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Up to two billion times acceleration of scientific simulations with deep neural architecture search MUHAMMAD KASIM, DUNCAN WATSON-PARRIS, LUCIA DEACONU, SOPHY OLIVER, PETER HATFIELD, University of Oxford, DUSTIN FROULA, University of Rochester, GIANLUCA GREGORI, MATT JARVIS, SAMAR KHATIWALA, JUN KORENAGA, JACOB TOPP-MUGGLESTONE, University of Oxford, ELEONORA VIEZZER, University of Seville, SAM VINKO, University of Oxford — Computer simulations are one of the main ways in studying plasma systems. Employing simulation enable researcher to perform indirect measurement of systems from observation as well as to explore parameter space. However, accurate simulations are often slow to execute, which limits their applicability to extensive parameter exploration, large-scale data analysis, and uncertainty quantification. A promising route to accelerate simulations by building fast emulators with machine learning requires large training datasets, which can be prohibitively expensive to obtain with slow simulations. Here we present a method based on neural architecture search to build accurate emulators even with a limited number of training data. The method successfully accelerates simulations by up to 2 billion times in 10 scientific cases including 4 cases in plasma physics. Our approach also inherently provides emulator uncertainty estimation, adding further confidence in their use. We anticipate this work will accelerate research involving expensive simulations, allow more extensive parameters exploration, and enable new, previously unfeasible computational discovery.

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