



## Nanophotonic Simulation and Inverse Design using Fast High-order Chebyshev-based Nyström Methods

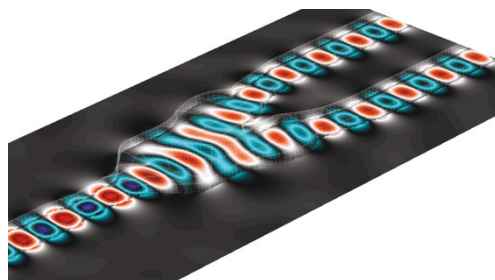
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The majority of electromagnetic devices for practical nanophotonic applications are tedious and challenging to design and analyze due to the lack of analytical solutions, necessitating fully vectorial three-dimensional solutions of Maxwell's equations. Unfortunately, these devices are often also difficult to solve numerically due to being electrically large (spanning many wavelengths in size) and often having subwavelength feature sizes. Time domain approaches, such as the Finite-Difference Time-Domain (FDTD) method, are often the only viable algorithms for simulating most nanophotonic devices, such as grating couplers, power and mode conversion splitters, tapers, and long waveguides. This is because volumetric frequency-domain methods such as the Finite Element Method (FEM) or the Finite-Difference Frequency-Domain (FDFD) method result in prohibitively large and poorly conditioned linear systems which become intractable even for modestly sized problems. In this work, we present a fast, high-order 3D integral equation solver based on the Nyström method [1], which can be used to simulate large electromagnetic devices efficiently and rapidly in the frequency domain, including nanophotonic devices with semi-infinite waveguides [2]. We will introduce the Chebyshev-based discretization scheme, which is leveraged by the solver to discretize a stable, well-conditioned N-Müller integral formulation, and discuss recent acceleration techniques that we have developed, including utilizing GPU computing, incorporating a sparse block-diagonal preconditioning strategy, and implementing a matrix-free approach for computing the transpose operator required by the discrete adjoint method. We will also present our most recent advancements, including automated high-order surface meshing of electromagnetic structures, adaptive integration of singular and near interactions for automated error control, and a new approach for efficiently launching unidirectional modes in waveguides.

Plane-wave, gaussian beam, and dipole-based incident source excitations are typically straightforward to implement in the context of integral equation solvers due to the availability of analytical field solutions. However, such sources are typically suboptimal for exciting waveguide-based devices and can lead to poor modal excitation efficiency, significant radiation fields, and potentially higher-order mode excitation in the case of multi-mode waveguides. A new technique will be introduced for efficiently launching unidirectional modes in waveguides by utilizing a single-trace indirect N-Müller formulation. All the energy in the incident field is coupled into a single direction of any desired propagating mode of the waveguide without any field leakage or nonspecific coupling into other modes.

A variety of examples of realistic nanophotonic devices simulated and inverse designed using our framework will be presented, including a nonadiabatic taper, a 50:50 power splitter (Fig. 1), and a directional coupler. The authors gratefully acknowledge support by the Air Force Office of Scientific Research (FA9550-20-1-0087) and the National Science Foundation (CCF-2047433).



**Figure 1.** Real part of  $E_z$  of inverse designed 50:50 silicon power splitter excited by the fundamental mode

1. Hu, Jin, Emmanuel Garza, and Constantine Sideris. "A Chebyshev-based high-order-accurate integral equation solver for Maxwell's equations." *IEEE Transactions on Antennas and Propagation* 69.9 (2021): 5790-5800.
2. Garza, Emmanuel, Constantine Sideris, and Oscar P. Bruno. "A boundary integral method for 3D nonuniform dielectric waveguide problems via the windowed Green function." *IEEE Transactions on Antennas and Propagation* (2023).