Fast Machine Learning for Science
Real-time and accelerated ML for fundamental sciences
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Real-Time Machine Learning in Materials Microscopy and Spectroscopy

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Materials have marked human evolution throughout history. The next technological advancement will inevitably be based on a groundbreaking material. Future discovery and application of materials in technology necessitates precise methods capable of creating long-range, non-equilibrium structures with atomic accuracy. To achieve this, we need enhanced analysis tools and swift automated synthesis. Although machine learning is gradually making inroads into materials science, most analysis happens well after the experiment, making the insights less actionable. Furthermore, most models applied are purely data-driven and thus do not necessarily adhere to the principles of physics. In this paper, we delve into our advancements in creating machine learning algorithms, informed and constrained by physics, implemented on FPGAs for detailed materials analysis. Firstly, we explore the use of 4D scanning transmission electron microscopy, where an electron beam produces a 2D image from 2D diffraction patterns with sub-atomic accuracy. We introduce a spatial transforming autoencoder that outperforms existing algorithms in determining crystallographic strain, shear, and orientation. We deploy these models on FPGAs via HLS4ML, achieving latencies less than 29 s, surpassing current imaging rate (˜1 kHz). This advancement provides capabilities for triggering systems that permit detection-controlled imaging modes that reduce damage during electron microscopy, preserving the natural state of sensitive materials. Secondly, we discuss real-time analysis of multimodal in situ spectroscopies in pulsed-laser deposition. This process involves a laser ablating a targeting a low-pressure oxidizing atmosphere, forming a plasma plume that is deposited on a heated substrate. We demonstrate how this process can be monitored using direct imaging of the plasma dynamics and reflection high-energy electron diffraction at >500 Hz to observe surface crystallography and diffusion. We show how hard-physics constrained machine learning methods deployed on FPGAs can serve as real-time approximates of processes providing a pathway towards autonomous synthesis.

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