High-Performance FDTD Simulations with Sub-Cell/Conformal Meshing in RSoft FullWAVE

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Introduction

The finite-difference time-domain (FDTD) method is an advanced, rigorous solution to Maxwell's equations that does not have any approximations or theoretical restrictions. It is a full-vectorial method that yields all electric and magnetic field components and can account for omni-directional propagation and scattering. Moreover, the FDTD method can include the effects of material dispersion, anisotropy and nonlinearities. Because of its generic nature, broadband aspects and massive parallelizability, the FDTD method is a widely used propagation solution for a variety of integrated photonics applications. A major limitation is that it can require a large amount of memory storage and extremely long computation times to obtain accurate, converged results. Moreover, standard FDTD introduces staircasing when mapping material interfaces onto a Cartesian grid that can degrade accuracy from second order to first order and lead to slower convergence, especially for curved interfaces.

Several techniques have been proposed in the literature for enhancing accuracy and improving convergence [1,2]. All RSoft™ simulation tools, including the FullWAVE™ [3] tool, use a proprietary sub-cell meshing technology (also called conformal meshing) when the simulation grid does not conform to the actual shape of the geometry. The RSoft sub-cell meshing technology builds on the techniques from the literature and includes proprietary enhancements. The RSoft proprietary technology provides significantly higher accuracy and smoother convergence when compared to commonly used staircase approximations. In this white paper, the RSoft sub-cell meshing technology will be referred to as RSoft SCM. To illustrate the performance and accuracy benefits of RSoft SCM over the staircase approach, this white paper presents four case studies: a multilayer stack structure; an SOI-based ring resonator; scattering from a dielectric cylinder; and a photonic crystal.

Case Study 1: Multilayer Stack Structure

The first test structure is a stack consisting of silicon, transparent conductive oxide (TCO) and air. The reference result is computed using RSoft DiffractMOD™, which provides a quick and exact solution for this simple test case and is further verified against analytic solutions. The RMS error of the FullWAVE results in reflection plus transmission compared to the reference results is calculated over a bandwidth of 600 nm.

Figure 1 shows the RMS error as a function of grid points per wavelength. The blue line shows the RMS error obtained with RSoft SCM and the green line shows the error obtained with a staircase meshing scheme. As can be seen in Figure 1, the results from RSoft SCM scheme have significantly lower error than the traditional staircase meshing scheme and converge much quicker. For example, to obtain an RMS error smaller than 0.015 in this example, the staircase meshing scheme would require 50 grid points per wavelength, whereas RSoft SCM obtains superior results with 16 grid points per wavelength. Since the computational time for FDTD calculations scale as $(1/grid\_size)^3$ in 2D and $(1/grid\_size)^4$ in 3D, this translates to a time savings of ~30x in 2D and ~95x in 3D with RSoft SCM.
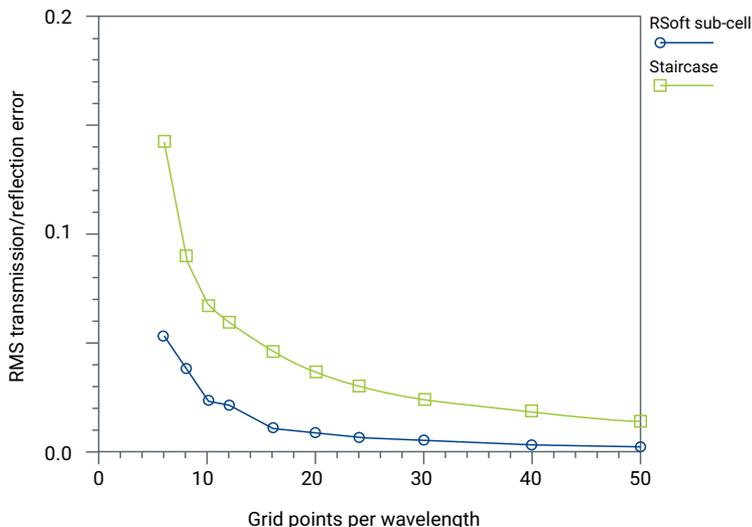

Figure 1: RMS transmission plus reflection error for a multilayer stack

Case Study 2: SOI-Based Ring Resonator

Ring resonators are critical components for silicon photonics applications, including wavelength channel add/drop multiplexing and filtering operations. Resonant modes of the ring form at certain wavelengths (Figure 2(a)) when the wavelength of the light fits an integer number of times in the optical path length of the ring; conversely, the light that does not meet this resonant condition is transmitted through the bus waveguide (Figure 2(b)).
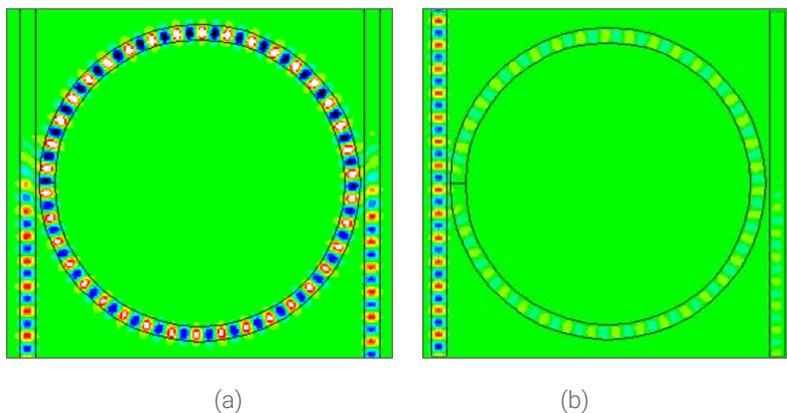

(a) (b)

Figure 2: Field distribution in the SOI-based ring resonator: (a) at resonance; (b) off resonance
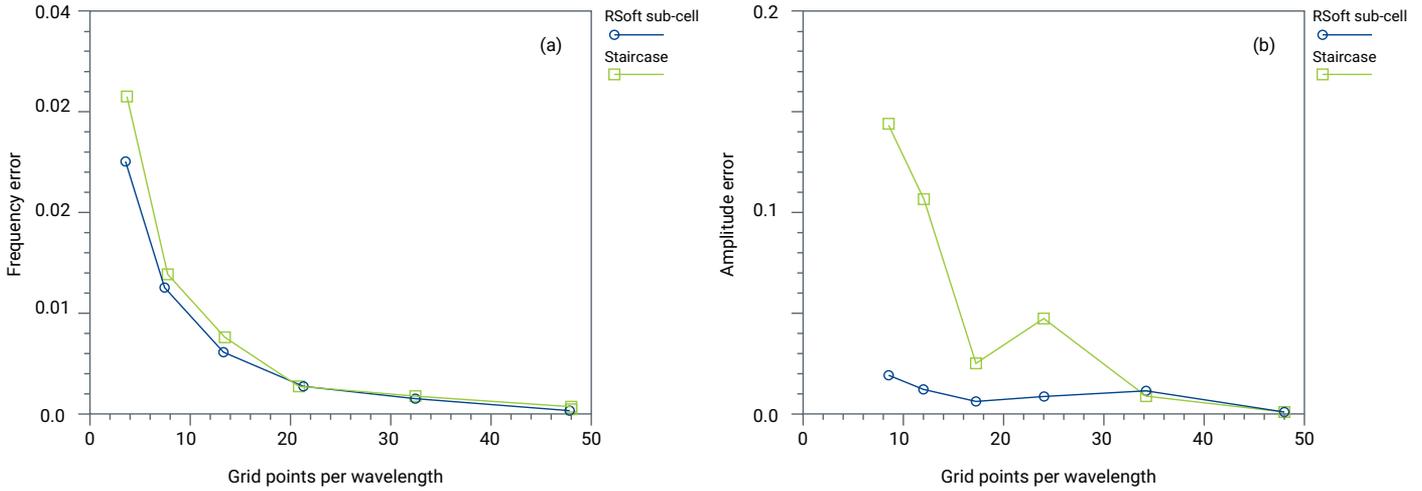
Figure 3: Results for SOI-based ring resonator: (a) frequency error; (b) amplitude error

Figures 3(a) and 3(b) show the convergence versus grid points per wavelength of the frequency and amplitude errors, respectively, for a typical SOI-based ring resonator. The blue line shows the results obtained with RSoft SCM and the green line shows the results obtained with a staircase meshing scheme. As can be seen in the figures, the error in the amplitude (Figure 3(b)) is far more sensitive compared to the error in the resonant frequency (Figure 3(a)). This is because the error in the resonant frequency is dominated by the phase propagation along the arc, which does not have any discontinuities along its axis. On the other hand, the amplitude error is limited by artificial scattering and RSoft SCM outperforms the staircase meshing scheme substantially both in terms of accuracy and smoother convergence. For example, to obtain an amplitude error smaller than 0.015, the staircase meshing scheme requires 34 grid points per wavelength. RSoft SCM requires only 12 grid points per wavelength to obtain the same result, which translates to a substantial time savings of ~22x in 2D and ~64x in 3D.

Case Study 3: Scattering from a Dielectric Cylinder

The third case study measures Mie scattering from a dielectric cylinder with a radius of 800 nm at a wavelength of 550 nm. An enclosed planewave launch encompassing the cylinder is excited and the power scattered by the cylinder outside the boundaries of the enclosed launch is measured.
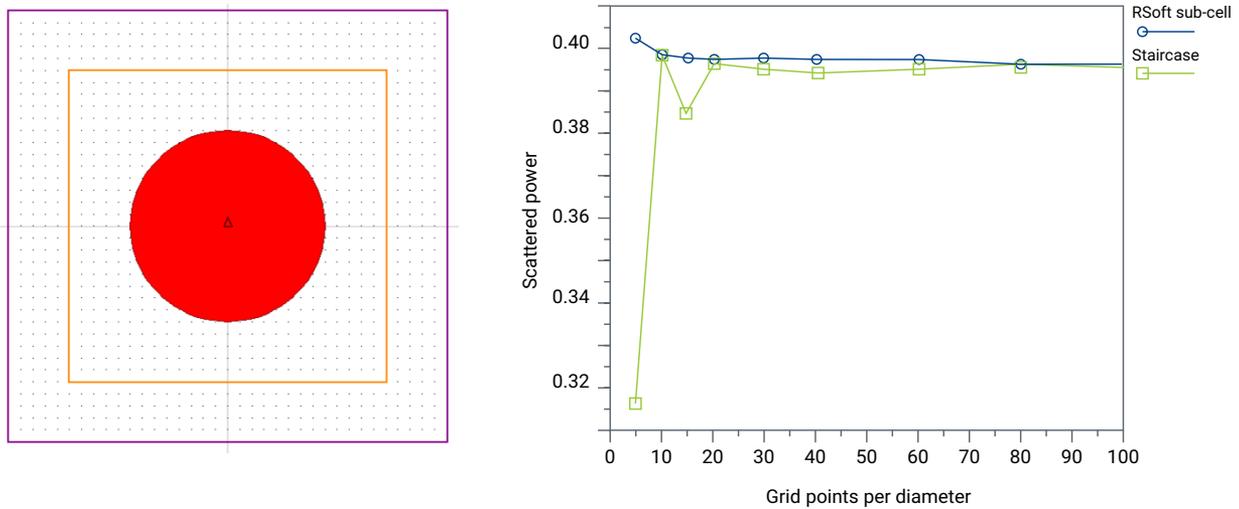

Figure 4: (a) The schematic of the simulated structure showing the dielectric cylinder, enclosed plane wave launch region (orange box) and the measurement region for the scattered power (purple box); (b) power scattered by a Mie cylinder

Figure 4(b) shows the scattered power as a function of grid points per diameter. The blue line shows the scattered power obtained with RSoft SCM and the green line shows the power obtained with a traditional staircase meshing scheme. As can be seen, the results from RSoft SCM display a much faster and smoother convergence compared to the staircase meshing scheme.

Case Study 4: Band Diagram for a Photonic Crystal

Photonic crystals can be seen as the optical analog of semiconductors; that is, photonic band gap (PBG) materials display gaps in their photon density of states. 2D and 3D photonic crystals at optical frequencies have been fabricated over the past decade. Several optical device applications have been proposed and demonstrated, including efficient waveguiding, transmitting light around sharp corners with relatively small losses and resonant microcavities that can be used to efficiently couple light into PBG-based waveguides. These applications can potentially lead to the design of new compact integrated optoelectronic and photonic integrated circuits.
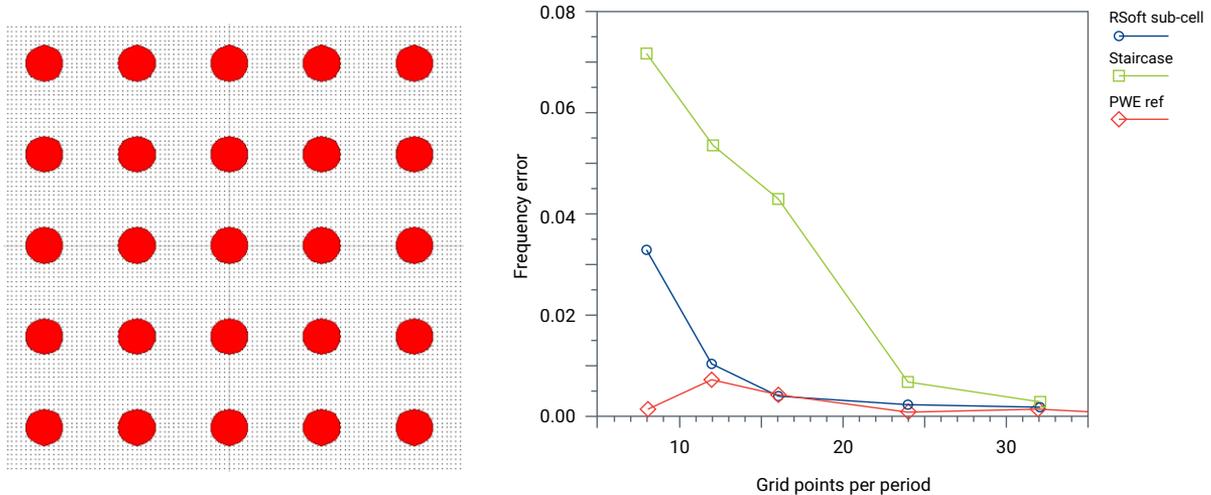

Figure 5: (a) 2D photonic crystal with a radius of 0.2 μm and a period of 1 μm; (b) frequency error in the photonic band calculation

Figure 5(b) shows the convergence versus grid size of the frequency error in the photonic band calculation and compares three different numerical approaches. The blue line shows the results obtained with RSoft SCM; the green line shows the results obtained with a staircase meshing scheme; and the red line shows the frequency error calculated using the RSoft BandSolve™ tool based on the Plane Wave Expansion (PWE) technique, which is useful for analyzing PBG applications. As can be seen, the results obtained with RSoft SCM show a significantly smaller error compared to the staircase meshing scheme. In addition, RSoft SCM achieves similar accuracy to the PWE technique, but much quicker than the staircase meshing scheme. For example, to obtain a frequency error smaller than 0.015, the staircase meshing scheme would require 24 grid points per wavelength, whereas RSoft SCM requires 12 grid points per wavelength, which translates to a time savings of ~8x in 2D and ~16x in 3D with RSoft SCM.

Summary

Because of the computationally intensive nature of the FDTD method, improved accuracy and convergence are critical for its practical use as a design algorithm in applications where numerous design variants need to be explored. In this white paper, four case studies are presented that demonstrate significantly higher accuracy and smoother convergence obtained with the RSoft proprietary sub-cell meshing (SCM) technique, also called conformal meshing, when compared to the commonly used staircase meshing approach.

References

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[2] Ardavan F. Oskooi, Chris Kottke, and Steven G. Johnson, "Accurate finite-difference time-domain simulation of anisotropic media by subpixel smoothing," *Opt. Lett*. 34, 2778-2780 (2009).

[3] *FullWAVE User Guide*, Synopsys, Inc., RSoft Products (2017).