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AI for complex physical simulation and inverse design

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In science and engineering, fundamental problems include the forward problem of simulating the evolution of complex physical systems, and the inverse design/inverse problem of optimizing/inferring the system's high-dimensional parameters. Traditional numerical simulation and optimization methods often require extensive computation due to complex physical dynamics. In this talk, I will introduce our method for addressing these challenges with graph neural networks (GNN) and generative models. For accelerating simulation, I introduce a GNN-based architecture that can perform large-scale fluid simulation with more than 10 million nodes, and another method that can simultaneously optimize computation by adding/removing nodes while predicting the system evolution. For inverse design, I introduce the CinDM method based on diffusion generative models. CinDM combines simulation and inverse design/problem into a single task, and learns the joint probability distribution (represented as energy function) of state trajectory and system parameters. In inference, by composing the learned energy function, it can generalize to simulation and inverse tasks more complex than in training. We demonstrate CinDM ’ s capability in 1D PDE and 2D airfoil design tasks.

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