Machine Learning for the simulation of strained-film growth: tackling long-time scales with Finite Element Method accuracy.

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In recent years Machine Learning (ML) has proven to be an effective tool to approximate computationally expensive tasks in materials simulations while retaining a high degree of accuracy [1]. Here we present an application of Neural Networks (NNs) to continuum models describing the morphological evolution of thin heteroepitaxial films. The dynamics of this class of system is determined, through Partial Differential Equations [2], by the (generalized) chemical potential. This, in turns, contains surface energy, strain effects and interactions with the underlying substrate. From a computational study perspective, elastic contributions due to the possible mismatch between the film and substrate lattice are the most expensive ones to calculate, as closed form analytical expressions are available only in the small-slope limit [3]. For a generic free surface profile, however, the elastic equilibrium problem should be solved, e.g. through Finite Element Method (FEM). This is the principal computational bottleneck, as a single full evolution may require several hundreds of thousands of FEM calls [4], hindering the study of large systems over long timescales. We show that an accurate and efficient NN model can be trained to surrogate the full FEM solution, with a speed up of ~4 orders of magnitude for simulations. Importantly, building the dataset required for the training procedure has a computational cost which is comparable to a single, small computational cell evolution.

For simplicity, the 2D, isotropic case will be discussed, using Ge on Si(001) as a prototypical system [5], although the method generalize to more complex scenarios. Once the NN is trained, it may be used to run simulations involving coarsening and growth with a several orders of magnitude reduction in the computational costs, pushing forward the limits of tractable systems both in terms of time and spatial scales.

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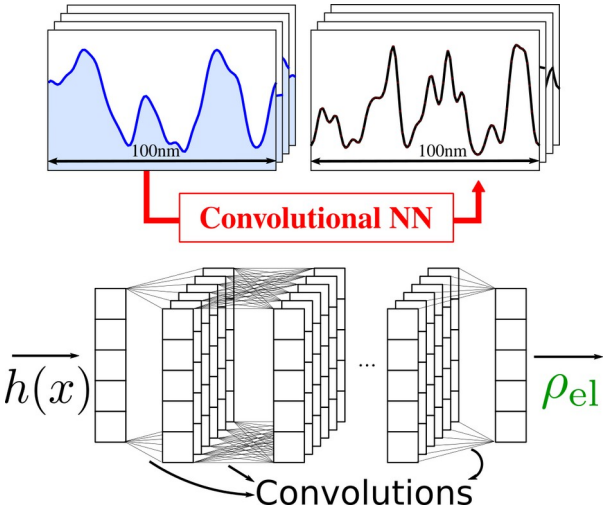

Figure 1: Neural Network (NN) scheme. The NN is used to approximate the mapping between the free surface profile h(x) and the elastic energy density ρ

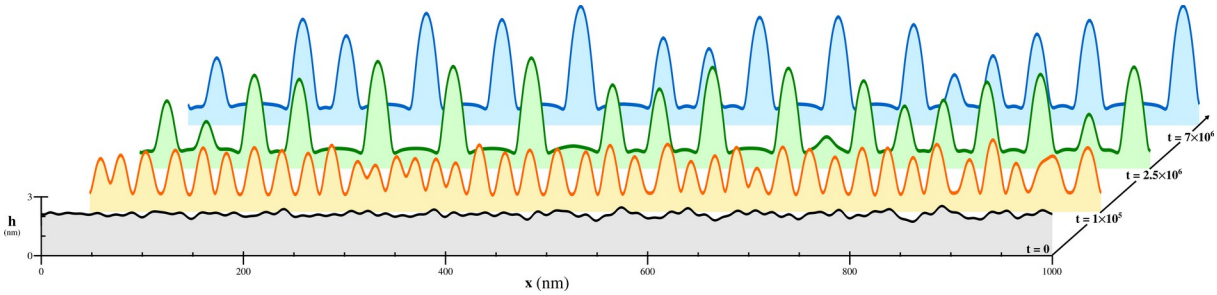

Figure 2: Once the NN is trained, it can be used to perform simulations over larger computational cells at a reduced computational cost, reaching longer time scales