PHyMOS

Accelerating the simulation of equation-based models by replacing non-linear algebraic loops with error-controlled machine learning surrogates

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Why non-linear Loops?

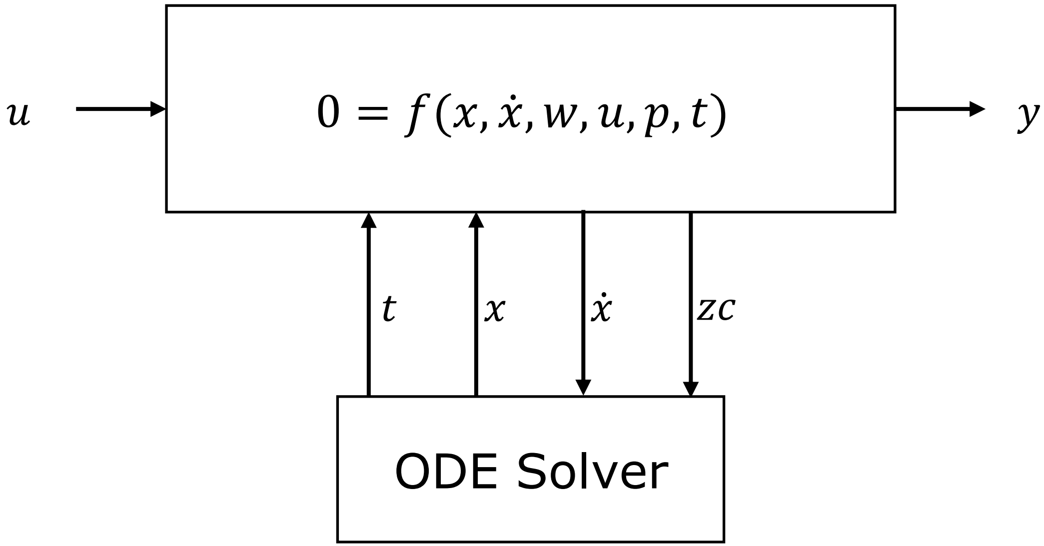
A.k.a. non-linear equation systems / strong components

Replacing Strong Components

Why replace non-linear algebraic loops?

- Expensive to solve
- Error control possible
- Improve ODE solver step size
- Learning task easier than learning whole ODE
- Improved start values for classic NLS solver
- Keep most of the physics

Replacing Strong Components



t	time
p	parameters
$u(t)$	inputs
$x(t)$	continuous states
$w(t)$	local variables
$y(t)$	outputs
$zc(t)$	event indicators

Replacing Strong Components

$$z(t) := \begin{pmatrix} \dot{x}(t) \\ w(t) \end{pmatrix} \text{ system unknowns}$$

$$\begin{aligned} f_1(z_3, z_4) &= 0 \\ f_2(z_2) &= 0 \\ f_3(z_2, z_3, z_5) &= 0 \\ f_4(z_1, z_2) &= 0 \\ f_5(z_1, z_3, z_5) &= 0 \end{aligned}$$

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$$\begin{array}{c} \\ f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \end{array} \begin{array}{c} \begin{array}{ccccc} z_1 & z_2 & z_3 & z_4 & z_5 \end{array} \\ \begin{pmatrix} 0 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 1 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 \end{pmatrix} \end{array}$$

$$\begin{array}{c} \\ f_2 \\ f_4 \\ f_3 \\ f_5 \\ f_1 \end{array} \begin{array}{c} \begin{array}{ccccc} z_2 & z_1 & z_3 & z_5 & z_4 \end{array} \\ \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & \boxed{1 \quad 1} & & 0 \\ 0 & 1 & \boxed{1 \quad 1} & & 0 \\ 0 & 0 & 1 & 0 & 1 \end{pmatrix} \end{array}$$

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$$\begin{aligned} f_2(z_2) &= 0 \\ f_4(z_1, z_2) &= 0 \\ f_{NLS}(z_1, z_2, z_3, z_5) &= 0 \\ f_1(z_3, z_4) &= 0 \end{aligned}$$

Machine learning surrogate f_S →

$$\begin{aligned} f_2(z_2) &= 0 \\ f_4(z_1, z_2) &= 0 \\ f_S(z_1, z_2) &= z_3, z_5 \\ f_1(z_3, z_4) &= 0 \end{aligned}$$

$$\begin{array}{c|ccccc} & z_1 & z_2 & z_3 & z_4 & z_5 \\ \hline f_1 & 0 & 0 & 1 & 1 & 0 \\ f_2 & 0 & 1 & 0 & 0 & 0 \\ f_3 & 0 & 1 & 1 & 0 & 1 \\ f_4 & 1 & 1 & 0 & 0 & 0 \\ f_5 & 1 & 0 & 1 & 0 & 1 \end{array}$$

$$\begin{array}{c|ccccc} & z_2 & z_1 & z_3 & z_5 & z_4 \\ \hline f_2 & 1 & 0 & 0 & 0 & 0 \\ f_4 & 1 & 1 & 0 & 0 & 0 \\ f_3 & 1 & 0 & 1 & 1 & 0 \\ f_5 & 0 & 1 & 1 & 1 & 0 \\ f_1 & 0 & 0 & 1 & 0 & 1 \end{array}$$

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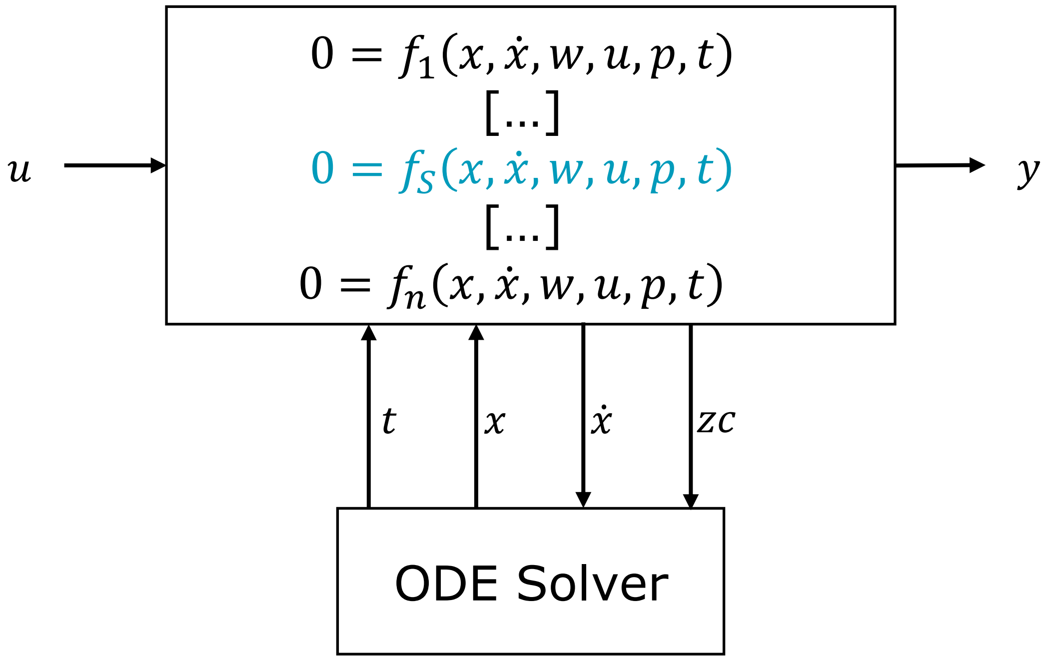
Replacing Strong Components



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Example

Simple Loop with two unknowns

Example: Simple Loop
Intersection between Circle and Line

Non-linear system (solve for x, y):

$$r^2 = x^2 + y^2$$
$$rs + b = x + y$$

Tearing

Transformed into:

Inner equation { $x = rs + b - y$

Residual equation { $0 = y^2 + x^2 - r^2$

2 Unknowns: x, y

1 Iteration variable: y

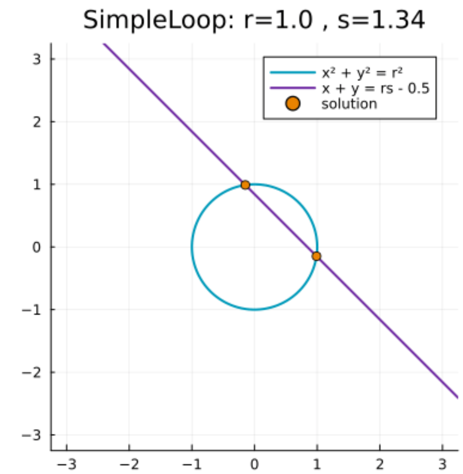
Parameters: b

Knowns: r, s

```
model simpleLoop
  Real r(min = 0);
  Real s(min = -sqrt(2), max = sqrt(2));
  Real x(start=1.0), y(start=0.5);
  parameter Real b = -0.5;
equation
  r = 1+time;
  s = sqrt((2-time)*0.9);

  r^2 = x^2 + y^2;
  r*s + b = x + y;
end simpleLoop;
```

Example: Simple Loop
Intersection between Circle and Line



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Residual equation $\{ \quad 0 = y^2 + x^2 - r^2$

2 Unknowns:	x, y
1 Iteration variable:	y
Parameters:	b
Knowns:	r, s

ML Surrogate:

$$y = f_S(r, s, b)$$
$$x = rs + b - y$$

Inputs:	r, s, b
Outputs:	y
Evaluate Inner Equations:	x

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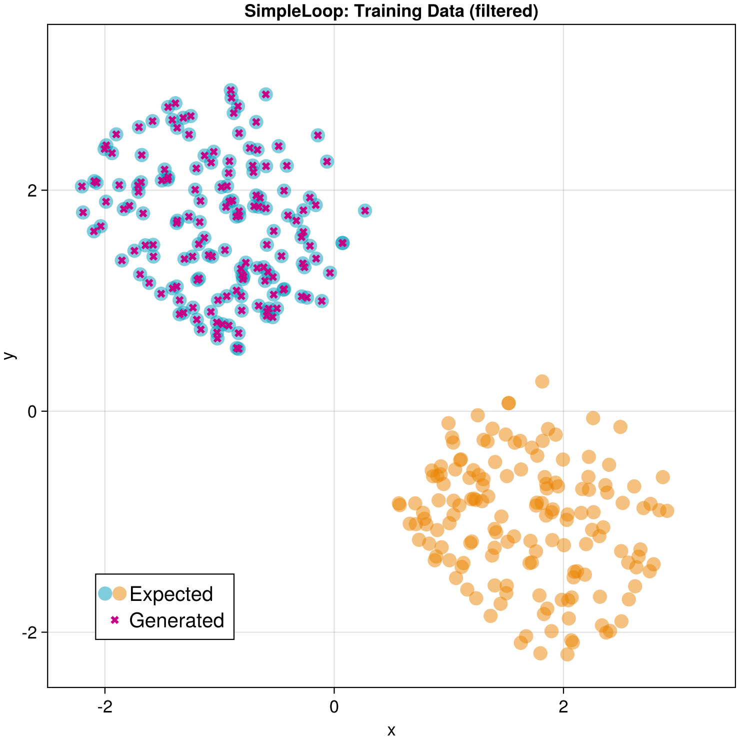
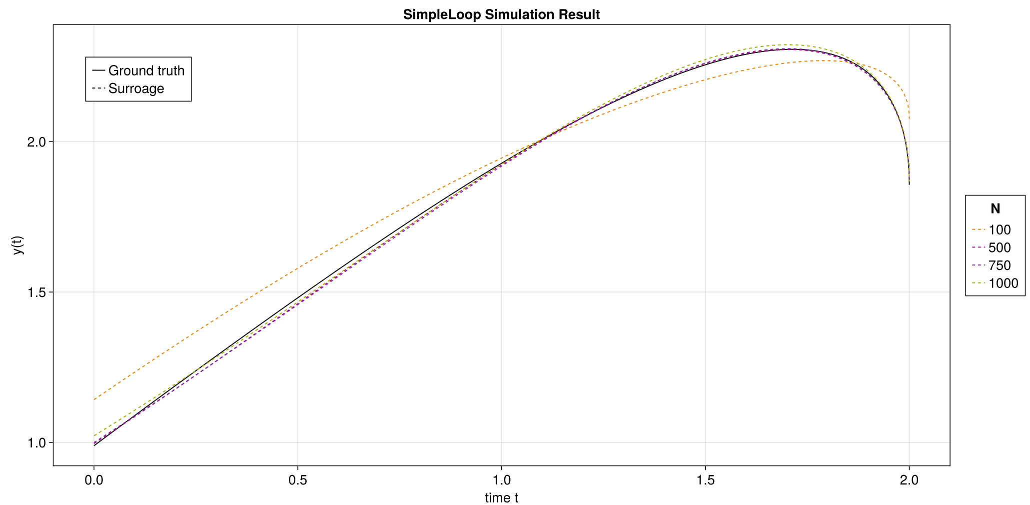
Example: Simple Loop
Intersection between Circle and Line





Requirements on the Surrogate

Classic Newton–Raphson method

- Quadratic convergence
  - Each step doubles number of correct decimals
  - Start values extrapolated from previous solution
- Complexity: $\mathcal{O}(N^3)$

Surrogate f_S needs to be:

- Sufficiently faster than NLS solver
- Accurate
- Independent of solver step size
- Trained on relevant input space

Method Overview

Method Overview

1. Identify slow equation sets
2. Generate training data
3. Train ANN surrogate
4. Replace equation set with ANN surrogate

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Automated Profiling

1. Simulate with Profiling

- `-d=infoXmlOperations` and `-clock=CPU -cpu`
- Profiling information and reference data

2. Process profiling JSON file

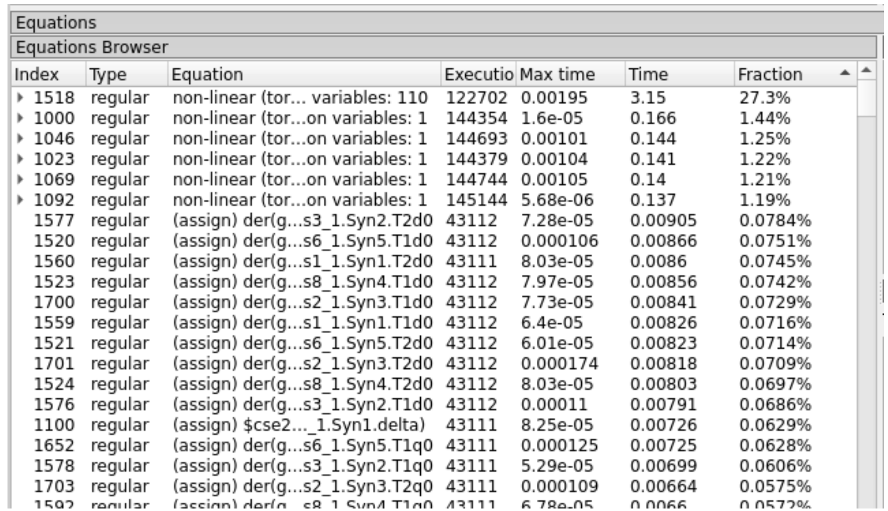
- Sort for total time
- Return equation systems over threshold

3. Process info JSON file

- Get dependent variables of equation

4. Process reference results

- Get min/max values of input variables



Equations
Equations Browser

Index	Type	Equation	Executio	Max time	Time	Fraction
1518	regular	non-linear (tor... variables: 110	122702	0.00195	3.15	27.3%
1000	regular	non-linear (tor...on variables: 1	144354	1.6e-05	0.166	1.44%
1046	regular	non-linear (tor...on variables: 1	144693	0.00101	0.144	1.25%
1023	regular	non-linear (tor...on variables: 1	144379	0.00104	0.141	1.22%
1069	regular	non-linear (tor...on variables: 1	144744	0.00105	0.14	1.21%
1092	regular	non-linear (tor...on variables: 1	145144	5.68e-06	0.137	1.19%
1577	regular	(assign) der(g...s3_1.Syn2.T2d0	43112	7.28e-05	0.00905	0.0784%
1520	regular	(assign) der(g...s6_1.Syn5.T1d0	43112	0.000106	0.00866	0.0751%
1560	regular	(assign) der(g...s1_1.Syn1.T2d0	43111	8.03e-05	0.0086	0.0745%
1523	regular	(assign) der(g...s8_1.Syn4.T1d0	43112	7.97e-05	0.00856	0.0742%
1700	regular	(assign) der(g...s2_1.Syn3.T1d0	43112	7.73e-05	0.00841	0.0729%
1559	regular	(assign) der(g...s1_1.Syn1.T1d0	43112	6.4e-05	0.00826	0.0716%
1521	regular	(assign) der(g...s6_1.Syn5.T2d0	43112	6.01e-05	0.00823	0.0714%
1701	regular	(assign) der(g...s2_1.Syn3.T2d0	43112	0.000174	0.00818	0.0709%
1524	regular	(assign) der(g...s8_1.Syn4.T2d0	43112	8.03e-05	0.00803	0.0697%
1576	regular	(assign) der(g...s3_1.Syn2.T1d0	43112	0.00011	0.00791	0.0686%
1100	regular	(assign) $cse2..._1.Syn1.delta)	43111	8.25e-05	0.00726	0.0629%
1652	regular	(assign) der(g...s6_1.Syn5.T1q0	43111	0.000125	0.00725	0.0628%
1578	regular	(assign) der(g...s3_1.Syn2.T1q0	43111	5.29e-05	0.00699	0.0606%
1703	regular	(assign) der(g...s2_1.Syn3.T2q0	43111	0.000109	0.00664	0.0575%
1592	regular	(assign) der(g...s8_1.Syn4.T1q0	43111	6.78e-05	0.0066	0.0572%

Automated Profiling

Model:
OpenIPSL.Examples.IEEE14.IEEE_14_Buses
OpenIPSL version 3.0.1

- Non-linear system 1403:
  - Unknowns: 204
    - Iteration variables: 110
    - Inner equations: 94
  - Knowns: 16 (time and states)

Index	Time [s]	Fraction [%]
1403	1.31	13.70
1594	0.06	0.61
1686	0.05	0.57
1640	0.05	0.56
1617	0.05	0.56
1663	0.05	0.55

Automated Profiling

1. Identify slow equation sets ☑
2. Generate training data ☐
3. Train ANN surrogate ☐
4. Replace equation set with ANN surrogate ☐

Generation of Training Data

1. Generate 2.0 ME C Source-Code FMU

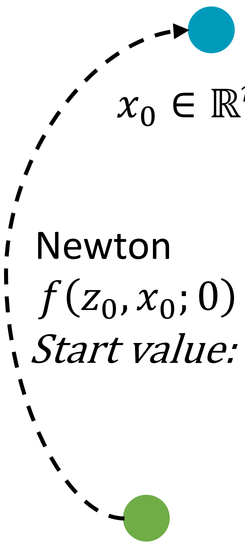
2. Add C extension

- Make it possible to evaluate single equations
- Re-compile FMU with changed sources

3. Generate training data

- Instantiate, setup experiment & initialize system
- Evaluate loop for used Variables (input) and initial values for iteration variables
- Save training data to CSV

Generation of Training Data



$x_0 \in \mathbb{R}^{n_{itter}}$

Newton

$f(z_0, x_0; 0) = 0$

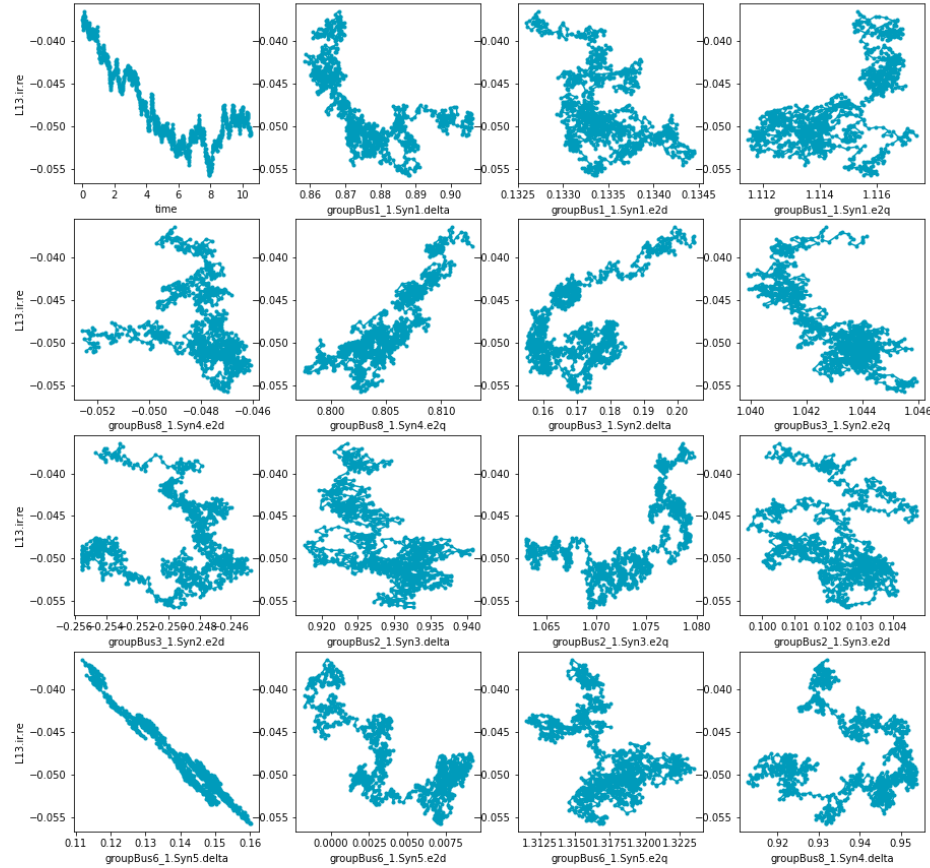
Start value: $0 \in R^{n_{itter}}$

$z_0 \in \mathbb{R}^{n_{input}}$ random

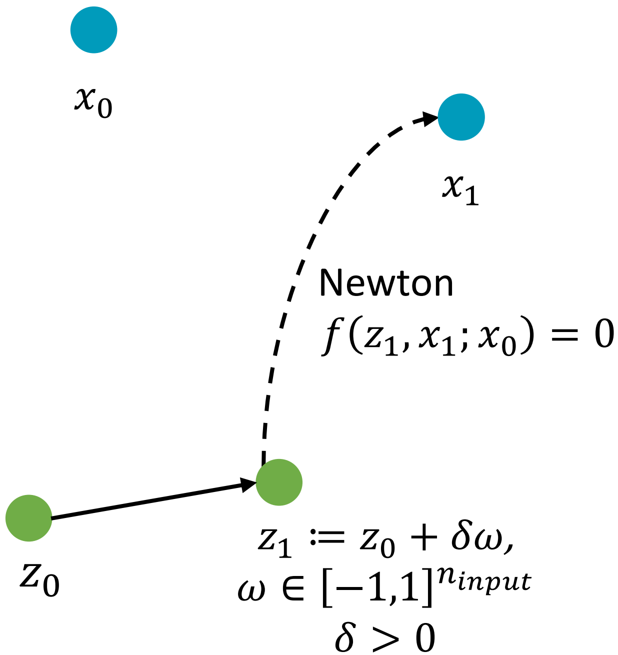
Save (z_0, x_0)

IEEE_14_Buses

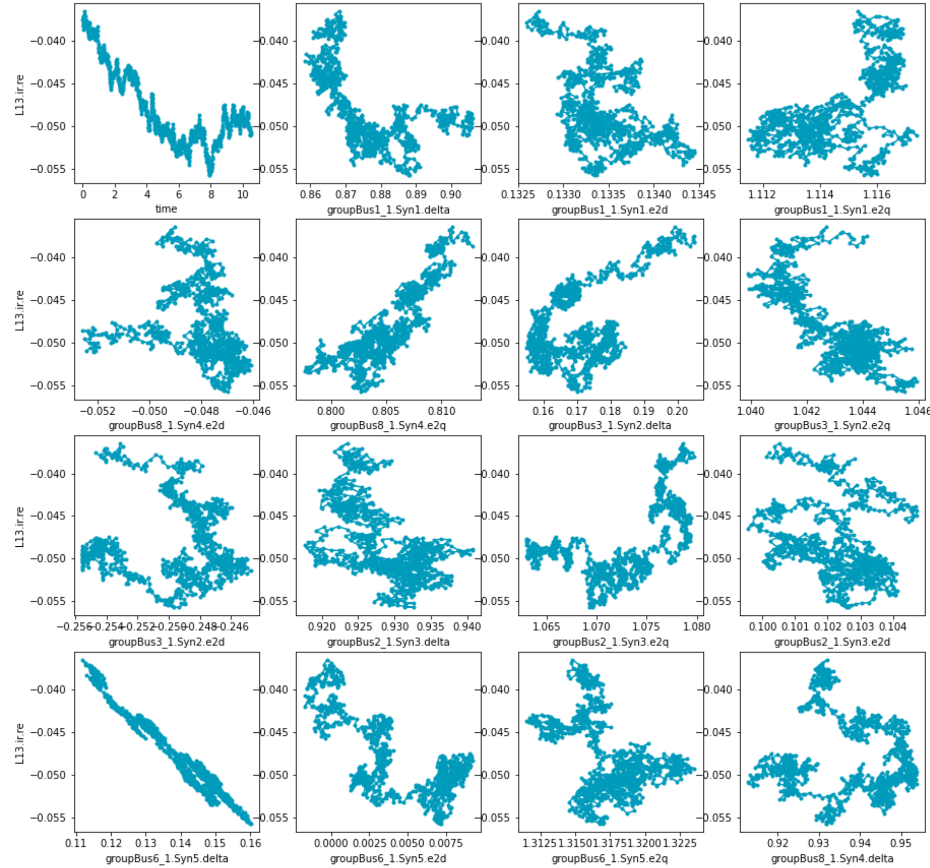
Inputs z_i vs Output $x_{i,1}$



Generation of Training Data



IEEE_14_Buses
Inputs z_i vs Output $x_{i,1}$



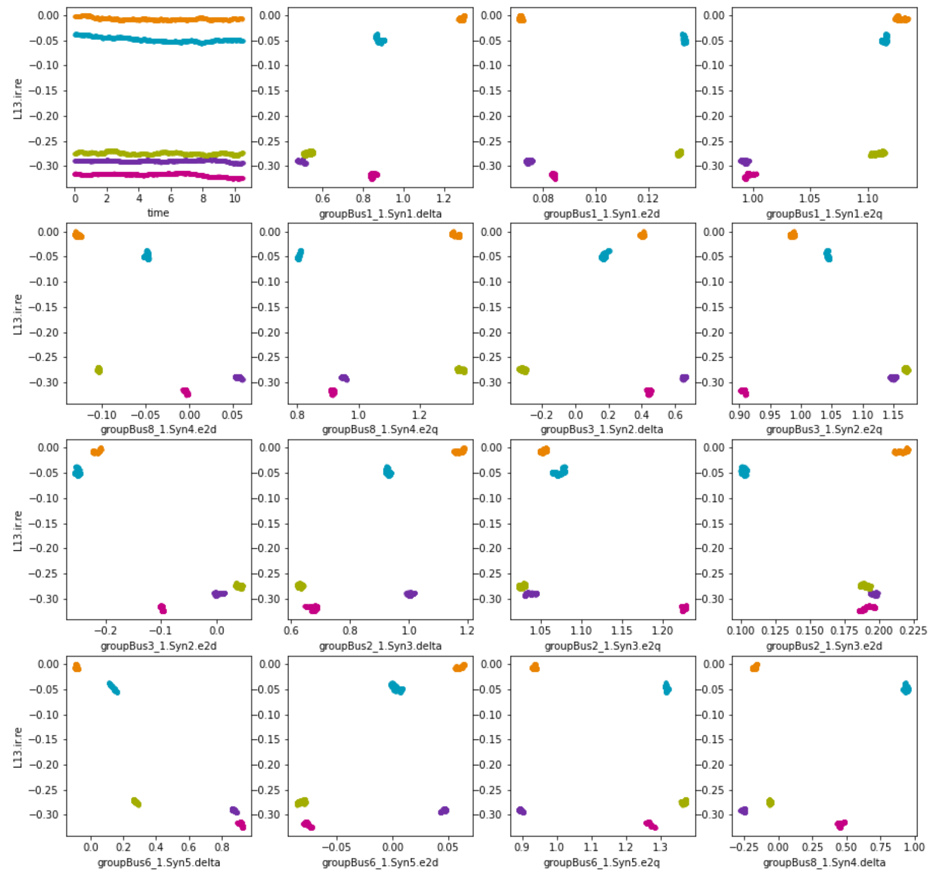
Generation of Training Data

Data generation is fast:

- Parallelized
- Only evaluating non-linear system equations.
- Start values for Newton iteration close to solution.

IEEE_14_Buses

Inputs z_i vs Output $x_{i,1}$



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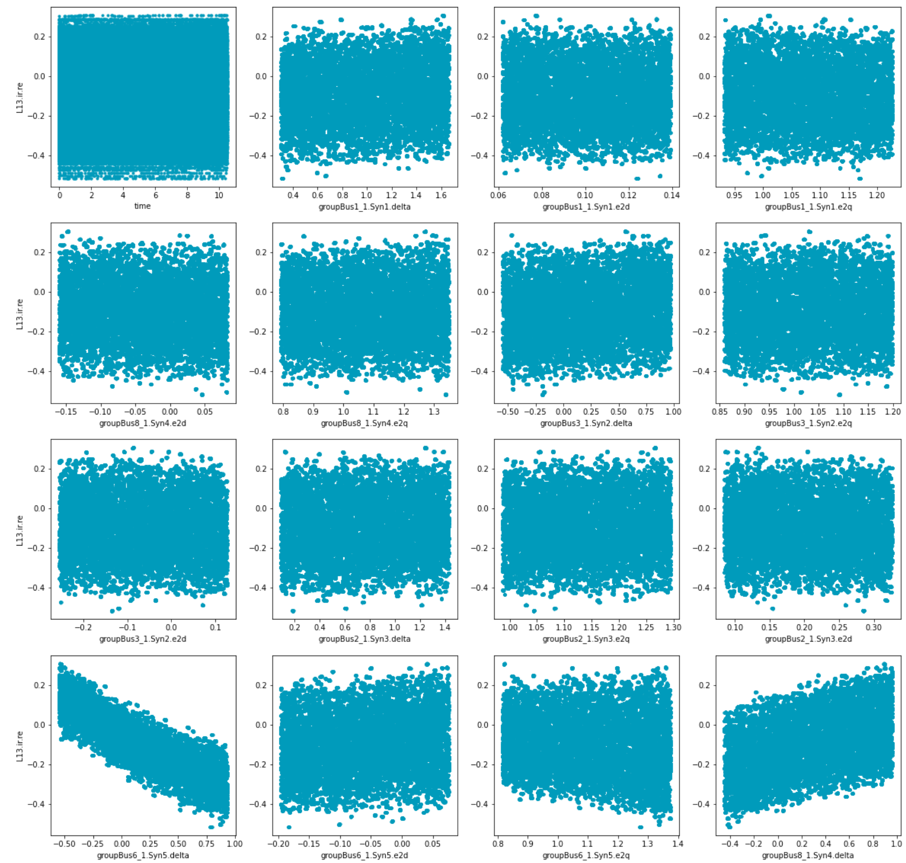
Generation of Training Data

IEEE_14_Buses

Inputs z_i vs Output $x_{i,1}$



Data generation is fast:

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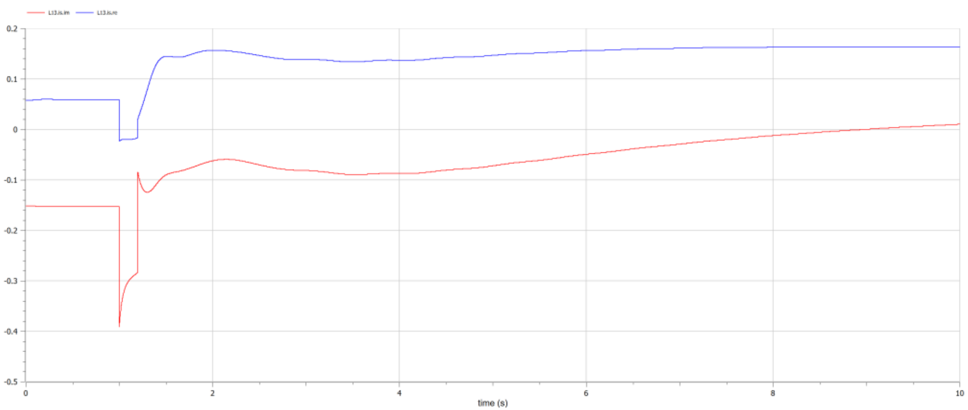
Generation of Training Data

- Possible to have complicated equations inside residuum equations
  - Events at 1s and 1.124s

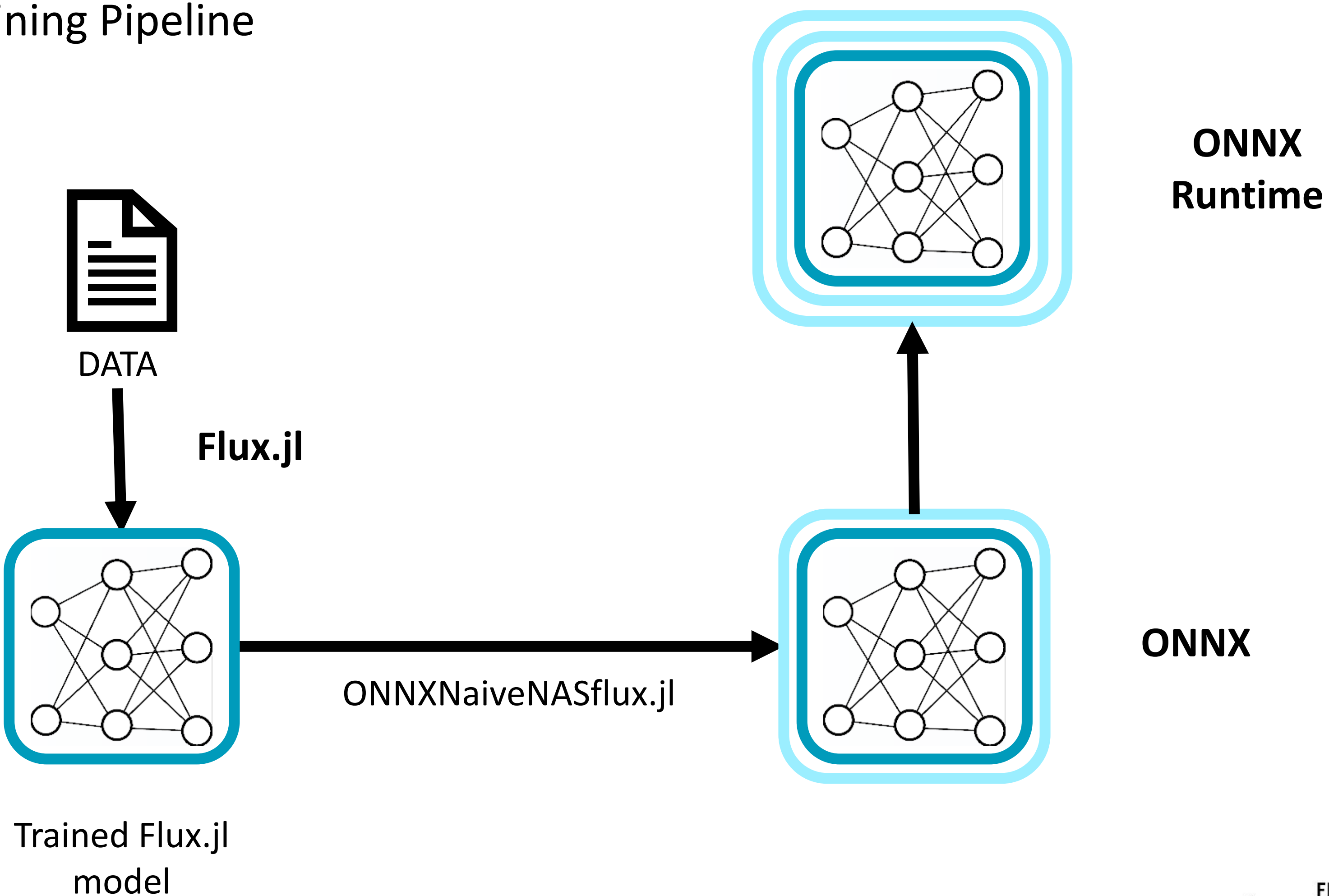



```
model OpenIPSL.Electrical.Branches.PwLine
  [...]
  if time >= t1 and time < t2 then
    if opening == 1 then
      is = Complex(0);
      ir = Complex(0);
    elseif opening == 2 then
      is = Complex(0);
      ir = (vr - ir*Z)*Y;
    else
      ir = Complex(0);
      is = (vs - is*Z)*Y;
    end if;
  else
    vs - vr = Z*(is - vs*Y);
    vr - vs = Z*(ir - vr*Y);
  end if;
end OpenIPSL.Electrical.Branches.PwLine;
```

Generation of Training Data

1. Identify slow equation sets ☑
2. Generate training data ☑
3. Train ANN surrogate ☐
4. Replace equation set with ANN surrogate ☐

Training Pipeline



Surrogate strategy

If $z_{t_i} \in TrainedArea \subset \mathbb{R}^{n\_input}$ then:

$\tilde{x} := f_S(z_{t_i})$

If $|f_{NLS}(z_{t_i}, \tilde{x})| > \epsilon$ then:

Newton: Solve $0 = f_{NLS}(z_{t_i}, x; \tilde{x})$ for x

$x_{t_i} := x$

Else:

$x_{t_i} := \tilde{x}$

Else:

$\tilde{x} := extrapolate(x_{t_{i-1}}, x_{t_{i-2}})$

Newton: Solve $0 = f_{NLS}(z_{t_i}, \mathrm{x}; \tilde{x})$ for x

$x_{t_i} := x$

ML Surrogate (first block)

Default NLS process (second block)

Replace Strong Component

Pros:

- Ensure correct solution up to given precision.
- Ensure performance outside of trained are (use default solver).
- Evaluation (mostly) independent of step-size / distance to previous solution.

Cons:

- Too slow to justify training effort:
  - Additional overhead for loading ONNX.
  - Evaluating default solver anyway.
- Solution not smooth enough rendering ODE solver step-size control useless.

Replacing Strong Components

1. Identify slow equation sets ☑
2. Generate training data ☑
3. Train ANN surrogate ☑
4. Replace equation set with ANN surrogate ☑

Ongoing Work

Problems and what‘s next

Problems with Prototype
Training and use-case

- Simple models
  - Precise, but too slow
- Large models
  - Training difficult, maybe fast
  - Speed-up potential not as high as expected
- Finding use-cases:
  - Large non-linear systems not best-practice
  - Large non-linear loops hard to train

Student project: Sensitivity analysis used vars <-> iteration variables

Problems with Prototype
FMI Standard

- Using FMU’s to evaluate only a part of the equations
  - Not always allowed to call fmi2SetXXX in FMU state
  - Variable time is special, can’t use arbitrary values

    → Don’t rely on FMI / Create simpler runtime for strong components

Next Steps

- Improve net topology
- Improve training process
  - Linear interpolation as additional input to ANN
- Improve data generation
  - Less post-processing
- Publish results
  - Julia package NonLinearSystemNeuralNetworkFMU.jl

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Proper **H**ybrid **M**odels for **S**marter **V**ehicles

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Questions Remarks Comments

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