

CEMRACS 2023 mini-project proposal

Title: Interpretable data-driven finite volume numerical flux for conservation laws

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1. Context

Since the explosive growth of machine learning methods in the 2010s, much work has been undertaken in order to build numerical methods integrating machine learning for hyperbolic PDEs. Examples include Ray, Discacciati and Hesthaven's work on the detection of oscillations [1] or the construction of artificial viscosities [2]. For more complex systems, such as those describing two-phase problems, it would be interesting to build new, less diffusive numerical fluxes to increase the accuracy of the numerical schemes.

A first approach, similar to [2], could be to learn the best among known fluxes, according to the local solution. However, this approach does not take stability into account, even though it is a critical property when simulating hyperbolic systems.

Another approach, proposed in [3, 4], is to learn by running the scheme over a large number of time steps, evaluating the recovered solution, and computing the gradient of the result with respect to the network weights. This approach is called « differentiable physics » and requires differentiating a composition of hundreds of functions within the scheme. This is made possible by robust machine learning libraries, such as PyTorch or Tensorflow. Work in progress [5] has shown that, in practice, this method enhances stability, but without any theoretical stability guarantees. In addition, such methods based on neural networks are unfortunately not interpretable.

2. Description and objectives

In this project, we propose to investigate a strategy to obtain, via machine learning, **new simple and interpretable numerical fluxes**. In addition, we could correct the obtained fluxes to ensure entropy stability. To ensure good numerical flux properties, such as consistency, we suggest **learning the viscosity matrix** rather than the whole flux.

To obtain new interpretable viscosities with good empirical stability properties, we propose to couple the differentiable physics approach with the SINDy method [6], rewriting this method under the framework of a neural network training. The SINDy approach consists in representing the numerical flux as a sparse linear combination of nonlinearities: **the end goal is therefore to obtain an interpretable formula for the numerical viscosity**. Once this approach has been validated, we wish to correct the viscosity matrix given by SINDy to obtain entropy inequalities, in the spirit of [7]. In the project, we will first test the approach on Burgers' equation, and then extend it to the shallow water equations, with or without source term.

3. Proposed methodology

We propose the following outline:

- 1) Write the scheme in the PyTorch framework with a classical viscosity or a neural network viscosity.
- 2) Learn a viscosity using a classical neural network, to validate the differentiable physics approach for the Burgers equation.
- 3) Replace the classical neural network by the SINDy approach, and learn a viscosity for Burgers' equation.
- 4) Extend the approach to the shallow water equations, and propose an entropy correction for the flux obtained for Burgers' equation.

4. Software requirements

To complete the project, the Python language and its PyTorch library will be used.

5. References

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