Learned simulators that satisfy the laws of Thermodynamics

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ICLR 2021 Workshop
Deep Learning for Simulation (simDL)

We learn physics from data…

- When data refer to phenomena that conserve some quantities (typically, energy), it is easy to enforce this conservation.
- This can be done by enforcing the symplectic (Hamiltonian) structure of the dynamics:

$$\frac{dz}{dt} = \boldsymbol{L}\frac{\partial E}{\partial z},$$

with E the energy of the system and $\boldsymbol{L}$ the symplectic (Poisson) matrix.
- But, how to proceed with dissipative phenomena?

… while enforcing the right thermodynamic structure

- This can be done by enforcing a metriplectic structure on the dynamics:

$$\frac{dz}{dt} = \boldsymbol{L}\frac{\partial E}{\partial z} + \boldsymbol{M}\frac{\partial S}{\partial z}.$$

- with $\boldsymbol{L}$ skew-symmetric and $\boldsymbol{M}$ symmetric, positive semi-definite.
- An additional constraint is necessary (*degeneracy conditions*):

$$\boldsymbol{L}\frac{\partial S}{\partial z} = \boldsymbol{M}\frac{\partial E}{\partial z} = \boldsymbol{0}.$$

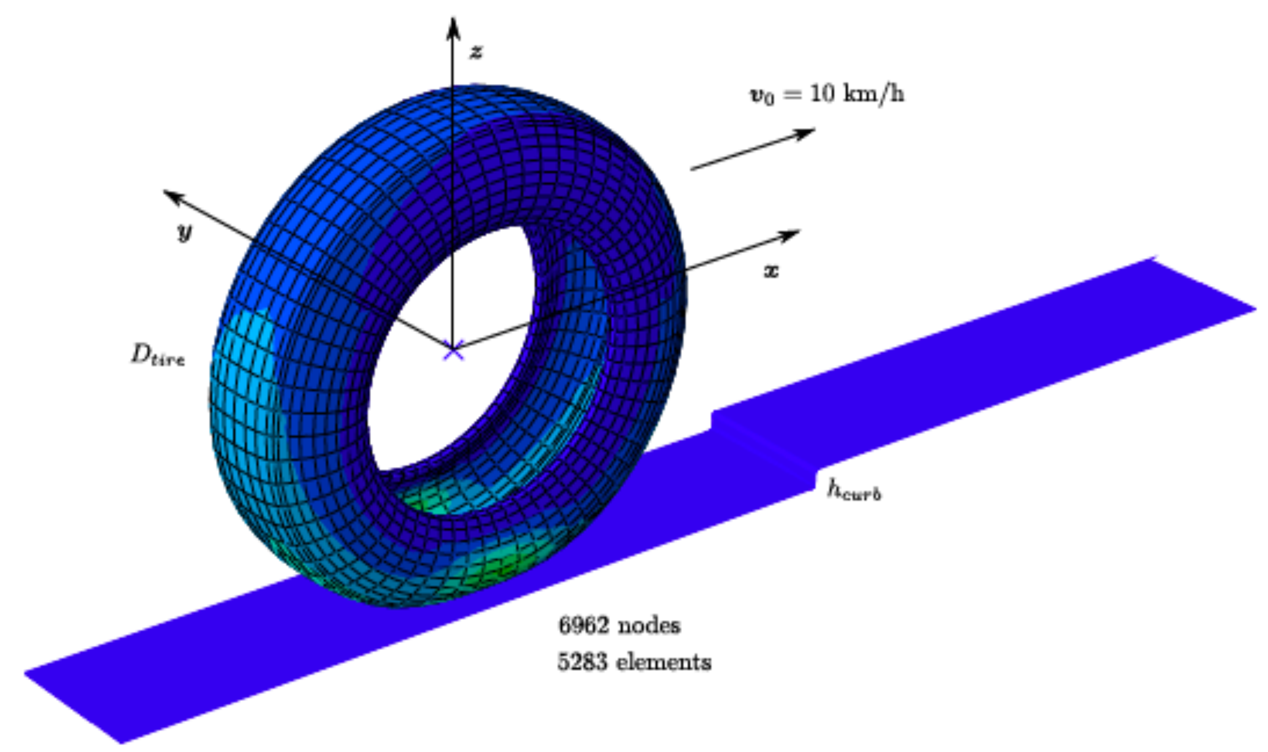
- This ensures the fulfillment of the first and second principles of thermodynamics.
- This is the so-called GENERIC formalism (Grmela and Oettinger, 1997).
- We augment the loss function with the fulfillment of the degeneracy conditions:

$$\mathcal{L}_n^{\text{degen}} = ||\mathsf{L}_n \cdot \mathsf{DS}_n||_2^2 + ||\mathsf{M}_n \cdot \mathsf{DE}_n||_2^2.$$

- Together with error and regularization terms, gives rise to

$$\mathcal{L}^{\text{SPNN}} = \frac{1}{N_{\text{train}}}\sum_{n=0}^{N_{\text{train}}}(\lambda_d^{\text{SPNN}}\mathcal{L}_n^{\text{data}} + \mathcal{L}_n^{\text{degen}}) + \lambda_r^{\text{SPNN}}\mathcal{L}^{\text{reg}}.$$

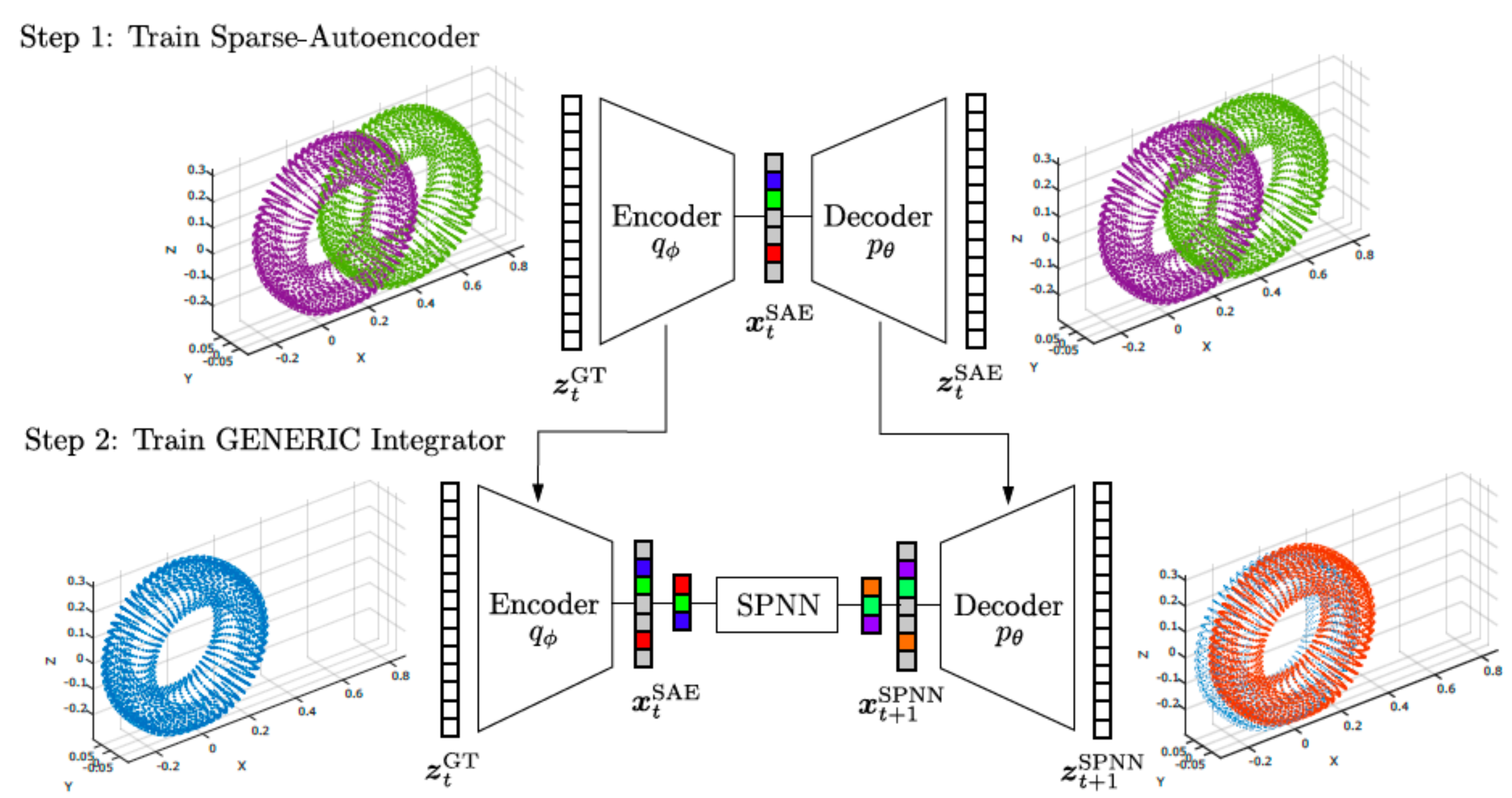
Example: tire facing a step



- As a proof-of-concept, we consider the problem of a non-linear, viscous-hyperelastic tire facing a step.
- Pseudo-data are taken from high-fidelity simulations.

Architecture of the network

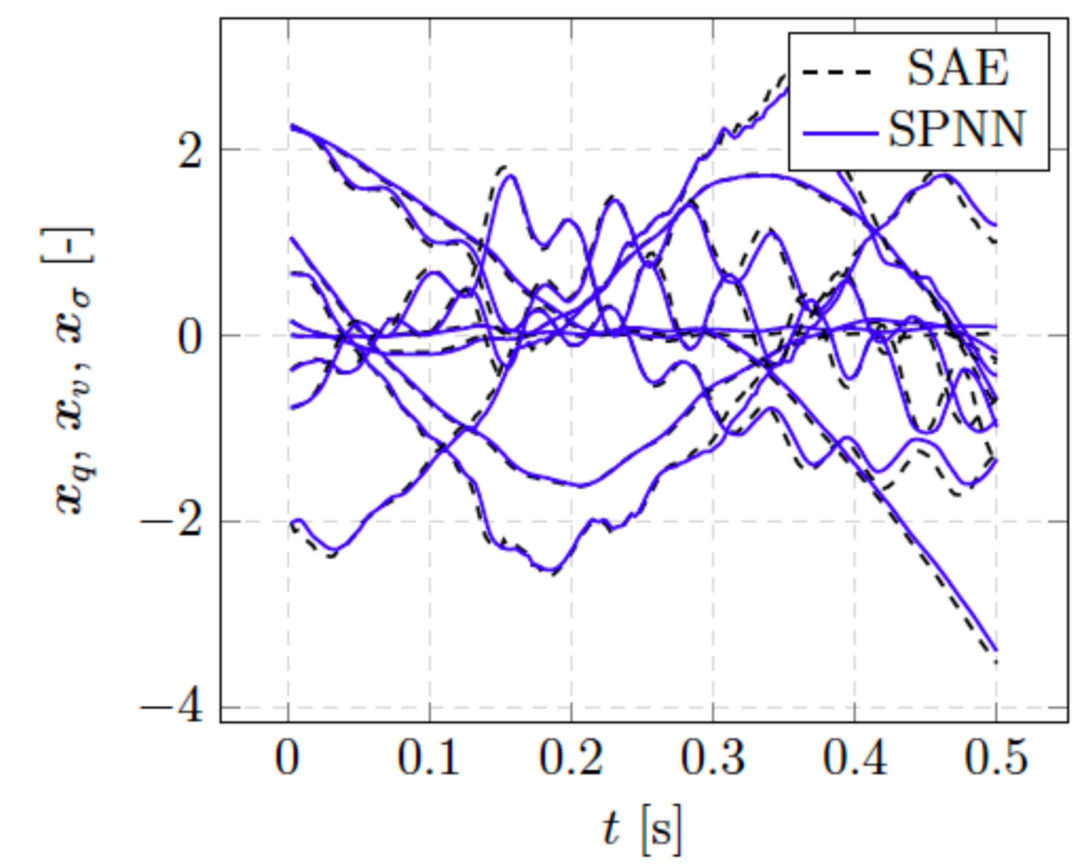
- We first unveil the intrinsic dimensionality of data with a sparse autoencoder (step 1).



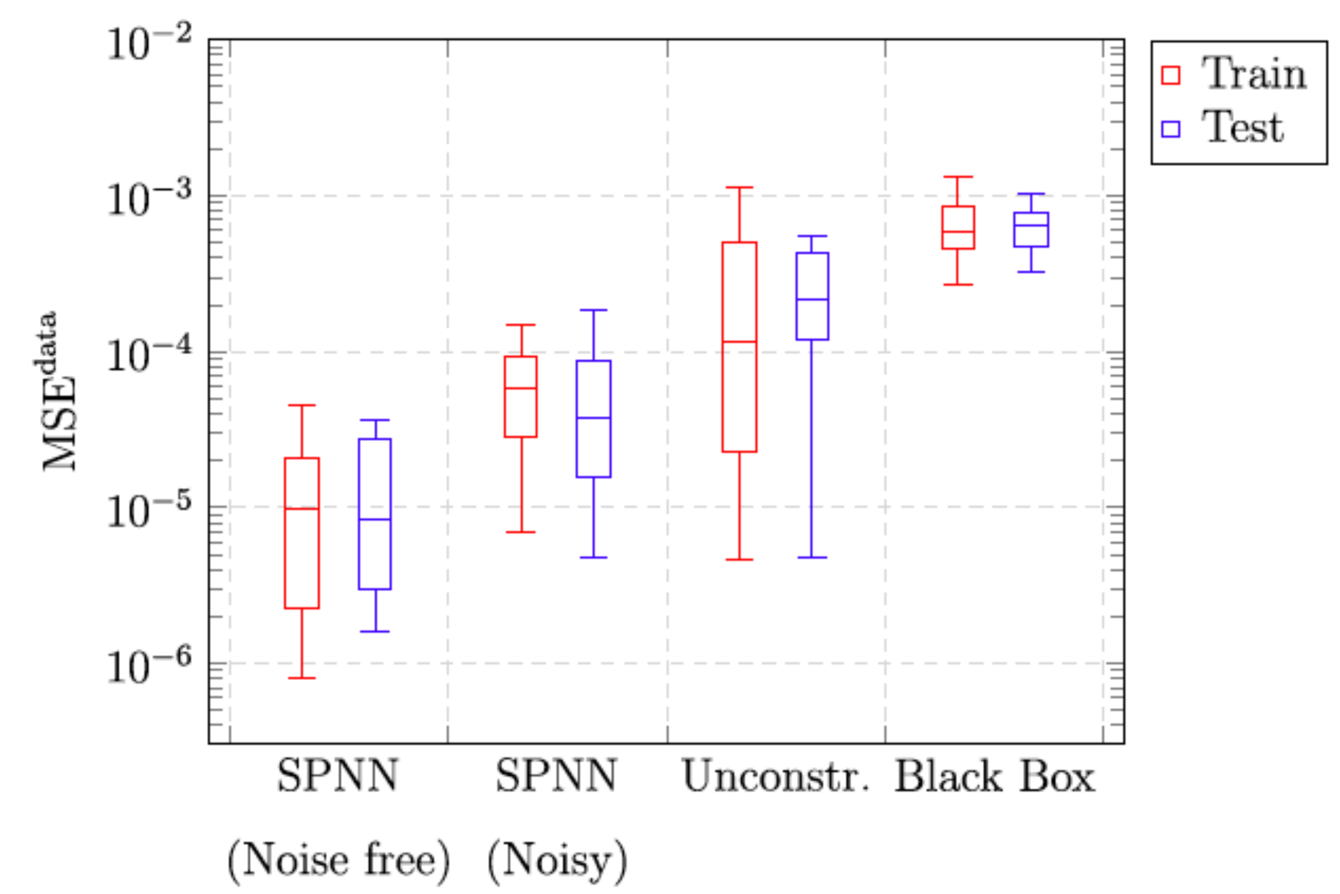
- We then learn a ***structure-preserving neural network*** (SPNN) on these low-dimensional data (step 2).
- This SPNN behaves as an energy-entropy-momentum integrator.
- Given the (low-dimensional) variables x at time t, it produces x at time $t+1$.

Results

- Error $\mathcal{O}(10^{-4})$ with only 9 dofs, compared with the original 49680 dofs.



- The more physics you enforce, the more accurate results you obtain and the less data you will need:



References

Miroslav Grmela and Hans Christian Oettinger. Dynamics and thermodynamics of complex fluids. I. Development of a general formalism. In: Physical Review E, 56(6):6620, 1997.

Q. Hernandez, A. Badias, D. Gonzalez, F. Chinesta, E. Cueto. Structure-preserving neural networks. In: Journal of Computational Physics, Volume 426, 109950, 2021.

Quercus Hernandez, Alberto Badias, David Gonzalez, Francisco Chinesta, Elias Cueto. Deep learning of thermodynamics-aware reduced-order models from data. In: Computer Methods in Applied Mechanics and Engineering, accepted for publication, 2021.

Drafts and links to GitHub of the project:

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