

FDTD Formulation for The General Dispersion Model Using the Z Transform Method

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Abstract

The Finite-Difference Time-Domain(FDTD) scattered field formulation for dispersive materials is developed and presented in this paper. A new model, referred to as the General Model is proposed for modeling of dispersive materials in visible wavelength range using the FDTD method with high efficiency. A parameter estimation method is introduced for the general model to fit material permittivity functions fast and accurately. The FDTD formulation is based on the Z transform method and models the frequency-dependent dispersive nature of permittivity as well. We introduce one frequency approximations design. These design techniques will be used to construct approximations to the general model. The implemented FDTD method is verified by the transient reflected and transmitted fields from a gold slab due to the incidence of a gaussian pulse. To validate our approach, we consider the light interaction with an infinite gold nanocylinder and compute the scattering cross section(SCS) and compare it with the analytical solution.

MathematicsSubjectClassification:

Keywords: FDTD, General Model, Z transform method

1 Introduction

The Finite-Difference Time-Domain (FDTD) method is an efficient, robust and easy to implement technique which solves Maxwell's equations in time domain [1]. Dispersive materials, such as semiconductors and metals, are widely used in optical devices. Also FDTD method is one of the most common choices for simulating such devices in a wide frequency rang. One of the most important advantages of the FDTD method is that the broadband response can be accurately obtained in only one simulation run[2]. Several simple phenomenological models, such as Debye, Drude, and Lorentz models, have been widely adopted for modeling dispersive materials using the FDTD method [3-7].

The General Model, referred in this paper for efficiently modeling of arbitrary linear dispersive materials. The proposed model is much more efficient than the conventional Drude, Lorentz and etc, models; because it offers more degrees of freedom in parameter estimation. In addition, a generally applicable parameter estimation method is proposed for this model to efficiently and accurately fit the permittivity function. The general model is implemented in the FDTD method.

Material dispersion is modeled by the Z transform technique. One frequency approximations designis introduced in Section 2. These design techniques will be used to construct approximations to the general model. The implemented FDTD method is verified by the transient reflected and transmitted fields from a gold slab due to the incidence of a gaussian pulse. Also, the application of the proposed model to analyze optical properties of nanocylinder is demonstrated in section 3.

2 The General Dispersion Model

Assuming the time harmonic dependence $\exp(j\omega t)$, the general model is proposed to describe the dispersive material's relative permittivity expressed by the rational fraction form as

$$\varepsilon(\omega) = \frac{a_0 + a_1(j\omega) + a_2(j\omega)^2 + \dots + a_n(j\omega)^n}{b_0 + b_1(j\omega) + b_2(j\omega)^2 + \dots + b_n(j\omega)^n} \quad (1)$$

Where a_n and b_n are real numbers and $j = \sqrt{-1}$, the fraction form is the ratio of two polynomials $\sum_{k=1}^n a_k(j\omega)^k$ and $\sum_{k=1}^n b_k(j\omega)^k$, where the highest order of the denominator is the same as that of the numerator. The parameters a_n and b_n of the two polynomials can be estimated accurately and quickly by a frequency-approximation design.

2.1 FDTD Formulation Using The Z Transform Technique

The method, which uses the Z transforms in order to obtain FDTD updating equations, is named the "Z transform method" and was first introduced by Sullivan

[8]. It should be noted that the transform method is not the only option to model the kind of dispersion considered here. Other techniques such as Auxiliary Differential Equation(ADE) method [9], the Piecewise-Linear RecursiveConvolution (PLRC) technique [10] andRecursive Convolution(RC) method [11] may also be used.

One of the most important methods of approximating a desired continuous-time system is frequency approximation [12]. There are four conventional frequency approximation design as, forward difference, backward difference, centered differenceand bilinear transform [13]. Using of this designs, value of “ $j\omega$ ” with the Z Transform technique are calculated. Then, we obtain relative permittivity constant values in Z space.

2.1.1 Backward Difference

In going from the frequency to the Z domain, there are times when it is difficult to break the frequency domain function into separate terms. There are methods to directly go from ω to z, but they are approximations.

It can be shown that if

$$F\{f(t)\} = F(\omega) \tag{2}$$

Then

$$F\left\{\frac{df(t)}{dt}\right\} = j\omega F(\omega)$$

A derivative can be approximated by

$$\frac{df(t)}{dt} \cong \frac{f(t)-f(t-\Delta t)}{\Delta t} \tag{3}$$

As long as Δt is small compared to how fast $f(t)$ is changing. As these may be thought of as two discrete points, we can take the Z transform

$$Z\left\{\frac{f(t)-f(t-\Delta t)}{\Delta t}\right\} = \frac{F(z)-z^{-1}F(z)}{\Delta t} = \frac{1-z^{-1}}{\Delta t} F(z) \tag{4}$$

So at least as an approximation, we can say that $j\omega$ in the frequency domain Becomes $(1 - Z^{-1})/\Delta t$ in the Z domain. This is known as the backward difference approximation[8]. So

$$j\omega = \frac{1-Z^{-1}}{\Delta t} \tag{5}$$

From (1) and (5) equation, we obtain

$$\mathcal{E}(z) = \frac{c_0 + c_1 z^{-1} + c_2 z^{-2} + \cdots + c_n z^{-n}}{d_0 + d_1 z^{-1} + d_2 z^{-2} + \cdots + d_n z^{-n}} \quad (6)$$

where

$$\begin{aligned} c_0 &= (-1)^0 \left[\binom{0}{0} a_0 \Delta t^n + \binom{1}{0} a_1 \Delta t^{n-1} + \binom{2}{0} a_2 \Delta t^{n-2} + \cdots + \binom{n}{0} a_n \right] \\ c_1 &= (-1)^1 \left[0 + \binom{1}{1} a_1 \Delta t^{n-1} + \binom{2}{1} a_2 \Delta t^{n-2} + \cdots + \binom{n}{1} a_n \right] \\ c_2 &= (-1)^2 \left[0 + 0 + \binom{2}{2} a_2 \Delta t^{n-2} + \cdots + \binom{n}{2} a_n \right] \\ &\vdots \\ &\vdots \\ &\vdots \\ c_n &= (-1)^n a_n \end{aligned} \quad (7)$$

and

$$\begin{aligned} d_0 &= (-1)^0 \left[\binom{0}{0} b_0 \Delta t^n + \binom{1}{0} b_1 \Delta t^{n-1} + \binom{2}{0} b_2 \Delta t^{n-2} + \binom{3}{0} b_3 \Delta t^{n-3} + \cdots + \binom{n}{0} b_n \right] \\ d_1 &= (-1)^1 \left[0 + \binom{1}{1} b_1 \Delta t^{n-1} + \binom{2}{1} b_2 \Delta t^{n-2} + \binom{3}{1} b_3 \Delta t^{n-3} + \cdots + \binom{n}{1} b_n \right] \\ d_2 &= (-1)^2 \left[0 + 0 + \binom{2}{2} b_2 \Delta t^{n-2} + \binom{3}{2} b_3 \Delta t^{n-3} + \cdots + \binom{n}{2} b_n \right] \\ &\vdots \\ &\vdots \\ &\vdots \\ d_n &= (-1)^n b_n \end{aligned} \quad (8)$$

2.1.2 Forward Difference

Similarly, we have

$$j\omega \approx \frac{(Z-1)}{\Delta t} \quad (9)$$

where

$$\begin{aligned}
 C_n &= (-1)^n \left[(-1)^0 \binom{0}{0} a_0 \Delta t^n + (-1)^1 \binom{1}{0} a_1 \Delta t^{n-1} + (-1)^2 \binom{2}{0} a_2 \Delta t^{n-2} + \dots + (-1)^n \binom{n}{0} a_n \right] \\
 C_{n-1} &= (-1)^{n-1} \left[0 + (-1)^1 \binom{1}{1} a_1 \Delta t^{n-1} + (-1)^2 \binom{2}{1} a_2 \Delta t^{n-2} + \dots + (-1)^n \binom{n}{1} a_n \right] \\
 C_{n-2} &= (-1)^{n-2} \left[0 + 0 + (-1)^2 \binom{2}{2} a_2 \Delta t^{n-2} + \dots + (-1)^n \binom{n}{2} a_n \right] \\
 &\vdots \\
 &\vdots \\
 &\vdots \\
 C_0 &= (-1)^0 \left[(-1)^n a_n \right] = a_n
 \end{aligned} \tag{10}$$

and

$$\begin{aligned}
 d_n &= (-1)^n \left[(-1)^0 \binom{0}{0} b_0 \Delta t^n + (-1)^1 \binom{1}{0} b_1 \Delta t^{n-1} + (-1)^2 \binom{2}{0} b_2 \Delta t^{n-2} + \dots + (-1)^n \binom{n}{0} b_n \right] \\
 d_{n-1} &= (-1)^{n-1} \left[0 + (-1)^1 \binom{1}{1} b_1 \Delta t^{n-1} + (-1)^2 \binom{2}{1} b_2 \Delta t^{n-2} + \dots + (-1)^n \binom{n}{1} b_n \right] \\
 d_{n-2} &= (-1)^{n-2} \left[0 + 0 + (-1)^2 \binom{2}{2} b_2 \Delta t^{n-2} + \dots + (-1)^n \binom{n}{2} b_n \right] \\
 &\vdots \\
 &\vdots \\
 &\vdots \\
 d_0 &= (-1)^0 \left[(-1)^n b_n \right] = b_n
 \end{aligned} \tag{11}$$

2.1.3 Centered Difference

The central difference is given by

$$j\omega \approx \frac{(z - z^{-1})}{2\Delta t} \tag{12}$$

where

$$\begin{aligned}
 c_0 &= (-1)^0 \binom{n}{0} 2^0 a_n \Delta t^n = a_n \Delta t^n \\
 c_1 &= (-1)^1 \binom{n-1}{0} 2^1 a_{n-1} \Delta t^{n-1} = 2a_{n-1} \Delta t^{n-1} \\
 c_2 &= (-1)^1 \binom{n}{1} 2^0 a_n \Delta t^n + (-1)^0 \binom{n-2}{0} 2^2 a_{n-2} \Delta t^{n-2} = -na_n \Delta t^n + 4a_{n-2} \Delta t^{n-2}
 \end{aligned}$$

$$\begin{aligned}
 & \cdot \quad \cdot \quad \quad \quad \cdot \quad \quad \quad \cdot \quad \cdot \\
 & \cdot \quad \cdot \quad \quad \quad \cdot \quad \quad \quad \cdot \quad \cdot \\
 & \cdot \quad \cdot \quad \quad \quad \cdot \quad \quad \quad \cdot \quad \cdot \\
 c_n &= (-1)^{n/2} \binom{n}{n/2} 2^0 a_n \Delta t^n + (-1)^{n/2-1} \binom{n-2}{n/2-1} 2^2 a_{n-2} \Delta t^{n-2} + \dots + 2^n a_0 \\
 c_{n+1} &= (-1)^{n/2} \binom{n-1}{n/2} 2^1 a_{n-1} \Delta t^{n-1} + (-1)^{n/2-1} \binom{n-3}{n/2-1} 2^3 a_{n-3} \Delta t^{n-3} + \dots + (-1)^1 \binom{1}{1} 2^{n-1} a_1 \Delta t \\
 & \hspace{20em} (13) \\
 c_{n+2} &= (-1)^{n/2+1} \binom{n}{n/2+1} 2^0 a_n \Delta t^n + (-1)^{n/2} \binom{n-2}{n/2} 2^2 a_{n-2} \Delta t^{n-2} + \dots + (-1)^2 \binom{2}{2} 2^{n-2} a_2 \Delta t^2 \\
 & \cdot \quad \quad \quad \cdot \quad \quad \quad \cdot \quad \quad \quad \cdot \\
 & \cdot \quad \quad \quad \cdot \quad \quad \quad \cdot \quad \quad \quad \cdot \\
 & \cdot \quad \quad \quad \cdot \quad \quad \quad \cdot \quad \quad \quad \cdot \\
 c_{2n} &= (-1)^n \binom{n}{n} 2^0 a_n \Delta t^n = a_n \Delta t^n
 \end{aligned}$$

2.1.4 Bilinear Transform

The following transform is the equivalent of using a trapezoidal approximation (bilinear) to a derivative

$$j\omega \approx \frac{2}{\Delta t} \cdot \frac{(z-1)}{(z+1)} \tag{14}$$

where

$$\begin{aligned}
 c_0 &= \alpha_{00} a_0 2^0 \Delta t^n + \alpha_{01} a_1 2^1 \Delta t^{n-1} + \alpha_{02} a_2 2^2 \Delta t^{n-2} + \dots + \alpha_{0n} a_n 2^n \\
 c_1 &= \alpha_{10} a_0 2^0 \Delta t^n + \alpha_{11} a_1 2^1 \Delta t^{n-1} + \alpha_{12} a_2 2^2 \Delta t^{n-2} + \dots + \alpha_{1n} a_n 2^n \\
 c_2 &= \alpha_{20} a_0 2^0 \Delta t^n + \alpha_{21} a_1 2^1 \Delta t^{n-1} + \alpha_{22} a_2 2^2 \Delta t^{n-2} + \dots + \alpha_{2n} a_n 2^n \\
 & \vdots \quad \quad \quad \vdots \quad \quad \quad \vdots \quad \quad \quad \vdots \quad \quad \quad \vdots \\
 & \vdots \quad \quad \quad \vdots \quad \quad \quad \vdots \quad \quad \quad \vdots \quad \quad \quad \vdots
 \end{aligned} \tag{15}$$

$$c_n = \alpha_{n0} a_0 2^0 \Delta t^n + \alpha_{n1} a_1 2^1 \Delta t^{n-1} + \alpha_{n2} a_2 2^2 \Delta t^{n-2} + \dots + \alpha_{nn} a_n 2^n$$

Where

$$\alpha_{00} = \binom{n}{0} \quad ; \quad \alpha_{01} = \alpha_{02} = \alpha_{03} = \dots = \alpha_{0n} = 1 \quad : c_0$$

dimensional (1-D) case of a plane wave traveling in the x direction. The general model FDTD algorithm may be summarized as follows:

$$E^{n+1} = \frac{1}{c_0} \begin{pmatrix} d_0 D^{n+1} + d_1 D^n + d_2 D^{n-1} + \dots + d_p D^{n-p} \\ -c_1 E^n - c_2 E^{n-1} - \dots - c_p E^{n-p} \end{pmatrix} \quad (19)$$

Where the electric field E and flux density D are evaluated.

We illustrate minimum storage implementations of the E^{n+1} dispersive algorithms. For (19) equation, we assume for demonstration a four-order permittivity model. Dropping the space dependence for notational convenience, (19) becomes

$$E^{n+1} = \frac{1}{c_0} (d_0 D^{n+1} + d_1 D^n + d_2 D^{n-1} + d_3 D^{n-2} + d_4 D^{n-3} - c_1 E^n - c_2 E^{n-1} - c_3 E^{n-2} - c_4 E^{n-3}) \quad (20)$$

A direct implementation of (20) above would required nine storage arrays: $d_0 D^{n+1}$, $d_1 D^n$, $d_2 D^{n-1}$, $d_3 D^{n-2}$, $d_4 D^{n-3}$, $c_1 E^n$, $c_2 E^{n-1}$, $c_3 E^{n-2}$ and $c_4 E^{n-3}$. Equation (20) above may be rewritten in the form of the following equations:

$$\begin{cases} W_4^{n+1} = \frac{1}{\epsilon_0} d_4 D_x^{n+1} - C_4 E_x^{n+1} \\ W_3^{n+1} = \frac{1}{\epsilon_0} d_3 D_x^{n+1} - C_3 E_x^{n+1} + W_4^n \\ W_2^{n+1} = \frac{1}{\epsilon_0} d_2 D_x^{n+1} - C_2 E_x^{n+1} + W_3^n \\ W_1^{n+1} = \frac{1}{\epsilon_0} d_1 D_x^{n+1} - C_1 E_x^{n+1} + W_2^n \\ E_x^{n+1} = \frac{1}{\epsilon_0} (D_x^{n+1} + W_1^n) \end{cases} \quad (21)$$

the explicit update equations represented by (21). Note that (21) do not require previous time storage of the E_x or D_x field, but do require storage of W_1 to W_4 and at time step n only, since W_1 to W_4 overwrite their own previous time values. Hence, (20) may be implemented using eight storage arrays instead of nine.

2.3 Extraction of Drude Model From General Model

At optical wavelengths, it may be important to treat electromagnetic wave interactions with metals using a dispersive formulation to properly account for the physics of internal electron motion. At the macroscopic scale, the Drude model

has become widely used for such modeling. The Drude model permittivity function is written as [1],

$$\epsilon_D = \epsilon_\infty + \frac{\omega_D^2}{\omega(j\gamma - \omega)} \quad (22)$$

Where ω_D is the plasma frequency and γ is the damping coefficient. It can be written

$$\epsilon_D(\omega) = \frac{a_0 + a_1(j\omega) + a_2(j\omega)^2}{b_1(j\omega) + b_2(j\omega)^2} \quad (23)$$

Where

$$\begin{cases} a_0 = \omega_D^2 \\ a_1 = \epsilon_\infty \gamma \\ a_2 = \epsilon_\infty \end{cases} ; \begin{cases} b_0 = 0 \\ b_1 = \gamma \\ b_2 = 1 \end{cases}$$

So, Drude model is a special case of the general model. For the four-order General model, the permittivity function is of the form,

$$\epsilon(\omega) = \frac{a_0 + a_1(j\omega) + a_2(j\omega)^2 + a_3(j\omega)^3 + a_4(j\omega)^4}{a_0 + a_1(j\omega) + a_2(j\omega)^2 + a_3(j\omega)^3 + a_4(j\omega)^4} \quad (24)$$

Where

$$\begin{cases} a_0 = (\omega_D \omega_L)^2 \\ a_1 = \gamma(\epsilon_\infty + \Delta\epsilon)\omega_L^2 + 2\delta\omega_D^2 \\ a_2 = \omega_D^2 + (\epsilon_\infty + \Delta\epsilon)\omega_L^2 + 2\delta\gamma\epsilon_\infty ; \\ a_3 = \epsilon_\infty(\gamma + 2\delta) \\ a_4 = \epsilon_\infty \end{cases} \begin{cases} b_0 = 0 \\ b_1 = \gamma\omega_L^2 \\ b_2 = \omega_L^2 + 2\delta\gamma \\ b_3 = (\gamma + 2\delta) \\ b_4 = 1 \end{cases}$$

Where ω_L is the resonant frequency and δ is the damping coefficient in the Lorentz model[1].

3 Validation of the FDTD Method with the General Model

In this section, FDTD formulation is used to calculate the transient reflected and transmitted fields from a gold slab due to the incidence of a gaussian pulse. The real and imaginary parts of the gold permittivity calculated with the Drude and general models, are, respectively, plotted. Furthermore, scattering from a finite nanocylinder has been calculated, and results are compared with the Mie theory [14].

3.1 Reflected and Transmitted Transient Fields From A Slab

The developed dispersive media FDTD formulation is used to obtain of Propagation of electric field in the time domain due to the scattering from a 100 nm-thick gold slab illuminated by an incident plane wave of gaussian waveform, as shown in Figure 1. The material parameters for the gold slab are obtained to be in table 1. values of Z Transform the parameters used for the Drude and the general models in table 2. We obtain values of table 2 using from Backward Difference Approximation.

Table 1. Values of the parameters used for the Drude and the General models in frequency domain.

Model	a_0	a_1	a_2	a_3	a_4	b_0	b_1	b_2	b_3	b_4
Drude	1.83×10^8	1.04×10^{18}	9.07	0	0	0	1.15×10^{17}	1.00	0	0
General	3.74×10^{63}	1.82×10^{47}	3.51×10^{32}	5.70×10^{15}	5.83	0	2.48×10^{45}	2.18×10^{31}	1.19×10^{15}	1.00

Table 2. Values of the parameters used for the Drude and the General models in Z domain.

Model	c_0	c_1	c_2	c_3	c_4	d_0	d_1	d_2	d_3	d_4
Drude	10.80	-19.87	9.07	0	0	1.19	-2.19	1.00	0	0
General	5.84	-23.35	35.01	-23.33	5.83	1.00	-4.00	6.00	-4.00	1.00

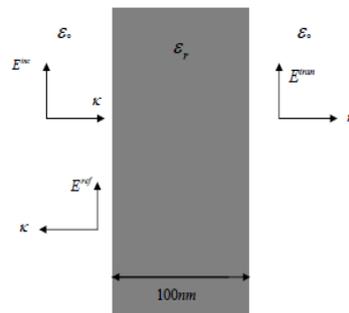


Figure1 gold slab and directions of the incident, reflected, and transmitted fields.

The reflected and transmitted fields due to the incidence of a plane wave of Gaussian waveform are calculated in the one-dimensional computation space. Figure2 shows how the field propagate. It can be seen that field is generated while the Gaussian wave propagates through the slab. The transient reflected and transmitted fields are calculated. The one-dimensional FDTD computation space consists of 2000 cells and has 1000 nm length. Thus, the time step value used is $\Delta t = \Delta x/c$ and the 100 nm-thick slab is 200 cells wide. A cell size of 1/10 of the wavelength is recommended [8]:

$$\Delta x = \lambda_0 / 10$$

Where λ_0 is the free space wavelength in the simulation domain. The transmitted field is calculated at 300 nm away from the right boundary of the slab and the reflected fields are calculated at 600 nm away from the left boundary of the slab.

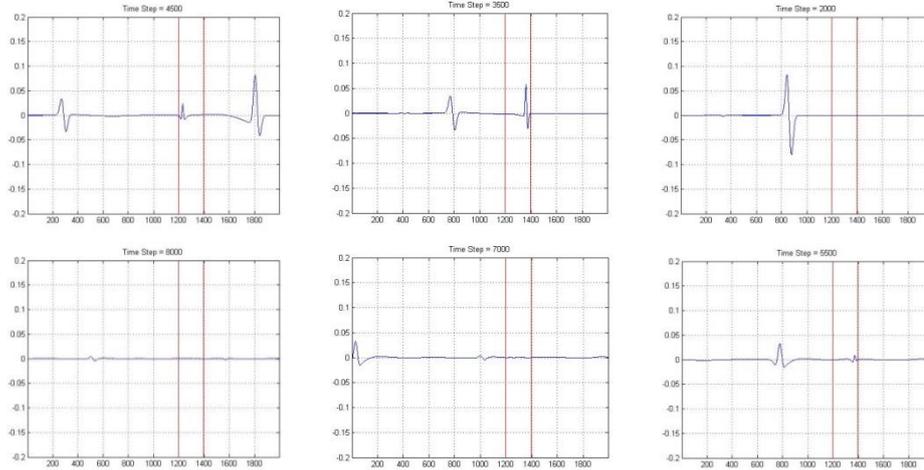


Figure2 Propagation of Pulse reflected and transmitted from gold slab.

We will calculate the coefficient of transmission in amplitude for the electric field using the formulas that appear in reference14, for a slab. In Figure 3, we present the results obtained considering a slab of thickness 20 nm. The absolute values of the transmission coefficient, computed through the FDTD implementation of the General Model. It can be observed in Figure3 that the agreement between the General Model and the analytical one is quite good.

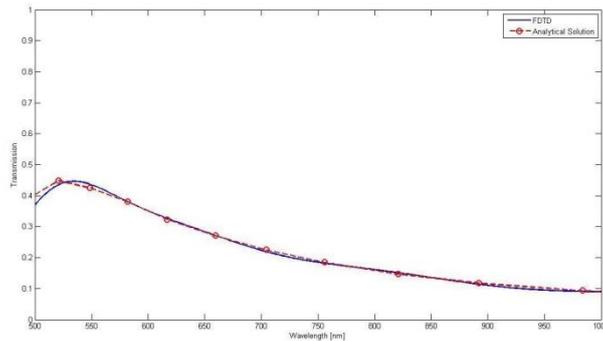


Figure3 Coefficient of transmission through a layer of 20 nm of gold, respectively, calculated analytically, with the general model.

The real and imaginary parts of the permittivity, calculated with the general model. In order to find the best set of parameters and the best fit of ϵ we employ the same optimization scheme as we did for the Drude model. The new parameters are presented in the second row of Table I and II. Figures 4 and 5

compares the relative permittivity of gold obtained from Drude model with the general model. In the near infrared, Drude model gives an acceptable description of the permittivity of gold. However, it can not accurately describe the dispersion function of gold in the optical range. Although a good agreement is achieved for wavelengths above 700nm, there exists a strong discrepancy for shorter wavelengths. This can be explained by the fact that in Drude model, the inter-band transitions are not considered.

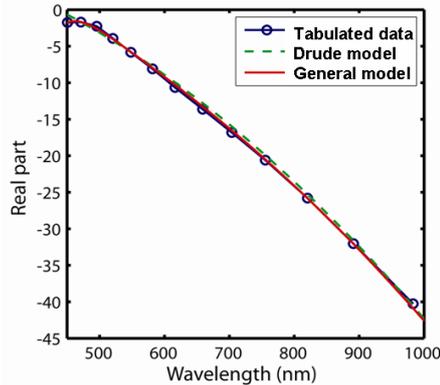


Figure 4 Real part of the permittivity of gold calculated with the Drude model and calculated with the general model.

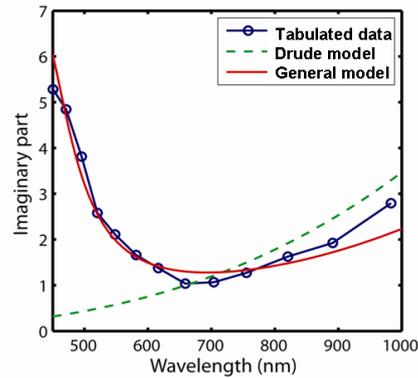


Figure 5 Imaginary part of the permittivity of gold calculated with the Drude model and calculated with the general model.

3.2 Light Scattering From A Nanoparticle

In order to validate our approach, we consider the scattering of a TE polarized plane wave by an infinite gold cylinder with circular cross section of radius 50 nm ($0.05 \mu\text{m}$). We compute the scattering cross section (SCS) and compare it with the analytical solution calculated by Mie theory in reference 14. To concentrate on the error related to the dispersion model, we choose very fine mesh ($dx = 1 \text{ nm}$) to reduce the staircasing error. Figure 6 depicts the computed SCS for Drude, General and Mie theory using the permittivity obtained from General model and those published in reference 16. It is observed that the agreement between the Drude model and the analytical solution decreases for wavelength below 700 nm, while the general model shows quite good agreement with the analytical solution. This behavior can be visualized further by plotting the relative error on the SCS for Drude and general models. The logarithmic plot in Figure 7 illustrates that the General leads to a very small error on a wide spectrum, while the Drude model accuracy is out of discussion around the resonance which is the most important part of the spectrum.

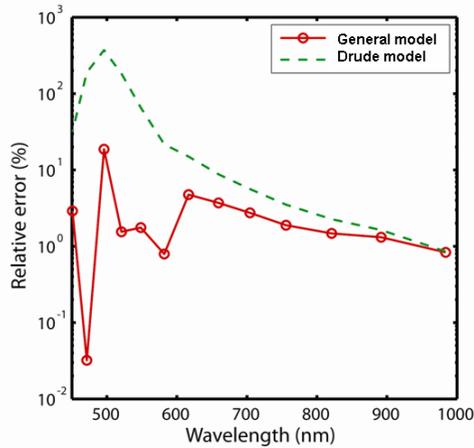


Figure 6 the computed SCS for Drude model, general model and Mie theory.

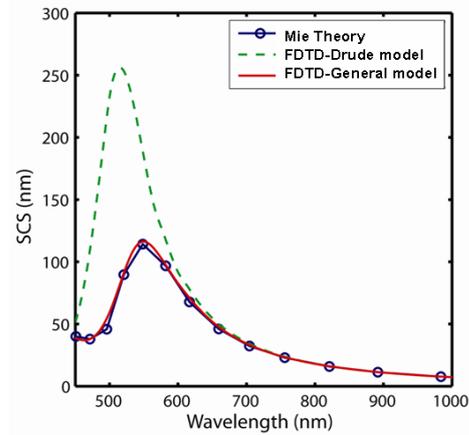


Figure 7 the relative error on the SCS for Drude and general models.

4 Conclusion

A new scattered FDTD formulation for dispersive materials are developed using the Z transform and frequency approximation methods. The General Model is proposed in this paper for simulation of dispersive materials in a visible wavelength range. It is shown that the quite good agreement between general model and the analytical solution in region of visible wavelengths. This behavior is illustrated further by plotting the relative error on the SCS for Drude and general model.

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