HAMLET
How to Apply Machine Learning to Experimental & Theoretical PHYSICS
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MetalAI - Atomic structure calculations guided by machine learning

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The advent of gravitational wave astronomy has enabled the direct study of the synthesis of heavy elements such as rare earths, lanthanides, and actinides. This was exemplified by the kilonova AT2017gfo/GW170817, where several heavy element emission lines were confirmed. The primary challenge in advancing this research is the lack of accurate and complete atomic data for these elements in ionization stages I-IV.

Our project, part of the ERC-funded HeavyMetal collaboration, aims to address this by using the GRASP atomic structure code to calculate theoretical atomic data. GRASP, known for its accuracy, requires extensive manual input and is time-consuming. The process involves iteratively adding Configuration State Functions (CSFs) and running GRASP to check for convergence. Each additional CSF can improve accuracy but also significantly increases computational time, making it critical to determine the optimal set of CSFs.

We propose to use machine learning to automate this iterative decision-making process. We will develop a transformer-based surrogate model to predict the convergence of GRASP for a given set of CSFs and the improvement in output accuracy. This model will enable a reinforcement learning esque approach to efficiently explore CSF combinations, optimizing for both accuracy and computational time.

This project will significantly reduce the manual effort required for GRASP calculations and use computational resources more efficiently, through the use of machine learning, enabling more rapid and comprehensive studies of the heaviest elements synthesized in neutron star mergers.

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