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ON THE EMPLOY OF INDUCTIVE BIASES FOR THE DEVELOPMENT OF LEARNED SIMULATORS

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Learned simulators are interesting due to their cheap (online) computational cost, and their excellent performance for many-query and real time problems. However, it is well known that neural networks often behave like a black box, are sensitive to noise and often show biased results.

Recently, the use of inductive biases—those that indicate the network how to proceed in unseen situations—has gained popularity. For instance, if the physics under analysis shows any type of conservative character (typically, conservation of energy), Lagrangian or Hamiltonian formalisms can be employed as inductive biases, thus ensuring by construction that they will be fulfilled.

In this work we study and compare several options for the construction of useful inductive biases. For problems showing dissipation, we employ metriplectic formalisms, that combine a Hamiltonian part so as to impose conservation of energy in closed systems with non-negative entropy production. Similarly, to cope with geometric symmetries, we employ graph-neural networks. Results will be presented that show the advantages of both types of biases.

REFERENCES

[1] Deep learning of thermodynamics-aware reduced-order models from data. Quercus Hernandez, Alberto Badias, David Gonzalez, Francisco Chinesta, Elias Cueto. Computer Methods in Applied Mechanics and Engineering, Volume 379, 113763, 2021.

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