach to Operator Inference; arXiv
W Uy, D Hartmann, B Peherstorfer(2023): Operator inference with roll outs for learning reduced models from scarce and low-quality data; Comput. Math. Appl..

SIEMENS

Example: Complex Cooling Flow



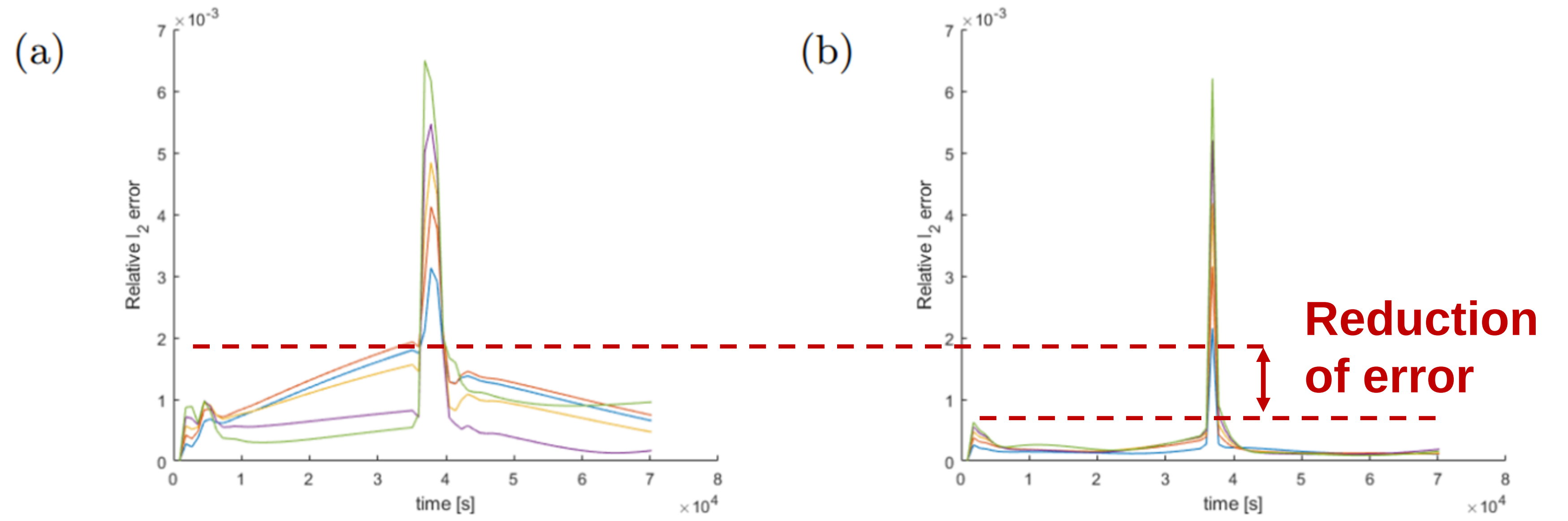
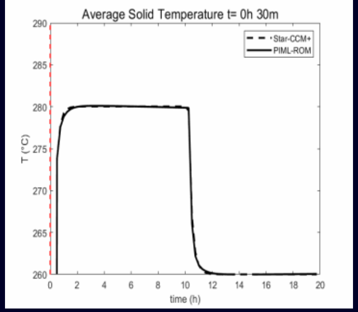


Figure: Operator Inference plus DEIM using 8 modes each: (a) Relative mean squared error of the dynamics predicted using stabilized operator inference (with stabilization parameter $\lambda = 1.0$) and (b) the same error after additional operator calibration (all 5 data sets, encoded in different color).

Source: D. Hartmann, L. Failer (2021): A Differentiable Solver Approach to Operator Inference; arXiv

SIEMENS

Example: Complex Cooling Flow



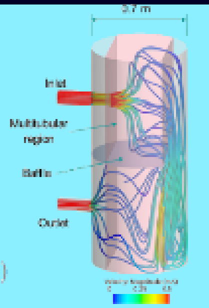
3D Physics with 400k DoF

$$\rho_c \left(\frac{\partial v}{\partial t} + (v \cdot \nabla) v \right) = -\nabla p + \mu \Delta v + \alpha(x) v$$

$$\nabla \cdot v = 0$$

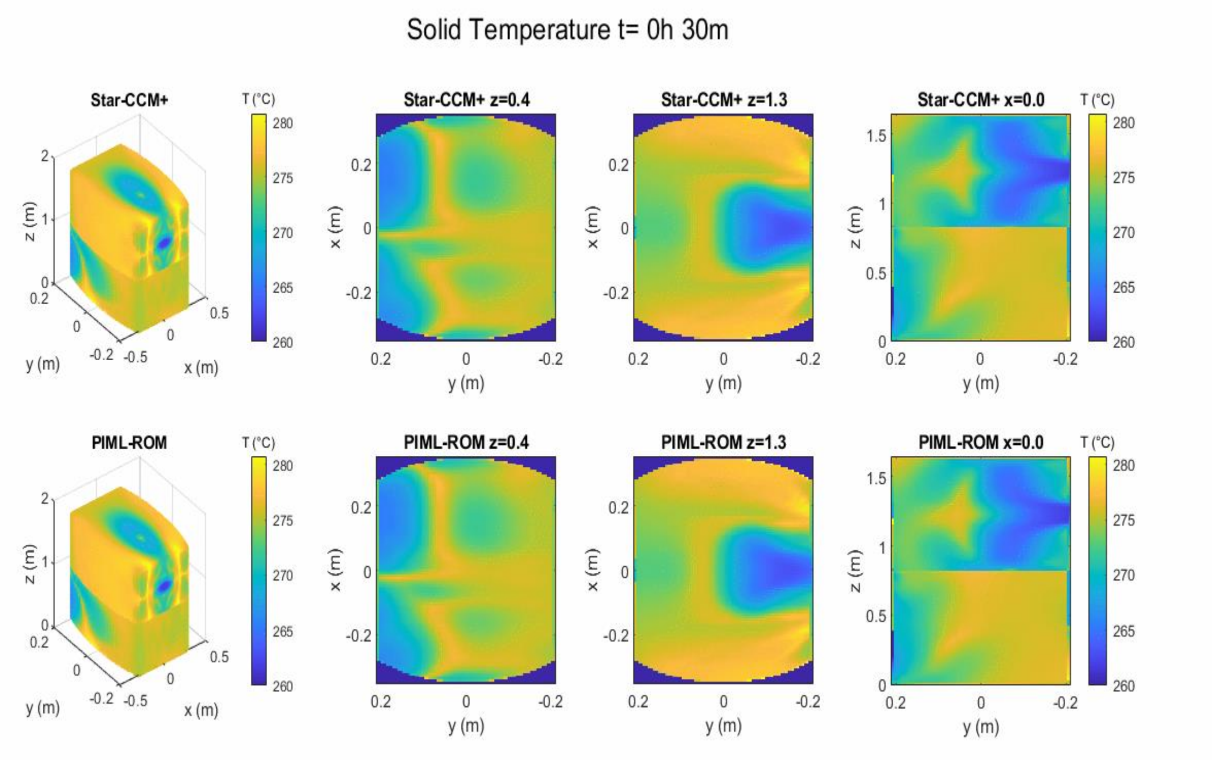
$$\rho_c c_{p,c} \left(\frac{\partial T_c}{\partial t} + (v \cdot \nabla) T_c \right) = \nabla \cdot (K_c \nabla T_c) + \chi_{\Omega_s} q (T_s - T_c)$$

$$\rho_s c_{p,s} \frac{\partial T_s}{\partial t} = \nabla \cdot (K_s \nabla T_s) - q (T_s - T_c) + \mathcal{P}(t, T_s)$$



ODE with 8 DoF

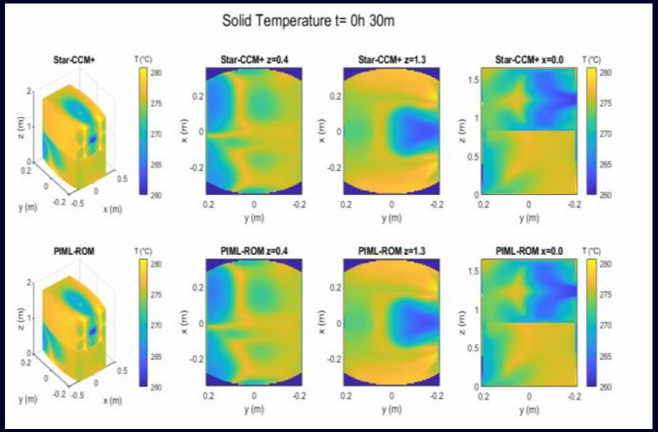
$$\dot{s} = \boldsymbol{A} \boldsymbol{s} + R(t)\ A\ \boldsymbol{P}_1\ \exp(B / (\boldsymbol{P}_2 \boldsymbol{s}))$$



Source: D. Hartmann, L. Failer (2021): A Differentiable Solver Approach to Operator Inference; arXiv

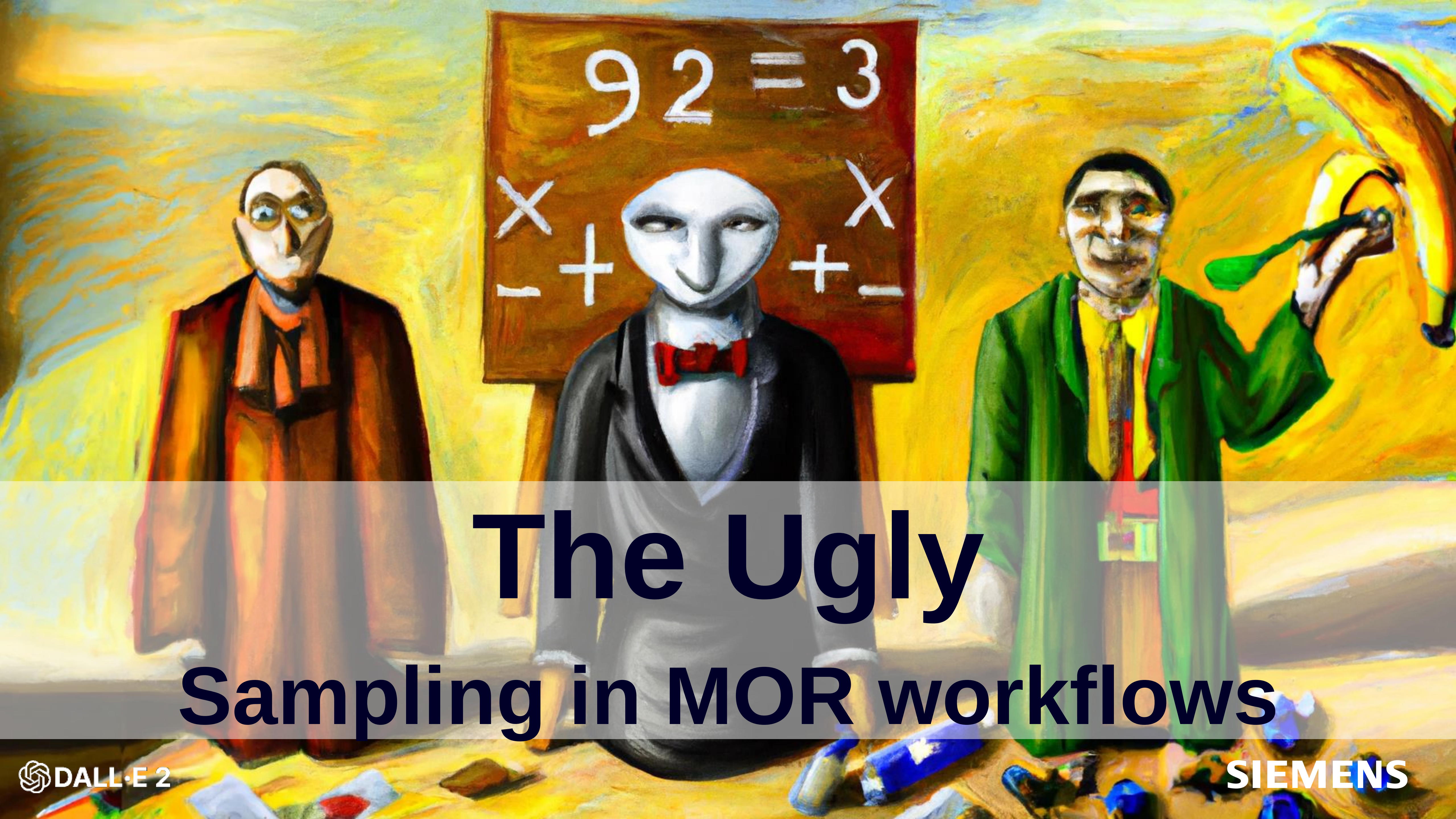
SIEMENS

Operator Inference



- ✓ Acceleration of prediction by orders of magnitude not loosing accuracy
- ✓ Explicit form of equations allows to be reused in many tools / systems
- ✓ Differentiable solver technology in not only key for machine learning applications
- ✗ Data generation can be quite cumbersome

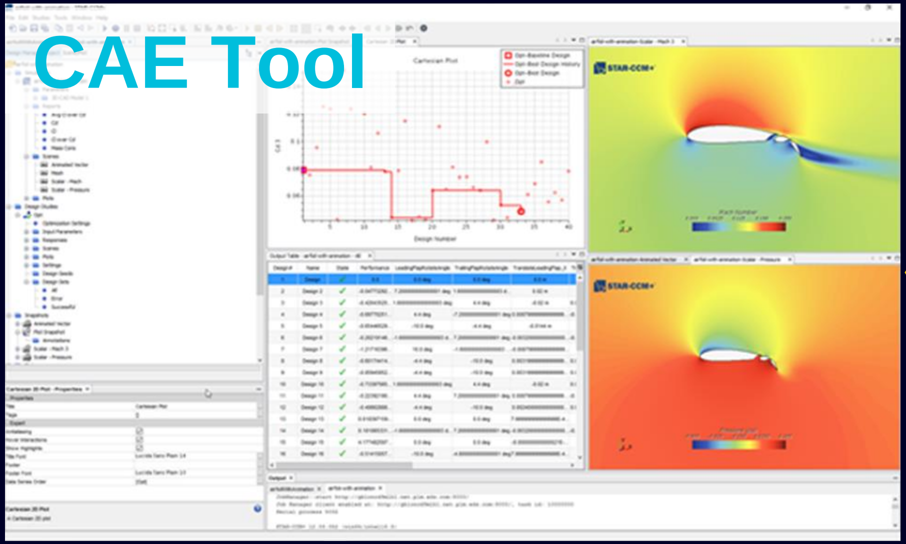
SIEMENS



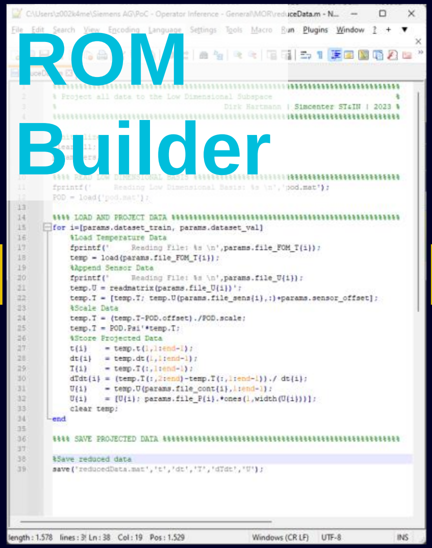
The Ugly

Sampling in MOR workflows

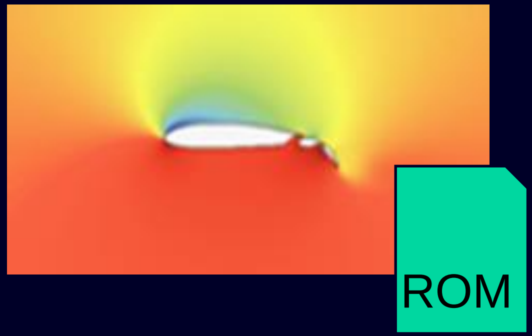
Industrial Model Order Reduction Workflows



Sample

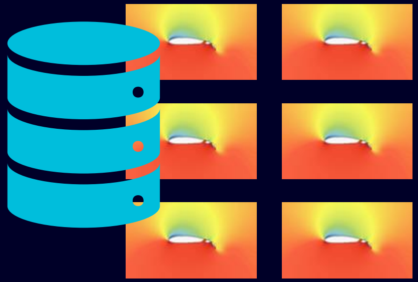


Export



Plus appropriate model management across the whole life cycle

FOM Snapshots



SIEMENS

How to sample effectively

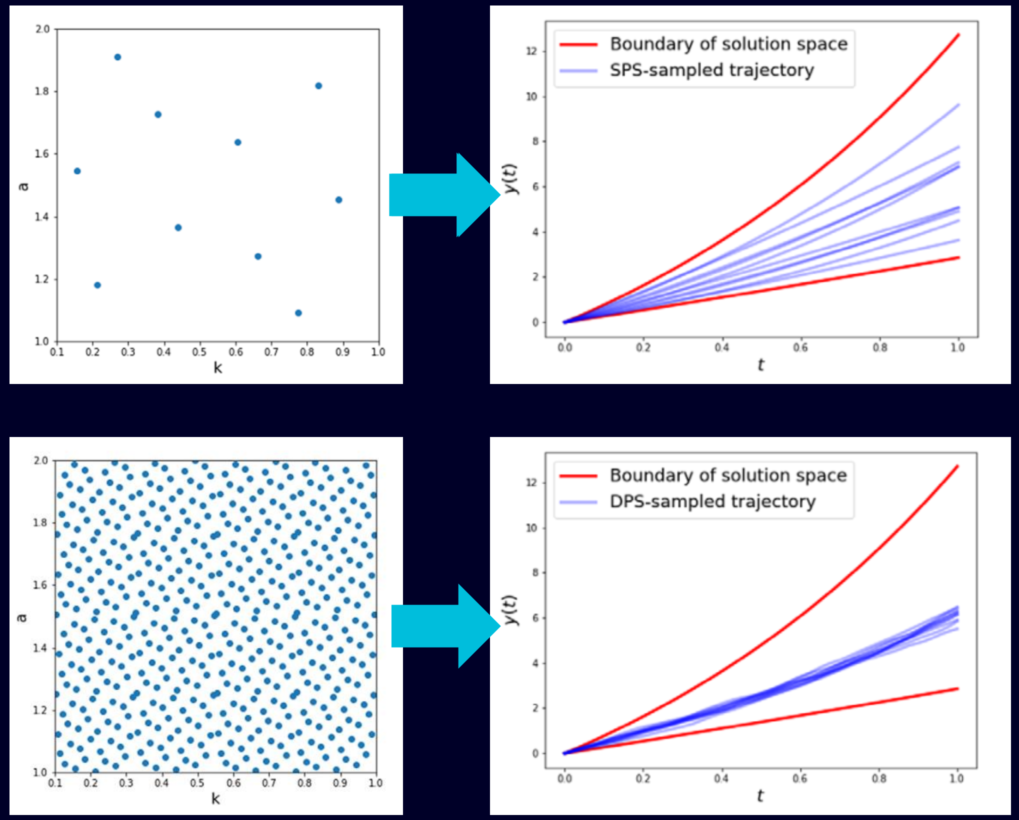
- Static vs. Dynamic Parameter Sampling
- One long trajectory vs many small trajectories
- …

Example:

$$\dot{y} = k(t)y + e^{a(t)}$$

Static Sampl.

Dynamic Sampl.



Source: Q Zhuang, D Hartmann, HJ Bungartz, JM Lorenzi,(2021): Active-learning-based nonintrusive model order reduction; Data-centric Eng

SIEMENS

Active Learning Heuristic for industrial ROM

Preparation

Full Order Model

Static sampling $\mathcal{M} = \left[\mu^{(1)}, \cdots, \mu^{(k)}\right]$

Snapshots $\boldsymbol{\mathcal{Y}} = \left[\boldsymbol{Y}_1^{(1)}, \boldsymbol{Y}_2^{(1)}, \cdots, \boldsymbol{Y}_m^{(k)}\right]$

Estimate joint space $\boldsymbol{\mathcal{J}} = \boldsymbol{\mathcal{Y}} \times \boldsymbol{\mathcal{M}}$

Data pool $\mathcal{J}_{all} \subset \mathcal{J}$

PAC[1] **validator**

1) Probably approximately correct

Active Learning / Sampling

Data pool $\mathcal{J}_{all}$

Sample $\mathcal{J}_s = \left[J^{(1)}, J^{(2)}, \cdots\right]$

(FOM) Training Data

ROM, e.g., NN

PAC

ROM

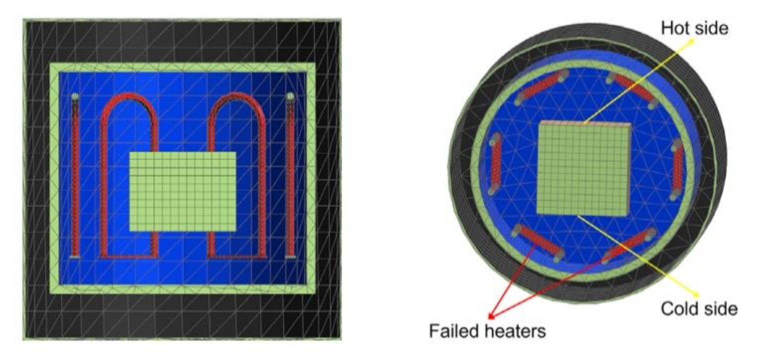
ROM

Error of ROM snapshots

Error estimator, e.g. $\mathcal{GP}$

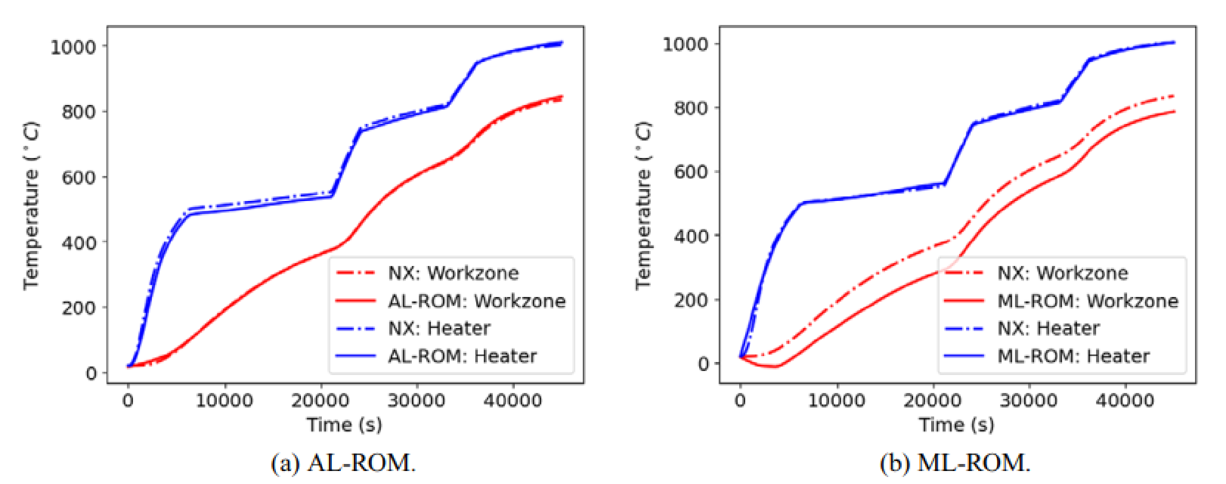
Source: Q Zhuang, D Hartmann, HJ Bungartz, JM Lorenzi,(2021): Active-learning-based nonintrusive model order reduction; Data-centric Eng

Active Learning Heuristic for industrial ROM

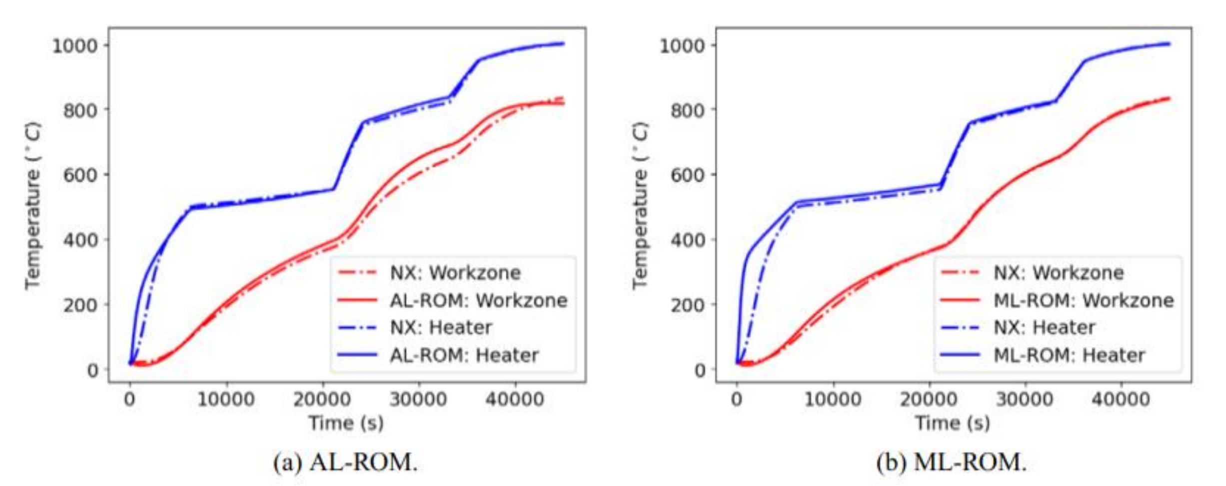


Test Case: Vacuum furnace

Euler Neural Network



Operator Inference

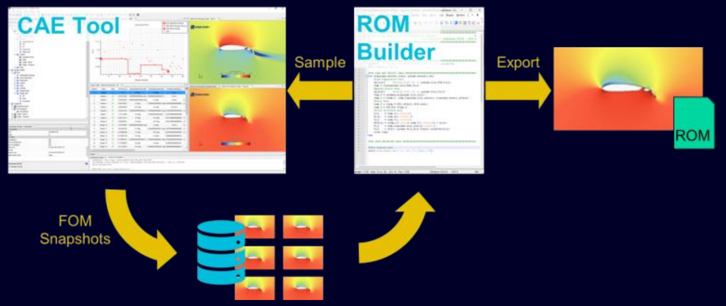


97%-confident ROM Error (PAC)

	#Samples	AL-ROM	ML-ROM
NN	20 000	1,00%	13,07%
OI	5 000	1,00%	7,54%

SIEMENS

Industrial Model Order Reduction Workflows



- ✔ Industrial workflows require a high degree of automation.
- ✔ Active learning strategies allow to achieve “optimal” ROMs.
- ✔ First heuristic strategies are available

- ✘ Analytic guarantees

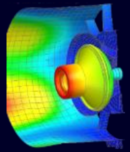
SIEMENS

4

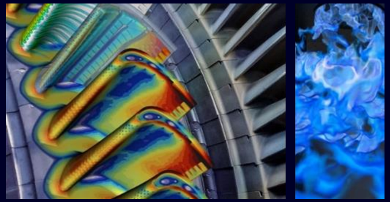
Wrap Up

Digital Twin - *A new age of computational paradigms*

Model Pioneers



CAx Sunrise



R&D Pervasion

Digital Twin Era

Industrial Metaverse

~1985 **~2000** **~2015** **~2022**

- Geometry
- Single-Physics

- Computer-Aided Tools in R&D
- Multi-Physics

- Collaborative
- Model-based Engineering

- Model-based Operations
- X-as-a-service

- Democratization
- Realtime++ Predictions

CAx: Computer Aided Design, Engineering, & Manufacturing

Contact

Dr. Dirk Hartmann
Technical Fellow
Siemens Digital Industries Software
Simulation and Test Solutions
Otto-Hahn-Ring 6
81739 Munich
Germany

Mobile +49 173 2537709
E-mail hartmann.dirk@siemens.com

The Art of the Possible – Blog
https://blogs.sw.siemens.com/art-of-the-possible

SIEMENS