Funny things may happen when using NNs to solve PDEs

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One way to think about the 'coarse-graining' of an evolution equation is as the restriction of a given evolution to some manifold of candidate solutions. While the classical manifolds are linear, as e.g. in the (Petrov-)Galerkin method, the manifolds used in e.g. Smooth Particle Hydronamics or neural-network approximations are inherently nonlinear. In the case of neural networks, the large class of 'Physics-Informed Neural Networks' and their siblings is a good example of this.

For some of these parametrized candidate solution sets, the parametrization may be smooth while the actual set is non-smooth, and this set may even change dimension from point to point. This leads to various problems in simulation, which in some cases can be severe. Existing solutions to these problems consist of modifying the projected evolution to make it regular, with the disadvantage of solving a different evolution than the original one.

In this talk we report on recent work for the specific case of gradient-flow evolutions. We treat the non-smooth set of candidate solutions as a metric space in its own right, and apply the theory of metric-space gradient flows to obtain a convergence theorem for time-discretized solutions. In the process we discover various non-trivial properties of the set of candidate solutions that are implicitly defined by neural networks.

This is joint work with Olga Mula (Vienna) and Daan Bon and Benjamin Caris (Eindhoven).