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Fourier spectral simulations and Gegenbauer reconstructions for electromagnetic waves in the presence of a metal nanoparticle

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Abstract

We describe Fourier pseudospectral time-domain simulations, carried out in order to study light interacting with a metallic nanoscale object. The difficulty of using Fourier methods to accurately predict the electromagnetic scattering in such problems arises from the discontinuity in the dielectric function along the surface of the metallic object. Standard Fourier methods lead to oscillatory behavior in approximating solutions that are nonsmooth or that have steep gradients. By applying the Gegenbauer reconstruction technique as a postprocessing method to the Fourier pseudospectral solution, we successfully reduce the oscillations after postprocessing.

Our computational results, including comparison with finite-difference time-domain simulations, demonstrate the efficiency and accuracy of the method.

Keywords: Fourier pseudospectral method; Gegenbauer reconstruction; Postprocessing

1. Introduction

Metallic nanostructures, such as metal nanoparticles and nanoholes in thin metal films, are of considerable interest because of the possibility of creating surface plasmon excitations when interacting with light [2,23]. Surface plasmons are collective electronic excitations that effectively concentrate and confine light energy [4]. The manipulation of surface plasmons could lead to novel nanoscale optoelectronic devices.

Numerical simulations help us to understand and predict the basic physics of such nanophotonics problems and also provide cost-effective tools for prototyping design of potential devices. Among general computational techniques employed in such simulations, Fourier methods have been naturally considered for problems with periodic features, such as planar waveguides and photonic crystal structures for integrated photonic devices. Computational implementations and their error estimates have been analyzed in the literature [9,26]. In this

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paper, we show how such Fourier methods can be applied to light interacting with metal nanostructures that do not possess periodic features. Our focus is on mathematical reconstruction techniques for Fourier pseudospectral simulation data for which one might consider Fourier–Padé or Gegenbauer approximations [6,16,24,26,27].

As a first step, we study light interacting with a small metallic cylinder or nanowire of diameter of 50 nm and infinite length in a vacuum. Before presenting detailed mathematical formulae, we give a brief overview of the mechanism behind surface plasmon excitation in such a system. Imagine the circular cross-section of the nanowire to be in the x–y plane with its long axis parallel to the z-axis. Incident light traveling along the x-axis with y-polarization is then capable of inducing dipolar (and higher-order) charge oscillations near the metal surfaces. These charge oscillations are associated with collective excitations of electrons near the metal surfaces and can lead to electromagnetic surface waves that are highly localized (evanescent) near surfaces, namely, surface plasmons. A complex-valued dielectric constant is used to describe the metallic response to radiation. More detailed analysis shows that this dielectric constant must have a negative real part for surface plasmons to be reasonably excited. Absorption of radiation by the metal can also occur, which involves introducing an imaginary part to the dielectric constant. In addition to being highly localized, the field intensities of surface plasmon excitations can be extremely large near the metal surfaces.

Many approaches exist for solving the relevant Maxwell's wave equations. In this paper we are concerned with time-domain methods that involve grids in space and time. The advantages of such methods include conceptual simplicity and the ability to model a variety of complex system architectures. The most popular time-domain approach is the finite-difference time-domain (FDTD) method [31,30]. It involves low-order finite differencing to accomplish both spatial and time derivatives. In order to describe surface plasmon behavior accurately, however, very fine grids in both space and time are required. An alternative to FDTD that can lead to better accuracy with larger grid spacings would be to evaluate the spatial derivatives with Fourier methods. Such pseudospectral time-domain (PSTD) methods have been proposed and studied in the context of nonplasmonic systems [21,27]. However the abrupt, sharp changes in magnitudes of the electromagnetic fields near the metal surfaces as a result of surface plasmons is problematic for PSTD methods. In particular, nonphysical oscillations, called Gibbs oscillations, can occur that contaminate the solution over a wide range of coordinate space. However, the finite Fourier data contains enough information about the original solution that one can reexpress the data as a Padé or Gegenbauer finite expansion and can thus reduce the oscillations. In both cases, the reconstructions require obtaining the coefficients for the reconstructed approximations in terms of the Fourier coefficients. Implementations with Fourier–Padé reconstructions in [26] have successfully reduced the oscillations for Fourier pseudospectral solutions of nonlinear partial differential equations such as Burgers' and Boussinesq equations.

Here, we apply the Gegenbauer reconstruction to Fourier pseudospectral time-domain simulations [21] of Maxwell's equations. The computational results show that the Gegenbauer reconstructions successfully reduce the noise in the Fourier pseudospectral simulations.

This paper is organized as follows. Section 2 gives the formulation of Maxwell's equations and the auxiliary differential equation [18,30] for the current term from the Drude model. Section 3 presents our numerical discretizations in space and time and the setup of parameters for PSTD simulations. Section 4 introduces cost-effective Gegenbauer reconstructions in one and two dimensions as postprocessing methods for PSTD solutions. Their convergence behaviors are demonstrated for some piecewise analytic functions in one dimension. CPU times for simulations are also discussed. Section 5 demonstrates the PSTD solutions from the nanoparticle scattering simulations and their postprocessed results. FDTD results computed on very finer grids are also provided for comparison with reconstructed results. Section 6 discusses the remaining issues concerning computational automation, with an appropriate error estimate for reconstructed solutions varying with free parameters. Section 7 briefly summarizes our research.

2. Maxwell's equations for metal nanoparticles

We consider the electrodynamics of metal nanosystems, such as those in [2,4,18,19,23], which are composed of (nonmagnetic) metals and dielectric materials. The frequency-domain Maxwell's equations for the electric and magnetic field vectors, $\tilde{E}$ and $\tilde{H}$, may then be taken to be [4]: