The formation of the large-scale structure, the evolution and distribution of galaxies, quasars, and dark matter on cosmological scales, requires numerical simulations. Differentiable simulations provide gradients of the cosmological parameters, that can accelerate the extraction of physical information from statistical analyses of observational data. The deep learning revolution has brought not only myriad powerful neural networks, but also breakthroughs including automatic differentiation (AD) tools and computational accelerators like GPUs, facilitating forward modeling of the Universe with differentiable simulations. Because AD needs to save the whole forward evolution history to backpropagate gradients, current differentiable cosmological simulations are limited by memory. Using the adjoint method, with reverse time integration to reconstruct the evolution history, we develop a differentiable cosmological particle-mesh (PM) simulation library \textit{pmwd} (particle-mesh with derivatives) with a low memory cost. Based on the powerful AD library \textit{JAX}, \textit{pmwd} is fully differentiable, and is highly performant on GPUs.

![pmwd logo](https://example.com/pmwd_logo.png)

\textbf{Figure 1:} \textit{pmwd} logo. The C2 symmetry of the name symbolizes the reversibility of the model, which helps to dramatically reduce the memory cost together with the adjoint method.
Statement of Need

Current established workflows of statistical inference from cosmological datasets involve reducing cleaned data to summary statistics like the power spectrum, and predicting these statistics using perturbation theories, semi-analytic models, or simulation-calibrated emulators. Rapid advances in accelerator technology like GPUs opens the possibility of direct simulation-based forward modeling and inference (Cranmer, Brehmer, and Louppe 2020), even at level of the fields before their compression into summary statistics. The forward modeling approach naturally account for the cross-correlation of different observables, and can easily incorporate systematic errors. In addition, model differentiability can accelerate parameter constraint with gradient-based optimization and inference. A differentiable field-level forward model combines the two features and is able to constrain physical parameters together with the initial conditions of the Universe.

The first differentiable cosmological simulations, such as BORG and ELUCID (Jasche and Wandelt 2013; Wang et al. 2014), were developed before the advent of modern AD systems, and were based on implementations of analytic derivatives. Later codes including FastPM and FlowPM (Seljak et al. 2017; Modi, Lanusse, and Seljak 2021) compute gradients using AD engines, namely vmad (written by the same authors) and TensorFlow, respectively. Both analytic differentiation and AD backpropagate the gradients through the whole history, thus requires saving the states at all time steps in memory. Therefore, they are subject to a trade-off between time and space/mass resolution, and typically can integrate for only tens of time steps, unlike the standard non-differentiable simulations.

Alternatively, the adjoint method provides systematic ways of deriving model gradients under constraints (Pontryagin 1962), such as the N-body equations of motion in the simulated Universe (Li et al. 2022). The adjoint method evolves a dual set of equations backward in time, dependent on the states in the forward run, which can be recovered by reverse time integration for reversible dynamics, thereby dramatically reducing the memory cost (Chen et al. 2018). Our logo in Figure 1 is inspired by such reversibility as well as the JAX artistic style. Furthermore, we take the discretize-then-optimize approach (e.g., Gholami, Keutzer, and Biros 2019) to ensure gradients propagate backward along the same discrete trajectory as taken by the forward time integration. We derive and validate our adjoint method in Li et al. (2022) in more details. The table below compares the differentiable cosmological simulation codes.

| code     | OSS | gradient | mem efficient | hardware  |
|----------|-----|----------|---------------|-----------|
| BORG     | analytic |         | CPU           |           |
| ELUCID   | analytic |         | CPU           |           |
| FastPM-vmad ✓ | AD |         | CPU           |           |
| FlowPM   ✓ | AD |         | GPU/CPU       |           |
| pmwd ✓ | adjoint ✓ |         | GPU/CPU       |           |

Being both computation and memory efficient, pmwd enables larger and more accurate forward modeling, thus will improve gradient based optimization and inference. Differentiable analytic, semi-analytic, and deep learning components can run based on or in parallel with pmwd simulations. Examples include a growth function emulator (Kwan et al. 2022) and our ongoing work on spatiotemporal optimization of the PM gravity solver (Zhang et al. in prep). In the future, pmwd will also facilitate the modeling of various cosmological observables and the understanding of the astrophysics at play.

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