# Simulating non-linear third order effects with the adapted complex Jacobi iteration method

P. Vandersteegen, B. Maes, P. Bienstman, R. Baets

INTEC, UGent-IMEC, Sint-Pietersnieuwstraat 41, B-9000 Gent

We present a numerical method to simulate the third order Kerr effect in wavelength scale dielectric structures. This is done by extending the recently introduced complex Jacobi Iteration method. This method solves the Helmholtz equation in a discrete finite simulation space by an iterative proces. This technique refines the field values during each iteration step, until a desired accuracy is achieved. Adjustment of the discrete field operators allows the use of the total field/scattered field formalism and PMLs as absorbing boundaries. Extending the iterative process with an extra calculation step allows simulating materials with the non-linear third order Kerr effect.

## **1** Introduction

The instantaneous Kerr non-linear effect shows a large potential to achieve all-optical signal processing. It can be modelled as an intensity dependent refractive index change which typically requires high intensities. These high intensities can be achieved by the increased confinement of light in advanced dielectric structures, e.g. photonic crystals and photonic wires. Modelling of these non-linear devices requires an accurate integration of the Helmholtz equation.

The complex Jacobi method ([1]) integrates the Helmholtz equation. The found amplitudes - in the frequency domain- are invariant in time, save a phase factor.

Our extensions to this method include the total field/scattered field (TFSF), perfectly matched layers (PML) and Kerr based materials. PML ([4]) allows good absorption at the boundaries. Injecting a field profile in the simulation area is achieved by an adjusted TFSF. ([2]) Although the basic complex Jacobi method is a fully vectorial solver in 3 dimensions, the proposed extensions have only been tested for the scalar 2D Helmholtz equation.

# 2 Linear complex Jacobi Method



(a) Simulation box with 'total field/scattered field' as field (b) Interface at index i' between source and PMLs as absorbing boundary conditions. scattered field - total field.

Figure 1: Simulation setup.

The basic complex Jacobi method [1] is an iterative method which only calculates the fields at equidistant points. The derivatives in the Helmholtz equation are replaced by central differences:

$$\frac{\partial}{\partial x}e_{i,j} \equiv \frac{e_{i+1,j}-e_{i-1,j}}{2\Delta x}$$

The field  $e_{i,j}$  is located at the point  $(i\Delta x, j\Delta y)$ , *i* and *j* are integers,  $\Delta x$  is the discretization step in x and y directions.

The complex Jacobi method refines the field-amplitudes with the following update equation until a desired accuracy for the Helmholtz equation has been achieved:

$$e_{i,j}^{n+1} = e_{i,j}^{n} + \left(2\alpha_1(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2})\right)^{-1} \left((\delta_x^2 + \delta_y^2 + (\frac{2\pi}{\lambda}n_{i,j})^2)e_{i,j}\right)$$
(1)

The superscript n is the iteration step. The wavelength in free space is  $\lambda$ ,  $n_{i,j}$  is the position dependent refractive index. The iteration process consists of repeatedly updating the fields with this equation, firstly with  $\alpha_1$ , then with  $\alpha_2$ , until a desired accuracy is achieved. Using  $exp(-j\omega t)$  as convention for the time dependent phase factor of the invariant field amplitudes results in the following optimal constants:  $\alpha_1 = \sqrt{3} - 1j$  and  $\alpha_2 = -\alpha_1^*$ .

#### 3 Linear extensions: total field/scattered field formalism and PML

Derivation of these optimal values for  $\alpha_1$  and  $\alpha_2$  can be found in the original paper [1].

**TFSF** injects a desired wave in the simulation space, Fig.1(a). In the scattered field region only the scattered field, i.e. the total field without the exciting field is calculated. The calculation of an amplitude at the interface (location i', Fig. 1(b)) uses:

Amplitudes  $e_{(i'-1,j),source}$  and  $e_{(i',j),source}$  are the amplitudes of the exciting wave at respective positions (i'-1,j) and (i',j). Substituting equation 2 in the update equation 1 in order to calculate  $e_{(i'-1,j),scatt}^n$  and  $e_{(i',j),tot}^n$  gives the required update equations.

With these adjusted update formulae it becomes possible to inject any desired field. **PML** eliminates reflections at the boundaries of a finite simulation box.We use a PML based on complex coordinate stretching [4].

$$\delta_x^2 e = \frac{1}{s_x} \left( \frac{\partial}{\partial x} \frac{1}{s_x} \right) \frac{\partial}{\partial x} e + \frac{1}{s_x^2} \frac{\partial^2}{\partial x^2} e$$
$$= \frac{1}{s_{x,i}} \left( \frac{\frac{1}{s_{x,i+1}} - \frac{1}{s_{x,i-1}}}{2\Delta x} \right) \left( \frac{e_{i+1} - e_{i-1}}{2\Delta x} \right) + \frac{1}{s_{x,i}^2} \frac{e_{i+1} + e_{i-1} - 2e_i}{\Delta x^2}$$

For  $s_x = 1.0$  the previous formulae reduce to the classical Helmholtz equation. A complex function  $s_y$  for  $\delta_y$  results in absorption in the y-direction. In our experience, optimal absorption was achieved with linearly increasing PML from  $s_x = 1.0$  to  $s_x = 1.0 + 0.25j$  over 30 grid-points.



(a) Two Bragg mirrors encapsulate a cavity. ( $\lambda_{resonance} = 1.56 \mu m, n_a = 2.6, n_b = 2.36.$   $d_a = \lambda_{resonance}/4n_a, d_b = \lambda_{resonance}/4n_b$  and  $d_{cavity} = \lambda_{resonance}/2n_b$ )



(b) Power Tranmission and Reflection for (c) Comparison between EME en Complex the linear structure Jacobi, both linear as non-linear case.

Figure 2: Power Transmission and Reflection of 2(a)

#### **4** Extending the iterative proces to simulate Kerr non-linearities

The implementation for the Kerr effect uses an extra update-step for the refractive index after each iteration step. The instantaneous Kerr effect, modelled by  $n = n_{lin} + n_2 |E|^2$ , results in: This results in:

$$\boldsymbol{\varepsilon}_{i,j}^{n} = \left(n_{i,j,lin} + n_{i,j,2}|e_{i,j}|^{2}\right)^{2}$$
(3)

#### 5 Comparison with non-linear eigenmode expansion

Comparison with eigenmode expansion (EME) has been done by simulating the onedimensional structure of figure 2(a). This structure basically is a cavity encapsulated by two Bragg mirrors.

The central cavity causes a resonance peak in the middle of the bandgap. (Fig. 2(b)) A non-linear material in the central cavity causes a shift of the central resonance wavelength to a higher wavelength. Figure 2(c) illustrates a good agreement between nonlinear eigenmode expansion (EME, [3]) and the non-linear complex Jacobi method (CJ). The incoming plane wave has an amplitude  $e = 1\frac{V}{m}$ . The non-linear cavity uses  $n_2 = 5 \times 10^{-3} \frac{m^2}{V^2}$ ,  $n_2$  as defined in formule 3.

EME uses an iterative proces for the non-linear sections. The recalculation of eigenmodes in the non-linear sections quickly becomes a bottleneck for a large amount of non-linear sections. CJ is very well suited for structures where the non-linearity is present in a large portion of the simulation domain.



Figure 3: Injection of a gaussian field profile in a linear and non-linear medium. ( (a): diffraction in linear medium, (b): soliton in non-linear medium)

## 6 Soliton in a non-linear Kerr-material

We have validated our extensions by simulating a soliton in non-linear space. In linear space, the injection of a gaussian field profile by the total field/scattered field formalism results in a diffraction pattern. Both effects can be seen in figure 3. The gaussian field profile is described by  $e = 1.0e^{\frac{x^2}{2*0.25^2}} \frac{V}{\mu m}$ . The material is described by the refractive index n = 3.6 and  $n_2 = 0.2 \frac{m^2}{V^2}$ .

## 7 Conclusion

Our extensions to the recently introduced complex Jacobi method allow the simulation of 2D-components with Kerr-based materials in the frequency domain. Our proposed extension to the complex Jacobi method is very well suited for structures where the non-linearity is present in a large portion of the simulation domain.

## 8 Acknowledgements

Bjorn Maes and Peter Bienstman acknowledge the Flemish Fund for Scientific Research (FWO-Vlaanderen) for their postdoctoral fellowships. Parts of this work were performed in the context of the Belgian DWTC project IAP-Photon.

## References

- [1] Hadley, Ronald G. "A complex Jacobi iterative method for the indefinite Helmholtz equation", *Journal of computational physics*, 203(1):358–370, February 10 2005.
- [2] Taflove, Allen., "Computational Electrodynamics The Finite-Difference Time-Domain Method", *Artech House Boston-London*, 108–109, 1995.
- [3] Maes B., Bienstman P. and Baets R. "Modeling of Kerr nonlinear photonic components with mode expansion", *optical and quantum electronics*, 36(1-3):15–24, January-February 2005
- [4] Chew, Weng Cho and Weedon, William H. "A 3D perfectly matched medium from modified Maxwell's equations with stretched coordinates", *Microwave and optical technology letters*, 7:599–604, September 1994.