The Analysis of Optical Properties of Nanoparticles Using General Model

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Abstract

In this paper, a dispersion model, referred to as the general model, is proposed for modeling dispersive materials in wide wavelength range using the Finite-Difference Time-Domain (FDTD) method. A parameter estimation method is introduced for the general model to fit material permittivity functions fast and accurately. The improved FDTD method with the general model is implemented and verified in simulation of the nanowires. The scattering cross-section (SCS) spectrum characteristics of different nanoparticles are systematically studied by employing the implemented method. The optical properties such as SCS and electric field enhancement of nano-ellipses are simulated by the accelerated 2D FDTD method and those of nano-ellipsoids are simulated by the accelerated 3D FDTD method.

Keywords: FDTD, general model, nanoparticles.

1. Introduction

Dispersive materials, such as metals, are widely used in optical devices. The Finite-Difference Time-Domain (FDTD) method [1] is one of the most common choices for simulating such devices in a wide frequency range. 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 dispersion models, such as multi-pole Debye, Drude, and Lorentz models, have been widely adopted for modeling dispersive materials using the FDTD method [3]. To fit permittivity function of a given material accurately in a wide frequency range, a large number of poles are required in these models. Rakic and Djurisic used the Durde model with up to five Lorentzian terms to fit the permittivity functions of eleven metals [4]. Hao and Nordlander proposed an improved model consisting of four Lorentzian terms to fit dielectric data of gold [5]. All the proposed multi-pole models archived good fit to the measure data. However, using a dispersion model with a large number of poles not only requires a lot of efforts for modal parameter estimation but also dramatically increases the memory and computational costs of the FDTD method [6]. Han, Dutton and Fan proposed a complex-conjugate pole-residue pair model and implemented it in the FDTD method to increase the modeling efficiency [7, 8]. However, these authors did not propose an efficient method for the parameters estimation. The FDTD formulation for dispersive materials are developed using the Z transform and frequency approximation methods [9]. In this paper, a dispersion model, referred to as the general model with a parameter estimation method is proposed for the simulation of optical properties of arbitrary linear dispersive media over a wide wavelength range. The conventional Debye, Drude and Lorentz models are derivable from this general model. The time domain properties of the proposed model are analyzed. It is demonstrated that the model can fit the relative permittivity data of a material accurately and efficiently in a wide wavelength range and the parameters of this model can be estimated requiring
no initial guess. The general model is implemented in the FDTD method as a powerful and computationally efficient tool for simulating nanoparticles of dispersive materials in a wide wavelength range of light. By employing this model, a systematic study of the optical properties of different nanoparticles gives a good reference for designs of optical devices utilizing the cross-section spectra characteristics of nanoparticles.

2. General Dispersion Model

Assuming the time harmonic dependence, $e^{j\omega t}$, the general model is proposed to describe the dispersive material’s relative permittivity expressed by the fraction form as

$$\varepsilon_r(\omega) = \frac{\sum_{k=1}^{N} a_k(j\omega)^k}{\sum_{k=1}^{N} b_k(j\omega)^k}$$

Where $a_k, b_k$ are real numbers. 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. To be conveniently adopted by the FDTD method, the general model is represented by its partial fraction expansion described by

$$\varepsilon_r(\omega) = \varepsilon_\infty + \sum_{k=1}^{L} \chi_k(\omega)$$

Where

$$\chi_k(\omega) = \frac{\sum_{n=0}^{L_k} c_n(j\omega)^n}{\sum_{n=0}^{L_k} d_n(j\omega)^n}$$

Where $C_k, D_k$ are real numbers.

Or,

$$\chi_k(\omega) = \begin{cases} \frac{r_k}{j\omega-p_k} &; \text{if } p_k \text{ is real} \\ \frac{r_k}{j\omega-p_k} + \frac{r_k^*}{j\omega-p_k^*} &; \text{if } p_k \text{ is complex} \\ \sum_{u=1}^{L_k} \frac{r_{ku}}{(j\omega-p_k)^u} &; \text{if } p_k \text{ is a multiple root} \end{cases}$$

Where $\varepsilon_\infty, r_k$, and $p_k$ are the direct coefficient, residue, and pole, respectively. The partial fraction term $\chi_k(\omega)$, is the frequency domain susceptibility function. It has three forms depending on the properties of the pole $p_k$: 1) a real fraction term with a real residue and a real pole, when $p_k$ is a real number; 2) two complex fraction terms consist of complex conjugate residue and pole pairs, when $p_k$ is a complex number; and 3) a summation of fraction terms which contains high order (>1) of $j\omega$, when $p_k$ is a multiple root of the denominator $\sum_{k=1}^{N} b_k(j\omega)^k$. It is observed that the third expression of $p_k$ should be avoided in the parameter estimation procedure because the high order (the order of $j\omega$ is higher than one) partial fraction terms make it difficult to implement this model in the FDTD method. If there are $L_1$ real poles and $L_2$ complex conjugate pole pairs, the upper bound of the summation in equation (2) is $L = L_1 + L_2$, and the total pole number is $N = L_1 + 2L_2$.

Table 1 shows relationships of the general model with other dispersion models. It shows that Debye, Drude, and Lorentz models are all special cases of general model with specified parameters. The general model treats the Debye, Drude, and Lorentz materials in a unified.
### Table 1: Coefficients of dispersion models.

<table>
<thead>
<tr>
<th>Model</th>
<th>$\varepsilon_0(\omega)$</th>
<th>$L$</th>
<th>$p_k$</th>
<th>$r_k$</th>
<th>$p_{k+1}$</th>
<th>$r_{k+1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Debye</td>
<td>$\varepsilon_0 + \sum_{p=1}^{N_p} \frac{\Delta \varepsilon_p}{j\omega \gamma_p + 1}$</td>
<td>$N_p$</td>
<td>$-1/\gamma_k$</td>
<td>$\frac{\Delta \varepsilon_k}{\gamma_k}$</td>
<td>$-$</td>
<td>$-$</td>
</tr>
<tr>
<td>Drude</td>
<td>$\varepsilon_0 + \sum_{p=1}^{N_p} \frac{\alpha_p^2}{\omega^2 + j\omega \gamma_p}$</td>
<td>$2N_p$</td>
<td>$0$</td>
<td>$\frac{\alpha_p^2}{\gamma_p}$</td>
<td>$-\gamma_p$</td>
<td>$\frac{\alpha_p^2}{\gamma_p}$</td>
</tr>
<tr>
<td>Lorentz</td>
<td>$\varepsilon_0 + \sum_{p=1}^{N_p} \frac{\Delta \varepsilon_p \alpha_p^2}{\omega^2 + 2j\omega \gamma_p + \omega_p^2}$</td>
<td>$N_p$</td>
<td>$-\gamma_p - j\sqrt{\omega^2 - \gamma_p^2}$</td>
<td>$\frac{\Delta \varepsilon_k \alpha_k^2}{2\sqrt{\omega^2 - \gamma_p^2}}$</td>
<td>$-$</td>
<td>$-$</td>
</tr>
<tr>
<td>Complex-conjugate pole-residue pair</td>
<td>$\varepsilon_0 + \sum_{p=1}^{N_p} \frac{r_k}{\omega - p_k} + \frac{r_k^<em>}{\omega - p_k^</em>}$</td>
<td>$N_p$</td>
<td>Complex number</td>
<td>Complex number</td>
<td>$-$</td>
<td>$-$</td>
</tr>
</tbody>
</table>

Formulation, which simplifies the implementation of dispersion models in numerical simulation algorithms, such as the FDTD method. It also shows that when, $p_k$ is a complex number, the partial fraction form of the general model is the same as the complex conjugate pole-residue pair model.

To study properties of the general model in time domain, the inverse Fourier transformation is performed on the frequency domain susceptibility function $\chi_k(\omega)$ defined in equation $(2b)$. If $p_k$ is a real number, the time domain susceptibility is expressed by

$$
\chi_k(t) = r_k e^{p_k t} U(t)
$$

Where, $U(t)$ is the unit step function. It shows that when $p_k > 0$, the susceptibility is exponentially growing with time, which contradicts the phenomenon that the light wave is decaying when propagating in lossy materials, such as metals. Thus, the parameter $p_k$ should not be greater than zero when modeling lossy materials in this model. If $p_k$ is a complex number, the frequency domain susceptibility can be reformed as

$$
\chi_k(\omega) = \frac{(-r_k p_k p_k^* - \alpha_k \alpha_k^*)}{-\omega^2 - (p_k^2 + p_k \alpha_k^*)/\omega + p_k^* p_k} + \frac{(r_k + r_k^*)}{-\omega^2 - (p_k^2 + p_k \alpha_k^*)/\omega + p_k^* p_k}
$$

The time domain susceptibility is obtained by taking the inverse Fourier transformation, as expressed by

$$
\chi_k(t) = \xi_k e^{-\alpha_k t} \sin(\kappa_k t) U(t) + \frac{d}{dt} \left[ \xi_k e^{-\alpha_k t} \sin(\kappa_k t) U(t) \right]
$$

Where

$$
\alpha_k = \frac{-(p_k^2 + p_k)}{2}, \quad \kappa_k = \sqrt{p_k^2 p_k - \alpha_k^2}, \quad \xi_k = \frac{-(r_k p_k^2 - p_k r_k^*)}{\kappa_k}, \quad \xi_k^* = \frac{(r_k + r_k^*)}{2}
$$

It is noteworthy that when the real part of $p_k$ is positive, the parameter $\alpha_k$ is negative ($\alpha_k < 0$). The time domain susceptibility $\chi_k(t)$ will grow exponentially with time, which contradicts the property of the lossy materials. The above analysis comes out a natural conclusion that the real part of the pole parameter $p_k$ should not be bigger than zero $\alpha_k > 0$, when using the general model to model lossy dispersive materials.
The general model can be easily and efficiently implemented in the FDTD method with an auxiliary differential equation (ADE) scheme. In Maxwell’s equations, Ampere’s law in frequency domain is expressed by

\[ j\omega\varepsilon_0\varepsilon_\infty \vec{E} + \sigma\vec{E} + \sum_{k=1}^{L} \vec{J}_k = \nabla \times \vec{H} \]  

(6)

Where, \( \vec{J}_k \) is the polarization current related with each term in the summation of the general model, defined by

\[ \vec{J}_k = \begin{cases} 
    j\omega\varepsilon_0 \vec{E} \frac{r_k}{j\omega-p_k} & \text{if } p_k \text{ is real} \\
    j\omega\varepsilon_0 \vec{E} \left( \frac{r_k}{j\omega-p_k} + \frac{r_k^*}{j\omega-p_k^*} \right) & \text{if } p_k \text{ is complex}
\end{cases} \]  

(7)

As mentioned previously, the multiple-root \( p_k \) should be avoided in the parameter estimation procedure, so that it would not be concerned with the difficult implementation of polarization current in the multiple-root \( p_k \) case. If \( p_k \) is real, \( r_k \) is also real. Then the time-domain polarization current is real and given by

\[ \frac{\partial I_k}{\partial t} - p_k I_k = r_k \varepsilon_0 \frac{\partial E}{\partial t} \]  

(8)

If \( p_k \) is complex, \( r_k \) is also complex. The time-domain polarization current has two parts \( I_k \) and \( I_k' \), corresponding to the two complex poles in equation (7). The two polarization currents are all complex and given by

\[ \frac{\partial I_k}{\partial t} - p_k I_k = r_k \varepsilon_0 \frac{\partial E}{\partial t} \]  

(9)

\[ \frac{\partial I_k'}{\partial t} - p_k^* I_k' = r_k^* \varepsilon_0 \frac{\partial E}{\partial t} \]  

(10)

Because \( E(t) \) is real, if the initial values for the two polarizations current are the same, the two parts are mutual complex conjugate, i.e. \( I_k = I_k' \). Only one complex equation, either equation (9) or (10), needs to be computed in the FDTD calculation. In the following derivation, equation (9) is employed. Therefore, when \( p_k \) is real, the real part of the time domain polarization current is \( \text{Re} \left[ F^{-1}(\vec{J}_k) \right] = 2 \text{ Re } (J_k) \). By applying the inverse Fourier transform on both sides of equation (6), the time domain Ampere’s curl equation is obtained as

\[ \varepsilon_0 \varepsilon_\infty \frac{\partial}{\partial t} E + \sigma E + \sum_{k=1}^{L} m \text{Re}(J_k) = \nabla \times H \]  

(11)

Where \( m = 1 \) if \( p_k \) is real; \( m = 2 \) if \( p_k \) is complex. The time domain polarization current equation and Ampere’s curl equation are combined together and discretized in the explicit FDTD scheme, yielding

\[ E^{n+1/2} = C_a E^{n-1/2} + C_b [\nabla \times H]^n - \text{Re} \left( \sum_{k=1}^{L} \frac{m}{2} (1 + p_k) |J_k|^{n-1/2} \right) \]  

(12)

\[ J_k^{n+1/2} = \kappa_k |J_k|^{n-1/2} + \beta_k \left( \frac{E^{n+1/2} - E^{n-1/2}}{\Delta t} \right) \]  

(13)

Where
The discretization of the magnetic field $\mathbf{H}^{n+1/2}$ is the same as it is in the standard FDTD algorithm [10]. This is an efficient implementation of the general model in the FDTD method. With the same number of poles, the general model takes no additional memory and computational costs for updating the auxiliary equations of the polarization currents compared with the conventional dispersion models such as multi-pole Lorentz-Drude model. However, the general model offers more degrees of freedom in fitting a permittivity function in the parameter estimation process. Thus, the implementation of the general model in the FDTD method is far more computationally efficient compared to those of Lorentz-Drude model. The general model is an analytical function that describes the relative permittivity of a dispersive material. To fit a given relative permittivity curve accurately and quickly, a parameter estimation procedure is highly demanded in obtaining a good initial guess for the starting point and locating a good approximation to the global optimum.

The advantage of the fraction form of the general model in equation (1a) lies in the fact that a very good initial guess of parameters $a_k$ and $b_k$ can be quickly obtained using the rational approximation method [11, 12]. After that, the initial values of the residues $r_k$, poles $p_k$, and direct coefficient $\varepsilon_\infty$ are obtained from the parameters $a_k$ and $b_k$ by converting the general model from the rational fraction form to the partial fraction form. Finally, the initial values are employed in a simulated annealing algorithm [13] to find the optimized values of parameters; $\varepsilon_\infty$, $p_k$ and $r_k$. The high efficiency of the general model is demonstrated in modeling metal materials Au (gold in a wide range of wavelength from 400 to 1100 nm). The measured relative permittivity of these three metals [14] is fitted using four dispersion models: the $4$-pole Lorentz-Drude model ($1$ Drude pole pair and $1$ Lorentz pole pair), the $6$-pole Lorentz-Drude model ($1$ Drude pole pair and $2$ Lorentz pole pairs), the general model with $4$ poles, and the general model with $6$ poles. The Lorentz-Drude model is expressed in the equation:

\[
\begin{align*}
\varepsilon_f(\omega) &= \varepsilon_\infty + \frac{\alpha_b}{-\omega^2 + j\omega\gamma_B} + \sum_{l=1}^{N_L} \frac{\Delta\varepsilon_l\omega_l^2}{-\omega^2 + 2j\omega\gamma_l + \omega_l^2} \\
\end{align*}
\]  

(15)

Where, the numbers of Drude, and Lorentz pole pairs are one, and $N_L$ respectively. As it is shown in Figure 1, both the Lorentz-Drude model and the general model achieve better accuracy with more number of poles. However, the general model overwhelms the Lorentz-Drude model with significant improvement of accuracy while having the same number of poles. Moreover, for some materials such as Au, the general model with $4$ poles fits the experimental data to a higher accuracy than that of the $6$-pole Lorentz-Drude model, while having much lower computational cost. The general model with $6$ poles performs a much more accurate fit than the $6$-pole Lorentz-Drude model, while having the same computational cost. black circles are experimental data taken from [13]; the black dot and dash lines are fitting curves with $4$-pole Lorentz-Drude model ($1$ Drude pole pair and $1$ Lorentz pole pair) and $6$-pole Lorentz-Drude model ($1$ Drude pole pair and $2$ Lorentz pole pairs), respectively; the solid red and blue lines are the fitting curves with $4$-pole and $6$-pole general model, respectively.

To demonstrate the advantages of the general model in terms of the modeling accuracy, a convergence test of the general model is performed on the three metal materials Au. The convergence of the general model is studied by measuring the relative errors of the modeled permittivity with increasing the number of poles. The relative error of the modeled permittivity to the experimental data is defined by

\[
\varepsilon_{rel}(dB) = 5[log(\sum_i^N|e^{exp}(\omega_i) - \varepsilon(\omega_i)|^2) - log(\sum_i^N|e^{exp}(\omega_i)|^2)]
\]  

(16)
Figure 1: (a) Real and (b) imaginary parts of the permittivity function of Au.

Figure 2, depicts the relative errors of the general model and the Lorentz-Drude mode in modeling the permittivity of the metal materials Au. It shows that increasing the number of poles, both the general model and the Lorentz-Drude model reduce the relative error. However, the general model converges faster than the Lorentz-Drude model. The parameters of the Lorentz-Drude model and the general model for modeling material Au are listed in Table 2 and Table 3, respectively.

Figure 2: Relative errors of modeled permittivity of Au.

Table 2: Values of the parameters for the Lorentz-Drude Model (Au).

<table>
<thead>
<tr>
<th>Parameters</th>
<th>1 Drude</th>
<th>2 Drude</th>
<th>3 Drude</th>
<th>4 Drude</th>
<th>5 Drude</th>
<th>1 Lorentz</th>
<th>2 Lorentz</th>
<th>3 Lorentz</th>
<th>4 Lorentz</th>
<th>5 Lorentz</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\varepsilon_0$</td>
<td>6.07</td>
<td>5.06</td>
<td>2.54</td>
<td>1.00</td>
<td>1.00</td>
<td>8.83</td>
<td>8.74</td>
<td>8.65</td>
<td>8.23</td>
<td>8.22</td>
</tr>
<tr>
<td>$\omega_p (eV)$</td>
<td>5.62e-2</td>
<td>6.27e-2</td>
<td>6.60e-2</td>
<td>1.04e-7</td>
<td>3.54e-8</td>
<td>1.93</td>
<td>7.36e-1</td>
<td>8.83e-1</td>
<td>1.19</td>
<td>5.32e-1</td>
</tr>
<tr>
<td>$\Delta \varepsilon_1$</td>
<td>3.04</td>
<td>2.75</td>
<td>3.08</td>
<td>3.09</td>
<td>2.68</td>
<td>5.03e-1</td>
<td>2.86e-1</td>
<td>3.05e-1</td>
<td>3.87e-1</td>
<td>2.64e-1</td>
</tr>
<tr>
<td>$\omega_1 (eV)$</td>
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<td>1.31</td>
<td>1.91</td>
<td>2.9</td>
<td>2.89</td>
<td>-</td>
<td>3.32</td>
<td>3.93</td>
<td>4.29</td>
<td>4.28</td>
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<tr>
<td>$\omega_2 (eV)$</td>
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<td>3.49e-1</td>
<td>5.86e-9</td>
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<td>1.89e-7</td>
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<td>6.52e-1</td>
<td>5.29e-1</td>
<td>1.18</td>
<td>-</td>
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<tr>
<td>$\Delta \varepsilon_2$</td>
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<td>1.18</td>
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<td>$\omega_3 (eV)$</td>
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<td>2.69</td>
<td>2.68</td>
<td>3.09</td>
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<td>$\omega_4 (eV)$</td>
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<td>$\Delta \varepsilon_3$</td>
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<tr>
<td>$\omega_6 (eV)$</td>
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<tr>
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</tr>
</tbody>
</table>
3. Numerical Simulations

In this section, the general model is employed for modeling material properties of metal nanoparticles in the light wave range with the FDTD method. It improves the accuracy of material modeling while does not increase the computing cost of the FDTD method. The optical properties such as scattering cross-section and electric field enhancement of nano-ellipses are simulated by the accelerated 2D FDTD method and those of nano-ellipsoids are simulated by the accelerated 3D FDTD method. The parameters employed for modeling the gold material with the general model in the FDTD method are similar to what is listed in Table 3. 6 poles are used in the general model for all the simulations.

### 3.1 Simulation of Nano-ellipsoid

The simulation results of the optical scattering properties of a gold nano-ellipsoid with different radii surrounding by air are produced by the three-dimensional (3D) FDTD method combined with the general model. In the 3D FDTD simulation, a uniform mesh size of 1.0 nm is employed and 30,000 time steps are performed. In Figure 3, the scattering cross-section spectrum of nano-ellipsoid with above four different configurations are compared and depicted. Figure 3, shows that the scattering effect is enhanced by the volume of the nanoparticle.

![Figure 3: Scattering cross section spectrum of gold nano-ellipsoids with different radii and incident wave polarizations.](image)

### 3.2 Simulation of Nano-ellipse

The optical properties such as the scattering cross section of a gold nano-ellipse with different configurations regarding the differences of sizes, incident wave angle and background materials are simulated using the 2D FDTD method accelerated by the high performance GPU hardware with parallel computing technique. The TM polarization is used in the 2D FDTD simulations. The structure of the nano-ellipse is showed in Figure 4. It has a longer radius $r_2$ and a shorter radius $r_1$. The nano-
ellipse is illuminated by an incident plane wave propagating toward it with an angle of alpha to the $r_2$ axis. The optical properties of this particle are studied in three cases. In the first case, the nano-ellipse with a longer radius $r_2 = 20$ nm and a shorter radius $r_1 = 10$ nm is surrounded by air. The plane wave propagates toward it from different directions, which means the angle alpha changes to different values. In the Figure 5a, scattering cross section increases when angle alpha varying from 0 degree to 90 degree. It shows that the peak of the scattering cross section increases when angle size changes from 0 to 90 degrees. When the longer axis of the nano-ellipse aligns with electric field polarization direction (alpha=90 degrees), the peaks reach the maximum. However, the peak positions in the spectra do not change in the simulations.

Figure 4: Structure of a single nano-ellipse illuminated by an incident plane wave.

Figure 5: Scattering cross section spectrum of a nano-ellipse: a) with incident wave illuminating from different directions, b) surrounded by different materials.

In the second case, the nano-ellipse has the same size as that in the first case and the electric field of the incident wave is polarized to the direction in the radius axis (alpha=90 degrees). However, different surrounded materials such as air (index=1.0), water (index=1.33), silica (index=1.42), Polymethyl Methacrylate (index=1.49) and silicon (index=3.2) are used in the simulations. The scattering cross sections are depicted in Figure 5b. It shows that peak of the scattering cross section increase along with the increase of the background material refractive index. With the increase of the background refractive index, the peak positions in the spectra will shift to the long wavelengths (red shift).

3.3 Non-regular cross section

We study the variation of SCS due to the nanoparticle shape. We consider three simple shapes, namely a rectangle, equilateral triangle, and right triangle. Figure 6, compares the SCS for these shapes. As it is shown, changing the shape affects the SCS amplitude, the resonance shift and line width. It is worth recalling the SCS dependence on the illumination direction which is actually stronger when the symmetry of the particle is reduced.

3.4 Circular cross section

As the last test, the FDTD method is a rigorous numerical tool for simulating nanoparticle problems by solving Maxwell’s equations accurately. However, it is extremely memory and time consuming.
when dealing with metal nanostructures in the wavelength range of light due to two reasons: 1) the small feature size of the structure requires very fine meshes and time steps; and 2) the complicated dispersion property dramatically increases the implementation complexity and computational cost. Therefore, it is strongly desired to have a simulation tool, which can accurately model the wide band dispersion properties, yet taking an affordable computation effort.

To exam the efficiency of the general model with different numbers of poles, the light wave scattering phenomenon of an Au nanowire with 40 nm diameter surrounded by air is simulated by the 2D FDTD method using the general model in a wide wavelength range from 400 to 1100 nm. A uniform mesh size of 0.5 nm is employed and 20,000 time steps are performed. Figure 7, shows the cross section curves calculated using the analytical solution, the FDTD method with 1 Drude pole pair and 2 Lorentz pole pairs (scheme 1), the FDTD method with the 4-pole general model (scheme 2), and the FDTD method with the 6-pole general model (scheme 3), respectively.

Table 4, lists the memory and computational costs of different FDTD schemes, as well as the relative errors of the extinction cross-section compared with the analytical solution. It shows that compared with the conventional Lorentz-Drude model, the FDTD method with the 4-pole General Model achieves a smaller relative error while taking much less computational effort, and the FDTD method with the 6-pole achieves even better accuracy yet maintaining a comparable computational cost.

<table>
<thead>
<tr>
<th>Scheme</th>
<th>Memory (mega-byte)</th>
<th>Computation time (second)</th>
<th>Relative error (dB) (Extinction cross section)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Scheme 1 (1 Drude pole pair and 2 Lorentz pole pairs)</td>
<td>6.600</td>
<td>694.58</td>
<td>-23.97</td>
</tr>
<tr>
<td>Scheme 2 (4 General Model poles)</td>
<td>5.872</td>
<td>599.26</td>
<td>-25.31</td>
</tr>
<tr>
<td>Scheme 3 (6 General Model poles)</td>
<td>6.604</td>
<td>702.04</td>
<td>-26.04</td>
</tr>
</tbody>
</table>

It proves that the general model is more efficient in terms of memory and computational costs in modeling dispersive materials in comparison with conventional models. It is a powerful and efficient tool for simulating broadband optical phenomena of nanoparticles with dispersive materials.
Figure 7: Scattering cross section: the black circles are analytical solution with experimental data [13]; the black dash line is the FDTD solution with 1 Drude pole pair and 2 Lorentz pole pairs; the solid red and blue lines are the FDTD solutions with 4-pole and 6-pole, respectively.

Conclusion

The general model with a parameter estimation method is proposed in this paper for simulation of dispersive materials in a wide wavelength range. The general model is proven to be more efficient in terms of memory and computational costs in comparison with conventional phenomenological models. The general model is implemented in the FDTD method, forming a powerful and efficient tool for simulating broadband optical phenomena of nanoparticles with dispersive materials. This method is applied to analyze the optical properties of gold nanoparticles. The characteristics of the cross section spectra affected by the geometry and background material of the nanoparticles are carefully studies. This systematic study of the optical properties of different nanoparticles gives a good reference for design of optical devices utilizing the cross section spectra characteristics of nanoparticles.

References