Project Results Summary

24.09.2024

PHyMoS

01.03.2021 – 31.08.2024

Oliver Lenord[1],
with contributions from all partners[2]

1) Robert Bosch GmbH, Germany
2) ESI Germany GmbH
   HSBI (Hochschule Bielefeld)
   LTX Simulation GmbH
   Modelon Deutschland GmbH
   TLK-Thermo GmbH
   TUBS (TU Braunschweig)
   UNA (Universität Augsburg)
   XRG Simulation GmbH

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NextGenerationEU

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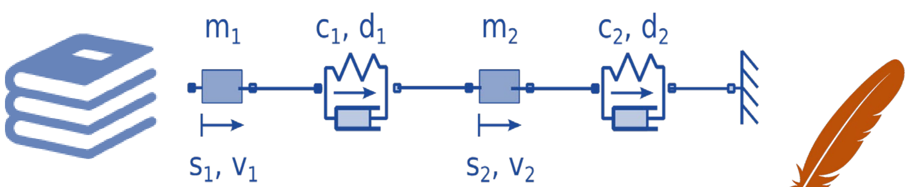
on the basis of a decision by the German Bundestag

Content

- Motivation and Problem Statement
- State-of-the-Art
- Vision and Project Goal
- Project Achievements
  - Demonstrators
  - Methods & Tools
- Summary and Outlook

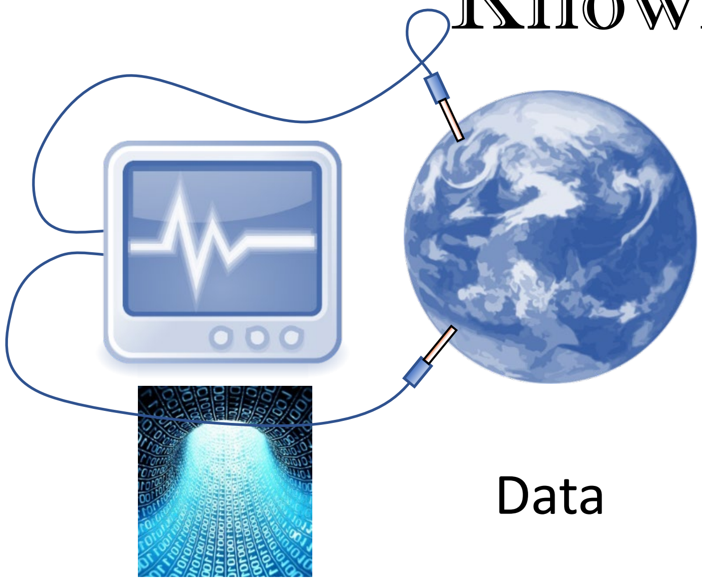
Motivation



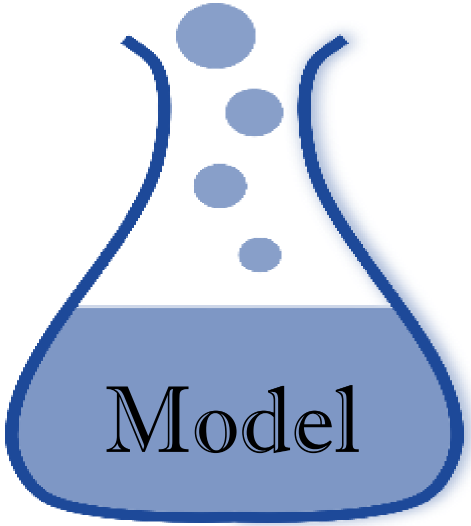
$$m_1\ddot{s_1} = c_1(s_2 - s_1) + d_1(\dot{s_2} - \dot{s_1})$$

Physics

Knowledge



Data

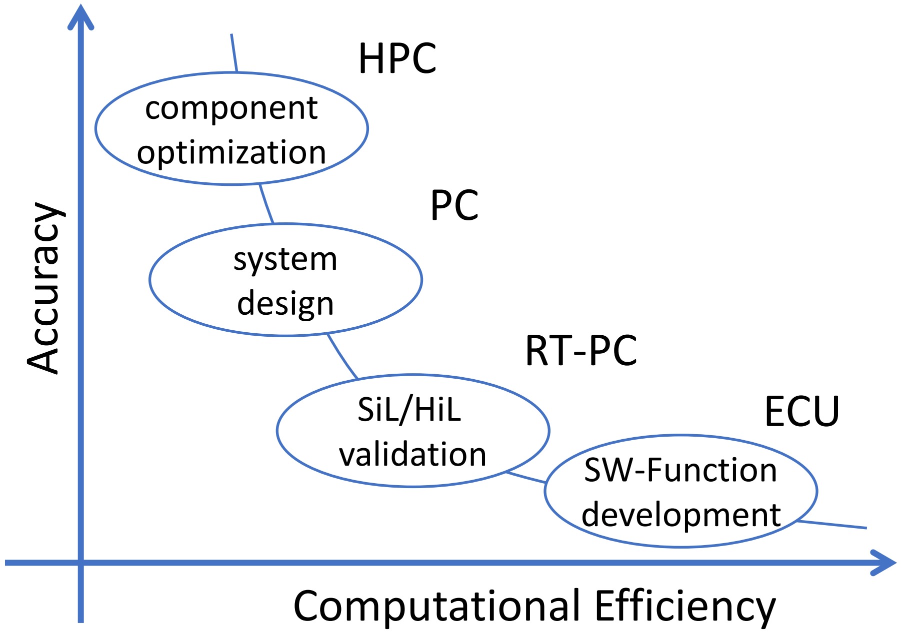


Simulation
MiL/SiL/HiL
Embedded Function

Problem Statement

Creating a „Proper Model“

- There is no “*One-size-fits-all* ” model.
- Trade-off between Accuracy and Runtime.
- Weighting depends on:
  - Model requirements,
  - Target environment,
  - Data availability (parameters, measurements)



➔ Reuse of models is often inadequate, if not impossible.

State-of-the-Art

Proper Model Creation

Classical Modeling	**Challenges**
• Conditional phys. effects (on/off)	• Binary logic (no gradual adjustment, trial and error, high expertise and experience
• Alternative models of phys. effects (replace component)	• Availability, compatibility, expertise
• Data-based characteristics (Look-up Table)	• Calibration effort, data quality, data volume
• Variable spatial discretization (component model)	• Applicability, Scalability
• Alternative formulation of the fundamental equations (model library)	• Compatibility
• Variable time discretization/error tolerance (numerical solver)	• Stability, limited effectiveness

State-of-the-Art

Proper Model Creation

Machine Learning

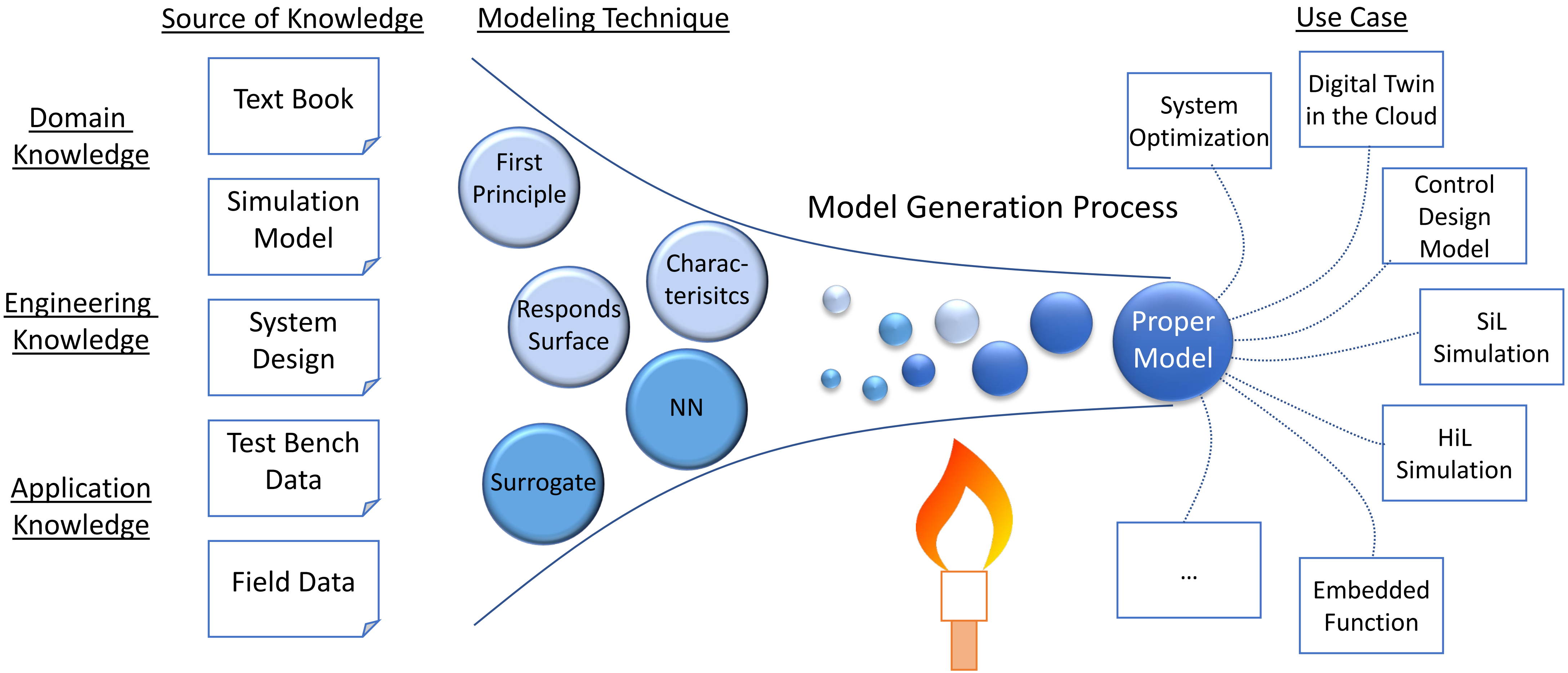
- Generic approaches
  - static relations (e.g. FFNN)
  - dynamics (e.g. LSTM, RNN)
- Hybrid approaches
  - PiNN
  - Problem spec. architectures

Challenges

- Training
  - Data availability (volume, quality, feature extraction, validation)
  - Convergence of the optimizer
  - Computational cost
- Behavior
  - Interpolation (Over-fitting)
  - Extrapolation (poor, unpredictable)
  - Stability at variable step size
- Architecture
  - Problem specific expertise
  - Data engineering expertise
  - Realization effort / integration effort

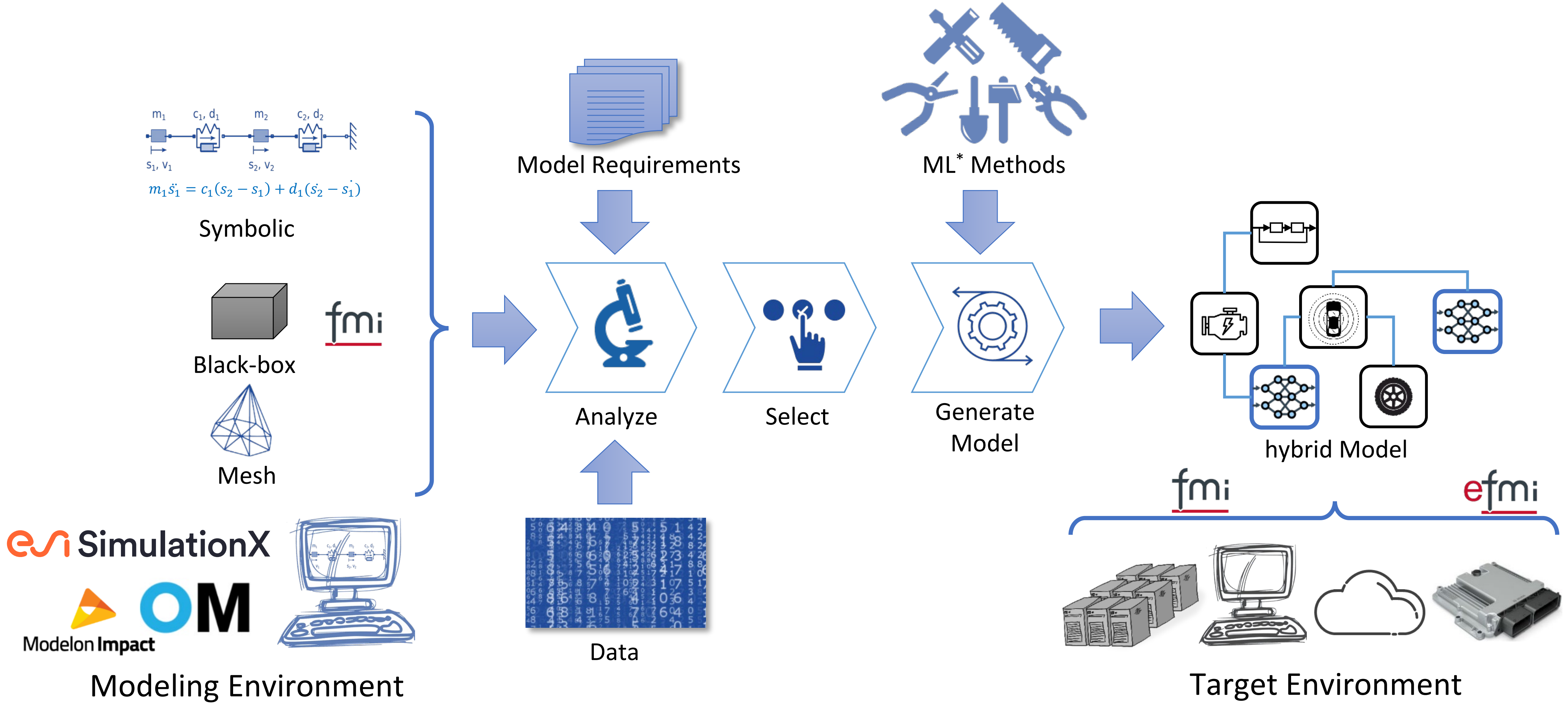
➔ Risky, not easily <u>accessible</u> to M&S engineers.

Vision



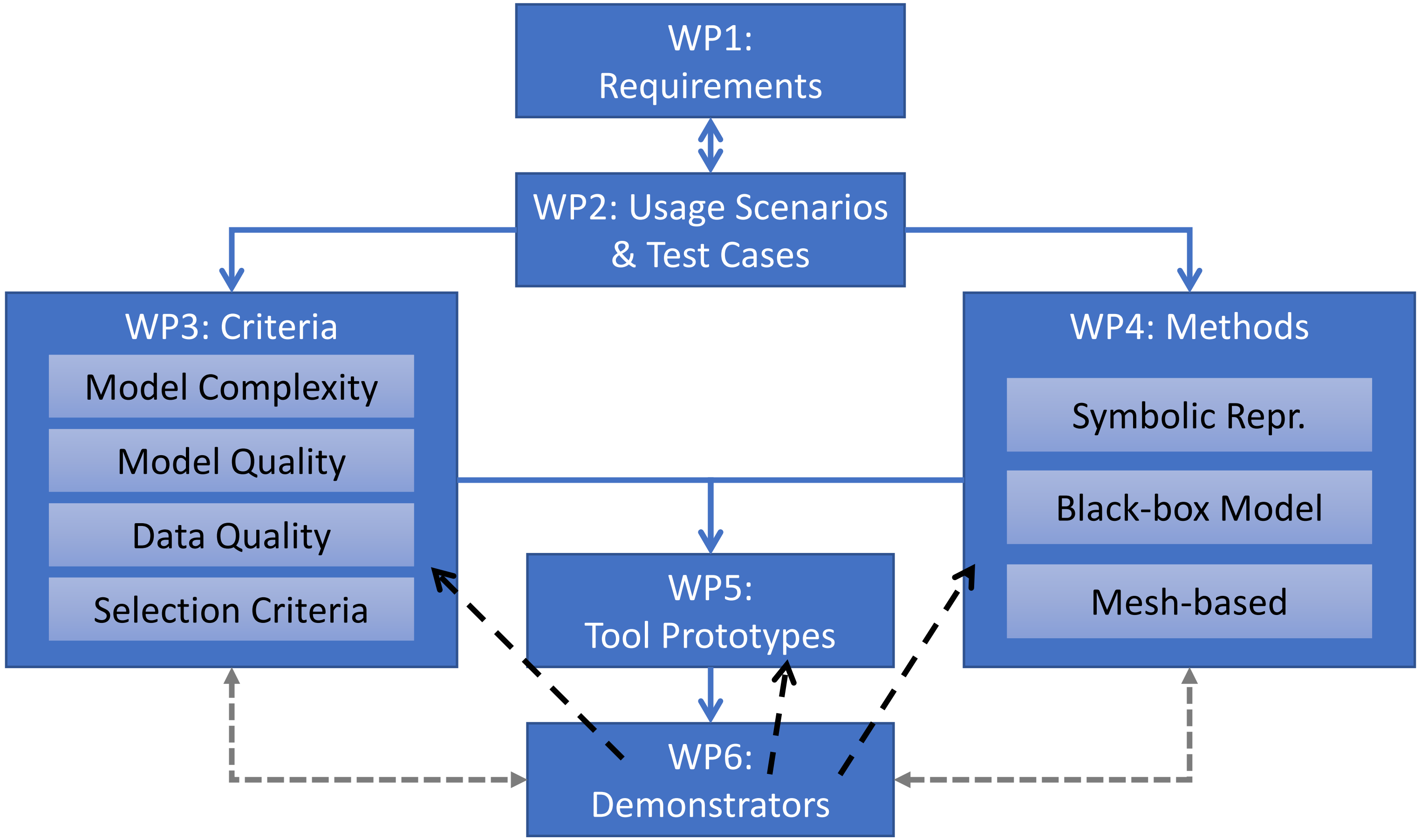
Source of Knowledge
Modeling Technique
Use Case
Domain Knowledge
Engineering Knowledge
Application Knowledge
Text Book
Simulation Model
System Design
Test Bench Data
Field Data
First Principle
Charac-terisitcs
Responds Surface
NN
Surrogate
Model Generation Process
Proper Model
System Optimization
Digital Twin in the Cloud
Control Design Model
SiL Simulation
HiL Simulation
Embedded Function
...

Project Goal (PHyMoS-Workflow)



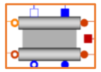
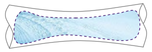
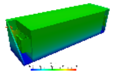
ML: Machine Learning

Project Structure → Results



WP: Work Packages

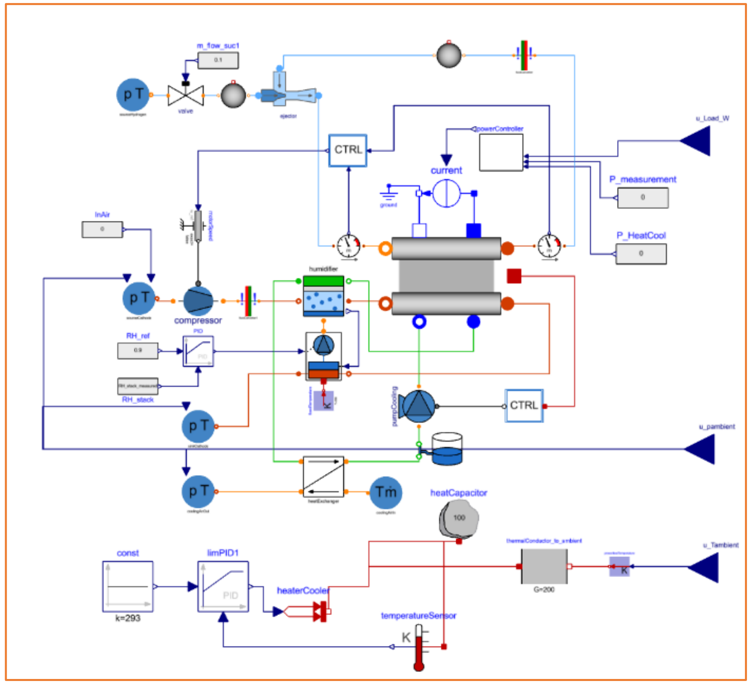
Demonstrators and Methods

		static	dynamic						symbolic			probabilistic				mesh based		
		FFNN	NODE	NDDE	NFMU	RNN	LSTM	PiNN	ALR	Sym. Reg.	egg	Bayes Flow	BNN	PBNN	MDN	MGN	DMDc	POD
	Fuel Cell	x																
	Heat Pump	x	x															
	Hyd. Pipe	x	x	x					x							x		
	Hyd. Drive				x	x	x											
	Jet Pump								x	x								
	MEMS							x				x	x	x	x			
	HVAC Cabin		x									x				x	x	
	Battery	x																x

FFNN: Feed-forward Neural Network
NODE: Neural Ordinary Differential Equations
NDDE: Neural Delay Differential Equations
NFMU: Neural Functional Mock-up Unit
RNN: Recursive Neural Network
LSTM: Long short-term memory
PiNN: Physics informed Neural Network
ALR: Algebraic Loop Replacement
egg: equality graphs good
BNN: Bayesian Neural Network
PBNN: Probabilistic Bayesian Network
MDN: Mixture Density Network
MGN: Mesh Graph Nets
DMDc: Dynamic Mode Decomposition w/ control
POD: Proper Orthogonal Decomposition

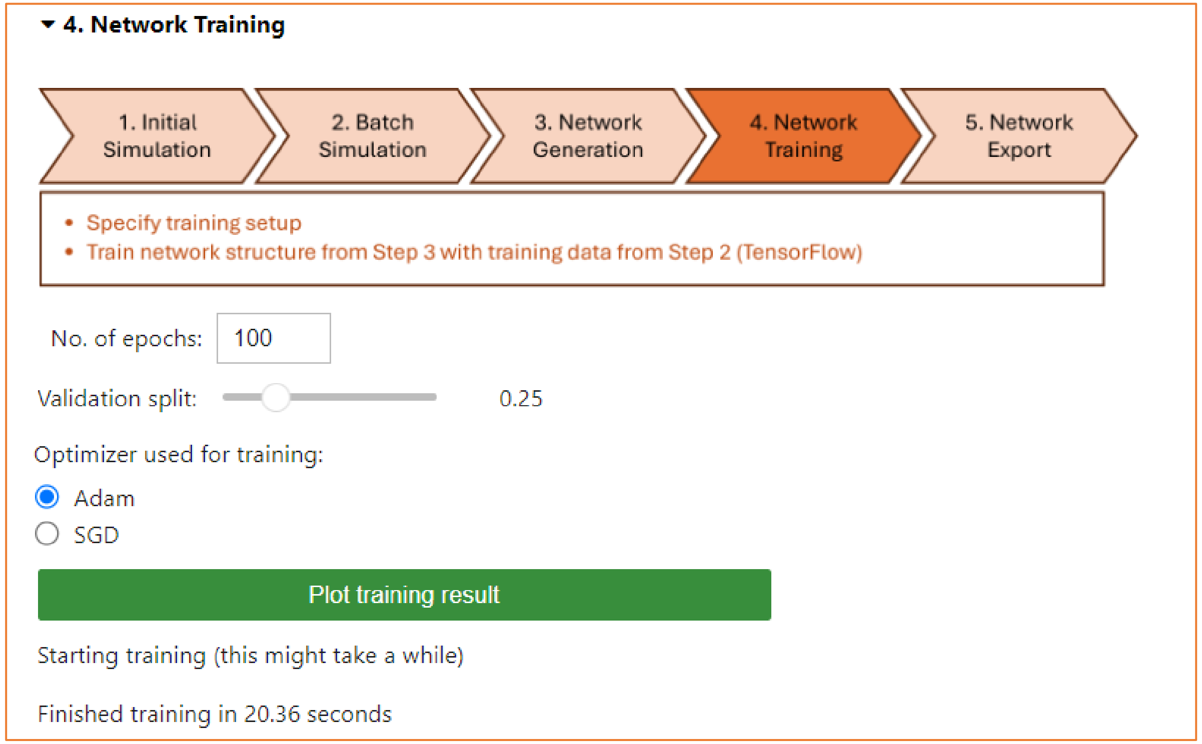
Modelon – Fuel Cell System

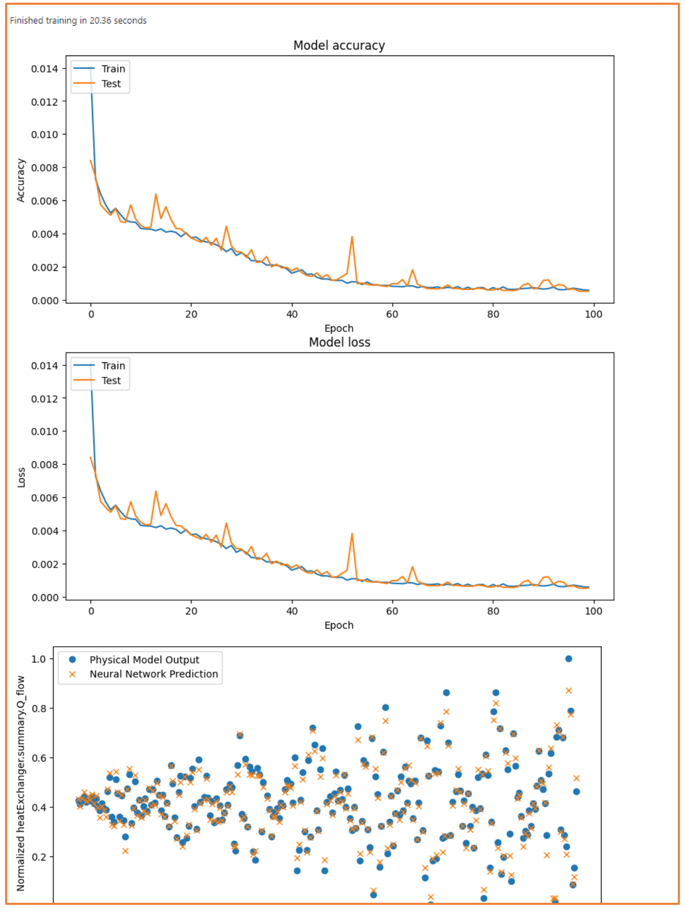
- Use Case:
  - Detailed Fuel Cell System Model
- Goal:
  - Significant simulation speed-up by replacing components or subsystems with surrogate models.
  - Easy-to-use integrated workflow.



• Continuous states:	82
• Variables:	2572
• Linear equation blocks:	13
• Non-linear equation blocks:	4

Demonstration in Modelon Impact

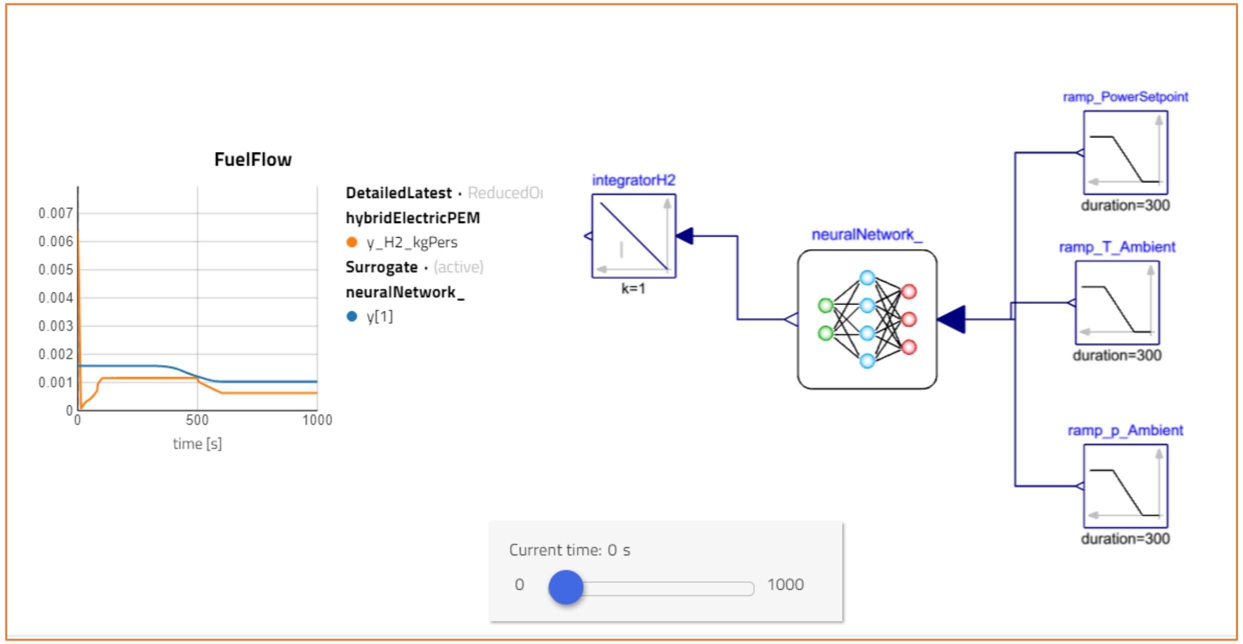




Hübel, Moritz, Nirmala Nirmala, Michael Deligant, and Lixiang Li. 2022. "Hybrid physical-AI based system modeling and simulation approach demonstrated on an automotive fuel cell.", In Modelica Conferences, pp. 157-163. 2022. https://doi.org/10.3384/ecp193157

Modelon – Results

- Methods:
  - FFNN, to be extended
- Integrated workflow
  - covering all stages from data generation to model training
  - creates Modelica compliant NN1) block of the surrogate
- Performance
  - Speed-up x5 – x500
  - error 1-5%
  - 2 times differentiable



1) NeuralNetwork Modelica library
https://github.com/AMIT-HSBI/NeuralNetwork

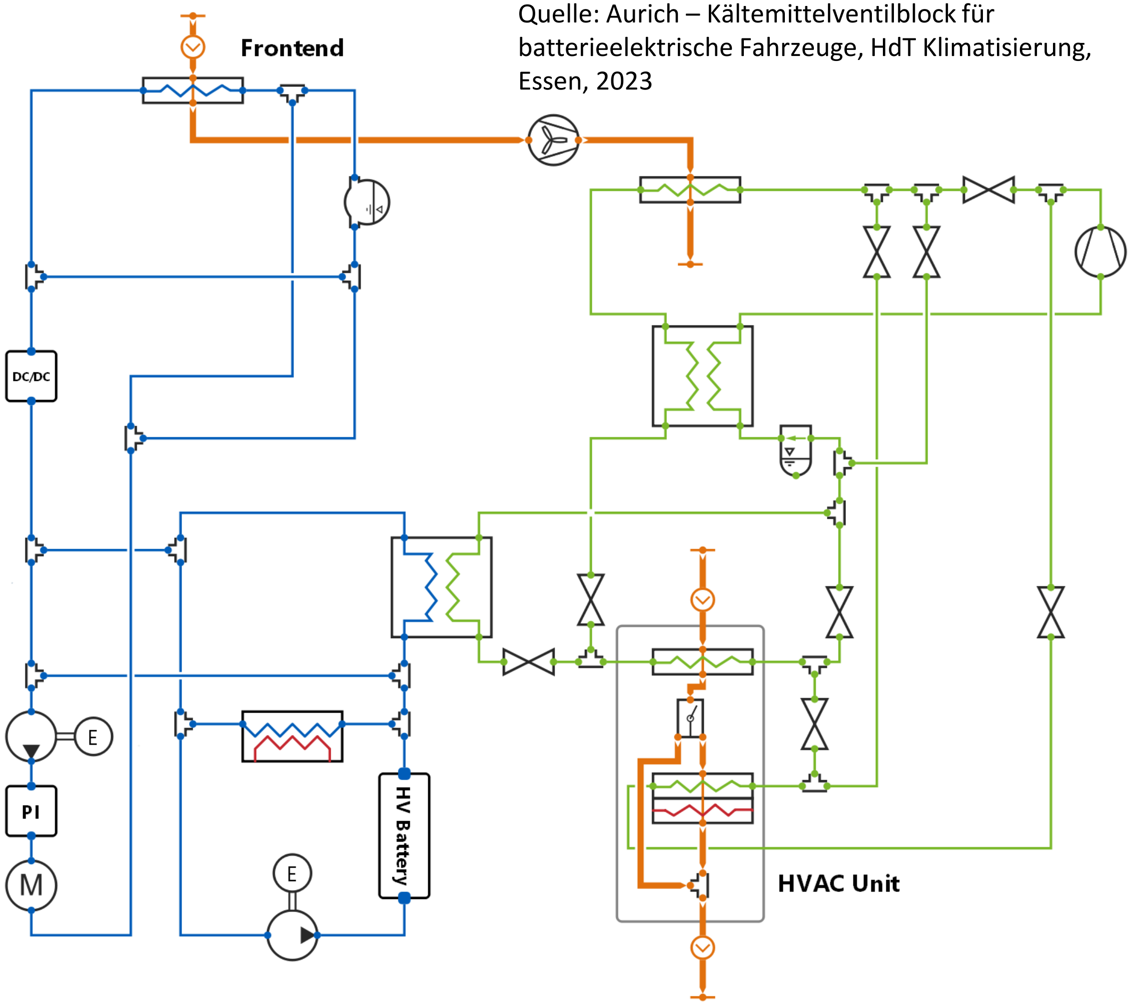
TLK – BEV Heat Pump

- Heating, cooling and dehumidifying of passenger compartment
- Electric drive train and battery cooling (waste heat utilization)
- Largest electrical auxiliary consumer

→ Safety (e.g. defogging)
→ Comfort
→ Range

→ Multiple control targets and complex interactions

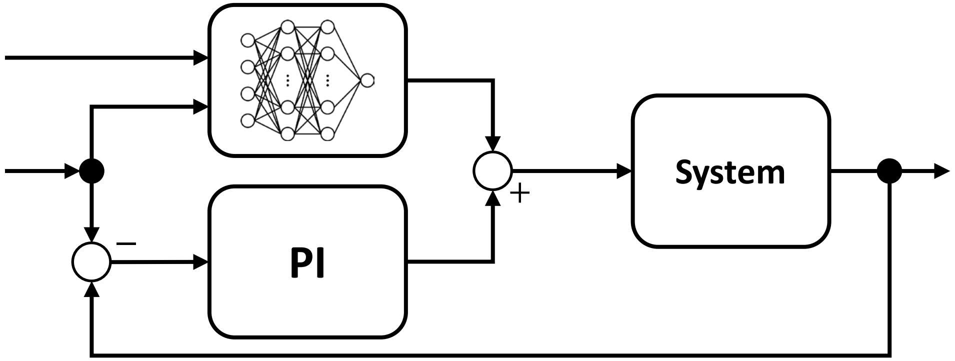
Quelle: Aurich – Kältemittelventilblock für batterieelektrische Fahrzeuge, HdT Klimatisierung, Essen, 2023



Demonstrator Use Cases

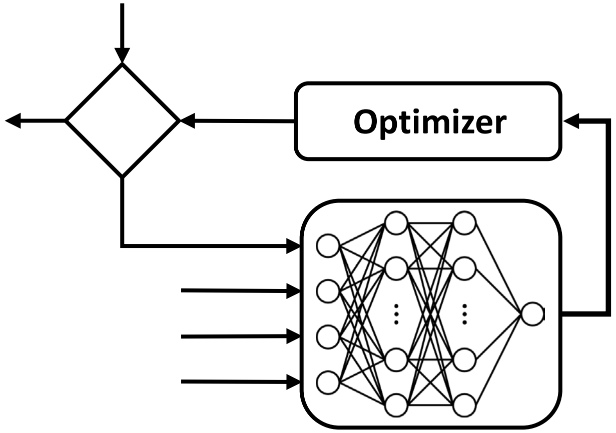
Static surrogates

- Simple feedforward control of compressor speed
- Reference variable optimization of heat rejection pressure



Dynamic surrogates

- Model-based control engineering
- Actuating variable optimization



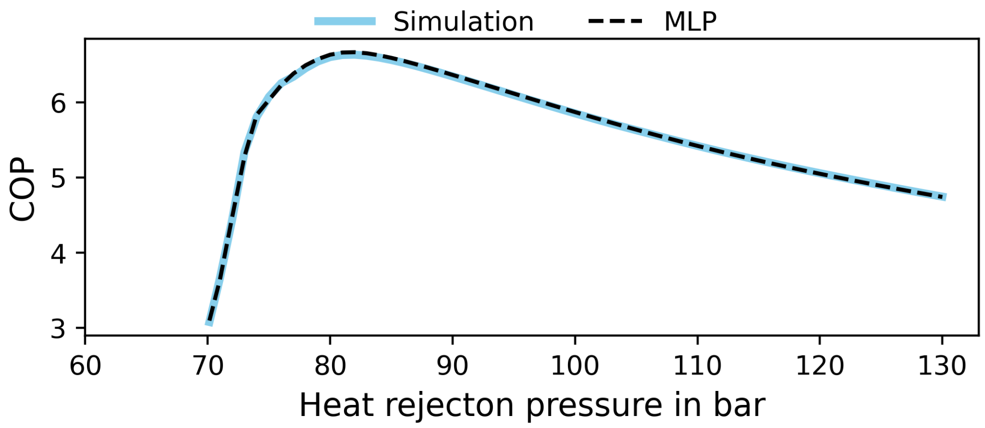
Demonstrator Results

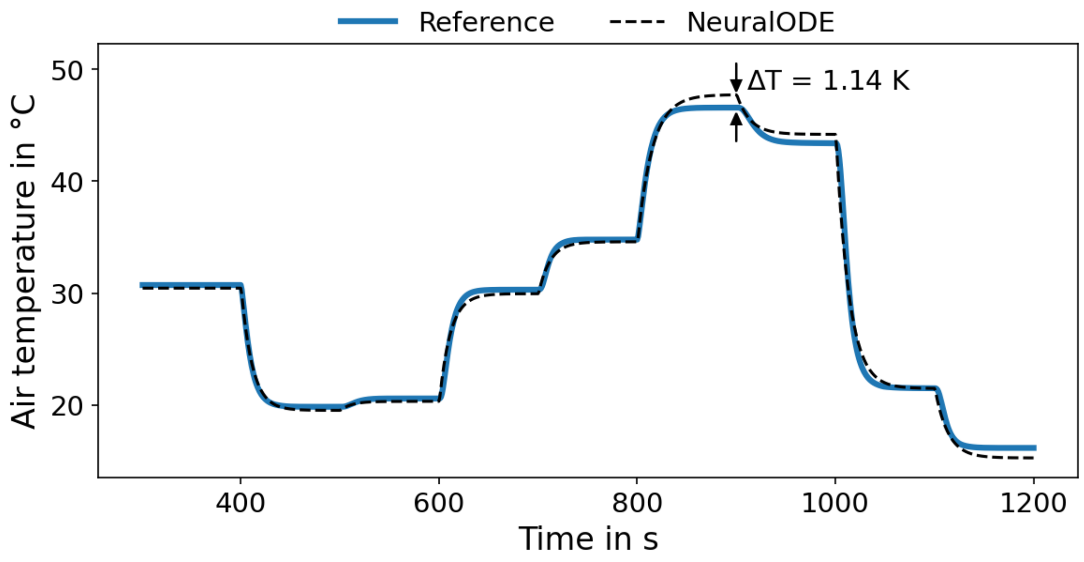
Static surrogates

- FFNN to estimate COP depending on operating point
- Enables online setpoint optimization

Dynamic surrogates

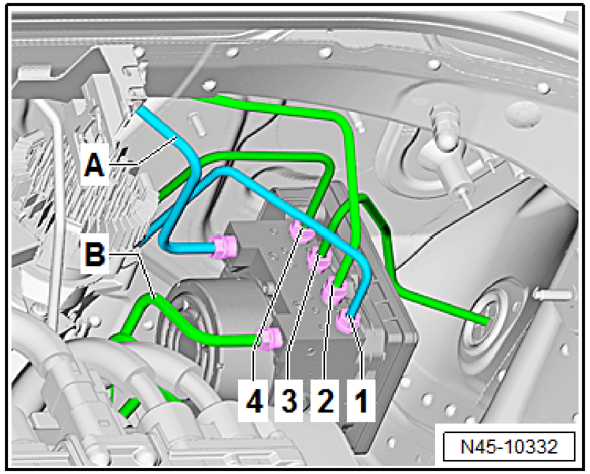
- NeuralODE for control targets
  - Model speed-up >x100
- Vehicle system simulation in co-simulation setup
  - Detailed heat exchanger model speed-up >x 1000
  - Overall speed-up >x2



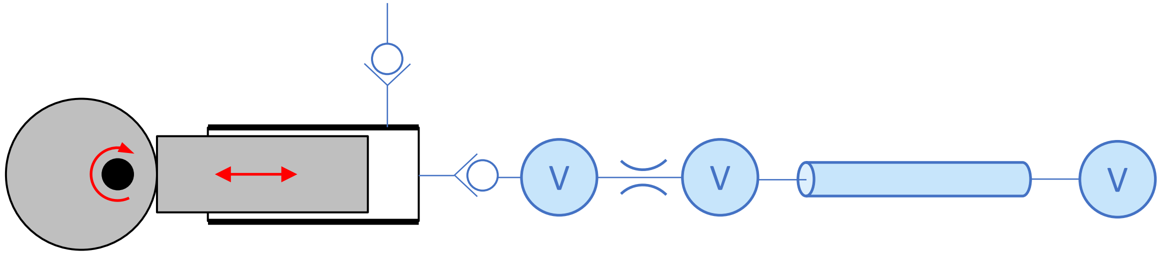


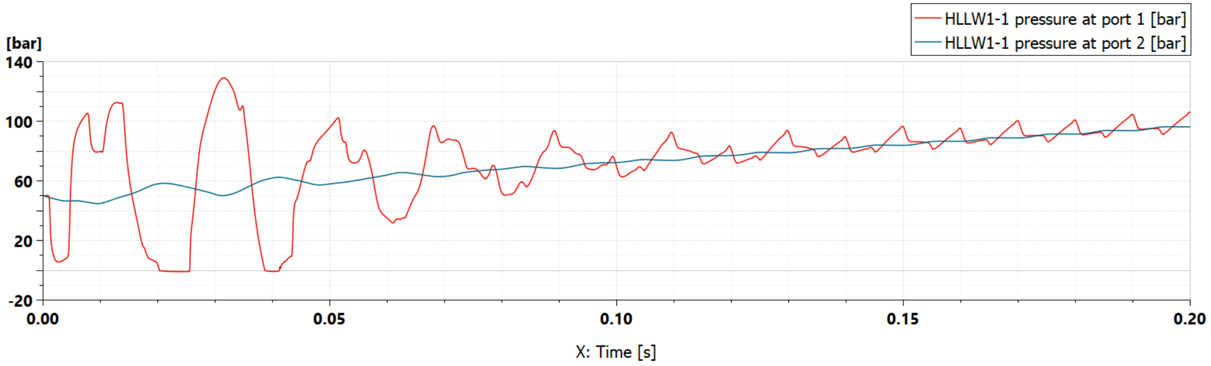
Bosch – Hydraulic Line

- Complex 2-phase dynamics considering cavitation
- High accuracy requirements
- 1D CFD Lax-Wendroff
  - High effort due to co-simulation setup
- ClaRa.PipeAdvancedVCM by XRG
  - Shows similar accuracy as Lax-Wendroff
  - Selected as base line for PHyMoS-benchmark



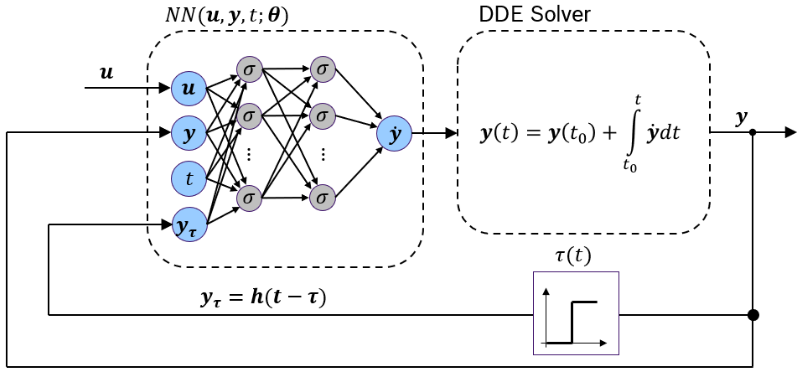
Hydraulic lines connecting central pump with braking cylinders at the wheels.

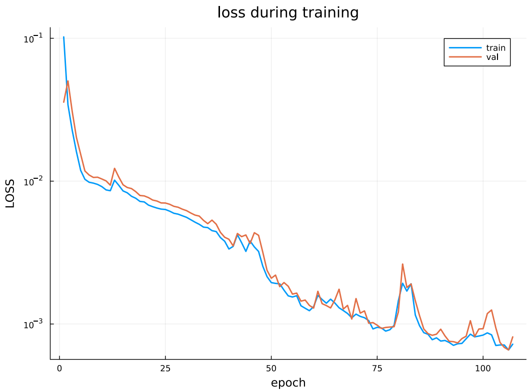


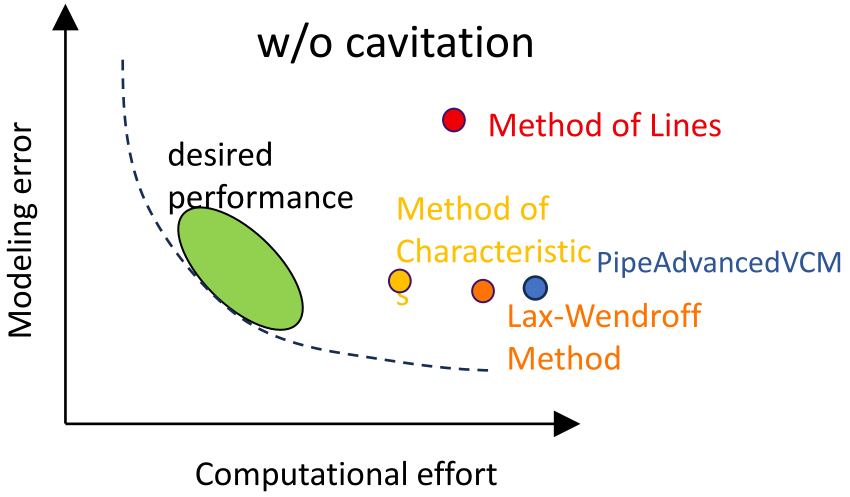


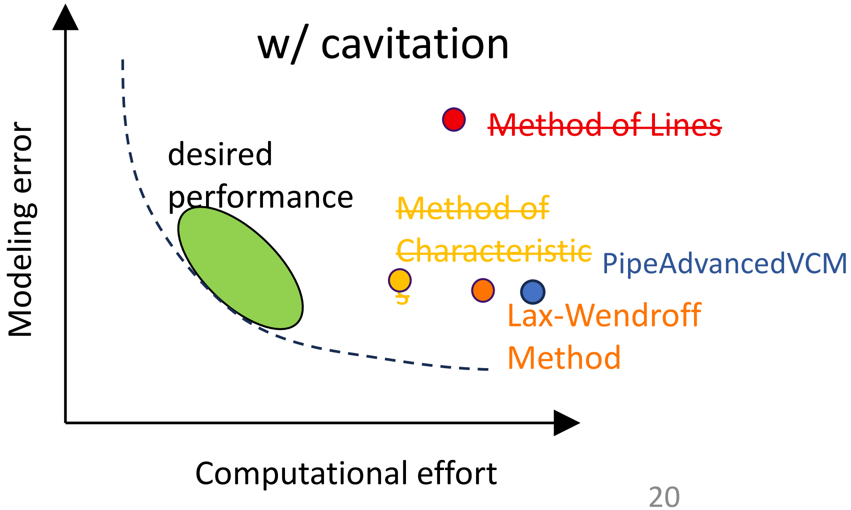
Bosch – Hydraulic Line

- PHyMoS Pipe Benchmark
  - Comprehensive data generated for 3 excitations
  - Test data of realistic braking scenario in system context
- Methods under test:
  - NDDE, NODE, ALR, MGNN
- First results of NDDE approach w/o cavitation



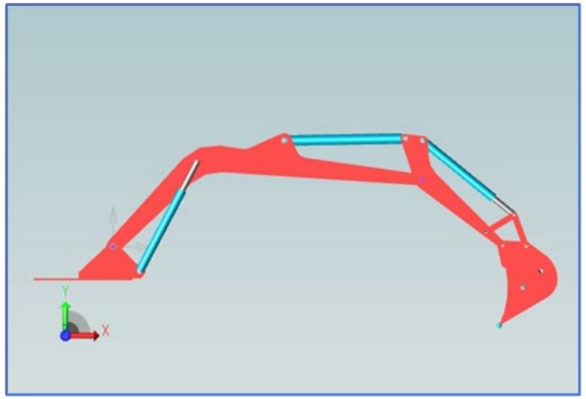


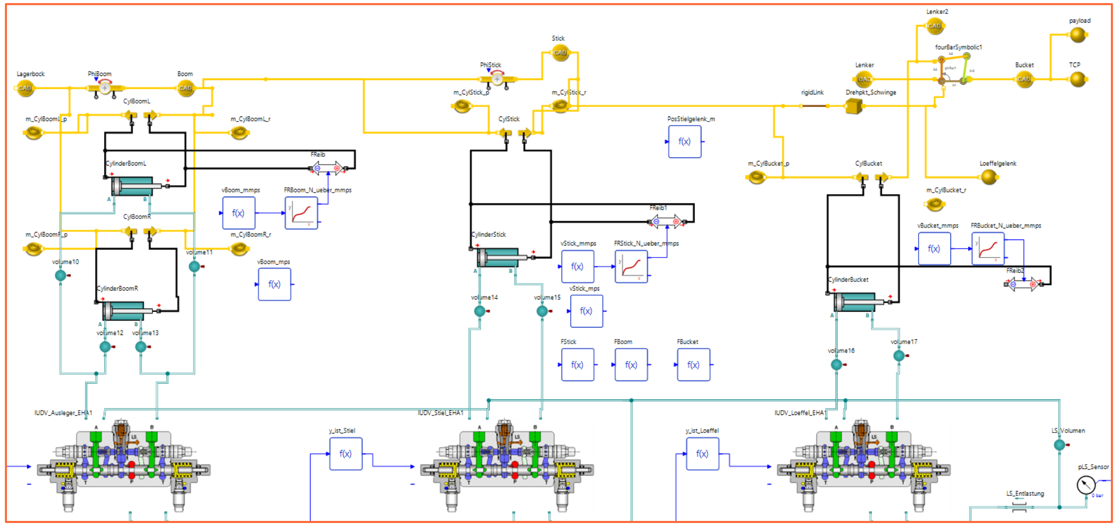




ESI – Hydro-mechanical Drive

- Use Case:
  - Hydro-mechanical system
  - Digital twin of real system with highly accurate cylinder positions and pressures
- Goal
  - Increase model accuracy of the bucket cylinder based on measurements
- Methods
  - NeuralFMU
  - RNN, LSTM

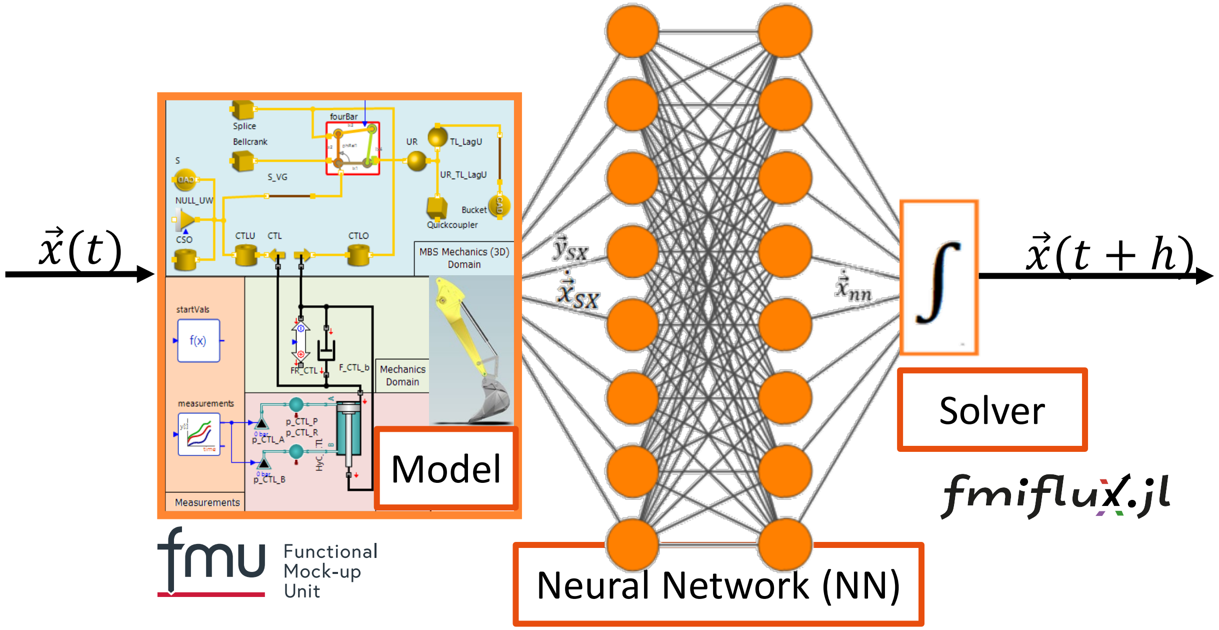




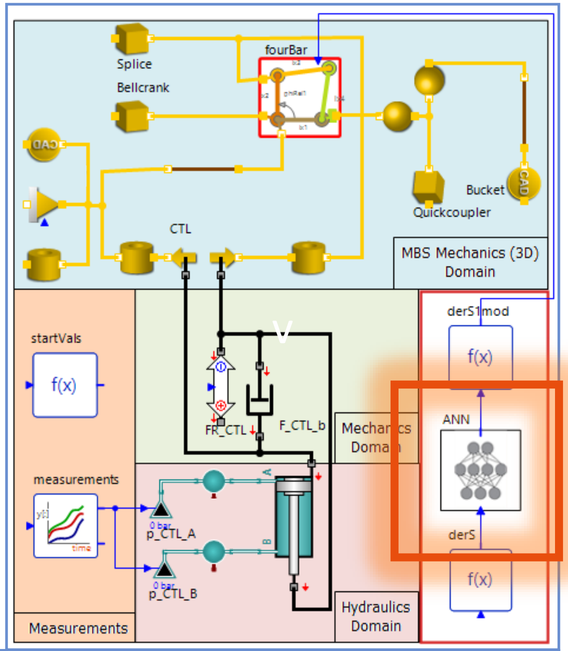
Thummerer, Tobias, Artem Kolesnikov, Julia Gundermann, Denis Ritz, and Lars Mikelsons. 2023. "Paving the way for Hybrid Twins using Neural Functional Mock-Up Units.", In Proceedings of the 15th International Modelica Conference, on October 9-11, 2023, in Aachen, Germany. https://doi.org/10.3384/ecp204141

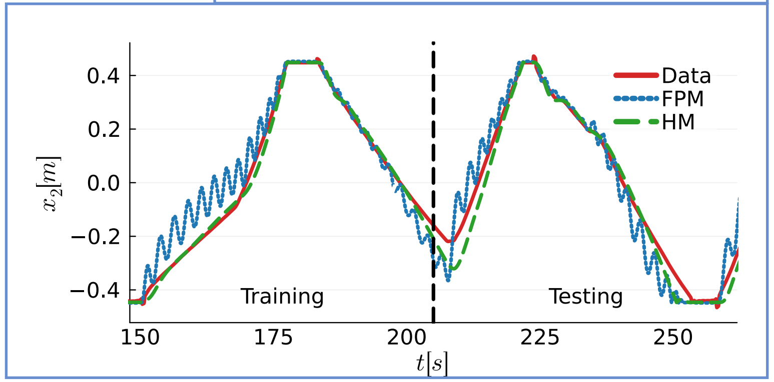
ESI – Hydro-mechanical Drive

- Hybrid Model (HM) architecture
  - FMU + NN + ODE Solver
  - Trained as a whole



- Results
  - Integration of NN via ONNX-Import
  - Accuracy compared with original model (FPM) improved by 67%





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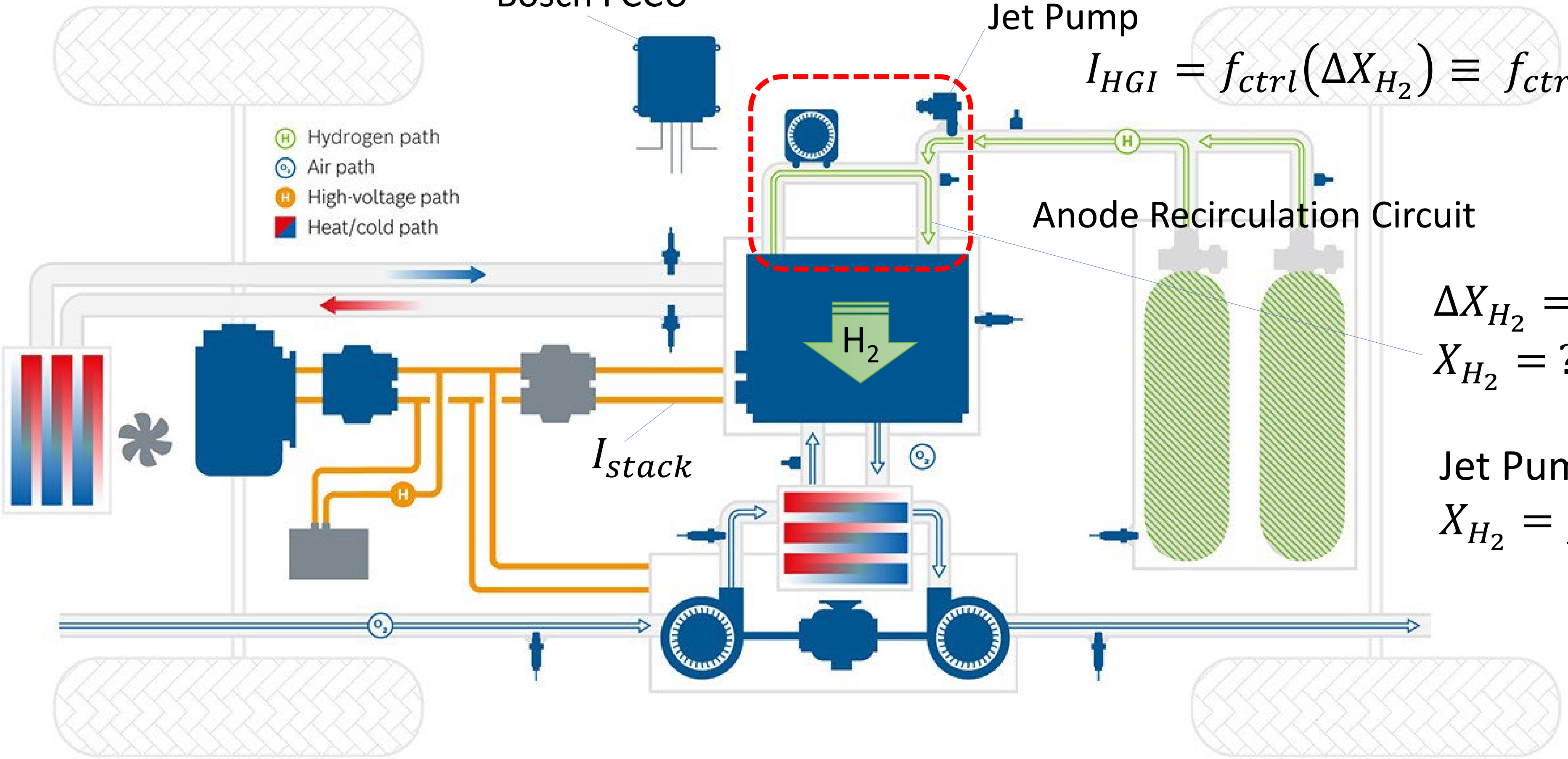
Bosch – Jet Pump

Bosch FCCU*

Jet Pump

$$I_{HGI} = f_{ctrl}(\Delta X_{H_2}) \equiv f_{ctrl}(p_i, T_i, I_{stack})$$

Anode Recirculation Circuit



I_{stack}

$$\Delta X_{H_2} = X_{H_2,\mathrm{set}} - X_{H_2}$$

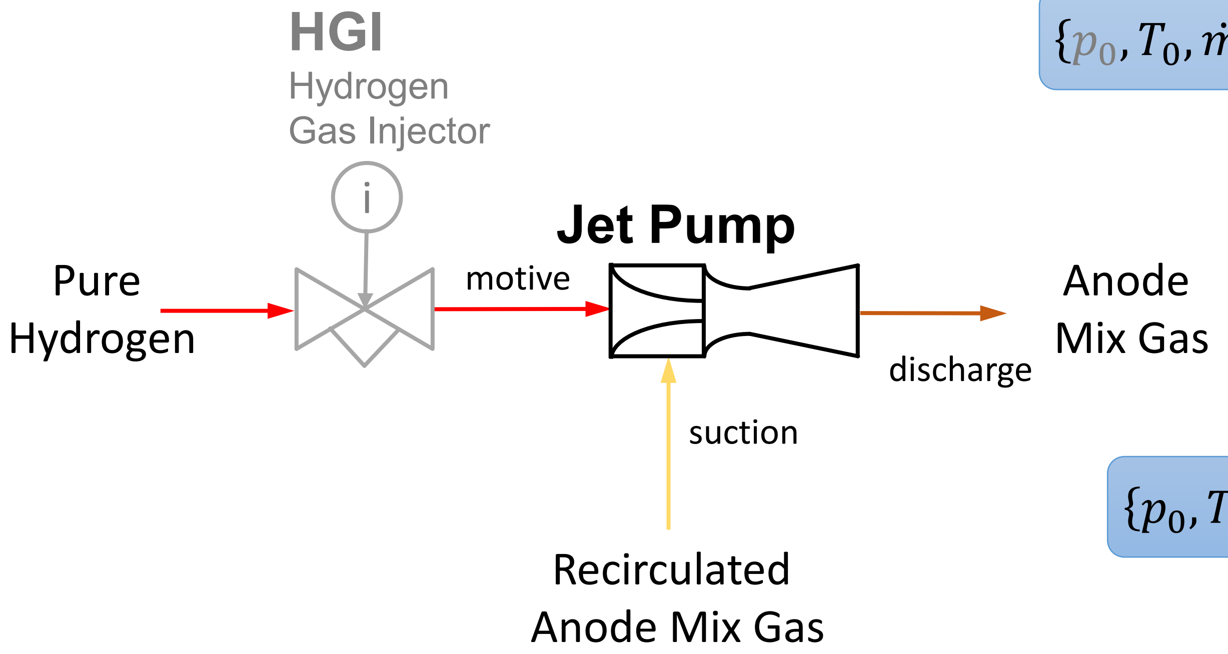
$$X_{H_2} = ?$$

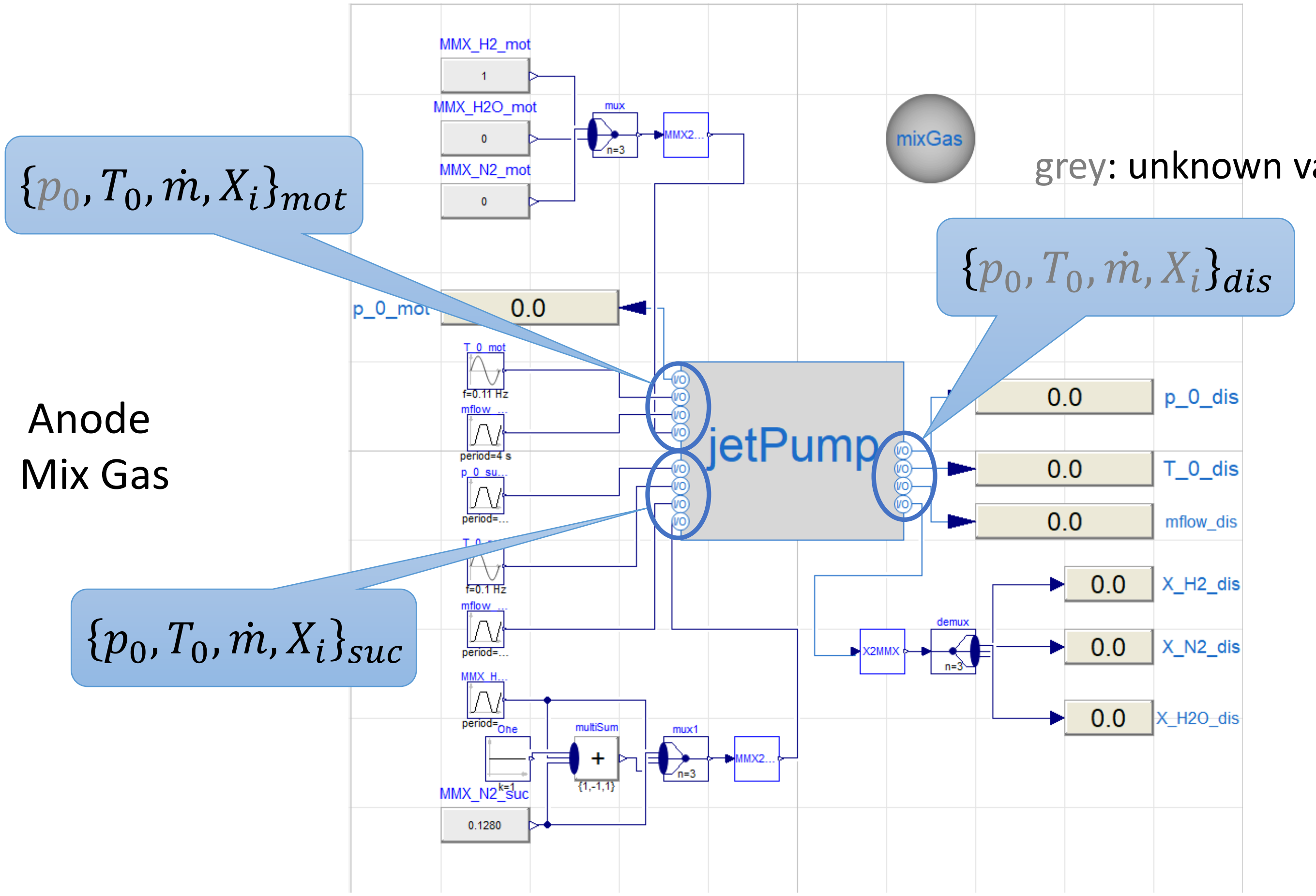
Jet Pump Model:

$$X_{H_2} = f_{JP}(p_{1,2,3}, T_{1,2,3}, X_{i_{reci}})$$

Fuel cell electric drive system from Bosch Mobility Solutions

Bosch – Jet Pump Use Case





grey: unknown variable

Bosch – Jet Pump Use Case

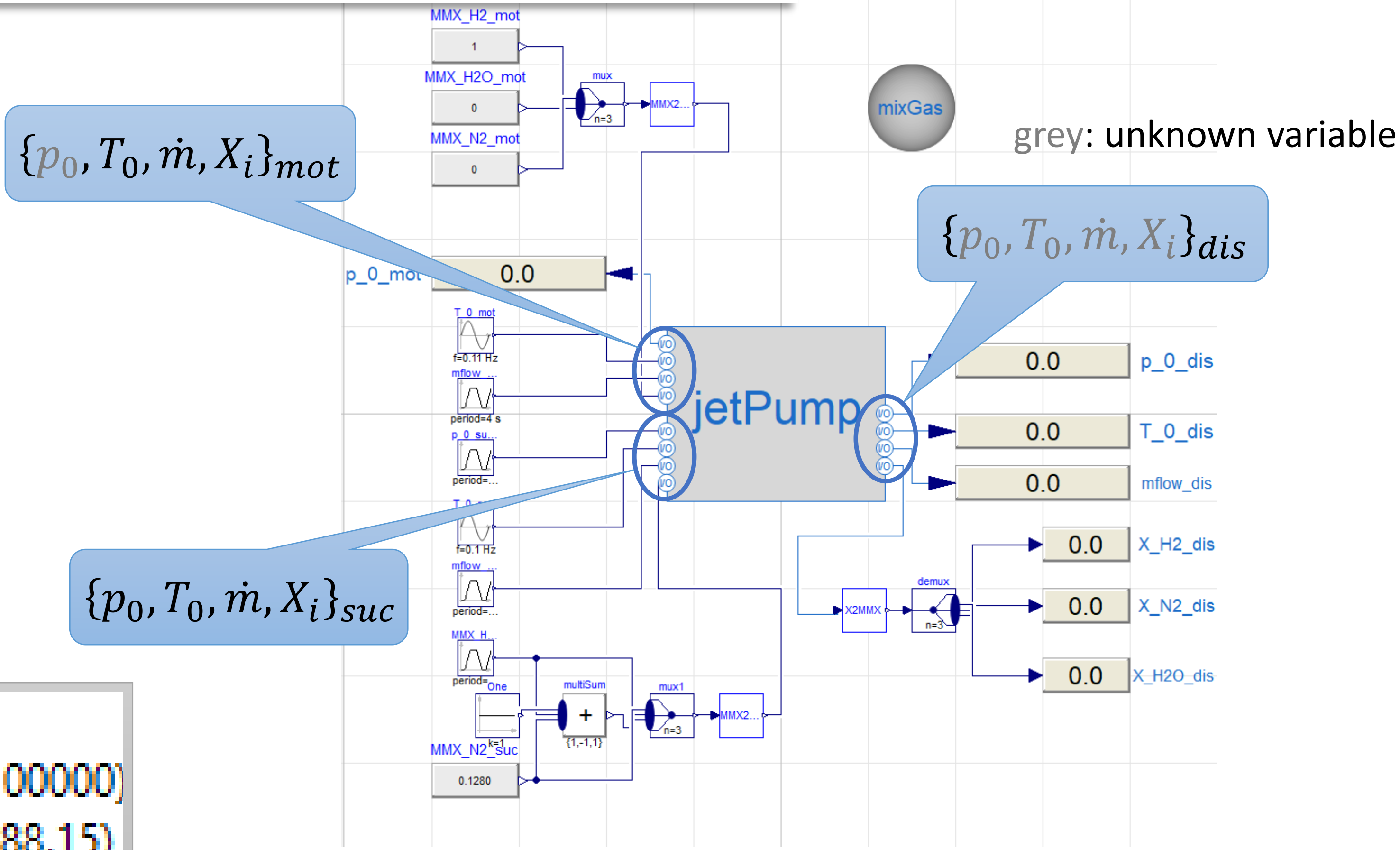
Translated Model
Co...
Fre...
Pa...
Tir...
Ali...
Nu...
Siz...
Sizes after manipulation of the linear syste...
Sizes of nonlinear systems of equations: {5, 4, 1, 1}
Sizes after manipulation of the nonlinear systems: {2, 1, 0, 0}
Number of numerical Jacobians: 0

...equations: {5, 4, 1, 1}
...e nonlinear systems: {2, 1, 0, 0}
...ans: 0

Variables appearing in the nonlinear systems of equations
System simulation.nonlinear[1]:
The equation system depends on the following timevarying variables:
jetPump._mflow_suc
jetPump._p_0_suc
jetPump._T_0_suc
Iteration variables:
jetPump.suctionFlow.p(start = 100000)
jetPump.suctionFlow.T(start = 288.15)
System simulation.nonlinear[...
The equation system de... ...wing timevarying variables:
jetPump._...
jetPump.m...
jetPump.su...
Iteration va...
jetPump._...

Iteration variables:
jetPump.suctionFlow.p(start = 100000)
jetPump.suctionFlow.T(start = 288.15)

➔Not applicable as embedded control function!



Algebraic Loop Replacement

```
model Scenario_01
  // [...]
equation
  // [...]
  p_0 / p = (1.0 + (k - 1.0) / 2.0 * Ma ^ 2.0) ^ (k / (k - 1.0)) "eq. 85";
  T_0 / T = 1.0 + (k - 1.0) / 2.0 * Ma ^ 2.0                     "eq. 86";
  v = R_s * mflow / A * T / p                                    "eq. 87";
  c = sqrt(k * R_s * T)                                          "eq. 88";
  Ma = v / c                                                     "eq. 89";
  I = v * mflow                                                  "eq. 91";
end Scenario_01;
```

Automatic:
- detection
- isolation
- data generation

$$p = f(Ma)$$
$$T = f(Ma)$$
$$Ma = f(p, T)$$

https://github.com/AMIT-HSBI/NonLinearSystemNeuralNetworkFMU.jl

Heuermann, Andreas, Philip Hannebohm, Matthias Schäfer, and Bernhard Bachmann. 2023. "Accelerating the Simulation of Equation-Based Models by Replacing Non-Linear Algebraic Loops with Error-Controlled Machine Learning Surrogates." In Proceedings of the 15th International Modelica Conference, on October 9-11, 2023, in Aachen, Germany. https://doi.org/10.3384/ecp204275

Algebraic Loop Replacement

$$p = f(Ma)$$
$$T = f(Ma)$$
$$Ma = f(p, T)$$

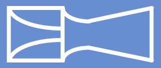
Symbolic Regression

$$p = f_{S1}(mflow, p_0, T_0)$$
$$T = f_{S2}(mflow, p_0, T_0)$$
$$Ma = f(p, T)$$

```
model Scenario_01_surrogate
  // [...]
equation
  // [...]
  p = 1.0421704 * (p_0 + (-1.8165398 * mflow * (1.1583588e6 + (-1 * p_0) + T_0 + (T_0 ^ 2))))           „eq. 85 surrogate";
  T = 11.234316 + (5.9411494e-5 * p_0) + T_0 + (-1 * (sqrt(T_0) + (3.287046 * mflow * (1.8603506 + T_0)))) "eq. 86 surrogate";
  v = R_s * mflow / A * T / p                                                                            "eq. 87";
  c = sqrt(k * R_s * T)                                                                                  "eq. 88";
  Ma = v / c                                                                                             "eq. 89";
  I = v * mflow                                                                                          "eq. 91";
end Scenario_01_surrogate;
```

Oliver Lenord, Andreas Heuermann, Alexander Fischer. “Nonlinear Loop Replacement Applied to Realtime Capable Jet Pump Model”. Center for Model-Based Cyber-Physical Product Development, vol. 33, no. 18, Apr. 2024, https://wcc.ep.liu.se/index.php/MODPROD/article/view/1237.

AlgLoopRepl. w/ Symbolic Regression Results



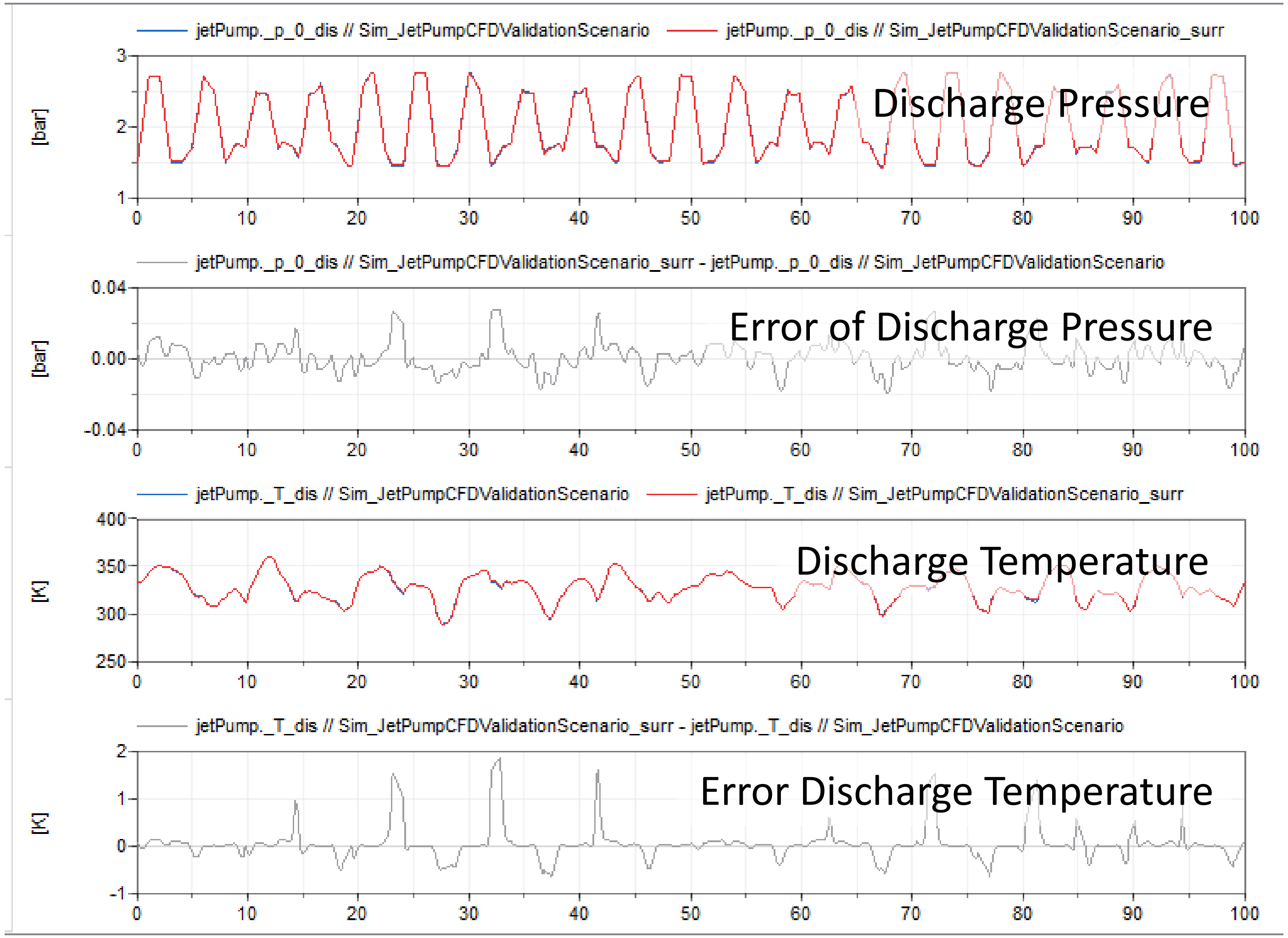
jetPump vs. jetPump_surr

- Max error abs. (rel.):
  - p_0_dis = 0.028bar (2.1%)[1)]
  - T_0_dis = 1.8K (2.6%)[1)]
- Mean error abs. (rel.)
  - p_0_dis = 0.006bar (0.46%)[1)]
  - T_0_dis = 0.97K (1.4%)[1)]

	size NLS	CPU time[2)]	speed-up
jetPump	{2,1]	12ms	-
jetPump_surr	{0,1}	6ms	x2

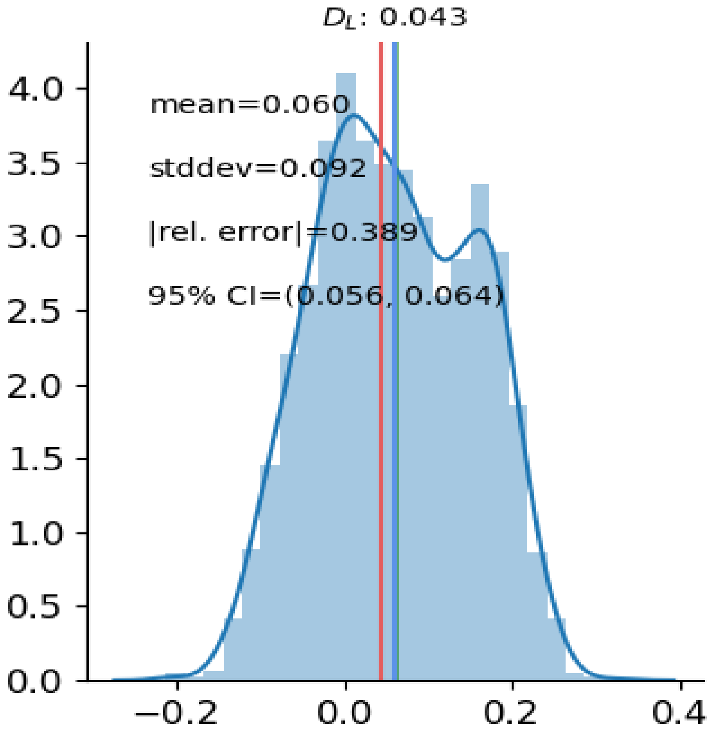
[1)] with respect to size of value range

[2)] Euler solver, PC



Probabilistic Methods

- Probabilistic Methods
  - applicable to physical parameters
  - return a distribution instead of a single value
    - mean → predicted value
    - accuracy → error of prediction and ground truth
    - precision → width of distribution
    - confidence → probability that the predicted value is within the defined confidence interval (e.g. 95%)



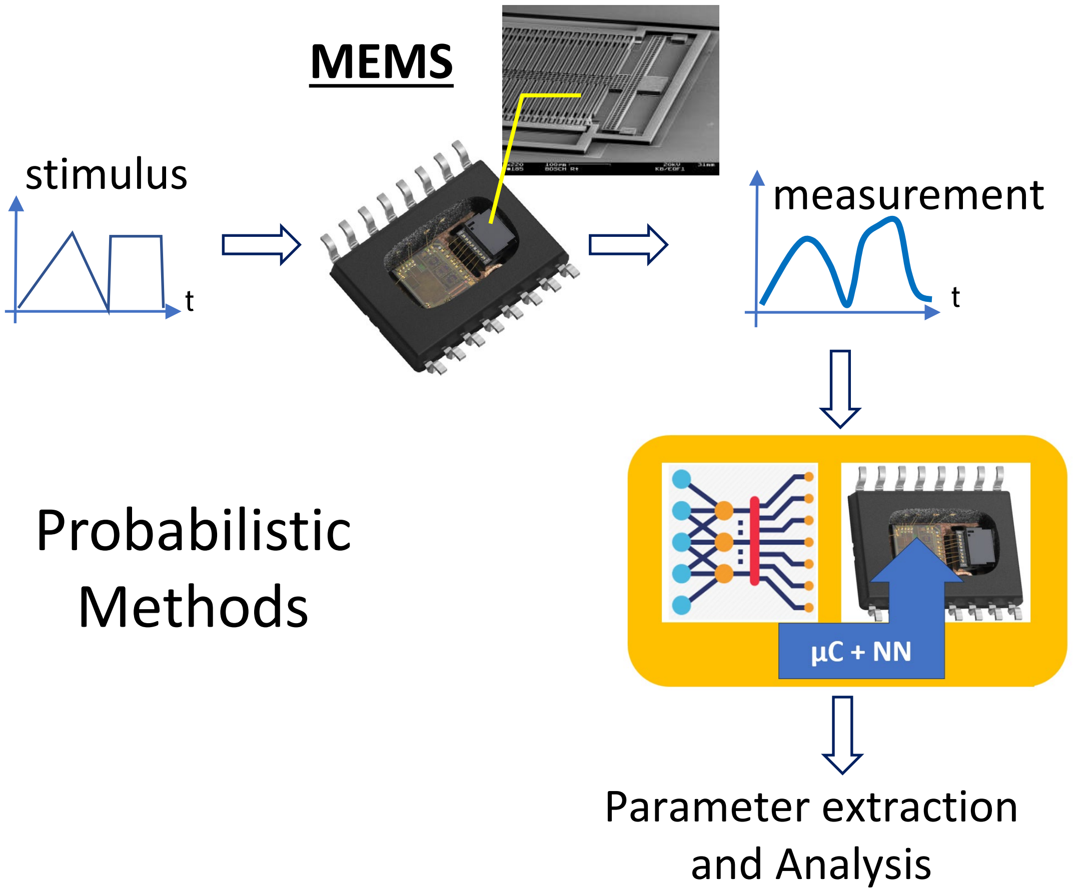
Enables educated decision making,
vs. blind trust in a black box output.

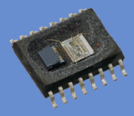
Bosch – MEMS

End-of-line testing time reduction

- fast, robust and precise extraction of parameters set from dynamic tests
  - within ms
  - no outliers (no false positives)
  - plausibility checks of physically interpretable parameters
  - determination of process parameters

Probabilistic Methods

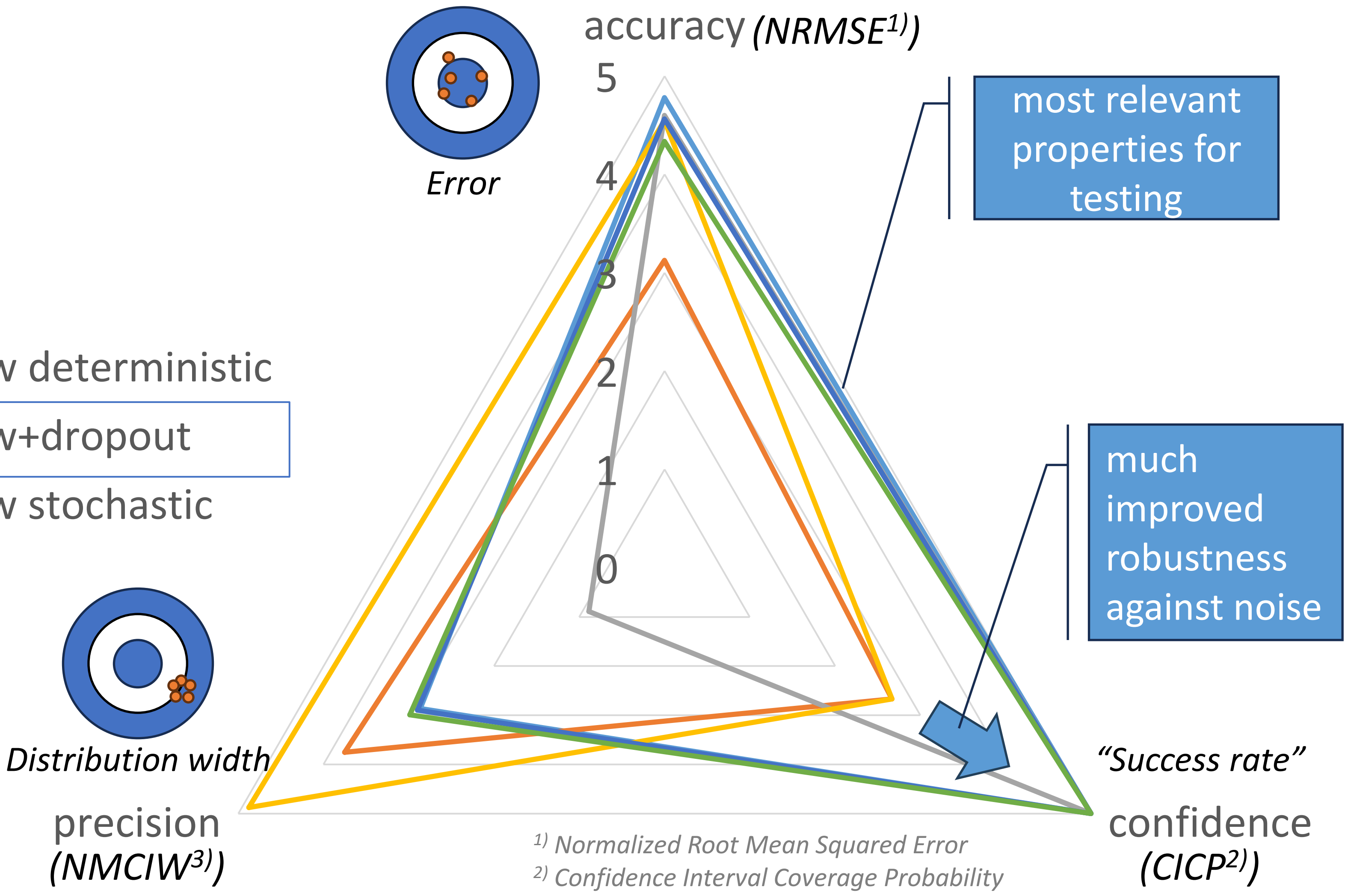




Bosch – MEMS Results

D_L

- BNN
- MDN
- PBNN
- BayesFlow deterministic
- BayesFlow+dropout
- BayesFlow stochastic



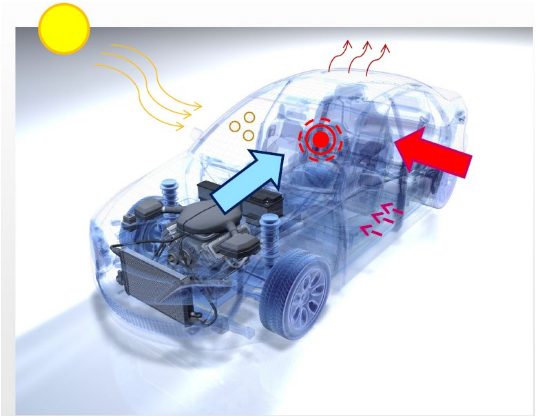
[1] Normalized Root Mean Squared Error
[2] Confidence Interval Coverage Probability
[3] Normalized Mean Confidence Interval Width

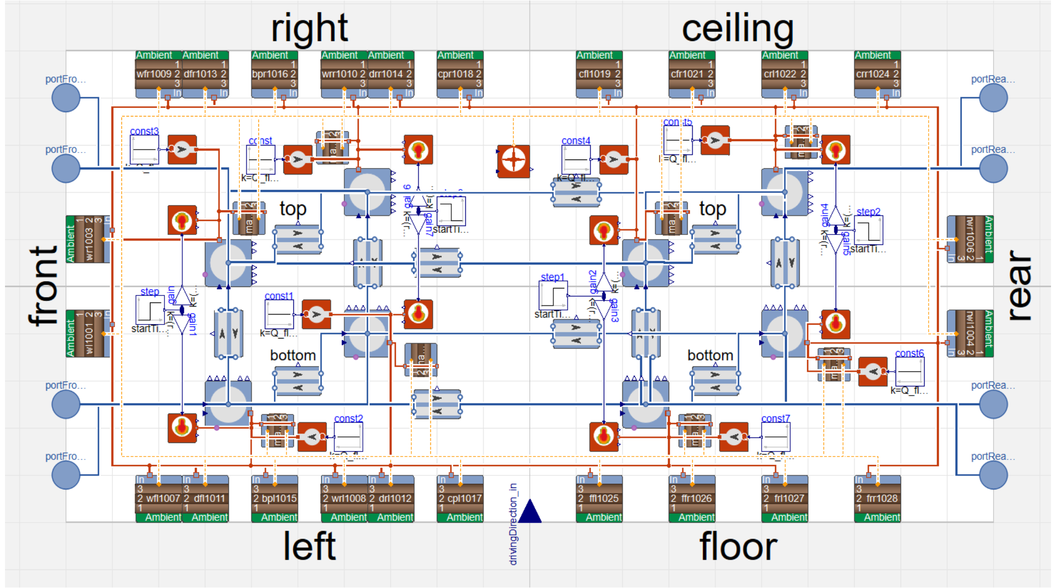
Heringhaus, Monika E., Yi Zhang, André Zimmermann, and Lars Mikelsons. 2022. "Towards Reliable Parameter Extraction in MEMS Final Module Testing Using Bayesian Inference" Sensors 22, no. 14: 5408. https://doi.org/10.3390/s22145408

Zhang, Yi, Lars Mikelsons. 2023. "Solving Stochastic Inverse Problems with Stochastic Normalizing Flows", 2023 IEEE/ASME International Conference on Advanced Intelligent Mechatronics (AIM), on June 27-July 1 (Tue-Sat), 2023, in Seattle, Washington, USA. DOI:10.1109/AIM46323.2023.10196190

XRG – Cabin Model: BayesFlow Results

- Use Case:
  - Physics-based system model of car cabin.
  - calibration of eight idea mixed volumes
- Approach:
  - Sensitivity Guided Iterative Parameter Identification for Model Calibration (PELS-VAE + BayesFlow)
- Results:
  - Very good accuracy (Calibration error: 0.108°C)
  - Much improved productivity.

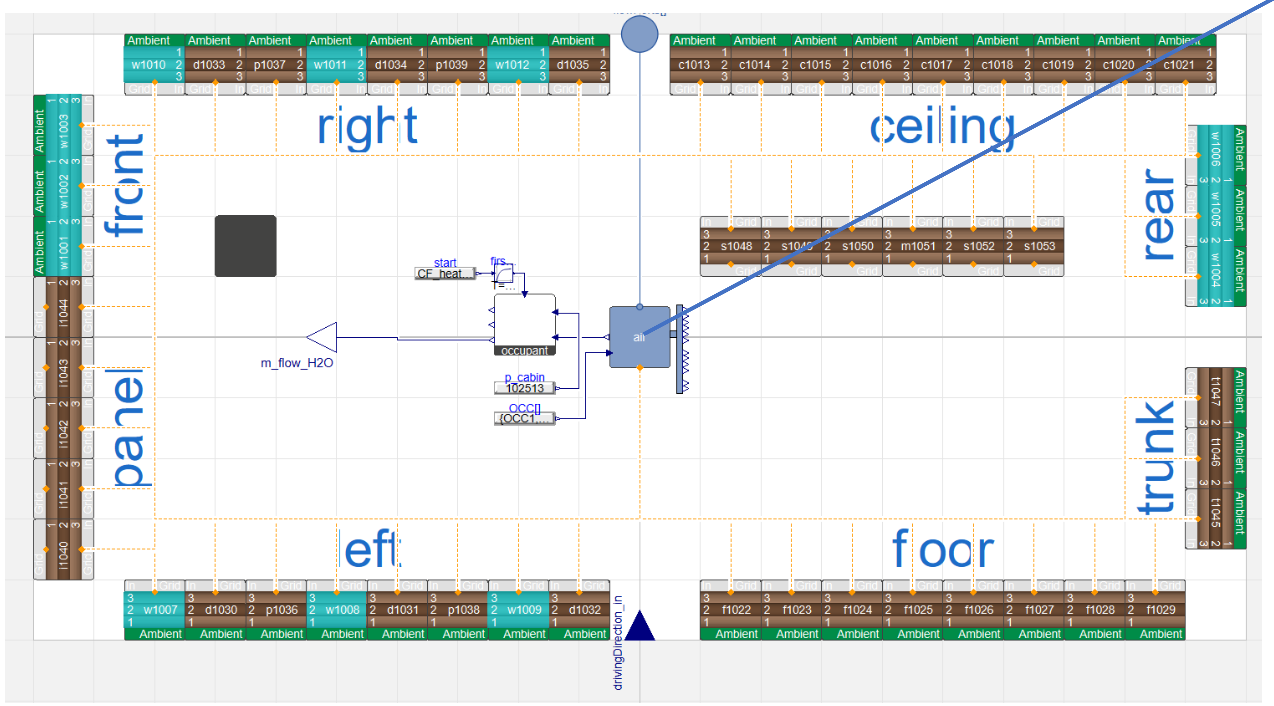


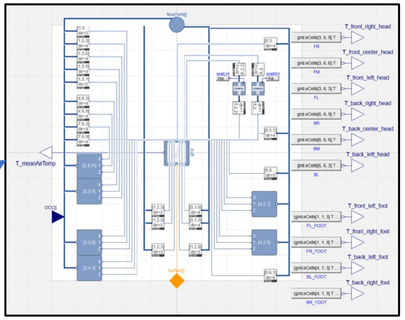


Zhang, Yi, Lars Mikelsons. "Sensitivity-Guided Iterative Parameter Identification and Data Generation with BayesFlow and PELS-VAE for Model Calibration", Adv. Model. and Simul. in Eng. Sci. 10, 9 (2023). https://doi.org/10.1186/s40323-023-00246-y

Julius Aka, Johannes Brunnemann, Svenne Freund, and Arne Speerforck. 2023. "Efficient Global Multi Parameter Calibration for Complex System Models Using Machine-Learning Surrogates.", In Proceedings of the 15th International Modelica Conference, on October 9-11, 2023, in Aachen, Germany. https://doi.org/10.3384/ecp204107

XRG – Cabin Model: Surrogate





CFD Grid model with 528 cells

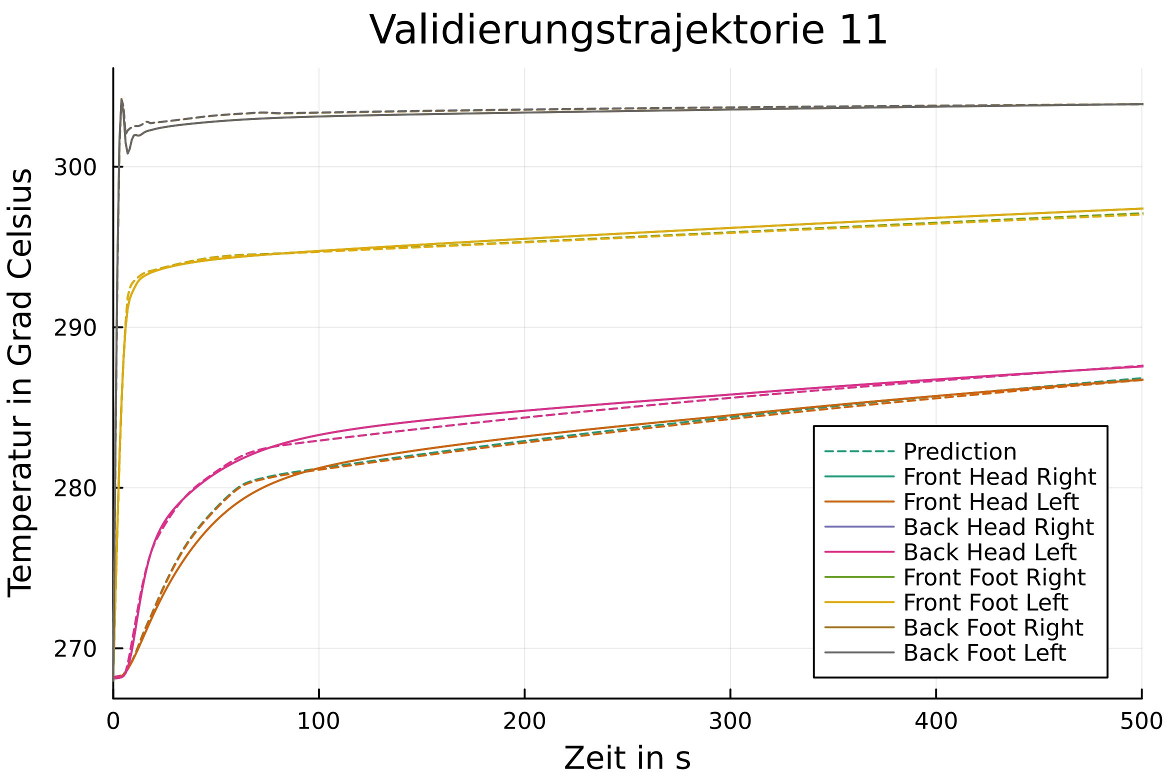
NeuralODE
Fast Surrogate

DMDc
Fast Surrogate

Mesh Graph Neural Network
Fast Surrogate

XRG – Cabin Model Results

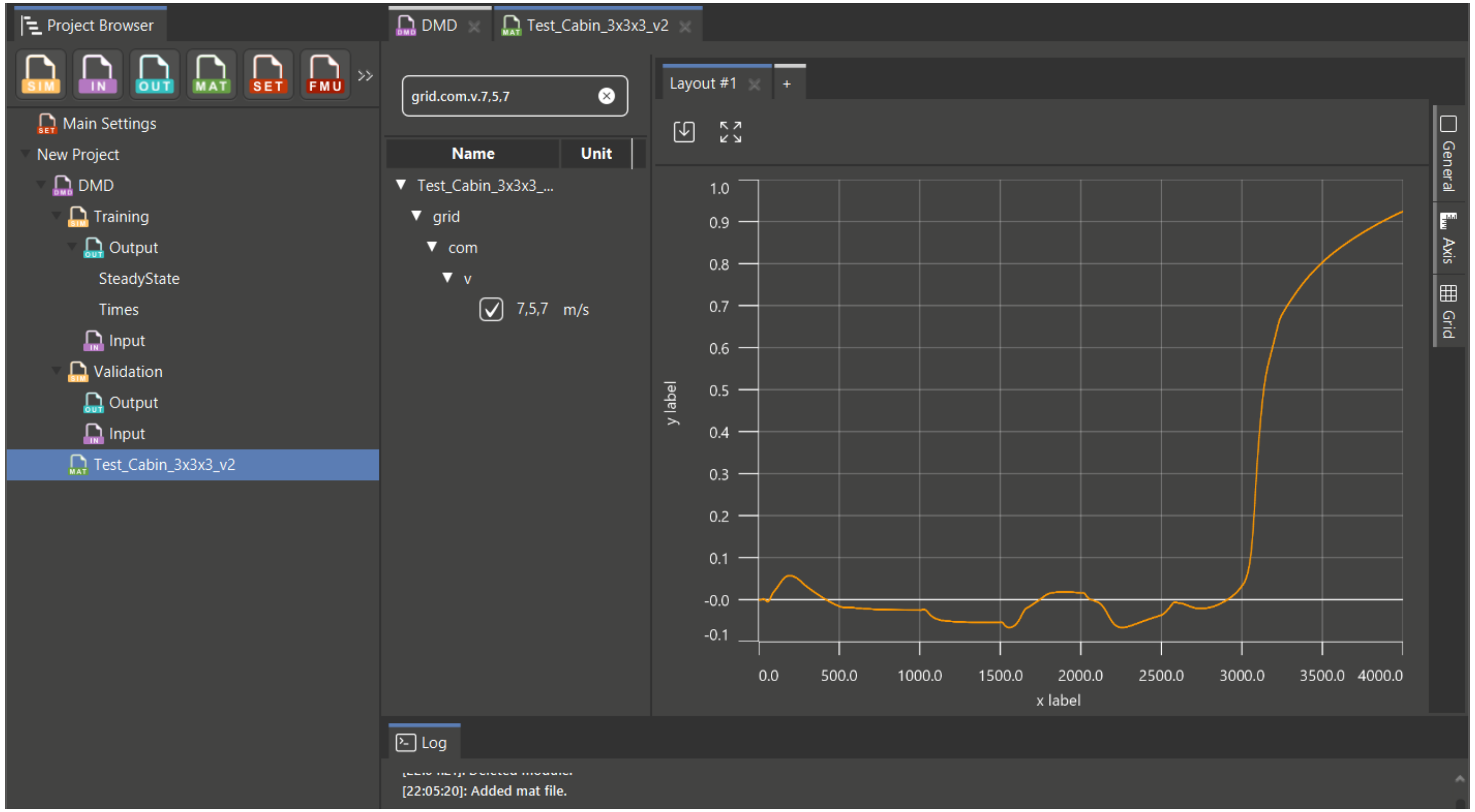
- DMDc
  - Speed-up: >x60
  - Accuracy: ΔT < [2, 3.5]K
- Mesh Graph Nets
  - Speed-up: ~x9
  - Accuracy: ΔT < 1K
- NeuralODE
  (head and foot temp. only)
  - Speed-up: ~x20.000
  - Accuracy:



XRG – Demonstration JSCORE

Tool for Automated Surrogate Generation and Model Calibration

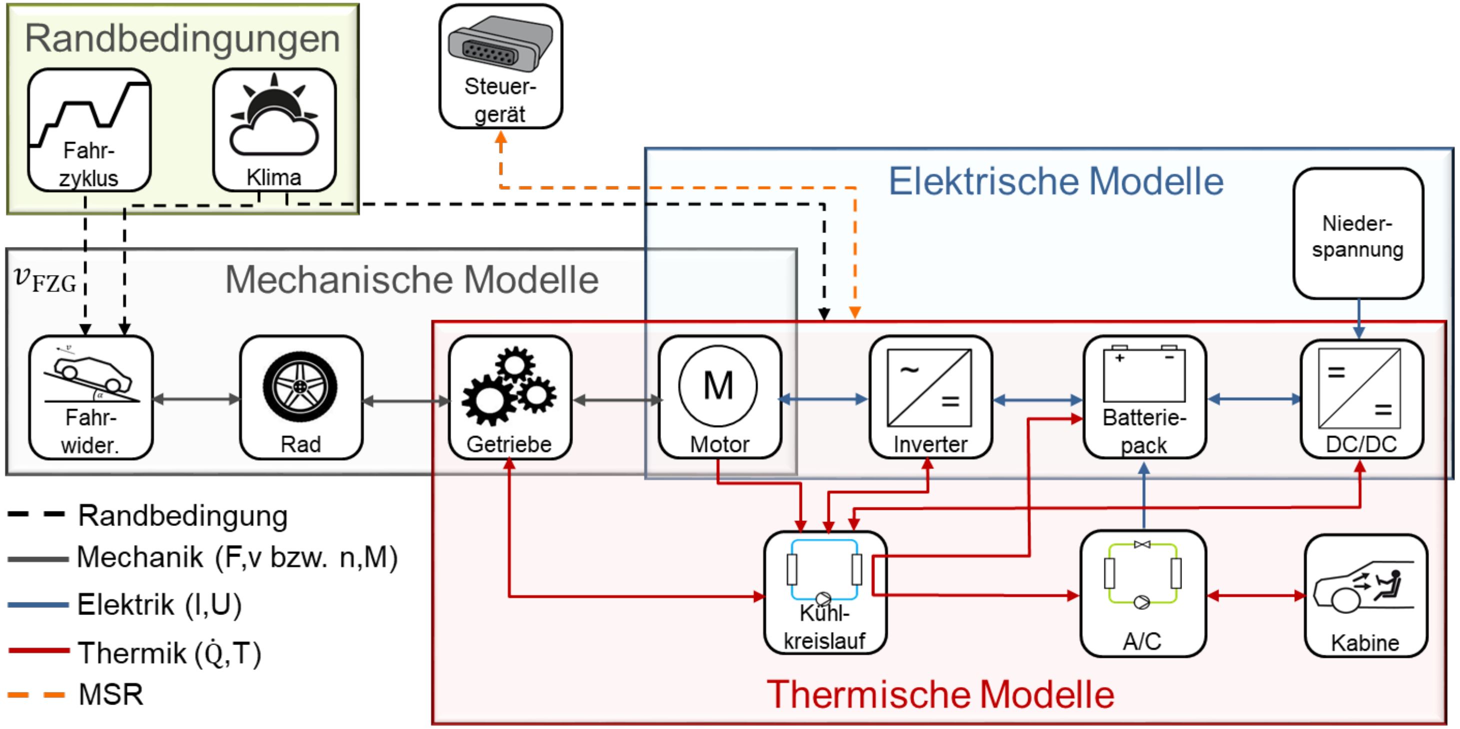
- Assisted method selection and training process definition
- Automated data generation
    - locally, on server, distributed over network
- Result evaluation and comparison to original model
- Model export to Python, Modelica or FMU

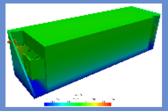


JSCORE user interface with result evaluation for DMDc method applied to car cabin use case

1. Motivation and Project Goal

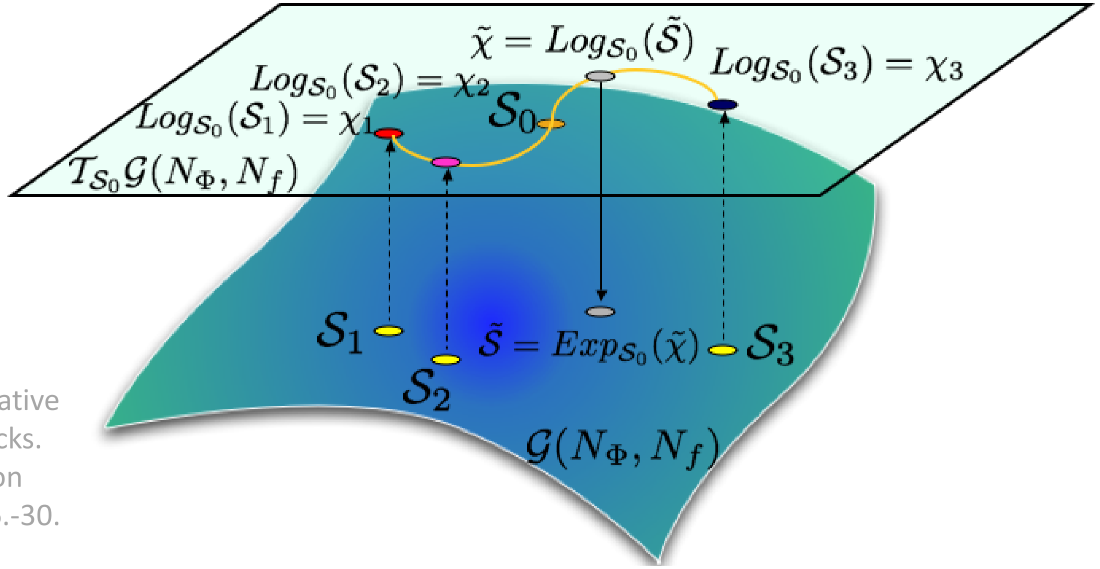
- Evaluation of the thermo management, aging and safety of battery cells and battery packs in the context of a full vehicle simulation.





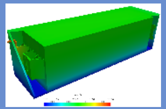
3. POD-G + POD-I of Battery Cell

- Dimension reduction $\mathbb{R}^{10.000} \rightarrow \mathbb{R}^3$
- POD-G applied to transient processes → Projection of the transport equations
- POD-I applied to stationary processes → Projection of the states
- Grassmann-Interpolation applied to optimal subspace



Steeb M., Sarge S.M., Tegethoff W., Köhler J.: Thermal investigation of inhomogenities in aged batteries using an isoperibolic calorimeter. Die 25. Kalorimetrietage, Braunschweig, 31. Mai - 02. Juni 2023

Hellmuth, J. F., Steeb, M., Pollak, M., Jäger, F., Tegethoff, W., Koehler, J.: Innovative thermal management operating strategies for battery-electric heavy-duty trucks. The 36th International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems, Las Palmas de Gran Canaria, 26.-30. Juni 2023, doi: doi.org/10.24355/dbbs.084-202310260841-0

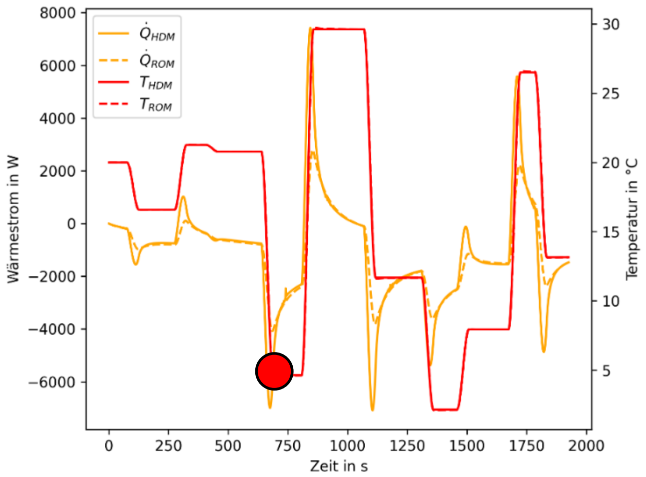


3. POD-G + POD-I of Battery Pack

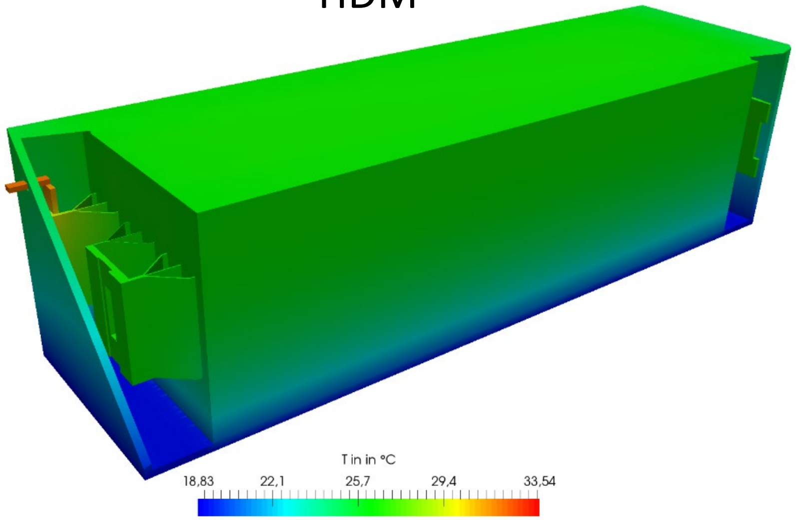
	Battery Cell	Battery Pack
Speed-up of simulation time	x 2,5	x 120

→ Extrapolation capable

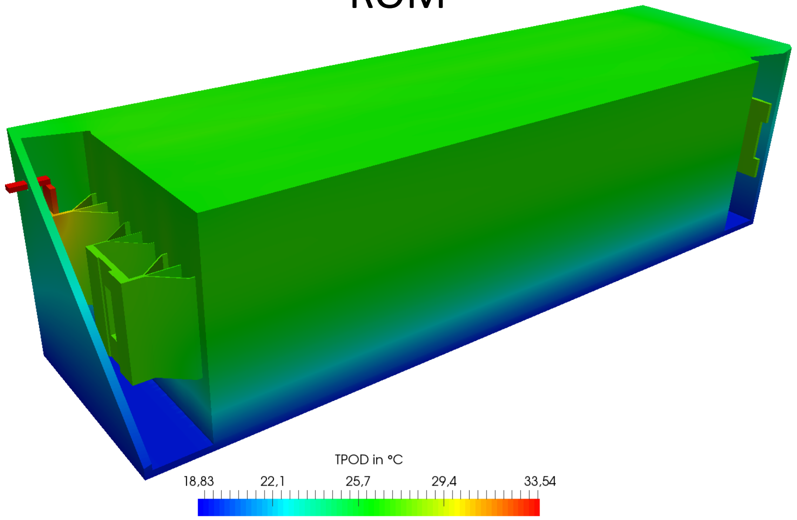
→ Sufficiently accurate (mean < +/- 1K, Max ~ +/- 2K)



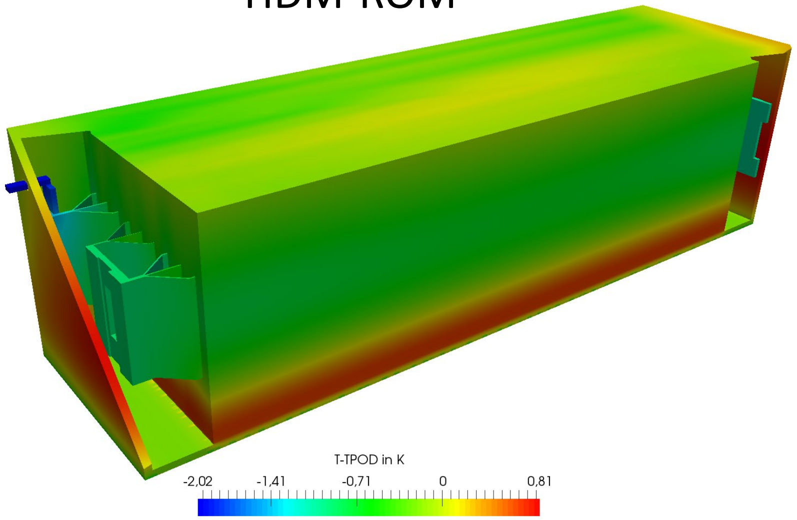
HDM



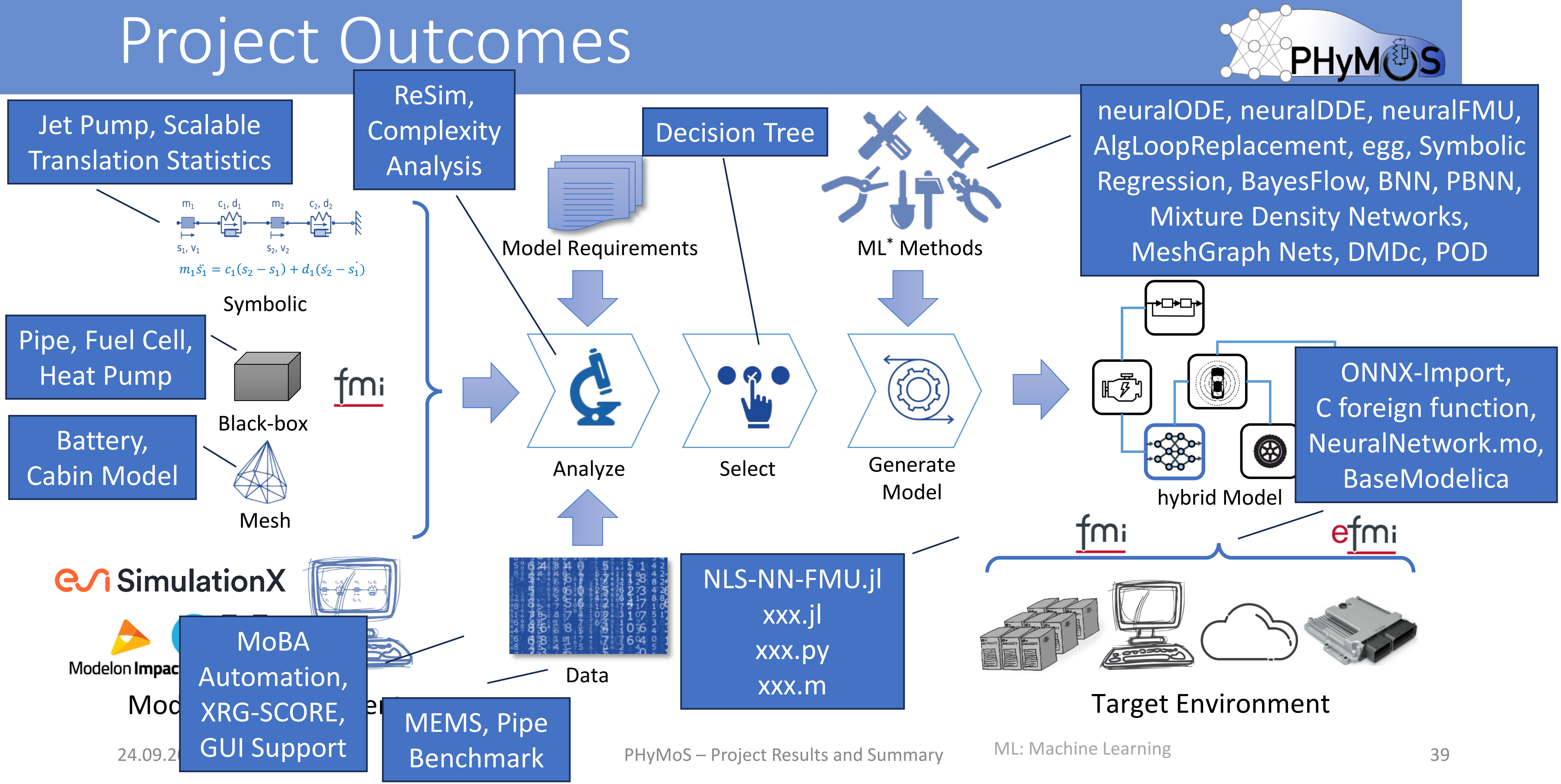
ROM



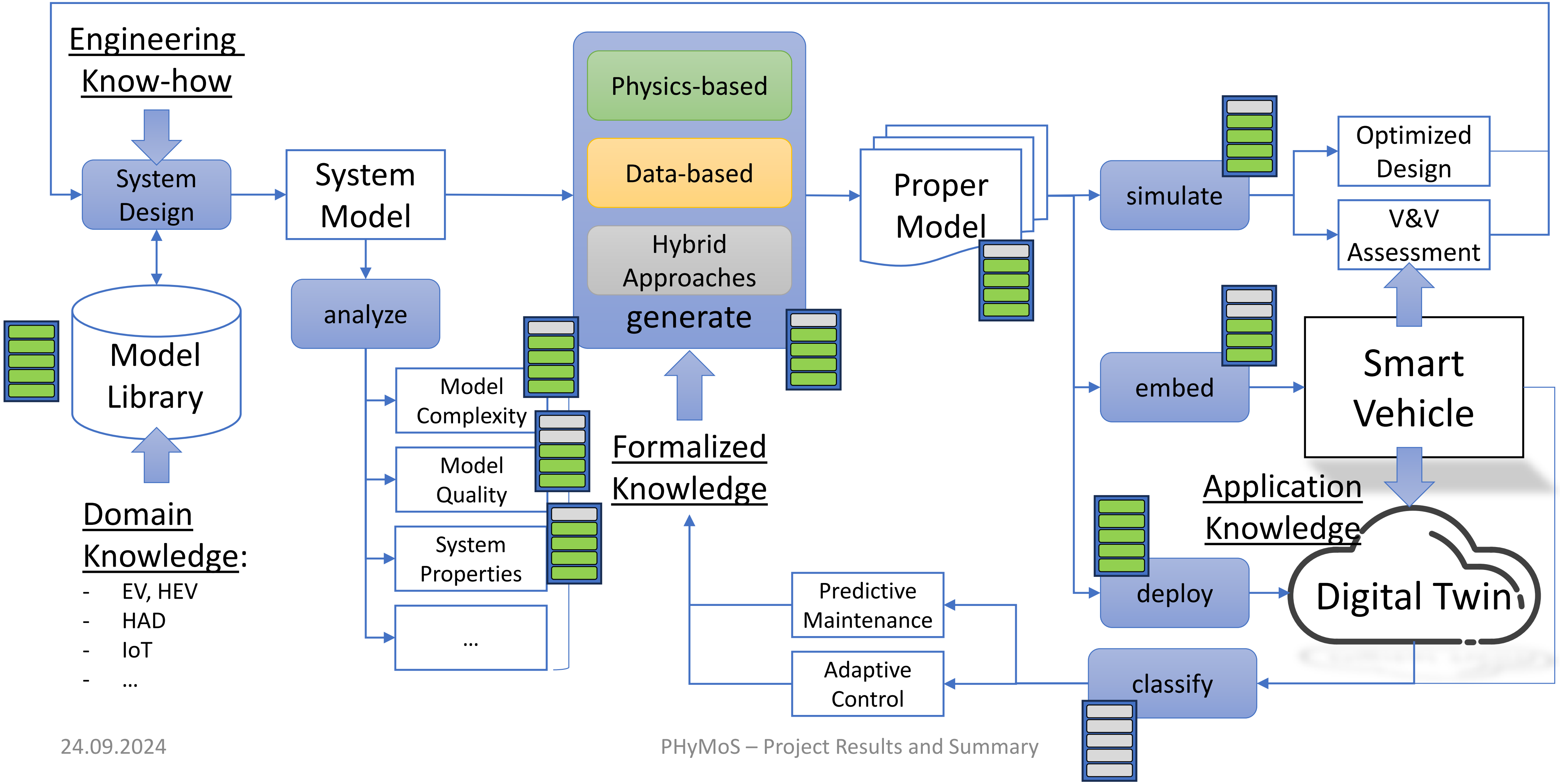
HDM-ROM



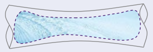
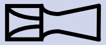
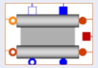
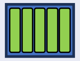
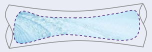
Project Outcomes



Target Achievement



Tool Prototypes

Organization	Tool	Description	Demonstrators	TRL
ESI Germany GmbH	Model Complexity, ONNX-Import	Complexity analysis and output, Integration of Proper Models into simulation models		6, 5
HSBI (Hochschule Bielefeld)	NonLinearSystemNeuralNetworkFMU.jl	OS packages for ALR with OpenModelica	 	6
LTX Simulation GmbH	ReSim	Regression Testing (VV of Proper Models)		6
Modelon Deutschland GmbH	Modelon Impact Reduced Order App	Integrated Proper Model Generation workflow		6
TLK-Thermo GmbH	MoBA Automation	Support of Proper Model Generation in customizable workflows		6-7
TUBS (TU Braunschweig)	POD	Projection based model order reduction		5
UNA (Universität Augsburg)	BayesFlow, MGN	OS packages enabling NFMU workflows		7, 6
Robert Bosch GmbH		NDDE/NODE training environment		6
XRG Simulation GmbH	Calibration Tool Box, JSCORE	Auto. Calibration, Proper Model Generation Workflow		7, 4

Summary

PHyMOS

Demonstrators

- 8 different applications
  - x2 enabling embedded application
  - x1.000 enabling full vehicle system co-simulation
  - x20.000 enabling high fidelity component model in system level simulation
  - +67% gain in accuracy
  - testing with confidence
  - significant gain in calibration productivity
- Know-how build-up
  - Machine learning skills
  - Hybrid architectures
  - Prerequisites and recommendations

Methods and Tool Prototypes

- New methods
- Improved methods
- Training scripts and OS packages
- Integrations in 5^{+} M+S tools

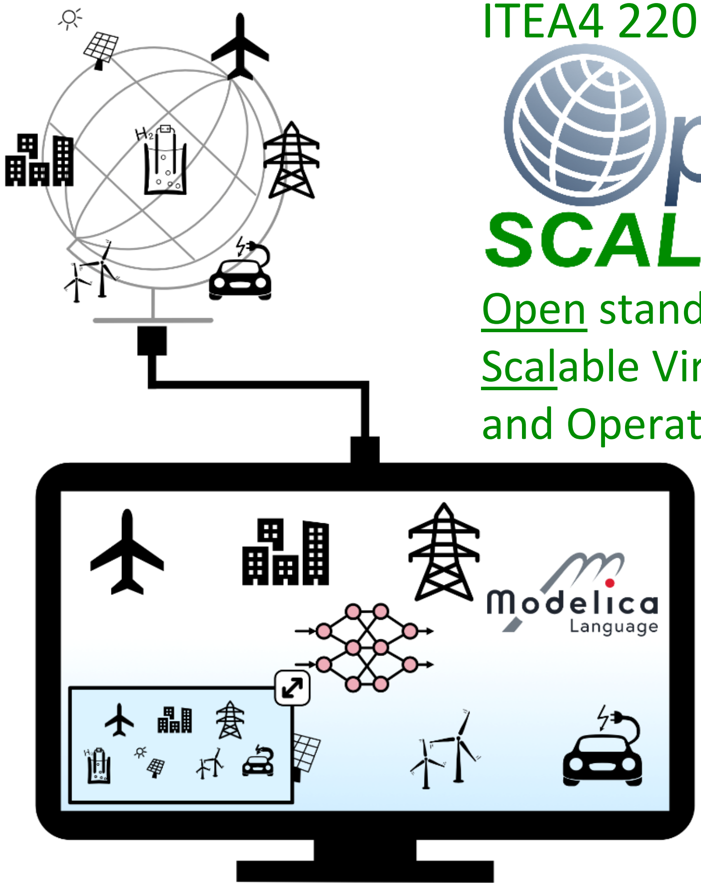
Publications

- Journals: 2
- Conferences: 11
- Workshops: 5

https://phymos.de/en/page/publications/

Outlook

- Future tool releases
- Further workflow automation
  - Method selection
  - Training configuration
  - Generation of training data
- Enhance modeling standards
  - FMI for Machine Learning
  - Standardized UQ (Modelica, FMI, SSP)
  - NN representations
- Improve training methods
  - Reliability of the models
  - Convergence of the training
- Further improve surrogate modeling
  - Heat Pump Systems



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