Using FMI for AI applications

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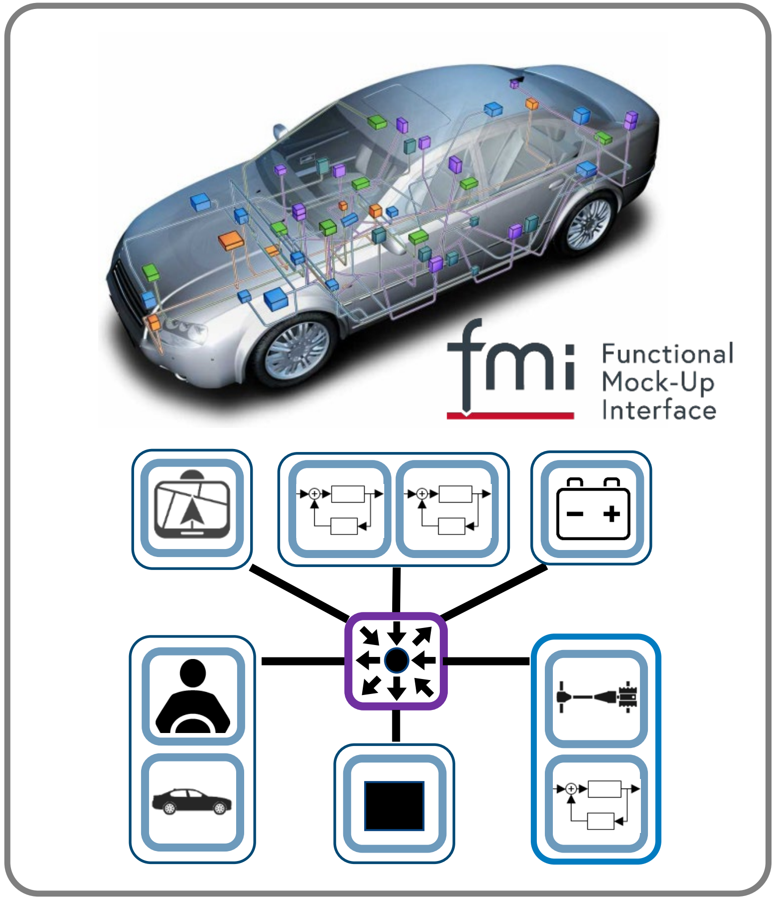
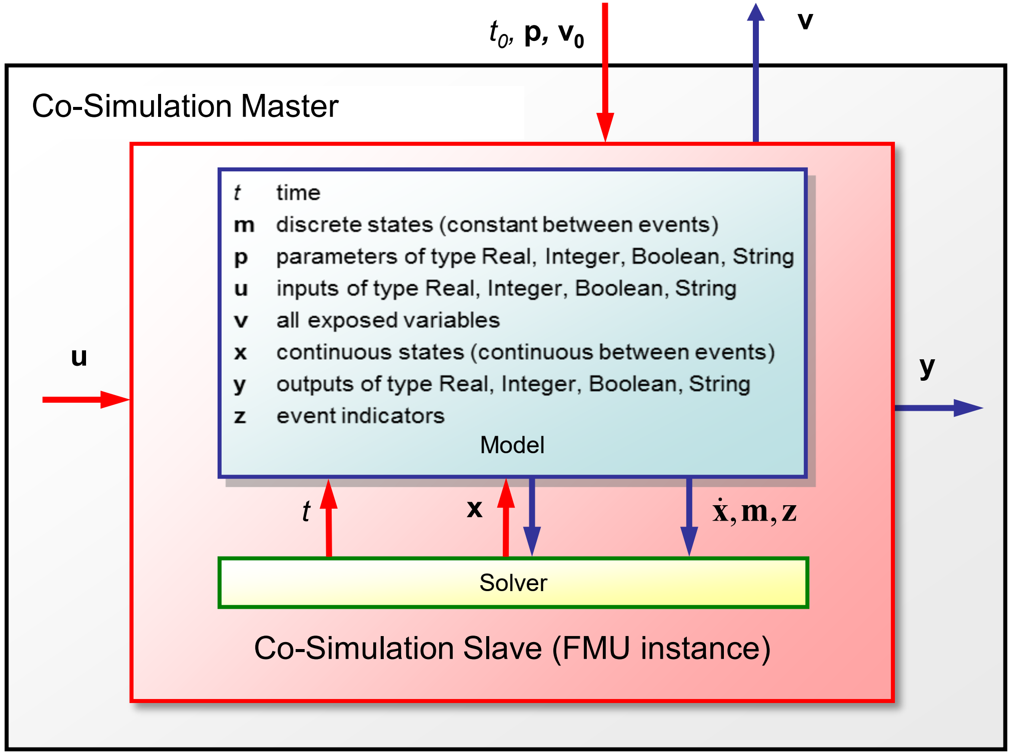
Using FMI for AI applications
FMI for “classical” system simulation

- Functional Mock-up Interface (FMI)
  https://fmi-standard.org/
  - Evaluate the functional properties of a system
  - by means of a virtual assembly of its parts
  - based on a standardized interface.
- Benefits:
  - Tool-independent model exchange format.
  - Coupling of solvers through co-simulation using the FMI-CS interface:
    - e.g., through a co-simulation middle ware.
  - Integration of black-box models through FMI-ME interface:
    - e.g., for IP protection,
    - or reuse of models in another simulation tool.



Using FMI for AI applications
FMI Interfaces

- FMI for Co-Simulation (CS)
  - Subsystems solved independently.
  - Data exchange restricted to discrete communication points.
  - Asynchronous execution is possible.
  - Execution of a time step:
    `fmiStatus` **`fmiDoStep`**`(fmi_cmpnt, t_curr, dt, newStep)`
  - `newStep = fmiTrue` if last step was accepted.
  - Return values are:
    `fmiOK, fmiDiscard, fmiError, fmiPending`
  - Calling sequence depends on the capabilities of the slave.

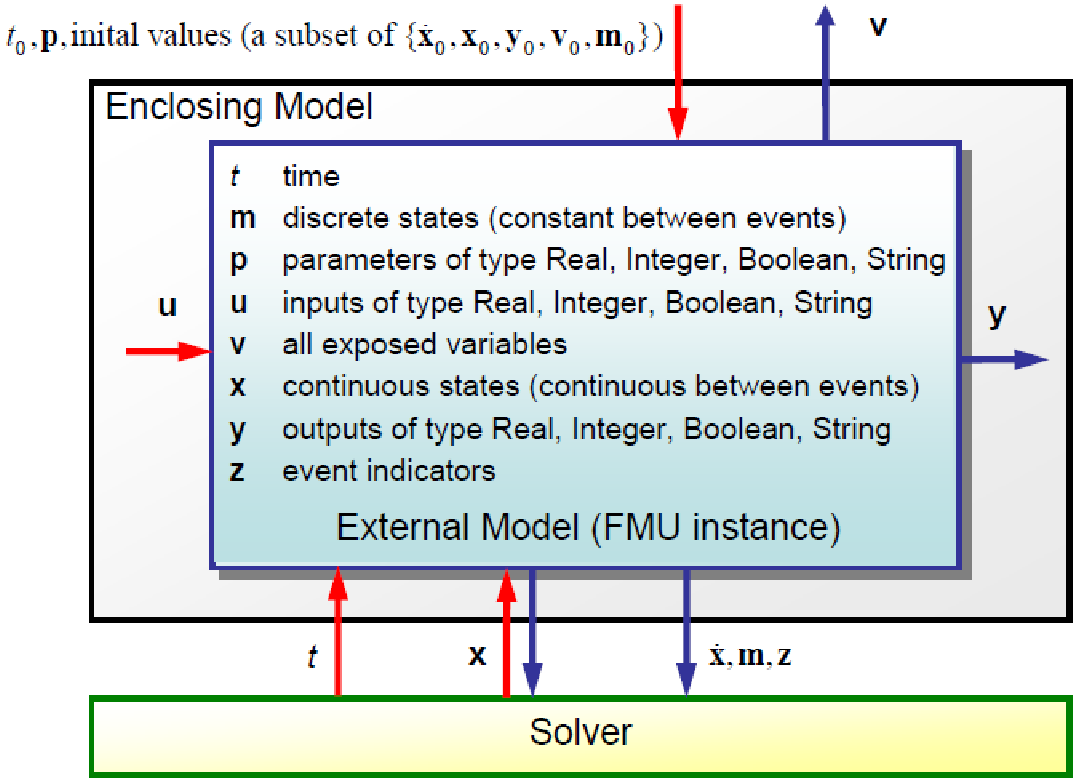


https://github.com/modelica/fmi-standard/releases/download/v2.0.4/FMI-Specification-2.0.4.pdf

Using FMI for AI applications
FMI Interfaces

- FMI for Model Exchange (ME)
  - described by
    - differential-, algebraic-, discrete equations,
    - with time-, state, and step-events
  - Typical calling sequence from solver:

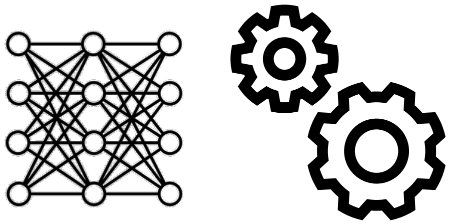
```
// Set input arguments
fmiSetTime(m, time);
fmiSetReal(m, id_u1, u1, nu1);
fmiSetContinuousStates(m, x, nx);
// Get results
fmiGetContinuousStates(m, derx, nx);
fmiGetEventIndicators (m, z, nz);
```



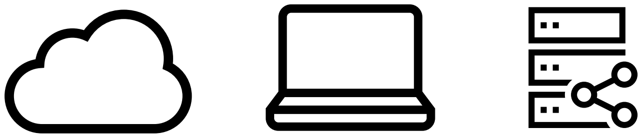
https://github.com/modelica/fmi-standard/releases/download/v2.0.4/FMI-Specification-2.0.4.pdf

Using FMI for AI applications
State of the art machine learning environments

- Python environment for data preparation, feature engineering, training of ML models



- Deployment to targets (cloud, PC, ECU, …)



  – Specialized solutions for embedded targets
    e.g. MILEA from Bosch for
    https://www.youtube.com/watch?v=0sdOI9RgS0Q

Using FMI for AI applications
State of the art ML+M&S Interaction

- Machine Learning, AI Community
  - python™ · Gymnasium · Keras · PyTorch · TensorFlow · julia · LUX.JL
- Exchange format:
  - ONNX

- Exchange formats:
  - Black box: fmi Functional Mock-Up Interface
    - FMPy https://github.com/CATIA-Systems/FMPy
    - PyFMI https://github.com/modelon-community/PyFMI
    - fmi.jl https://github.com/ThummeTo/FMI.jl
  - White box
    - BaseModelica* Modelica
- "Classical" Modelling and Simulation
  - MATLAB SIMULINK · DYMOLA · SC AME · OpenModelica

*Kurzbach, Gerd, Oliver Lenord, Hans Olsson, Martin Sjölund, and Henrik Tiedefelt. "Design Proposal of a Standardized Base Modelica Language," n.d. https://doi.org/10.3384/ecp204.

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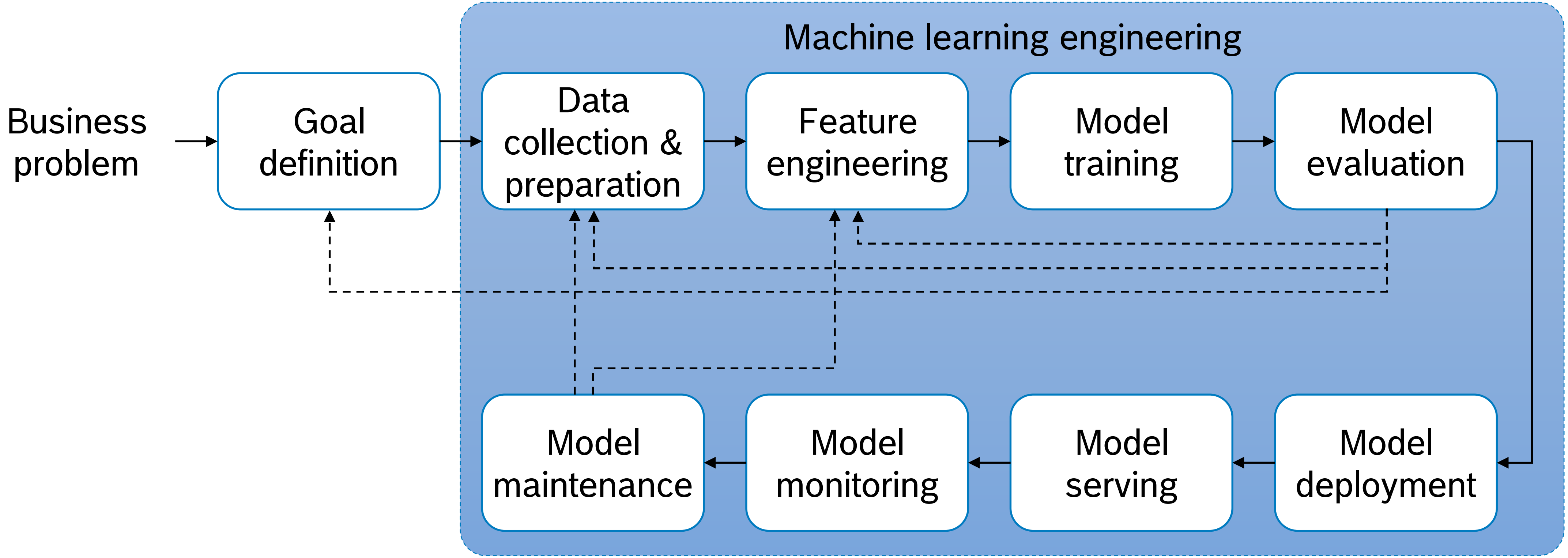
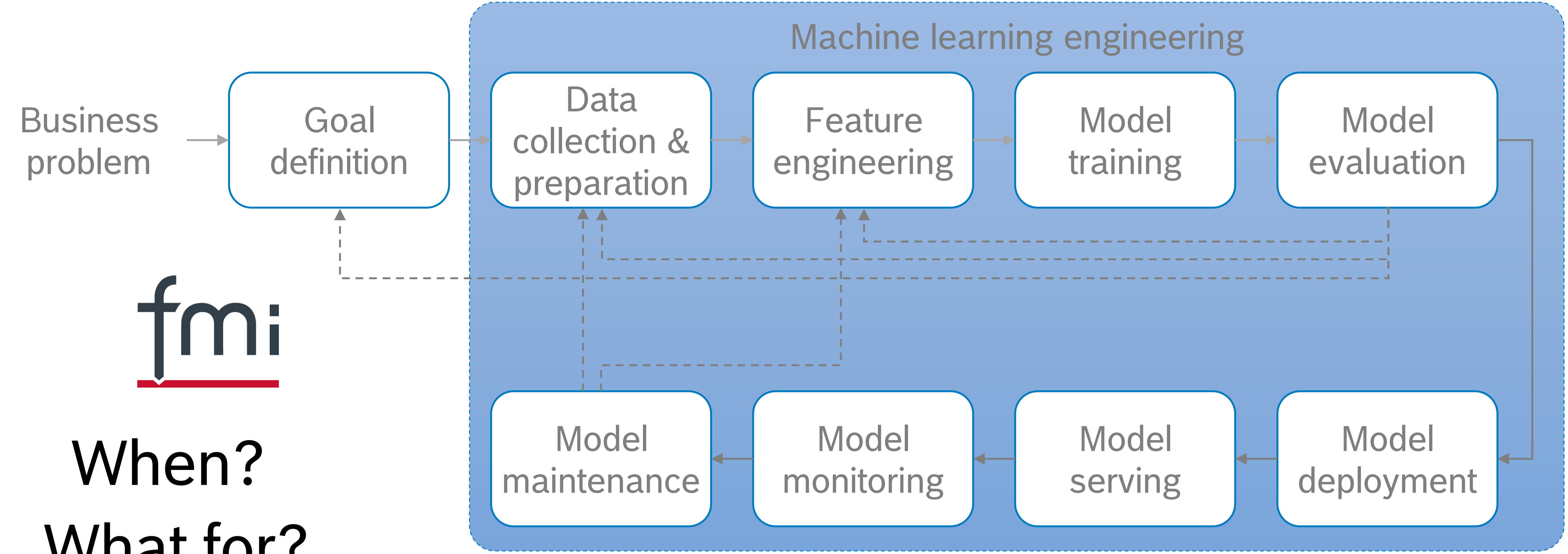
Using FMI for AI applications
State of the art machine learning (ML)



Burkov, A. (2020). Machine learning engineering (Vol. 1). Montreal, QC, Canada: True Positive Incorporated.

Using FMI for AI applications
Usage scenarios of FMI for machine learning (ML)



When?
What for?

Burkov, A. (2020). Machine learning engineering (Vol. 1). Montreal, QC, Canada: True Positive Incorporated.

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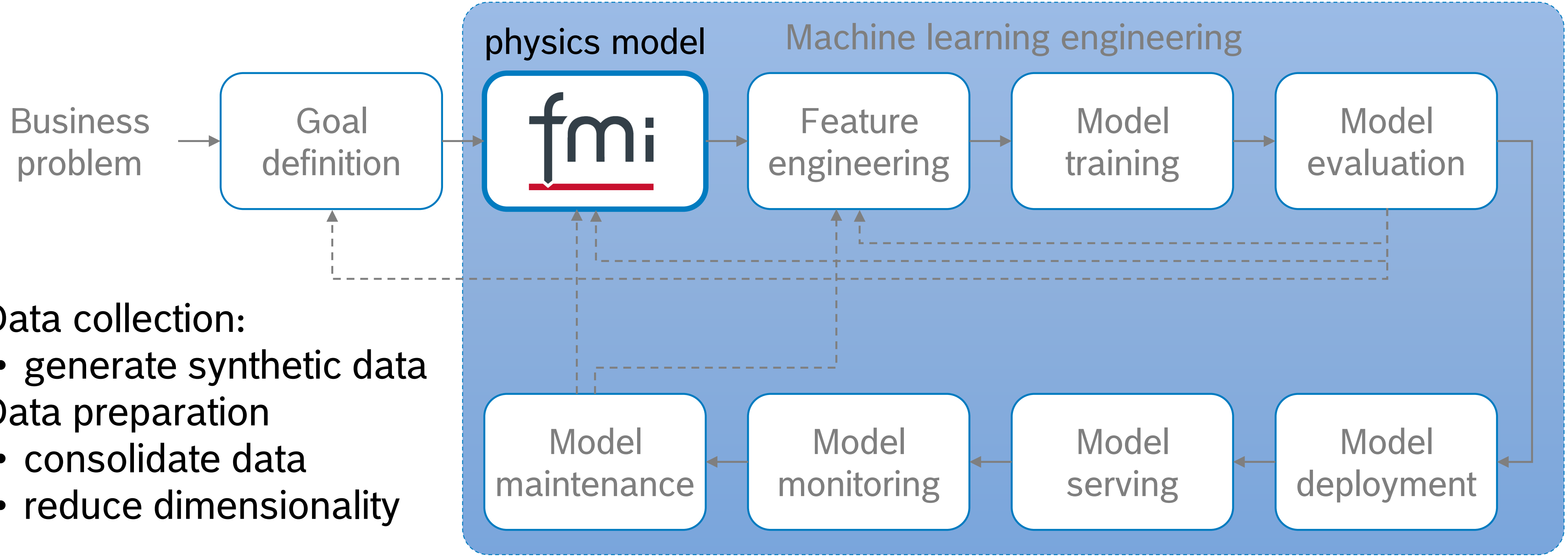

Data collection:
- generate synthetic data

Data preparation
- consolidate data
- reduce dimensionality

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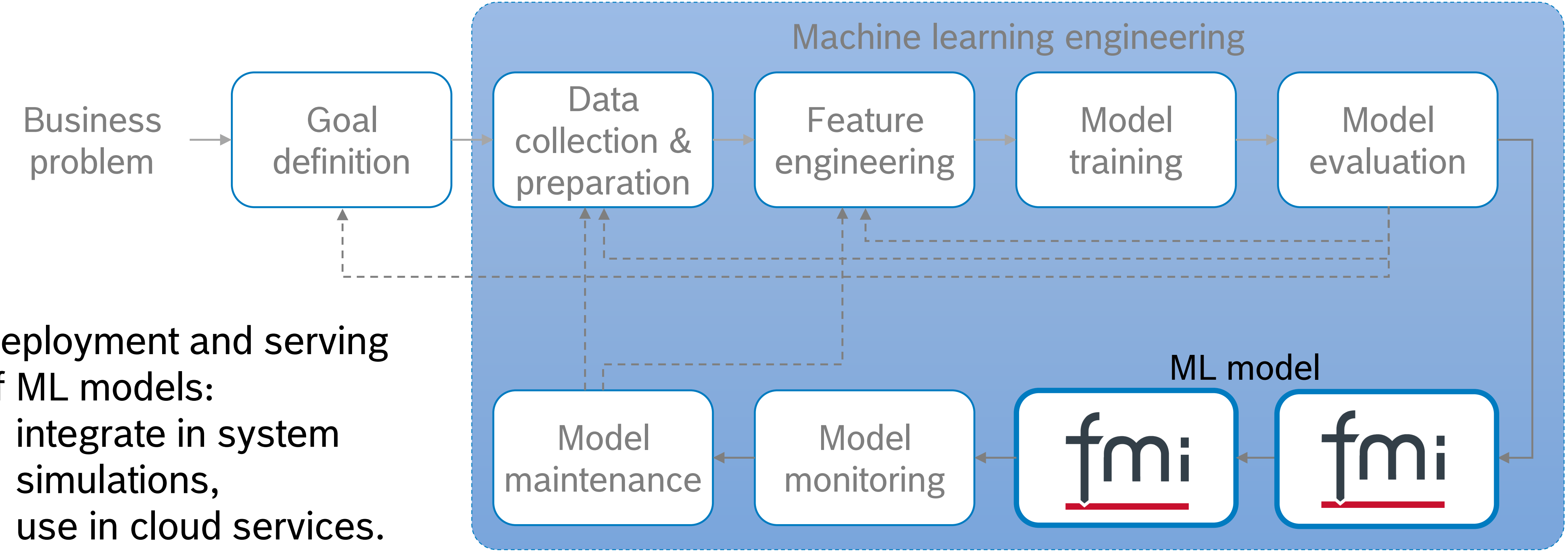
Using FMI for AI applications
Usage scenarios of FMI for machine learning (ML)



Deployment and serving of ML models:
- integrate in system simulations,
- use in cloud services.

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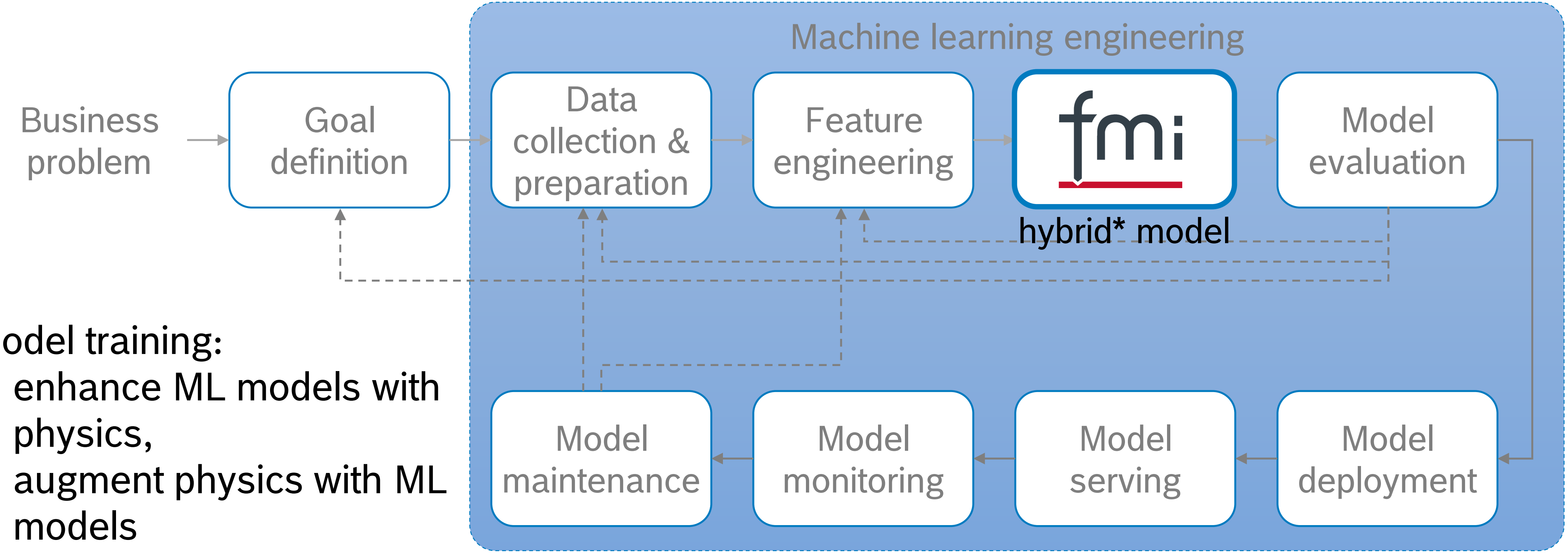
Using FMI for AI applications
Usage scenarios of FMI for machine learning (ML)



Model training:
- enhance ML models with physics,
- augment physics with ML models

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hybrid = physics + data-based

Using FMI for AI applications
Use Cases and benefits of physics + data-based (hybrid) modeling

- Improve existing physics simulation models by including AI parts to
  - reduce model error (accuracy)
  - reduce simulation effort (runtime efficiency)

- Improve training of ML models by physics models to
  - increase the range of validity (robustness)
  - increase physical soundness (explainability)
  - reduce training effort through reduction of training samples, pre-training or faster convergence (training efficiency)

- How?

Using FMI for AI applications

Frequent design patterns of hybrid* models

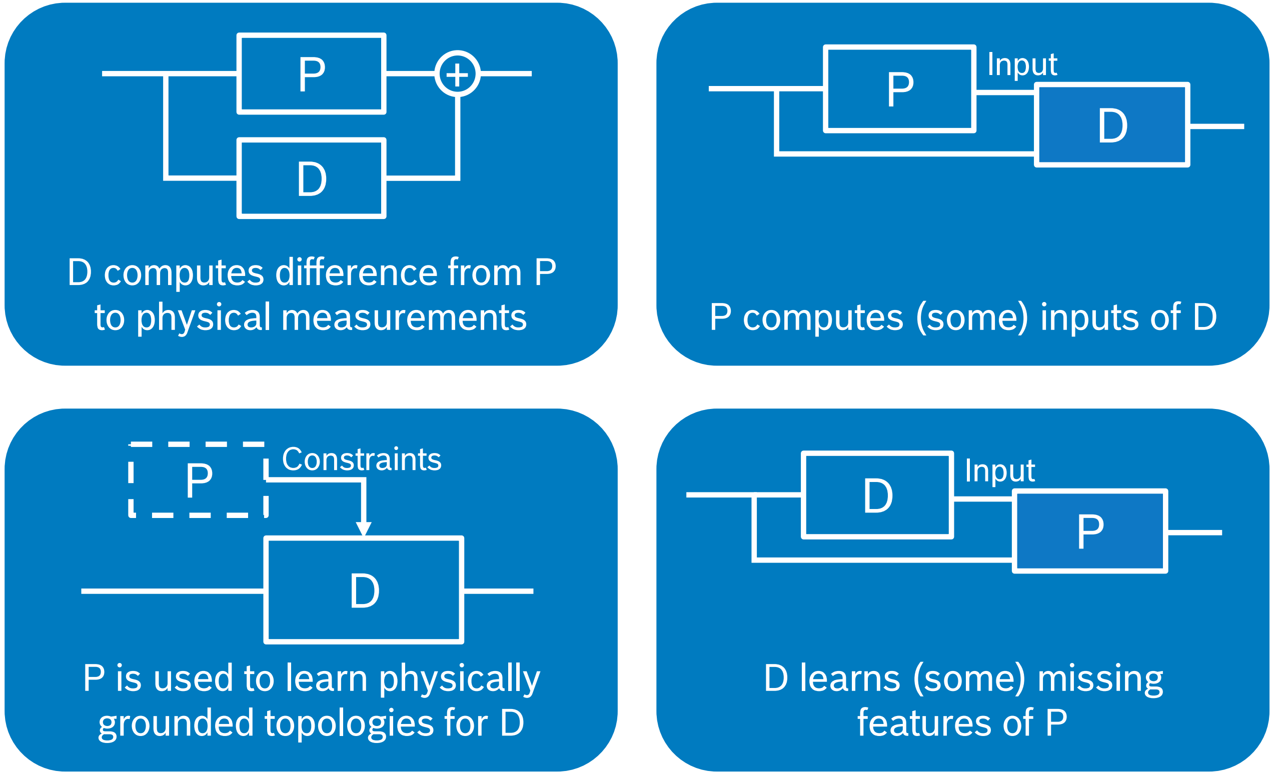
*physics + data-based models

Delta Model

Physics-based Pre-processing

Physical Constraints

Feature Learning



P = first Principle-based model, D = Data-based model

Rudolph, Maja, Stefan Kurz, and Barbara Rakitsch. “Hybrid Modeling Design Patterns,” 2024. https://doi.org/10.48550/ARXIV.2401.00033.

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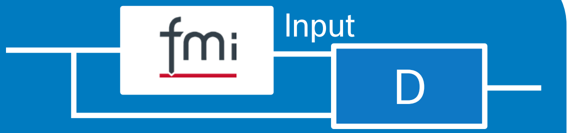
Using FMI for AI applications

Frequent design patterns of hybrid* models with fmi ≡ P

*physics + data-based models

Delta Model

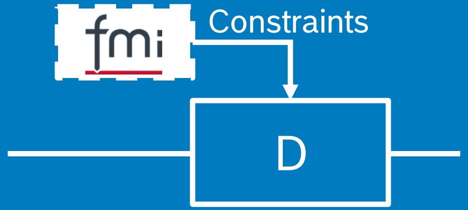
D computes difference from P to physical measurements



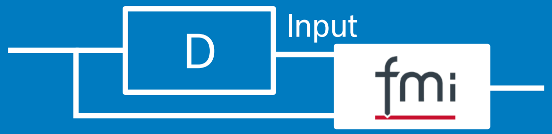
P computes (some) inputs of D

Physics-based Pre-processing

Physical Constraints



P is used to learn physically grounded topologies for D



D learns (some) missing features of P

Feature Learning

P = first Principle-based model, D = Data-based model

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Using FMI for AI applications

Frequent design patterns of hybrid* models with fmi ≡ D

*physics + data-based models

Delta Model

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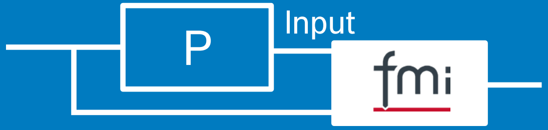

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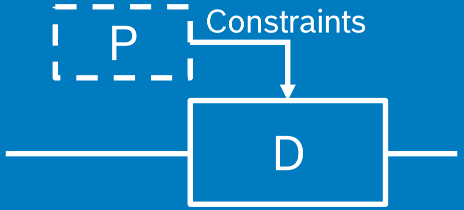
Physics-based Pre-processing

Physical Constraints



P is used to learn physically grounded topologies for D

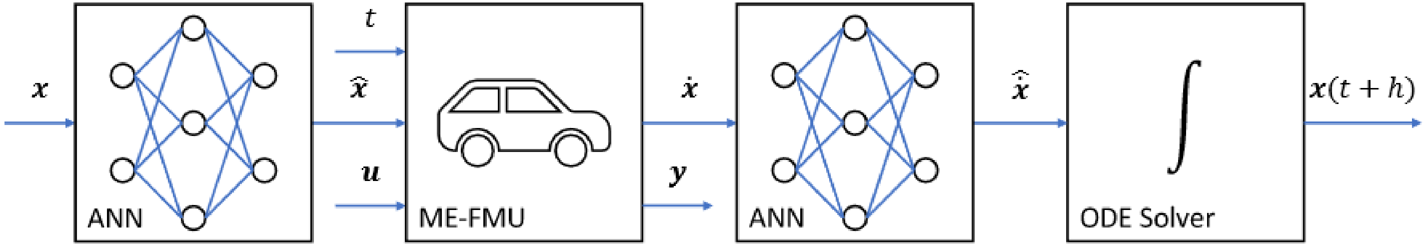
D learns (some) missing features of P

Feature Learning

P = first Principle-based model, D = Data-based model

Using FMI for AI applications
Generic architecture combining physics + data-based models

- FMU becomes part of the trained model architecture
  - is not only evaluated,
  - but has to backpropagate the losses to the parameters (weights) of the neural network.



Thummerer, Tobias, Johannes Stoljar, and Lars Mikelsons. "NeuralFMU: Presenting a Workflow for Integrating Hybrid NeuralODEs into Real World Applications." arXiv, September 8, 2022. http://arxiv.org/abs/2209.03933.

  - Successfully applied to a hydraulic excavator model with drastically improved accuracy.

Tobias Thummerer, Artem Kolesnikov, Julia Gundermann, Denis Ritz, Lars Mikelsons "Paving the way for Hybrid Twins using Neural Functional Mock-Up Units", Modelica Conference 2023

Using FMI for AI applications
FMI features supporting machine learning

- FMI for the evaluation of ML-Models
  - ME FMI 2.0: no continuous states, no numerical solver to be called, direct feedthrough
  - CS FMI 2.0 FMUs: most tool support, one has to accept a timestep “delay” between input setting and getting outputs
- Forward Sensitivity Analysis:
  - compute the directional derivatives: $\mathbf{v}_{sensitivity} = \mathbf{J} \cdot \mathbf{v}_{seed}$
  - `fmi2GetDirectionalDerivatives(V)`
    `fmi3GetDirectionalDerivatives(V)`
- Backward Sensitivity Analysis:
  - calculate the adjoint derivatives: $\mathbf{v}^{\mathbf{T}}_{sensitivity} = \mathbf{v}^{\mathbf{T}}_{seed} \cdot \mathbf{J}$
  - `fmi3GetAdjointDerivatives(V)*`

https://fmi-standard.org/docs/3.0.1/#partial-derivatives

Remark: Fast JVP operations require efficient implementations, e.g. automatic differentiation, caching,…

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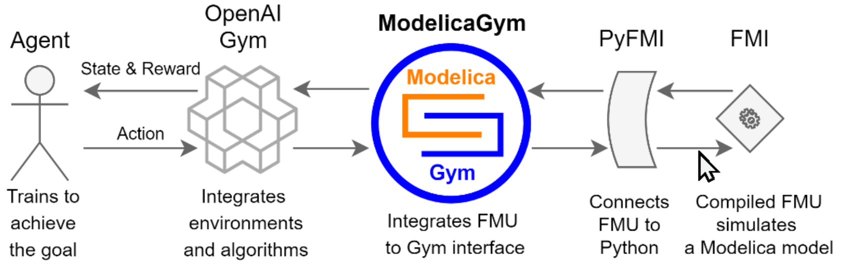
Using FMI for AI applications
Example: FMI for reinforcement learning

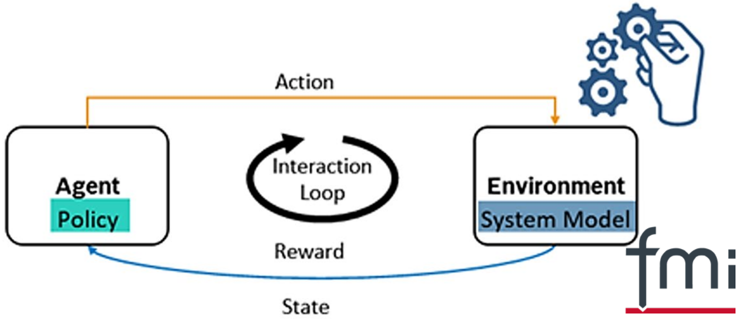
- Environment
  - Gym / Gymnasium by OpenAI:
    Open source Python library for developing and comparing **reinforcement learning** algorithms

Gymnasium



- Use FMI to bring Simulation models to Gym environment
  - Several open source and in-house solutions available, e.g., ModelicaGym*

- Successfully applied by Bosch in a similar setup
  - Reinforcement Learning for controller development.
  - FMI to generate training data based on dynamic models
  - Enables training that would be to risky on the real system



* Lukianykhin, Oleh, and Tetiana Bogodorova. "ModelicaGym: Applying Reinforcement Learning to Modelica Models." In *Proceedings of the 9th International Workshop on Equation-Based Object-Oriented Modeling Languages and Tools*, 27–36, 2019. https://doi.org/10.1145/3365984.3365985.

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Using FMI for AI applications
Conclusions & Outlook

- In “classical” simulation FMI is the de-facto industry standard for tool-independent model exchange and model deployment for

- FMI is the ideal exchange format to bridge the gap between ML and classical simulation
  → **Should be used more, especially in the ML community!**
- New features such as adjoint derivatives support very generic architectures.

Outlook:

- Lack of tool support and further improvements shall be addressed in the ITEA4 project 22013: (11/2023 - 10/2026)

https://itea4.org/project/openscaling.html

FMI,
the way to exchange models
of any kind!

Thank you for you attention!

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