HS'BI

Hochschule Bielefeld

University of Applied Sciences and Arts

NeuralNetwork 3.0: A library for representing PeNODEs

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iDaS

Institute for Data Science Solutions

- PeNODE
  - Definition
  - Example
  - Training
- NeuralNetwork Library
  - Structure
  - Example
- Future

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Closing the Sim-to-Real Gap with Physics-enhanced Neural ODEs

Tobias Kamp[1] [a], Johannes Ultsch[1] [b] and Jonathan Brembeck[1] [c]
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Keywords: Dynamical Systems, Hybrid Modelling, Neural Ordinary Differential Equations, Scientific Machine Learning, Physics-enhanced Neural ODEs

Abstract: A central task in engineering is the modelling of dynamical systems. In addition to first-principle methods, data-driven approaches leverage recent developments in machine learning to infer models from observations. Hybrid models aim to inherit the advantages of both, white- and black-box modelling approaches by combining the two methods in various ways. In this sense, Neural Ordinary Differential Equations (NODEs) proved to be a promising approach that deploys state-of-the-art ODE solvers and offers great modelling flexibility. In this work, an exemplary NODE setup is used to train low-dimensional artificial neural networks with physically meaningful outputs to enhance a dynamical model. The approach maintains the physical integrity of the model and offers the possibility to enforce physical laws during the training. Further, this work outlines how a confidence interval for the learned functions can be inferred based on the deployed training data. The robustness of the approach against noisy data and model uncertainties is investigated and a way to optimize model parameters alongside the neural networks is shown. Finally, the training routine is optimized with mini-batching and sub-sampling, which reduces the training duration in the given example by over 80 %.

1 INTRODUCTION

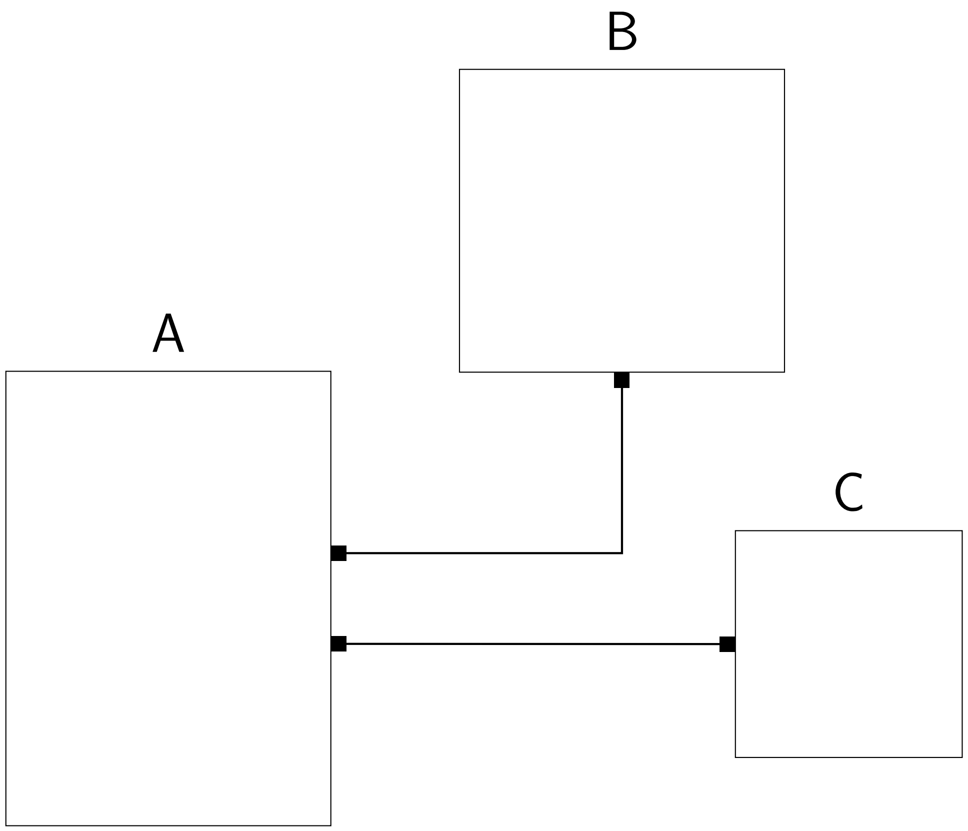
The modelling of dynamical systems is an important and challenging engineering task which forms

introduced by Chen (Chen et al., 2018), pose another promising approach. NODEs only approximate the right-hand side of the differential equations with neural networks (NNs) and benefit from the us-

DEFINITION

Physics-enhanced Neural ODE

physically meaningful neural components

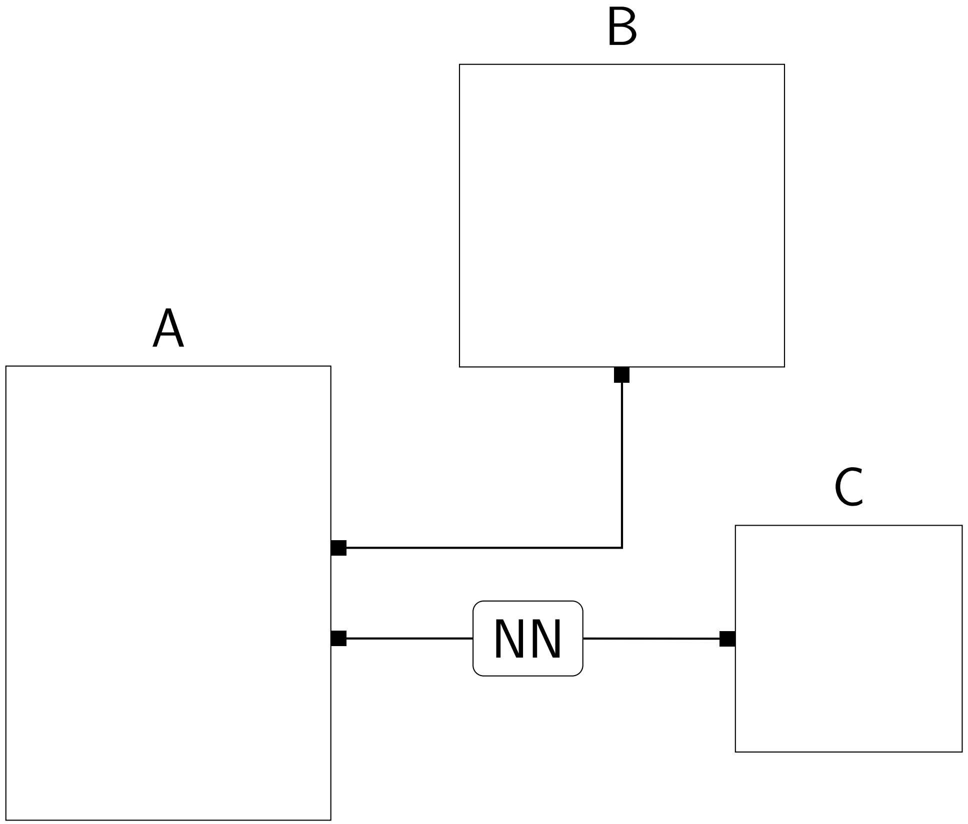


DEFINITION

Physics-enhanced Neural ODE

physically meaningful neural components

- Neural Network



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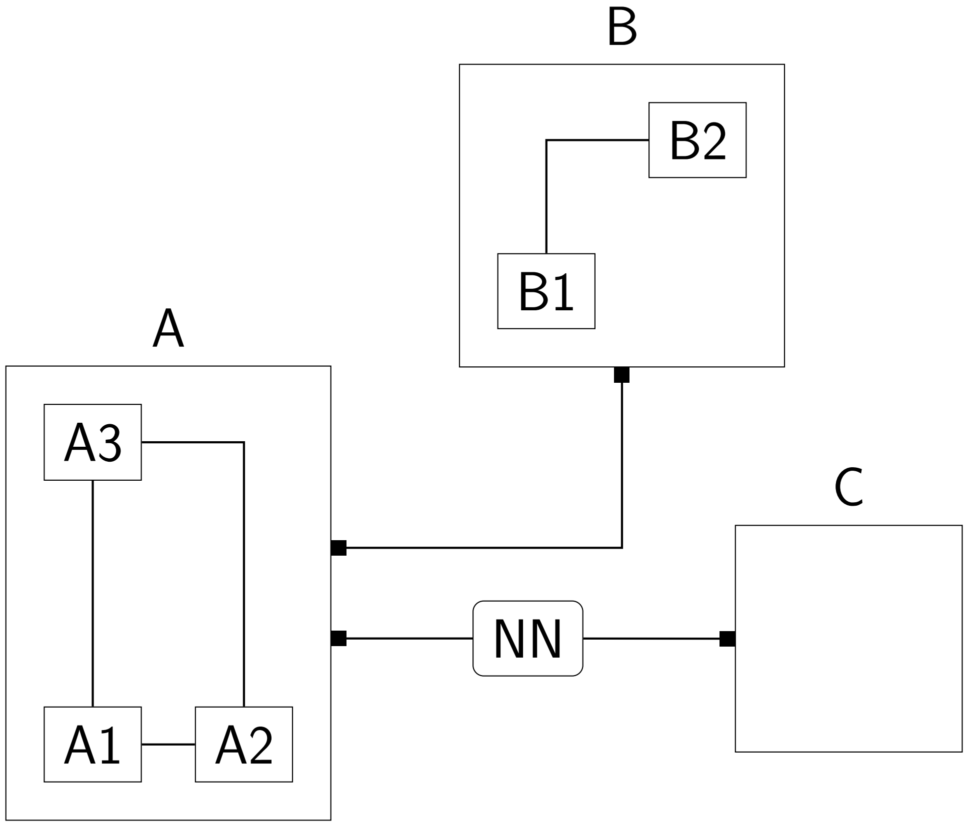
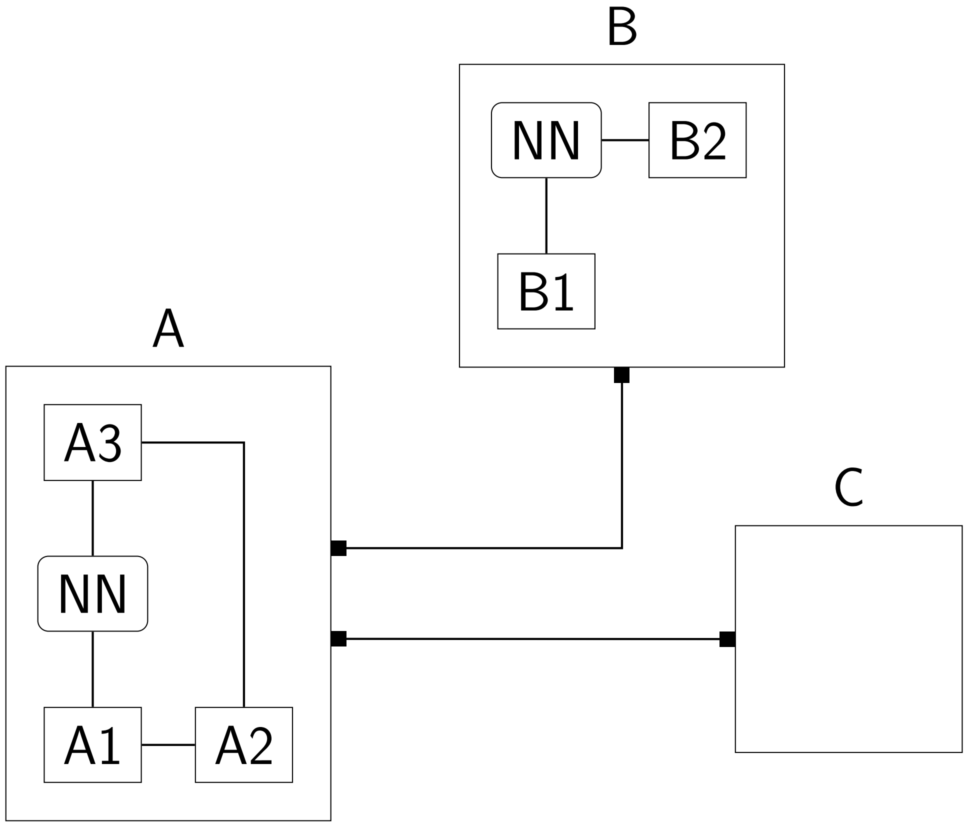


DEFINITION

Physics-enhanced Neural ODE

physically meaningful neural components

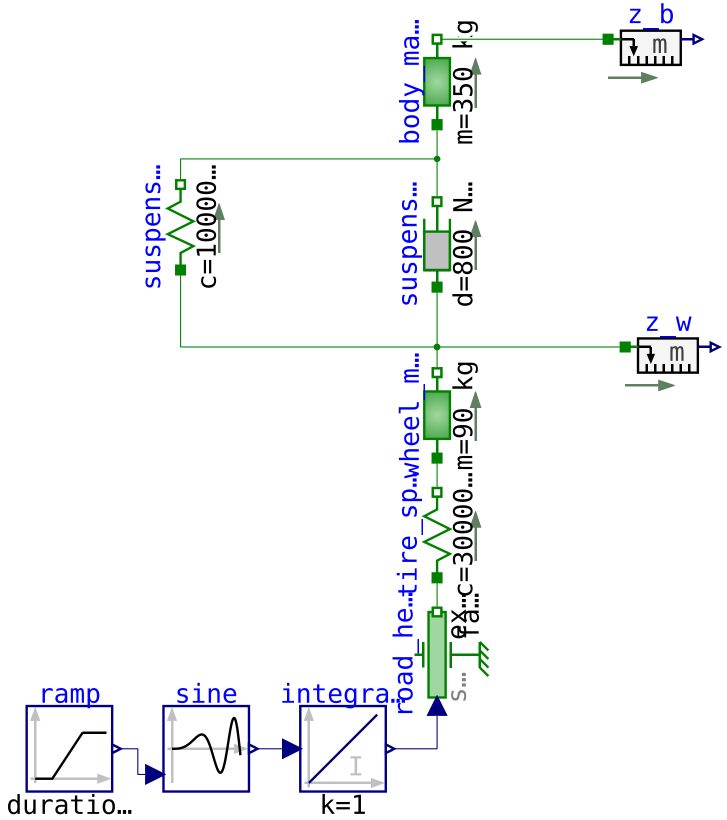
- Neural Network
- in-between other blocks
- usually relatively small



EXAMPLE: NEURAL QVM

Quarter Vehicle Model

- masses connected with spring



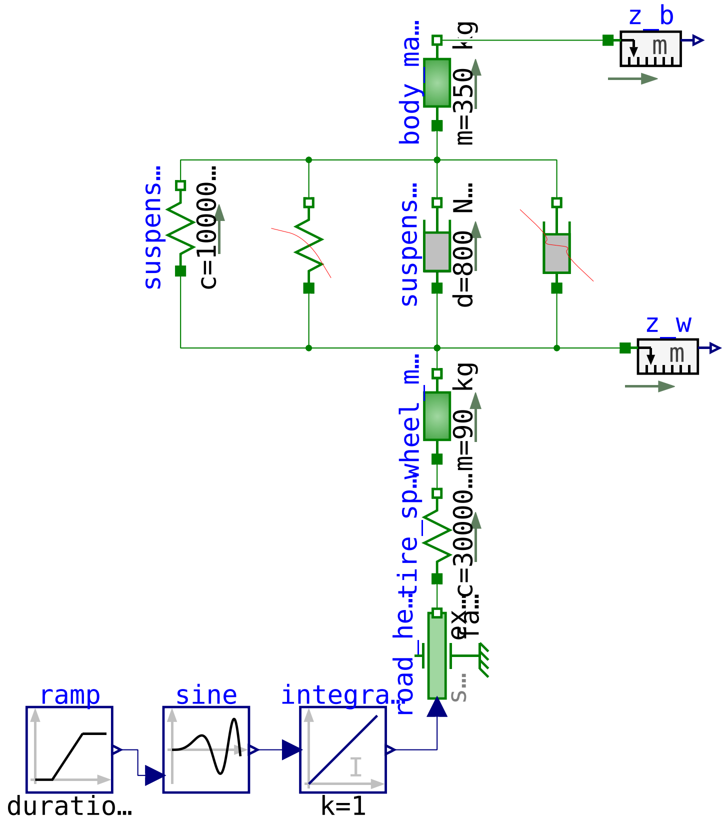
[1] T. Kamp et. al. *Closing the Sim-to-Real Gap with Physics-Enhanced Neural ODEs.* ICINCO 2023.

https://elib.dlr.de/200100/

EXAMPLE: NEURAL QVM

Quarter Vehicle Model

- masses connected with spring
- nonlinearities



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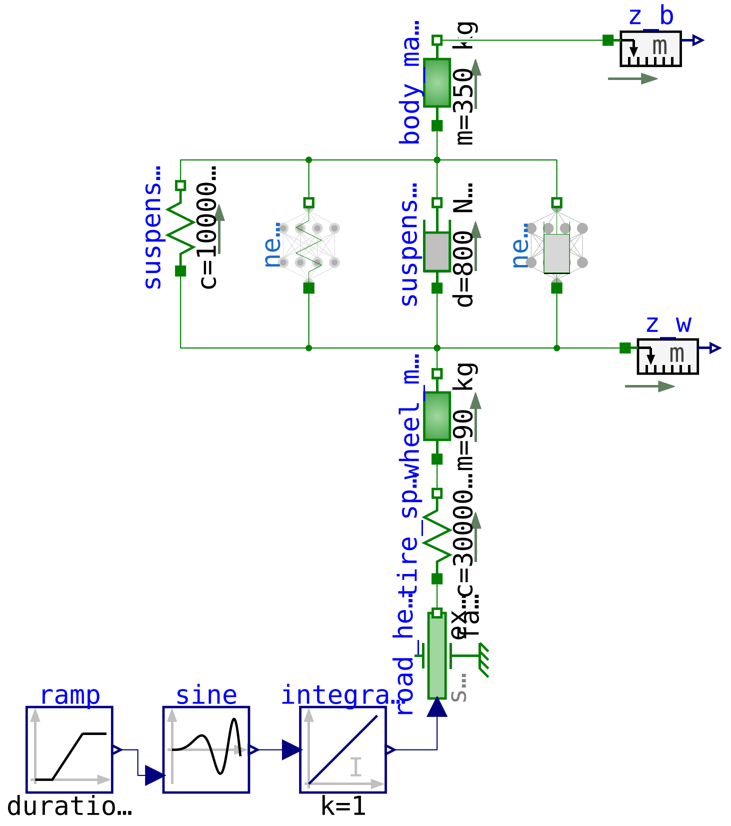
EXAMPLE: NEURAL QVM

Quarter Vehicle Model

- masses connected with spring
- nonlinearities
- approximate by trained surrogate



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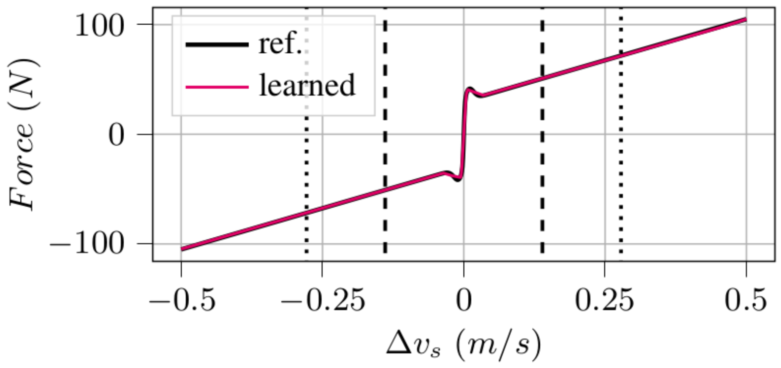
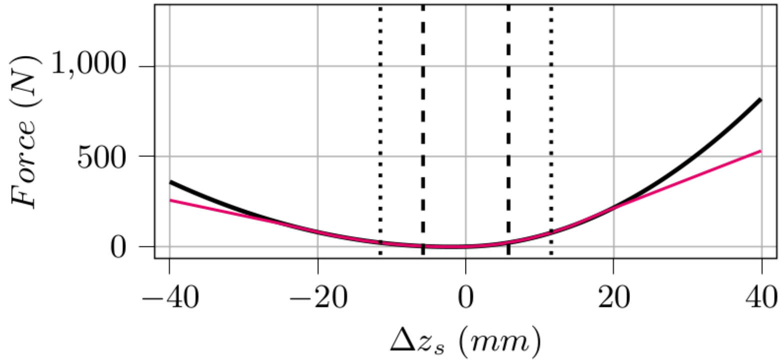
DO OR DO NOT, THERE IS NO TRAINING

Training outside of the library!

- use pre-trained models
- ...or perform parameter optimization (dynamic optimization)



(a) Friction Force



Images taken from [1]

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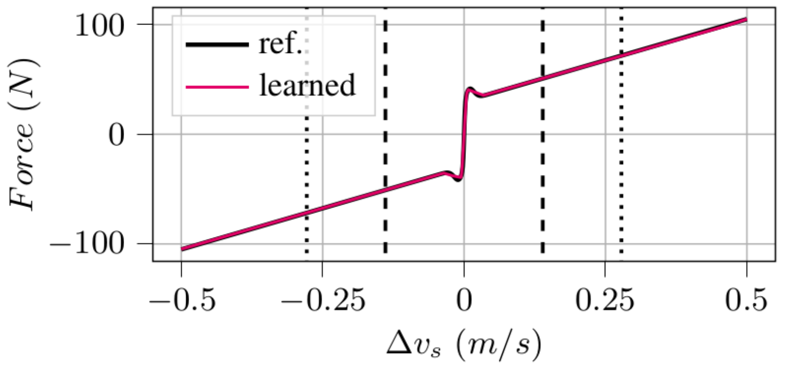
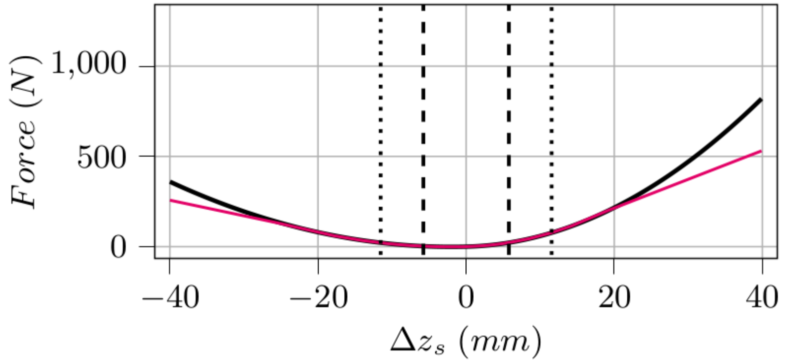
Use cases

data driven $\rightarrow$ accuracy
reference model $\rightarrow$ speed



(a) Friction Force



Images taken from [1]

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LIBRARY STRUCTURE

- NeuralNetwork
  - Layer
    - Interfaces
    - Preprocessing
    - Dense
    - LSTM
  - ActivationFunctions
  - Networks
    - Interfaces
      - Network
      - SISO
      - MISO
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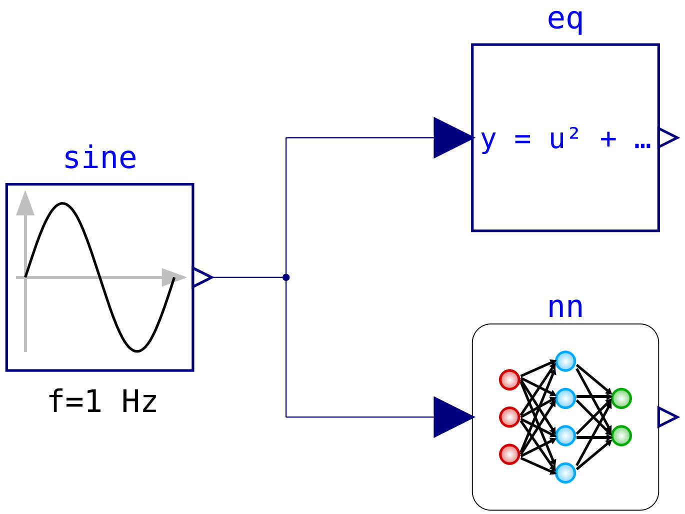
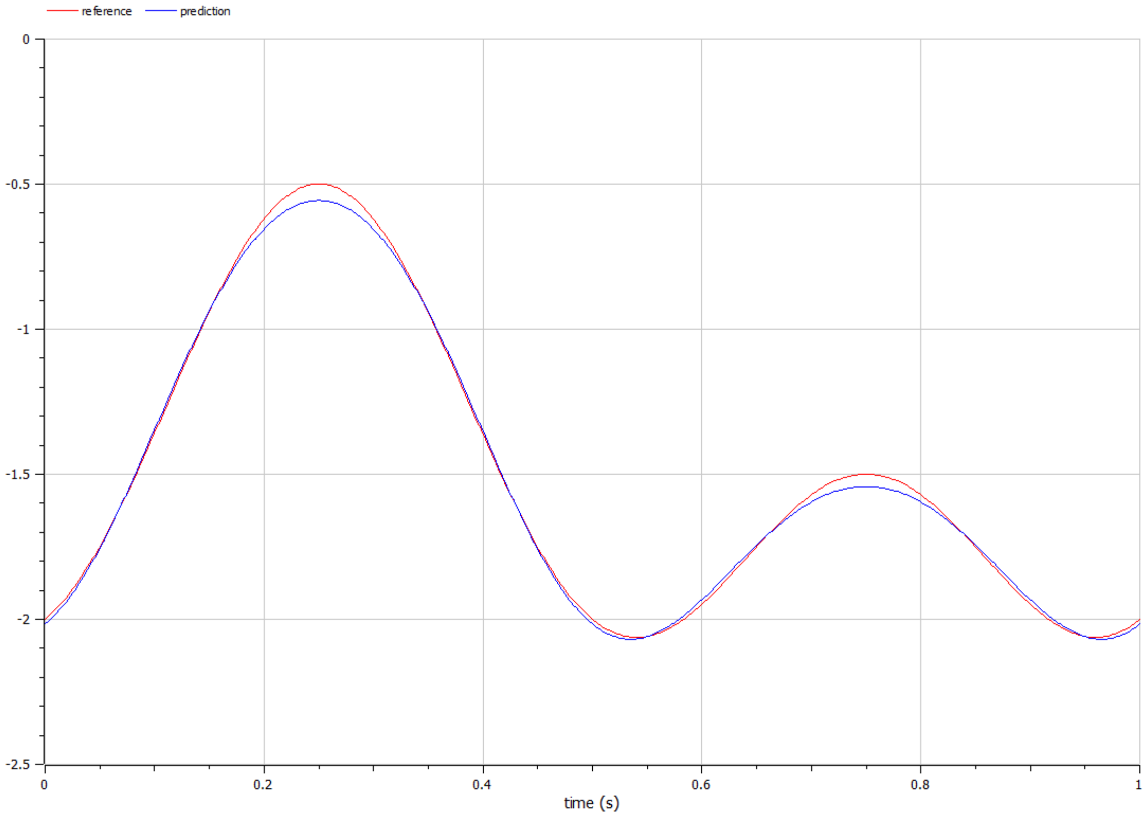
and it's open source (BSD-3)

`https://github.com/AMIT-HSBI/NeuralNetwork`

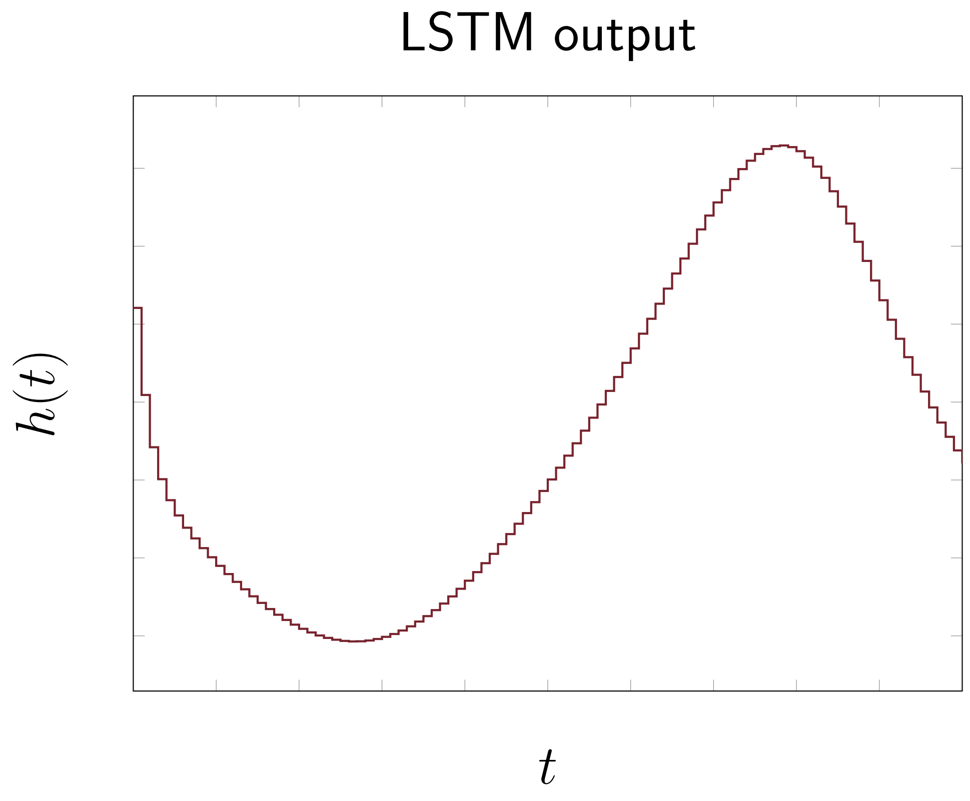
HELLO WORLD


eq
y = u² + …
sine
f=1 Hz
nn


reference
prediction
0
-0.5
-1
-1.5
-2
-2.5
0
0.2
0.4
0.6
0.8
1
time (s)

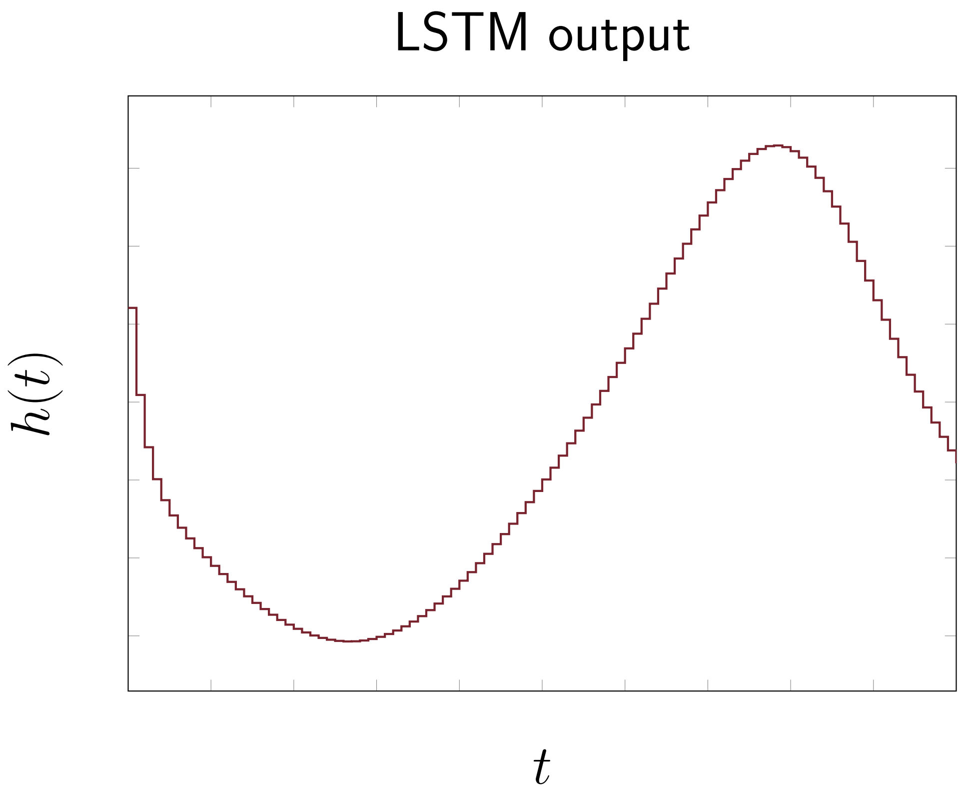
LSTM (WIP)

$$f_t = \sigma_g(W_f x_t + U_f h_{t-1} + b_f)$$
$$i_t = \sigma_g(W_i x_t + U_i h_{t-1} + b_i)$$
$$o_t = \sigma_g(W_o x_t + U_o h_{t-1} + b_o)$$
$$\tilde{c}_t = \sigma_c(W_c x_t + U_c h_{t-1} + b_c)$$
$$c_t = f_t \odot c_{t-1} + i_t \odot \tilde{c}_t$$
$$h_t = o_t \odot \sigma_h(c_t)$$



LSTM (WIP)

```
y = hold(h) "output";
when clk then
  x  = sample(u) "input";
  hp = previous(h);
  f  = sigma_g(Wf*x + Uf*hp + bf);
  i  = sigma_g(Wi*x + Ui*hp + bi);
  o  = sigma_g(Wo*x + Uo*hp + bo);
  ca = sigma_c(Wc*x + Uc*hp + bc);
  c  = f.*previous(c) + i.*ca;
  h  = o.*sigma_h(c);
end when;
```



USER BASE

- Modelon impact since v2.1.0 (PHyMoS)
- starting to use it for e-fmi (OpenSCALING)

We are looking forward to get feedback!

WHAT'S NEXT FOR THE LIBRARY?

recent development

- simpler interface with SISO, MISO
- recurrent networks (LSTM)
- new training approach

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current development

- more examples
- replaceable components
- release 3.0.0

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- simpler interface with SISO, MISO
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(possibly) upcoming development

- convolutional networks, other structures
- flexible weights import (SSP?)
- sparse matrices