

## Differentiable Physics Simulators for AI-Accelerated Engineering Optimization

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Optimization and inverse problems play a crucial role in engineering design and analysis. Traditional methods for calculating derivatives through forward simulations are computationally expensive and prone to numerical instability. Moreover, these simulations cannot be easily integrated into machine learning models for optimization due to their inability to compute gradients with respect to input parameters. To address these challenges, we propose a novel Differentiable Programming simulator that combines automatic reverse differentiation with second-order gradient-based optimization algorithms, such as L-BFGS, resulting in a fully-differentiable Material Point Method (MPM) simulator.

Our approach identifies input material properties by iteratively updating parameters to minimize a loss function, typically defined as the norm of the difference to the target observation. The gradient is then minimized using a second-order optimization algorithm. Solving exact PDEs approximates environment dynamics more accurately than model-agnostic reinforcement learning methods. We successfully apply this approach to estimate input parameters for colliding deformable bodies. The differentiable MPM simulator provides gradients through simulation, enabling integration with machine learning algorithms for real-time decision-making and optimization in robotics.

Extending our approach, we introduce physics-embedded Differentiable Graph Network Simulators (GNS) to accelerate particulate and fluid simulations further. GNS represents domains as graphs with particles as nodes and learned interactions as edges, allowing for the learning of localized physics and improving generalization. This method achieves over 165x speedup for granular flow prediction compared to parallel CPU simulations.

We also propose a novel hybrid GNS/MPM approach that interleaves GNS with MPM to conserve momentum and minimize errors, achieving a 24x speedup compared to purely numerical simulations. This differentiable GNS solves inverse problems through automatic differentiation, such as identifying material parameters for target runout distances in granular flows.

Furthermore, we have developed techniques to derive material parameters and loads from videos by constructing 3D point clouds using Neural Radiance Fields (NeRFs). This allows us to iteratively minimize differentiable simulation results to determine material properties and loading conditions.