Operator Splitting Methods for Non-Autonomous Systems and its Application to the Numerical Solution of the Maxwell Equations in Time-Varying Media

I. Faragó, Á. Havasi, R. Horváth

Eötvös Loránd University
Budapest, Hungary
faragois@cs.elte.hu, hagi@nimbus.elte.hu

University of Technology and Economics Budapest
Budapest, Hungary
rhorvath@math.bme.hu

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Motivation

Operator splitting

Operator splitting techniques applied to systems of ODEs turned to be very efficient in analyzing and constructing schemes for the Maxwell equations.

- Unconditional stability of the ADI-FDTD scheme [Horváth 2002, Lee, Fornberg 2003, Darms et al. 2002]
- New efficient chemes [Kole, Figge, de Raedt 2001, Fornberg 2003, Horváth 2006]
- Handling of source terms [Botchev, Faragó, Horváth 2009]

Time-varying media

How to handle time varying media?

- such as sudden ionization of a gas,
- plasma or semiconductor crystal,
- transience induced by laser pulse excitation,
- ball lightning explosion,
- electric arc discharge,
- etc.

There are some results but they allow only the conductivity to change.

Taylor, Lam, Sumpert, Int. Notes, MSU, 1968.
Lee, Kalluri, IEEE Tr. Ant. Prop. 1999.
Ren, Gao, M. M. Wave Techn. 2000.

Outline

- Magnus expansion
- Magnus expansion and the classical splitting schemes
- Classical FDTD scheme
- Semi-discretized Maxwell equations
- Solution of the Maxwell equations in time-varying media
- Numerical test

Magnus expansion

Magnus series

$$\begin{aligned} \frac{\mathrm{d}\mathbf{y}}{\mathrm{d}t} &= \mathbf{A}(t)\mathbf{y} + \mathbf{g}(t), \quad t \in (t_0, T] \\ \mathbf{y}(t_0) &= \mathbf{y}_0, \end{aligned}$$

Consider only the homogeneous part

$$\begin{aligned} \frac{\mathrm{d}\mathbf{y}}{\mathrm{d}t} &= \mathbf{A}(t)\mathbf{y}, \quad t \in (t_0, T] \\ \mathbf{y}(t_0) &= \mathbf{y}_0, \end{aligned}$$

The fundamental solution can be written in the form

$$\mathbf{Y}(t) = \exp(\mathbf{\Omega}_{\mathbf{A}}(t, t_0)), \ldots$$

Magnus series

... where $\mathbf{\Omega}_{\mathbf{A}}(t, t_0) = \mathbf{\Omega}_{\mathbf{A},1}(t, t_0) + \mathbf{\Omega}_{\mathbf{A},2}(t, t_0) + \ldots$

Magnus series

$$\mathbf{\Omega}_{\mathbf{A},1}(t, t_0) = \int_{t_0}^{t} \mathbf{A}(s) ds,$$

$$\mathbf{\Omega}_{\mathbf{A},2}(t, t_0) = \frac{1}{2} \int_{t_0}^{t} \int_{t_0}^{s_1} [\mathbf{A}(s_1), \mathbf{A}(s_2)] \, ds_2 \, ds_1, \; \ldots .$$

The solution of the inhomogeneous equation can be written as

$$\mathbf{y}(t) = \mathbf{Y}(t) \left(\int_{t_0}^{t} \mathbf{Y}^{-1}(s) \mathbf{g}(s) \, \mathrm{d}s + \mathbf{y}(t_0) \right).$$

Magnus series

Using only the the first term we have a second order approximation

$$\mathbf{y}(t) = \exp(\boldsymbol{\Omega}_{\mathbf{A},1}(t;t_0)) \left(\int_{t_0}^{t} \exp(-\boldsymbol{\Omega}_{\mathbf{A},1}(s;t_0))\mathbf{g}(s)\mathrm{d}s + \mathbf{y}(t_0) \right) + \mathcal{O}((t-t_0)^3)$$

The integral can be approximated by the second midpoint or trapezoidal rules

$$\begin{aligned}\Omega_{\mathbf{A},1}(t;t_0) &= (t-t_0)\mathbf{A}((t-t_0)/2) + \mathcal{O}((t-t_0)^3)\\ &= (t-t_0)\frac{\mathbf{A}(t)+\mathbf{A}(t_0)}{2} + \mathcal{O}((t-t_0)^3).\end{aligned}$$

Magnus series

Important in the Maxwell case that if

$$[\mathbf{A}(s_1), \mathbf{A}(s_2)] = \mathbf{0}, \ \forall \ s_1, s_2 \in (t_0, T]$$

then

$$\mathbf{Y}(t) = \exp\left(\int_{t_0}^{t} \mathbf{A}(s)\, ds\right).$$

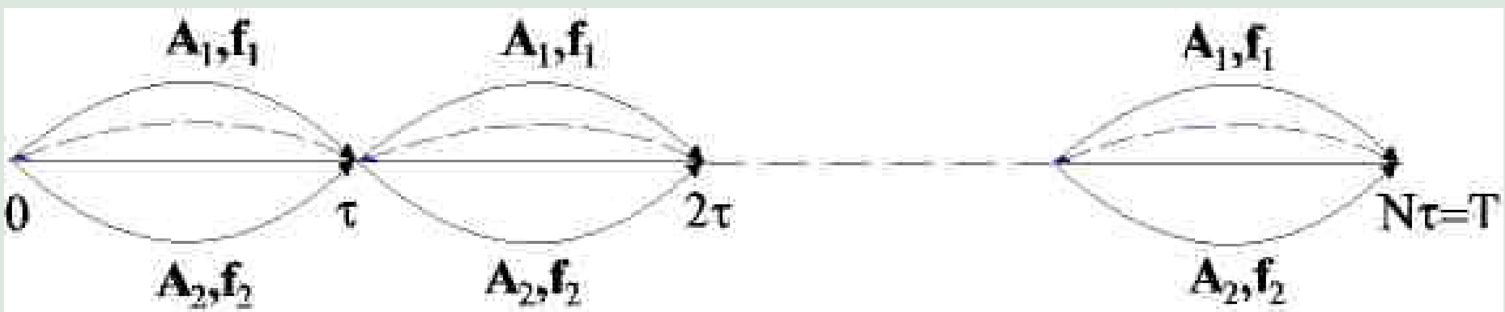
Magnus expansion and classical splitting schemes

Classical splitting schemes

$$\frac{\mathrm{d}\mathbf{y}}{\mathrm{d}t} = \mathbf{A}(t)\mathbf{y} + \mathbf{g}(t)$$

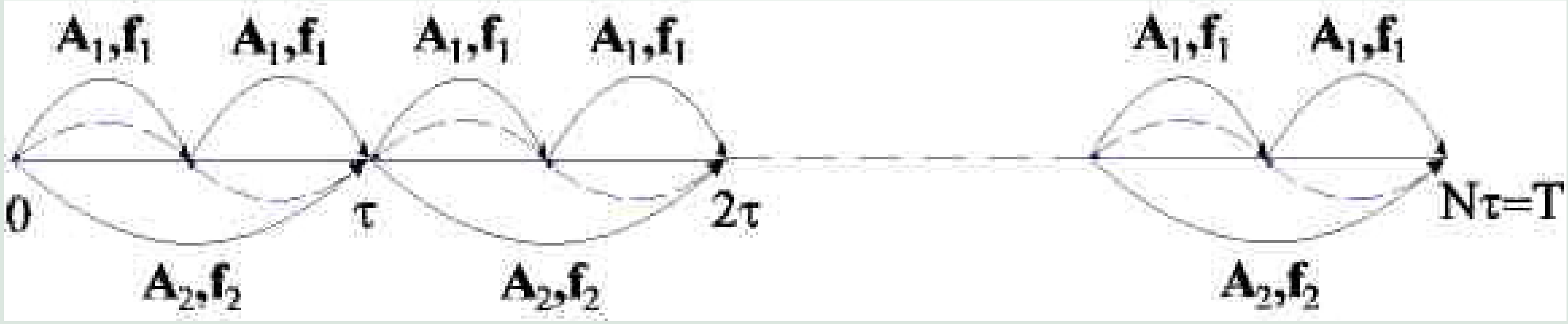
$$\frac{d\mathbf{y}_1}{dt} = \mathbf{A}_1(t)\mathbf{y}_1 + \mathbf{f_1}(t) \qquad \frac{d\mathbf{y}_2}{dt} = \mathbf{A}_2(t)\mathbf{y}_2 + \mathbf{f_2}(t),$$

Sequential splitting (first order local spl. error)



Classical splitting schemes

Strang-Marchuk splitting (second order)



The above splitting schemes preserve their order also to non-autonomous equations (proof was carried out using the Magnus expansion).

[Faragó, Havasi, Horváth, submitted to IJNAM.]

Classical FDTD scheme

Maxwell equations

$$\frac{\partial(\varepsilon \mathbf{E})}{\partial t} = \nabla \times \mathbf{H} - \sigma \mathbf{E} - \mathbf{J_e},$$

$$\frac{\partial(\mu \mathbf{H})}{\partial t} = -\nabla \times \mathbf{E},$$

Curl equations

$$\nabla(\varepsilon \mathbf{E}) = \mathbf{0},$$

$$\nabla(\mu \mathbf{H}) = \mathbf{0},$$

Divergence equations

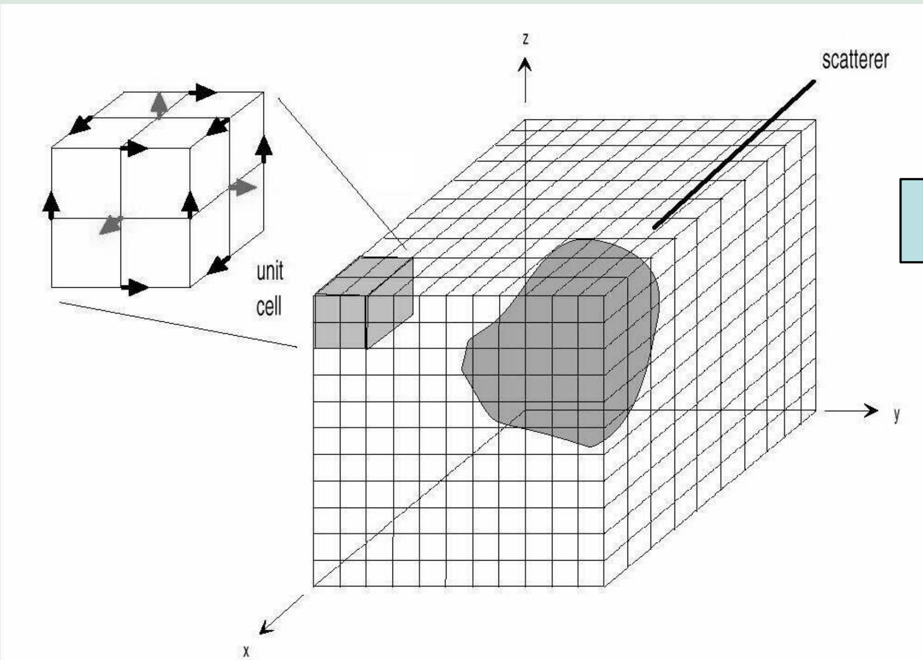
Known:

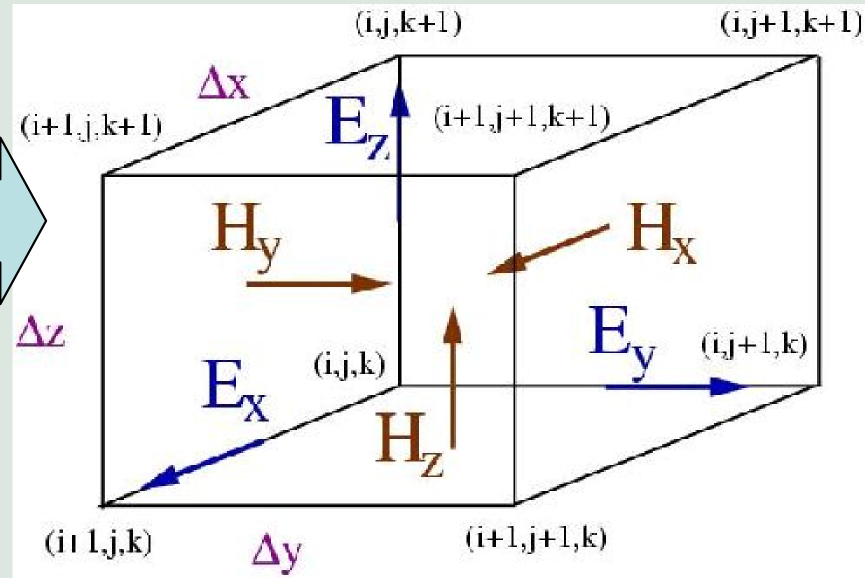
$$\begin{aligned} \varepsilon &= \varepsilon(x,y,z,t), \mu = \mu(x,y,z,t), \\ \sigma &= \sigma(x,y,z,t), \mathbf{J}_e = \mathbf{J}_e(x,y,z,t) \end{aligned}$$

Unknown: $\mathbf{E} = \mathbf{E}(x,y,z,t), \mathbf{H} = \mathbf{H}(x,y,z,t),$

Spatial discretization

The Finite Difference Time Domain method (FDTD) was published in 1966 by K. Yee.

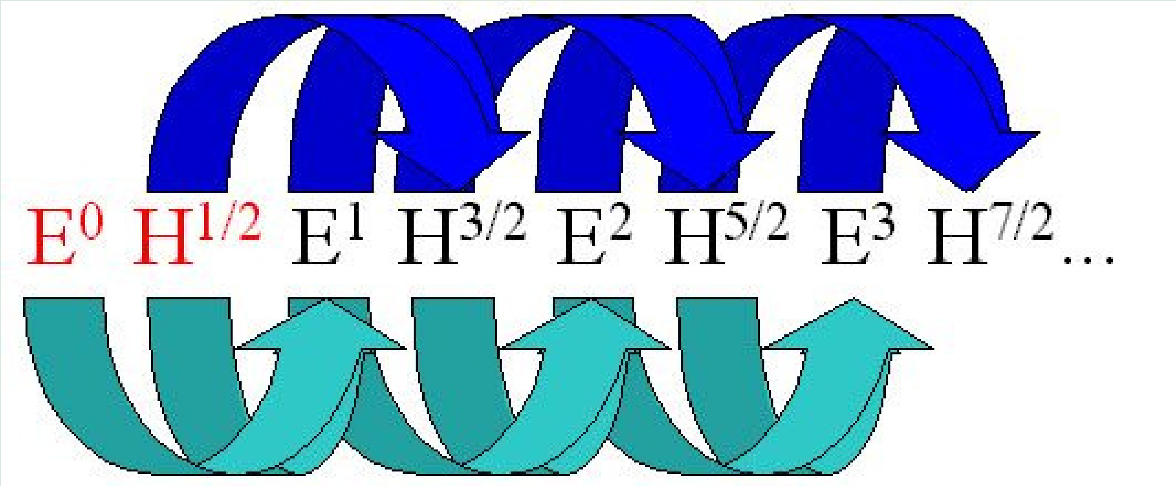




Yee-cell

Time discretization

The leapfrog scheme is used. $\Delta t > 0$



Pros and cons

- simple (explicit)
- time-domain method
- flexible choice of material parameters

- strict stability condition

$$\Delta t \approx \frac{\text{mesh size}}{\text{speed of light}}$$

- material parameters are independent of time

Semi-discretized Maxwell equations

Spatial discretization

Introducing $\mathcal{E} := \sqrt{\varepsilon}\mathbf{E}$, $\mathcal{H} := \sqrt{\mu}\mathbf{H}$, $\mathcal{J}_e := (1/\sqrt{\varepsilon})\mathbf{J}_e$
we have

$$\frac{\partial}{\partial t}\left[\begin{array}{c}\mathcal{E}\\ \mathcal{H}\end{array}\right] = \mathcal{A}\cdot\left[\begin{array}{c}\mathcal{E}\\ \mathcal{H}\end{array}\right] - \left[\begin{array}{c}\mathcal{J}_e\\ 0\end{array}\right],$$

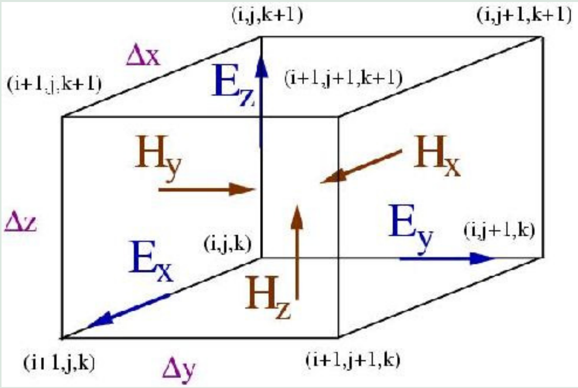
with

$$\mathcal{A} = \left[\begin{array}{cc}-\sigma/\varepsilon - \varepsilon'/(2\varepsilon) & (1/\sqrt{\varepsilon\mu})\nabla\times\\ -(1/\sqrt{\varepsilon\mu})\nabla\times & -\mu'/(2\mu)\end{array}\right].$$

Define the real functions

$$\mathcal{E}_x|_{i,j,k}(t) = \mathcal{E}(i\Delta x/2, j\Delta y/2, k\Delta z/2, t)$$

i is odd, *j*,*k* are even, etc.



Spatial discretization

After this semi-discretization we have

$$
\begin{aligned}
\mathcal{E}_x|'_{i,j,k}(t) &= \frac{1}{\Delta y\sqrt{\varepsilon(t)\mu(t)}}\mathcal{H}_z|_{i,j+1,k}(t) - \frac{1}{\Delta y\sqrt{\varepsilon(t)\mu(t)}}\mathcal{H}_z|_{i,j-1,k}(t) \\
&\quad + \frac{1}{\Delta z\sqrt{\varepsilon(t)\mu(t)}}\mathcal{H}_y|_{i,j,k-1}(t) - \frac{1}{\Delta z\sqrt{\varepsilon(t)\mu(t)}}\mathcal{H}_y|_{i,j,k+1}(t) \\
&\quad - \left(\frac{\sigma(t)}{\varepsilon(t)} + \frac{\varepsilon'(t)}{2\varepsilon(t)}\right)\mathcal{E}_x|_{i,j,k}(t) - (\mathcal{J}_e)_x|_{i,j,k}(t), \\
\mathcal{H}_z|'_{i,j+1,k}(t) &= \frac{1}{\Delta y\sqrt{\varepsilon(t)\mu(t)}}\mathcal{E}_x|_{i,j+2,k}(t) - \frac{1}{\Delta y\sqrt{\varepsilon(t)\mu(t)}}\mathcal{E}_x|_{i,j,k}(t) \\
&\quad + \frac{1}{\Delta x\sqrt{\varepsilon(t)\mu(t)}}\mathcal{E}_y|_{i-1,j+1,k}(t) - \frac{1}{\Delta x\sqrt{\varepsilon(t)\mu(t)}}\mathcal{E}_y|_{i+1,j+1,k}(t) \\
&\quad - \frac{\mu'(t)}{2\mu(t)}\mathcal{H}_z|_{i,j+1,k}(t)
\end{aligned}
$$

etc.

Splitting of the Cauchy-problem

Writing these equations into a compact form we arrive at the Cauchy-problem

$$\mathbf{w}'(t) = \mathbf{Z}(t)\mathbf{w}(t) + \mathbf{f}(t), \quad \mathbf{w}(0) \text{ is given.}$$

$$\mathbf{f}(t) = \mathbf{f}_1(t) + \underbrace{\mathbf{f}_2(t)}_{\equiv 0}$$

$$\mathbf{Z}(t) = \mathbf{M}(t) + \mathbf{D}(t) \in \mathbb{R}^{N \times N}$$

$$\mathbf{D}(t) = \mathbf{D}_1(t) + \mathbf{D}_2(t)$$

skew-symmetric ($\mathbf{M}(t)$) diagonal ($\mathbf{D}(t)$)

In $\mathbf{M}_1, \mathbf{M}_2$ the rows of the magnetic and electric fields are zeroed, respectively. $\mathbf{Z} = \mathbf{M}_1 + \mathbf{M}_2$

Some properties of the subsystems

$$\mathbf{M}_i(s_1)\mathbf{M}_i(s_2) = \mathbf{0},\ \forall s_1, s_2 \in [0, T]$$

⇩

Solution of the CP

$$\mathbf{w}'(t) = \mathbf{M}_i(t)\mathbf{w}(t),\ t \in (0, T],\ \mathbf{w}(0) \text{ is given } (i = 1, 2)$$

is

$$\mathbf{w}(t) = \left(\mathbf{I} + \int_0^t \mathbf{M}_i(s)\,\mathrm{d}s\right)\mathbf{w}(0),\ t \in (0, T].$$

$$\mathbf{M}_i(s_1)\mathbf{D}_i(s_2) = \mathbf{0}\ (i = 1, 2),\ \forall s_1, s_2 \in (0, T]$$

Some properties of the subsystems

Solution of the CP

$$\mathbf{w}'(t) = \mathbf{D}_i(t)\mathbf{w}(t),\ t \in (0,T],\ \mathbf{w}(0) \text{ is given } (i = 1,2)$$

is

$$\mathbf{w}(t) = \mathbf{E}_{\mathbf{D}_i}(t)\mathbf{w}(0),\ t \in (0,T]$$

with

$$(\mathbf{E}_{\mathbf{D}_i}(t))_{jj} = \exp\left(\int_0^t (\mathbf{D}_i(s))_{jj}\,\mathrm{d}s\right),\ j = 1,\ldots,6N.$$

Solution of the homogeneous subs.

Solution of the CP

$$\mathbf{w}'(t) = (\mathbf{D}_i(t) + \mathbf{M}_i(t))\mathbf{w}(t),\ \ t \in (0, T]$$

can be computed numerically with the second order scheme

$$\mathbf{w}^{n+1} = \left(\mathbf{I} - \frac{\Delta t}{2}\mathbf{D}_i((n+1)\Delta t)\right)^{-1}\left(\mathbf{I} + \frac{\Delta t}{2}\mathbf{D}_i(n\Delta t) + \Delta t\mathbf{M}_i((n+1/2)\Delta t)\right)\mathbf{w}^n$$

if $\varepsilon(t), \mu(t)$ are three times continuously differentiable and $\sigma(t)$ is twice continuously differentiable and

$$\varepsilon(t), \mu(t) \geq a_0 > 0,\ \ t \in [0, T].$$

The finial form of the scheme

We solve the subsystems

$$\begin{aligned}
\mathbf{w}_1'(t) &= (\mathbf{M}_1(t) + \mathbf{D}_1(t))\mathbf{w}_1(t), \\
\mathbf{w}_2'(t) &= (\mathbf{M}_2(t) + \mathbf{D}_2(t))\mathbf{w}_2(t), \\
\mathbf{w}_3'(t) &= \mathbf{f}_1(t),
\end{aligned}$$

using the Strang-Marchuk splitting (second order) and the previous second order numerical schemes. For the third equation the midpoint or trapezoidal rule is applied.

Properties of the scheme

- If the material parameters do not depend on time then we get back the classical FDTD scheme.

- The method is explicit. Only a diagonal matrix must be inverted.

- Similarly to the classical FDTD scheme, the method is conditionally stable.

Numerical test

1D example – problem setting

We solve the 1D problem

$$\frac{\partial(\varepsilon E)}{\partial t} = \frac{\partial H}{\partial x} - J,$$
$$\frac{\partial(\mu H)}{\partial t} = \frac{\partial E}{\partial x},$$

on $[0, \pi]$. The material parameters are chosen as

$$\mu = 1, \varepsilon(t) = e^t$$

and

$$J(t, x) = \sin x(e^t(\sin t - \cos t) - \sin t).$$

1D example – problem setting

Initial

$$E(0,x) = \sin x, \;\; H(0,x) = 0$$

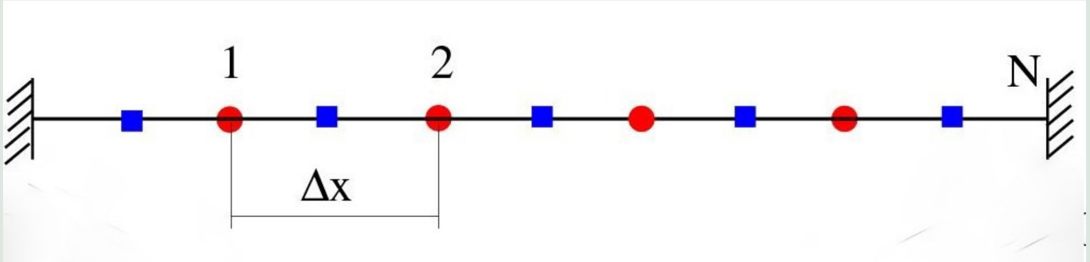
and boundary conditions

$$E(t,0) = E(t,\pi) = 0, \;\; H(t,0) = \sin t, \;\; H(t,\pi) = -\sin t.$$

Exact solution

$$E(t,x) = \cos t \sin x, \;\; H(t,x) = \sin t \cos x.$$

The error of the electric field component is measured at $T=5$ in l_2 norm. N is the number of Yee-cells.



1D example – Results

N	Δt	Error	order
10	$5/20$	$1.3811e-3$	
20	$5/40$	$3.4118e-4$	2.0172
40	$5/80$	$8.5018e-5$	2.0047
80	$5/160$	$2.1238e-5$	2.0011
160	$5/320$	$5.3086e-6$	2.0002
320	$5/640$	$1.3271e-6$	2.0001
640	$5/1280$	$3.3176e-7$	2.0001

The end

Thank you for your attention