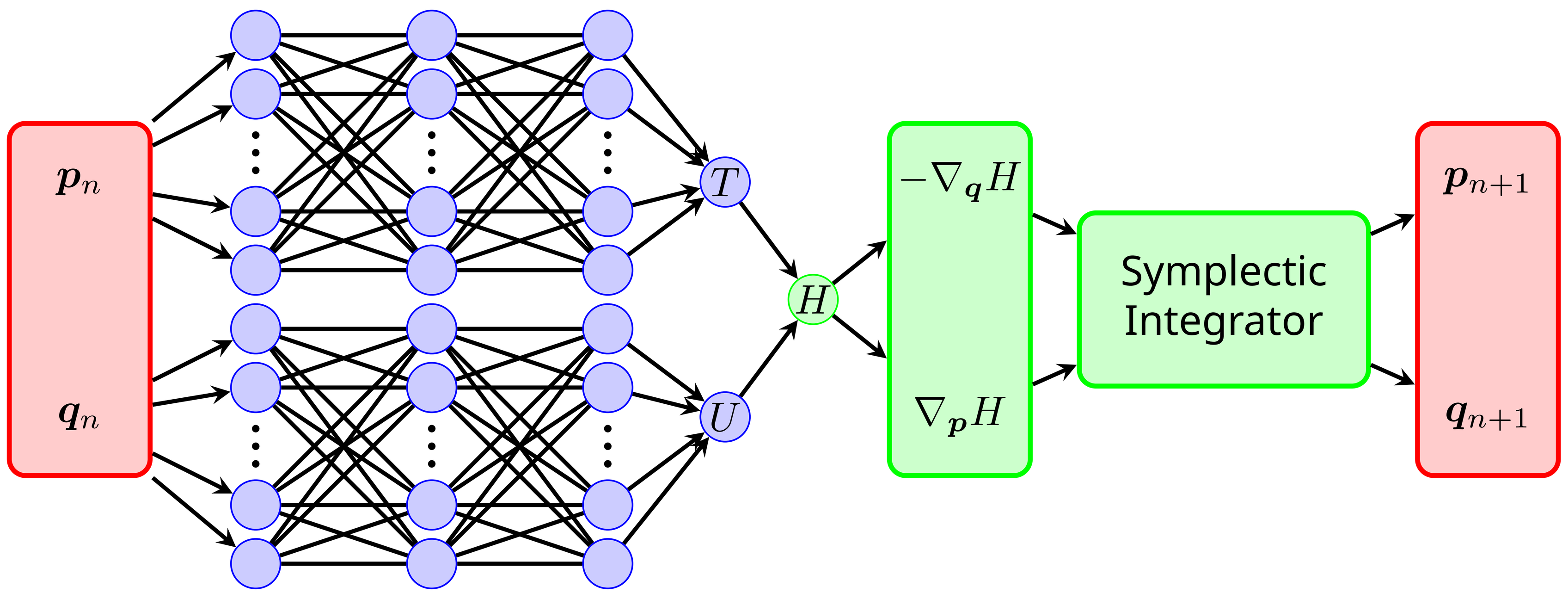
A Generalized Framework of Neural Networks for Hamiltonian Systems (GHNN)

Philipp Horn and Barry Koren (Eindhoven University of Technology)
Veronica Saz Ulibarrena and Simon Portegies Zwart (Leiden Observatory)

Symplectic Recurrent Neural Networks by Chen *et al.* [1]

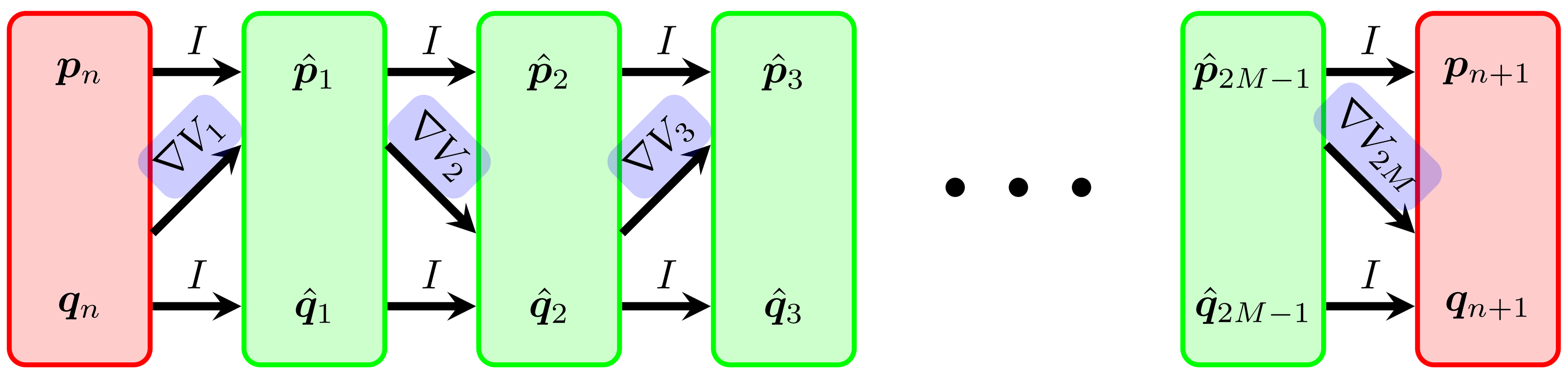
SRNNs can be used to predict trajectories of Hamiltonian systems by learning their flow map. They learn a separable Hamiltonian and embed a symplectic numerical integrator inside their topology.



Schematic of a Symplectic Recurrent Neural Network.

SympNets by Jin *et al.* [2]

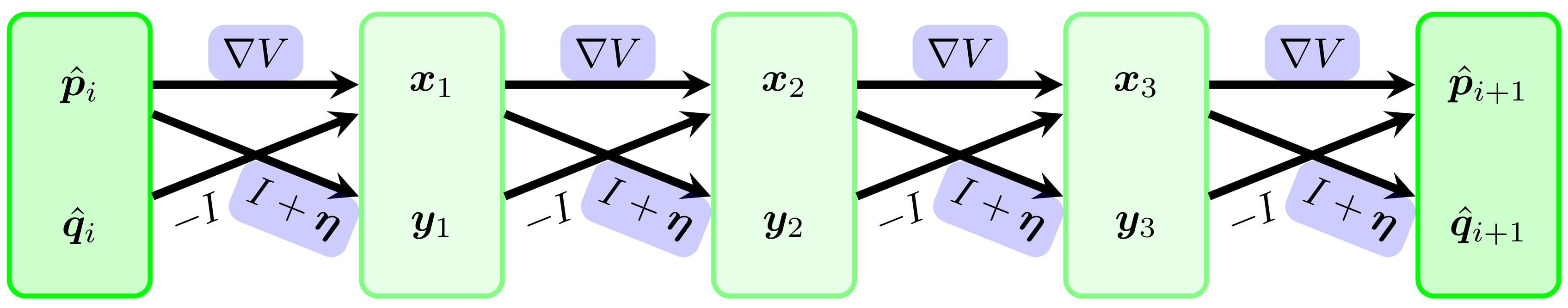
Alternatively, SympNets directly focus on learning any symplectic map, like the flow map of a Hamiltonian system, without the need to learn a separable Hamiltonian. This is achieved by learning unit triangular updates.



Schematic of a SympNet.

HénonNets by Burby *et al.* [3]

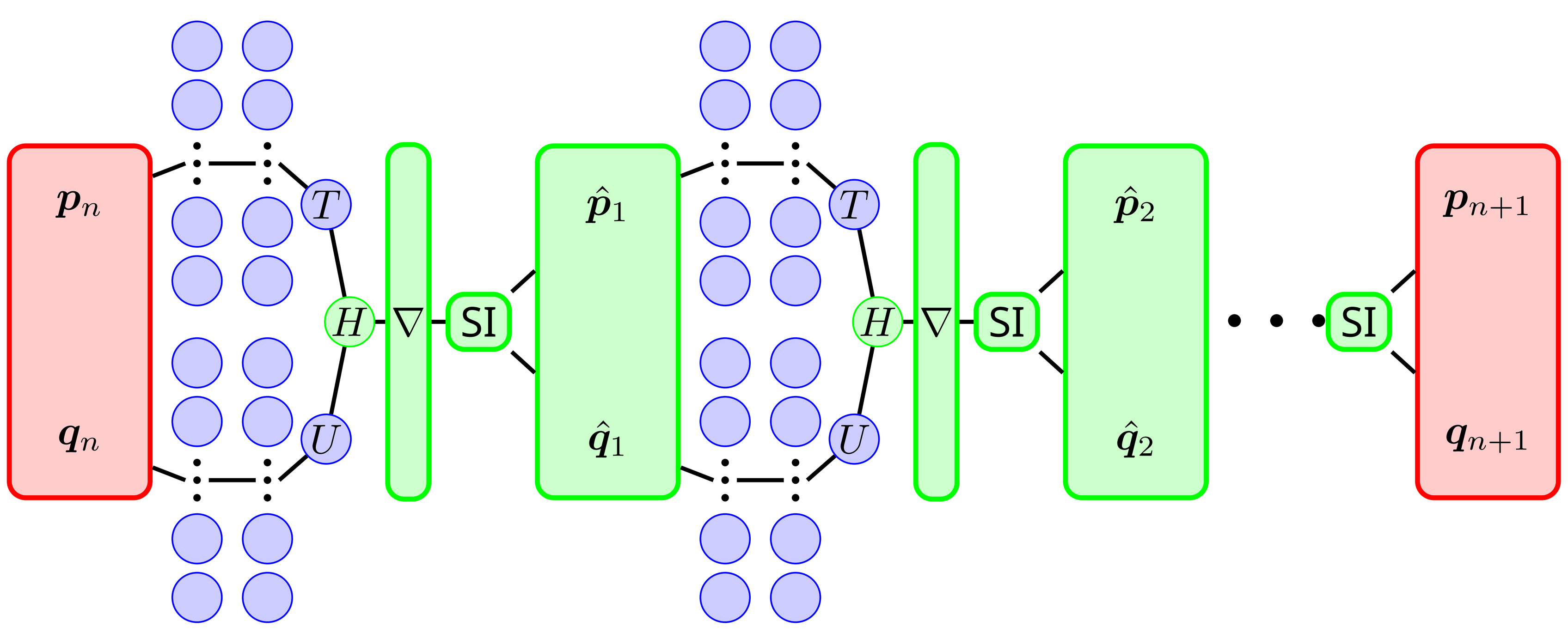
Also, a HénonNet directly focuses on learning symplectic maps by concatenating multiple so-called Hénon layers, based on Hénon-like map.



Schematic of a single Hénon layer.

Generalized Hamiltonian Neural Networks

A general framework of NNs for Hamiltonian systems can be introduced. This framework includes SRNNs, SympNets and HénonNets as edge cases. The more flexible framework allows the creation of NNs that are superior to SRNNs, SympNets and HénonNets.

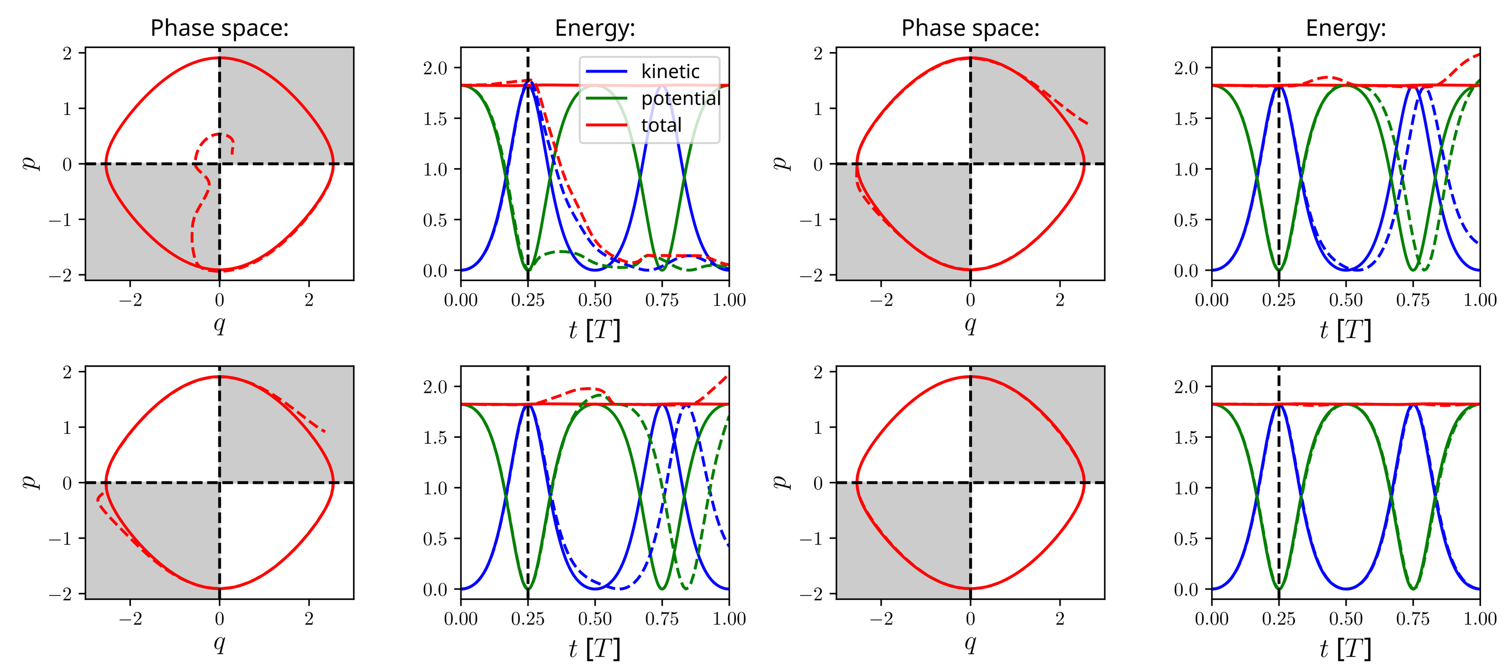


Schematic of a Generalized Hamiltonian Neural Network that is not an SRNN, SympNet or HénonNet.

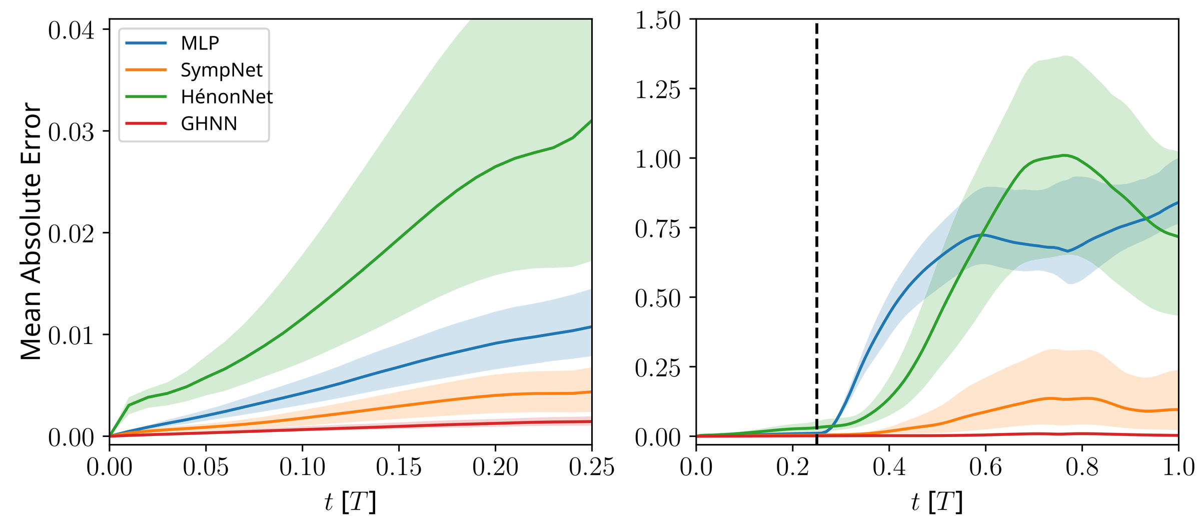
Numerical Experiments

The performance of the different NN architectures is analyzed using data of three different Hamiltonian systems. While the NNs are only trained on data until a certain cut-off, they are used to predict for longer times.

The single Pendulum

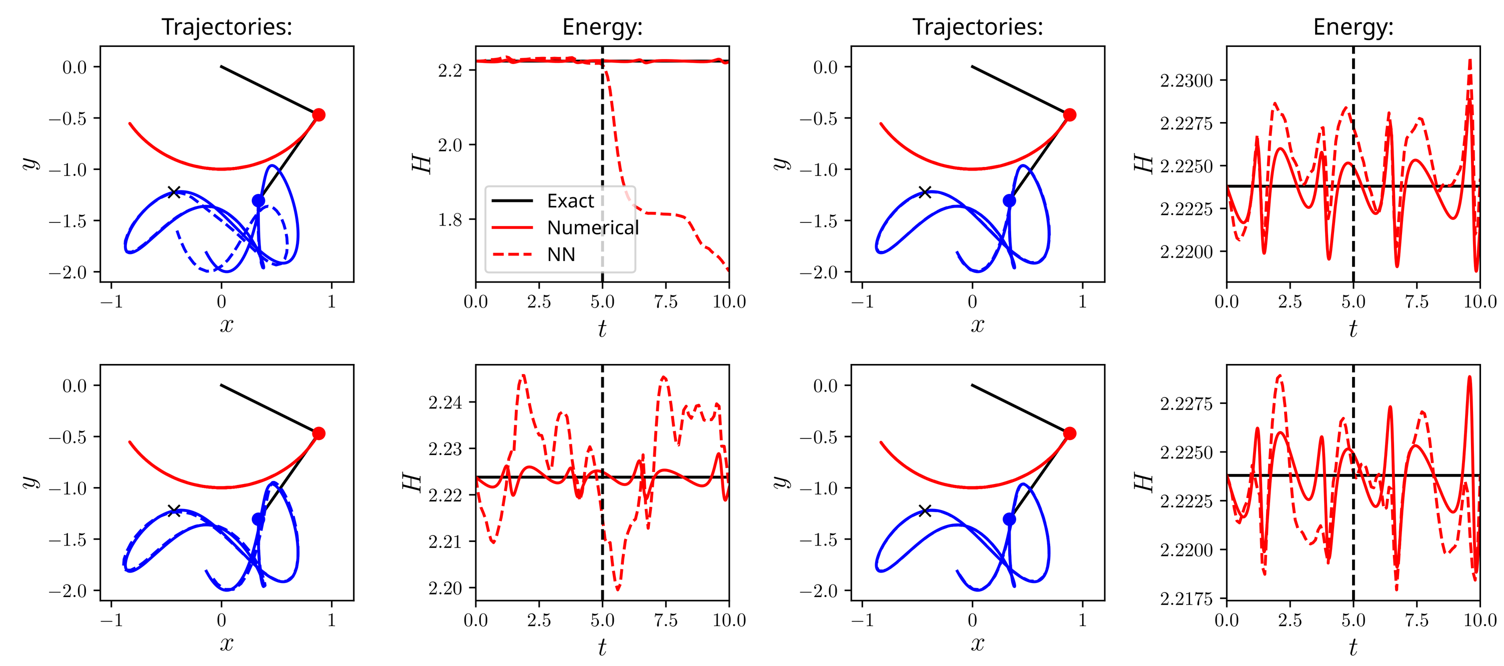


MLP, SympNet, HénonNet and GHNN (left-to-right then top-to-bottom).



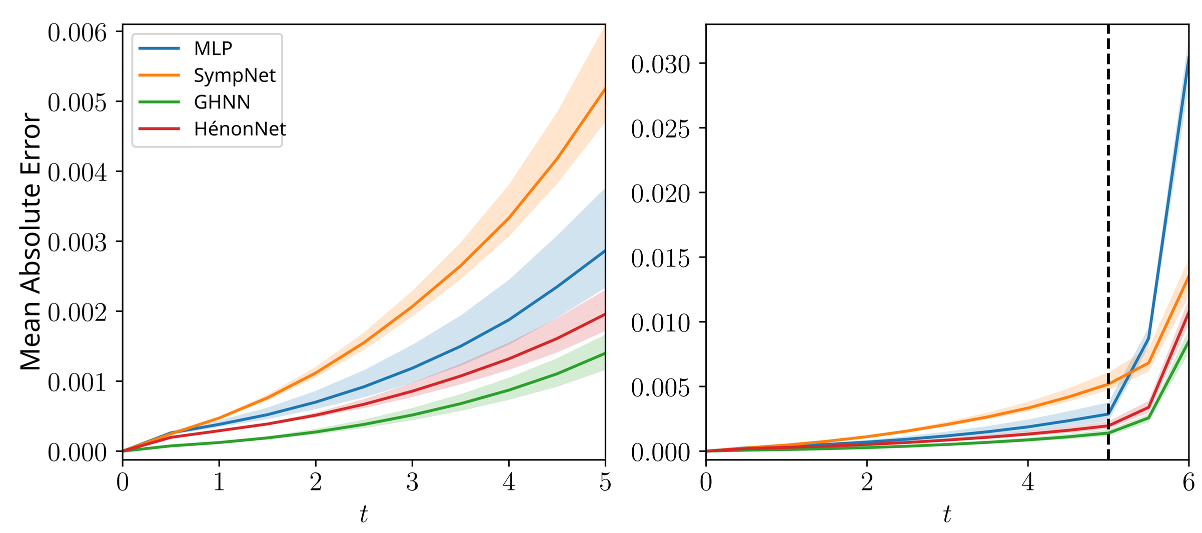
MAE inside the training data range and outside (after dashed line).

The double Pendulum



MLP, SympNet, HénonNet and GHNN (left-to-right then top-to-bottom).

The 3-body Problem



MAE inside the training data range and outside (after dashed line).

Not every symplectic NN is necessarily more accurate than a physics-unaware MLP. However, they are all more stable outside the training data. GHNNs consistently outperform all other NNs.

References

[1] Z. Chen *et al.*, Symplectic recurrent neural networks, *8th International Conference on Learning Representations*, ICLR, 2020.

[2] P. Jin *et al.*, SympNets: Intrinsic structure-preserving symplectic networks for identifying Hamiltonian systems, *Neural Networks*, Vol. **132**, 2020.

[3] J. Burby *et al.*, Fast neural Poincaré maps for toroidal magnetic fields, *Plasma Physics and Controlled Fusion*, Vol. **63**, 2021.

Mathematics and Computer Science