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ML-Based Solid Boundary Treatment for Meshfree Particle Methods

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ABSTRACT

Meshfree particle methods (MPM), such as Moving Particle Semi-implicit (MPS) and Smoothed Particle Hydrodynamics (SPH), discretize continuum using a set of moving particles (computational nodes with no connectivity) over which field variables and their derivatives are approximated through a kernel smoothing process. The mesh-free Lagrangian nature of these methods gives them the flexibility to deal with highly deformed or fragmented interfaces. However, near solid boundaries, these methods require special treatments to address kernel incompleteness and enforce boundary conditions. Common approaches include the ghost particle method, repulsive force method, and polygon-based boundary conditions, but these techniques often introduce significant computational costs and implementation challenges, particularly for complex geometries.

This research proposes a machine learning (ML) model to predict boundary contributions in the MPS method, significantly reducing computational costs compared to traditional boundary treatment techniques. More specifically, the ML model learns from the ghost particle approach to estimate boundary effects in the MPS approximation of field values and their derivatives. The proposed model is a deep neural network (DNN) that integrates a convolutional neural network (CNN) for feature extraction with a fully connected neural network (FCNN) for prediction. The input features include geometric properties (e.g., particle position relative to the boundary and boundary shape), kernel properties, and field variables, and the model's output provides boundary contributions to the MPS approximation of particle number density, gradients, divergence, and Laplacians. The model is trained using synthetic datasets with different geometric complexities and predefined field variations, then tested on unseen cases involving 2D unsteady pure diffusion, advection-diffusion, and Navier-Stokes equations. Comparisons with the ghost particle approach demonstrate the accuracy of the proposed ML model, making it a promising alternative for efficient boundary treatment in MPS simulations.