

# A Generalized Framework of Neural Networks for Hamiltonian Systems

Philipp Horn<sup>1</sup>, Veronica Saz Ulibarrena<sup>2</sup>, Barry Koren<sup>1</sup>, Simon Portegies Zwart<sup>2</sup>

<sup>1</sup>) Eindhoven University of Technology, Centre for Analysis, Scientific Computing and Applications (CASA), PO Box 513, 5600 MB Eindhoven, Netherlands  
p.horn@tue.nl

<sup>2</sup>) Leiden University, Leiden Observatory, PO Box 9513, 2300 RA Leiden, Netherlands

When solving Hamiltonian systems using numerical integrators, preserving the symplectic structure is crucial [4]. At the same time, solving chaotic problems requires integrators to approximate the trajectories with extreme precision. This can be very computationally expensive. However, for example in [1] it was shown that a neural network can be a viable alternative to numerical integrators. Offering high accuracy solutions for the chaotic N-body problem many orders of magnitudes faster.

To understand when it is useful to add physics constraints into neural networks, we analyze three well-known neural network topologies that include a symplectic structure inside the NN architecture [3, 6, 2]. Between these neural network topologies many similarities can be found [5]. This allows us to formulate a generalized framework for these topologies. With the new framework, we can find novel topologies by transitioning between the established ones.

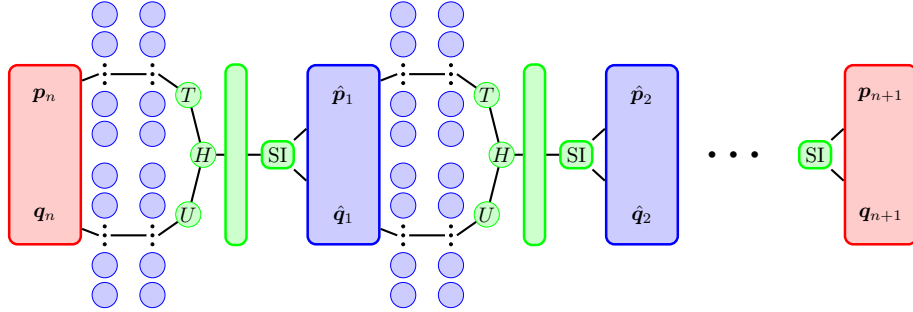


Figure 1: A visualization of the generalized framework of neural networks for Hamiltonian systems. (GHNN)

We compare these new Generalized Hamiltonian Neural Networks (GHNN) against the already established SympNets and HénonNets and physics-unaware multilayer perceptrons. This comparison is performed with data from a pendulum, a double pendulum and a gravitational three-body problem. A special focus lies on the generalization capabilities outside the training data. We found that the GHNN outperforms all other neural network architectures.

## References

- [1] P.G. Breen, C.N. Foley, T. Boekholt and S. Portegies Zwart, 2020. Newton versus the machine: solving the chaotic three-body problem using deep neural networks, *Monthly Notices of the Royal Astronomical Society*, Vol. **494**, pp. 2465-2470.
- [2] J. Burby, Q. Tang and R. Maulik, 2021. Fast neural Poincaré maps for toroidal magnetic fields, *Plasma Physics and Controlled Fusion*, Vol. **63**.
- [3] Z. Chen, J. Zhang, M. Arjovsky and L. Bottou, 2020. Symplectic Recurrent Neural Networks, *Proceedings of the 8th International Conference on Learning Representations*.
- [4] E. Hairer, C. Lubich and G. Wanner, 2006. Geometric Numerical Integration - Structure-Preserving Algorithms for Ordinary Differential Equations, Springer Berlin.
- [5] P. Horn, V. Saz Ulibarrena, B. Koren and S. Portegies Zwart, 2022. Structure-Preserving Neural Networks for the N-body Problem, *Proceedings of ECCOMAS*.
- [6] P. Jin, Z. Zhang, A. Zhu, Y. Tang and G.E. Karniadakis, 2020. SympNets: Intrinsic structure-preserving symplectic networks for identifying Hamiltonian systems, *Neural Networks*, Vol. **132**, pp. 166-179.