Accelerating Stiff Nonlinear Systems using Continuous Time Echo State Networks

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General, data-driven method to produce accurate surrogates

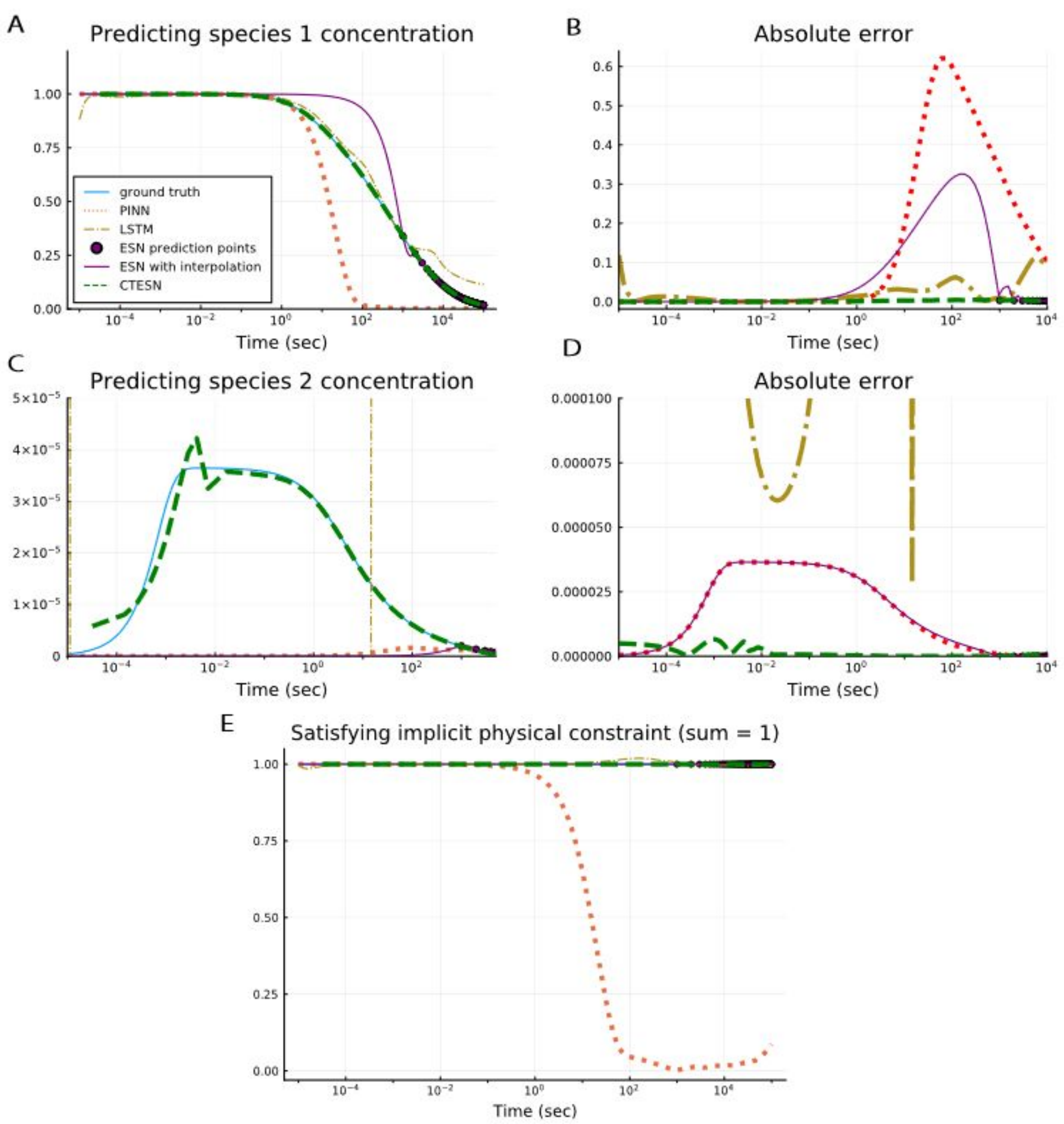
$$A \xrightarrow{0.04} B$$
$$B + B \xrightarrow{3\times10^7} C + B$$
$$B + C \xrightarrow{10^4} A + C$$

which lead to the ordinary differential equations:

$$\dot{y}_1 = -0.04y_1 + 10^4 y_2 \cdot y_3 \quad (6)$$
$$\dot{y}_2 = 0.04y_1 - 10^4 y_2 \cdot y_3 - 3 \cdot 10^7 y_2^2 \quad (7)$$
$$\dot{y}_3 = 3 \cdot 10^7 y_2^2 \quad (8)$$

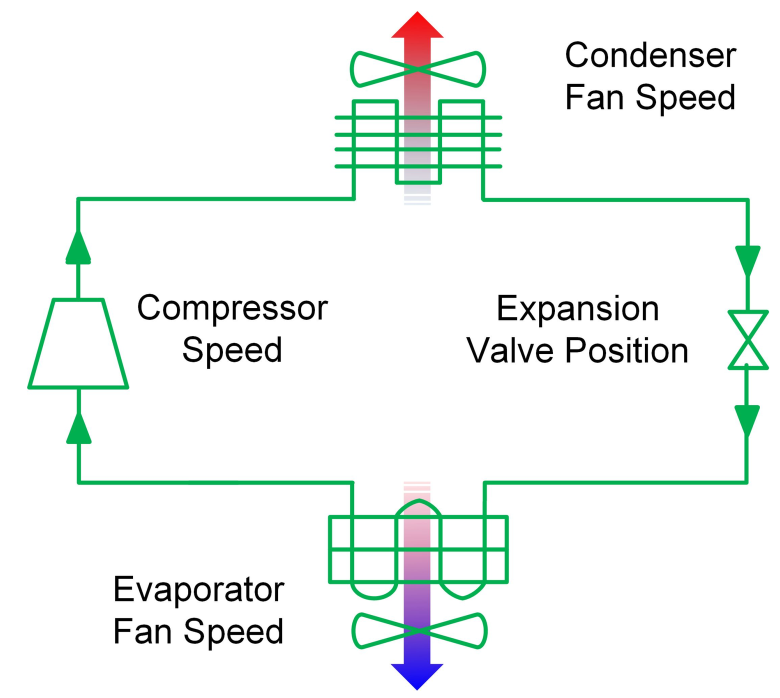
Robertson's equations:
Classic stiff problem with **slow reactions and fast transients in the same system**. Time constant scale of separation = 10^9.

Breaks many existing surrogate model methods.



Comparison of Physics Informed Neural Networks vs (Discrete) Echo State Networks vs CTESN on Robertson's Equations -
CTESNs are able to capture both slow and fast transients, improving on the current state of the art.
CTESN uses infromation from the ODE solver during training, which enables it to capture multi-scale dynamics

Scales to real world systems

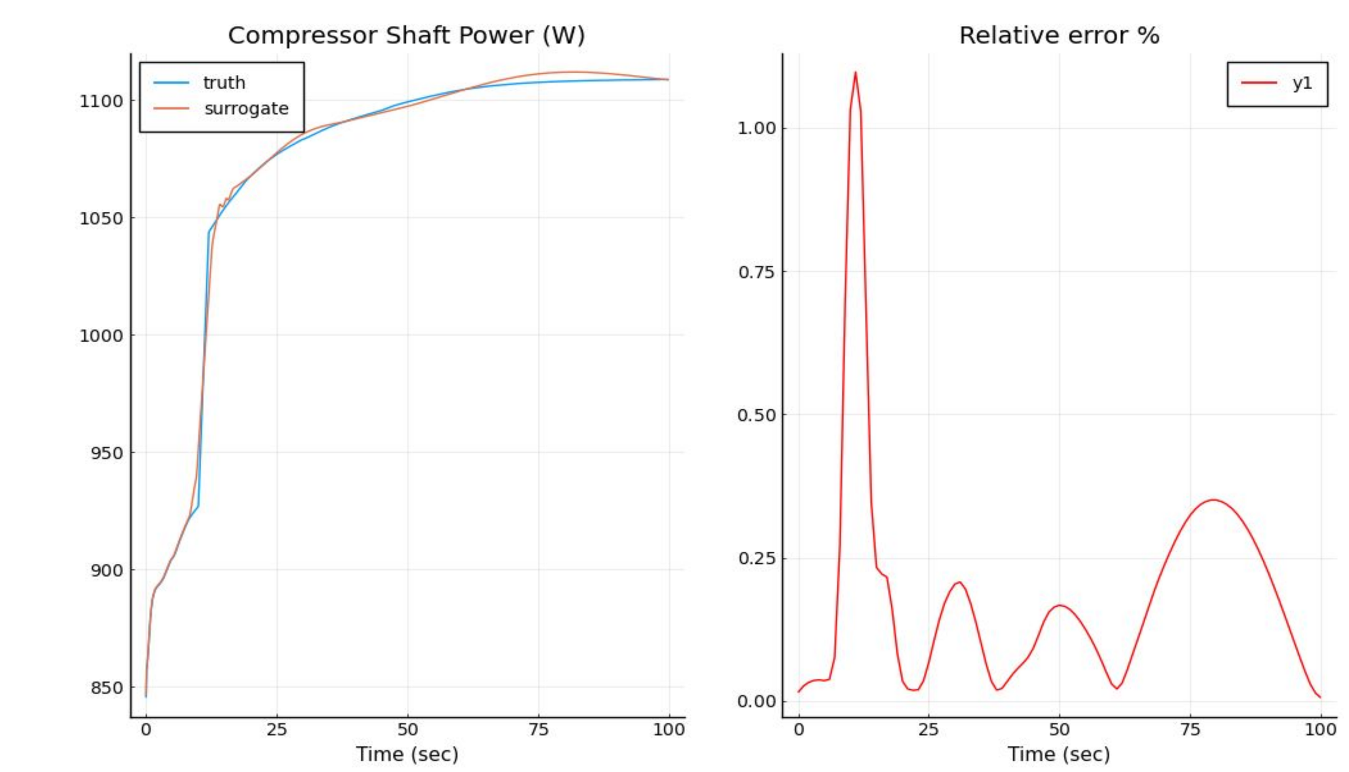


8,134 equation vapor-compression cycle model

The Julia implementation is 6x faster than Dymola for the full cycle simulation.

- `Dymola reference model: 35.3 s`
- `Surrogate model: 0.06 seconds.`

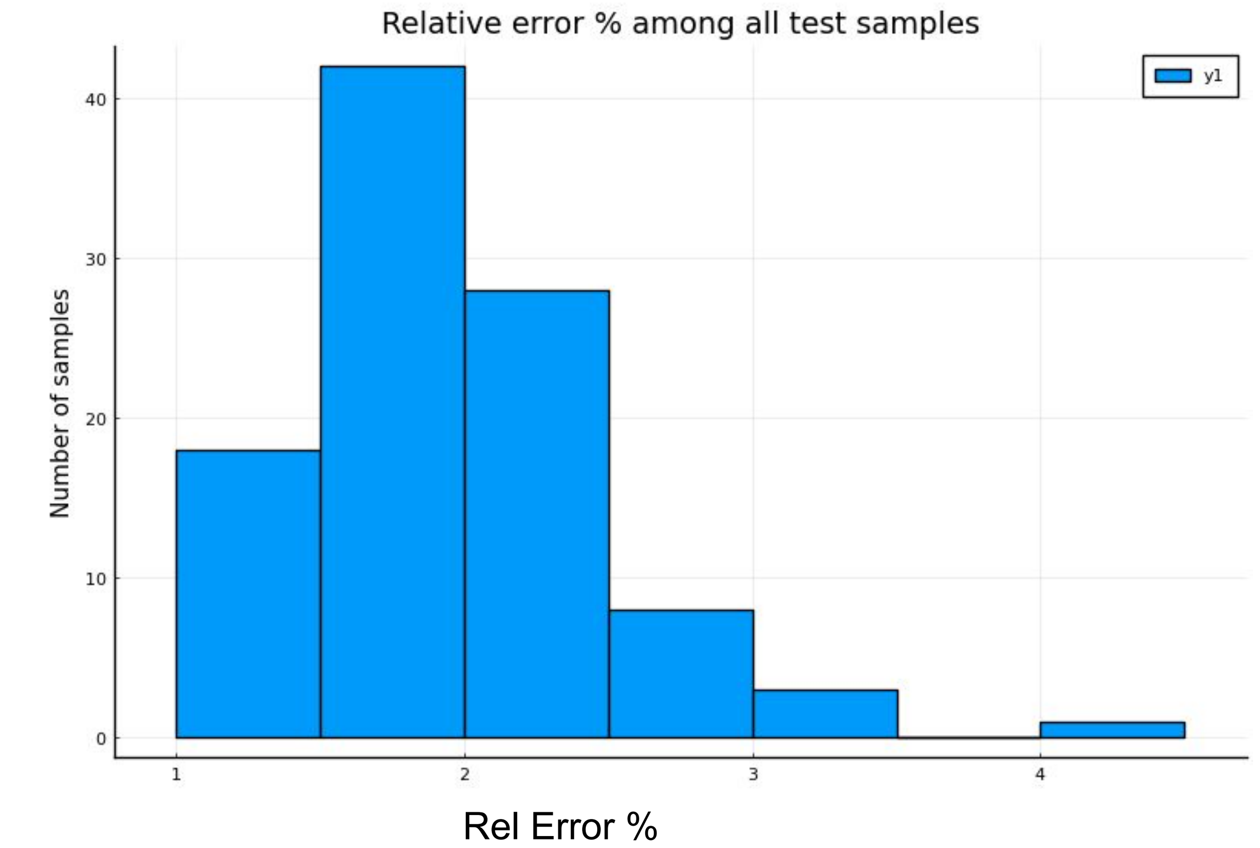
Speedup = 570x , error is < 5%.



(Above) Predicted time series for a given output quantity at a test point.

(Below) Max relative errors across time series for all output quantities at a test point.

No.	Output	Error (%)	No.	Output	Error (%)
1	Compressor inlet pressure	0.788	9	Condenser heat flow rate	0.792
2	Compressor outlet pressure	0.732	10	Evaporator heat flow rate	2.28
3	LEV inlet pressure	0.811	11	Coefficient of Performance	0.281
4	LEV outlet pressure	0.378	12	Condenser outlet air temperature	0.009
5	LEV outlet specific enthalpy	2.65	13	Evaporator outlet air temperature	0.002
6	Compressor refrigerant mass flow rate	2.21	14	Compressor power consumption	1.097
7	LEV refrigerant mass flow rate	1.839	15	Compressor inlet specific enthalpy	1.858
8	Evaporator superheat temperature	2.33	16	Compressor outlet specific enthalpy	1.978



Reliability of surrogate through entire parameter space. Predictions were made at 100 sample test points from throughout parameter space and then average relative error across output quantities was calculated for each test.

Deploy to accelerate optimization and coupled simulations

Given a cartesian input space P, we can generate the following surrogate equations using the ModelingToolkit package.

The CTESN works by predicting projections from a non-stiff differential equation, which is faster to simulate. We can deploy the surrogate by generating the non-stiff differential equation given below and embed a prediction in a larger code base

$$r' = f(Ar + W_{fb}x(p^*, t)) \quad (5.1)$$
$$x(t) = g(W_{out}(p)r(t)) \quad (5.2)$$

where $p^* \in P$ is a fixed parameter, A and W_{fb} are fixed matrices, and $W_{out}(p)$ is a learned projection function determined by the training process.

The surrogate may be deployed as a component of a larger system, reducing the O(N^3) cost of computation of stiff dynamical systems.

References

Anantharaman, Ranjan, et al. "Accelerating Simulation of Stiff Nonlinear Systems using Continuous-Time Echo State Networks." *arXiv preprint arXiv:2010.04004* (2020).

Ma, Yingbo, et al. "ModelingToolkit: A Composable Graph Transformation System For Equation-Based Modeling." *arXiv preprint arXiv:2103.05244* (2021).