

Chapter 33

Computer Simulations of Solar Energy Systems

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ABSTRACT

In recent years, computer simulation has become a standard tool for analyzing solar energy systems. The interaction of light with nanoscale matter can provide greater functionality for photonic devices and render unique information about their structural and dynamical properties. As the field of nanophotonics continues to experience phenomenal growth at both the fundamental research and applications level, computational modeling is essential both for interpreting experiments and for suggesting new directions – for example, in designing of thin-film photovoltaic cells. The demand for computer simulation continues to increase as researchers and developers tackle the tough challenges of designing new generation devices and optimizing current generation devices. This chapter is devoted to the development and application of the Finite-Difference Time-Domain (FDTD) method to solar energy systems. In addition, new models covering the latest advances in nanophotonics technologies, as well as key improvements to the numeric solvers and new usability features, are introduced in this chapter.

INTRODUCTION

Thin-film solar cells offer the possibility to improve efficiencies and lower costs in next generation photovoltaic devices. Further, light trapping is the standard technique for improving solar cell efficiencies and for harvesting the spectrum of incoming sunlight.

In order to describe the propagation and scattering of sunlight within the solar cell and optimize the process, Maxwell's equations have to be rigorously solved. Some of the well-adopted simulations for optical simulations are the finite difference time domain (FDTD) method (Qiu and He, 2000; Farjadpour *et al.*, 2006; Ong *et al.*, 2007; Tsakalakos *et al.*, 2007), the transfer matrix (TM) method (Hu and Chen, 2007), and scattering theory (Street *et al.*, 2008).

DOI: 10.4018/978-1-4666-5125-8.ch033

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FINITE DIFFERENCE TIME DOMAIN (FDTD) METHOD

The FDTD method numerically solves Maxwell's curl equations by representing time and spatial derivatives as finite differences. The basic Maxwell's curl equations in a three dimensional (3D) domain are expressed as (Taflove & Hagness, 2000):

$$\frac{\partial \vec{E}}{\partial t} = \frac{1}{\varepsilon} \nabla \times \vec{H} - \frac{\sigma}{\varepsilon} \vec{E} \quad (1)$$

$$\frac{\partial \vec{H}}{\partial t} = -\frac{1}{\mu} \nabla \times \vec{E} \quad (2)$$

where both the electric field $\vec{E}$ and magnetic field $\vec{H}$ describe the interaction between light and the solar cell. The solar cell is described by its permittivity ε and permeability μ . The parameters, $\varepsilon = \varepsilon_r \varepsilon_o$ and σ describe the optical properties of the solar cell. Expanding the curl operator in (1) and (2) and equating their respective vector components on each side appropriately, these equations can be represented with the following six equations in a Cartesian coordinate system (x, y, z):

$$\frac{\partial H_x}{\partial t} = -\frac{1}{\mu} \left[\frac{\partial E_z}{\partial y} - \frac{\partial E_y}{\partial z} \right] \quad (3)$$

$$\frac{\partial H_y}{\partial t} = -\frac{1}{\mu} \left[\frac{\partial E_z}{\partial x} - \frac{\partial E_x}{\partial z} \right] \quad (4)$$

$$\frac{\partial H_z}{\partial t} = -\frac{1}{\mu} \left[\frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} \right] \quad (5)$$

$$\frac{\partial E_x}{\partial t} = \frac{1}{\varepsilon} \left[\frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} - \sigma E_x \right] \quad (6)$$

$$\frac{\partial E_y}{\partial t} = \frac{1}{\varepsilon} \left[\frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} - \sigma E_y \right] \quad (7)$$

$$\frac{\partial E_z}{\partial t} = \frac{1}{\varepsilon} \left[\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} - \sigma E_z \right] \quad (8)$$

The FDTD algorithm divides the problem geometry into a spatial grid where electric and magnetic field components are placed at certain discrete positions in space, and it solves Maxwell's equations in time at discrete time instances (Taflove & Brodwin, 1975; Yee, 1966). Grid coordinates on a uniform, rectangular FDTD mesh are defined as:

$$(i, j, k) = (i\Delta x, j\Delta y, k\Delta z) \quad (9)$$

in which Δx , Δy , and Δz represent the physical dimensions of each grid cell. Furthermore, any function with temporal and spatial variations can be generally expressed as:

$$s_{i,j,k}^n = (i\Delta x, j\Delta y, k\Delta z) \quad (10)$$

with Δt denoting the time-step and n the corresponding time index. Using this notation, the time and space derivatives of s in central-difference form can be written as:

$$\frac{\partial s_{i,j,k}^n}{\partial x} = \frac{s_{i+\frac{1}{2},j,k}^n - s_{i-\frac{1}{2},j,k}^n}{\Delta x} + O\left[(\Delta x)^2\right] \quad (11)$$

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