Solutions for exercises to chapter 3

“Finite-difference time-domain method”

Exercise 3.1: *Derive a fourth-order central-difference scheme for* $\partial u/_{\partial x}$*using the Taylor series expansion of function u(x) around point x.*

For the 4th order accuracy we must expand the stencil for the finite difference operator to four points $\{x-2h, x-h, x+h, x+2h\}$ around basic point *x*. Then using the Taylor expansions and combining them for points symmetrical over *x* we have:

$$u(x+2h)-u(x-2h)=4u'(x)h+8/3u'''(x)h^3+O(h^5),$$
$$u(x+h)-u(x-h)=2u'(x)h+1/3u'''(x)h^3+O(h^5).$$

To get rid of the third derivative we have to take into account factor 8 between two expressions. Finally it will give:

$$\frac{\partial u}{\partial x}=\frac{-u(x+2h)+8u(x+h)-8u(x-h)+u(x-2h)}{12h}+O(h^4).$$

Exercise 3.2: *Derive a second-order central difference scheme for* ${}^{2}u/_{x^{2}}$*Eq. (3.10). Use h/2 discretization and central difference approximations for function* $\partial u/_{\partial x}$.

Rewriting the second derivative as a sequence of first order derivatives and applying the central difference operator for each of them we obtain:

$$\frac{\partial^2 u}{\partial x^2}=\frac{\partial}{\partial x}\frac{\partial u}{\partial x}=D_x^c\left.\frac{\partial u}{\partial x}\right|_x+O(h^2)=\frac{1}{h}\left(\left.\frac{\partial u}{\partial x}\right|_{x+h/2}-\left.\frac{\partial u}{\partial x}\right|_{x-h/2}\right)+O(h^2)=$$
$$\frac{1}{h}\left(D_x^c u\big|_{x+h/2}-D_x^c u\big|_{x-h/2}\right)+O(h^2)=\frac{1}{h}\left(\frac{u(x+h)-u(x)}{h}-\frac{u(x)-u(x-h)}{h}\right)+O(h^2)=$$
$$\frac{u(x+h)-2u(x)+u(x-h)}{h^2}+O(h^2)$$

Exercise 3.3: *Consider one-dimensional propagation of an electromagnetic wave in vacuum. Solve the 1D dispersion Eq. (3.44) regarding the wavenumber analytically. Find the conditions for the wavenumber to be real or complex. What kind of waves do such wavenumbers describe? Use Eq. (3.52) if needed.*

We start with the 1D dispersion equation (3.44), rewriting it in the form suitable for extracting the wavenumber

$$\cos k\delta x = 1 + \frac{1}{Q^2}\left(\cos\ \omega\delta t - 1\right). \tag{3.1}$$

It can be formally solved regarding *k*:

$$k = \frac{1}{\delta x}\arccos\left[1 + \frac{1}{Q^2}\left(\cos\ \frac{2\pi Q}{N_\lambda} - 1\right)\right], \tag{3.2}$$

where we introduce grid sampling $N_\lambda = \lambda/\delta x$ - number of grid points per wavelength in vacuum. We used it in the following substitution $\omega\delta t = \frac{2\pi c_0}{\lambda}\frac{Q\delta x}{c_0} = \frac{2\pi Q}{\lambda/\delta x} = \frac{2\pi Q}{N_\lambda}$. Accordingly to a value of the expression in the brackets, let's call it ξ, *k* can be either real ($|\xi| \le 1$) or complex ($|\xi| > 1$) depending on the interplay between parameters Q and N_λ. It cannot reach the upper limit ξ = 1, because then $\frac{2\pi Q}{N_\lambda} = 0,\ 2\pi,\ 4\pi,...$, which is not the case for 0 < Q ≤ 1 and $N_\lambda \ge 1$. At another extreme, there are solutions of equation ξ = -1 or $\cos\frac{2\pi Q}{N_\lambda} = 1 - 2Q^2$, which depend on particular choice of Q and grid sampling. For example, for Q = 0.5, the border between *k* being real and $k = k' + ik''$ being complex is at $N_\lambda = 3$.

Real *k* certifies a case of propagating waves, while complex *k* points for attenuated waves with exponentially decaying amplitude. To remind you the propagation happens in vacuum and the result of attenuation is completely a numerical artifact of the too coarse grid specification.

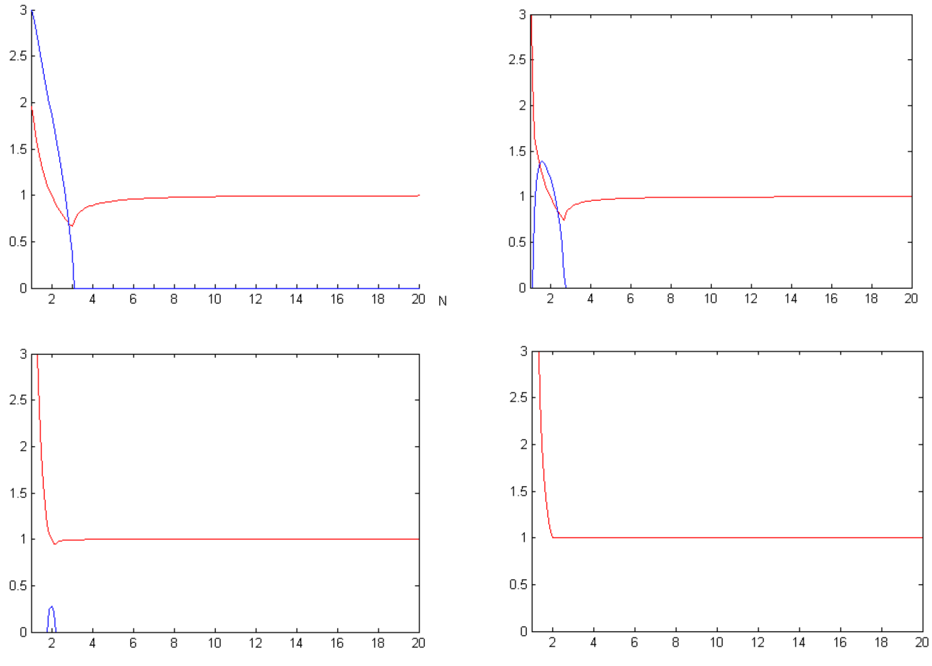
Exercise 3.4: *In this exercise we study superluminal ($v_p > c_0$) and subluminal ($v_p < c_0$) numerical light propagation in vacuum. Show that* $\omega\delta t = \frac{2\pi Q}{N_\lambda}$ *where* $N_\lambda = \lambda/\delta x$ *is a grid sampling (number of grid points per wavelength in vacuum) defined by formula (3.60). Derive the expression for the phase velocity of a plane wave on a 1D grid. Plot the phase velocity normalized by the speed of light in vacuum in dependence of the grid sampling. Take the Courant stability factor: Q=0.4; 0.6; 0.8; 0.9; 0.99; 1.0 and grid sampling from 1.0 (extremely course mesh) to 20 (moderate-to-fine meshing). Use analytical results from Exercise 3. Define grid samplings for the superluminal and subluminal propagation*.

By definition $v_p = \omega/k = 2\pi c_0/\lambda k$. Accounting for the possible complex character of the wavenumber, the real part of *k* must be used instead. By inserting Eq. (3.2) in the definition of the phase velocity and normalizing the latter by the speed of light in vacuum we obtain:

$$\frac{v_p}{c_0} = \frac{2\pi}{N_\lambda \operatorname{Re}\left(\arccos\left[1 + \frac{1}{Q^2}\left(\cos\frac{2\pi Q}{N_\lambda} - 1\right)\right]\right)}. \tag{4.1}$$

A short MATLAB routine is given below.

```
clc
format compact
hold all
f=1;
for Q=[0.4 0.6 0.8 0.9 0.99 1.0];
figure(f);f=f+1;
Nlambda=1:0.1:20;
xi=1+(1/Q^2)*(cos(2*pi*Q./Nlambda)-1);
k=acos(xi);
vpn=(2*pi./Nlambda)./real(k);
k2=imag(k);

p=plot(Nlambda,vpn,'r',...
    Nlambda,-k2,'b');
end
```



Results of calculations are plotted in figures above. The first row: Q = 0.4 (left) and Q = 0.8 (right). The second row: Q = 0.99 (left) and Q = 1.0 (right). Phase velocity is given by the red curves. As a rule with a coarse mesh a light wave first exhibits superluminal and then subluminal properties, which slowly converge to normal behavior with a fine meshing.

Exercise 3.5: *In this exercise we study numerical losses of light in vacuum. If the wavenumber k is complex, then the plane wave is attenuated, unless an unstable FDTD algorithm is used with Q > 1. Wave's amplitude is exponentially decreasing during the propagation. Find an analytical formula* *for the attenuation constant, which characterizes such decay, in dependence of the grid sampling* N_λ. *Take Courant stability factors: Q = 0.4; 0.6; 0.8; 0.9; 0.99; 1.0 and grid sampling from 1.0 (extremely course mesh) to 20 (moderate-to-fine meshing). Use analytical results from Exercise 3.*

The attenuation of a light wave is defined by the imaginary part of the wavenumber *k*. When *k* is real, no attenuation is presented as we expect for light propagation in vacuum. So, it is enough to plot Im(*k*) versus N_λ for various values of parameter *Q*. Taking Eq. (3.2) we notice that it is convenient to plot not the wavenumber alone, but its product with the grid size:

$$\mathrm{Im}(k)\delta x = \mathrm{Im}\left(\arccos\left[1 + \frac{1}{Q^2}\left(\cos \frac{2\pi Q}{N_\lambda} - 1 \right) \right] \right). \tag{5.1}$$

Such combination gives the attenuation of the wave amplitude on the grid interval. The MATLAB routine is pretty much the same as in Exercise 4, see above. Attenuation characteristics accordingly to Eq. (5.1) are given with blue curves in the figures.

Exercise 3.6: *Analyze numerical dispersion in the case of one-dimensional wave propagation with the Courant stability factor Q = 1.0. Explain, why the time step* $\delta t = h/c_0$ *is called the magic step.*

The wave propagation is accurately characterized (with no spurious losses and super- or subluminal propagation) with the magic step *Q* = 1.0 (see plots in the previous exercise). Dispersion equation (3.1) becomes a “trivial” vacuum case: $\frac{\delta x}{\delta t} = \frac{\omega}{k} = v_p$ and equation (4.1) provides $\frac{v_p}{c_0} = 1$. So, it means that the numerical dispersion is cancelled by such choice of the time step, and numerical solutions of a one-dimensional wave equation are exact. This is why it is called a “magic step”.

Exercise 3.7: *Show that the finite-difference scheme applied on the 3D Yee-grid is divergence-free for the computed magnetic fields.*

The solution here can be derived in analogy with the proof of divergence-free nature of the Yee scheme for the electric fields (see Subsection 3.2.3). As we mentioned there, a robust numerical method for solving Maxwell's equations must obey discrete equations (2.4), (2.5). Failure of nullifying the divergence operator $\nabla \cdot \mathbf{B} = 0$ means that the algorithm generates such spurious charges, what is definitely is unphysical.

We need to show that the evolution scheme does not change the initial value of $\nabla \cdot \mathbf{B}$, which is supposed to be equal to 0. Applying the Gauss theorem to a divergence operator we get

$$\frac{\partial}{\partial t}\int_V \nabla \cdot \mathbf{B} dV = \frac{\partial}{\partial t}\oint_S \mathbf{B} \cdot \mathbf{n} dS = \oint_S \frac{\partial}{\partial t}\mathbf{B} \cdot \mathbf{n} dS = 0$$

We choose one unit cell of the Yee grid Fig.3.4. Then

$$\oint_S \frac{\partial}{\partial t}\mathbf{B}\cdot\mathbf{n}dS = \left(\partial_t B_x\big|_{i+1\,j+1/2\,k+1/2} - \partial_t B_x\big|_{ij+1/2\,k+1/2}\right)\delta y\delta z + \left(\partial_t B_y\big|_{i+1/2\,j+1\,k+1/2} - \partial_t B_y\big|_{i+1/2\,jk+1/2}\right)\delta x\delta z + \left(\partial_t B_z\big|_{i+1/2\,j+1/2\,k+1} - \partial_t B_z\big|_{i+1/2\,j+1/2\,k}\right)\delta x\delta y \tag{7.1}$$

Now taking into account Faraday's Law

$$\partial_t B_x = \partial_z E_y - \partial_y E_z, \quad \partial_t B_y = \partial_x E_z - \partial_z E_x, \quad \partial_t B_z = \partial_y E_x - \partial_x E_y$$

for each of the terms in parentheses in (7.1), produces the following expressions

$$(\text{First})\delta y\delta z = \left(\frac{E_y\big|_{i+1\,j+1/2\,k+1} - E_y\big|_{i+1\,j+1/2\,k}}{\delta z} - \frac{E_z\big|_{i+1\,j+1\,k+1/2} - E_z\big|_{i+1\,jk+1/2}}{\delta y} - \frac{E_y\big|_{ij+1/2\,k+1} - E_y\big|_{ij+1/2\,k}}{\delta z} + \frac{E_z\big|_{ij+1\,k+1/2} - E_z\big|_{ij+k+1/2}}{\delta y}\right)\delta y\delta z$$

$$(\text{Second})\delta x\delta z = \left(\frac{E_z\big|_{i+1\,j+1\,k+1/2} - E_z\big|_{ij+1\,k+1/2}}{\delta x} - \frac{E_x\big|_{i+1/2\,j+1\,k+1} - E_x\big|_{i+1/2\,j+1\,k}}{\delta z} - \frac{E_z\big|_{i+1\,jk+1/2} - E_z\big|_{ijk+1/2}}{\delta x} + \frac{E_x\big|_{i+1/2\,jk+1} - E_x\big|_{i+1/2\,jk}}{\delta z}\right)\delta x\delta z$$

$$(\text{Third})\delta x\delta y = \left(\frac{E_x\big|_{i+1/2\,j+1\,k+1} - E_x\big|_{i+1/2\,jk+1}}{\delta y} - \frac{E_y\big|_{i+1\,j+1/2\,k+1} - E_y\big|_{ij+1/2\,k+1}}{\delta x} - \frac{E_x\big|_{i+1/2\,j+1\,k} - E_x\big|_{i+1/2\,jk}}{\delta y} + \frac{E_y\big|_{i+1\,j+1/2\,k} - E_y\big|_{ij+1/2\,k}}{\delta x}\right)\delta x\delta y$$

To avoid the cumbersome arithmetic we suggest tracing one component of the electric field, e.g. E_y in expression (7.1):

$$E_y\big|_{i+1\,j+1/2\,k+1} - E_y\big|_{i+1\,j+1/2\,k} - E_y\big|_{ij+1/2\,k+1} + E_y\big|_{ij+1/2\,k} - E_y\big|_{i+1\,j+1/2\,k+1} + E_y\big|_{ij+1/2\,k+1} + E_y\big|_{i+1\,j+1/2\,k} - E_y\big|_{ij+1/2\,k} = 0$$

Thus, we have shown the divergence-free character of the finite differences scheme on the Yee mesh.

Exercise 3.8: *Prove that in the limit of infinitesimal spatial grid meshing $h \to 0$ and time stepping $\delta t \to 0$ dispersion equation (3.41) converges to the conventional light dispersion equation in a uniform dielectric (3.32).*

If we repeat the whole derivation in Subsection 3.2.1 to the case of a uniform dielectric with material parameters ε and μ, this just bring $\varepsilon\mu$ product to the left-hand part of Eq.(3.41). Further we employ the well-known expression $\lim\limits_{x\to 0}\frac{\sin ax}{x}=a$. Then, evidently, Eq.(3.41) tends to $\frac{\varepsilon\mu\omega^2}{2c_0^2}=\frac{k_x^2+k_y^2+k_z^2}{2}$ or $\varepsilon\mu\omega^2=c_0^2\left(k_x^2+k_y^2+k_z^2\right)$.

Exercise 3.9: *Derive the 2D numerical dispersion equation*

$$\frac{\varepsilon\mu}{c_0^2\delta t^2}\sin^2\frac{\omega\delta t}{2}=\frac{1}{\delta x^2}\sin^2\frac{k_x\delta x}{2}+\frac{1}{\delta y^2}\sin^2\frac{k_y\delta y}{2} \tag{9.1}$$

for uniform dielectric by completing the steps of substituting TM traveling waves into the 2D FDTD scheme

$$\begin{aligned}
&\frac{H_x\big|_{ij+1/2}^{n+1/2}-H_x\big|_{ij+1/2}^{n-1/2}}{\delta t}=-\frac{1}{\mu_0\mu}\frac{E_z\big|_{ij+1}^{n}-E_z\big|_{ij}^{n}}{\delta y},\\
&\frac{H_y\big|_{i+1/2j}^{n+1/2}-H_y\big|_{i+1/2j}^{n-1/2}}{\delta t}=\frac{1}{\mu_0\mu}\frac{E_z\big|_{i+1j}^{n}-E_z\big|_{ij}^{n}}{\delta y},\\
&\frac{E_z\big|_{ij}^{n+1}-E_z\big|_{ij}^{n}}{\delta t}=\frac{1}{\varepsilon_0\varepsilon}\left(\frac{H_y\big|_{i+1/2j}^{n+1/2}-H_y\big|_{i-1/2j}^{n+1/2}}{\delta x}-\frac{H_x\big|_{ij+1/2}^{n+1/2}-H_x\big|_{ij-1/2}^{n+1/2}}{\delta y}\right)
\end{aligned} \tag{9.2}$$

To avoid confusion between indices and $i=\sqrt{-1}$ we designate grid indices with capital letters. So a plane TM wave propagating on a 2D grid has components:

$$H_x\big|_{IJ}^{n}=H_xe^{i(\omega n\delta t-k_xI\delta x-k_yJ\delta y)},\quad H_y\big|_{IJ}^{n}=H_ye^{i(\omega n\delta t-k_xI\delta x-k_yJ\delta y)},\quad E_z\big|_{IJ}^{n}=E_ze^{i(\omega n\delta t-k_xI\delta x-k_yJ\delta y)}$$

Then, substitution of these formulas in the first equation (9.2) gives:

$$\frac{H_xe^{i(\omega n\delta t-k_xI\delta x-k_yJ\delta y)}e^{-ik_y\delta y/2}(e^{i\omega\delta t/2}-e^{-i\omega\delta t/2})}{\delta t}=-\frac{1}{\mu_0\mu}\frac{E_ze^{i(\omega n\delta t-k_xI\delta x-k_yJ\delta y)}\left(e^{-ik_y\delta y}-1\right)}{\delta y},$$

what can be transformed to

$$\frac{H_x\sin(\omega\delta t/2)}{\delta t}=\frac{1}{\mu_0\mu}\frac{E_z\sin\left(k_y\delta y/2\right)}{\delta y}. \tag{9.3}$$

In the same manner the second equation (9.2) gives

$$\frac{H_y \sin(\omega\delta t/2)}{\delta t} = -\frac{1}{\mu_0 \mu} \frac{E_z \sin\left(k_x \delta x/2\right)}{\delta x}. \tag{9.4}$$

And the last

$$\frac{E_z \sin(\omega\delta t/2)}{\delta t} = \frac{1}{\varepsilon_0 \varepsilon}\left(\frac{H_y \sin\left(k_x \delta x/2\right)}{\delta x} - \frac{H_x \sin\left(k_y \delta y/2\right)}{\delta y}\right) \tag{9.5}$$

Expressing H_x and H_y from (9.3), (9.4) and gathering everything in (9.5) yields dispersion equation in the form of expression (9.1).

Exercise 3.10: *Solving numerically 2D dispersion equation (3.172) on a square grid, prove that even an empty grid-defined space exhibits anisotropy for light propagation, when phase velocity depends on the direction of propagation. Choose appropriate numerical parameters on your own.*

2D dispersion equation (3.172) for the empty space

$$\frac{1}{c_0^2 \delta t^2}\sin^2\frac{\omega\delta t}{2} = \frac{1}{\delta x^2}\sin^2\frac{k_x \delta x}{2} + \frac{1}{\delta y^2}\sin^2\frac{k_y \delta y}{2}$$

can be solved regarding the absolute value k of a wavevector **k**, where $k_x = k\cos\varphi$, $k_y = k\sin\varphi$ and angle φ characterizing direction of wave propagation on a 2D square grid ($\delta x = \delta y = h$) is measured from the x-axis. Introducing parameters N_λ and $Q = c_0\delta t/h$ we can rewrite the dispersion equation as an implicit equation $F(kh) = 0$, which can be easily solved by MATLABs routine “fzero”:

$$\frac{1}{Q^2}\sin^2\frac{\pi Q}{N_\lambda} - \sin^2\frac{kh\cos\varphi}{2} - \sin^2\frac{kh\sin\varphi}{2} = 0.$$

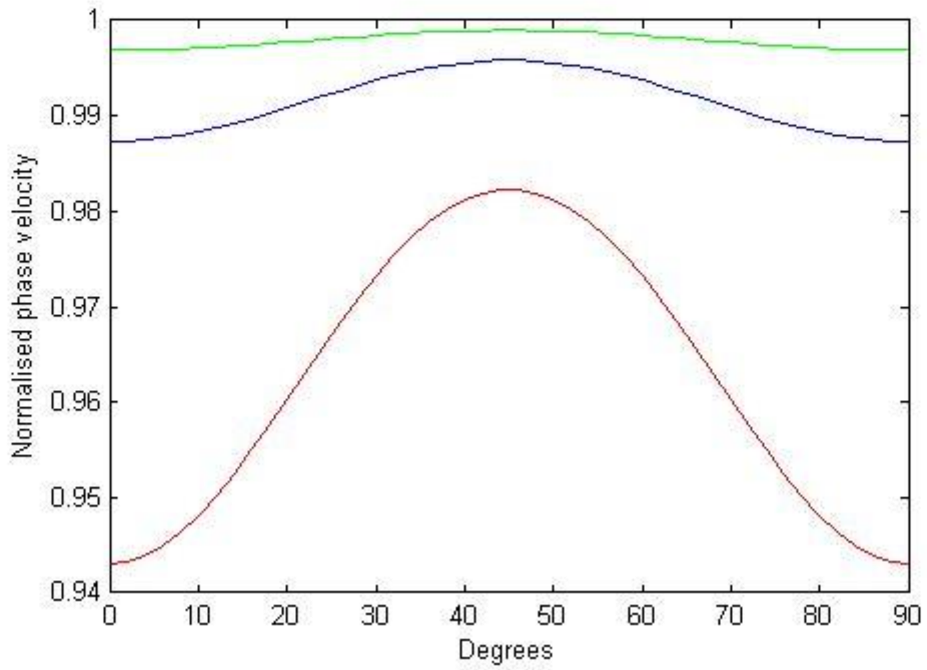
Then, similar to how we already have considered phase velocity issues in Exercise 4, we plot normalized phase velocity $\frac{v_p}{c_0} = \frac{2\pi}{N_\lambda kh}$ as function of the angle of propagation. The MATLAB routine is below

---

```
clc
clear all
format compact

Q=0.7;

Nlambda=5;
phid=0:2:90;
values=phid;

for ip=1:length(phid);
 phi=phid(ip)*pi/180;
```

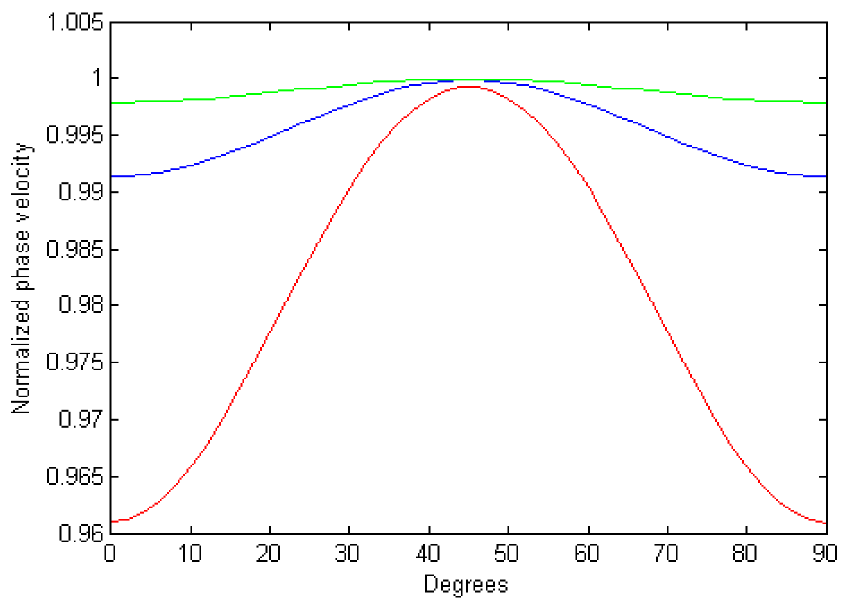
```
 [k0 val]=fzero(@(k)((1/Q^2)*(sin(pi*Q/Nlambda))^2 - (sin(k*cos(phi)/2))^2 -
(sin(k*sin(phi)/2))^2),1);
 vpn=(2*pi./Nlambda)./real(k0);
 values(ip)=vpn;
end

figure(1);
hold off
p=plot(phid,values,'r');

Nlambda=10;
values=phid;

for ip=1:length(phid);
 phi=phid(ip)*pi/180;
 [k0 val]=fzero(@(k)((1/Q^2)*(sin(pi*Q/Nlambda))^2 - (sin(k*cos(phi)/2))^2 -
(sin(k*sin(phi)/2))^2),1);
 vpn=(2*pi./Nlambda)./real(k0);
 values(ip)=vpn;
end

figure(1);
hold on
p=plot(phid,values,'b');

Nlambda=20;
values=phid;

for ip=1:length(phid);
 phi=phid(ip)*pi/180;
 [k0 val]=fzero(@(k)((1/Q^2)*(sin(pi*Q/Nlambda))^2 - (sin(k*cos(phi)/2))^2 -
(sin(k*sin(phi)/2))^2),1);
 vpn=(2*pi./Nlambda)./real(k0);
 values(ip)=vpn;
end

figure(1);
p=plot(phid,values,'g');
```

We consider three cases: a coarse grid with $N_\lambda = 5$ (red curve), an intermediate grid with $N_\lambda = 10$ (blue curve), and a fine grid with $N_\lambda = 20$ (green curve). Parameter $Q = 0.5$.

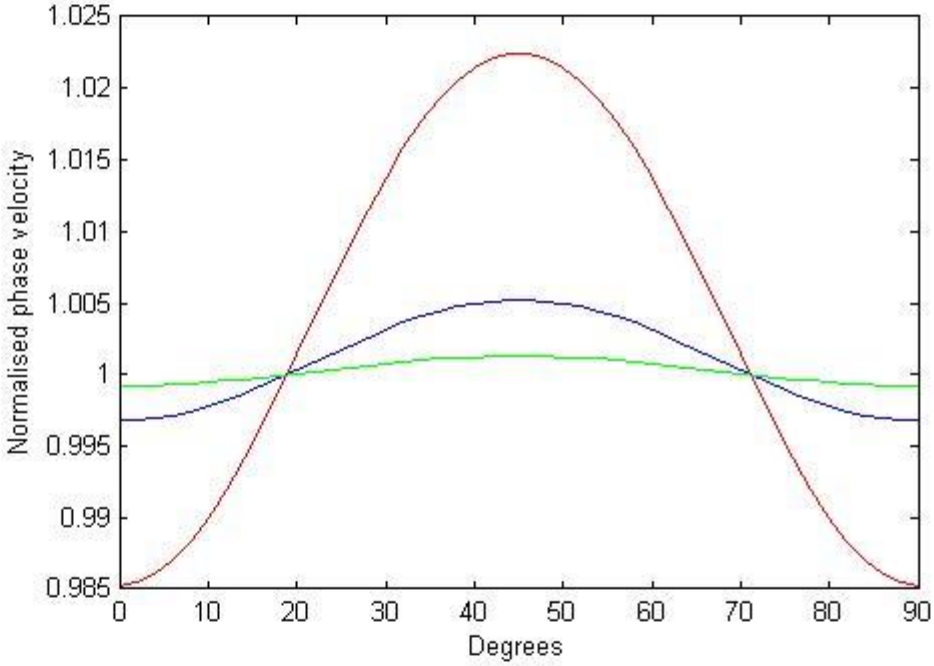


Anisotropy (numerical artifact) is obvious for the coarse and even for intermediate grids. To mitigate the spurious anisotropy the finer meshing can be recommended, where difference in the phase velocity as function of the angle of propagation is minimized to a couple of percent.

It is interesting to play with parameter Q. For the 2D square mesh it has to obey the inequality (3.50). Next figure is plotted with Q = 0.7, what is rather close to the stability limit.



The last case investigates what happen with the phase velocity anisotropy if we break the stability criteria and take Q = 0.9.



Now, not only subluminal, but also superluminal propagation of a light wave on the coarse and intermediate grids is presented. However, the fine mesh drastically decreases the spurious anisotropy on the grid.

Exercise 3.11: *Assume the 1D empty space numerical domain from i = 1 to i =11. All initial electric* $E_i^{1/2}$ *and magnetic* $H_{i+1/2}^{0}$ *fields are nullified, except* $E_6^{1/2} = 1.0$. *Calculate analytically electric and magnetic fields in the nine consequent time steps δt/2 and fill up a table with the field amplitudes in space points (coordinates in rows) in different time moments (time steps in columns). Take Q = 1.0.*

For simplicity we consider updating equations (3.19) and (3.23) of the 1D FDTD method transformed for the renormalized electric field accordingly to formula (3.26). In the case of the magic step they become extremely simple:

$$E_i^{n+1/2} = E_i^{n-1/2} - H_{i+1/2}^{n} + H_{i-1/2}^{n}, \quad H_{i+1/2}^{n+1} = H_{i+1/2}^{n} - E_{i+1}^{n+1/2} + E_i^{n+1/2}.$$

Here we omit the cap over the electric field for convenience. Now by filling the table we get:

	1	3/2	4/2	5/2	6/2	7/2	8/2	9/2	10/2	11/2	12/2	13/2	14/2	15/2	16/2	17/2	18/2	19/2	20/2	21/2	22/2
0		0		0		0		0		0		0		0		0		0		0	
1/2	0		0		0		0		0		1		0		0		0		0		0
1		0		0		0		0		-1		1		0		0		0		0	
3/2	0		0		0		0		1		-1		1		0		0		0		0
2		0		0		0		-1		1		-1		1		0		0		0	
5/2	0		0		0		1		-1		1		-1		1		0		0		0
3		0		0		-1		1		-1		1		-1		1		0		0	
7/2	0		0		1		-1		1		-1		1		-1		1		0		0
4		0		-1		1		-1		1		-1		1		-1		1		0	
9/2	0		1		-1		1		-1		1		-1		1		-1		1		0
5		-1		1		-1		1		-1		1		-1		1		-1		1	

Exercise 3.12: *Write down a script implementing the numerical scheme of a 1D FDTD method. Make your choice of parameter Q and the size of the domain. Implement a monochromatic source (continuous wave - CW) as the right end and a perfect magnetic conductor (PMC) as the left boundary conditions terminating the domain. Test the script for a homogeneous medium, $\varepsilon = \mu = 1$ observing*

a) fields E_i^n, H_i^n in all coordinate points at several time moments, for example n = 100, 200, 500;

b) fields E_i^n, H_i^n at all time-steps in several points, for example i = 20, 50, 200;

c) choose $Q \geq 1.0$ and observe unlimited growth of the fields.

The simplest 1D FDTD code is below. We choose rather fine mesh with $N_\lambda = 40$. The number of grid points is given by *ngrid*; positions of the monitors to store fields as functions of time – by *monpos*.

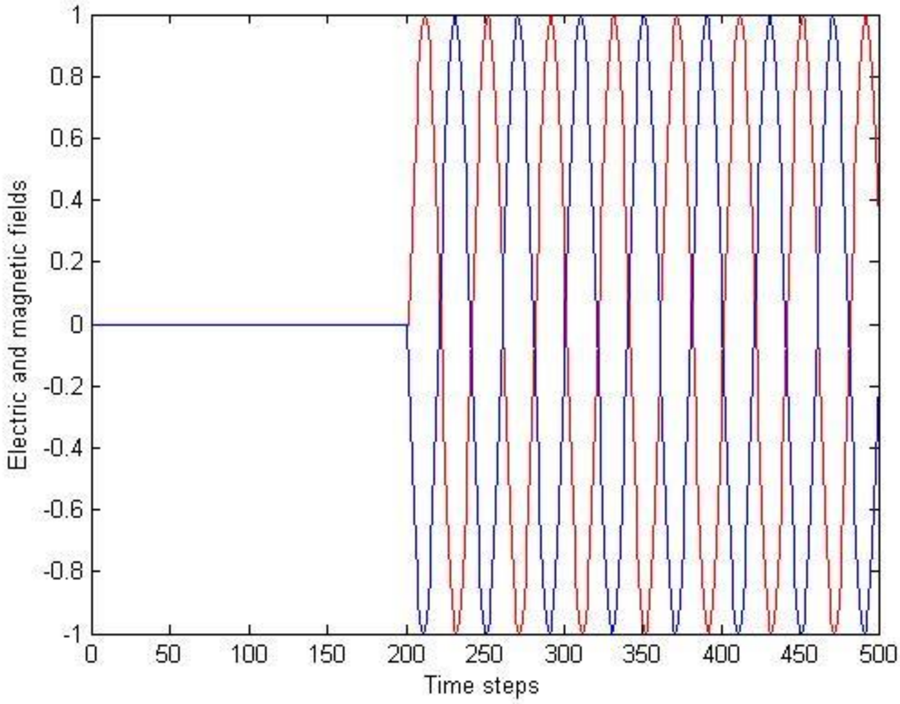
```
clc
clear all
format compact

Q=1.00;
Nlambda=40; %%parameter N_lambda
timepoints=500; %%number of time steps
ngrid=402; %%dimension of the domain
%% Initialization of grid, material parameters and monitors
grid=1:ngrid;
eps(1:ngrid)=1.0;
mu(1:ngrid)=1.0;

monitorE=1:timepoints;
monitorH=1:timepoints;
monpos=200; %%position of monitors
```

```
sourcepos=ngrid; %%position of source

Efield=zeros(1,ngrid);
Hfield=zeros(1,ngrid);
%% Main cycle
for it=1:timepoints

    Esource=sin(it*2*pi*Q/Nlambda); %CW source

 for i=2:ngrid-1
   Efield(i)=Efield(i)-(Q/eps(i))*(Hfield(i)-Hfield(i-1));
 end
   Efield(sourcepos)=Esource;
 for i=2:ngrid-1
   Hfield(i)=Hfield(i)-(Q/mu(i))*(Efield(i+1)-Efield(i));
 end
  monitorE(it)=Efield(monpos);
  monitorH(it)=Hfield(monpos);
end

%% a) plot E- and H-fields in all grid points at time step n = 500
hold all
%  plot(grid,Efield,'r')
%  plot(grid,Hfield,'b')
 hold off

%% b) plot E- and H-fields at monitors (i = 200) in all time steps
 plot(1:timepoints,monitorE,'r',1:timepoints,monitorH,'b')
```

Notice that we realize the PMC condition by keeping the initial nullified magnetic field not updated in the point $i = 1$.

Here we plot normalized electric (red) and magnetic (blue) fields captured in all time steps by the monitors positioned at point $i = 200$ (question b). To plot fields in all points at certain time steps use commented commands just above.

Exercise c) is very easy to check just by changing parameter Q to, e.g. 1.01, but remember that the number of time steps must be enough for the radiation emitted by the most-right CW source to reach your monitors: in our example it must be at least over 200.



Exercise 3.13: *Repeat exercise 3.12 but with a hard CW source positioned in the middle of the domain with $\varepsilon = 9$, $\mu = 1$ and an additional perfect electric conductor (PEC) as the right boundary condition terminating the domain. Describe the changes in the field pictures you observe? Try to violate the Courant stability condition. Does the limit value depend on ε?*

The script is pretty much the same as the previous routine. We recommend to calculate the position in the middle of the domain by operation: `sourcepos=round(ngrid/2+0.5),` which rounds numbers larger than, for example 100.5 to 101, but numbers smaller than 100.5 to 100. The electric field generated by the source is updated by the CW formula and is excluded from the FDTD field evolving scheme.

It is easy to check that parameter Q can be extended to 3.0 (corrected by $\sqrt{\varepsilon}$). And over this threshold the FDTD algorithm breaks. However, be aware that such simple rule is applied only in the case of one dimensional homogeneous computational domain.

Exercise 3.14: *Implement a pulse current source from the very right end of the numerical domain, generating a pulse like $\sin(\omega t)\sin(\Omega t)$. Take two cases: $\varepsilon = \mu = 1$ and $\varepsilon = 9$, $\mu = 1$.*

a) Trace the pulse propagation in time and space.

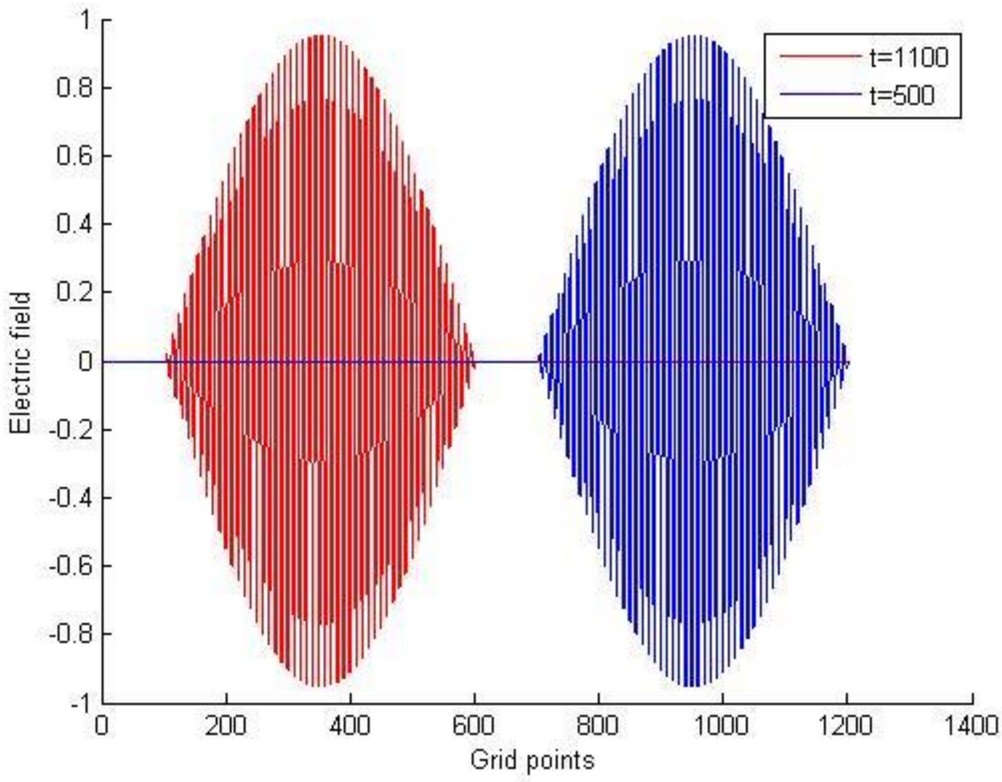
b) Check the peak value and pulse shape.

c) Determine the group velocity of the pulse, defined as the speed of the pulse peak propagation.

The changes in the program are connected with implementation of the pulse source. This is the script:

```
%% Main cycle
for it=1:timepoints  %%pulse source switched for a half of the period
     if it*2*Q/NNLambda < 1
        Esource=sin(it*2*pi*Q/Nlambda)*sin(it*2*pi*Q/NNLambda);
     else
        Esource=0;
     end
```

The source is active a half of the period connected with the envelope frequency *Ω*. This frequency is controlled by parameter `NNLambda=100*Nlambda,` which is taken here to be 100 times larger than N_λ. Thus $\Omega=100\omega$. The spatial picture of the pulse (electric field) in two time moments is shown below.



We see that the shape of the pulse and its peak value are preserved (question b) during propagation in homogeneous dispersionless dielectric. To find the group velocity we should estimate the distance between two positions of the peak and divide it by the time interval. Approximately, $\Delta x = 600\delta x$ and $\Delta t = 600\delta t$. Hence $v_g = \dfrac{\Delta x}{\Delta t} = \dfrac{\delta x}{\delta t} = \dfrac{c_0}{Q} = c_0$. It is also the consequences of propagation in a dispersionless uniform medium, where the group velocity is equal to the phase velocity. You can change permittivity and notice the correspondent changes in the group velocity of the pulse.

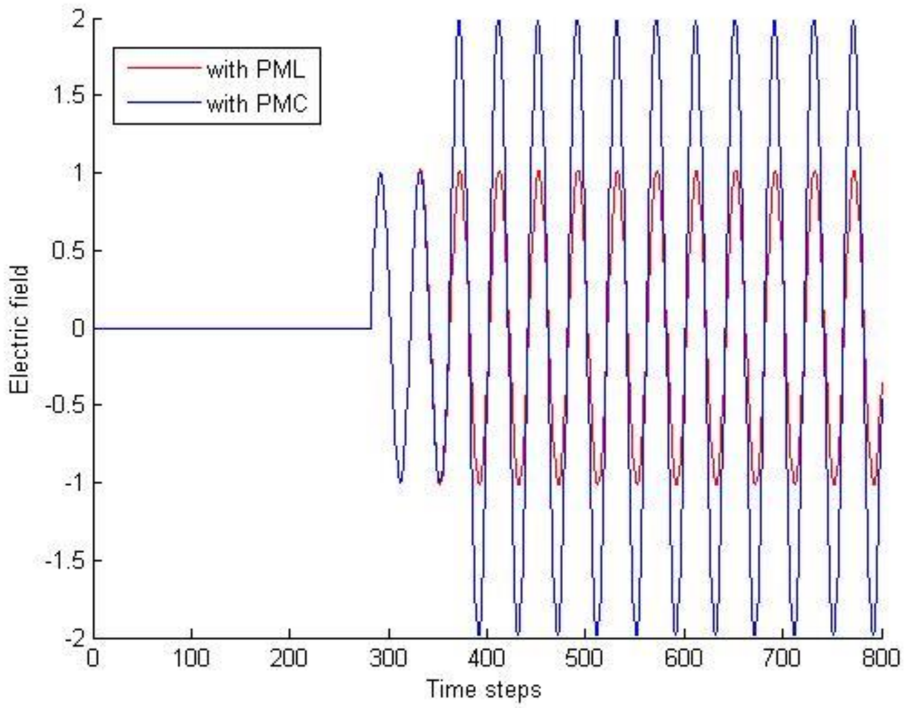
Exercise 3.15: *Implement a 1D PML from one side of the domain opposite to the position of the CW source. Observe propagation of the wave front before and after reflection from the PML. Wait for the steady state conditions. Quantify the PML performance as an ABC by comparing amplitudes of the reflected waves with the perfect conductor boundary condition and PML.*

We slightly rearrange the program to unify the field evolution algorithm in the physical domain and in the PMLs regions. Now the unique update scheme is applied to all computational domain, but outside the PML region the control parameter of the strength of the PML w0 is nullified.

```
clc
clear all
format compact

Q=1.00;
Nlambda=40;
timepoints=800;
d_PML=20; %% PML layer thickness in grid points
ngrid=302+d_PML;

%% Initialization of grid, material parameters and monitors
grid=1:ngrid;
eps(1:ngrid)=1.0;
mu(1:ngrid)=1.0;
monitorE=1:timepoints;
monitorH=1:timepoints;
monpos=40; %%position of monitors
sourcepos=ngrid; %%position of source

%% Initializing PML
we(ngrid)=0;
wm(ngrid)=0;
w0=0.0 %% PMC condition
%w0=1.50; %% PML condition
m=2;
for i=1:d_PML
    we(i)=w0*((d_PML-i)/d_PML)^m;
    wm(i)=w0*((d_PML-i)/d_PML)^m;
    %wm(i)=w0*((d_PML-i-1/2)/d_PML)^m;
    if d_PML-i-1/2<0 wm(i)=0;
    end
end

%% Initializing fields
Efield=zeros(1,ngrid);
Hfield=zeros(1,ngrid);

%% Main cycle
for it=1:timepoints

    Esource=sin(it*2*pi*Q/Nlambda); %CW source
```

```
 for i=2:ngrid
   Efield(i)=(1-we(i))*Efield(i)/(1+we(i))-(Q/eps(i))*(Hfield(i)-Hfield(i-1))/(1+we(i));
 end
   Efield(1)=(1-we(1))*Efield(1)/(1+we(1))-(Q/eps(1))*(Hfield(1)-0)/(1+we(1));
%% PMC for Hfield(0)
   Efield(sourcepos)=Esource;
 for i=1:ngrid-1
   Hfield(i)=(1-wm(i))*Hfield(i)/(1+wm(i))-(Q/mu(i))*(Efield(i+1)-Efield(i))/(1+wm(i));
 end

  monitorE(it)=Efield(monpos);
  monitorH(it)=Hfield(monpos);
end

%%plot E- and H-fields in all grid points
hold all
%   plot(grid,Efield,'r')
%   plot(grid,Hfield,'b')
hold off
%%plot E- and H-fields at monitors in all time steps
%plot(1:timepoints,monitorE,'r',1:timepoints,monitorH,'b')
hold all
plot(1:timepoints,monitorE,'b')
```

To check for the effectiveness of the PML as an absorbing boundary condition we compare PMC and PML behavior observing, e.g. an electric field at the monitor point in the time interval long enough such that the signal from the CW crosses the domain, experiences reflection from the utmost left side and passes again through the monitor. Results are shown in the figure below.



When the wave is totally reflected by the PMC, its amplitude at the monitor is doubled (blue line) due to the in-phase interference with the incoming wave (remember that we have a CW source). When the PML is switched on, then no any observable changes of the amplitude at the monitor point is traced certifying that back reflection from the PML is very small. For quantification of the PML reflection we recommend either to use time-limited CW signal to avoid the interference effects or to apply a pulse source.

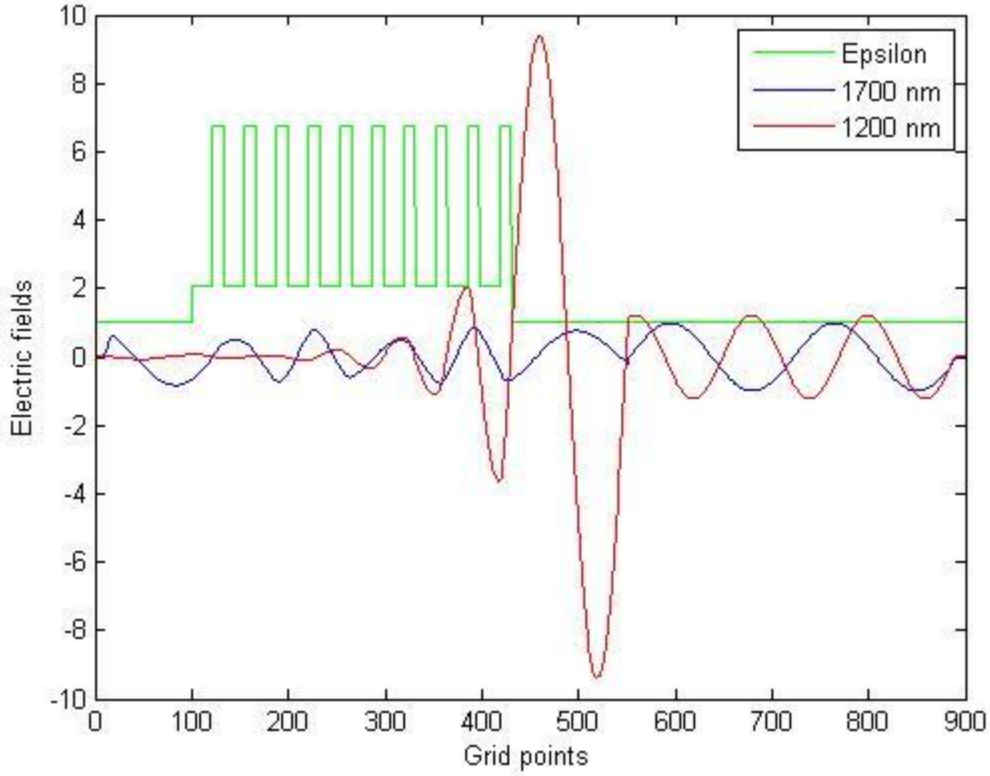
Exercise 3.16: *Somewhere in the middle of the domain make a Bragg grating with parameters: 10 periods; thicknesses of the layers obey condition:* $\sqrt{\varepsilon_1}l_1 = \sqrt{\varepsilon_2}l_2 = \lambda_0/4$ *with* λ_0 *= 1200nm,* $\sqrt{\varepsilon_1} = 1.45$, and $\sqrt{\varepsilon_2} = 2.60$. *Put a CW source at one side of the Bragg grating. Observe transmission through the Bragg grating at different wavelengths.*

We know that on the central wavelength of the Bragg grating, transmission should be very low. So we implement a hard source some distance away from the grating. The grating is initialized by this script:

```
lambda=1200; %%CW wavelength in nanometers
dz=10 %% mesh size in nanometers
d_PML=20; %% PML layer thickness in grid points
z_bragg0=100; %% the first grid point of the grating
n_periods=10; %% number of periods in the Bragg grating
lambdaBragg=1200; %% wavelength in nanometers
l1=lambdaBragg/4/n1; %% 1st layer thickness in nanometers
l2=lambdaBragg/4/n2; %% 2nd layer thickness in nanometers
z_bragg1=round(l1/dz+0.5); %% 1st layer thickness in grid points
z_bragg2=round(l2/dz+0.5); %% 2nd layer thickness in grid points
z_period=z_bragg1+z_bragg2; %% One Bragg period thickness in grid points
ngrid=2*d_PML+2*z_bragg0+2*n_periods*z_period; %% total numerical domain
thickness

%% Initialization of grid, material parameters and monitors
grid=1:ngrid;
eps(1:ngrid)=1.0;
mu(1:ngrid)=1.0;

timepoints=4000;
monitorE=1:timepoints;
monitorH=1:timepoints;
monpos=50; %%position of monitor
sourcepos=round(ngrid/2+0.5)+100 %%position of source. Check that it is outside
the Bragg grating

%% Initialization of Bragg grating

for i=1:n_periods
  eps(z_bragg0+z_period*(i-1)+1:z_bragg0+z_period*(i-1)+z_bragg1)=eps1;
  eps(z_bragg0+z_period*(i-1)+z_bragg1+1:z_bragg0+z_period*(i-1)+z_period)=eps2;
end
plot(1:ngrid,eps,'g')
```

It is important to emphasize that as soon as we get the precise spatial parameter, in our case the central Bragg wavelength λ_0, all previous dimensionless parameters must be scaled in length units: mesh size, layers thicknesses, etc.

We use a hard CW source with two wavelengths: λ = 1200 nm and λ = 1700 nm. The electric field distribution in the numerical domain after 5000 time steps is shown in the figure.



We see that on λ = 1200 nm the highly reflecting Bragg grating (profile of the dielectric permittivity in the domain is shown by the green line) and the hard source (i = 551) form a cavity. So the amplitude is growing up with time. However, transmission of the Bragg grating is poor (red line). In contrary, at 1700 nm reflection is low, transmission is high, and thus no any cavity effect is observed.

Exercise 3.17: *Implement PMLs from both sides of the domain. Put your source in the middle between two Bragg gratings with the same parameters. Trace CW and pulse propagation in the frequency ranges with good (passband) and poor (stopband) transmission*

The code now includes two PMLs terminating the physical domain from the left and right sides. Be aware that we shift the absorption profile for the magnetic field by one half of a grid remembering the staggered grid realization. We prepare also two options of the source: CW and pulse. One of them must be commented during execution to avoid multisource operation. The duration of pulses is controlled by the parameter `lambda_envelope`, where a constant wavelength `lambda_0` is used. Thus changing the wavelength of the modulated signal we keep the pulse duration unchanged.

Bragg gratings are described separately, that helps to tune them individually as it is asked in Exercise 3.18.

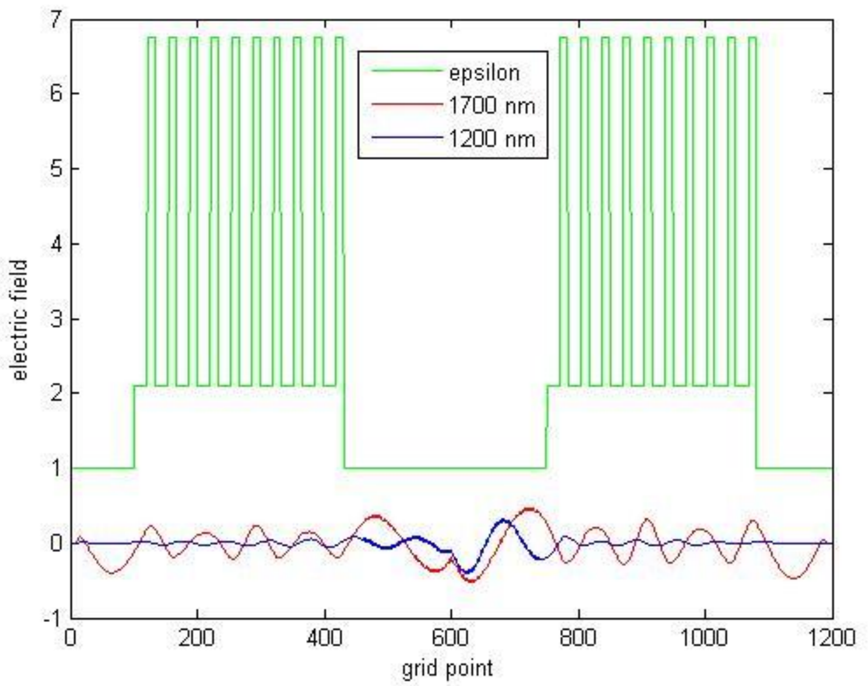
We realize the current source concept, where current as a function of time is added in the field updating scheme directly. Position of the source now is defined by the position of non-zero element/elements in array `source`. The output again can be done in terms of plotting a time-dependent field in a specified mesh point or observing fields in the whole domain in a prescribed time point. The switching is done by commenting/uncommenting the output operators.

```
clc
clear all
format compact

%% Geometrical and material parameters
Q=1.0;
n1=1.45; %%first refractive index
eps1=n1*n1;
n2=2.60; %%second refractive index
eps2=n2*n2;
lambda=1200; %wavelength in nanometers
lambda_0=1200; %reference wavelength in nanometers
lambda_envelope=lambda_0*100;% envelope wavelength in nanometers
dz=10 %% mesh size in nanometers
d_PML=20; %% PML layer thickness in grid points
z_bragg01=100; %% beginning of the first Bragg grating
delta_gratings=300; %%distance between gratings
n_periods=10; %% number of periods in Bragg grating

%% Bragg grating parameters
%% First Bragg grating
lambdaBragg1=1200; %% operational wavelength in nanometers
l11=lambdaBragg1/4/n1 %% 1st layer thickness in nanometers
l21=lambdaBragg1/4/n2 %% 2nd layer thickness in nanometers
z_bragg11=round(l11/dz+0.5) %% 1st layer thickness in grid points
z_bragg21=round(l21/dz+0.5) %% 2nd layer thickness in grid points
z_period1=z_bragg11+z_bragg21 %% first Bragg period thickness in grid points

%% Second Bragg grating
lambdaBragg2=1200; %% operational wavelength in nanometers
l12=lambdaBragg2/4/n1 %% 1st layer thickness in nanometers
l22=lambdaBragg2/4/n2 %% 2nd layer thickness in nanometers
z_bragg12=round(l12/dz+0.5) %% 1st layer thickness in grid points
z_bragg22=round(l22/dz+0.5) %% 2nd layer thickness in grid points
z_period2=z_bragg12+z_bragg22 %%  second Bragg period thickness in grid points
z_bragg02=d_PML+z_bragg01+n_periods*z_period1+delta_gratings; %% beginning of
the second grating

%% Initialization of grid, material parameters and monitors
ngrid=2*d_PML+2*z_bragg01+n_periods*(z_period1+z_period2)+delta_gratings%% total
numerical domain thickness
grid=1:ngrid;
eps(1:ngrid)=1.0;
mu(1:ngrid)=1.0;

timepoints=7000;
```

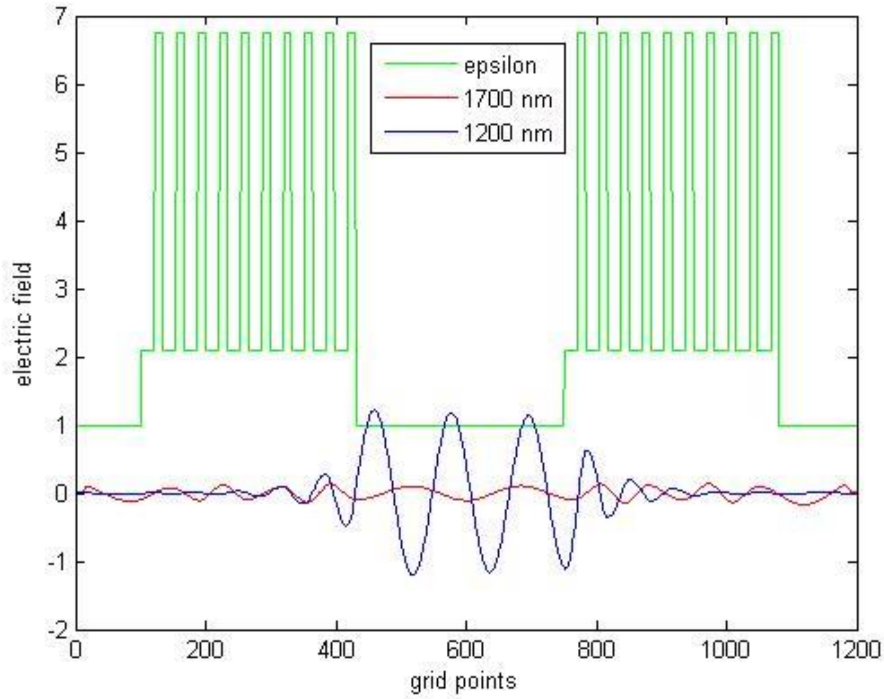
```
monitorE=1:timepoints;
monitorH=1:timepoints;
sourcepos=round(ngrid/2+0.5)
monpos=50;
%% Initialization of Bragg gratings

for i=1:n_periods
  eps(z_bragg01+z_period1*(i-1)+1:z_bragg01+z_period1*(i-1)+z_bragg11)=eps1;
  eps(z_bragg01+z_period1*(i-1)+z_bragg11+1:z_bragg01+z_period1*(i-
1)+z_period1)=eps2;
end

for i=1:n_periods
  eps(z_bragg02+z_period2*(i-1)+1:z_bragg02+z_period2*(i-1)+z_bragg12)=eps1;
  eps(z_bragg02+z_period2*(i-1)+z_bragg12+1:z_bragg02+z_period2*(i-
1)+z_period2)=eps2;
end
%plot(1:ngrid,eps,'g') %%plot profile of dielectric permittivity
%% Initialization of PMLs

we(ngrid)=0;
wm(ngrid)=0;
w0=1.5;
m=2;
%% Left PML
for i=1:d_PML
    we(i)=w0*((d_PML-i)/d_PML)^m;
    %wm(i)=w0*((d_PML-i)/d_PML)^m;
    wm(i)=w0*((d_PML-i-1/2)/d_PML)^m;
    if d_PML-i-1/2<0 wm(i)=0;
    end
end
%% Right PML
for i=ngrid-d_PML:ngrid
    we(i)=w0*((i-ngrid+d_PML)/d_PML)^m;
    %wm(i)=w0*((d_PML-i)/d_PML)^m;
    wm(i)=w0*((i-ngrid+d_PML-1/2)/d_PML)^m;
    if i-ngrid+d_PML-1/2<0 wm(i)=0;
    end
end

%%Initialization of fields and source arrays
Efield=zeros(1,ngrid);
Hfield=zeros(1,ngrid);
source=zeros(1,ngrid);

%% Main cycle
for it=1:timepoints %%Pulse source
    if it*2*Q*dz/lambda_envelope < 1

source(sourcepos)=sin(it*2*pi*Q*dz/lambda)*sin(it*2*pi*Q*dz/lambda_envelope);
    else
       source(sourcepos)=0;
    end

 %   source(sourcepos)=sin(it*2*pi*Q*dz/lambda); %CW source
```

```
 for i=2:ngrid
   Efield(i)=(1-we(i))*Efield(i)/(1+we(i))-(Q/eps(i))*(Hfield(i)-Hfield(i-1)+source(i))/(1+we(i)); %% realization of current source
 end
   Efield(1)=(1-we(1))*Efield(1)/(1+we(1))-(Q/eps(1))*(Hfield(1)-0)/(1+we(1));
%% PMC for Hfield(0)
   %Efield(sourcepos)=Esource;
 for i=1:ngrid-1
   Hfield(i)=(1-wm(i))*Hfield(i)/(1+wm(i))-(Q/mu(i))*(Efield(i+1)-Efield(i))/(1+wm(i));
 end
   Hfield(ngrid)=(1-wm(ngrid))*Hfield(ngrid)/(1+wm(ngrid))-(Q/mu(ngrid))*(0-Efield(ngrid))/(1+wm(ngrid));

  monitorE(it)=Efield(monpos);
  monitorH(it)=Hfield(monpos);
end

%% Output block
hold all
plot(grid,Efield,'b') %%plot the last updated fields in all grid points
% plot(grid,Hfield,'b')
% hold off

%plot(1:timepoints,monitorE,'r',1:timepoints,monitorH,'b')
%plot(1:timepoints,monitorE,'r') %%plot field as function of time at the monitor
```

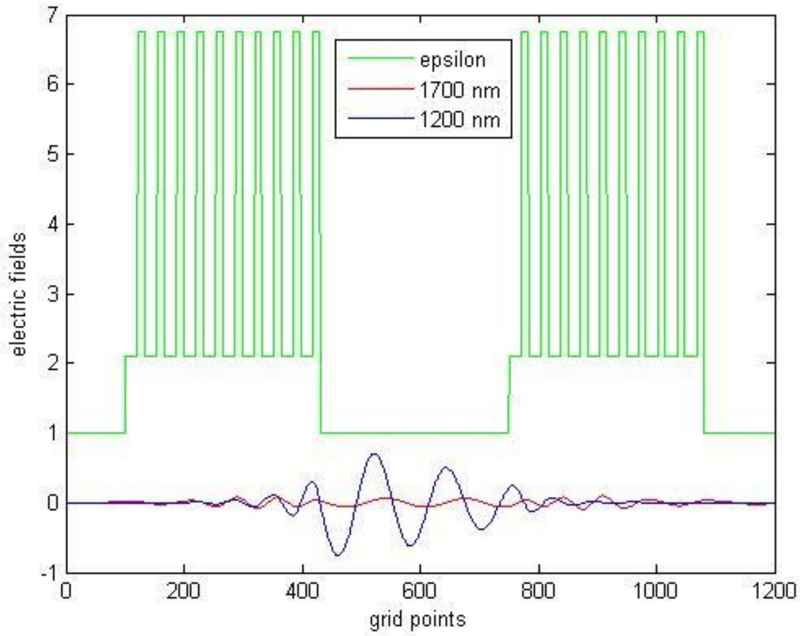
Results of the program execution are given below. The electric field in the whole domain in the case of a CW source:



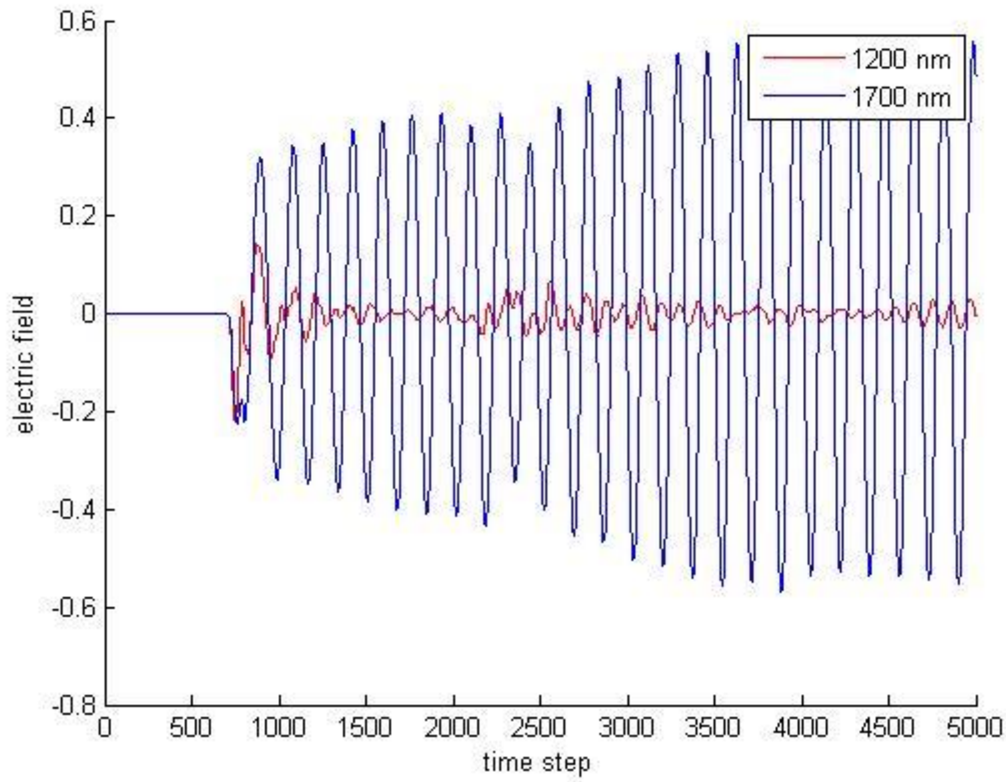
The electric field in the whole domain in the case of a long (narrow band) pulse source. The Bragg gratings serve as a cavity walls for the pulse centered around 1200 nm:



The electric field in the whole domain in the case of a short (broad band) pulse source. The Bragg gratings serve as a cavity walls, but reflection properties worsened.



The electric field from the monitor placed outside the cavity formed with the Bragg gratings. It is interesting to observe the transient behavior of the CW signal front. Even in case of the stopband wavelength the first cycle easily passes the Bragg mirror.



Exercise 3.18: *Tune the left Bragg mirror on wavelength λ_1 = 1500nm. Generate a CW,*

short (broadband) and long (narrowband) pulses with the (central) frequencies matching with either the left or right Bragg gratings stopbands. Observe and describe its propagation through the structures.

The code given in 3.17 suited for this exercise. Playing with the source and Bragg grating parameters we can either let or stop waves/pulses to propagate through the gratings. In terms of pulses with a finite bandwidth propagation may not be blocked in the stopband completely.