Scientific machine learning

https://doi.org/10.1038/s42256-026-01238-4

Neural operators for free-boundary problems

Constantinos Siettos

Free boundary problems, such as modelling glacier melt, are difficult to capture with neural operators. A new framework addresses this challenge by leveraging the mathematical principle of topological conjugacy.

Learning operators — mappings between infinite-dimensional function spaces — from data has become one of the most challenging problems in contemporary scientific machine learning (SciML). With the development of DeepONet[1] in 2021, neural operators entered mainstream SciML, catalysing a wave of research in the field of learning solution operators of partial differential equations (PDEs). Yet, an important class of problems remains particularly challenging, and comparatively underexplored in the neural operator setting: free boundary problems (FBPs), in which the domain of the solution is itself unknown. Such problems arise across high-impact real-world systems, including glacier melt under global warming; multiphase flows in which moving liquid–gas or liquid–liquid interfaces evolve, merge or break up (for example, bubbles, droplets and sprays); tumour growth with expanding boundaries coupled to diffusion–reaction and mechanics; and mechanotransduction, where deforming tissues interact with stress–strain fields to regulate growth and cell state. Although deep neural networks and physics-informed SciML[2] have been used to model free-boundary dynamics[3], extending neural operator learning to this setting remains challenging — especially when one seeks to learn the infinite-dimensional input–output map in a fully data-driven manner, without relying on an explicit knowledge (or part) of the governing PDEs and interface laws. This gap reflects a core mismatch: neural operators are typically formulated on a prescribed domain; FBPs break this assumption because the solution field 'lives' on an a priori unknown, evolving domain. Research by Long et al.[4] in this issue of *Nature Machine Intelligence* addresses this challenge, introducing a major step for learning neural operators for FBPs.

The proposed FBNO builds on MIONet[5], a generalization of the DeepONet for learning multiple-input operators — but adds a crucial ingredient: a learned geometric (conjugate) transformation that links dynamics on the unknown, evolving domain $\Omega(t)$, in response to the solution field $u(x,t)$, $x \in \Omega(t)$, to dynamics on a fixed reference domain Ω_{ref} (Fig. 1).

This transformation can be viewed as a continuous and reversible stretching or bending of a shape — one that does not tear it apart or creates holes. In particular, the FBNO learns two coupled operators: (i) an evolution operator $\mathcal{G}$ on a fixed reference domain Ω_{ref}, and (ii) a geometry operator $\mathcal{H}$ (a homeomorphism/diffeomorphism) that provides a bijective (reversible) mapping between the evolving free-boundary domain $\Omega(t)$ and Ω_{ref}. The evolving boundary $\partial\Omega(t)$ is obtained by mapping the reference boundary through the composed operators $\mathcal{H}$ and $\mathcal{G}$. A key theoretical contribution is a tailored universal approximation theorem for this construction, covering solutions in Sobolev spaces $\mathcal{W}^{k,2}(\Omega)$ — that is, functions with square-integrable

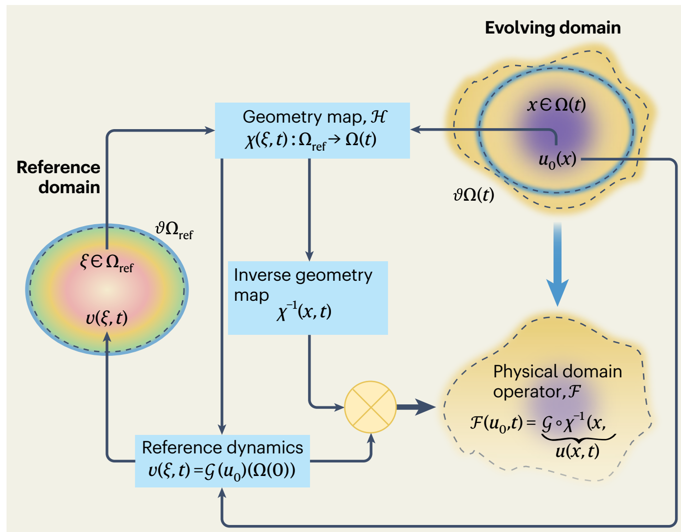

Fig. 1 | Schematic of the free-boundary neural operator conjugacy framework. Given points ξ in the reference Ω_{ref} and x in the evolving domain Ω(t), with corresponding free boundary $\partial\Omega(t)$, the FBNO learns a geometry map (a diffeomorphism) $\chi(\xi,t)$: $\Omega_{ref} \rightarrow \Omega$ and an operator $\mathcal{G}$ on Ω_{ref} that evolves an initial condition u_0 sampled from a Banach space. The resulting dynamics in Ω_{ref} are mapped back via the inverse of χ to recover the physical-domain operator $\mathcal{F}$. The inverse coordinates can, for example, be obtained via an autoencoder. This learned diffeomorphism has a similar role to an isoparametric mapping in finite elements — a change of variables from a reference to a physical domain — but here the map is global, time-dependent, and data-driven. The gradient colours illustrate the distribution of a field.

weak derivatives up to order k, typical of systems with moving interfaces and sharp fronts. Once trained, the FBNO can rapidly predict both the solution fields and the associated moving interfaces. The efficiency of FBNO is demonstrated via a set of benchmark studies in one, two and three spatial dimensions, including Stefan-type models describing the evolution of the interface between two phases of a material undergoing a phase transition, such as in ice melting.

Several challenges remain open at the intersection of FBPs and neural operators. Free boundaries can involve irreversible topological changes (merging or breaking interfaces), in which a diffeomorphic mapping breaks down. Even when topology is preserved, identifiability and stability questions arise: how sensitive is the recovered interface to the level and type of noise in the training data, and how do errors in the geometry map propagate into solution errors over long time horizons? Importantly, in many real-world settings, data are sparse — few snapshots, irregular sampling, and partial observations — neural operators often assume dense sampling. A promising solution is to incorporate local neural operators[6], which learn short-horizon or patch-wise mappings, improving robustness and computational efficiency under sparse data.

We have reached a point where achieving scientific breakthroughs requires genuinely interdisciplinary advances to build a new generation of SciML methods. In particular, neural operators that can overcome the curse of dimensionality, which still limits reliable, generalizable models of high-dimensional, real-world complex systems under sparce data and limited computational resources. Meeting this challenge will require new mathematical theories. This need is urgent and important: progress must extend beyond simplified test cases to high-impact problems with sharp, potentially irreversible (catastrophic) transitions, from glacier melting driven by global warming, to abrupt shifts in the evolving tumour–host interface during cancer therapy.

Constantinos Siettos

Dipartimento di Matematica e Applicazioni "Renato Caccioppoli", University of Naples Federico II, Naples, Italy.

e-mail: constantinos.siettos@unina.it

Published online: 21 May 2026

References

1. Lu, L., Jin, P., Pang, G., Zhang, Z. & Karniadakis, G. E. *Nat. Mach. Intell.* **3**, 218–229 (2021).
2. Karniadakis, G. E. et al. *Nat. Rev. Phys.* **3**, 422–440 (2021).
3. Wang, S. & Perdikaris, P. *J. Comput. Phys.* **428**, 109914 (2021).
4. Long, Z., Zhou, Q., Zhu, A., Dai, D. & Liu, Y. *Nat. Mach. Intell.* https://doi.org/10.1038/s42256-026-01233-9 (2026).
5. Jin, P., Meng, S. & Lu, L. *SIAM J. Sci.Comput.* **44**, A3490–A3514 (2022).
6. Fabiani, G., Vandecasteele, H., Goswami, S., Siettos, C. & Kevrekidis, I. G. Preprint at https://doi.org/10.48550/arXiv.2505.02308 (2025).

Competing interests

The author declares no competing interests.