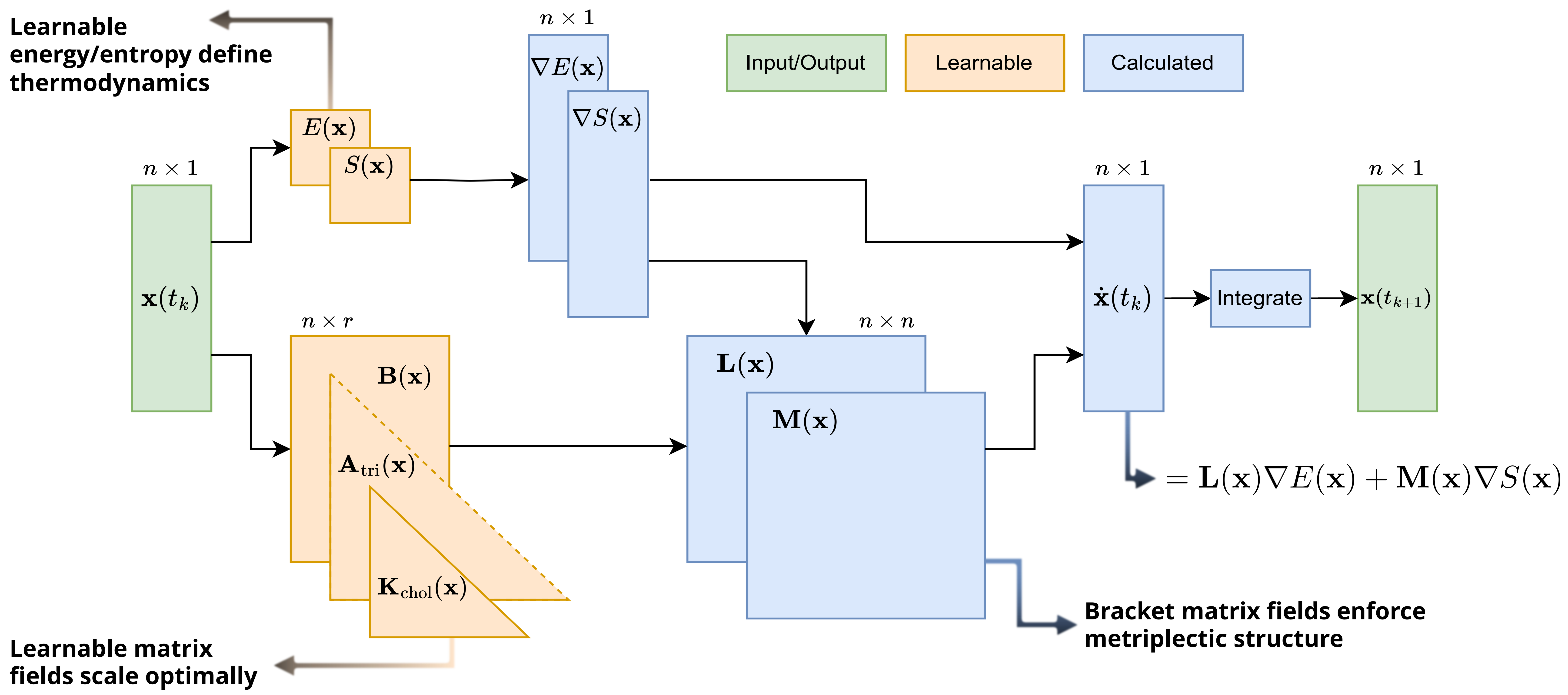
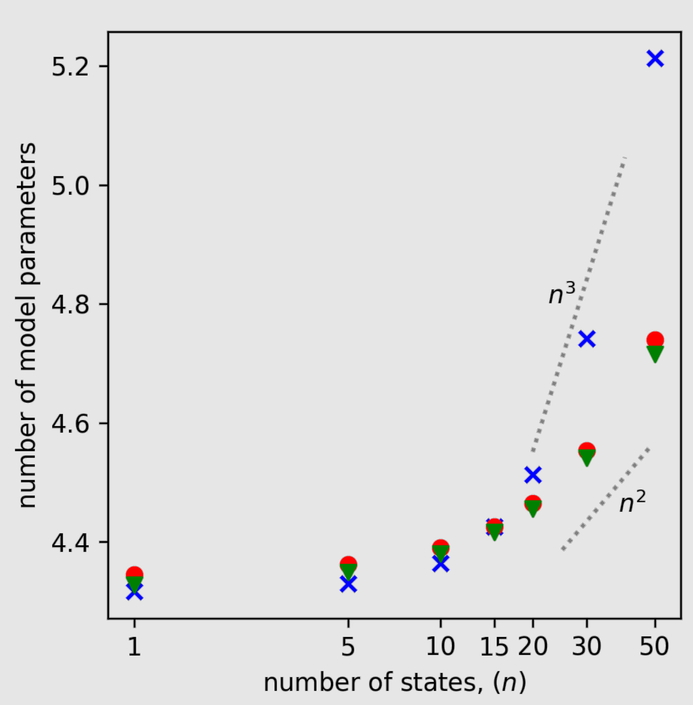
Efficiently Parameterized Neural Metriplectic Systems

Anthony Gruber[1], Kookjin Lee[2], Haksoo Lim[3], Noseong Park[4], Nathaniel Trask[5]

Given simulated or experimental data, infer a metriplectic model which **respects fundamental thermodynamic principles**.

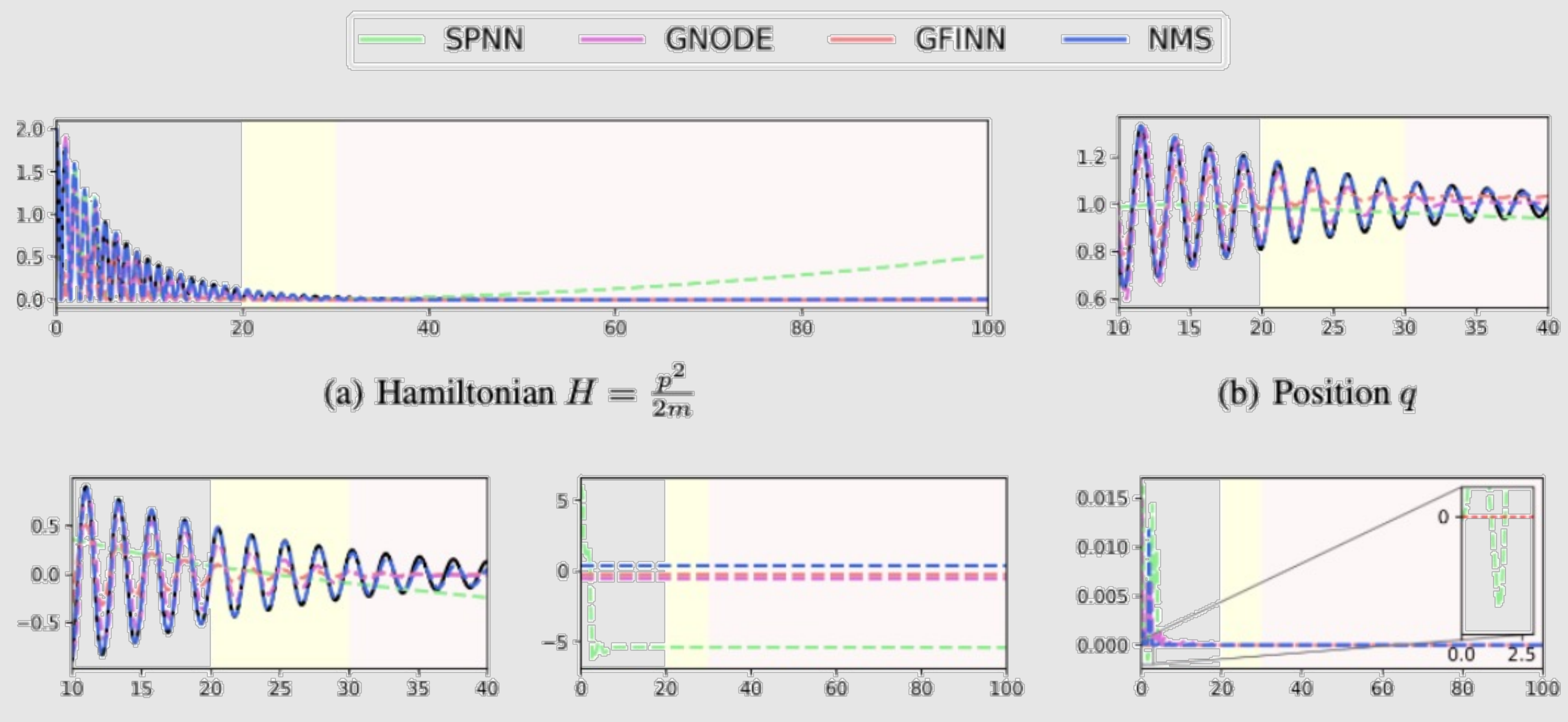
- Guaranteed energy conservation and entropy generation laws.
- Universal approximation properties.
- Rigorous bounds on generalization error.
- Better predictive performance.





Our method (NMS) exhibits better predictive performance at reduced cost.

Optimal (quadratic) scaling in the number of states (n) is retained.



(a) Hamiltonian $H = \frac{p^2}{2m}$ (b) Position q (c) Momentum p (d) Energy $E = H + \sum_i E_i$ (e) Instantaneous Entropy $\dot{S}$

How this works: *Exterior algebra*

- Metriplectic structure parameterized via multivector fields with symmetries.
- Energy conservation and entropy generation guaranteed **independent of training quality.**

Check out our paper here!

adgrube@sandia.gov

https://www.agrubertx.github.io

Provable guarantees on network performance

- Universal approximation of any nondegenerate metriplectic system.
- Computable *a posteriori* error estimate bounding generalization error in time.

$$\left(\int_0^T |\mathbf{x} - \tilde{\mathbf{x}}|^2 \, dt\right)^{\frac{1}{2}} \leq \varepsilon \left|\frac{b}{a}\right| \sqrt{e^{2aT} - 2e^{aT} + T + 1},$$

Rigorous statements on energy/entropy stability and learnable conservation laws.

Well-behaved and **stable** feature propagation.

Better data efficiency, interpretability, and **predictive performance.**

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

SAND2025-03078C

[1]Sandia National Laboratories
[2]Arizona State University
[3]Yonsei University
[4]Korea Advanced Institute of Science and Technology
[5]University of Pennsylvania