SIMULATING ENERGETIC PARTICLE DYNAMICS USING OPERATOR NEURAL NETWORKS WITH SPATIAL TRANSLATION INVARIANCE

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1. INTRODUCTION

The rapid evolution of artificial intelligence has opened new avenues for overcoming computational bottlenecks inherent in traditional simulation methods. In the context of energetic particle dynamics, conventional single-particle tracking algorithms rely heavily on precise numerical solvers for long-term evolution processes, leading to prohibitive computational costs in large-scale systems or high-temporal-resolution scenarios. Neural networks, as surrogate models, offer a transformative potential to replace these resource-intensive methods at a fraction of the computational cost. While recent studies—such as Linlin Zhong et al.'s physics-informed neural networks (PINNs) for transient-state predictions in low-temperature plasmas, Diogo D. Carvalho et al.'s graph neural networks for 1D plasma dynamics, and Vignesh Gopakumar et al.'s Fourier neural operators for magnetohydrodynamic plasma modeling—demonstrate progress, these approaches predominantly rely on soft physical constraints through optimization, resulting in approximations that may deviate from strict physical consistency. This limitation underscores a critical gap in enforcing structural-level physical priors within neural architectures.

2. INNOVATIVE INTEGRATION OF SYMMETRY PRINCIPLES

Recent advances in deep learning have revealed that embedding explicit *symmetries*—fundamental invariants pervasive in mathematical and physical systems—into neural architectures significantly enhances model generalizability. Pioneering works across domains, such as Clebsch-Gordan decomposition-based Lorentz group-equivariant networks for relativistic particle physics, rotation-invariant convolutional networks for Navier-Stokes equations, and tensor-basis neural networks (TBNNs) for turbulence modeling, collectively demonstrate that symmetry-aware architectures outperform conventional models in both accuracy and interpretability. Despite these strides, existing symmetry-driven frameworks predominantly focus on geometric or algebraic invariants (e.g., permutation equivariance, rotational invariance in graph networks, or parity symmetry), often neglecting *spatiotemporal symmetries*—such as spatial translation invariance—that govern fundamental conservation laws in physics. This oversight highlights a critical opportunity for innovation.

3. METHODOLOGICAL AND TECHNICAL

This study pioneers a symmetry-hardened neural operator framework for charged particle dynamics simulation, explicitly embedding spatial translation invariance—a cornerstone symmetry governing conservation of momentum and system evolution—into the network architecture. Unlike prior works that either approximate symmetries via loss function (e.g., Hamiltonian/Lagrangian neural networks) or focus on non-physical invariants, our approach rigorously enforces symmetry constraints at the structural level, ensuring strict adherence to physical laws. Key innovations include:

Theoretical Foundation: A mathematical formulation of the necessary conditions for spatial translation invariance in neural operators, bridging abstract symmetry principles with implementable architectural designs.

Architectural Innovation: A novel neural operator architecture that intrinsically satisfies translation invariance, eliminating reliance on ad-hoc regularization.

Validation Paradigm: Comprehensive numerical benchmarks against state-of-the-art methods (e.g., baseline neural operators, symmetry-regularized HNN/LNN variants), demonstrating superior accuracy and generalizability to unseen field configurations.

4. BROADER IMPLICATIONS

By unifying deep learning with Noether's theorem—the profound link between symmetries and conservation laws—this work establishes a paradigm shift in physics-informed AI. It not only advances energetic particle simulations but also provides a blueprint for embedding fundamental physical principles into neural architectures, with transformative potential for plasma physics, astrophysics, and quantum system modeling. The methodology's success in maintaining physical consistency while achieving computational efficiency (10-20× speedup vs. traditional solvers) positions it as a critical tool for next-generation multiscale simulations in fusion research and plasma physics.

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