Comparison of Time Integration Schemes in FDTD Simulations in Two Dimensions

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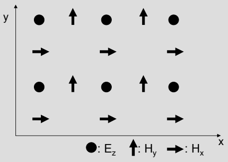
Motivation

- Conventional finite difference time domain methods (FDTD) are only conditionally stable. Because space discretization is defined in principle by the geometry and properties of matter in the simulation region, time step size is limited.
- Stability becomes a crucial subject in nonlinear problems. Therefore the use of alternative time integration schemes becomes attractive for such problems.
- Optimization of photonic structures is a subject which needs a combination of fast and reliable calculation schemes for the photonic structures and effective optimization strategies. Conventional FDTD solvers do not completely fulfill those requirements.

Space Discretization

Yee-Grid in two dimensions [S1]:

- Widely used spatial discretization scheme
- Meshs for electrical and magnetical fields are shifted by a half step
- Fields are divergence-free
- Finite difference expressions are central
- Easy to implement



[S1] Yee, K.S., „Numerical solution of initial boundary value problems involving Maxwell's equations in isotropic media", *IEEE Trans. Antennas Propagat., Vol. 14, 1966 pp.302-307*

Time Discretization

Classical approach:	Specialized methods like symplectic methods (e.g. leap frog) for Maxwell equations in standard applications
Open problem:	More general physical models include, e.g., anisotropic effects, dissipation, nonlinearities and different materials.

➡ General purpose solvers required which
  - can deal with large dimensions and
  - have good stability properties (unconditional stability).

Novel approach: Stable integrators combined with iterative methods of numerical linear algebra (Krylov subspace methods) [T1, T2, T3]

Properties:

- Avoid the time consuming evaluation of the Jacobian using iterative methods based on matrix-vector products that are approximated by finite differences (matrix-free methods).
- Applicable for general problems, also on nonuniform meshes.
- Good stability properties, time stepsize restricted by accuracy requirements, only.
- Time stepsizes adapted automatically to meet user defined error bounds.
- User friendly black box implementation, the user has to provide only the space discretization of the Maxwell equations.

VODPK

- Approved Krylov subspace code [T1] combining BDF and GMRES
- Drawback: A-stable only for low order time discretization ($p \leq 2$).

ROWMAP

- Krylov subspace code [T2] with ROW-method + multiple Arnoldi process
- The user can choose among different ROW-methods of order $p = 4$ including A-stable methods (no stepsize restriction for stability reasons).

DOPRI5

- Standard explicit Runge-Kutta solver ($p = 5$) for problems with low stability requirements, used as reference.

References

[T1] G.D. Byrne: *Pragmatic experiments with Krylov methods in the stiff ODE-setting*. - In: Computational ordinary differential equations, Clarendon Press, Oxford, 1992, pp. 323-356.

[T2] R. Weiner, B.A. Schmitt and H. Podhaisky: *ROWMAP – a ROW-code with Krylov techniques for large stiff ODEs.* – Appl. Num. Math. **25** (1997), 303-319.

[T3] M.A. Botchev , D. Harutyunyan, J. J. W. van der Vegt: *The Gautschi time stepping scheme for edge finite element discretizations of the Maxwell equations*. - J. of Comput. Phys. **216** (2006), 654-686.

Implementation

Input: Physical structure and simulation parameters are defined in a **XML-file**

- Human- and machine-readable
- Generation of complex structures with a few lines
  - Define materials, rods, arrays of those and defects
- Ready for extensions as new functionality is required

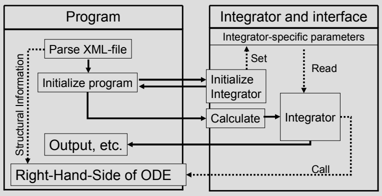
Time Integration:

- Provide common interface for each integrator
- Compile program with support for one specific integrator

⇒No changes in main program
⇒Easy implementation of new integrators

Program structure:

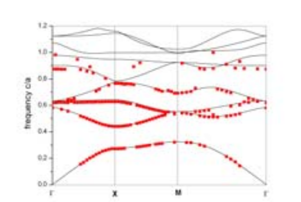
- Implemented in FORTRAN95
- Can be used as a FORTRAN module in other programs



Test of the Method

Photonic Bandstructure – Periodic Boundary Conditions

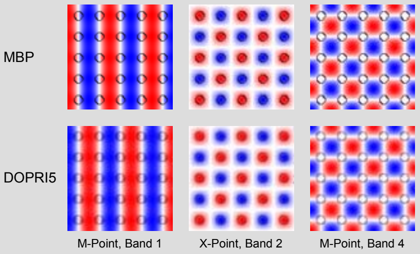
- Integrator for test: DOPRI5
- Task: Calculate bandstructure of dielectric rods in air (ε= 8.9, r/a = 0.2)
- Excite field with Gauss distributed specturm of frequencies (mean frequency=0.5, FWHM=2.0)
- Calculate electrical field, measure w.r.t. time and analyze spectrum with HARMINV



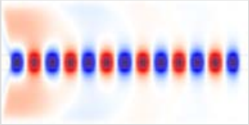
Comparison MPB (-) and DOPRI5 (■)

Electrical Field Patterns – Periodic Boundary Conditions

- Integrator for test: DOPRI5
- Task: Calculate electrical field pattern
- Excite field with narrow-band spectrum near eigenfrequency
- Output of electrical fields as a color encoded image considering the boundary conditions

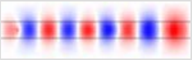


Fields in a straight Waveguide – Absorbing Boundary Conditions (PML)



MEEP

- Integrator for test: DOPRI5
- Excite electrical field with continuous wave
- Wavelength and width of waveguide are chosen such that one expects field propagation along the waveguide
- Taken from the MEEP tutorial

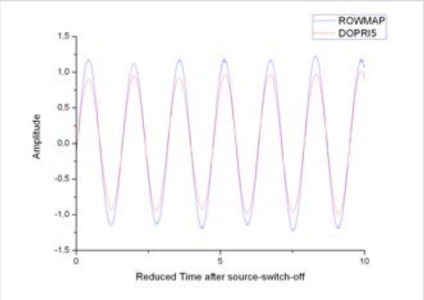


DOPRI5

MPB S.G. Johnson, J.D. Joannopoulos, *Block-iterative frequency-domain methods for Maxwell's equations in a plane wave basis,* Optics Express **8**, 173 (2001)
MEEP (*MIT Electromagnetic Equation Propagation*), FDTD simulation software package developed at MIT
HARMINV Program to perform harmonic inversion developed by S.G. Johnson

Comparison of Time Integration Methods

Time evolution of electrical field in one point

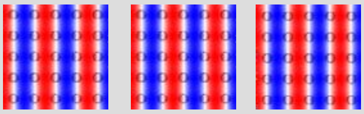


Comments

- Unlike Leap-Frog the integration methodes used here require several parameters, such as tolerances, Krylov dimension, maximum order, etc.
- Each integrator requires specific parameters
- Setting up parameters correctly requires some experience
- Extension to nonlinear problems straightforward

- VODPK less efficient because of missing A-stability
- Extension: Preconditioning in ROWMAP and VODPK for improved performance

Again Electrical Field Patterns



DOPRI5 ROWMAP VODPK

Performance and CPU-Time in seconds

Resolution	DOF	DOPRI5	ROWMAP
10x10	800	20.6	71.0
20x20	3200	183.4	554.0
40x40	12800	1616.4	4931.7

Comparing the calculated Eigenfrequencies

	MPB	DOPRI5	ROWMAP	VODPK
M-Point Band 1	0.32453	0.320285	0.320287	0.320287
X-Point Band 2	0.44407	0.439949	0.439949	0.439949
M-Point Band 4	0.69351	0.691867	0.691867	0.691867

Conclusions and Outlook

- We have combined the discretization in real space using the Yee method with different time integration schemes in one module. We have demonstrated the method using a standard two dimensional photonic crystal. The results have been compared with other programs.
- The method will be further developed to optimize performance.
- We will include the calculation of several quantities which can be measured directly like transmission and reflection coefficients.
- The extension to three dimensions is possible.
- The method will be used as a building block in optimization procedures (genetic algorithms).
- Our approach will be helpful in the investigation of nonlinear phenomena and coherent control of light guidance on the nanoscale (Sukharev, Seidemann, J. Chem. Phys. **124** (2006), 144707-1)