Stabilizing PDE—ML Coupled Systems

Pacific Northwest NATIONAL LABORATORY

Scientific Achievement

- Studied the mechanisms underlying instabilities in PDE—ML coupled systems and proposed strategies for stabilizing them while maintaining their accuracy

Significance and Impact

- PDE-ML coupled systems combine physically accurate models with ML surrogates but are notoriously unstable when solved numerically.
- By studying a prototype problem that exhibits similar behavior, we explore strategies for stabilizing it and improving its accuracy.
- Similar approaches can be applied to more complex systems, thus enabling the replacement of computationally expensive parameterizations by ML surrogates.

Technical Approach

- Replacing the diffusion term in the viscous Burgers' equation by a feedforward network leads to an unstable system; this is because of *spectral bias*, the inability of neural networks to adequately learn high frequencies: the learnt diffusion term cannot suitably damp the high frequencies created by the convective term.
- Applying a low-pass filter to the nonlinear term prevents the cascade of energy to high-frequency modes, effectively yielding a stable low resolution Galerkin treatment (Fig 1).
- We complement this with memory terms suggested by the *Mori-Zwanzig identity*: these are convolutions over time of values of the resolved variables with memory kernels, and whose accurate calculation helps correct the low-resolution solutions (Fig 2).

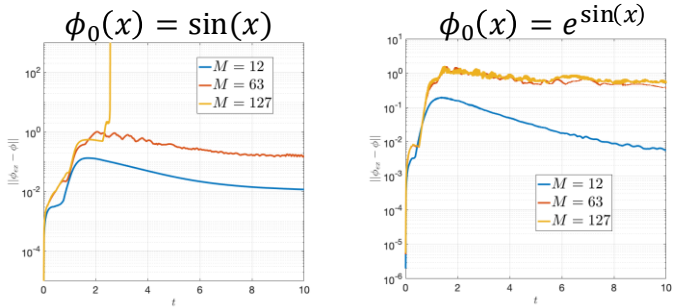

Figure 1: Error evolution while applying low-pass filters at varying thresholds M to the convective term. Observe that $M = 127$ (no band-limiting) gives either instabilities or $O(1)$ errors, whereas $M = 12$ improves both stability and accuracy.

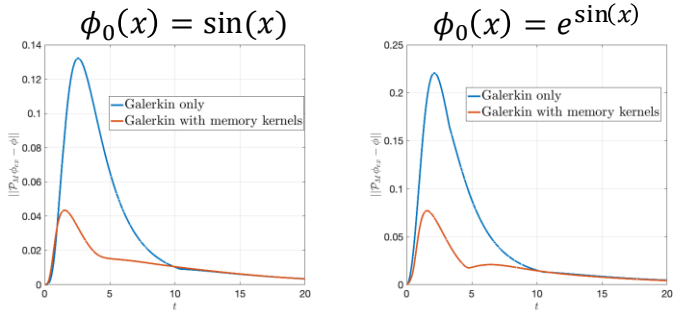

Figure 2: Evolution of error with and without the inclusion of memory terms. Note that complementing the Galerkin treatment with memory terms helps improve the accuracy of the solutions.

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Publication(s) for this work: Qadeer S, Wan H, Stinis P. Stabilizing PDE--ML Coupled Systems. arXiv preprint arXiv:2506.19274