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Peer Review

# Review of: "Inverse Evolution Data Augmentation for Neural PDE Solvers"

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The focus of the article is on enriching the data sets; the context of the enrichment is to improve the training of neural operators. The neural operators are then used to approximate solutions of time-varying partial differential equations (PDEs). The novelty of the proposed approach is to use intuition from inverse processes to generate additional data efficiently from random initialisation to augment the original data.

The authors outline the computational burden in obtaining solutions of spatio-temporal PDEs and thereby situate their approach to addressing this problem. Previous and prevailing approaches utilise surrogate models and deep-learning neural networks to gain solutions rapidly; further, the authors indicate that neural operators are emerging as promising approaches to solve such PDEs. In these data-driven approaches, reliable and trusted training data is needed. In section 2, the authors briefly describe the neural operator training process, thereby situating their approach within the training process. Although the Inverse Evolution is succinctly described, the text around Eqs 3 and 4 is complex to follow. Perhaps adding a flow diagram to visualise the proposed scheme would help clarify the description.

The remaining part of Section 2 develops the Data Generation and Initialisation schemes, with a brief, but sufficient, introduction to the high-order schemes for inverse evolution. The discussions on the authors' Inverse Evolution and the Original Evolution help to summarise the benefits of the approach. Two additional cases are described; viz. a) schemes for dealing with sharp interfaces, and b) the potential benefits of pseudo-spectral over the finite difference methods for spatial discretisation.

In section 3, the authors compare and contrast their methods on four case studies (the heat diffusion equation, the Burger's equation, the Allen-Cahn equation, and the Navier-Stokes equation). The Viscous Burger's equation is of particular interest because at small values of the diffusion coefficient, the solution


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of the equation exhibits sharp (discontinuous) shock solutions. Table 3 shows that the proposed methods are able to provide accurate solutions, even in this case.

Questions arising:

1. On page 7, the authors introduce the constants $\lambda_j$ and $C$ to create a large number of initialisations with a small set of original data points. How are the values of these determined?
2. On page 12, the authors state that spatial discretisation methods include finite
difference, finite element, finite volume, and spectral methods (including the pseudo-spectral methods). How does one choose which method to use for a particular PDE? Is there a pattern emerging on when to use the finite X approaches and when to use the pseudo-spectral approach? Or is this a topic for further work?
3. How are uncertainties in the data accounted for in the inverse evolution approach? This may be relevant when the original data is obtained, for example, through physical experiments or through in-service sensors (i.e., data for some aspect of a "digital twin").

## Declarations

**Potential competing interests:** No potential competing interests to declare.