

## Chapter 8 Partial Differential Equations

### 8-1 Elliptic Partial Differential Equations

Solve  $\frac{\partial^2 u(x, y)}{\partial x^2} + \frac{\partial^2 u(x, y)}{\partial y^2} = f(x, y), \quad \forall (x, y) \in R; \quad u(x, y) = g(x, y), \quad \forall (x, y) \in S$ , where

$R = \{(x, y): a \leq x \leq b, c \leq y \leq d\}$ , and  $S$  is the boundary of  $R$ .

Set  $x_i = a + ih, y_j = c + jk, h = (b-a)/n, k = (d-c)/m, i = 0, 1, 2, \dots, n$ , and  $j = 0, 1, 2, \dots, m$ .

**Central difference method:**

$$\frac{u(x_{i+1}, y_j) - 2u(x_i, y_j) + u(x_{i-1}, y_j))}{h^2} + \frac{u(x_i, y_{j+1}) - 2u(x_i, y_j) + u(x_i, y_{j-1}))}{k^2} = f(x_i, y_j)$$

and  $u(x_0, y_j) = g(x_0, y_j), u(x_n, y_j) = g(x_n, y_j), j = 0, 1, 2, \dots, m-1; u(x_i, y_0) = g(x_i, y_0), u(x_i, y_m) = g(x_i, y_m), i = 0, 1, 2, \dots, n-1$

$$\Rightarrow 2 \left[ \left( \frac{h}{k} \right)^2 + 1 \right] u_{ij} - (u_{i+1,j} + u_{i-1,j}) - \left( \frac{h}{k} \right)^2 (u_{i,j+1} + u_{i,j-1}) = -h^2 f_{ij} \quad \text{and } u_{0j} = g_{0j}, u_{nj} = g_{nj},$$

$$u_{i0} = g_{i0}, u_{im} = g_{im}.$$

**Eg. Solve**  $\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0, \quad 0 \leq x \leq 0.5, \quad 0 \leq y \leq 0.5$  with  $u(0, y) = u(x, 0) = 0,$

$u(x, 1/2) = 200x, u(1/2, y) = 200y.$  (Exact solution:  $u(x, y) = 400xy$ )

(Sol.) We set  $n = m = 4$ , and then

$$h = k = \frac{1}{4} = \frac{1}{8}, \quad u_{ij} = u(x_i, y_j), \quad x_i = ih, \quad y_j = jk \Rightarrow \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2} + \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{k^2} = 0$$

$$\Rightarrow 2 \left[ \left( \frac{h}{k} \right)^2 + 1 \right] u_{ij} - (u_{i+1,j} + u_{i-1,j}) - \left( \frac{h}{k} \right)^2 (u_{i,j+1} + u_{i,j-1}) = 0$$

$$\Rightarrow \begin{cases} 4u_{13} - u_{23} - u_{12} = u_{14} = 200 \times \frac{1}{8} = 25 \\ 4u_{23} - u_{33} - u_{13} - u_{22} = u_{24} = 200 \times \frac{2}{8} = 50 \\ 4u_{33} - u_{23} - u_{32} = u_{43} + u_{34} = 200 \times \frac{3}{8} + 200 \times \frac{3}{8} = 150 \\ 4u_{12} - u_{22} - u_{13} - u_{11} = u_{02} = 0 \\ 4u_{22} - u_{32} - u_{12} - u_{23} - u_{21} = 0 \\ 4u_{32} - u_{22} - u_{33} - u_{31} = u_{42} = 200 \times \frac{2}{8} = 50 \\ 4u_{11} - u_{21} - u_{12} = u_{01} + u_{10} = 0 \\ 4u_{21} - u_{31} - u_{11} - u_{22} = u_{20} = 0 \\ 4u_{31} - u_{21} - u_{32} = u_{30} + u_{41} = 0 + 200 \times \frac{1}{8} = 25 \end{cases} \Rightarrow \begin{bmatrix} 4 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 4 & -1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 4 & 0 & 0 & -1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 4 & -1 & 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & -1 & 4 & -1 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 & -1 & 4 & 0 & 0 & -1 \\ 0 & 0 & 0 & -1 & 0 & 0 & 4 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & -1 & 4 & -1 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 4 \end{bmatrix} \begin{bmatrix} u_{13} \\ u_{23} \\ u_{33} \\ u_{12} \\ u_{22} \\ u_{32} \\ u_{11} \\ u_{21} \\ u_{31} \end{bmatrix} = \begin{bmatrix} 25 \\ 50 \\ 150 \\ 0 \\ 0 \\ 50 \\ 0 \\ 0 \\ 25 \end{bmatrix}$$

$$\Rightarrow u_{13} = 18.75, u_{23} = 37.5, \dots, u_{21} = 12.5, u_{31} = 18.75$$

In **MATLAB** language, we can use the following program to solve the partial differential equation:

```
>>A=[4,-1,0,-1,0,0,0,0,0;-1,4,-1,0,-1,0,0,0,0;0,-1,4,0,0,-1,0,0,0;-1,0,0,4,-1,0,-1,0,0;
0,-1,0,-1,4,-1,0,-1,0;0,0,-1,0,-1,4,0,0,-1;0,0,0,-1,0,0,4,-1,0;0,0,0,0,-1,0,-1,4,-1;
0,0,0,0,0,-1,0,-1,4];
>>B=[25;50;150;0;0;50;0;0;25];
>>rref([A,B])
```

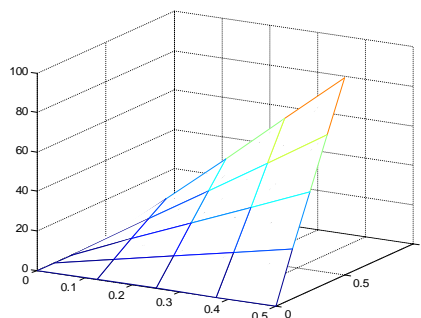
ans =

Columns 1 through 7

1.0000	0	0	0	0	0	0	0	0
0	1.0000	0	0	0	0	0	0	0
0	0	1.0000	0	0	0	0	0	0
0	0	0	1.0000	0	0	0	0	0
0	0	0	0	1.0000	0	0	0	0
0	0	0	0	0	1.0000	0	0	0
0	0	0	0	0	0	1.0000	0	0
0	0	0	0	0	0	0	1.0000	0
0	0	0	0	0	0	0	0	1.0000

Columns 8 through 10

0	0	18.7500
0	0	37.5000
0	0	56.2500
0	0	12.5000
0	0	25.0000
0	0	37.5000
0	0	6.2500
1.0000	0	12.5000
0	1.0000	18.7500



## 8-2 Parabolic Partial Differential Equations

Solve  $\frac{\partial u(x,t)}{\partial t} = \alpha^2 \cdot \frac{\partial^2 u(x,t)}{\partial x^2}$ ,  $0 \leq x \leq l$ ,  $t > 0$ , with  $u(0,t)=u(l,t)=0$ ,  $u(x,0)=f(x)$ .

Set  $h=l/m$ ,  $x_i=ih$ ,  $t_j=jk$ ,  $i=0, 1, 2, \dots, m$ , and  $j=0, 1, 2, \dots$

**Forward difference method:**  $\frac{u_{i,j+1} - u_{ij}}{k} - \alpha^2 \cdot \frac{u_{i+1,j} - 2u_{ij} + u_{i-1,j}}{h^2} = 0$

Set  $\lambda = \frac{\alpha^2 k}{h^2} \Rightarrow u_{i,j+1} = (1-2\lambda)u_{ij} + \lambda(u_{i+1,j} + u_{i-1,j})$  and  $u_{0j}=u_{mj}=0$ ,  $u_{i0}=f(x_i)$

$$\Rightarrow \begin{bmatrix} u_{1,j+1} \\ u_{2,j+1} \\ \vdots \\ \vdots \\ u_{m-1,j+1} \end{bmatrix} = \begin{bmatrix} (1-2\lambda) & \lambda & 0 & \dots & 0 \\ \lambda & (1-2\lambda) & \lambda & \ddots & \vdots \\ 0 & \lambda & (1-2\lambda) & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \lambda \\ 0 & \dots & 0 & \lambda & (1-2\lambda) \end{bmatrix} \begin{bmatrix} u_{1j} \\ u_{2j} \\ \vdots \\ \vdots \\ u_{m-1,j} \end{bmatrix}$$

We have

$$\begin{bmatrix} u_{11} \\ u_{21} \\ \vdots \\ \vdots \\ u_{m-1,1} \end{bmatrix} = \begin{bmatrix} (1-2\lambda) & \lambda & 0 & \dots & 0 \\ \lambda & (1-2\lambda) & \lambda & \ddots & \vdots \\ 0 & \lambda & (1-2\lambda) & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \lambda \\ 0 & \dots & 0 & \lambda & (1-2\lambda) \end{bmatrix} \begin{bmatrix} f(x_1) \\ f(x_2) \\ \vdots \\ \vdots \\ f(x_{m-1}) \end{bmatrix},$$

$$\begin{bmatrix} u_{12} \\ u_{22} \\ \vdots \\ \vdots \\ u_{m-1,2} \end{bmatrix} = \begin{bmatrix} (1-2\lambda) & \lambda & 0 & \dots & 0 \\ \lambda & (1-2\lambda) & \lambda & \ddots & \vdots \\ 0 & \lambda & (1-2\lambda) & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \lambda \\ 0 & \dots & 0 & \lambda & (1-2\lambda) \end{bmatrix} \begin{bmatrix} u_{11} \\ u_{21} \\ \vdots \\ \vdots \\ u_{m-1,1} \end{bmatrix},$$

$$\begin{bmatrix} u_{13} \\ u_{23} \\ \vdots \\ \vdots \\ u_{m-1,3} \end{bmatrix} = \begin{bmatrix} (1-2\lambda) & \lambda & 0 & \dots & 0 \\ \lambda & (1-2\lambda) & \lambda & \ddots & \vdots \\ 0 & \lambda & (1-2\lambda) & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \lambda \\ 0 & \dots & 0 & \lambda & (1-2\lambda) \end{bmatrix} \begin{bmatrix} u_{12} \\ u_{22} \\ \vdots \\ \vdots \\ u_{m-1,2} \end{bmatrix},$$

$$\begin{bmatrix} u_{14} \\ u_{24} \\ \vdots \\ \vdots \\ u_{m-1,4} \end{bmatrix} = \begin{bmatrix} (1-2\lambda) & \lambda & 0 & \dots & 0 \\ \lambda & (1-2\lambda) & \lambda & \ddots & \vdots \\ 0 & \lambda & (1-2\lambda) & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \lambda \\ 0 & \dots & 0 & \lambda & (1-2\lambda) \end{bmatrix} \begin{bmatrix} u_{13} \\ u_{23} \\ \vdots \\ \vdots \\ u_{m-1,3} \end{bmatrix}, \dots$$

**Backward difference method:**  $\frac{u_{ij} - u_{i,j-1}}{k} - \alpha^2 \cdot \frac{u_{i+1,j} - 2u_{ij} + u_{i-1,j}}{h^2} = 0$

$$\Rightarrow u_{i,j-1} = (1 + 2\lambda)u_{ij} - \lambda(u_{i+1,j} + u_{i-1,j})$$

$$\begin{bmatrix} (1+2\lambda) & -\lambda & 0 & \cdots & 0 \\ -\lambda & (1+2\lambda) & -\lambda & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & -\lambda \\ 0 & \cdots & 0 & -\lambda & (1+2\lambda) \end{bmatrix} \begin{bmatrix} u_{1j} \\ u_{2j} \\ \vdots \\ \vdots \\ u_{m-1,j} \end{bmatrix} = \begin{bmatrix} u_{1,j-1} \\ u_{2,j-1} \\ \vdots \\ \vdots \\ u_{m-1,j-1} \end{bmatrix}, \text{ where } u_{i0} = f(x_i).$$

We solve

$$\begin{bmatrix} (1+2\lambda) & -\lambda & 0 & \cdots & 0 \\ -\lambda & (1+2\lambda) & -\lambda & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & -\lambda \\ 0 & \cdots & 0 & -\lambda & (1+2\lambda) \end{bmatrix} \begin{bmatrix} u_{11} \\ u_{21} \\ \vdots \\ \vdots \\ u_{m-1,1} \end{bmatrix} = \begin{bmatrix} f(x_1) \\ f(x_2) \\ \vdots \\ \vdots \\ f(x_{m-1}) \end{bmatrix} \Rightarrow \begin{bmatrix} u_{11} \\ u_{21} \\ \vdots \\ \vdots \\ u_{m-1,1} \end{bmatrix} = ?$$

and then we solve

$$\begin{bmatrix} (1+2\lambda) & -\lambda & 0 & \cdots & 0 \\ -\lambda & (1+2\lambda) & -\lambda & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & -\lambda \\ 0 & \cdots & 0 & -\lambda & (1+2\lambda) \end{bmatrix} \begin{bmatrix} u_{12} \\ u_{22} \\ \vdots \\ \vdots \\ u_{m-1,2} \end{bmatrix} = \begin{bmatrix} u_{11} \\ u_{21} \\ \vdots \\ \vdots \\ u_{m-1,1} \end{bmatrix} \Rightarrow \begin{bmatrix} u_{12} \\ u_{22} \\ \vdots \\ \vdots \\ u_{m-1,2} \end{bmatrix} = ?$$

and then we solve

$$\begin{bmatrix} (1+2\lambda) & -\lambda & 0 & \cdots & 0 \\ -\lambda & (1+2\lambda) & -\lambda & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & -\lambda \\ 0 & \cdots & 0 & -\lambda & (1+2\lambda) \end{bmatrix} \begin{bmatrix} u_{13} \\ u_{23} \\ \vdots \\ \vdots \\ u_{m-1,3} \end{bmatrix} = \begin{bmatrix} u_{12} \\ u_{22} \\ \vdots \\ \vdots \\ u_{m-1,2} \end{bmatrix} \Rightarrow \begin{bmatrix} u_{13} \\ u_{23} \\ \vdots \\ \vdots \\ u_{m-1,3} \end{bmatrix} = ?$$

and then we solve

$$\begin{bmatrix} (1+2\lambda) & -\lambda & 0 & \cdots & 0 \\ -\lambda & (1+2\lambda) & -\lambda & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & -\lambda \\ 0 & \cdots & 0 & -\lambda & (1+2\lambda) \end{bmatrix} \begin{bmatrix} u_{14} \\ u_{24} \\ \vdots \\ \vdots \\ u_{m-1,4} \end{bmatrix} = \begin{bmatrix} u_{13} \\ u_{23} \\ \vdots \\ \vdots \\ u_{m-1,3} \end{bmatrix} \Rightarrow \begin{bmatrix} u_{14} \\ u_{24} \\ \vdots \\ \vdots \\ u_{m-1,4} \end{bmatrix} = ?$$

, ....

**Eg. Solve**  $\frac{\partial u(x,t)}{\partial t} - \frac{\partial^2 u(x,t)}{\partial x^2} = 0$ ,  $0 \leq x \leq 1$ ,  $t > 0$  with  $u(0,t)=u(1,t)=0$ , and  $u(x,0)=\sin(\pi x)$ .

(Sol.) Use the Backward-difference method, and choose  $m=10$ ,  $h=0.1$ ,  $k=0.01 \Rightarrow \lambda=1$ ,  $1+2\lambda=3$ ,  $x_i=0.1i$ ,  $t_j=0.01j$ , and then we have

$$\begin{bmatrix} 3 & -1 & 0 & \cdots & 0 \\ -1 & 3 & -1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & -1 \\ 0 & \cdots & 0 & -1 & 3 \end{bmatrix} \begin{bmatrix} u_{11} \\ u_{21} \\ \vdots \\ \vdots \\ u_{91} \end{bmatrix} = \begin{bmatrix} u_{10} \\ u_{20} \\ \vdots \\ \vdots \\ u_{90} \end{bmatrix} = \begin{bmatrix} \sin(\pi x_1) \\ \sin(\pi x_2) \\ \vdots \\ \vdots \\ \sin(\pi x_9) \end{bmatrix}$$

$$\Rightarrow \begin{bmatrix} u_{11} \\ u_{21} \\ \vdots \\ \vdots \\ u_{91} \end{bmatrix} = \begin{bmatrix} 3 & -1 & 0 & \cdots & 0 \\ -1 & 3 & -1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & -1 \\ 0 & \cdots & 0 & -1 & 3 \end{bmatrix}^{-1} \begin{bmatrix} \sin(\pi x_1) \\ \sin(\pi x_2) \\ \vdots \\ \vdots \\ \sin(\pi x_9) \end{bmatrix}, \text{ and}$$

$$\begin{bmatrix} 3 & -1 & 0 & \cdots & 0 \\ -1 & 3 & -1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & -1 \\ 0 & \cdots & 0 & -1 & 3 \end{bmatrix} \begin{bmatrix} u_{12} \\ u_{22} \\ \vdots \\ \vdots \\ u_{92} \end{bmatrix} = \begin{bmatrix} u_{11} \\ u_{21} \\ \vdots \\ \vdots \\ u_{91} \end{bmatrix} \Rightarrow \begin{bmatrix} u_{12} \\ u_{22} \\ \vdots \\ \vdots \\ u_{92} \end{bmatrix} = \begin{bmatrix} 3 & -1 & 0 & \cdots & 0 \\ -1 & 3 & -1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & -1 \\ 0 & \cdots & 0 & -1 & 3 \end{bmatrix}^{-1} \begin{bmatrix} u_{11} \\ u_{21} \\ \vdots \\ \vdots \\ u_{91} \end{bmatrix},$$

$$\begin{bmatrix} 3 & -1 & 0 & \cdots & 0 \\ -1 & 3 & -1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & -1 \\ 0 & \cdots & 0 & -1 & 3 \end{bmatrix} \begin{bmatrix} u_{13} \\ u_{23} \\ \vdots \\ \vdots \\ u_{93} \end{bmatrix} = \begin{bmatrix} u_{12} \\ u_{22} \\ \vdots \\ \vdots \\ u_{92} \end{bmatrix} \Rightarrow \begin{bmatrix} u_{13} \\ u_{23} \\ \vdots \\ \vdots \\ u_{93} \end{bmatrix} = \begin{bmatrix} 3 & -1 & 0 & \cdots & 0 \\ -1 & 3 & -1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & -1 \\ 0 & \cdots & 0 & -1 & 3 \end{bmatrix}^{-1} \begin{bmatrix} u_{12} \\ u_{22} \\ \vdots \\ \vdots \\ u_{92} \end{bmatrix},$$

$$\begin{bmatrix} 3 & -1 & 0 & \cdots & 0 \\ -1 & 3 & -1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & -1 \\ 0 & \cdots & 0 & -1 & 3 \end{bmatrix} \begin{bmatrix} u_{14} \\ u_{24} \\ \vdots \\ \vdots \\ u_{94} \end{bmatrix} = \begin{bmatrix} u_{13} \\ u_{23} \\ \vdots \\ \vdots \\ u_{93} \end{bmatrix} \Rightarrow \begin{bmatrix} u_{14} \\ u_{24} \\ \vdots \\ \vdots \\ u_{94} \end{bmatrix} = \begin{bmatrix} 3 & -1 & 0 & \cdots & 0 \\ -1 & 3 & -1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & -1 \\ 0 & \cdots & 0 & -1 & 3 \end{bmatrix}^{-1} \begin{bmatrix} u_{13} \\ u_{23} \\ \vdots \\ \vdots \\ u_{93} \end{bmatrix},$$

...

In **Matlab** language, we can use the following program to solve the partial differential equation:

```

>> A=[3,-1,0,0,0,0,0,0,0;-1,3,-1,0,0,0,0,0,0;-1,3,-1,0,0,0,0,0,0;-1,3,-1,0,0,0,0,0,0;
      0,0,0,-1,3,-1,0,0,0;0,0,0,0,-1,3,-1,0,0;0,0,0,0,0,-1,3,-1,0;0,0,0,0,0,0,-1,3,-1;
      0,0,0,0,0,0,0,-1,3];
>>pi=3.1415926;
>>B=[sin(0.1*pi);sin(0.2*pi);sin(0.3*pi);sin(0.4*pi);sin(0.5*pi);sin(0.6*pi);sin(0.7*pi)
);sin(0.8*pi);sin(0.9*pi)];
>>for i=1:5
      C=inv(A)*B
      B=C;
end
C =
      0.1765
      0.3356
      0.4620
      0.5431
      0.5710
      0.5431
      0.4620
      0.3356
      0.1765

C =
      0.1607
      0.3057
      0.4208
      0.4947
      0.5201
      0.4947
      0.4208
      0.3057
      0.1607

C =
      0.1464
      0.2785
      0.3833
      0.4506
      0.4737
      0.4506
      0.3833

```

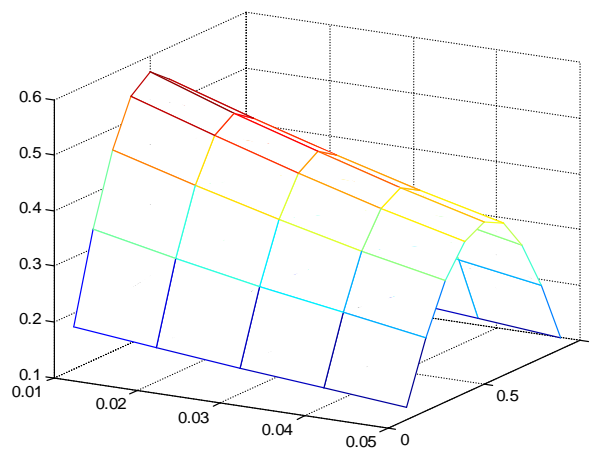
0.2785  
0.1464

C =

0.1333  
0.2536  
0.3491  
0.4104  
0.4315  
0.4104  
0.3491  
0.2536  
0.1333

C =

0.1215  
0.2310  
0.3180  
0.3738  
0.3930  
0.3738  
0.3180  
0.2310  
0.1215



**Richardson's method:** 
$$\frac{u_{i,j+1} - u_{i,j-1}}{2k} - \alpha^2 \frac{u_{i+1,j} - 2u_{ij} + u_{i-1,j}}{h^2} = 0.$$

**Note:** Forward difference method is conditional stable. Richardson's method has a serious stability problem.





### 8-3 Hyperbolic Partial Differential Equations

Solve  $\frac{\partial^2 u(x,t)}{\partial t^2} - \alpha^2 \frac{\partial^2 u(x,t)}{\partial x^2} = 0$ ,  $0 \leq x \leq l$ ,  $t > 0$  with  $u(0,t)=u(l,t)=0$ ,  $u(x,0)=f(x)$ ,

$$\frac{\partial u}{\partial t}(x,0) = g(x).$$

**Central difference method: Set  $h=l/m$ ,  $x_i=ih$ ,  $t_j=jk$ , and  $\lambda=ak/h$**

$$\Rightarrow \frac{u_{i,j+1} - 2u_{ij} + u_{i,j-1}}{k^2} - \alpha^2 \frac{u_{i+1,j} - 2u_{ij} + u_{i-1,j}}{h^2} = 0 \Rightarrow u_{i,j+1} = 2(1 - \lambda^2)u_{ij} + \lambda^2(u_{i+1,j} + u_{i-1,j}) - u_{i,j-1},$$

$$u_{i0}=f(x_i), u_{0j}=u_{mj}=0, \text{ and } u_{i1}=u_{i0}+kg(x_i) \approx (1 - \lambda^2)u_{i0} + \frac{\lambda^2}{2}[f(x_{i+1}) + f(x_{i-1})] + kg(x_i)$$

$$\Rightarrow \begin{bmatrix} u_{1,j+1} \\ u_{2,j+1} \\ \vdots \\ \vdots \\ u_{m-1,j+1} \end{bmatrix} = \begin{bmatrix} 2(1-\lambda^2) & \lambda^2 & 0 & \cdots & 0 \\ \lambda^2 & 2(1-\lambda^2) & \lambda^2 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \lambda^2 \\ 0 & \cdots & 0 & \lambda^2 & 2(1-\lambda^2) \end{bmatrix} \begin{bmatrix} u_{1j} \\ u_{2j} \\ \vdots \\ \vdots \\ u_{m-1,j} \end{bmatrix} - \begin{bmatrix} u_{1,j-1} \\ u_{2,j-1} \\ \vdots \\ \vdots \\ u_{m-1,j-1} \end{bmatrix}$$

We have

$$\begin{bmatrix} u_{12} \\ u_{22} \\ \vdots \\ \vdots \\ u_{m-1,2} \end{bmatrix} = \begin{bmatrix} 2(1-\lambda^2) & \lambda^2 & 0 & \cdots & 0 \\ \lambda^2 & 2(1-\lambda^2) & \lambda^2 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \lambda^2 \\ 0 & \cdots & 0 & \lambda^2 & 2(1-\lambda^2) \end{bmatrix} \begin{bmatrix} u_{11} \\ u_{21} \\ \vdots \\ \vdots \\ u_{m-1,1} \end{bmatrix} - \begin{bmatrix} f(x_1) \\ f(x_2) \\ \vdots \\ \vdots \\ f(x_{m-1}) \end{bmatrix},$$

$$\begin{bmatrix} u_{13} \\ u_{23} \\ \vdots \\ \vdots \\ u_{m-1,3} \end{bmatrix} = \begin{bmatrix} 2(1-\lambda^2) & \lambda^2 & 0 & \cdots & 0 \\ \lambda^2 & 2(1-\lambda^2) & \lambda^2 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \lambda^2 \\ 0 & \cdots & 0 & \lambda^2 & 2(1-\lambda^2) \end{bmatrix} \begin{bmatrix} u_{12} \\ u_{22} \\ \vdots \\ \vdots \\ u_{m-1,2} \end{bmatrix} - \begin{bmatrix} u_{11} \\ u_{21} \\ \vdots \\ \vdots \\ u_{m-1,1} \end{bmatrix},$$

$$\begin{bmatrix} u_{14} \\ u_{24} \\ \vdots \\ \vdots \\ u_{m-1,4} \end{bmatrix} = \begin{bmatrix} 2(1-\lambda^2) & \lambda^2 & 0 & \cdots & 0 \\ \lambda^2 & 2(1-\lambda^2) & \lambda^2 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \lambda^2 \\ 0 & \cdots & 0 & \lambda^2 & 2(1-\lambda^2) \end{bmatrix} \begin{bmatrix} u_{13} \\ u_{23} \\ \vdots \\ \vdots \\ u_{m-1,3} \end{bmatrix} - \begin{bmatrix} u_{12} \\ u_{22} \\ \vdots \\ \vdots \\ u_{m-1,2} \end{bmatrix}, \dots$$

**Eg. Solve**  $\frac{\partial^2 u(x,t)}{\partial t^2} - 4 \frac{\partial^2 u(x,t)}{\partial x^2} = 0$  ,  $0 \leq x \leq 1$ ,  $t > 0$  with  $u(0,t)=u(1,t)=0$ ,

$u(x,0)=\sin(\pi x)$ , and  $\frac{\partial u(x,0)}{\partial t} = 0$ .

(Sol.) Set  $m=10$ ,  $h=0.1$ ,  $k=0.05 \Rightarrow \lambda=1$ ,  $\lambda^2=1$ ,  $2(1-\lambda^2)=0$ ,  $x_i=0.1i$ ,  $t_j=0.05j$

$\Rightarrow u_{i0}=f(x_i)=\sin(\pi x_i)$ ,  $u_{0j}=u_{mj}=0$ ,

$$u_{i1} \approx \frac{1}{2}[f(x_{i+1}) + f(x_{i-1})] + 0.05g(x_i) = \frac{1}{2}[\sin(\pi x_{i+1}) + \sin(\pi x_{i-1})],$$

and then we have

$$\begin{bmatrix} u_{10} \\ u_{20} \\ \vdots \\ \vdots \\ u_{90} \end{bmatrix} = \begin{bmatrix} \sin(\pi x_1) \\ \sin(\pi x_2) \\ \vdots \\ \vdots \\ \sin(\pi x_9) \end{bmatrix}, \quad \begin{bmatrix} u_{11} \\ u_{21} \\ \vdots \\ \vdots \\ u_{91} \end{bmatrix} = \begin{bmatrix} \frac{1}{2}[\sin(\pi x_2) + \sin(\pi x_0)] \\ \frac{1}{2}[\sin(\pi x_3) + \sin(\pi x_1)] \\ \vdots \\ \vdots \\ \frac{1}{2}[\sin(\pi x_{10}) + \sin(\pi x_8)] \end{bmatrix},$$

$$\begin{bmatrix} u_{12} \\ u_{22} \\ \vdots \\ \vdots \\ u_{92} \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 1 & 0 & 1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & 1 \\ 0 & \cdots & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} \frac{1}{2}[\sin(\pi x_2) + \sin(\pi x_0)] \\ \frac{1}{2}[\sin(\pi x_3) + \sin(\pi x_1)] \\ \vdots \\ \vdots \\ \frac{1}{2}[\sin(\pi x_{10}) + \sin(\pi x_8)] \end{bmatrix} - \begin{bmatrix} \sin(\pi x_1) \\ \sin(\pi x_2) \\ \vdots \\ \vdots \\ \sin(\pi x_9) \end{bmatrix}$$

$$\Rightarrow \begin{bmatrix} u_{13} \\ u_{23} \\ \vdots \\ \vdots \\ u_{93} \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 1 & 0 & 1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & 1 \\ 0 & \cdots & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} u_{12} \\ u_{22} \\ \vdots \\ \vdots \\ u_{92} \end{bmatrix} - \begin{bmatrix} \frac{1}{2}[\sin(\pi x_2) + \sin(\pi x_0)] \\ \frac{1}{2}[\sin(\pi x_3) + \sin(\pi x_1)] \\ \vdots \\ \vdots \\ \frac{1}{2}[\sin(\pi x_{10}) + \sin(\pi x_8)] \end{bmatrix}$$

$$\Rightarrow \begin{bmatrix} u_{14} \\ u_{24} \\ \vdots \\ \vdots \\ u_{94} \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 1 & 0 & 1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & 1 \\ 0 & \cdots & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} u_{13} \\ u_{23} \\ \vdots \\ \vdots \\ u_{93} \end{bmatrix} - \begin{bmatrix} u_{12} \\ u_{22} \\ \vdots \\ \vdots \\ u_{92} \end{bmatrix}$$

$$\Rightarrow \begin{bmatrix} u_{15} \\ u_{25} \\ \vdots \\ \vdots \\ u_{95} \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 1 & 0 & 1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & 1 \\ 0 & \cdots & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} u_{14} \\ u_{24} \\ \vdots \\ \vdots \\ u_{94} \end{bmatrix} - \begin{bmatrix} u_{13} \\ u_{23} \\ \vdots \\ \vdots \\ u_{93} \end{bmatrix} \Rightarrow \dots$$

In **Matlab** language, we can use the following program to solve the partial differential equation:

```
>>A=[0,1,0,0,0,0,0,0,0;1,0,1,0,0,0,0,0,0;0,1,0,1,0,0,0,0,0;0,0,1,0,1,0,0,0,0;
      0,0,0,1,0,1,0,0,0;0,0,0,0,1,0,1,0,0;0,0,0,0,0,1,0,1,0;0,0,0,0,0,0,1,0,1;
      0,0,0,0,0,0,0,1,0];
>>pi=3.1415926;
>>B=[sin(0.1*pi);sin(0.2*pi);sin(0.3*pi);sin(0.4*pi);sin(0.5*pi);sin(0.6*pi);sin(0.7*pi)
);sin(0.8*pi);sin(0.9*pi)];
>>C=[(0+sin(0.2*pi))/2;(sin(0.1*pi)+sin(0.3*pi))/2;(sin(0.2*pi)+sin(0.4*pi))/2;(sin(0.
3*pi)+sin(0.5*pi))/2;(sin(0.4*pi)+sin(0.6*pi))/2;(sin(0.5*pi)+sin(0.7*pi))/2;(sin(0.6*pi
i)+sin(0.8*pi))/2;(sin(0.7*pi)+sin(0.9*pi))/2;(sin(0.8*pi)+sin(pi))/2];
>>for i=2:5
      D=A*C-B
      B=C;
      C=D;
end
```

```
D =
    0.2500
    0.4755
    0.6545
    0.7694
    0.8090
    0.7694
    0.6545
    0.4755
    0.2500
```

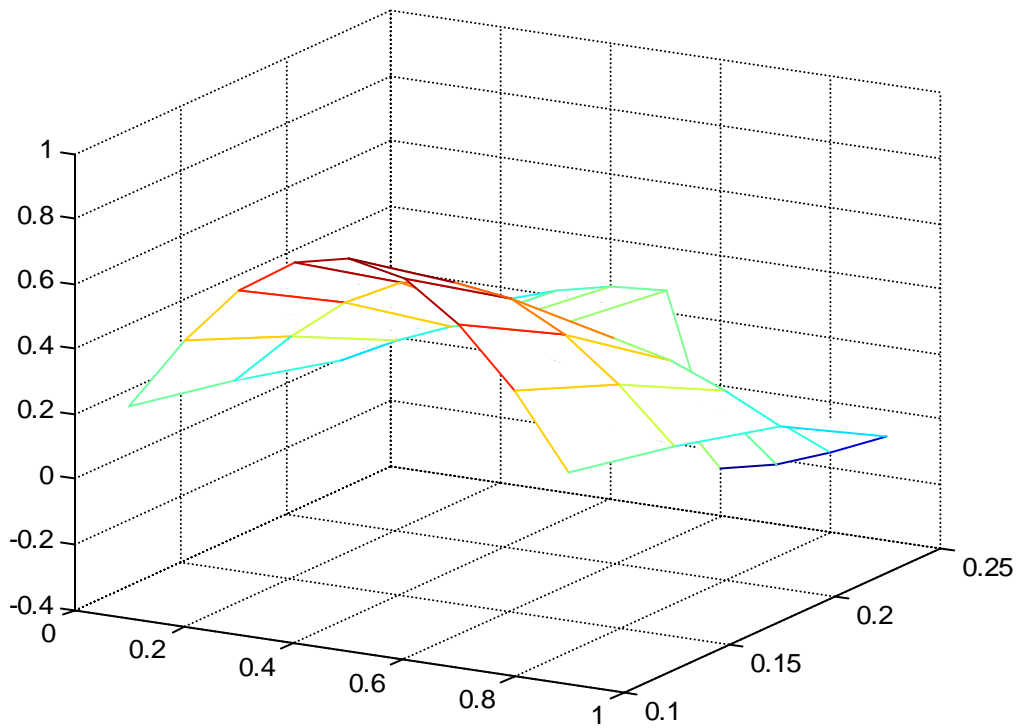
```
D =
    0.1816
    0.3455
    0.4755
    0.5590
    0.5878
    0.5590
    0.4755
    0.3455
    0.1816
```

```
D =
    0.0955
    0.1816
    0.2500
```

0.2939  
0.3090  
0.2939  
0.2500  
0.1816  
0.0955

D =  
1.0e-007 \*

0.0828  
0.1575  
0.2168  
0.2548  
0.2679  
-0.2548  
-0.2168  
-0.1575  
-0.0828



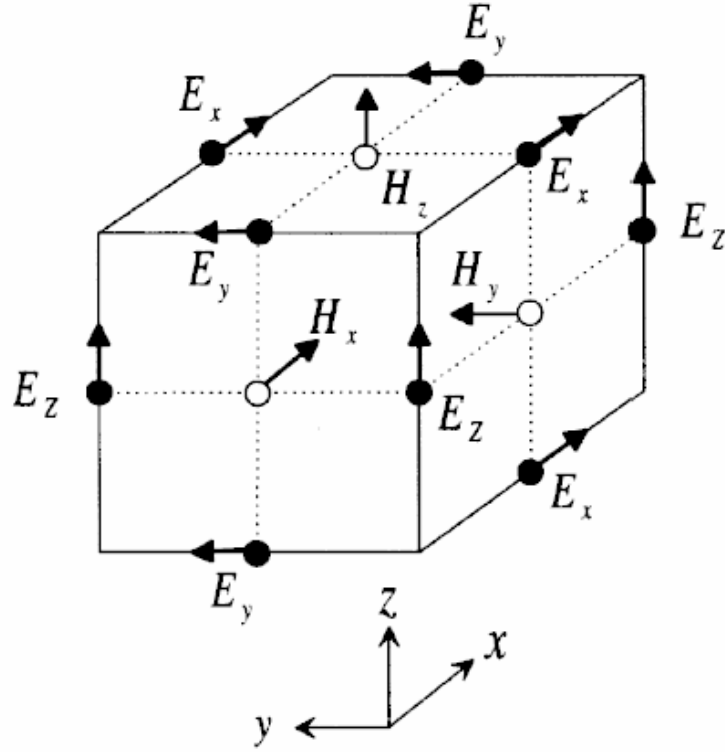
## 8-4 Finite-Difference Time-Domain (FDTD) Method of Solving Maxwell's Equations

### 3D Full-vector FDTD method (by Kane S. Yee, 1966):

Maxwell's equations in the source-free region:  $\nabla \times \vec{H} = \varepsilon \frac{\partial \vec{E}}{\partial t}$ ,  $\nabla \times \vec{E} = -\mu \frac{\partial \vec{H}}{\partial t}$

$$\Rightarrow \varepsilon \frac{\partial E_x}{\partial t} = \frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z}, \quad \varepsilon \frac{\partial E_y}{\partial t} = \frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x}, \quad \varepsilon \frac{\partial E_z}{\partial t} = \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y},$$

$$\mu \frac{\partial H_x}{\partial t} = \frac{\partial E_y}{\partial z} - \frac{\partial E_z}{\partial y}, \quad \mu \frac{\partial H_y}{\partial t} = \frac{\partial E_z}{\partial x} - \frac{\partial E_x}{\partial z}, \quad \mu \frac{\partial H_z}{\partial t} = \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x}$$



(Yee's cell)

Define the following notations:  $E(i\Delta x, j\Delta y, k\Delta z, l\Delta t) \equiv E(i, j, k, l) \equiv E^l(i, j, k)$  and  $H(i\Delta x, j\Delta y, k\Delta z, l\Delta t) \equiv H(i, j, k, l) \equiv H^l(i, j, k)$ . According to Yee's cell, we have

$$E_x \equiv E_x(i+1/2, j, k, l) \equiv E_x^l(i+1/2, j, k),$$

$$E_y \equiv E_y(i, j+1/2, k, l) \equiv E_y^l(i, j+1/2, k),$$

$$E_z \equiv E_z(i, j, k+1/2, l) \equiv E_z^l(i, j, k+1/2),$$

$$H_x \equiv H_x(i, j+1/2, k+1/2, l-1/2) \equiv H_x^{l-1/2}(i, j+1/2, k+1/2),$$

$$H_y \equiv H_y(i+1/2, j, k+1/2, l-1/2) \equiv H_y^{l-1/2}(i+1/2, j, k+1/2),$$

$$H_z \equiv H_z(i+1/2, j+1/2, k, l-1/2) \equiv H_z^{l-1/2}(i+1/2, j+1/2, k),$$

$$\frac{\partial E_x}{\partial t} \approx \frac{E_x(i + \frac{1}{2}, j, k, l+1) - E_x(i + \frac{1}{2}, j, k, l)}{\Delta t},$$

$$\frac{\partial E_y}{\partial t} \approx \frac{E_y(i, j + \frac{1}{2}, k, l+1) - E_y(i, j + \frac{1}{2}, k, l)}{\Delta t},$$

$$\frac{\partial E_z}{\partial t} \approx \frac{E_z(i, j, k + \frac{1}{2}, l+1) - E_z(i, j, k + \frac{1}{2}, l)}{\Delta t},$$

$$\frac{\partial E_x}{\partial y} \approx \frac{E_x(i + \frac{1}{2}, j, k, l) - E_x(i + \frac{1}{2}, j-1, k, l)}{\Delta y},$$

$$\frac{\partial E_x}{\partial z} \approx \frac{E_x(i + \frac{1}{2}, j, k, l) - E_x(i + \frac{1}{2}, j, k-1, l)}{\Delta z},$$

$$\frac{\partial E_y}{\partial x} \approx \frac{E_y(i, j + \frac{1}{2}, k, l) - E_y(i-1, j + \frac{1}{2}, k, l)}{\Delta x},$$

$$\frac{\partial E_y}{\partial z} \approx \frac{E_y(i, j + \frac{1}{2}, k, l) - E_y(i, j + \frac{1}{2}, k-1, l)}{\Delta z},$$

$$\frac{\partial E_z}{\partial x} \approx \frac{E_z(i, j, k + \frac{1}{2}, l) - E_z(i-1, j, k + \frac{1}{2}, l)}{\Delta x},$$

$$\frac{\partial E_z}{\partial y} \approx \frac{E_z(i, j, k + \frac{1}{2}, l) - E_z(i, j-1, k + \frac{1}{2}, l)}{\Delta y},$$

But

$$\frac{\partial H_x}{\partial t} \approx \frac{H_x(i, j + \frac{1}{2}, k + \frac{1}{2}, l + \frac{1}{2}) - H_x(i, j + \frac{1}{2}, k + \frac{1}{2}, l - \frac{1}{2})}{\Delta t},$$

$$\frac{\partial H_y}{\partial t} \approx \frac{H_y(i + \frac{1}{2}, j, k + \frac{1}{2}, l + \frac{1}{2}) - H_y(i + \frac{1}{2}, j, k + \frac{1}{2}, l - \frac{1}{2})}{\Delta t},$$

$$\frac{\partial H_z}{\partial t} \approx \frac{H_z(i + \frac{1}{2}, j + \frac{1}{2}, k, l + \frac{1}{2}) - H_z(i + \frac{1}{2}, j + \frac{1}{2}, k, l - \frac{1}{2})}{\Delta t},$$

$$\frac{\partial H_x}{\partial y} \approx \frac{H_x(i, j + \frac{1}{2}, k + \frac{1}{2}, l - \frac{1}{2}) - H_x(i, j - \frac{1}{2}, k + \frac{1}{2}, l - \frac{1}{2})}{\Delta y},$$

$$\frac{\partial H_x}{\partial z} \approx \frac{H_x(i, j + \frac{1}{2}, k + \frac{1}{2}, l - \frac{1}{2}) - H_x(i, j + \frac{1}{2}, k - \frac{1}{2}, l - \frac{1}{2})}{\Delta z},$$

$$\frac{\partial H_y}{\partial x} \approx \frac{H_y(i + \frac{1}{2}, j, k + \frac{1}{2}, l - \frac{1}{2}) - H_y(i - \frac{1}{2}, j, k + \frac{1}{2}, l - \frac{1}{2})}{\Delta x},$$

$$\frac{\partial H_y}{\partial z} \approx \frac{H_y(i + \frac{1}{2}, j, k + \frac{1}{2}, l - \frac{1}{2}) - H_y(i + \frac{1}{2}, j, k - \frac{1}{2}, l - \frac{1}{2})}{\Delta z},$$

$$\frac{\partial H_z}{\partial x} \approx \frac{H_z(i + \frac{1}{2}, j + \frac{1}{2}, k, l - \frac{1}{2}) - H_z(i - \frac{1}{2}, j + \frac{1}{2}, k, l - \frac{1}{2})}{\Delta x},$$

$$\frac{\partial H_z}{\partial y} \approx \frac{H_z(i + \frac{1}{2}, j + \frac{1}{2}, k, l - \frac{1}{2}) - H_z(i + \frac{1}{2}, j - \frac{1}{2}, k, l - \frac{1}{2})}{\Delta y}$$

$\Rightarrow$

$$E_x^{l+1}(i + \frac{1}{2}, j, k) = E_x^l(i + \frac{1}{2}, j, k) + C(i + \frac{1}{2}, j, k) \cdot$$

$$\left[ \frac{H_z^{l-\frac{1}{2}}(i + \frac{1}{2}, j + \frac{1}{2}, k) - H_z^{l-\frac{1}{2}}(i + \frac{1}{2}, j - \frac{1}{2}, k)}{\Delta y} - \frac{H_y^{l-\frac{1}{2}}(i + \frac{1}{2}, j, k + \frac{1}{2}) - H_y^{l-\frac{1}{2}}(i + \frac{1}{2}, j, k - \frac{1}{2})}{\Delta z} \right],$$

$$E_y^{l+1}(i, j + \frac{1}{2}, k) = E_y^l(i, j + \frac{1}{2}, k) + C(i, j + \frac{1}{2}, k) \cdot$$

$$\left[ \frac{H_x^{l-\frac{1}{2}}(i, j + \frac{1}{2}, k + \frac{1}{2}) - H_x^{l-\frac{1}{2}}(i, j + \frac{1}{2}, k - \frac{1}{2})}{\Delta z} - \frac{H_z^{l-\frac{1}{2}}(i + \frac{1}{2}, j + \frac{1}{2}, k) - H_z^{l-\frac{1}{2}}(i - \frac{1}{2}, j + \frac{1}{2}, k)}{\Delta x} \right],$$

$$E_z^{l+1}(i, j, k + \frac{1}{2}) = E_z^l(i, j, k + \frac{1}{2}) + C(i, j, k + \frac{1}{2}) \cdot$$

$$\left[ \frac{H_y^{l-\frac{1}{2}}(i + \frac{1}{2}, j, k + \frac{1}{2}) - H_y^{l-\frac{1}{2}}(i - \frac{1}{2}, j, k + \frac{1}{2})}{\Delta x} - \frac{H_x^{l-\frac{1}{2}}(i, j + \frac{1}{2}, k + \frac{1}{2}) - H_x^{l-\frac{1}{2}}(i, j - \frac{1}{2}, k + \frac{1}{2})}{\Delta y} \right],$$

$$H_x^{l+\frac{1}{2}}(i, j + \frac{1}{2}, k + \frac{1}{2}) = H_x^{l-\frac{1}{2}}(i, j + \frac{1}{2}, k + \frac{1}{2}) + D(i, j + \frac{1}{2}, k + \frac{1}{2}) \cdot$$

$$\left[ -\frac{E_z^l(i, j + 1, k + \frac{1}{2}) - E_z^l(i, j, k + \frac{1}{2})}{\Delta y} + \frac{E_y^l(i, j + \frac{1}{2}, k + 1) - E_y^l(i, j + \frac{1}{2}, k)}{\Delta z} \right],$$

$$H_y^{l+\frac{1}{2}}(i + \frac{1}{2}, j, k + \frac{1}{2}) = H_y^{l-\frac{1}{2}}(i + \frac{1}{2}, j, k + \frac{1}{2}) + D(i + \frac{1}{2}, j, k + \frac{1}{2}) \cdot$$

$$\left[ \frac{E_z^l(i + 1, j, k + \frac{1}{2}) - E_z^l(i, j, k + \frac{1}{2})}{\Delta x} - \frac{E_x^l(i + \frac{1}{2}, j, k + 1) - E_x^l(i + \frac{1}{2}, j, k)}{\Delta z} \right],$$

$$H_z^{l+\frac{1}{2}}(i+\frac{1}{2}, j+\frac{1}{2}, k) = H_z^{l-\frac{1}{2}}(i+\frac{1}{2}, j+\frac{1}{2}, k) + D(i+\frac{1}{2}, j+\frac{1}{2}, k) \cdot \left[ \frac{E_x^l(i+\frac{1}{2}, j+1, k) - E_x^l(i+\frac{1}{2}, j, k)}{\Delta y} - \frac{E_y^l(i+1, j+\frac{1}{2}, k) - E_y^l(i, j+\frac{1}{2}, k)}{\Delta x} \right],$$

where  $C(i, j, k) = \frac{\Delta t}{\varepsilon(i, j, k)}$ ,  $D(i, j, k) = \frac{\Delta t}{\mu(i, j, k)}$ , and the electromagnetic power distribution  $\propto |\vec{E}|^2 = (E_x^2 + E_y^2 + E_z^2)$ .

Stability criterion:  $\Delta t \leq \frac{1}{v_{\max} \sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}}$ , where  $v_{\max}$  is the maximal velocity

of EM wave propagating.



### 3D Scalar FDTD method (by Dr. Wei-Ping Huang, 1991):



**Dr. Wei-Ping Huang** was born in Beijing. He graduated from MIT and got his PhD degree. Now he is a professor in the ECE Department at the University of Waterloo, Canada. His research group is one of the leading groups internationally in photonics and computer aided design. Dr. Huang is creating new design tools to help develop the highly-efficient photonics systems required for large-scale broadband communication.

Consider a wave equation:  $\nabla^2\Psi + \frac{n^2}{c^2} \frac{\partial^2\Psi}{\partial t^2} = \frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2} + \frac{\partial^2\Psi}{\partial z^2} + \frac{n^2}{c^2} \frac{\partial^2\Psi}{\partial t^2} = 0$ ,

where  $\Psi(x,y,z,t)$  is the scalar field (approximation) and  $n(x,y,z)$  is the refractive index. Using  $\Psi(i\Delta x, j\Delta y, k\Delta z, l\Delta t) \equiv \Psi(i,j,k,l) \equiv \Psi^l(i,j,k)$ , where  $0 \leq i \leq I$ ,  $0 \leq j \leq J$ , and  $0 \leq k \leq K$ .

$$\text{Let } \frac{\partial^2\Psi}{\partial x^2} = \frac{\Psi^l(i+1,j,k) - 2\Psi^l(i,j,k) + \Psi^l(i-1,j,k)}{\Delta x^2},$$

$$\frac{\partial^2\Psi}{\partial y^2} = \frac{\Psi^l(i,j+1,k) - 2\Psi^l(i,j,k) + \Psi^l(i,j-1,k)}{\Delta y^2},$$

$$\frac{\partial^2\Psi}{\partial z^2} = \frac{\Psi^l(i,j,k+1) - 2\Psi^l(i,j,k) + \Psi^l(i,j,k-1)}{\Delta z^2},$$

$$\text{and } \frac{\partial^2\Psi}{\partial t^2} = \frac{\Psi^{l+1}(i,j,k) - 2\Psi^l(i,j,k) + \Psi^{l-1}(i,j,k)}{\Delta t^2}$$

$$\Rightarrow \Psi^{l+1}(i,j,k) = 2 \cdot \left[ 1 - \frac{\delta_x^2 + \delta_y^2 + \delta_z^2}{n^2(i,j,k)} \right] \cdot \Psi^l(i,j,k) - \Psi^{l-1}(i,j,k)$$

$$+ \frac{\delta_x^2}{n^2(i,j,k)} \cdot [\Psi^l(i+1,j,k) + \Psi^l(i-1,j,k)] + \frac{\delta_y^2}{n^2(i,j,k)} \cdot [\Psi^l(i,j+1,k) + \Psi^l(i,j-1,k)]$$

$$+ \frac{\delta_z^2}{n^2(i,j,k)} \cdot [\Psi^l(i,j,k+1) + \Psi^l(i,j,k-1)]$$

$$\text{where } \delta_x = \frac{c\Delta t}{\Delta x}, \quad \delta_y = \frac{c\Delta t}{\Delta y}, \quad \delta_z = \frac{c\Delta t}{\Delta z}.$$

The electromagnetic power distribution  $\propto |\Psi|^2$ .

The 3D scalar FDTD method may be incorporated with the Mur's absorbing boundary conditions.

### Mur's First-Order Absorbing Boundary Conditions:

$$\text{At } x=0, \quad \Psi^{l+1}(0,j,k) = \Psi^l(1,j,k) + \frac{c\Delta t - \Delta x}{c\Delta t + \Delta x} \cdot [\Psi^{l+1}(1,j,k) - \Psi^l(0,j,k)]$$

$$x=I\Delta x, \Psi^{l+1}(I, j, k) = \Psi^l(I-1, j, k) + \frac{c\Delta t - \Delta x}{c\Delta t + \Delta x} \cdot [\Psi^{l+1}(I-1, j, k) - \Psi^l(I, j, k)]$$

$$y=0, \Psi^{l+1}(i, 0, k) = \Psi^l(i, 1, k) + \frac{c\Delta t - \Delta y}{c\Delta t + \Delta y} \cdot [\Psi^{l+1}(i, 1, k) - \Psi^l(i, 0, k)]$$

$$y=J\Delta y, \Psi^{l+1}(i, J, k) = \Psi^l(i, J-1, k) + \frac{c\Delta t - \Delta y}{c\Delta t + \Delta y} \cdot [\Psi^{l+1}(i, J-1, k) - \Psi^l(i, J, k)]$$

$$z=0, \Psi^{l+1}(i, j, 0) = \Psi^l(i, j, 1) + \frac{c\Delta t - \Delta z}{c\Delta t + \Delta z} \cdot [\Psi^{l+1}(i, j, 1) - \Psi^l(i, j, 0)]$$

$$z=K\Delta z, \Psi^{l+1}(i, j, K) = \Psi^l(i, j, K-1) + \frac{c\Delta t - \Delta z}{c\Delta t + \Delta z} \cdot [\Psi^{l+1}(i, j, K-1) - \Psi^l(i, j, K)]$$

### 3D Semi-vectorial FDTD method (also by Dr. Wei-Ping Huang):

$$E_x^{l+1}(i, j, k) = 2 \cdot \left\{ 1 - \frac{[2 - \frac{T(i+1, j, k) + T(i-1, j, k)}{2}] \cdot \delta_x^2 + \delta_y^2 + \delta_z^2}{n^2(i, j, k)} \right\} \cdot E_x^l(i, j, k) - E_x^{l-1}(i, j, k)$$

$$+ \frac{\delta_x^2}{n^2(i, j, k)} \cdot [T(i+1, j, k) \cdot E_x^l(i+1, j, k) + T(i-1, j, k) \cdot E_x^l(i-1, j, k)]$$

$$+ \frac{\delta_y^2}{n^2(i, j, k)} \cdot [E_x^l(i, j+1, k) + E_x^l(i, j-1, k)] + \frac{\delta_z^2}{n^2(i, j, k)} \cdot [E_x^l(i, j, k+1) + E_x^l(i, j, k-1)]$$

$$E_y^{l+1}(i, j, k) = 2 \cdot \left\{ 1 - \frac{\delta_x^2 + [2 - \frac{T(i, j+1, k) + T(i, j-1, k)}{2}] \cdot \delta_y^2 + \delta_z^2}{n^2(i, j, k)} \right\} \cdot E_y^l(i, j, k) - E_y^{l-1}(i, j, k)$$

$$+ \frac{\delta_x^2}{n^2(i, j, k)} \cdot [E_y^l(i+1, j, k) + E_y^l(i-1, j, k)] + \frac{\delta_z^2}{n^2(i, j, k)} \cdot [E_y^l(i, j, k+1) + E_y^l(i, j, k-1)]$$

$$+ \frac{\delta_y^2}{n^2(i, j, k)} \cdot [T(i, j+1, k) \cdot E_y^l(i, j+1, k) + T(i, j-1, k) \cdot E_y^l(i, j-1, k)]$$

$$\text{where } T(i\pm 1, j, k) = \frac{2n^2(i\pm 1, j, k)}{n^2(i\pm 1, j, k) + n^2(i, j, k)} \quad \text{and} \quad T(i, j\pm 1, k) = \frac{2n^2(i, j\pm 1, k)}{n^2(i, j\pm 1, k) + n^2(i, j, k)}$$

The 3D Semi-vectorial FDTD method may be incorporated with the perfectly matched layer (PML) boundary conditions.

**Perfectly matched layer (PML) boundary conditions:**

In the  $x$ -direction:

$$\begin{aligned} \Psi^{l+1}(i, j, k) = & -\Psi^{l-1}(i, j, k) + 2 \left[ 1 - \frac{\delta_y^2 + \delta_z^2}{n^2(i, j, k)} \right] \Psi^l(i, j, k) \\ & + \frac{\delta_x^2}{n^2(i, j, k)} \left[ D_{2x}^{l+\frac{1}{2}}(i, j, k) - D_{2x}^{l-\frac{1}{2}}(i, j, k) \right] + \frac{\delta_y^2}{n^2(i, j, k)} \left[ \Psi^l(i, j+1, k) + \Psi^l(i, j-1, k) \right] \\ & + \frac{\delta_z^2}{n^2(i, j, k)} \left[ \Psi^l(i, j, k+1) + \Psi^l(i, j, k-1) \right], \text{ where } \delta_x = \frac{c\Delta t}{\Delta x}, \delta_y = \frac{c\Delta t}{\Delta y}, \delta_z = \frac{c\Delta t}{\Delta z} \end{aligned}$$

$$\begin{aligned} D_{1x}^{l+1}(i+1, j, k) = & \frac{a_x - \frac{\sigma_x \cdot \Delta t}{\epsilon_0 n^2(i+1, j, k)}}{a_x + \frac{\sigma_x \cdot \Delta t}{\epsilon_0 n^2(i+1, j, k)}} \cdot D_{1x}^{l-1}(i+1, j, k) \\ & + \frac{1}{a_x + \frac{\sigma_x \cdot \Delta t}{\epsilon_0 n^2(i+1, j, k)}} \cdot \left[ \Psi^l(i+1, j, k) - \Psi^l(i, j, k) \right] \end{aligned}$$

$$\begin{aligned} D_{2x}^{l+1}(i, j, k) = & \frac{a_x - \frac{\sigma_x \cdot \Delta t}{\epsilon_0 n^2(i+1, j, k)}}{a_x + \frac{\sigma_x \cdot \Delta t}{\epsilon_0 n^2(i+1, j, k)}} \cdot D_{2x}^{l-1}(i, j, k) \\ & + \frac{1}{a_x + \frac{\sigma_x \cdot \Delta t}{\epsilon_0 n^2(i+1, j, k)}} \cdot \left[ D_{1x}^{l+1}(i+1, j, k) - D_{1x}^{l+1}(i-1, j, k) \right. \\ & \left. - D_{1x}^{l-1}(i+1, j, k) + D_{1x}^{l-1}(i-1, j, k) \right], \end{aligned}$$

$$\sigma_x(x) = \left( \frac{x}{d} \right)^m \sigma_{x\max} = - \left( \frac{x}{d} \right)^m \frac{n_x^2 \epsilon_0 c (m+1) \ln(R_0)}{2d}$$

$d = n_x \Delta x$ : thickness of PML,  $m$ : order,  $R_0$ : reflection from PML at normal incidence

$$n_x = 8, R_0 = 10^{-2}, m=4$$

In the  $y$ -direction:

$$\begin{aligned}\Psi^{l+1}(i, j, k) = & -\Psi^{l-1}(i, j, k) + 2 \left[ 1 - \frac{\delta_x^2 + \delta_z^2}{n^2(i, j, k)} \right] \Psi^l(i, j, k) \\ & + \frac{\delta_x^2}{n^2(i, j, k)} [\Psi^l(i+1, j, k) + \Psi^l(i-1, j, k)] \\ & + \frac{\delta_y^2}{n^2(i, j, k)} \left[ D_{2y}^{l+\frac{1}{2}}(i, j, k) - D_{2y}^{l-\frac{1}{2}}(i, j, k) \right] + \frac{\delta_z^2}{n^2(i, j, k)} [\Psi^l(i, j, k+1) + \Psi^l(i, j, k-1)],\end{aligned}$$

where  $\delta_x = \frac{c\Delta t}{\Delta x}$ ,  $\delta_y = \frac{c\Delta t}{\Delta y}$ ,  $\delta_z = \frac{c\Delta t}{\Delta z}$

$$\begin{aligned}D_{1y}^{l+1}(i, j+1, k) = & \frac{a_y - \frac{\sigma_y \cdot \Delta t}{\epsilon_0 n^2(i, j+1, k)}}{a_y + \frac{\sigma_y \cdot \Delta t}{\epsilon_0 n^2(i, j+1, k)}} \cdot D_{1y}^{l-1}(i, j+1, k) \\ & + \frac{1}{a_y + \frac{\sigma_y \cdot \Delta t}{\epsilon_0 n^2(i, j+1, k)}} \cdot [\Psi^l(i, j+1, k) - \Psi^l(i, j, k)] \\ D_{2y}^{l+1}(i, j, k) = & \frac{a_y - \frac{\sigma_y \cdot \Delta t}{\epsilon_0 n^2(i, j+1, k)}}{a_y + \frac{\sigma_y \cdot \Delta t}{\epsilon_0 n^2(i, j+1, k)}} \cdot D_{2y}^{l-1}(i, j, k) \\ & + \frac{1}{a_y + \frac{\sigma_y \cdot \Delta t}{\epsilon_0 n^2(i, j+1, k)}} \cdot [D_{1y}^{l+1}(i, j+1, k) - D_{1y}^{l+1}(i, j-1, k) \\ & - D_{1y}^{l-1}(i, j+1, k) + D_{1y}^{l-1}(i, j-1, k)],\end{aligned}$$

$$\sigma_y(y) = \left(\frac{y}{d}\right)^m \sigma_{y\max} = -\left(\frac{y}{d}\right)^m \frac{n_y^2 \epsilon_0 c(m+1) \ln(R_0)}{2d}$$

$d = n_y \Delta y$ : thickness of PML,  $m$ : order

$R_0$ : reflection from PML at normal incidence

$n_y = 8$ ,  $R_0 = 10^{-2}$ ,  $m=4$

In the  $z$ -direction:

$$\begin{aligned}\Psi^{l+1}(i, j, k) = & -\Psi^{l-1}(i, j, k) + 2 \left[ 1 - \frac{\delta_x^2 + \delta_y^2}{n^2(i, j, k)} \right] \Psi^l(i, j, k) \\ & + \frac{\delta_x^2}{n^2(i, j, k)} [\Psi^l(i+1, j, k) + \Psi^l(i-1, j, k)] \\ & + \frac{\delta_y^2}{n^2(i, j, k)} [\Psi^l(i, j+1, k) + \Psi^l(i, j-1, k)] + \frac{\delta_z^2}{n^2(i, j, k)} \left[ D_{2z}^{l+\frac{1}{2}}(i, j, k) - D_{2z}^{l-\frac{1}{2}}(i, j, k) \right],\end{aligned}$$

where  $\delta_x = \frac{c\Delta t}{\Delta x}$ ,  $\delta_y = \frac{c\Delta t}{\Delta y}$ ,  $\delta_z = \frac{c\Delta t}{\Delta z}$

$$\begin{aligned}D_{1z}^{l+1}(i, j, k+1) = & \frac{a_z - \frac{\sigma_z \cdot \Delta t}{\epsilon_0 n^2(i, j, k+1)}}{a_z + \frac{\sigma_z \cdot \Delta t}{\epsilon_0 n^2(i, j, k+1)}} \cdot D_{1z}^{l-1}(i, j, k+1) \\ & + \frac{1}{a_z + \frac{\sigma_z \cdot \Delta t}{\epsilon_0 n^2(i, j, k+1)}} \cdot [\Psi^l(i, j, k+1) - \Psi^l(i, j, k)]\end{aligned}$$

$$\begin{aligned}\sigma_z(z) = & \left( \frac{z}{d} \right)^m \sigma_{z\max} = - \left( \frac{z}{d} \right)^m \frac{n_z^2 \epsilon_0 c (m+1) \ln(R_0)}{2d} \\ & + \frac{1}{a_z + \frac{\sigma_z \cdot \Delta t}{\epsilon_0 n^2(i, j, k+1)}} \cdot [D_{1z}^{l+1}(i, j, k+1) - D_{1z}^{l+1}(i, j, k-1) \\ & - D_{1z}^{l-1}(i, j, k+1) + D_{1z}^{l-1}(i, j, k-1)]\end{aligned}$$

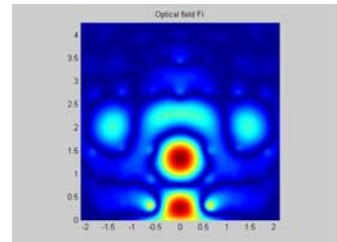
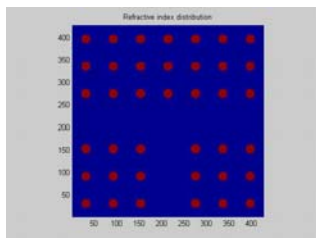
$$\sigma_z(z) = \left( \frac{z}{d} \right)^m \sigma_{z\max} = - \left( \frac{z}{d} \right)^m \frac{n_z^2 \epsilon_0 c (m+1) \ln(R_0)}{2d}$$

$d = n_z \Delta z$ : thickness of *PML*,  $m$ : order

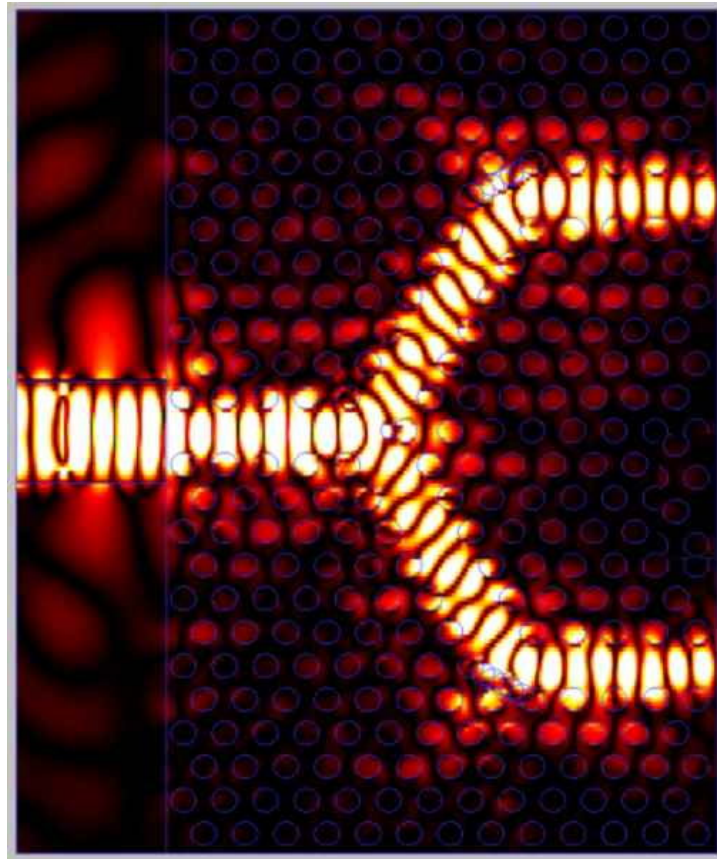
$R_0$ : reflection from *PML* at normal incidence

$n_z = 8$ ,  $R_0 = 10^{-2}$ ,  $m=4$

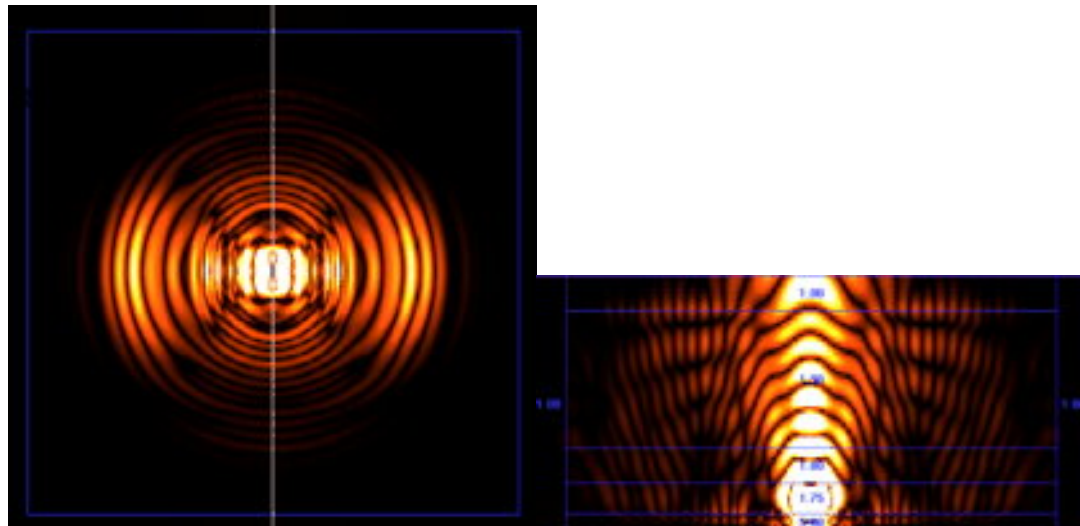
**Eg. Use FDTD method to simulate the characteristics of photonic crystal T-junction waveguide. (by Y. -J. Lin, 林宇仁)**



**Eg. Use FDTD method to simulate the characteristics of photonic crystal Y-junction waveguide.**



**Eg. Use FDTD method to simulate the characteristics of LED.**



## 8-5 Finite-difference Beam Propagation Method (FDBPM)

Consider that a light wave propagates along  $z$ -directional optical waveguide and set  $\vec{E} = \hat{x}E'_x + \hat{y}E'_y + \hat{z}E'_z$  in a source-free region.

**$E$ -formulation (by Dr. Wei-Ping Huang):**

$$\begin{aligned}\nabla \times \nabla \times \vec{E} - n^2 k^2 \vec{E} &= \nabla(\nabla \cdot \vec{E}) - \nabla^2 \vec{E} - n^2 k^2 \vec{E} = 0 \Rightarrow \nabla^2 \vec{E} + n^2 k^2 \vec{E} = \nabla(\nabla \cdot \vec{E}) \\ \Rightarrow \nabla^2 (\hat{x}E'_x + \hat{y}E'_y + \hat{z}E'_z) + n^2 k^2 (\hat{x}E'_x + \hat{y}E'_y + \hat{z}E'_z) &= \nabla \left( \frac{\partial E'_x}{\partial x} + \frac{\partial E'_y}{\partial y} + \frac{\partial E'_z}{\partial z} \right)\end{aligned}$$

$$\because \text{No source, } \therefore \nabla \cdot (\epsilon \vec{E}) = \nabla \cdot (n^2 \vec{E}) = 0 \Rightarrow \frac{\partial(n^2 E'_x)}{\partial x} + \frac{\partial(n^2 E'_y)}{\partial y} + \frac{\partial n^2 E'_z}{\partial z} + n^2 \frac{\partial E'_z}{\partial z} = 0$$

If the refractive index profile varies slowly along the  $z$ -axis,  $\partial n^2 / \partial z$  may be neglected.

$$\Rightarrow \frac{\partial E'_z}{\partial z} \approx -\frac{1}{n^2} \left[ \frac{\partial(n^2 E'_x)}{\partial x} + \frac{\partial(n^2 E'_y)}{\partial y} \right]$$

$$\begin{aligned}\nabla^2 (\hat{x}E'_x + \hat{y}E'_y + \hat{z}E'_z) + n^2 k^2 (\hat{x}E'_x + \hat{y}E'_y + \hat{z}E'_z) \\ = (\hat{x} \frac{\partial}{\partial x} + \hat{y} \frac{\partial}{\partial y} + \hat{z} \frac{\partial}{\partial z}) \left( \frac{\partial E'_x}{\partial x} + \frac{\partial E'_y}{\partial y} - \frac{1}{n^2} \left[ \frac{\partial(n^2 E'_x)}{\partial x} + \frac{\partial(n^2 E'_y)}{\partial y} \right] \right) \\ \Rightarrow \nabla^2 E'_x + n^2 k^2 E'_x = \frac{\partial}{\partial x} \left\{ \frac{\partial E'_x}{\partial x} + \frac{\partial E'_y}{\partial y} - \frac{1}{n^2} \left[ \frac{\partial(n^2 E'_x)}{\partial x} + \frac{\partial(n^2 E'_y)}{\partial y} \right] \right\},\end{aligned}$$

$$\text{and } \nabla^2 E'_y + n^2 k^2 E'_y = \frac{\partial}{\partial y} \left\{ \frac{\partial E'_x}{\partial x} + \frac{\partial E'_y}{\partial y} - \frac{1}{n^2} \left[ \frac{\partial(n^2 E'_x)}{\partial x} + \frac{\partial(n^2 E'_y)}{\partial y} \right] \right\}.$$

Assume that  $E'_x = E_x e^{-jn_0 k z}$  and  $E'_y = E_y e^{-jn_0 k z}$ , where  $k$  is the vacuum wave number and  $n_0 = \beta/k$  is the effective refractive index. With the assumption that the guided lightwave has a slow-varying envelop and is paraxially propagating; i.e.,

$$\left| \frac{\partial^2 E_x}{\partial z^2} \right| \ll 2n_0 k \left| \frac{\partial E_x}{\partial z} \right|, \quad \left| \frac{\partial^2 E_y}{\partial z^2} \right| \ll 2n_0 k \left| \frac{\partial E_y}{\partial z} \right| \Rightarrow \left| \frac{\partial^2 E_x}{\partial z^2} \right| \text{ and } \left| \frac{\partial^2 E_y}{\partial z^2} \right| \text{ are neglected.}$$

And then we have the following coupled equations

$$\begin{aligned}2jn_0 k \cdot \frac{\partial E_x(x, y, z)}{\partial z} &= \frac{\partial}{\partial x} \left\{ \frac{1}{n^2(x, y, z)} \cdot \frac{\partial}{\partial x} [n^2(x, y, z) E_x(x, y, z)] \right\} + \frac{\partial^2 E_x(x, y, z)}{\partial y^2} \\ &\quad + [n^2(x, y, z) - n_0^2] k^2 E_x(x, y, z) \\ &\quad + \frac{\partial}{\partial x} \left\{ \frac{1}{n^2(x, y, z)} \cdot \frac{\partial}{\partial y} [n^2(x, y, z) E_y(x, y, z)] \right\} - \frac{\partial^2 E_y(x, y, z)}{\partial x \partial y}\end{aligned}$$

and

$$\begin{aligned}
2jn_0k \cdot \frac{\partial E_y(x,y,z)}{\partial z} &= \frac{\partial^2 E_y(x,y,z)}{\partial x^2} + \frac{\partial}{\partial y} \left\{ \frac{1}{n^2(x,y,z)} \cdot \frac{\partial}{\partial y} [n^2(x,y,z)E_y(x,y,z)] \right\} \\
&\quad + [n^2(x,y,z) - n_0^2] k^2 E_y(x,y,z) \\
&\quad + \frac{\partial}{\partial y} \left\{ \frac{1}{n^2(x,y,z)} \cdot \frac{\partial}{\partial x} [n^2(x,y,z)E_x(x,y,z)] \right\} - \frac{\partial^2 E_x(x,y,z)}{\partial y \partial x}
\end{aligned}$$

These coupled equations are the basic formulas of the full-vector BPM. If we neglect the terms of  $A_{xy}$  and  $A_{yx}$ , then the equations are reduced to the formulas of the semi-vector BPM. In case the transverse variation of the refractive index is very small, and that is,  $\frac{1}{n^2} \frac{\partial}{\partial x} (n^2 E_x) \approx \frac{\partial E_x}{\partial x}$  and  $\frac{1}{n^2} \frac{\partial}{\partial y} (n^2 E_y) \approx \frac{\partial E_y}{\partial y}$ .

The formulas of the semi-vector BPM can be simplified into the following Fresnel equation, which is the formula of the scalar BPM.

### 3D Full-vector BPM involving the Runge-Kutta algorithm (by Y. -J. Lin):

The transverse components of the optical field fulfill the following coupled equations

$$\begin{aligned}
2jn_0k \cdot \frac{\partial E_x(x,y,z)}{\partial z} &= \frac{\partial}{\partial x} \left\{ \frac{1}{n^2(x,y,z)} \cdot \frac{\partial}{\partial x} [n^2(x,y,z)E_x(x,y,z)] \right\} + \frac{\partial^2 E_x(x,y,z)}{\partial y^2} \\
&\quad + [n^2(x,y,z) - n_0^2] k^2 E_x(x,y,z) \\
&\quad + \frac{\partial}{\partial x} \left\{ \frac{1}{n^2(x,y,z)} \cdot \frac{\partial}{\partial y} [n^2(x,y,z)E_y(x,y,z)] \right\} - \frac{\partial^2 E_y(x,y,z)}{\partial x \partial y}
\end{aligned}$$

and

$$\begin{aligned}
2jn_0k \cdot \frac{\partial E_y(x,y,z)}{\partial z} &= \frac{\partial^2 E_y(x,y,z)}{\partial x^2} + \frac{\partial}{\partial y} \left\{ \frac{1}{n^2(x,y,z)} \cdot \frac{\partial}{\partial y} [n^2(x,y,z)E_y(x,y,z)] \right\} \\
&\quad + [n^2(x,y,z) - n_0^2] k^2 E_y(x,y,z) \\
&\quad + \frac{\partial}{\partial y} \left\{ \frac{1}{n^2(x,y,z)} \cdot \frac{\partial}{\partial x} [n^2(x,y,z)E_x(x,y,z)] \right\} - \frac{\partial^2 E_x(x,y,z)}{\partial y \partial x}
\end{aligned}$$

According to the Runge-Kutta method, the transverse components of the propagating field are expressed by



$$\left\{ \begin{array}{l} E_x(m, n, l+1) = \left\{ \begin{array}{l} E_x(m, n, l) + \frac{K_1(m, n, l) + 2K_2(m, n, l) + 2K_3(m, n, l) + K_4(m, n, l)}{6} \\ + \left[ E_y(m, n, l) + \frac{O_1(m, n, l) + 2O_2(m, n, l) + 2O_3(m, n, l) + O_4(m, n, l)}{6} \right] \end{array} \right\} \\ E_y(m, n, l+1) = \left\{ \begin{array}{l} E_y(m, n, l) + \frac{J_1(m, n, l) + 2J_2(m, n, l) + 2J_3(m, n, l) + J_4(m, n, l)}{6} \\ + \left[ E_x(m, n, l) + \frac{P_1(m, n, l) + 2P_2(m, n, l) + 2P_3(m, n, l) + P_4(m, n, l)}{6} \right] \end{array} \right\} \end{array} \right. ,$$

where

$$\begin{aligned} K_1(m, n, l) = & \frac{\Delta z}{2jn_0k} \cdot \left\{ \frac{a}{\Delta x^2} \left[ E_x(m+1, n, l) \right] + \frac{-b}{\Delta x^2} \left[ E_x(m, n, l) \right] + \frac{c}{\Delta x^2} \left[ E_x(m-1, n, l) \right] \right. \\ & + \frac{1}{\Delta y^2} \left[ E_x(m, n+1, l) \right] + \frac{-2}{\Delta y^2} \left[ E_x(m, n, l) \right] + \frac{1}{\Delta y^2} \left[ E_x(m, n-1, l) \right] \\ & \left. + \left[ n^2(m, n, l) - n_0^2 \right] \cdot k^2 \cdot \left[ E_x(m, n, l) \right] \right\} \end{aligned}$$

$$\begin{aligned} K_2(m, n, l) = & \frac{\Delta z}{2jn_0k} \cdot \left\{ \frac{a}{\Delta x^2} \left[ E_x(m+1, n, l) + \frac{K_1(m+1, n, l)}{2} \right] \right. \\ & + \frac{-b}{\Delta x^2} \left[ E_x(m, n, l) + \frac{K_1(m, n, l)}{2} \right] + \frac{c}{\Delta x^2} \left[ E_x(m-1, n, l) + \frac{K_1(m-1, n, l)}{2} \right] \\ & + \frac{1}{\Delta y^2} \left[ E_x(m, n+1, l) + \frac{K_1(m, n+1, l)}{2} \right] + \frac{-2}{\Delta y^2} \left[ E_x(m, n, l) + \frac{K_1(m, n, l)}{2} \right] \\ & + \frac{1}{\Delta y^2} \left[ E_x(m, n-1, l) + \frac{K_1(m, n-1, l)}{2} \right] \\ & \left. + \left[ n^2(m, n, l) - n_0^2 \right] \cdot k^2 \cdot \left[ E_x(m, n, l) + \frac{K_1(m, n, l)}{2} \right] \right\} \end{aligned}$$

$$\begin{aligned} K_3(m, n, l) = & \frac{\Delta z}{2jn_0k} \cdot \left\{ \frac{a}{\Delta x^2} \left[ E_x(m+1, n, l) + \frac{K_2(m+1, n, l)}{2} \right] \right. \\ & + \frac{-b}{\Delta x^2} \left[ \hat{E}_x(m, n, l) + \frac{K_2(m, n, l)}{2} \right] + \frac{c}{\Delta x^2} \left[ \hat{E}_x(m-1, n, l) + \frac{K_2(m-1, n, l)}{2} \right] \\ & + \frac{1}{\Delta y^2} \left[ E_x(m, n+1, l) + \frac{K_2(m, n+1, l)}{2} \right] + \frac{-2}{\Delta y^2} \left[ E_x(m, n, l) + \frac{K_2(m, n, l)}{2} \right] \\ & + \frac{1}{\Delta y^2} \left[ E_x(m, n-1, l) + \frac{K_2(m, n-1, l)}{2} \right] \\ & \left. + \left[ n^2(m, n, l) - n_0^2 \right] \cdot k^2 \cdot \left[ E_x(m, n, l) + \frac{K_2(m, n, l)}{2} \right] \right\} \end{aligned}$$

$$K_4(m, n, l) = \frac{\Delta z}{2jn_0k} \cdot \left\{ \frac{a}{\Delta x^2} \left[ E_x(m+1, n, l) + K_3(m+1, n, l) \right] \right\}$$

$$\begin{aligned}
& + \frac{-b}{\Delta x^2} \left[ E_x(m, n, l) + K_3(m, n, l) \right] + \frac{c}{\Delta x^2} \left[ E_x(m-1, n, l) + K_3(m-1, n, l) \right] \\
& + \frac{1}{\Delta y^2} \left[ E_x(m, n+1, l) + K_3(m, n+1, l) \right] + \frac{-2}{\Delta y^2} \left[ E_x(m, n, l) + K_3(m, n, l) \right] \\
& \quad + \frac{1}{\Delta y^2} \left[ E_x(m, n-1, l) + K_3(m, n-1, l) \right] \\
& \quad + \left[ n^2(m, n, l) - n_0^2 \right] \cdot k^2 \cdot \left[ E_x(m, n, l) + K_3(m, n, l) \right] \}
\end{aligned}$$

$$\begin{aligned}
O_1(m, n, l) &= \frac{\Delta z}{8jn_0k\Delta x\Delta y} \left\{ E_y(m+1, n+1, l) \cdot \left[ \frac{n^2(m+1, n+1, l)}{n^2(m+1, n, l)} - 1 \right] \right. \\
& + E_y(m, n+1, l) \cdot \left[ -2 \frac{n^2(m, n+1, l)}{n^2(m, n, l)} + 2 \right] + E_y(m-1, n+1, l) \cdot \left[ \frac{n^2(m-1, n+1, l)}{n^2(m-1, n, l)} - 1 \right] \\
& + E_y(m+1, n-1, l) \cdot \left[ \frac{n^2(m+1, n-1, l)}{n^2(m+1, n, l)} - 1 \right] + E_y(m, n-1, l) \cdot \left[ -2 \frac{n^2(m, n-1, l)}{n^2(m, n, l)} + 2 \right] \\
& \left. + E_y(m-1, n-1, l) \cdot \left[ \frac{n^2(m-1, n-1, l)}{n^2(m-1, n, l)} - 1 \right] \right\} - 2E_y(m+1, n, l) + 4E_y(m, n, l) - \\
& 2E_y(m-1, n, l)
\end{aligned}$$

$$\begin{aligned}
O_2(m, n, l) &= \frac{\Delta z}{8jn_0k\Delta x\Delta y} \left\{ \right. \\
& \left[ E_y(m+1, n+1, l) + \frac{O_1(m+1, n+1, l)}{2} \right] \cdot \left[ \frac{n^2(m+1, n+1, l)}{n^2(m+1, n, l)} - 1 \right] \\
& \quad + \left[ E_y(m, n+1, l) + \frac{O_1(m, n+1, l)}{2} \right] \cdot \left[ -2 \frac{n^2(m, n+1, l)}{n^2(m, n, l)} + 2 \right] \\
& \quad + \left[ E_y(m-1, n+1, l) + \frac{O_1(m-1, n+1, l)}{2} \right] \cdot \left[ \frac{n^2(m-1, n+1, l)}{n^2(m-1, n, l)} - 1 \right] \\
& \quad + \left[ E_y(m+1, n-1, l) + \frac{O_1(m+1, n-1, l)}{2} \right] \cdot \left[ \frac{n^2(m+1, n-1, l)}{n^2(m+1, n, l)} - 1 \right] \\
& \quad + \left[ E_y(m, n-1, l) + \frac{O_1(m, n-1, l)}{2} \right] \cdot \left[ -2 \frac{n^2(m, n-1, l)}{n^2(m, n, l)} + 2 \right] \\
& \quad \left. + \left[ E_y(m-1, n-1, l) + \frac{O_1(m-1, n-1, l)}{2} \right] \cdot \left[ \frac{n^2(m-1, n-1, l)}{n^2(m-1, n, l)} - 1 \right] \right\} \\
& - 2 \cdot [E_y(m+1, n, l) + O_1(m+1, n, l)/2] + 4 \cdot [E_y(m, n, l) + O_1(m, n, l)/2] \\
& - 2 \cdot [E_y(m-1, n, l) + O_1(m-1, n, l)/2]
\end{aligned}$$

$$\begin{aligned}
O_3(m, n, l) = & \frac{\Delta z}{8jn_0k\Delta x\Delta y} \{ \\
& \left[ E_y(m+1, n+1, l) + \frac{O_2(m+1, n+1, l)}{2} \right] \cdot \left[ \frac{n^2(m+1, n+1, l)}{n^2(m+1, n, l)} - 1 \right] \\
& + \left[ E_y(m, n+1, l) + \frac{O_2(m, n+1, l)}{2} \right] \cdot \left[ -2 \frac{n^2(m, n+1, l)}{n^2(m, n, l)} + 2 \right] \\
& + \left[ E_y(m-1, n+1, l) + \frac{O_2(m-1, n+1, l)}{2} \right] \cdot \left[ \frac{n^2(m-1, n+1, l)}{n^2(m-1, n, l)} - 1 \right] \\
& + \left[ E_y(m+1, n-1, l) + \frac{O_2(m+1, n-1, l)}{2} \right] \cdot \left[ \frac{n^2(m+1, n-1, l)}{n^2(m+1, n, l)} - 1 \right] \\
& + \left[ E_y(m, n-1, l) + \frac{O_2(m, n-1, l)}{2} \right] \cdot \left[ -2 \frac{n^2(m, n-1, l)}{n^2(m, n, l)} + 2 \right] \\
& + \left[ E_y(m-1, n-1, l) + \frac{O_2(m-1, n-1, l)}{2} \right] \cdot \left[ \frac{n^2(m-1, n-1, l)}{n^2(m-1, n, l)} - 1 \right] \} \\
& - 2 \cdot [E_y(m+1, n, l) + O_2(m+1, n, l)/2] + 4 \cdot [E_y(m, n, l) + O_2(m, n, l)/2] \\
& - 2 \cdot [E_y(m-1, n, l) + O_2(m-1, n, l)/2]
\end{aligned}$$

$$\begin{aligned}
O_4(m, n, l) = & \frac{\Delta z}{8jn_0k\Delta x\Delta y} \{ \\
& \left[ E_y(m+1, n+1, l) + O_3(m+1, n+1, l) \right] \cdot \left[ \frac{n^2(m+1, n+1, l)}{n^2(m+1, n, l)} - 1 \right] \\
& + \left[ E_y(m, n+1, l) + O_3(m, n+1, l) \right] \cdot \left[ -2 \frac{n^2(m, n+1, l)}{n^2(m, n, l)} + 2 \right] \\
& + \left[ E_y(m-1, n+1, l) + O_3(m-1, n+1, l) \right] \cdot \left[ \frac{n^2(m-1, n+1, l)}{n^2(m-1, n, l)} - 1 \right] \\
& + \left[ E_y(m+1, n-1, l) + O_3(m+1, n-1, l) \right] \cdot \left[ \frac{n^2(m+1, n-1, l)}{n^2(m+1, n, l)} - 1 \right] \\
& + \left[ E_y(m, n-1, l) + O_3(m, n-1, l) \right] \cdot \left[ -2 \frac{n^2(m, n-1, l)}{n^2(m, n, l)} + 2 \right] \\
& + \left[ E_y(m-1, n-1, l) + O_3(m-1, n-1, l) \right] \cdot \left[ \frac{n^2(m-1, n-1, l)}{n^2(m-1, n, l)} - 1 \right] \} \\
& - 2 \cdot [E_y(m+1, n, l) + O_3(m+1, n, l)] + 4 \cdot [E_y(m, n, l) + O_3(m, n, l)] \\
& - 2 \cdot [E_y(m-1, n, l) + O_3(m-1, n, l)]
\end{aligned}$$

$$J_1(m, n, l) = \frac{\Delta z}{2jn_0k} \cdot \left\{ \frac{1}{\Delta x^2} \left[ E_y(m+1, n, l) \right] + \frac{-2}{\Delta x^2} \left[ E_y(m, n, l) \right] \right\}$$

$$\begin{aligned}
& + \frac{1}{\Delta x^2} \left[ E_y(m-1, n, l) \right] + \frac{d}{\Delta y^2} \left[ E_y(m, n+1, l) \right] + \frac{-e}{\Delta y^2} \left[ E_y(m, n, l) \right] + \\
& \quad \frac{f}{\Delta y^2} \left[ E_y(m, n-1, l) \right] \\
& \quad + \left[ n^2(m, n, l) - n_0^2 \right] \cdot k^2 \cdot \left[ E_y(m, n, l) \right] \} \\
J_2(m, n, l) &= \frac{\Delta z}{2jn_0k} \cdot \left\{ \frac{1}{\Delta x^2} \left[ E_y(m+1, n, l) + \frac{J_1(m+1, n, l)}{2} \right] \right. \\
& + \frac{-2}{\Delta x^2} \left[ E_y(m, n, l) + \frac{J_1(m, n, l)}{2} \right] + \frac{1}{\Delta x^2} \left[ E_y(m-1, n, l) + \frac{J_1(m-1, n, l)}{2} \right] \\
& + \frac{d}{\Delta y^2} \left[ E_y(m, n+1, l) + \frac{J_1(m, n+1, l)}{2} \right] + \frac{-e}{\Delta y^2} \left[ E_y(m, n, l) + \frac{J_1(m, n, l)}{2} \right] \\
& \quad + \frac{f}{\Delta y^2} \left[ E_y(m, n-1, l) + \frac{J_1(m, n-1, l)}{2} \right] \\
& \quad \left. + \left[ n^2(m, n, l) - n_0^2 \right] \cdot k^2 \cdot \left[ E_y(m, n, l) + \frac{J_1(m, n, l)}{2} \right] \right\} \\
J_3(m, n, l) &= \frac{\Delta z}{2jn_0k} \cdot \left\{ \frac{1}{\Delta x^2} \left[ E_y(m+1, n, l) + \frac{J_2(m+1, n, l)}{2} \right] \right. \\
& + \frac{-2}{\Delta x^2} \left[ E_y(m, n, l) + \frac{J_2(m, n, l)}{2} \right] + \frac{1}{\Delta x^2} \left[ E_y(m-1, n, l) + \frac{J_2(m-1, n, l)}{2} \right] \\
& + \frac{d}{\Delta y^2} \left[ E_y(m, n+1, l) + \frac{J_2(m, n+1, l)}{2} \right] + \frac{-e}{\Delta y^2} \left[ E_y(m, n, l) + \frac{J_2(m, n, l)}{2} \right] \\
& \quad + \frac{f}{\Delta y^2} \left[ E_y(m, n-1, l) + \frac{J_2(m, n-1, l)}{2} \right] \\
& \quad \left. + \left[ n^2(m, n, l) - n_0^2 \right] \cdot k^2 \cdot \left[ E_y(m, n, l) + \frac{J_2(m, n, l)}{2} \right] \right\} \\
J_4(m, n, l) &= \frac{\Delta z}{2jn_0k} \cdot \left\{ \frac{1}{\Delta x^2} \left[ E_y(m+1, n, l) + J_3(m+1, n, l) \right] \right. \\
& + \frac{-2}{\Delta x^2} \left[ E_y(m, n, l) + J_3(m, n, l) \right] + \frac{1}{\Delta x^2} \left[ E_y(m-1, n, l) + J_3(m-1, n, l) \right] \\
& + \frac{d}{\Delta y^2} \left[ E_y(m, n+1, l) + J_3(m, n+1, l) \right] + \frac{-e}{\Delta y^2} \left[ E_y(m, n, l) + J_3(m, n, l) \right] \\
& \quad + \frac{f}{\Delta y^2} \left[ E_y(m, n-1, l) + J_3(m, n-1, l) \right] \\
& \quad \left. + \left[ n^2(m, n, l) - n_0^2 \right] \cdot k^2 \cdot \left[ E_y(m, n, l) + J_3(m, n, l) \right] \right\}
\end{aligned}$$

$$\begin{aligned}
P_1(m, n, l) = & \frac{\Delta z}{8jn_0k\Delta x\Delta y} \left\{ E_x(m+1, n+1, l) \cdot \left[ \frac{n^2(m+1, n+1, l)}{n^2(m, n+1, l)} - 1 \right] \right. \\
& + E_x(m+1, n, l) \cdot \left[ -2 \frac{n^2(m+1, n, l)}{n^2(m, n, l)} + 2 \right] + E_x(m+1, n-1, l) \cdot \left[ \frac{n^2(m+1, n-1, l)}{n^2(m, n-1, l)} - 1 \right] \\
& + E_x(m-1, n+1, l) \cdot \left[ \frac{n^2(m-1, n+1, l)}{n^2(m, n+1, l)} - 1 \right] + E_x(m-1, n, l) \cdot \left[ -2 \frac{n^2(m-1, n, l)}{n^2(m, n, l)} + 2 \right] \\
& \left. + E_x(m-1, n-1, l) \cdot \left[ \frac{n^2(m-1, n-1, l)}{n^2(m, n-1, l)} - 1 \right] \right\} - 2E_x(m, n+1, l) + 4E_x(m, n, l) \\
& - 2E_x(m, n-1, l)
\end{aligned}$$

$$\begin{aligned}
P_2(m, n, l) = & \frac{\Delta z}{8jn_0k\Delta x\Delta y} \left\{ \right. \\
& \left[ E_x(m+1, n+1, l) + \frac{P_1(m+1, n+1, l)}{2} \right] \cdot \left[ \frac{n^2(m+1, n+1, l)}{n^2(m, n+1, l)} - 1 \right] \\
& + \left[ E_x(m+1, n, l) + \frac{P_1(m+1, n, l)}{2} \right] \cdot \left[ -2 \frac{n^2(m+1, n, l)}{n^2(m, n, l)} + 2 \right] \\
& + \left[ E_x(m+1, n-1, l) + \frac{P_1(m+1, n-1, l)}{2} \right] \cdot \left[ \frac{n^2(m+1, n-1, l)}{n^2(m, n-1, l)} - 1 \right] \\
& + \left[ E_x(m-1, n+1, l) + \frac{P_1(m-1, n+1, l)}{2} \right] \cdot \left[ \frac{n^2(m-1, n+1, l)}{n^2(m, n+1, l)} - 1 \right] \\
& + \left[ E_x(m-1, n, l) + \frac{P_1(m-1, n, l)}{2} \right] \cdot \left[ -2 \frac{n^2(m-1, n, l)}{n^2(m, n, l)} + 2 \right] \\
& \left. + \left[ E_x(m-1, n-1, l) + \frac{P_1(m-1, n-1, l)}{2} \right] \cdot \left[ \frac{n^2(m-1, n-1, l)}{n^2(m, n-1, l)} - 1 \right] \right\} \\
& - 2 \cdot [E_x(m, n+1, l) + P_1(m, n+1, l)/2] + 4 \cdot [E_x(m, n, l) + P_1(m, n, l)/2] \\
& - 2 \cdot [E_x(m, n-1, l) + P_1(m, n-1, l)/2]
\end{aligned}$$

$$\begin{aligned}
P_3(m, n, l) = & \frac{\Delta z}{8jn_0k\Delta x\Delta y} \left\{ \right. \\
& \left[ E_x(m+1, n+1, l) + \frac{P_2(m+1, n+1, l)}{2} \right] \cdot \left[ \frac{n^2(m+1, n+1, l)}{n^2(m, n+1, l)} - 1 \right] \\
& + \left[ E_x(m+1, n, l) + \frac{P_2(m+1, n, l)}{2} \right] \cdot \left[ -2 \frac{n^2(m+1, n, l)}{n^2(m, n, l)} + 2 \right] \\
& \left. + \left[ E_x(m+1, n-1, l) + \frac{P_2(m+1, n-1, l)}{2} \right] \cdot \left[ \frac{n^2(m+1, n-1, l)}{n^2(m, n-1, l)} - 1 \right] \right\}
\end{aligned}$$

$$\begin{aligned}
& + \left[ E_x(m-1, n+1, l) + \frac{P_2(m-1, n+1, l)}{2} \right] \cdot \left[ \frac{n^2(m-1, n+1, l)}{n^2(m, n+1, l)} - 1 \right] \\
& + \left[ E_x(m-1, n, l) + \frac{P_2(m-1, n, l)}{2} \right] \cdot \left[ -2 \frac{n^2(m-1, n, l)}{n^2(m, n, l)} + 2 \right] \\
& + \left[ E_x(m-1, n-1, l) + \frac{P_2(m-1, n-1, l)}{2} \right] \cdot \left[ \frac{n^2(m-1, n-1, l)}{n^2(m, n-1, l)} - 1 \right] \} \\
& - 2 \cdot [E_x(m, n+1, l) + P_2(m, n+1, l)/2] + 4 \cdot [E_x(m, n, l) + P_2(m, n, l)/2] \\
& - 2 \cdot [E_x(m, n-1, l) + P_2(m, n-1, l)/2]
\end{aligned}$$

$$\begin{aligned}
P_4(m, n, l) = & \frac{\Delta z}{8j_{n_0} k \Delta x \Delta y} \left\{ \left[ E_x(m+1, n+1, l) + P_3(m+1, n+1, l) \right] \cdot \left[ \frac{n^2(m+1, n+1, l)}{n^2(m, n+1, l)} - 1 \right] \right. \\
& + \left[ E_x(m+1, n, l) + P_3(m+1, n, l) \right] \cdot \left[ -2 \frac{n^2(m+1, n, l)}{n^2(m, n, l)} + 2 \right] \\
& + \left[ E_x(m+1, n-1, l) + P_3(m+1, n-1, l) \right] \cdot \left[ \frac{n^2(m+1, n-1, l)}{n^2(m, n-1, l)} - 1 \right] \\
& + \left[ E_x(m-1, n+1, l) + P_3(m-1, n+1, l) \right] \cdot \left[ \frac{n^2(m-1, n+1, l)}{n^2(m, n+1, l)} - 1 \right] \\
& + \left[ E_x(m-1, n, l) + P_3(m-1, n, l) \right] \cdot \left[ -2 \frac{n^2(m-1, n, l)}{n^2(m, n, l)} + 2 \right] \\
& + \left. \left[ E_x(m-1, n-1, l) + P_3(m-1, n-1, l) \right] \cdot \left[ \frac{n^2(m-1, n-1, l)}{n^2(m, n-1, l)} - 1 \right] \right\} \\
& - 2 \cdot [E_x(m, n+1, l) + P_3(m, n+1, l)] + 4 \cdot [E_x(m, n, l) + P_3(m, n, l)] \\
& - 2 \cdot [E_x(m, n-1, l) + P_3(m, n-1, l)]
\end{aligned}$$

$$a = \frac{1}{2} + \frac{n^2(m+1, n, l)}{2n^2(m, n, l)}, \quad b = 1 + \frac{n^2(m, n, l)}{2} \cdot \left[ \frac{1}{n^2(m+1, n, l)} + \frac{1}{n^2(m-1, n, l)} \right],$$

$$c = \frac{1}{2} + \frac{n^2(m-1, n, l)}{2n^2(m, n, l)}, \quad d = \frac{1}{2} + \frac{n^2(m, n+1, l)}{2n^2(m, n, l)},$$

$$e = 1 + \frac{n^2(m, n, l)}{2} \cdot \left[ \frac{1}{n^2(m, n+1, l)} + \frac{1}{n^2(m, n-1, l)} \right], \quad f = \frac{1}{2} + \frac{n^2(m, n-1, l)}{2n^2(m, n, l)}$$

$$\text{Power distribution} \propto |\vec{E}|^2 = (E_x^2 + E_y^2)$$

### 3D Semi-vector BPM involving the Runge-Kutta algorithm (by K. -Y. Lee):

The transverse components of the optical field  $E_x(x,y,z)$  and  $E_y(x,y,z)$  fulfill

$$2jn_0k \cdot \frac{\partial E_x(x,y,z)}{\partial z} = \frac{\partial}{\partial x} \left\{ \frac{1}{n^2(x,y,z)} \cdot \frac{\partial}{\partial x} [n^2(x,y,z)E_x(x,y,z)] \right\} + \frac{\partial^2 E_x(x,y,z)}{\partial y^2} \\ + [n^2(x,y,z) - n_0^2] k^2 E_x(x,y,z)$$

and

$$2jn_0k \cdot \frac{\partial E_y(x,y,z)}{\partial z} = \frac{\partial^2 E_y(x,y,z)}{\partial x^2} + \frac{\partial}{\partial y} \left\{ \frac{1}{n^2(x,y,z)} \cdot \frac{\partial}{\partial y} [n^2(x,y,z)E_y(x,y,z)] \right\} \\ + [n^2(x,y,z) - n_0^2] k^2 E_y(x,y,z)$$

The Runge-Kutta algorithm can be directly to obtain the propagating field components as

$$E_x(m,i,l+1) = E_x(m,i,l) + \frac{K_1(m,i,l) + 2K_2(m,i,l) + 2K_3(m,i,l) + K_4(m,i,l)}{6}$$

and

$$E_y(m,i,l+1) = E_y(m,i,l) + \frac{J_1(m,i,l) + 2J_2(m,i,l) + 2J_3(m,i,l) + J_4(m,i,l)}{6},$$

where

$$K_1(m,i,l) = \frac{\Delta z}{2jn_0k} \cdot \left\{ \frac{aE_x(m+1,i,l) - bE_x(m,i,l) + cE_x(m-1,i,l)}{\Delta x^2} \right. \\ \left. + \frac{E_x(m,i+1,l) - 2E_x(m,i,l) + E_x(m,i-1,l)}{\Delta y^2} + [n^2(m,i,l) - n_0^2] \cdot k^2 \cdot E_x(m,i,l) \right\}$$

$$K_2(m,i,l) = \frac{\Delta z}{2jn_0k} \cdot \left\{ \frac{d[E_x(m+1,i,l) + \frac{K_1(m+1,i,l)}{2}] - b[E_x(m,i,l) + \frac{K_1(m,i,l)}{2}] + c[E_x(m-1,i,l) + \frac{K_1(m-1,i,l)}{2}]}{\Delta x^2} \right. \\ \left. + \frac{E_x(m,i+1,l) + \frac{K_1(m,i+1,l)}{2} - 2[E_x(m,i,l) + \frac{K_1(m,i,l)}{2}] + E_x(m,i-1,l) + \frac{K_1(m,i-1,l)}{2}}{\Delta y^2} \right. \\ \left. + [n^2(m,i,l) - n_0^2] \cdot k^2 \cdot [E_x(m,i,l) + \frac{K_1(m,i,l)}{2}] \right\}$$

$$K_3(m,i,l) = \frac{\Delta z}{2jn_0k} \cdot \left\{ \frac{d[E_x(m+1,i,l) + \frac{K_2(m+1,i,l)}{2}] - b[E_x(m,i,l) + \frac{K_2(m,i,l)}{2}] + c[E_x(m-1,i,l) + \frac{K_2(m-1,i,l)}{2}]}{\Delta x^2} \right. \\ \left. + \frac{E_x(m,i+1,l) + \frac{K_2(m,i+1,l)}{2} - 2[E_x(m,i,l) + \frac{K_2(m,i,l)}{2}] + E_x(m,i-1,l) + \frac{K_2(m,i-1,l)}{2}}{\Delta y^2} \right. \\ \left. + [n^2(m,i,l) - n_0^2] \cdot k^2 \cdot [E_x(m,i,l) + \frac{K_2(m,i,l)}{2}] \right\}$$

$$K_4(m, i, l) = \frac{\Delta z}{2jn_0k} \cdot \left\{ \frac{a[E_x(m+1, i, l) + K_3(m+1, i, l)] - b[E_x(m, i, l) + K_3(m, i, l)] + c[E_x(m-1, i, l) + K_3(m, i, l)]}{\Delta x^2} \right.$$

$$+ \frac{E_x(m, i+1, l) + K_3(m, i+1, l) - 2[E_x(m, i, l) + K_3(m, i, l)] + E_x(m, i-1, l) + K_3(m, i-1, l)}{\Delta y^2}$$

$$\left. + [n^2(m, i, l) - n_0^2] \cdot k^2 \cdot [E_x(m, i, l) + K_3(m, i, l)] \right\}$$

$$J_1(m, i, l) = \frac{\Delta z}{2jn_0k} \cdot \left\{ \frac{E_y(m+1, i, l) - 2E_y(m, i, l) + E_y(m-1, i, l)}{\Delta x^2} \right.$$

$$+ \frac{dE_y(m, i+1, l) - eE_y(m, i, l) + fE_y(m, i-1, l)}{\Delta y^2}$$

$$\left. + [n^2(m, i, l) - n_0^2] \cdot k^2 \cdot E_y(m, i, l) \right\},$$

$$J_2(m, i, l) = \frac{\Delta z}{2jn_0k} \cdot \left\{ \frac{E_y(m+1, i, l) + \frac{J_1(m+1, i, l)}{2} - 2[E_y(m, i, l) + \frac{J_1(m, i, l)}{2}] + E_y(m-1, i, l) + \frac{J_1(m-1, i, l)}{2}}{\Delta x^2} \right.$$

$$+ \frac{d[E_y(m, i+1, l) + \frac{J_1(m, i+1, l)}{2}] - e[E_y(m, i, l) + \frac{J_1(m, i, l)}{2}] + f[E_y(m, i-1, l) + \frac{J_1(m, i-1, l)}{2}]}{\Delta y^2}$$

$$\left. + [n^2(m, i, l) - n_0^2] \cdot k^2 \cdot [E_y(m, i, l) + \frac{J_1(m, i, l)}{2}] \right\}$$

$$J_3(m, i, l) = \frac{\Delta z}{2jn_0k} \cdot \left\{ \frac{E_y(m+1, i, l) + \frac{J_2(m+1, i, l)}{2} - 2[E_y(m, i, l) + \frac{J_2(m, i, l)}{2}] + E_y(m-1, i, l) + \frac{J_2(m-1, i, l)}{2}}{\Delta x^2} \right.$$

$$+ \frac{d[E_y(m, i+1, l) + \frac{J_2(m, i+1, l)}{2}] - e[E_y(m, i, l) + \frac{J_2(m, i, l)}{2}] + f[E_y(m, i-1, l) + \frac{J_2(m, i-1, l)}{2}]}{\Delta y^2}$$

$$\left. + [n^2(m, i, l) - n_0^2] \cdot k^2 \cdot [E_y(m, i, l) + \frac{J_2(m, i, l)}{2}] \right\}$$

$$J_4(m, i, l) = \frac{\Delta z}{2jn_0k} \cdot \left\{ \frac{E_y(m+1, i, l) + J_3(m+1, i, l) - 2[E_y(m, i, l) + J_3(m, i, l)] + E_y(m-1, i, l) + J_3(m, i, l)}{\Delta x^2} \right.$$

$$+ \frac{d[E_y(m, i+1, l) + J_3(m, i+1, l)] - e[E_y(m, i, l) + J_3(m, i, l)] + f[E_y(m, i-1, l) + J_3(m, i-1, l)]}{\Delta y^2}$$

$$\left. + [n^2(m, i, l) - n_0^2] \cdot k^2 \cdot [E_y(m, i, l) + J_3(m, i, l)] \right\}$$



$$a = \frac{1}{2} + \frac{n^2(m+1,i,l)}{2n^2(m,i,l)}, \quad b = 1 + \frac{n^2(m,i,l)}{2} \cdot \left[ \frac{1}{n^2(m+1,i,l)} + \frac{1}{n^2(m-1,i,l)} \right], \quad c = \frac{1}{2} + \frac{n^2(m-1,i,l)}{2n^2(m,i,l)},$$

$$d = \frac{1}{2} + \frac{n^2(m,i+1,l)}{2n^2(m,i,l)}, \quad e = 1 + \frac{n^2(m,i,l)}{2} \cdot \left[ \frac{1}{n^2(m,i+1,l)} + \frac{1}{n^2(m,i-1,l)} \right], \quad f = \frac{1}{2} + \frac{n^2(m,i-1,l)}{2n^2(m,i,l)}$$

Note that coefficients  $b$  and  $e$  approach 2, but  $a$ ,  $c$ ,  $d$ , and  $f$  approach 1 as the transverse variations of the refractive index profiles are very small. In this case, the above semivectorial formulae for two types of polarizations are reduced into the same scalar expressions.

$$\text{Power distribution} \propto |\vec{E}|^2 = E_x^2 \quad \text{or} \quad E_y^2$$

### 3D Scalar BPM involving the Runge-Kutta algorithm (by K. -Y. Lee):

The scalar optical field  $\phi(x,y,z)$  can be described by the following Fresnel equation

$$2jn_0k \cdot \frac{\partial \phi(x,y,z)}{\partial z} = \frac{\partial^2 \phi(x,y,z)}{\partial x^2} + \frac{\partial^2 \phi(x,y,z)}{\partial y^2} + [n^2(x,y,z) - n_0^2]k^2 \phi(x,y,z),$$

Utilizing the finite difference scheme and the Runge-Kutta method, the propagating optical field at  $(x = m\Delta x, y = i\Delta y, z = (l+1)\Delta z)$  is expressed by

$$\phi(m,i,l+1) = \phi(m,i,l) + \frac{K_1(m,i,l) + 2K_2(m,i,l) + 2K_3(m,i,l) + K_4(m,i,l)}{6},$$

where

$$K_1(m,i,l) = \frac{\Delta z}{2jn_0k} \cdot \left\{ \frac{\phi(m+1,i,l) - 2\phi(m,i,l) + \phi(m-1,i,l)}{\Delta x^2} \right.$$

$$\left. + \frac{\phi(m,i+1,l) - 2\phi(m,i,l) + \phi(m,i-1,l)}{\Delta y^2} + [n^2(m,i,l) - n_0^2] \cdot k^2 \cdot \phi(m,i,l) \right\}$$

$$K_2(m,i,l) = \frac{\Delta z}{2jn_0k} \cdot \left\{ \frac{\phi(m+1,i,l) + \frac{K_1(m+1,i,l)}{2} - 2\phi(m,i,l) - K_1(m,i,l) + \phi(m-1,i,l) + \frac{K_1(m-1,i,l)}{2}}{\Delta x^2} \right.$$

$$\left. + \frac{\phi(m,i+1,l) + \frac{K_1(m,i+1,l)}{2} - 2\phi(m,i,l) - K_1(m,i,l) + \phi(m,i-1,l) + \frac{K_1(m,i-1,l)}{2}}{\Delta y^2} \right.$$

$$\left. + [n^2(m,i,l) - n_0^2] \cdot k^2 \cdot \left[ \phi(m,i,l) + \frac{K_1(m,i,l)}{2} \right] \right\}$$

$$K_3(m,i,l) = \frac{\Delta z}{2jn_0k} \cdot \left\{ \frac{\phi(m+1,i,l) + \frac{K_2(m+1,i,l)}{2} - 2\phi(m,i,l) - K_2(m,i,l) + \phi(m-1,i,l) + \frac{K_2(m-1,i,l)}{2}}{\Delta x^2} \right.$$

$$\left. + \frac{\phi(m,i+1,l) + \frac{K_2(m,i+1,l)}{2} - 2\phi(m,i,l) - K_2(m,i,l) + \phi(m,i-1,l) + \frac{K_2(m,i-1,l)}{2}}{\Delta y^2} \right.$$

$$+ [n^2(m, i, l) - n_0^2] \cdot k^2 \cdot [\phi(m, i, l) + \frac{K_2(m, i, l)}{2}] \}$$

and

$$K_4(m, i, l) = \frac{\Delta z}{2jn_0k} \cdot \left\{ \frac{\phi(m+1, i, l) + K_3(m+1, i, l) - 2\phi(m, i, l) - 2K_3(m, i, l) + \phi(m-1, i, l) + K_3(m, i, l)}{\Delta x^2} \right. \\ \left. + \frac{\phi(m, i+1, l) + K_3(m, i+1, l) - 2\phi(m, i, l) - 2K_3(m, i, l) + \phi(m, i-1, l) + K_3(m, i-1, l)}{\Delta y^2} \right. \\ \left. + [n^2(m, i, l) - n_0^2] \cdot k^2 \cdot [\phi(m, i, l) + K_3(m, i, l)] \right\}$$

On the other hand, the **transparent boundary condition (TBC)** is implemented in the computer programming for reducing extra numerical errors due to undesired wave reflections at the edges of computational windows.

### Transparent Boundary Conditions (TBC):

Define  $\alpha_{+x}$ ,  $\alpha_{-x}$ ,  $\beta_{+x}$ ,  $\beta_{-x}$ ,  $\alpha_{+y}$ ,  $\alpha_{-y}$ ,  $\beta_{+y}$ , and  $\beta_{-y}$  as

$$\alpha_{\pm x} + j\beta_{\pm x} \equiv \ln \left[ \frac{\phi(\pm M \mp 1, i, l)}{\phi(\pm M \mp 2, i, l)} \right] \quad \text{and} \quad \alpha_{\pm y} + j\beta_{\pm y} \equiv \ln \left[ \frac{\phi(m, \pm I \mp 1, l)}{\phi(m, \pm I \mp 2, l)} \right]$$

TBC shows that

$$\phi(\pm M, i, l) = \begin{cases} \frac{\phi(\pm M \mp 1, i, l)^2}{\phi(\pm M \mp 2, i, l)} & , \alpha_{\pm x} < 0 \\ \phi(\pm M \mp 1, i, l) \cdot \exp(j\beta_{\pm x}) & , \alpha_{\pm x} \geq 0 \end{cases}$$

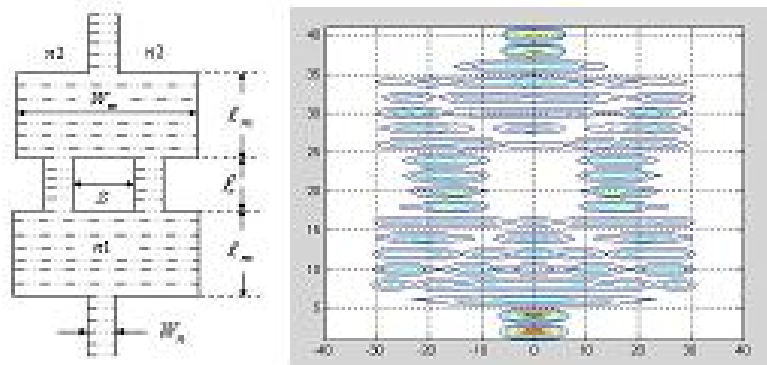
and

$$\phi(m, \pm I, l) = \begin{cases} \frac{\phi(m, \pm I \mp 1, l)^2}{\phi(m, \pm I \mp 2, l)} & , \alpha_{\pm y} < 0 \\ \phi(m, \pm I \mp 1, l) \cdot \exp(j\beta_{\pm y}) & , \alpha_{\pm y} \geq 0 \end{cases}$$

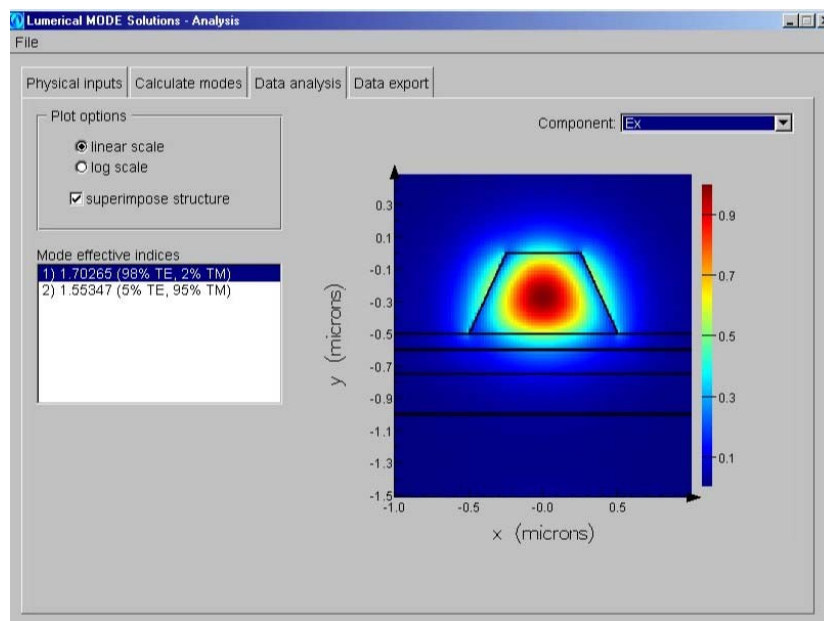
Similarly, the values  $K_1(\pm M, i, l)$ ,  $K_2(\pm M, i, l)$ ,  $K_3(\pm M, i, l)$ ,  $K_4(\pm M, i, l)$ ,  $K_1(m, \pm I, l)$ ,  $K_2(m, \pm I, l)$ ,  $K_3(m, \pm I, l)$ , and  $K_4(m, \pm I, l)$  at the edges of the computation windows are obtained by the same rules.

$$\text{Power distribution} \propto |\phi|^2$$

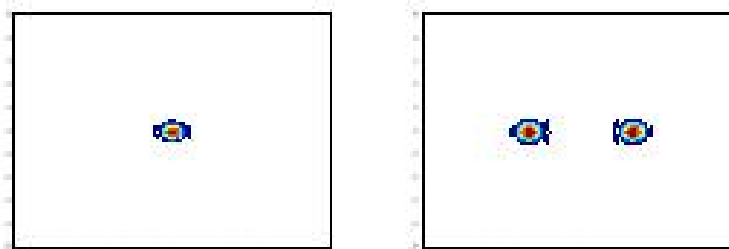
**Eg. A laser beam passes an MMI waveguide device.** (by K. Huang, 黃建智)



**Eg. Simulation of the fundamental mode of a single-mode ridge waveguide.**

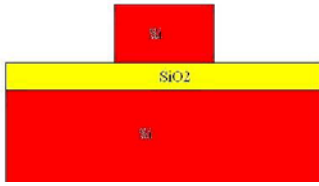


**Eg. Simulation of a  $10^\circ$ -Y-junction 3D waveguide.** (by K. -Y. Lee)

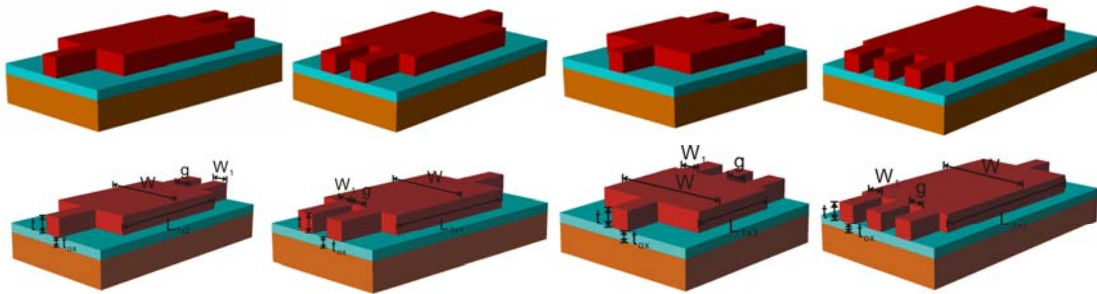


Input mode

Output light spots



Eg. For an  $n \times 1$  MMI optical combiner and a  $1 \times n$  MMI optical splitter, the BPM simulation shows that  $L_{n \times 1}/L_{1 \times n} \approx n-1$ , where  $L_{n \times 1}$  is the wide section length of the  $n \times 1$  MMI optical combiner and  $L_{1 \times n}$  is the wide section length of the  $1 \times n$  MMI optical splitter, respectively. Consider a SOI waveguide of  $n_{\text{core}}=3.45$ ,  $n_{\text{SiO}_2}=1.5$ ,  $\lambda=1.55\mu\text{m}$ . The thickness of oxide is  $2\mu\text{m}$ . The input single-mode waveguide has a  $5\mu\text{m} \times 5\mu\text{m}$  cross section.



1×2 MMI splitter

2×1 MMI combiner

1×3 MMI splitter

3×1 MMI combiner 3D

BPM simulation (by J. –R. Sze *et al.*):

$n$	2	3	4	5
$W$	$40\mu\text{m}$	$40\mu\text{m}$	$40\mu\text{m}$	$40\mu\text{m}$
$g$	$15\mu\text{m}$	$8.333\mu\text{m}$	$5\mu\text{m}$	$3\mu\text{m}$
$L_{n \times 1}$	$1772\mu\text{m}$	$2380\mu\text{m}$	$2684\mu\text{m}$	$2846\mu\text{m}$
$L_{1 \times n}$	$1805\mu\text{m}$	$1197\mu\text{m}$	$893\mu\text{m}$	$731\mu\text{m}$
$L_{n \times 1}/L_{1 \times n}$	<b><math>0.98 \doteq 1</math></b>	<b><math>1.98 \doteq 2</math></b>	<b><math>3.005 \doteq 3</math></b>	<b><math>3.89 \doteq 4</math></b>

