



# The Hong Kong Polytechnic University Department of Applied Mathematics

## Seminar

## Bridging scales with data-driven nonlocal models

### By

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#### Abstract

Nonlocal models are characterized by integral operators that embed lengthscales in their definition. As such, they are preferable to classical partial differential equation models in situations where the dynamics of a system is affected by the small scale behavior, yet the small scales would require prohibitive computational cost to be treated explicitly. In this sense, nonlocal models can be considered as coarse-grained, homogenized models that, without resolving the small scales, are still able to accurately capture the system's global behavior. However, nonlocal models depend on "kernel functions" that are often hand tuned.

We propose to learn optimal kernel functions from high fidelity data by combining machine learning algorithms, known physics, and nonlocal theory. This combination guarantees that the resulting model is mathematically well-posed and physically consistent. Furthermore, by learning the operator rather than a surrogate for the solution, these models generalize well to settings that are different from the ones used during training. We apply this learning technique to find homogenized nonlocal models for subsurface solute transport solely on the basis of breakthrough curves. We also apply the same kernel-learning technique to design new stable and resolution-independent deep neural networks, referred to as Nonlocal Kernel Networks (NKN). Stability of NKNs is obtained by imposing constraints derived from the nonlocal vector calculus, whereas deep training is performed by means of a shallow-to-deep initialization technique. We demonstrate the accuracy and stability of NKNs on PDE-learning and image-classification problems.



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Date: 11 May 2022 (Wednesday) Time: 11:00-12:00 (Hong Kong Standard Time GMT +8) Venue: Online Talk via Zoom (Meeting ID: 999 6025 0341) Speaker: Dr. Marta D'Elia, Sandia National Laboratories Host: Prof. Zhonghua Qiao, The Hong Kong Polytechnic University Click to join: https://polyu.zoom.us/j/99960250341?pwd=Tm9kZGlQeG8rMlAwNzg1ZTdUYm45dz09