Seminar series : **Mathematics of Data Science**

Organizers:
Assoc Prof. Martin Andersen (SC)
Assoc Prof. Jakob Lemvig (MAT)
Assoc Prof. Allan Peter Engsig-Karup (SC)

DTU Compute
Department of Applied Mathematics and Computer Science

Executable Digital Twin

Reimagining industrial operations through Scientific Machine Learning

MoDS Seminar, DTU | February 6th, 2024

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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

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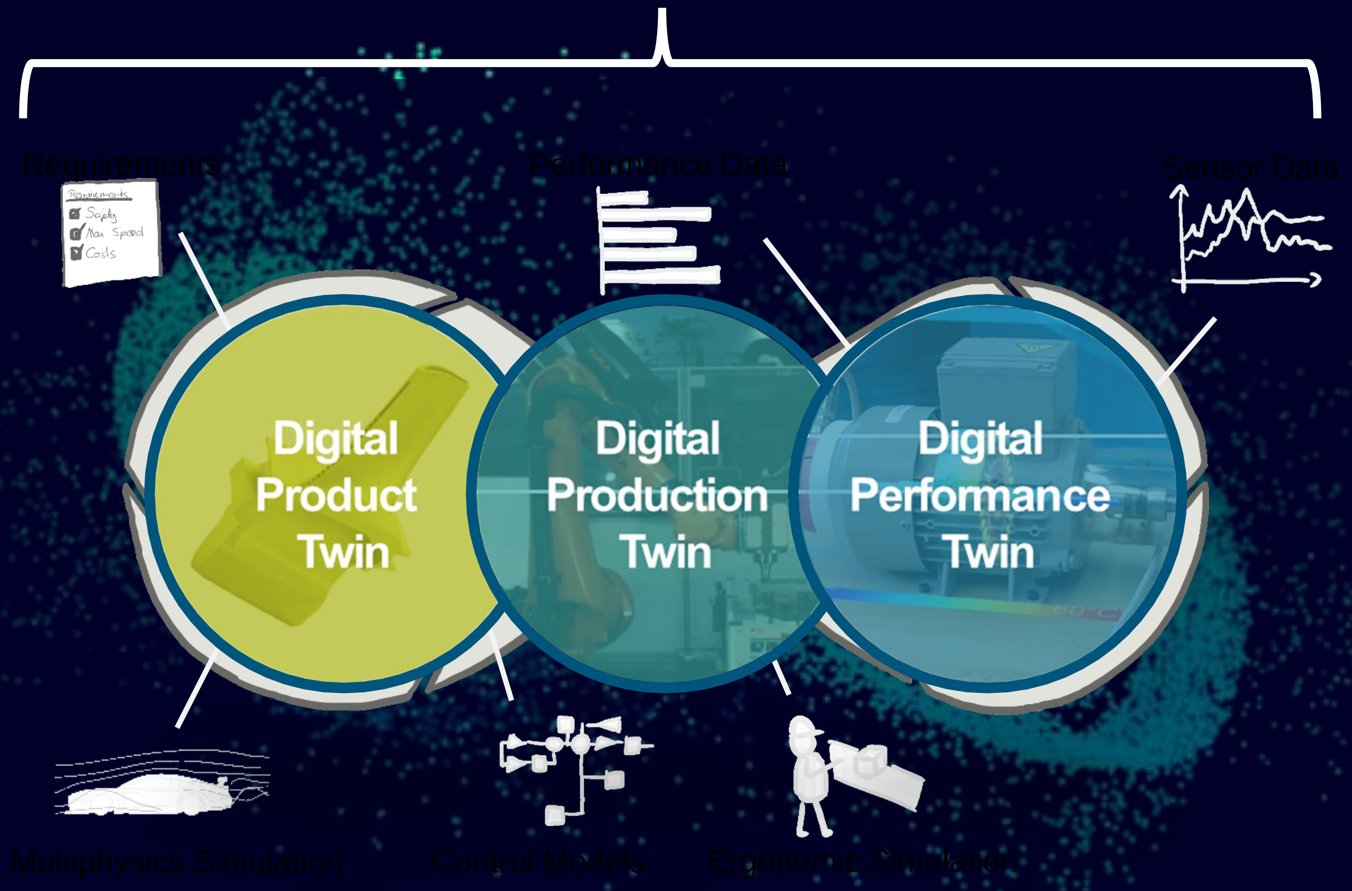
The comprehensive Digital Twin

Digital world



Real world

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1

Digital Twin

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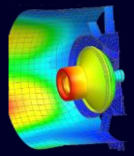
Digital Twin - *An old story!*

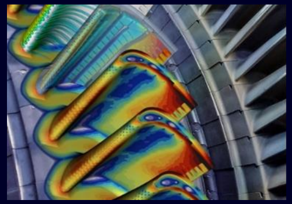
Model Pioneers



- Geometry
- Single-Physics

~1985

CAx Sunrise



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

~2000

R&D Pervasion

- Collaborative
- Model-based Engineering

CAx: Computer Aided Design, Engineering, & Manufacturing

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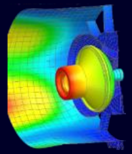
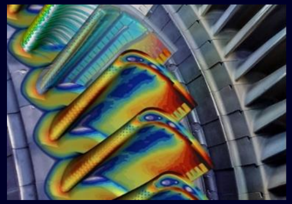
Digital Twin - *A new age of computational paradigms*

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

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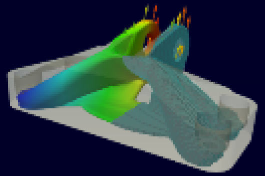
Why now? Drivers & Enablers

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

"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

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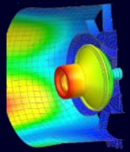
The Digital Twin Paradigm

"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.

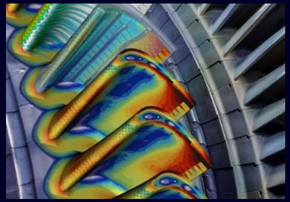
Dirk Hartmann (2023)

Digital Twin - *A new age of computational paradigms*

Model Pioneers



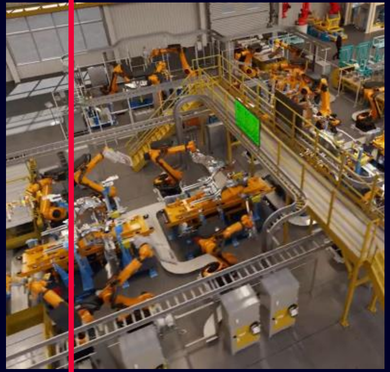
CAx Sunrise



R&D Pervasion

Digital Twin Era

Industrial Metaverse



~1985 | ~2000 | ~2015 | ~2022 | TODAY

Model Pioneers
- Geometry
- Single-Physics

CAx Sunrise (~1985)
- Computer-Aided Tools in R&D
- Multi-Physics

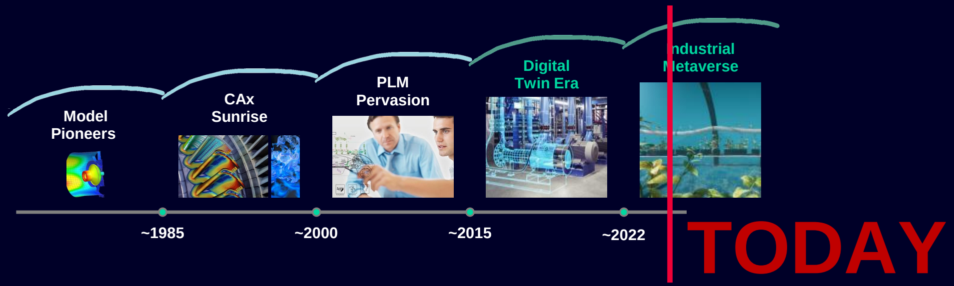
R&D Pervasion (~2000)
- Collaborative
- Model-based Engineering

Digital Twin Era (~2015)
- Model-based Operations
- X-as-a-service

Industrial Metaverse (~2022)
- 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

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Executable[1] Digital Twin

1) Scientific ML enabled

Major Challenges in Digital Twin based Operations

What are the major pain 😖 points for more and broader adoption of #DigitalTwins for #IndustrialOperation and #Service?

Lack of experts 👴	37%
Missing (real-time) models 📊 ✔	32%
Missing calculation power 💻	4%
Too complex software landscape	28%

249 votes

"Digital Twins are slow and bespoke!

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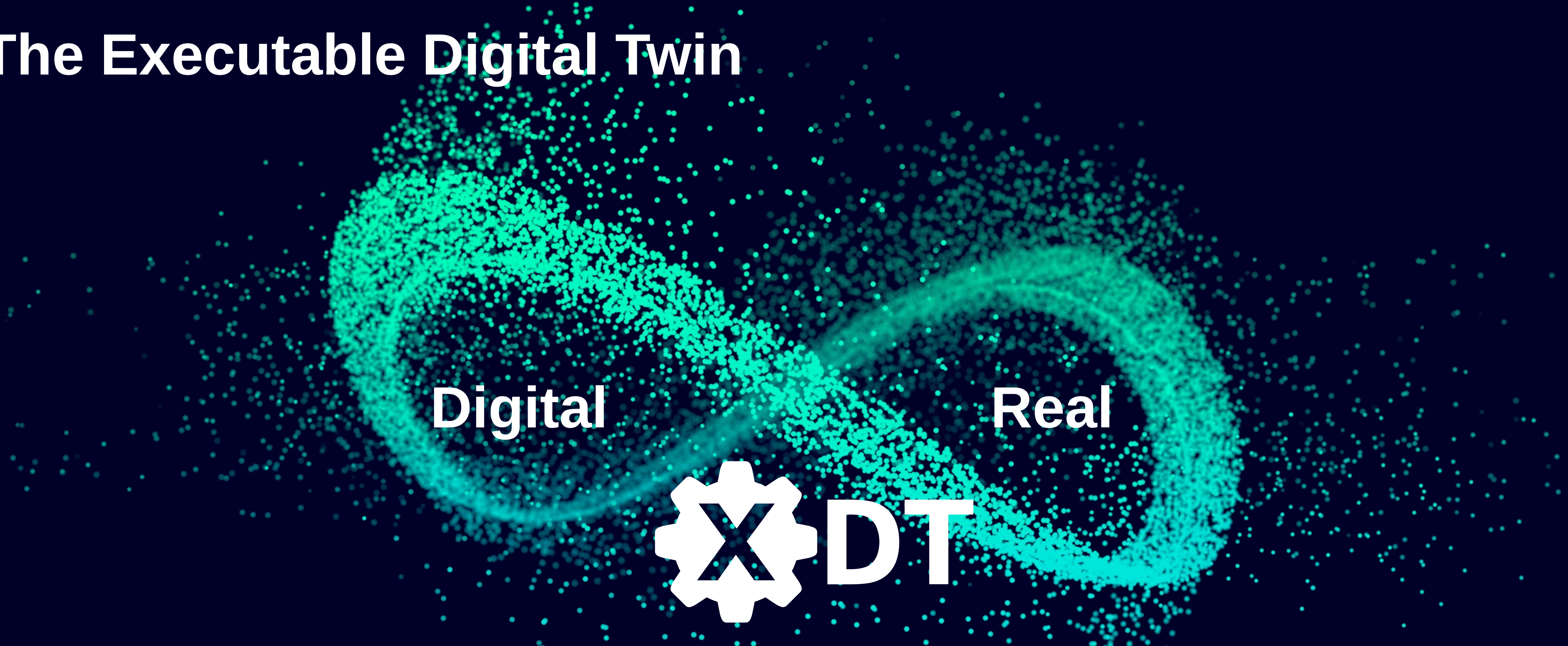
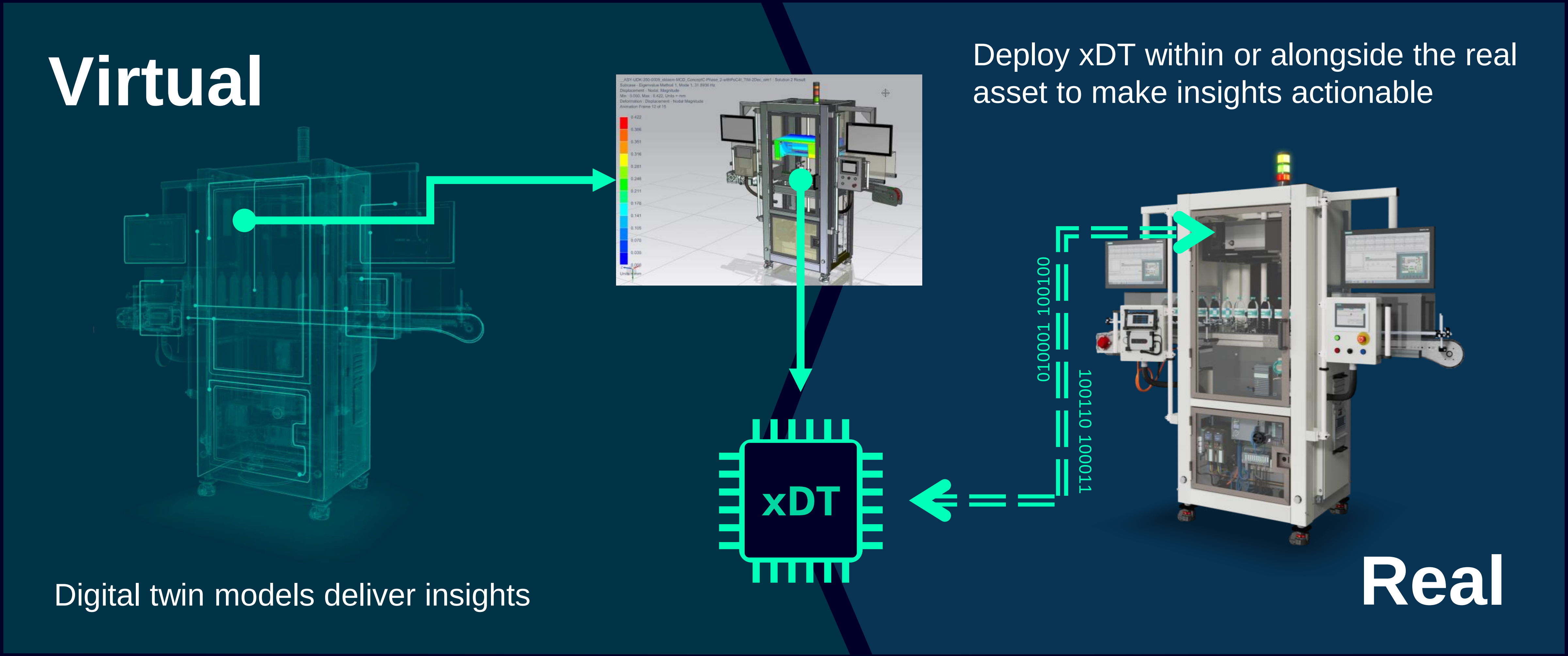
The Executable Digital Twin



Self-contained executable digital behavior of an asset

Leveraged by anyone at any point in lifecycle

Use xDT to bring virtual and real worlds together



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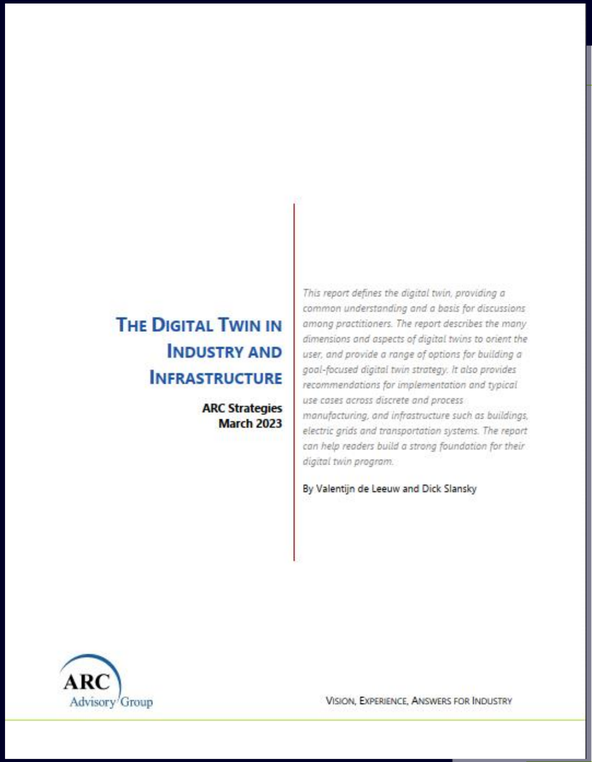
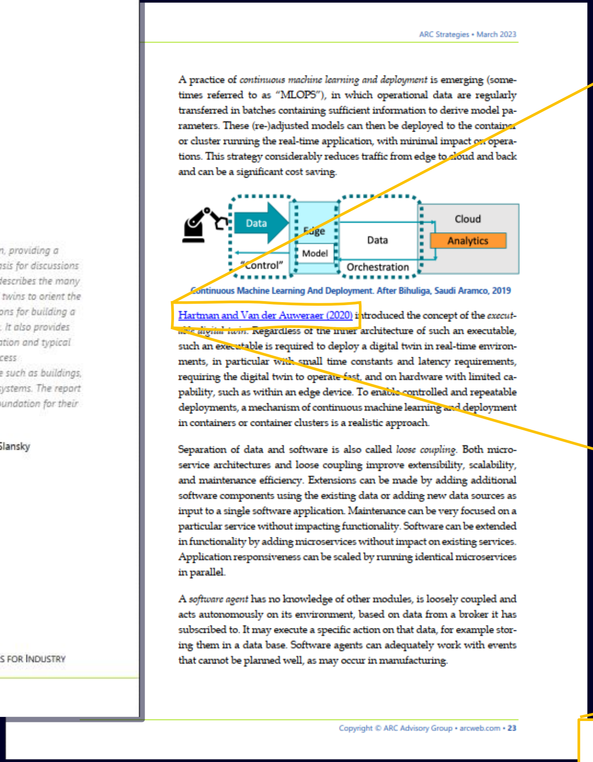
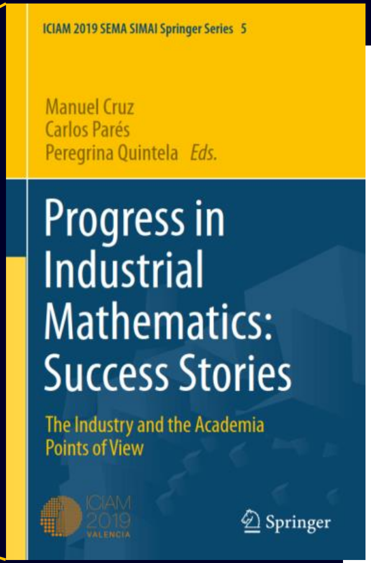
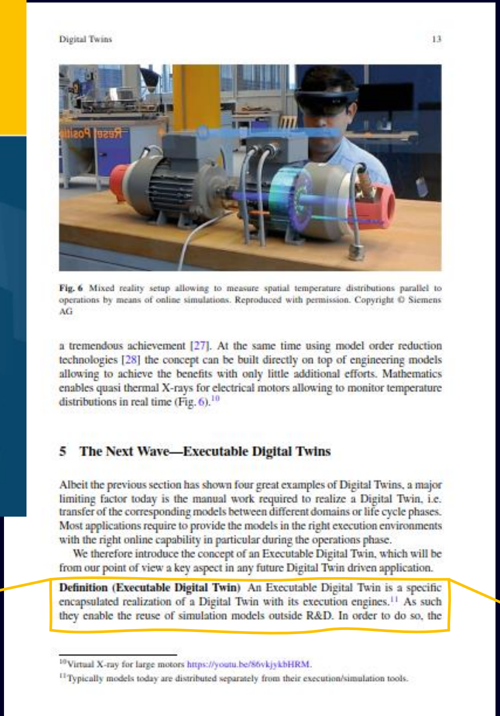
The "first" math paper quoted in an Industry Analyst paper









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

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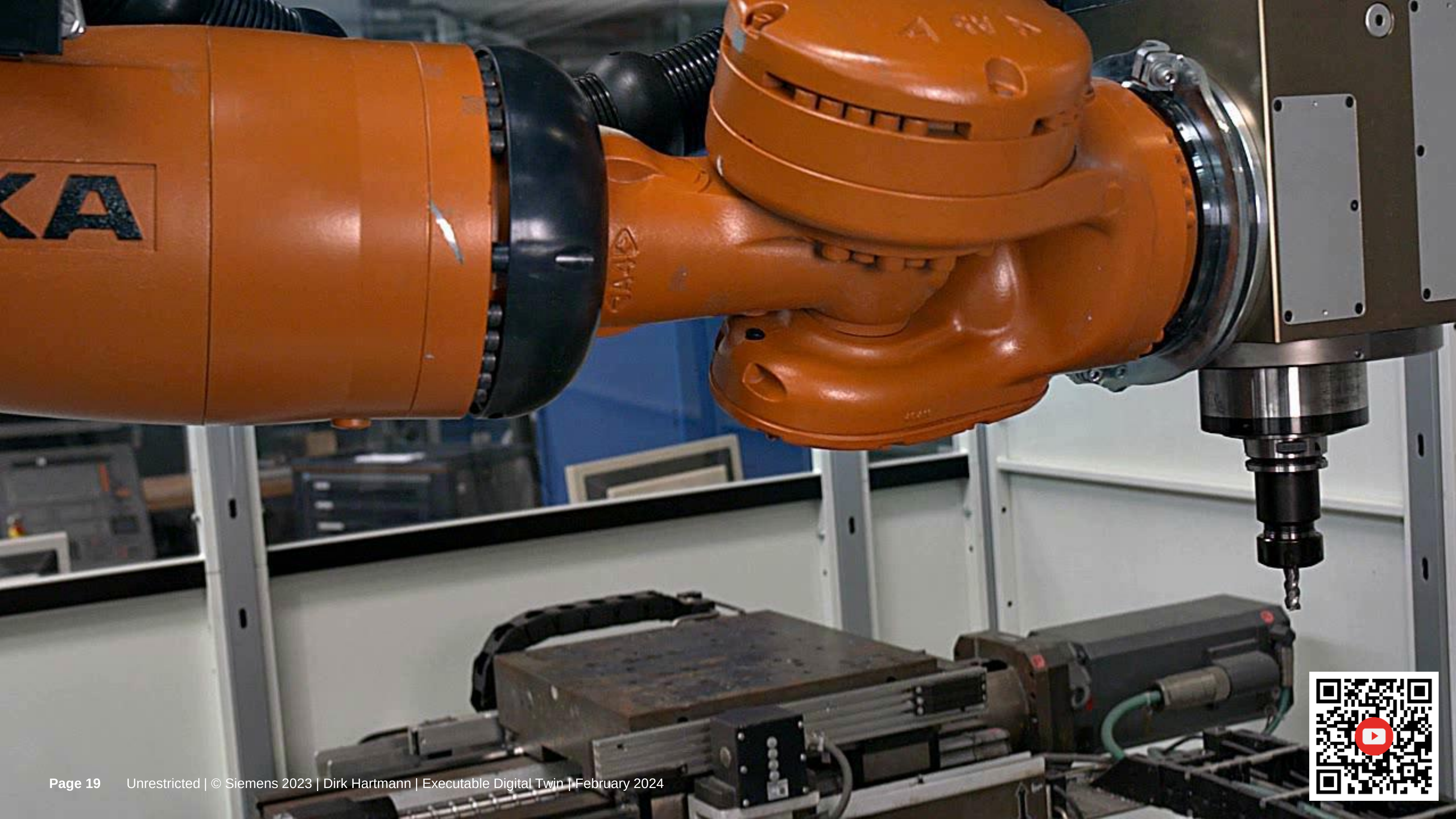

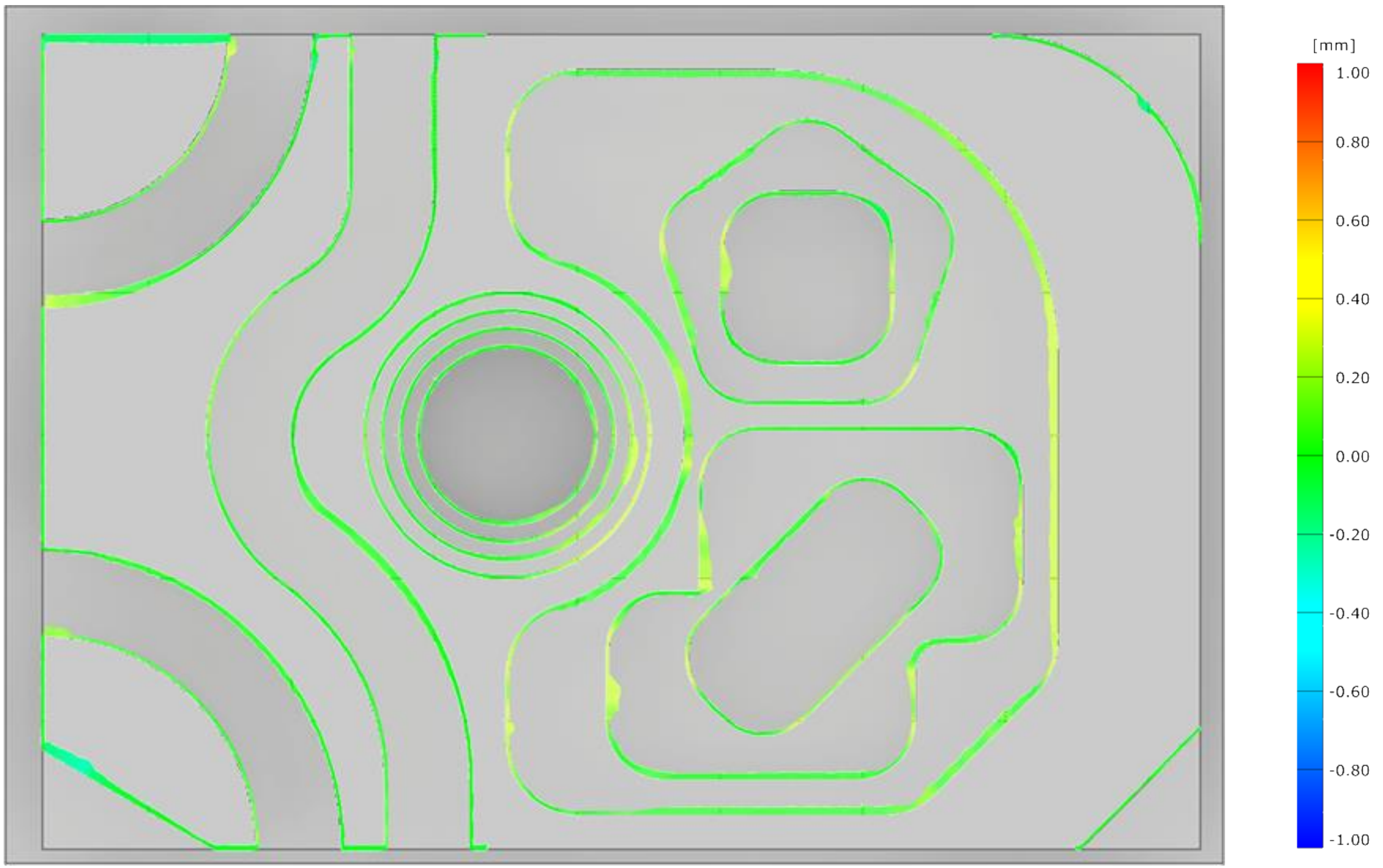
[mm]
1.00
0.80
0.60
0.40
0.20
0.00
-0.20
-0.40
-0.60
-0.80
-1.00


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on combined with
Augmented Monitoring
in real time during
r almost anything

3

Math Deep Dive

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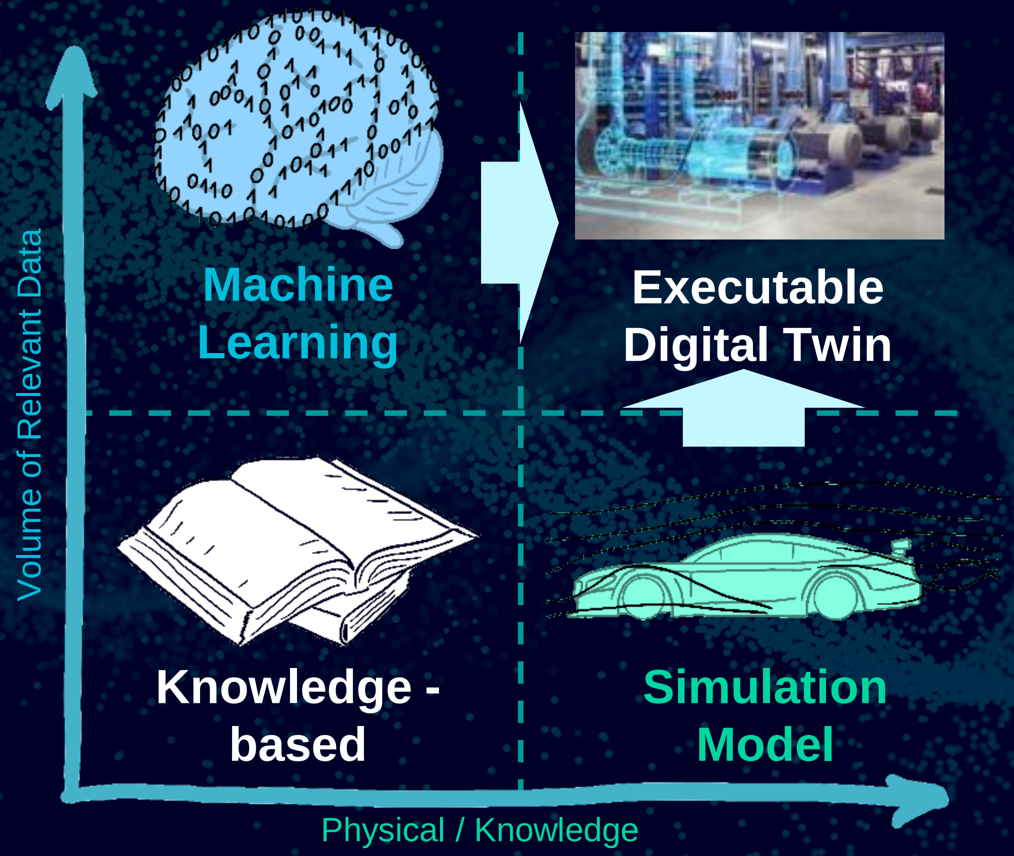
ML combined with Simulation enable the Executable Digital Twins at scale



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

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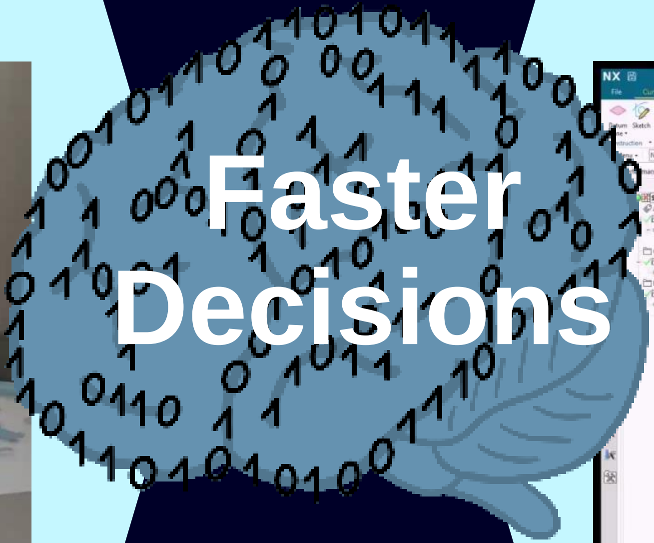
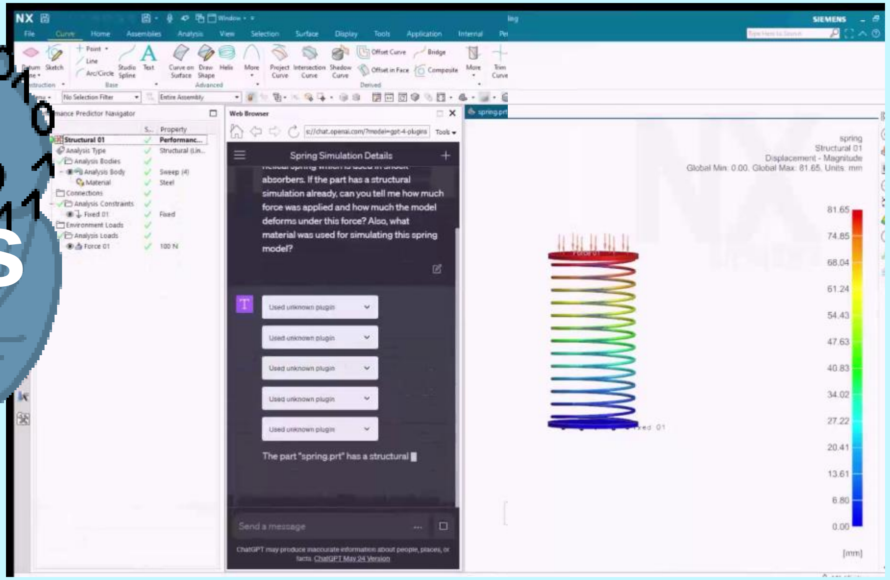
AI and ML boost Decisions in Engineering and Operation

Accelerate Predictions

High End CFD simulation of a car



Improve User Efficiency



PoC

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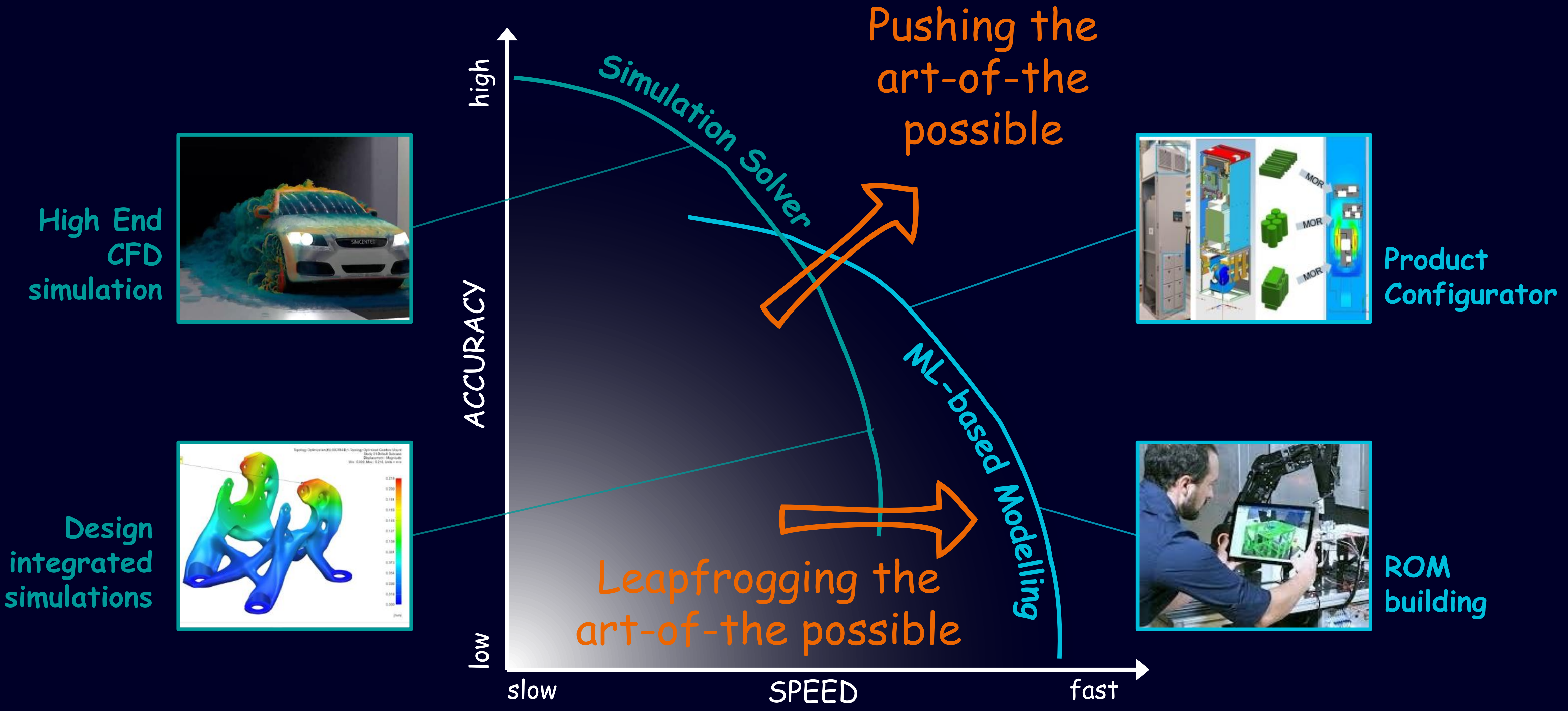
ML is challenging the Art of the Possible



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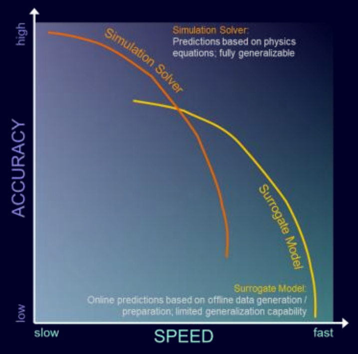
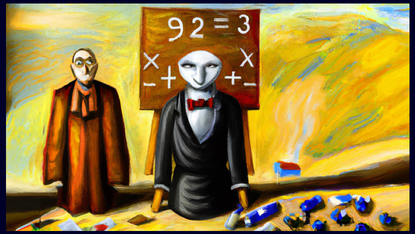
ML-accelerated Prediction Use Cases



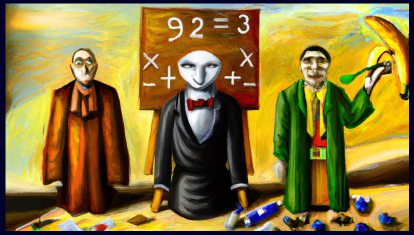
The Good

Acceleration of classical solvers



The Bad

Regression-based Model Order Reduction



The Ugly

Sampling strategies for industrial MOR workflows

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The Good

Acceleration of classical solvers

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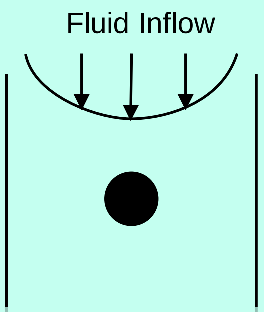
ML augmented CFD solver

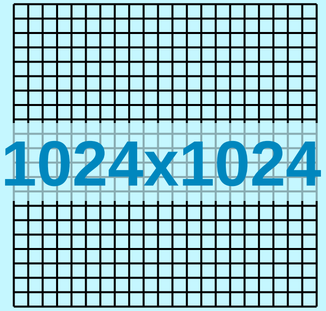
Simulation Task

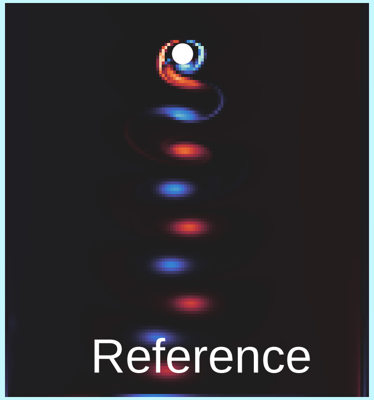


$$\rho \frac{D\vec{V}}{Dt} = -\nabla p + \mu \Delta \vec{V}$$

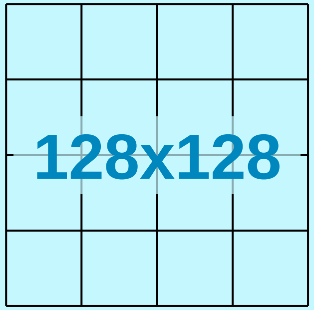
$$\nabla \cdot \vec{V} = 0$$

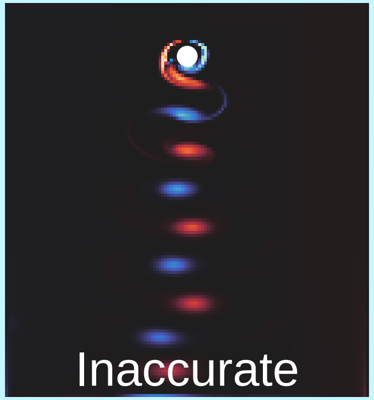
HiFi Simulation





LoFi Simulation





Using a coarser mesh allows a significant acceleration

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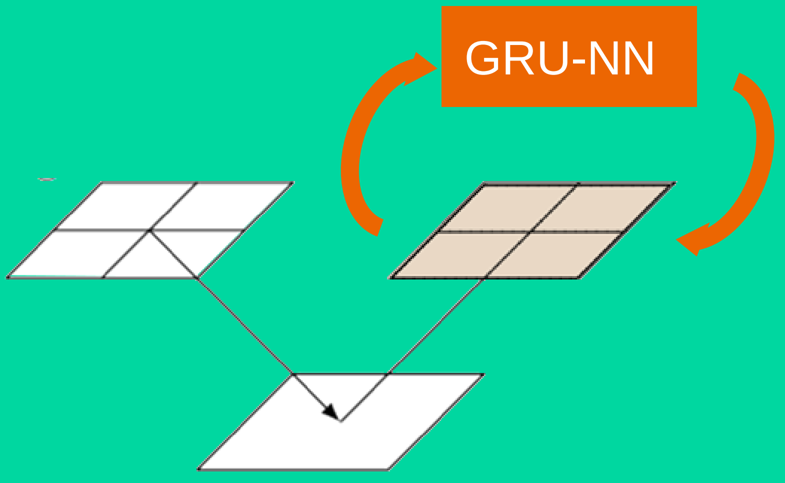
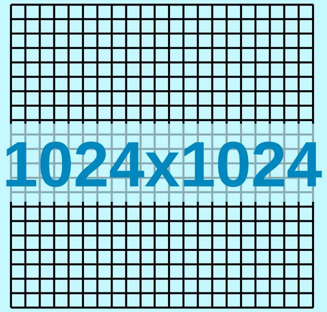
ML augmented CFD solver

NN-based Multigrid

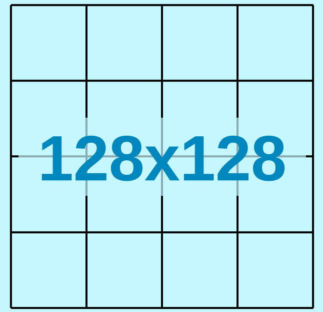


- Geometric multi-grid method
- NN-based smoother

HiFi Simulation



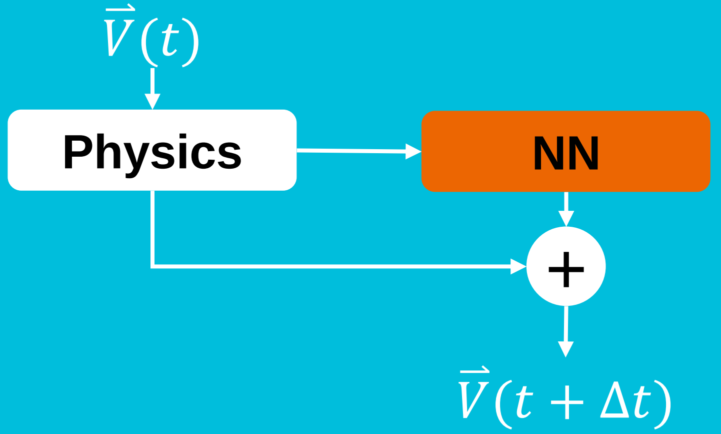
LoFi Simulation



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

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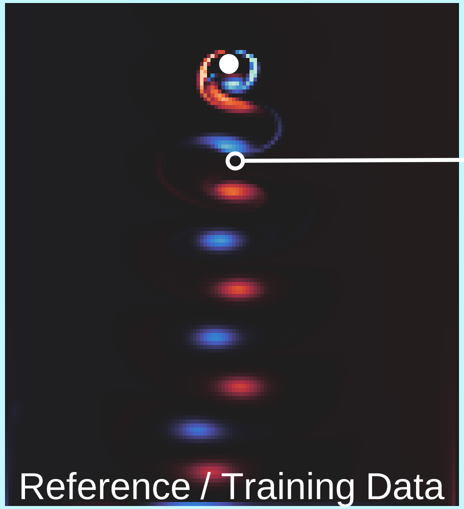
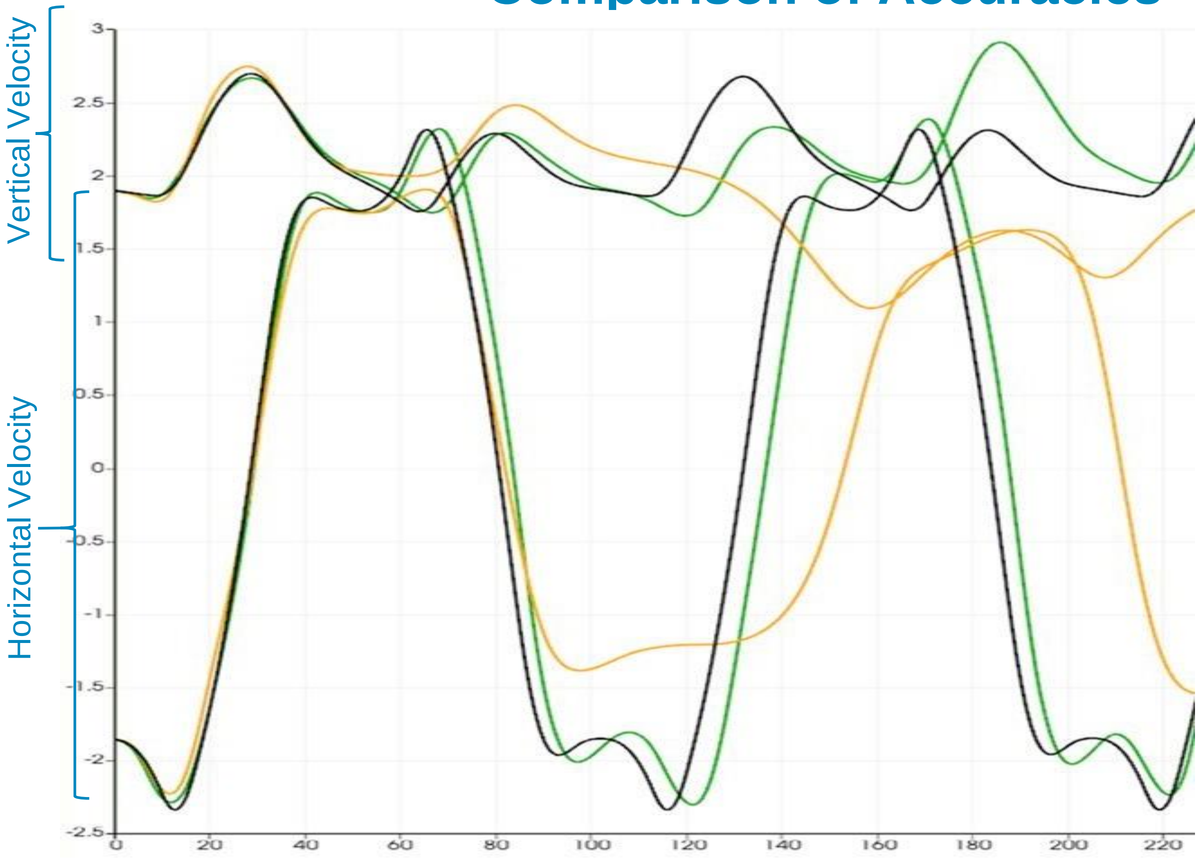
ML-based hybrid Modelling - Accuracy

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

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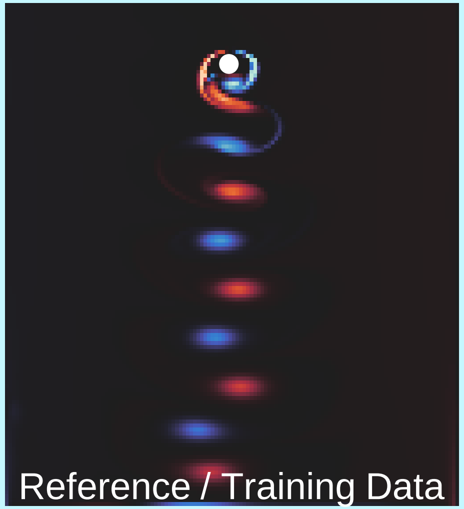
ML-based hybrid Modelling - Generalization

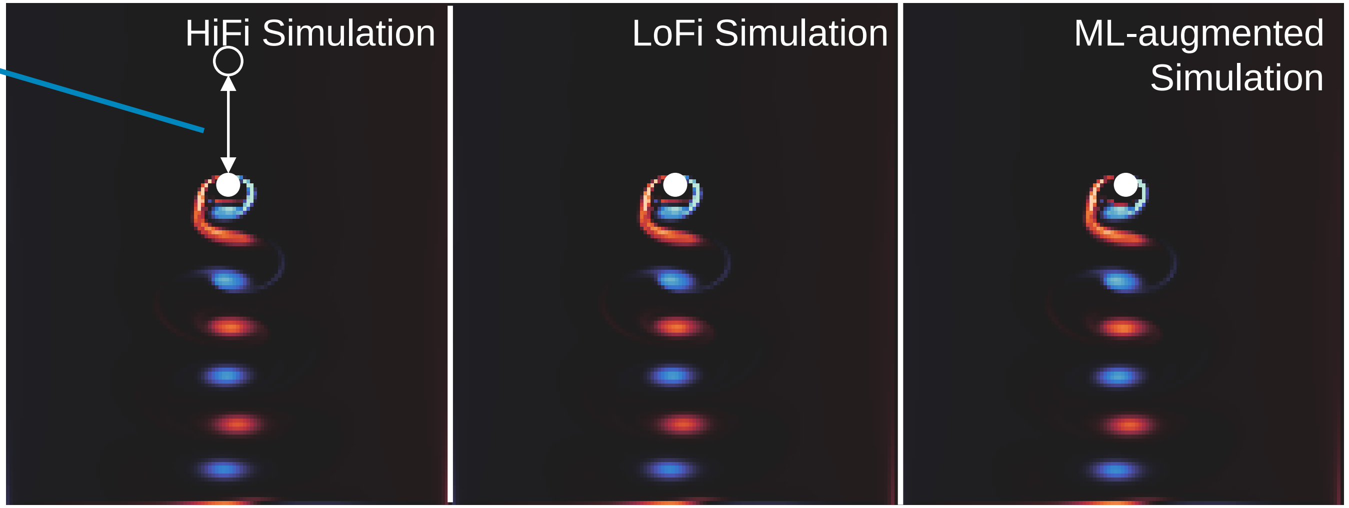
HiFi Simulation



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

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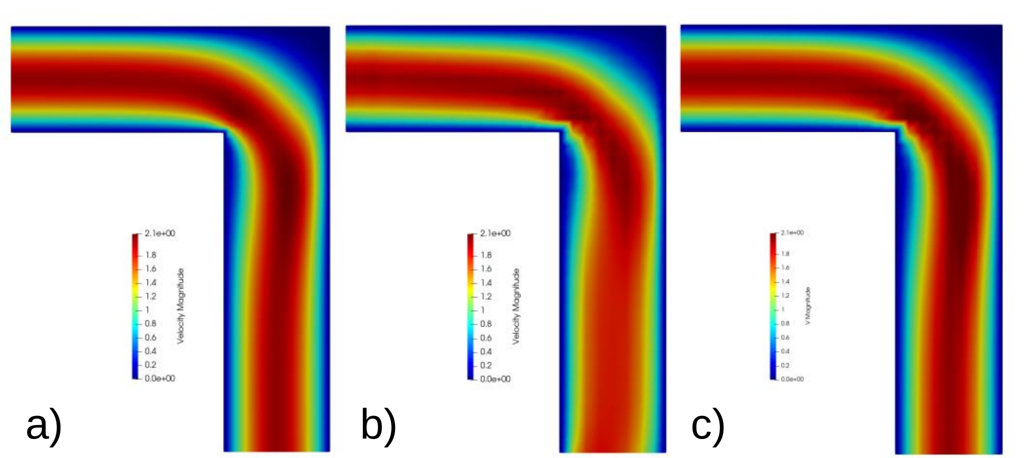
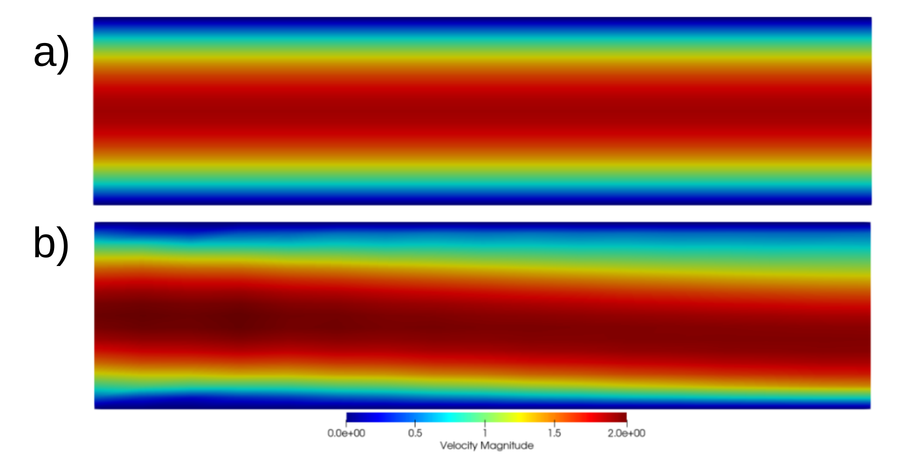
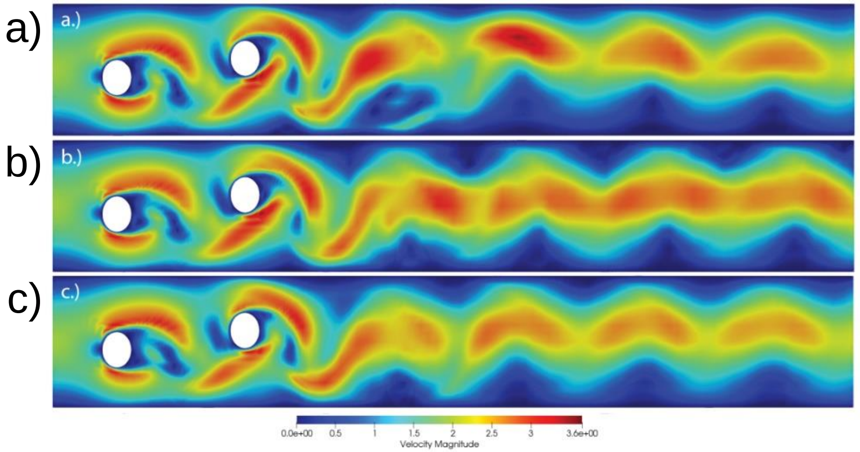
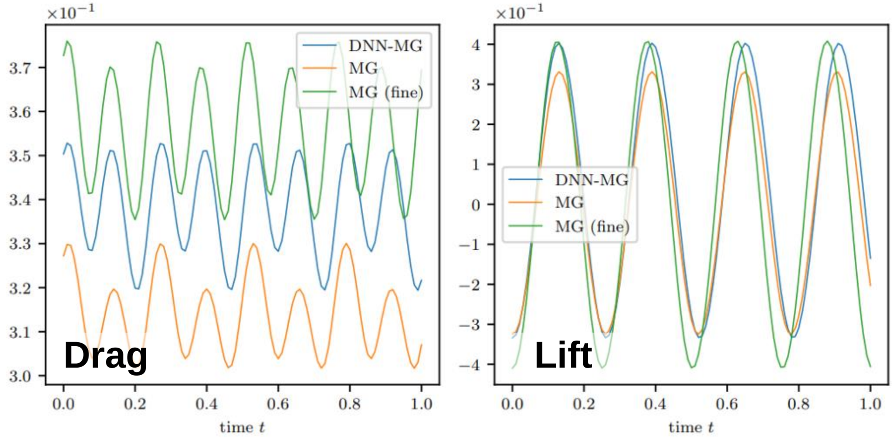
NN-based Multigrid Method - Generalization





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.

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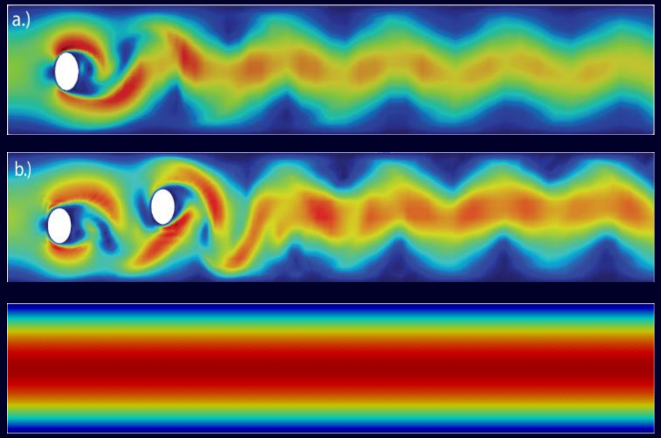
Intrusive Solver Acceleration



- ✔ 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

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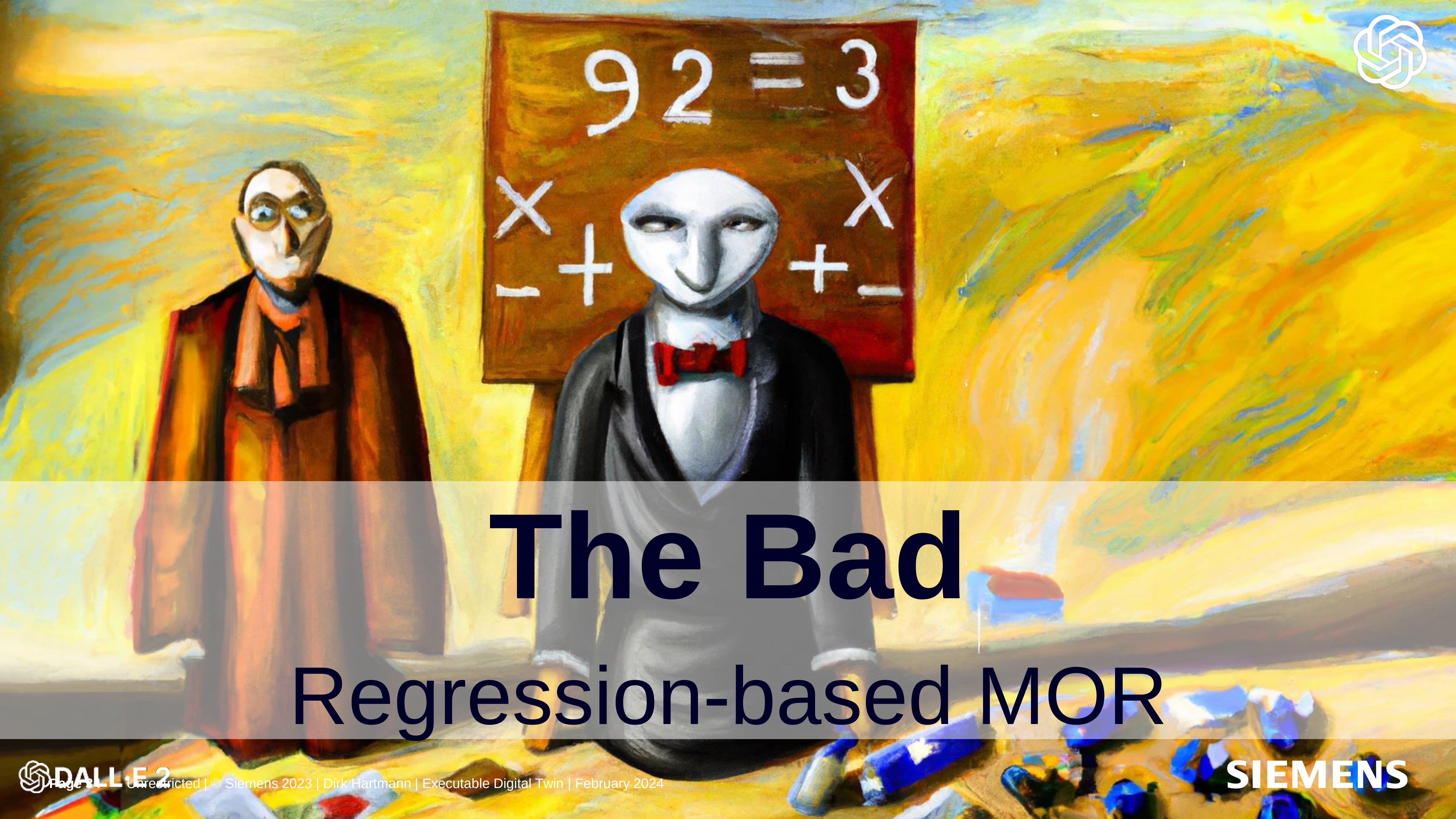
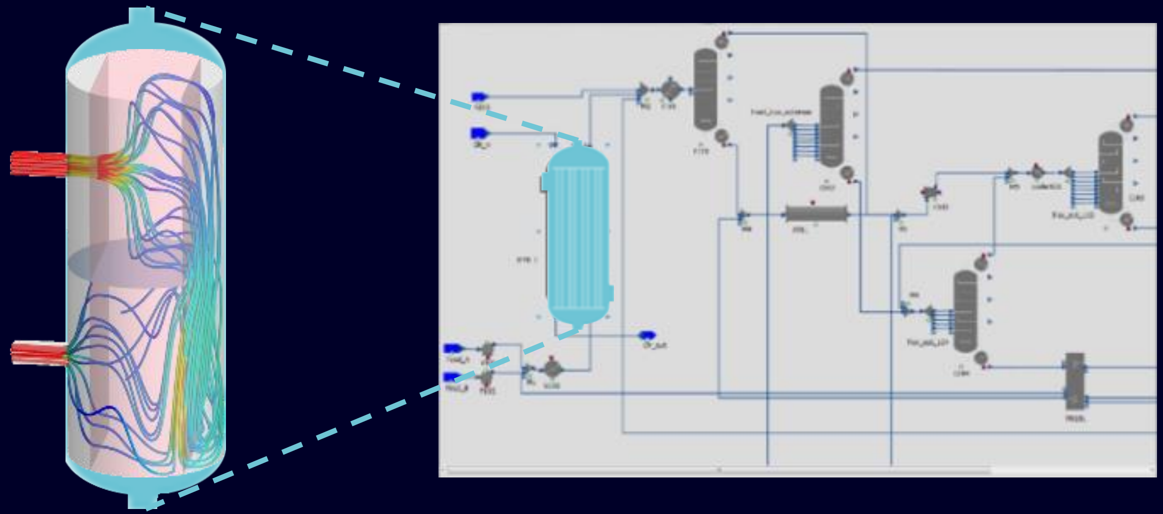


The Bad

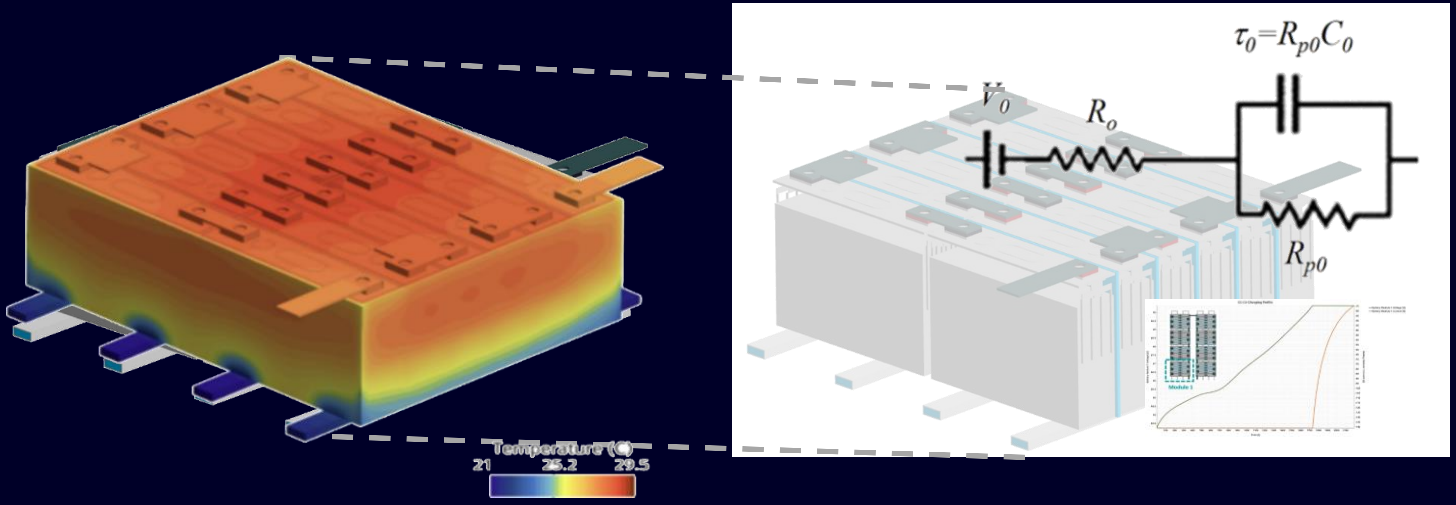
Regression-based MOR

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



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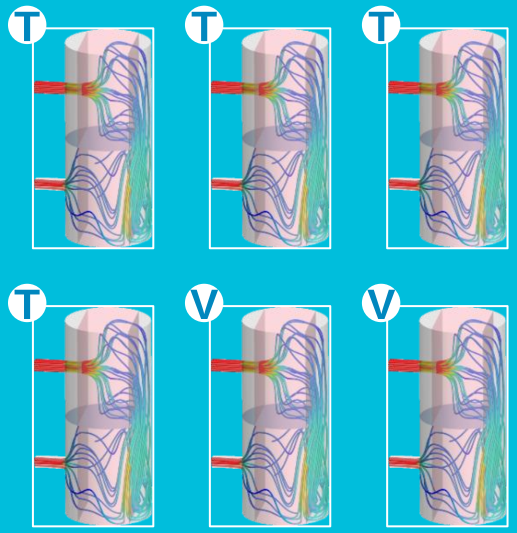
Non-linear Model Order Reduction in a nut-shell

Full Model Snapshots

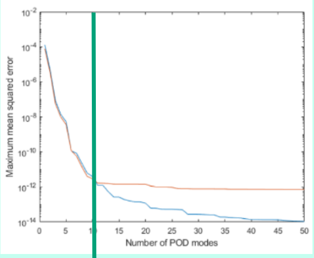


$x \in \mathbb{R}^n$

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

Latent Dimension Identification

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



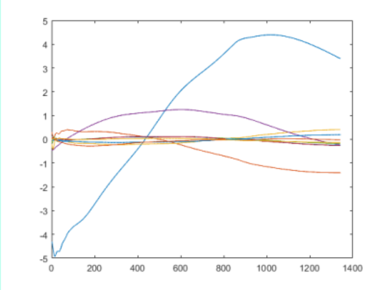
$\hat{x} \in \mathbb{R}^m$

with $m \sim 10 - 100$

Reduced Model Operator Discovery

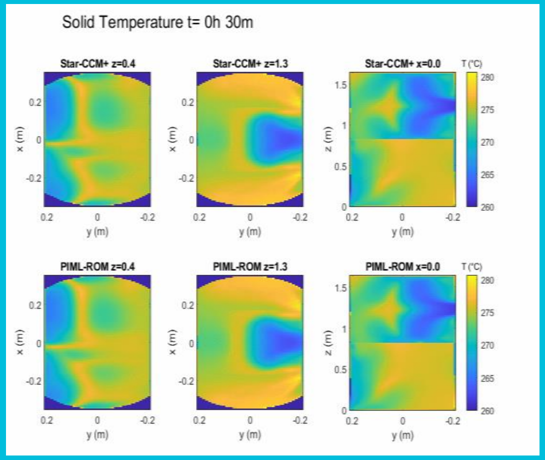
$$\partial_t \hat{x} = \hat{f}(\hat{x}, \mu)$$

- Discrete Empirical Interpolation
- Neural Networks
- Operator Inference



Reduced Coordinate trajectories

Reduced Model

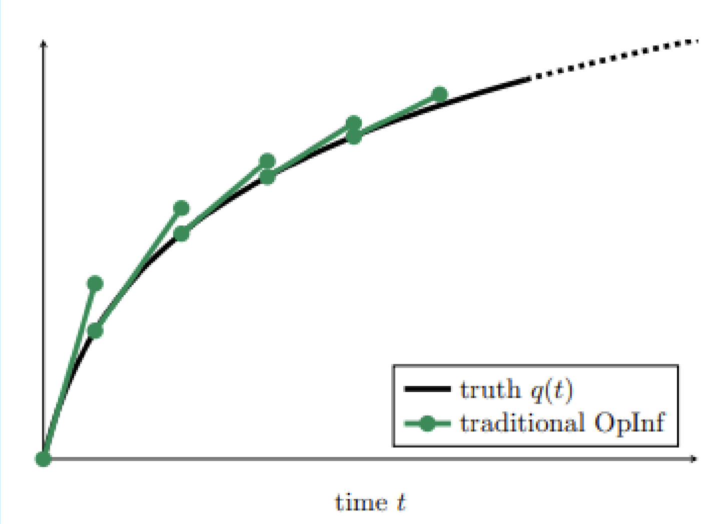


Real-time capable model, predicting the full field

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..

Solver-in-the-loop Model Order Reduction

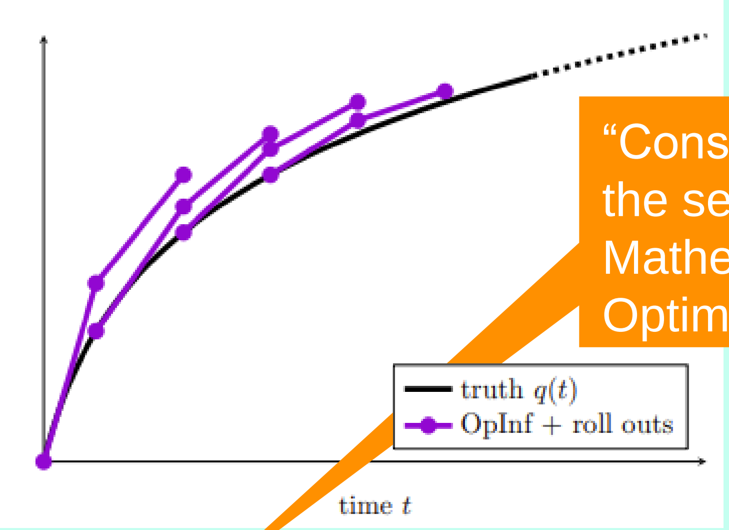
Classic Operator Inference



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



"Constrained" in the sense of Mathematical Optimization

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..

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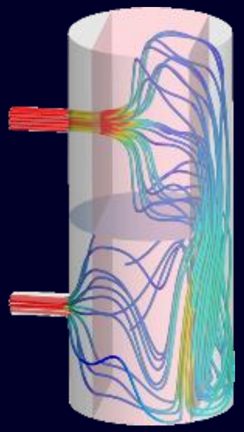
Example: Complex Cooling Flow



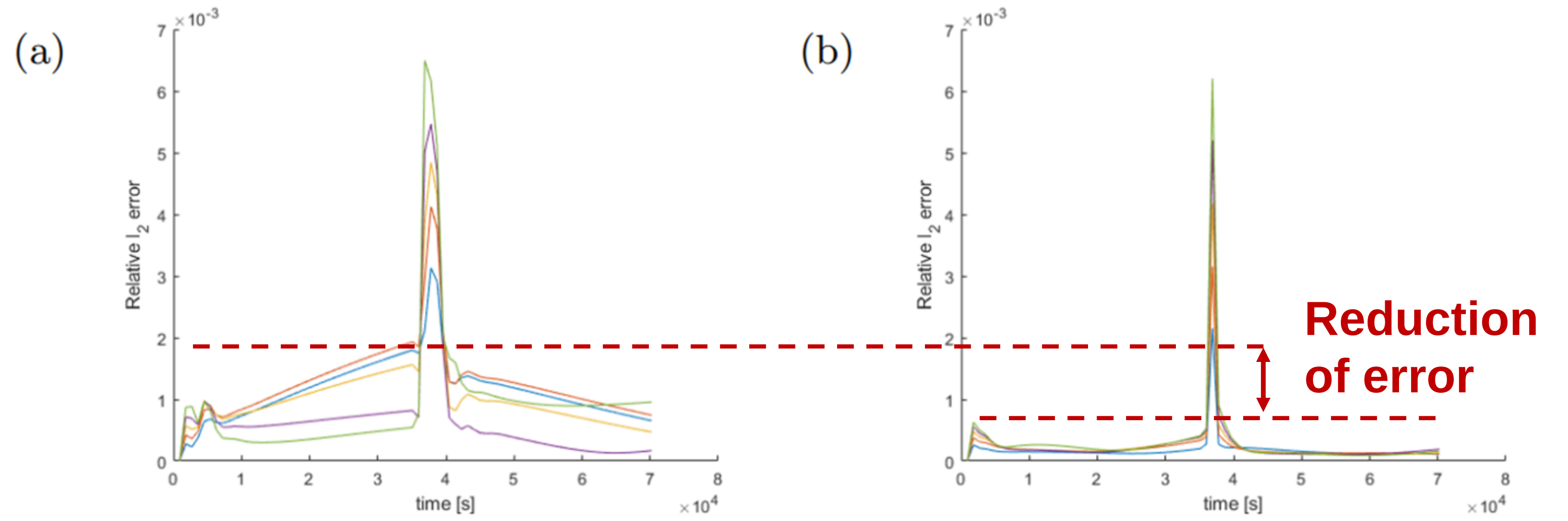
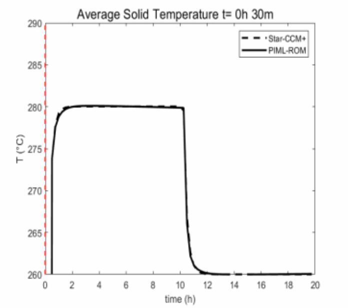


Figure: Operator Inference plus DEIM using 8 modes each: (a) Relative mean squared error of the dynamics predicted using stabilized operator inference (with stabilization parameter $\lambda = 1.0$) and (b) the same error after additional operator calibration (all 5 data sets, encoded in different color).

Example: Complex Cooling Flow



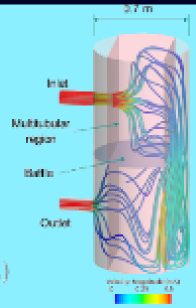
3D Physics with 400k DoF

$$\rho_0\left(\frac{\partial v}{\partial t} + (v\cdot\nabla)v\right) = -\nabla p + \mu\Delta v + \alpha(x)v$$

$$\nabla\cdot v = 0$$

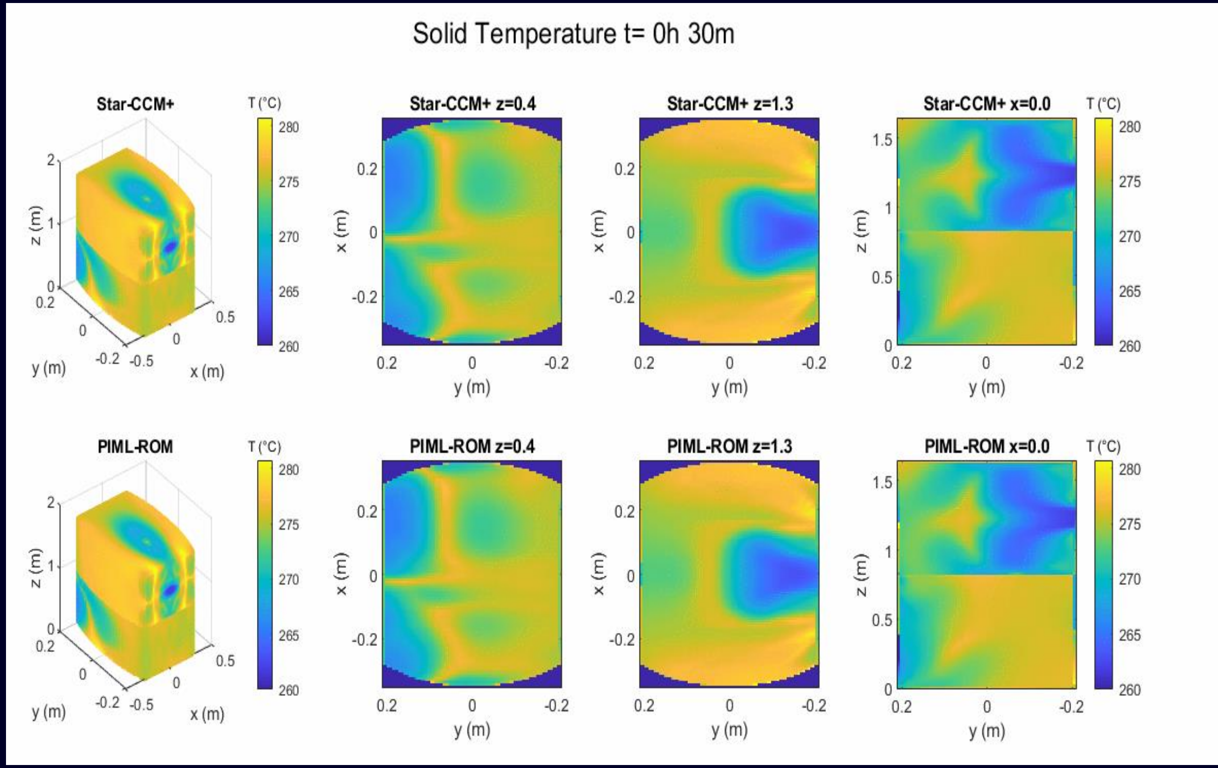
$$\rho_c c_{p,c}\left(\frac{\partial T_c}{\partial t} + (v\cdot\nabla)T_c\right) = \nabla\cdot(K_c\nabla T_c) + \chi_{\Omega_s} q(T_s - T_c)$$

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



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

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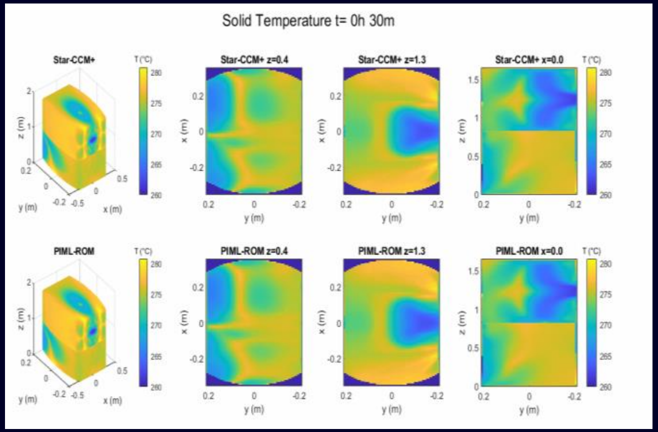
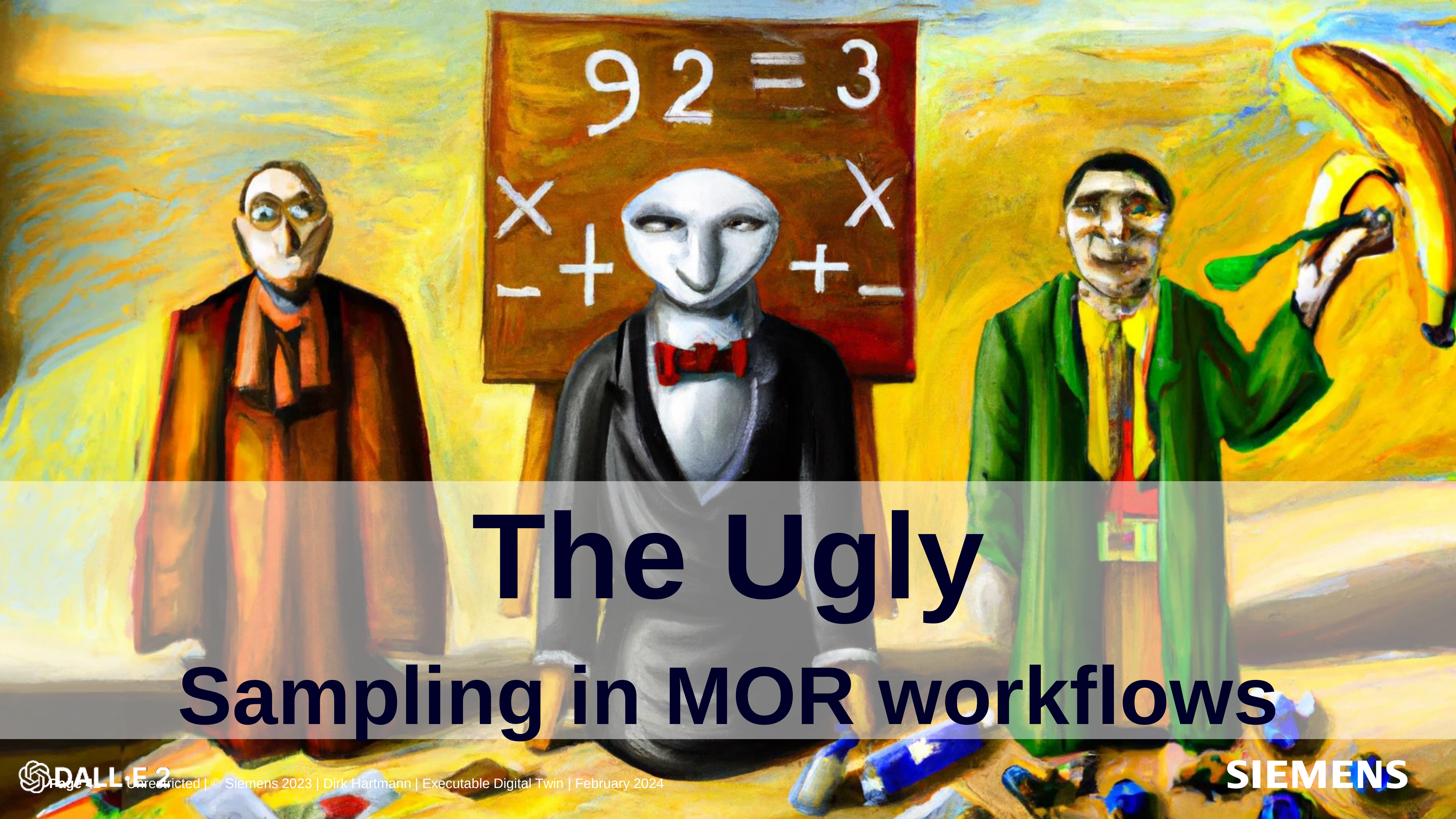
Operator Inference



- 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

The Ugly

Sampling in MOR workflows



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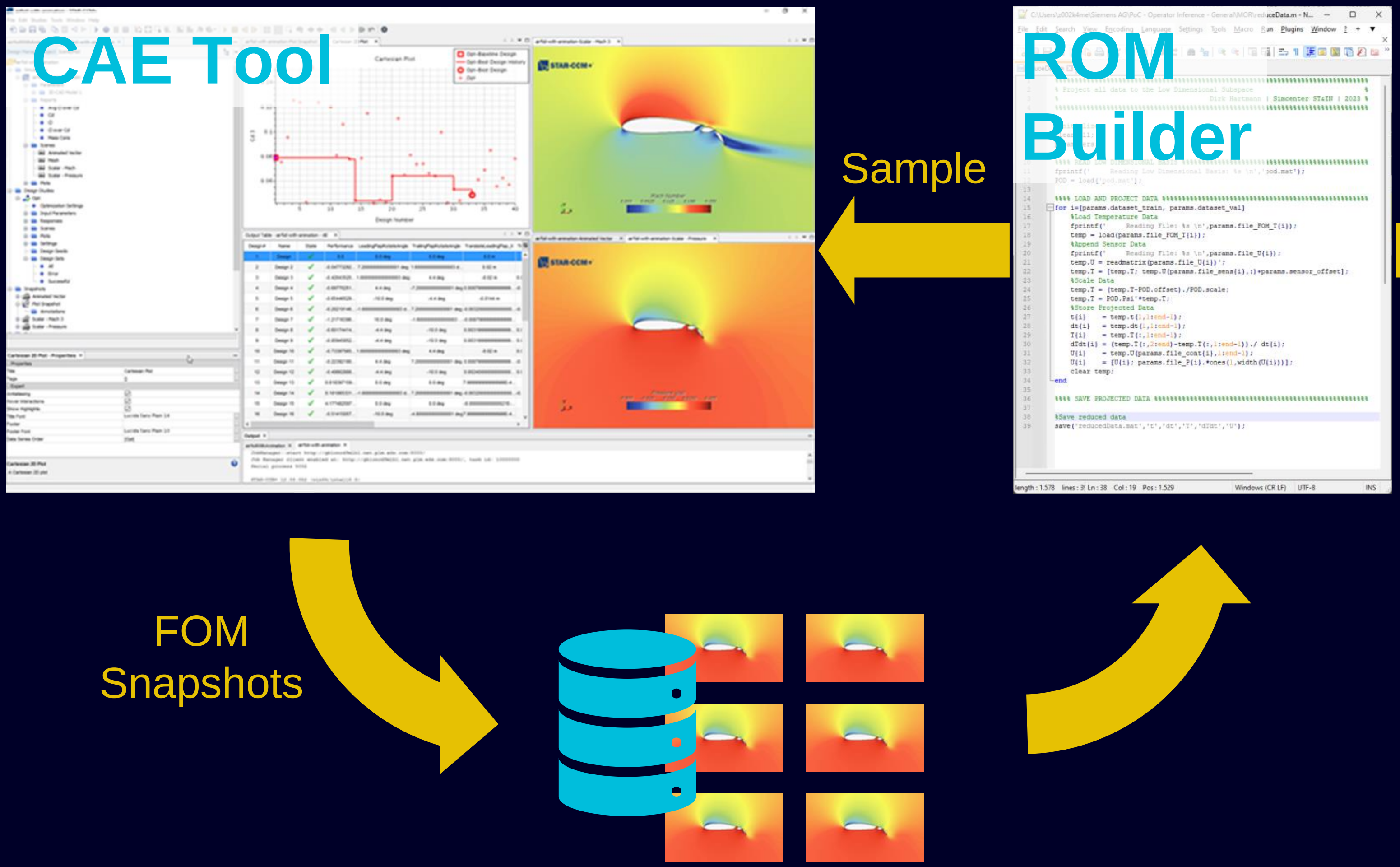
Industrial Model Order Reduction Workflows



Plus appropriate model management across the whole life cycle

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How to sample effectively

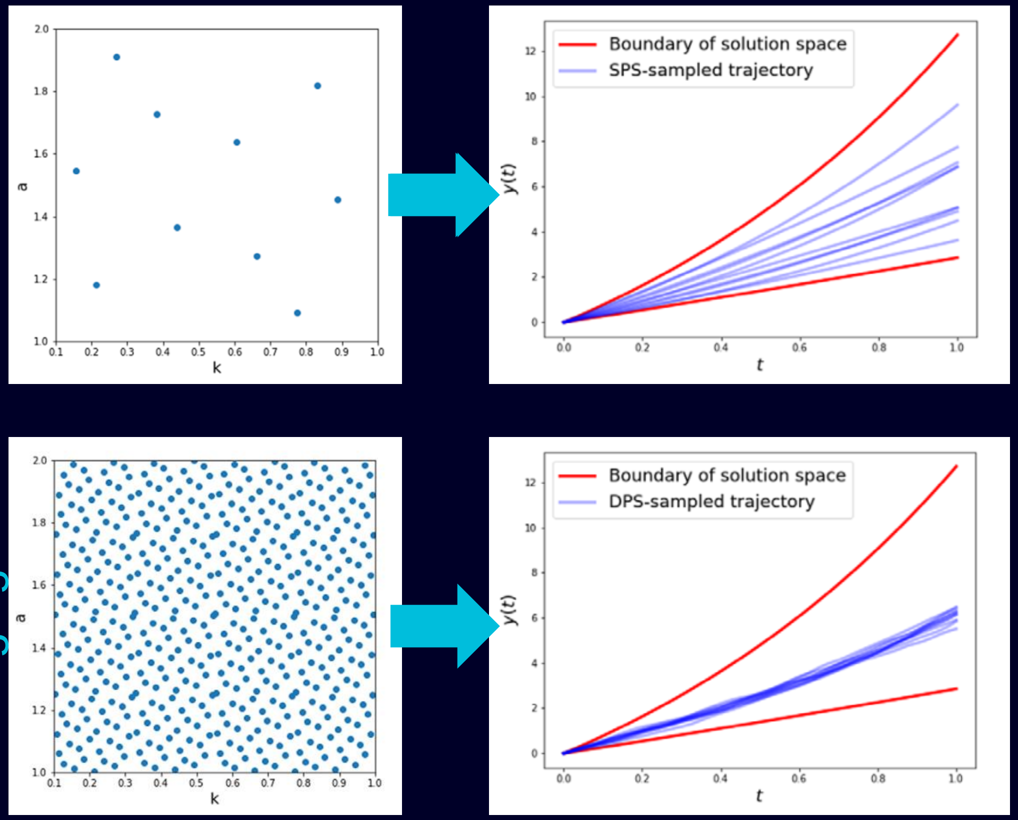
- Static vs. Dynamic Parameter Sampling
- One long trajectory vs many small trajectories
- …

Example:

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

Static Sampl.

Dynamic Sampl. changing in t



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

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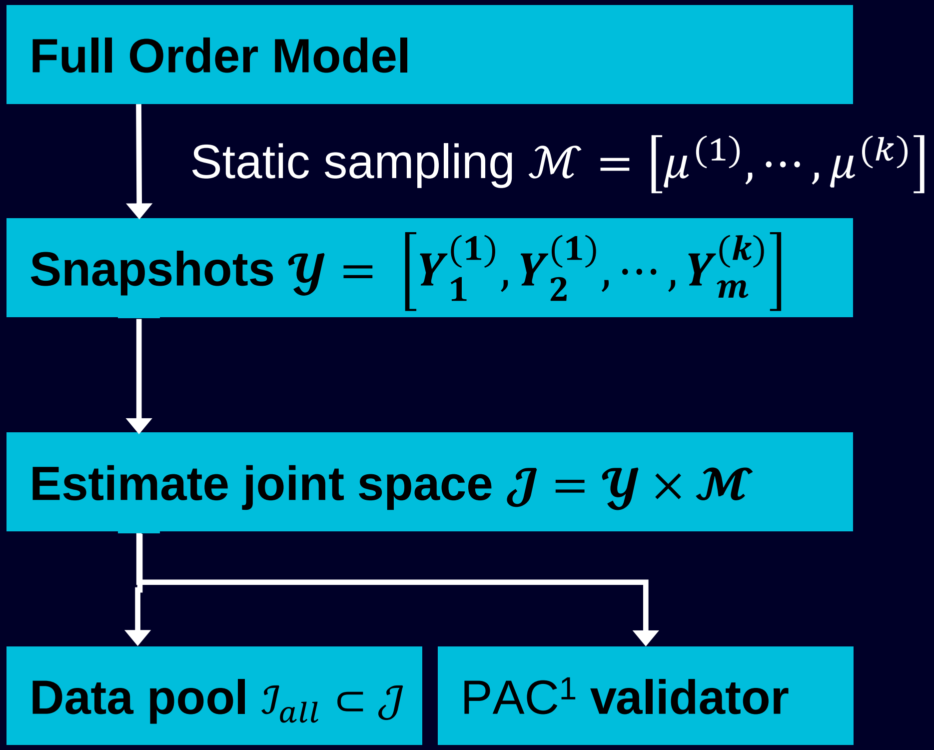
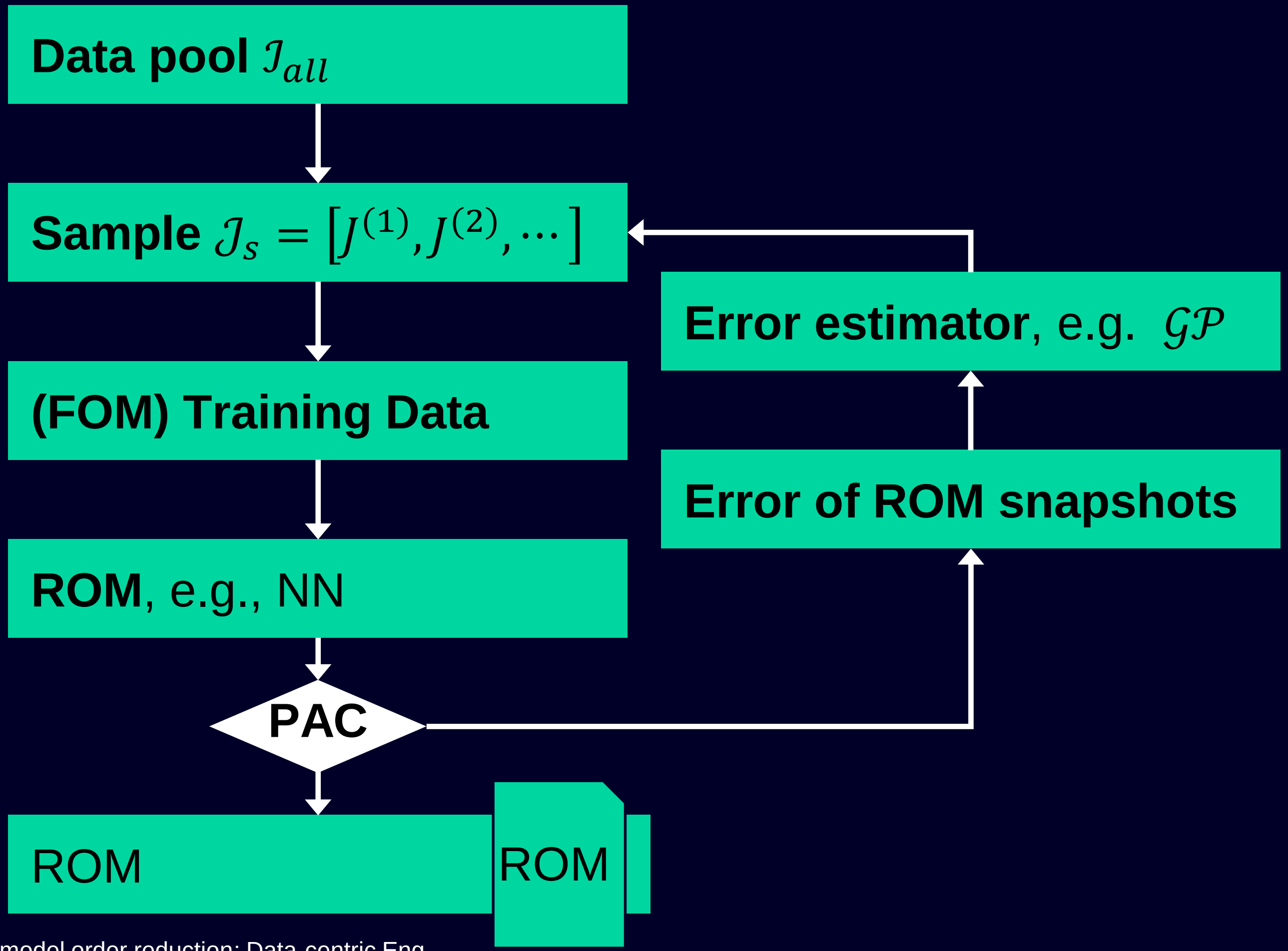
Active Learning Heuristic for industrial ROM

Preparation



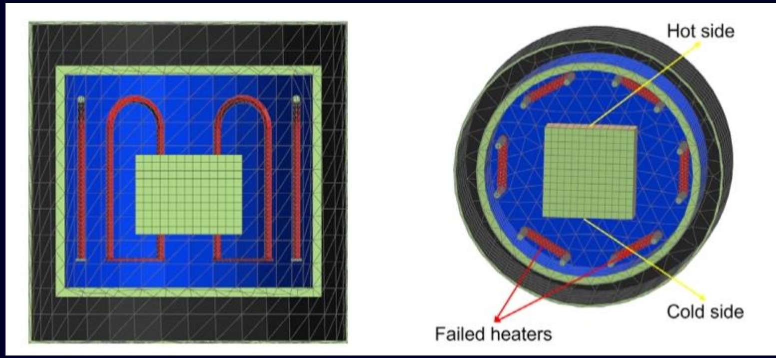
1) Probably approximately correct

Active Learning / Sampling



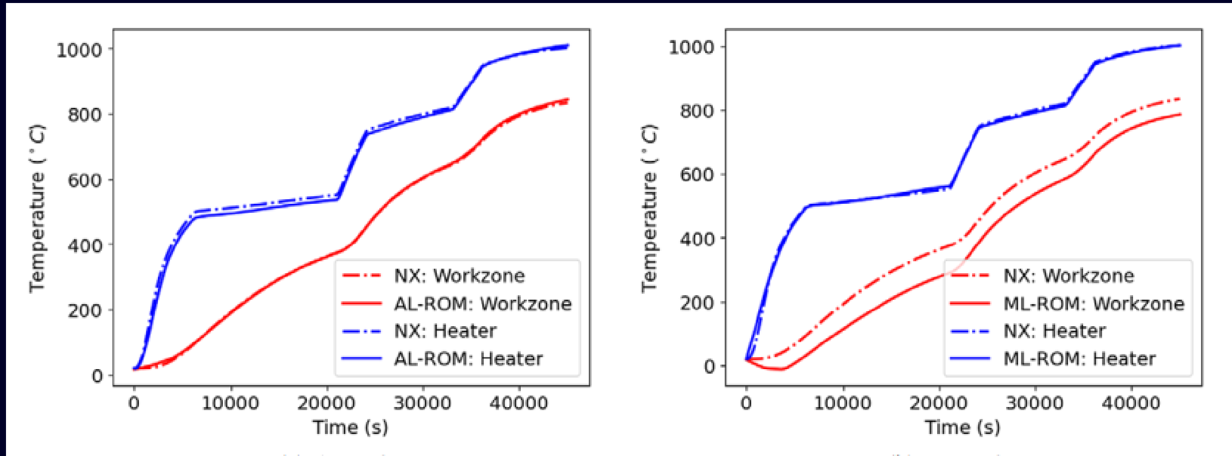
Source: Q Zhuang, D Hartmann, HJ Bungartz, JM Lorenzi,(2021): Active-learning-based nonintrusive model order reduction; Data-centric Eng

Active Learning Heuristic for industrial ROM



Test Case: Vacuum furnace

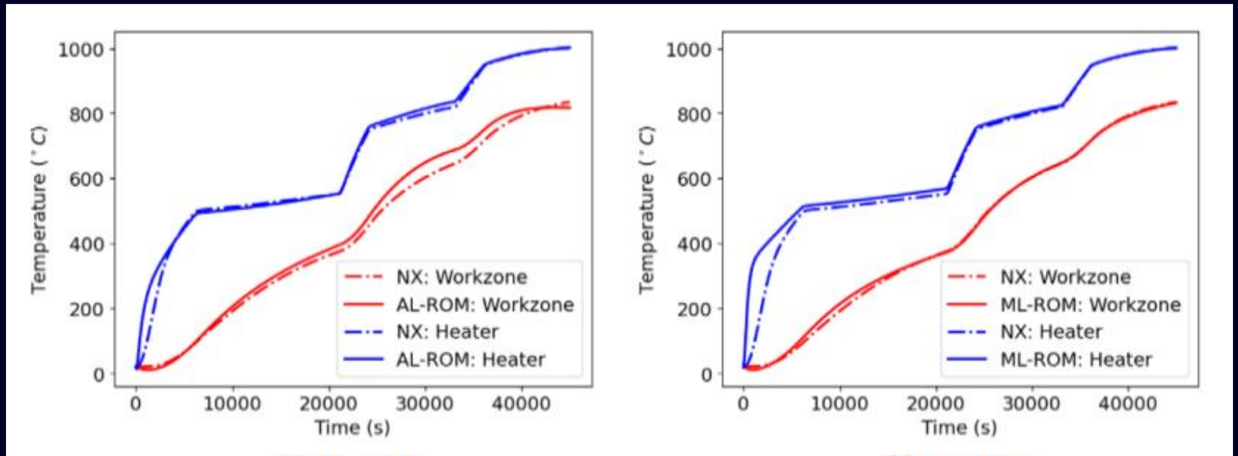
Euler Neural Network



(a) AL-ROM.

(b) ML-ROM.

Operator Inference



(a) AL-ROM.

(b) ML-ROM.

97%-confident ROM Error (PAC)

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

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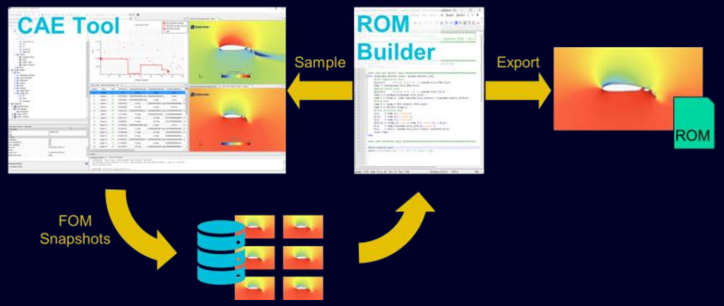
Industrial Model Order Reduction Workflows



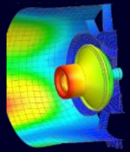
- ✓ Industrial workflows require a high degree of automation.
- ✓ Active learning strategies allow to achieve “optimal” ROMs.
- ✓ First heuristic strategies are available
- ✗ Analytic guarantees

4

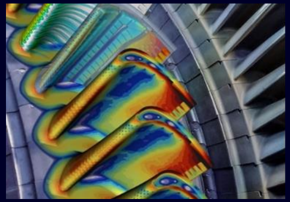
Wrap Up

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

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