Accelerating Proximity-Field Nanopatterning: GPU-Optimized Electromagnetic Solvers for Complex 3D Nanostructure Design

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Enhancing productivity in 3D nanoprinting is crucial for advancing applications in energy storage, sensors, photonic devices, and microrobotics. Among various techniques, proximity-field nanopatterning (PnP) stands out for its ability to balance high productivity with satisfactory spatial resolution. This method relies on coherent light passing through a phase mask to generate intricate 3D hologram patterns within a photoresist. However, traditional approaches for designing phase masks often result in low-contrast patterns, limiting the complexity of achievable nanostructures.
Recent developments integrating numerical simulations with optimization algorithms have addressed these challenges by enabling high-contrast patterns. Gradient-based optimization has proven effective for refining phase mask designs iteratively. However, designing large-scale phase masks remains computationally demanding, particularly for multi-layered structures requiring 3D simulations. Traditional methods like the finite-difference time-domain (FDTD) approach struggle with computational feasibility, making large-scale designs impractical.
Frequency-domain solvers provide simulation results using less computational resources by eliminating time-stepping and improving accuracy for steady-state scattering analysis. Even though those approaches have been validated in previous studies, they suffer from scalability issues, especially for simulating three-dimensional (3D) space.
This work proposes a convergent Born series frequency-domain solver that enhances computational efficiency and stability. This solver stably works for 3D simulation by ensuring mathematical stability. Coupled with GPU acceleration, this solver significantly reduces simulation time and extends the applicability of PnP for complex nanostructure fabrication.

References

1. Lee, Dohyeon, et al. "Fast Free-Form Phase Mask Design for Three-Dimensional Photolithography Using Convergent Born Series." ACS Photonics (2025).
2. Osnabrugge, Gerwin, Saroch Leedumrongwatthanakun, and Ivo M. Vellekoop. "A convergent Born series for solving the inhomogeneous Helmholtz equation in arbitrarily large media." Journal of Computational Physics 322 (2016): 113-124.
3. Vettenburg, Tom, Simon AR Horsley, and J. Bertolotti. "Calculating coherent light-wave propagation in large heterogeneous media." Optics Express 27.9 (2019): 11946-11967.
4. Nam, Sang-Hyeon, et al. "Photolithographic realization of target nanostructures in 3D space by inverse design of phase modulation." Science Advances 8.21 (2022): eabm6310.