Advanced Computation:
Computational Electromagnetics

Maxwell's Equations in Fourier Space

1

Outline

- Maxwell's Equations in Fourier Space
- Matrix form of Maxwell's equations in Fourier space
- Constructing convolution matrices
- Fast Fourier factorization
- Consequences of Fourier-space representation

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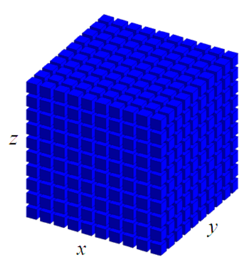
2

Maxwell's Equations in Fourier Space

Slide 3

3

What is Fourier Space?

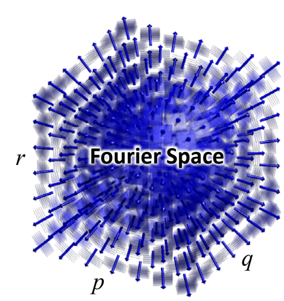


Real Space

So far, fields and devices were represented on an x-y-z grid where field values and material properties are defined at discrete points.

Fourier Space

In Fourier-space, fields are represented as a sum of plane waves at different angles and different wavelengths called *spatial harmonics*. Devices are also represented as the sum of sinusoidal gratings at different angles and periods.



Slide 4

4

Fourier-Space Vs. Frequency-Domain

$$\nabla \times \vec{E} = -\mu \frac{\partial \vec{H}}{\partial t}$$
$$\nabla \times \vec{H} = \varepsilon \frac{\partial \vec{E}}{\partial t}$$

Fourier transform x, y, and z to k_x, k_y, and k_z.

Fourier transform t to ω.

$$j\vec{k} \times \vec{E} = -\mu \frac{\partial \vec{H}}{\partial t}$$
$$j\vec{k} \times \vec{H} = \varepsilon \frac{\partial \vec{E}}{\partial t}$$

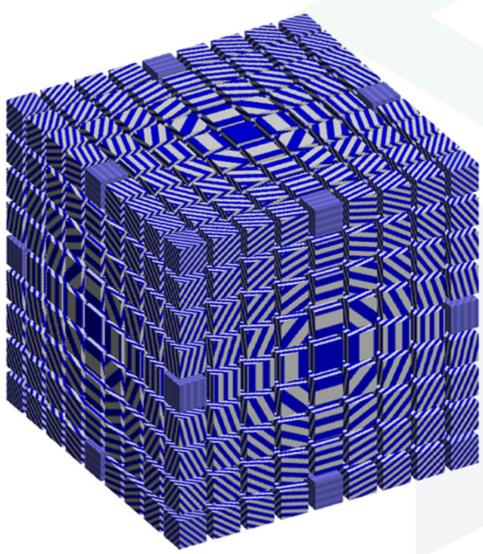
Fourier Space

$$\nabla \times \vec{E} = -j\omega\mu\vec{H}$$
$$\nabla \times \vec{H} = j\omega\varepsilon\vec{E}$$

Frequency Domain

	Real-Space	Fourier-Space
Time-Domain	FDTD, Discontinuous Galerkin	Pseudo-spectral FDTD
Frequency-Domain	FDFD, FEM, MoM, MoL	RCWA, SAM, PWEM, spectral domain

Visualizing the Spatial Harmonics



$$\vec{k}(p,q,r) = p\vec{T}_1 + q\vec{T}_2 + r\vec{T}_3$$

p, q, and r are the indices of the spatial harmonics.

$$p \equiv \text{integer} \quad -\infty,\ldots,-2,-1,0,1,2,\ldots,\infty$$
$$q \equiv \text{integer} \quad -\infty,\ldots,-2,-1,0,1,2,\ldots,\infty$$
$$r \equiv \text{integer} \quad -\infty,\ldots,-2,-1,0,1,2,\ldots,\infty$$

$\vec{T}_1$, $\vec{T}_2$, and $\vec{T}_3$ are the reciprocal lattice vectors.

Each of these plane waves will be assigned its own complex amplitude to convey its magnitude and phase.

Conventional Complex Fourier Series

Periodic functions can be expanded into a Fourier series.

For 1D periodic functions, this is

$$f(x)=\sum_{p=-\infty}^{\infty} a(p)e^{j\frac{2\pi px}{\Lambda}} \qquad a(p)=\frac{1}{\Lambda}\int_{-\Lambda/2}^{\Lambda/2} f(x)e^{-j\frac{2\pi px}{\Lambda}}dx$$

For 2D periodic functions, this is

$$f(x,y)=\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty} a(p,q)e^{j\left(\frac{2\pi px}{\Lambda_x}+\frac{2\pi qy}{\Lambda_y}\right)} \qquad a(p,q)=\frac{1}{A}\iint_A f(x,y)e^{-j\left(\frac{2\pi px}{\Lambda_x}+\frac{2\pi qy}{\Lambda_y}\right)}dA$$

For 3D periodic functions, this is

$$f(x,y,z)=\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty} a(p,q,r)e^{j\left(\frac{2\pi px}{\Lambda_x}+\frac{2\pi qy}{\Lambda_y}+\frac{2\pi rz}{\Lambda_z}\right)} \qquad a(p,q,r)=\frac{1}{V}\iiint_V f(x,y,z)e^{-j\left(\frac{2\pi px}{\Lambda_x}+\frac{2\pi qy}{\Lambda_y}+\frac{2\pi rz}{\Lambda_z}\right)}dV$$

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Slide 7

7

Generalized Complex Fourier Series

Fourier series can be written in terms of the reciprocal lattice vectors.

For 1D periodic functions, this is

$$f(x)=\sum_{p=-\infty}^{\infty} a(p)e^{jpTx} \qquad a(p)=\frac{1}{\Lambda}\int_{-\Lambda/2}^{\Lambda/2} f(x)e^{-jpTx}dx \qquad T=\frac{2\pi}{\Lambda}$$

For 2D periodic functions, this is

$$f(x,y)=\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty} a(p,q)e^{j\left(p\vec{T}_1+q\vec{T}_2\right)\bullet\vec{r}} \qquad a(p,q)=\frac{1}{A}\iint_A f(x,y)e^{-j\left(p\vec{T}_1+q\vec{T}_2\right)\bullet\vec{r}}dA$$

For 3D periodic functions, this is

$$f(\vec{r})=\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty} a(p,q,r)e^{j\left(p\vec{T}_1+q\vec{T}_2+r\vec{T}_3\right)\bullet\vec{r}} \qquad a(p,q,r)=\frac{1}{V}\iiint_V f(\vec{r})e^{-j\left(p\vec{T}_1+q\vec{T}_2+r\vec{T}_3\right)\bullet\vec{r}}dV$$

For rectangular, tetrahedral, or orthorhombic geometries, the reciprocal lattice vectors are:

$$\vec{T}_1=\frac{2\pi}{\Lambda_x}\hat{x} \qquad \vec{T}_2=\frac{2\pi}{\Lambda_y}\hat{y} \qquad \vec{T}_3=\frac{2\pi}{\Lambda_z}\hat{z}$$

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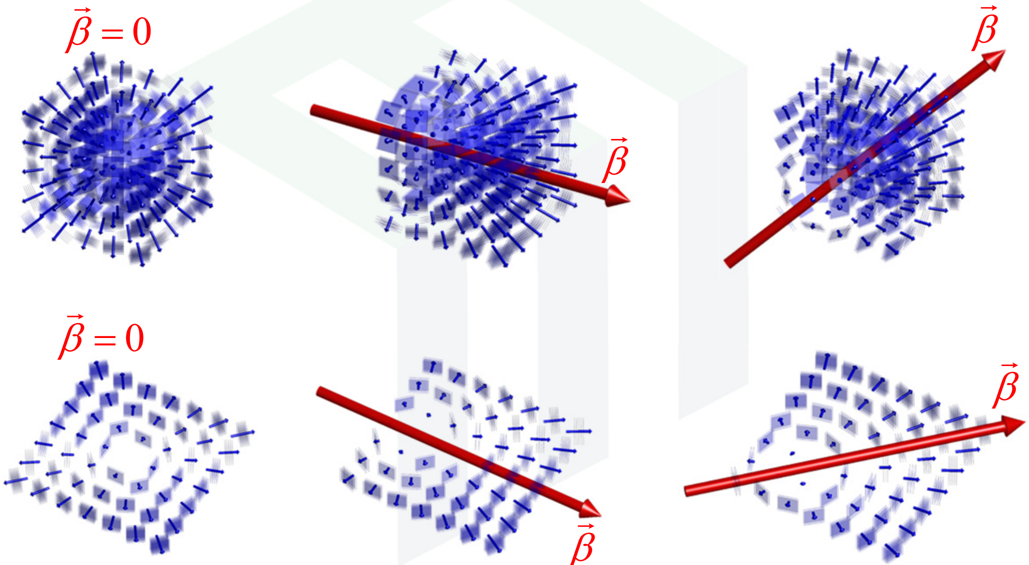
8

Visualizing Expansions with Different β's



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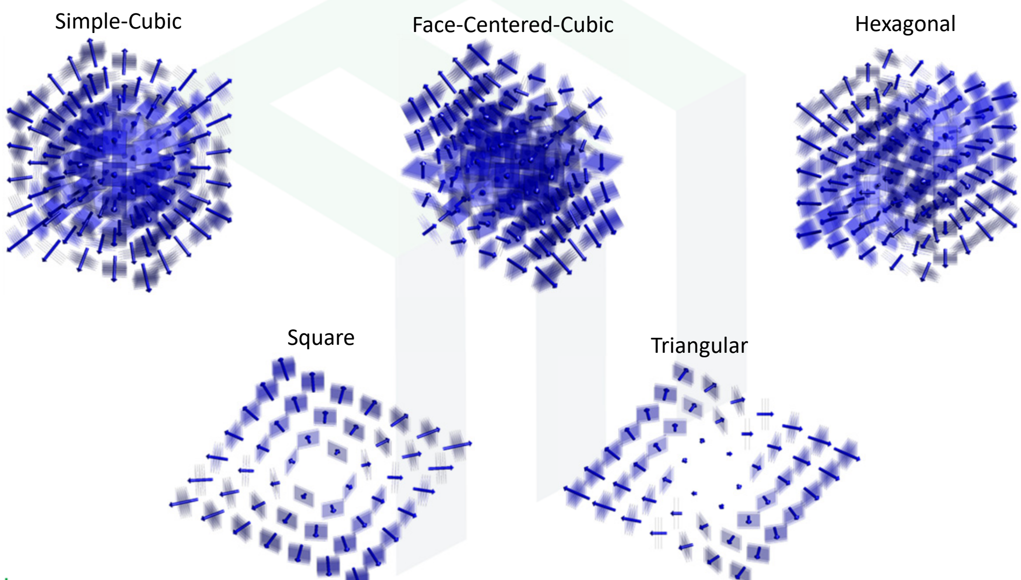
9

Visualizing Expansions with Different Symmetries



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10

Starting Point

Start with Maxwell's equations in the following form…

$$\frac{\partial E_z}{\partial y}-\frac{\partial E_y}{\partial z}=k_0\mu_r\tilde{H}_x \qquad \frac{\partial \tilde{H}_z}{\partial y}-\frac{\partial \tilde{H}_y}{\partial z}=k_0\varepsilon_r E_x$$

$$\frac{\partial E_x}{\partial z}-\frac{\partial E_z}{\partial x}=k_0\mu_r\tilde{H}_y \qquad \frac{\partial \tilde{H}_x}{\partial z}-\frac{\partial \tilde{H}_z}{\partial x}=k_0\varepsilon_r E_y$$

$$\frac{\partial E_y}{\partial x}-\frac{\partial E_x}{\partial y}=k_0\mu_r\tilde{H}_z \qquad \frac{\partial \tilde{H}_y}{\partial x}-\frac{\partial \tilde{H}_x}{\partial y}=k_0\varepsilon_r E_z$$

Recall that the magnetic field was normalized according to

$$\vec{\tilde{H}}=-j\sqrt{\frac{\mu_0}{\varepsilon_0}}\vec{H}$$

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11

Fourier Expansion of the Materials

Assuming the device is infinitely periodic in all directions, the permittivity and permeability functions can be expanded into a generalized Fourier Series.

$$\varepsilon_r(\vec{r})=\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}a(p,q,r)e^{j\left(p\vec{T}_1+q\vec{T}_2+r\vec{T}_3\right)\bullet\vec{r}}$$

$$a(p,q,r)=\frac{1}{V}\iiint_V \varepsilon_r(\vec{r})e^{-j\left(p\vec{T}_1+q\vec{T}_2+r\vec{T}_3\right)\bullet\vec{r}}dV$$

$$\mu_r(\vec{r})=\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}b(p,q,r)e^{j\left(p\vec{T}_1+q\vec{T}_2+r\vec{T}_3\right)\bullet\vec{r}}$$

$$b(p,q,r)=\frac{1}{V}\iiint_V \mu_r(\vec{r})e^{-j\left(p\vec{T}_1+q\vec{T}_2+r\vec{T}_3\right)\bullet\vec{r}}dV$$

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12

Fourier Expansion of the Fields

The field expansions are slightly different because a wave could be travelling in any direction $\vec{\beta}$. The expansions must satisfy the Floquet boundary conditions.

$$\vec{E}(\vec{r}) = e^{-j\vec{\beta}\bullet\vec{r}} \sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty} \vec{S}(p,q,r)\, e^{j\left(p\vec{T}_1+q\vec{T}_2+r\vec{T}_3\right)\bullet\vec{r}}$$

Think of $\vec{\beta}$ as $\vec{k}_{\text{inc}}$

$$= \sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty} \vec{S}(p,q,r)\, e^{-j\underbrace{\left(\vec{\beta}-p\vec{T}_1-q\vec{T}_2-r\vec{T}_3\right)}_{\text{Let this be } \vec{k}(p,q,r)}\bullet\vec{r}}$$

$e^{-j\vec{\beta}\bullet\vec{r}}$ was brought inside summation and combined with second exponential.

$$= \sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty} \vec{S}(p,q,r)\, e^{-j\vec{k}(p,q,r)\bullet\vec{r}}$$

This is clearly a set of plane waves with amplitudes $\vec{S}(p,q,r)$.

$$= \sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty} \vec{S}(p,q,r)\, e^{-j\left[k_x(p,q,r)x+k_y(p,q,r)y+k_z(p,q,r)z\right]}$$

$$\vec{k}(p,q,r) = \vec{\beta} - p\vec{T}_1 - q\vec{T}_2 - r\vec{T}_3$$

$$k_x(p,q,r) = \beta_x - pT_{1,x} - qT_{2,x} - rT_{3,x}$$
$$k_y(p,q,r) = \beta_y - pT_{1,y} - qT_{2,y} - rT_{3,y}$$
$$k_z(p,q,r) = \beta_z - pT_{1,z} - qT_{2,z} - rT_{3,z}$$

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13

Substitute Expansions into Maxwell's Equations

$$\tilde{H}_y(\vec{r}) = \sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty} U_y(p,q,r)\, e^{-j\left[k_x(p,q,r)x+k_y(p,q,r)y+k_z(p,q,r)z\right]}$$

$$\varepsilon_r(\vec{r}) = \sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty} a(p,q,r)\, e^{j\left(p\vec{T}_1+q\vec{T}_2+r\vec{T}_3\right)\bullet\vec{r}}$$

$$\tilde{H}_z(\vec{r}) = \sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty} U_z(p,q,r)\, e^{-j\left[k_x(p,q,r)x+k_y(p,q,r)y+k_z(p,q,r)z\right]}$$

$$E_x(\vec{r}) = \sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty} S_x(p,q,r)\, e^{-j\left[k_x(p,q,r)x+k_y(p,q,r)y+k_z(p,q,r)z\right]}$$

$$\frac{\partial \tilde{H}_z}{\partial y} - \frac{\partial \tilde{H}_y}{\partial z} = k_0 \varepsilon_r E_x$$

$$\Downarrow$$

$$\frac{\partial}{\partial y}\left[\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty} U_z(p,q,r)\, e^{-j\left[k_x(p,q,r)x+k_y(p,q,r)y+k_z(p,q,r)z\right]}\right] - \frac{\partial}{\partial z}\left[\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty} U_y(p,q,r)\, e^{-j\left[k_x(p,q,r)x+k_y(p,q,r)y+k_z(p,q,r)z\right]}\right]$$
$$= k_0\left[\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty} a(p,q,r)\, e^{j\left(p\vec{T}_1+q\vec{T}_2+r\vec{T}_3\right)\bullet\vec{r}}\right]\left[\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty} S_x(p,q,r)\, e^{-j\left[k_x(p,q,r)x+k_y(p,q,r)y+k_z(p,q,r)z\right]}\right]$$

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14

Algebra for the Left Side Terms

First ugly term…

$$\frac{\partial}{\partial y}\left[\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}U_z(p,q,r)e^{-j\left[k_x(p,q,r)x+k_y(p,q,r)y+k_z(p,q,r)z\right]}\right]=\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}U_z(p,q,r)\frac{\partial}{\partial y}e^{-j\left[k_x(p,q,r)x+k_y(p,q,r)y+k_z(p,q,r)z\right]}$$

$$=\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}U_z(p,q,r)\left[-jk_y(p,q,r)\right]e^{-j\left[k_x(p,q,r)x+k_y(p,q,r)y+k_z(p,q,r)z\right]}$$

$$=\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}-jk_y(p,q,r)U_z(p,q,r)e^{-j\left[k_x(p,q,r)x+k_y(p,q,r)y+k_z(p,q,r)z\right]}$$

Second ugly term…

$$\frac{\partial}{\partial z}\left[\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}U_y(p,q,r)e^{-j\left[k_x(p,q,r)x+k_y(p,q,r)y+k_z(p,q,r)z\right]}\right]=\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}U_y(p,q,r)\frac{\partial}{\partial z}e^{-j\left[k_x(p,q,r)x+k_y(p,q,r)y+k_z(p,q,r)z\right]}$$

$$=\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}U_y(p,q,r)\left[-jk_z(p,q,r)\right]e^{-j\left[k_x(p,q,r)x+k_y(p,q,r)y+k_z(p,q,r)z\right]}$$

$$=\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}-jk_z(p,q,r)U_y(p,q,r)e^{-j\left[k_x(p,q,r)x+k_y(p,q,r)y+k_z(p,q,r)z\right]}$$

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Slide 15

15

Algebra for the Right-Side Term

Third ugly term…

This term as the product of two triple summations.

$$\left[\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}a(p,q,r)e^{j\left(p\vec{T}_1+q\vec{T}_2+r\vec{T}_3\right)\bullet\vec{r}}\right]\left[\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}S_x(p,q,r)e^{-j\left[k_x(p,q,r)x+k_y(p,q,r)y+k_z(p,q,r)z\right]}\right]$$

This is called a Cauchy product and is handled as follows.

$$\left(\sum_{n=0}^{\infty}a_n\right)\cdot\left(\sum_{n=0}^{\infty}b_n\right)=\sum_{n=0}^{\infty}c_n \qquad c_n=\sum_{m=0}^{n}a_m b_{n-m}$$

Applying this rule to the triple summations, gives

$$\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}\left\{e^{-j\left[k_x(p,q,r)x+k_y(p,q,r)y+k_z(p,q,r)z\right]}\sum_{p'=-\infty}^{\infty}\sum_{q'=-\infty}^{\infty}\sum_{r'=-\infty}^{\infty}a(p-p',q-q',r-r')S_x(p',q',r')\right\}$$

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16

Combine the Terms Inside Summation

$$\frac{\partial}{\partial y}\left[\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}U_z(p,q,r)e^{-j\left[k_x(p,q,r)x+k_y(p,q,r)y+k_z(p,q,r)z\right]}\right]-\frac{\partial}{\partial z}\left[\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}U_y(p,q,r)e^{-j\left[k_x(p,q,r)x+k_y(p,q,r)y+k_z(p,q,r)z\right]}\right]$$
$$=k_0\left[\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}a(p,q,r)e^{j\left(p\vec{T}_1+q\vec{T}_2+r\vec{T}_3\right)\bullet\vec{r}}\right]\left[\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}S_x(p,q,r)e^{-j\left[k_x(p,q,r)x+k_y(p,q,r)y+k_z(p,q,r)z\right]}\right]$$

$$\Downarrow$$

$$\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}-jk_y(p,q,r)U_z(p,q,r)e^{-j\left[k_x(p,q,r)x+k_y(p,q,r)y+k_z(p,q,r)z\right]}-\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}-jk_z(p,q,r)U_y(p,q,r)e^{-j\left[k_x(p,q,r)x+k_y(p,q,r)y+k_z(p,q,r)z\right]}$$
$$=k_0\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}\left\{e^{-j\left[k_x(p,q,r)x+k_y(p,q,r)y+k_z(p,q,r)z\right]}\sum_{p'=-\infty}^{\infty}\sum_{q'=-\infty}^{\infty}\sum_{r'=-\infty}^{\infty}a(p-p',q-q',r-r')S_x(p',q',r')\right\}$$

The equation can now be brought inside a single triple summation.

$$\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}\left\{\begin{aligned}&-jk_y(p,q,r)U_z(p,q,r)e^{-j\left[k_x(p,q,r)x+k_y(p,q,r)y+k_z(p,q,r)z\right]}+jk_z(p,q,r)U_y(p,q,r)e^{-j\left[k_x(p,q,r)x+k_y(p,q,r)y+k_z(p,q,r)z\right]}\\&=k_0e^{-j\left[k_x(p,q,r)x+k_y(p,q,r)y+k_z(p,q,r)z\right]}\sum_{p'=-\infty}^{\infty}\sum_{q'=-\infty}^{\infty}\sum_{r'=-\infty}^{\infty}a(p-p',q-q',r-r')S_x(p',q',r')\end{aligned}\right\}$$

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17

Final Equation for $(p,q,r)^{\text{th}}$ Harmonic

$$\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}\left\{\begin{aligned}&-jk_y(p,q,r)U_z(p,q,r)e^{-j\left[k_x(p,q,r)x+k_y(p,q,r)y+k_z(p,q,r)z\right]}+jk_z(p,q,r)U_y(p,q,r)e^{-j\left[k_x(p,q,r)x+k_y(p,q,r)y+k_z(p,q,r)z\right]}\\&=k_0e^{-j\left[k_x(p,q,r)x+k_y(p,q,r)y+k_z(p,q,r)z\right]}\sum_{p'=-\infty}^{\infty}\sum_{q'=-\infty}^{\infty}\sum_{r'=-\infty}^{\infty}a(p-p',q-q',r-r')S_x(p',q',r')\end{aligned}\right\}$$

The equation inside the braces much be satisfied for each combination of (p,q,r).

$$-jk_y(p,q,r)U_z(p,q,r)e^{-j\left[k_x(p,q,r)x+k_y(p,q,r)y+k_z(p,q,r)z\right]}+jk_z(p,q,r)U_y(p,q,r)e^{-j\left[k_x(p,q,r)x+k_y(p,q,r)y+k_z(p,q,r)z\right]}$$
$$=k_0e^{-j\left[k_x(p,q,r)x+k_y(p,q,r)y+k_z(p,q,r)z\right]}\sum_{p'=-\infty}^{\infty}\sum_{q'=-\infty}^{\infty}\sum_{r'=-\infty}^{\infty}a(p-p',q-q',r-r')S_x(p',q',r')$$

Last, divide both sides by the common exponential term and move the j to the right-hand side.

$$k_y(p,q,r)U_z(p,q,r)-k_z(p,q,r)U_y(p,q,r)=jk_0\sum_{p'=-\infty}^{\infty}\sum_{q'=-\infty}^{\infty}\sum_{r'=-\infty}^{\infty}a(p-p',q-q',r-r')S_x(p',q',r')$$

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18

Alternate Derivation

Start with

$$\frac{\partial \tilde{H}_z}{\partial y} - \frac{\partial \tilde{H}_y}{\partial z} = k_0 \underbrace{\varepsilon_r E_x}$$

Point-by-point multiplication in real-space…

Fourier-transform this equation in x, y, and z resulting in

$$k_y(p,q,r)U_z(p,q,r) - k_z(p,q,r)U_y(p,q,r) = jk_0 \underbrace{a * S_x}$$

…becomes a convolution in Fourier-space.

$a = \text{FT}\{\varepsilon_r\}$

$S_x = \text{FT}\{E_x\}$

It can now be seen that the strange triple summation remaining in the equation is actually a 3D convolution in Fourier space!

$$a * S_x \quad \rightarrow \quad \sum_{p'=-\infty}^{\infty} \sum_{q'=-\infty}^{\infty} \sum_{r'=-\infty}^{\infty} a(p-p', q-q', r-r') S_x(p', q', r')$$

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19

Summary of Maxwell's Equations in Fourier Space

Real-Space

$$\frac{\partial \tilde{H}_z}{\partial y} - \frac{\partial \tilde{H}_y}{\partial z} = k_0 \varepsilon_r E_x$$

$$\frac{\partial \tilde{H}_x}{\partial z} - \frac{\partial \tilde{H}_z}{\partial x} = k_0 \varepsilon_r E_y$$

$$\frac{\partial \tilde{H}_y}{\partial x} - \frac{\partial \tilde{H}_x}{\partial y} = k_0 \varepsilon_r E_z$$

Fourier-Space

$$\boxed{\begin{aligned} k_y(p,q,r)U_z(p,q,r) - k_z(p,q,r)U_y(p,q,r) &= jk_0 a(p,q,r) * S_x(p,q,r) \\ k_z(p,q,r)U_x(p,q,r) - k_x(p,q,r)U_z(p,q,r) &= jk_0 a(p,q,r) * S_y(p,q,r) \\ k_x(p,q,r)U_y(p,q,r) - k_y(p,q,r)U_x(p,q,r) &= jk_0 a(p,q,r) * S_z(p,q,r) \end{aligned}}$$

$$\vec{k}(p,q,r) = k_x(p,q,r)\hat{a}_x + k_y(p,q,r)\hat{a}_y + k_z(p,q,r)\hat{a}_z = \vec{\beta} - p\vec{T}_1 - q\vec{T}_2 - r\vec{T}_3$$

$$p = -\infty, \cdots, -2, -1, 0, 1, 2, \cdots, \infty$$

$$q = -\infty, \cdots, -2, -1, 0, 1, 2, \cdots, \infty$$

$$r = -\infty, \cdots, -2, -1, 0, 1, 2, \cdots, \infty$$

$$\frac{\partial E_z}{\partial y} - \frac{\partial E_y}{\partial z} = k_0 \mu_r \tilde{H}_x$$

$$\frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x} = k_0 \mu_r \tilde{H}_y$$

$$\frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} = k_0 \mu_r \tilde{H}_z$$

$$\boxed{\begin{aligned} k_y(p,q,r)S_z(p,q,r) - k_z(p,q,r)S_y(p,q,r) &= jk_0 b(p,q,r) * U_x(p,q,r) \\ k_z(p,q,r)S_x(p,q,r) - k_x(p,q,r)S_z(p,q,r) &= jk_0 b(p,q,r) * U_y(p,q,r) \\ k_x(p,q,r)S_y(p,q,r) - k_y(p,q,r)S_x(p,q,r) &= jk_0 b(p,q,r) * U_z(p,q,r) \end{aligned}}$$

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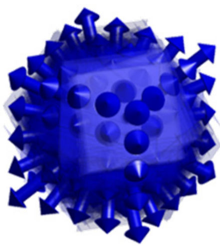
20

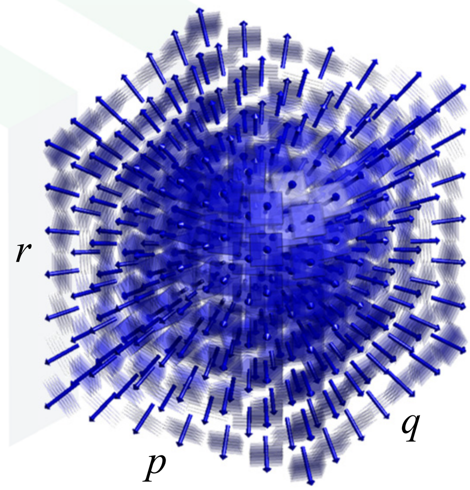
Visualizing Maxwell's Equations in Fourier Space

In real-space, the field values are known at discrete points.

In Fourier-space, amplitudes are known of discrete plane waves.

A less clear, but more accurate picture is when all the plane waves overlap.





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Slide 21

21

Matrix Form of Maxwell's Equations in Fourier Space

Slide 22

22

Conversion to Matrix Form

The following equation is written once for each spatial harmonic.

$$k_y(p,q,r)U_z(p,q,r)-k_z(p,q,r)U_y(p,q,r)=jk_0\sum_{p'=-\infty}^{\infty}\sum_{q'=-\infty}^{\infty}\sum_{r'=-\infty}^{\infty}a(p-p',q-q',r-r')S_x(p',q',r')$$

total # spatial harmonics = $P\cdot Q\cdot R$

This large set of equations can be written in matrix form as

$$\mathbf{K}_y\mathbf{u}_z-\mathbf{K}_z\mathbf{u}_y=jk_0[\![\varepsilon_\mathrm{r}]\!]\mathbf{s}_x$$

$$\mathbf{K}_i=\begin{bmatrix} k_i(1,1,1) & & & 0 \\ & k_i(1,1,2) & & \\ & & \ddots & \\ 0 & & & k_i(P,Q,R)\end{bmatrix}$$

The $\mathbf{K}$ terms are diagonal matrices containing all the wave vector components along its center diagonal.

Only Toeplitz for 1D

$$[\![\varepsilon_\mathrm{r}]\!]=\begin{bmatrix}\text{Toeplitz}\end{bmatrix}$$

Convolution matrix

$$\mathbf{u}_i=\begin{bmatrix}U_i(1,1,1)\\U_i(1,1,2)\\\vdots\\U_i(P,Q,R)\end{bmatrix}\qquad \mathbf{s}_i=\begin{bmatrix}S_i(1,1,1)\\S_i(1,1,2)\\\vdots\\S_i(P,Q,R)\end{bmatrix}$$

$\mathbf{u}_i$ and $\mathbf{s}_i$ are column vectors containing the amplitudes of each spatial harmonic in the expansion.

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Slide 23

23

Matrix Form of Maxwell's Equations in Fourier Space

Analytical Equations

$$k_y(p,q,r)U_z(p,q,r)-k_z(p,q,r)U_y(p,q,r)=jk_0a(p,q,r)*S_x(p,q,r)$$
$$k_z(p,q,r)U_x(p,q,r)-k_x(p,q,r)U_z(p,q,r)=jk_0a(p,q,r)*S_y(p,q,r)$$
$$k_x(p,q,r)U_y(p,q,r)-k_y(p,q,r)U_x(p,q,r)=jk_0a(p,q,r)*S_z(p,q,r)$$

$$k_y(p,q,r)S_z(p,q,r)-k_z(p,q,r)S_y(p,q,r)=jk_0b(p,q,r)*U_x(p,q,r)$$
$$k_z(p,q,r)S_x(p,q,r)-k_x(p,q,r)S_z(p,q,r)=jk_0b(p,q,r)*U_y(p,q,r)$$
$$k_x(p,q,r)S_y(p,q,r)-k_y(p,q,r)S_x(p,q,r)=jk_0b(p,q,r)*U_z(p,q,r)$$

Matrix Equations

$$\mathbf{K}_y\mathbf{u}_z-\mathbf{K}_z\mathbf{u}_y=jk_0[\![\varepsilon_\mathrm{r}]\!]\mathbf{s}_x$$
$$\mathbf{K}_z\mathbf{u}_x-\mathbf{K}_x\mathbf{u}_z=jk_0[\![\varepsilon_\mathrm{r}]\!]\mathbf{s}_y$$
$$\mathbf{K}_x\mathbf{u}_y-\mathbf{K}_y\mathbf{u}_x=jk_0[\![\varepsilon_\mathrm{r}]\!]\mathbf{s}_z$$

$$\mathbf{K}_y\mathbf{s}_z-\mathbf{K}_z\mathbf{s}_y=jk_0[\![\mu_\mathrm{r}]\!]\mathbf{u}_x$$
$$\mathbf{K}_z\mathbf{s}_x-\mathbf{K}_x\mathbf{s}_z=jk_0[\![\mu_\mathrm{r}]\!]\mathbf{u}_y$$
$$\mathbf{K}_x\mathbf{s}_y-\mathbf{K}_y\mathbf{s}_x=jk_0[\![\mu_\mathrm{r}]\!]\mathbf{u}_z$$

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Slide 24

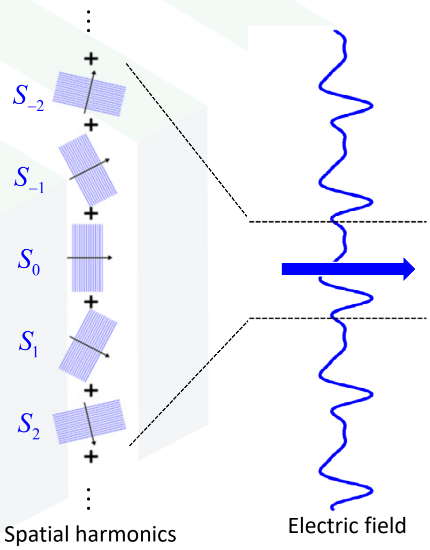
24

Interpreting the Column Vectors

Each element of the column vector $\mathbf{u}_i$ is the complex amplitude of a spatial harmonic.

$$\mathbf{s}_i = \begin{bmatrix} \vdots \\ S_{-2} \\ S_{-1} \\ S_0 \\ S_1 \\ S_2 \\ \vdots \end{bmatrix}$$

Column vector



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Slide 25

25

Constructing the Convolution Matrices

Slide 26

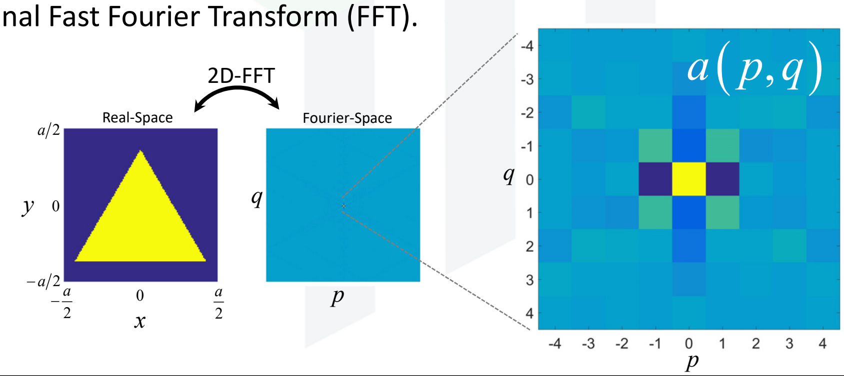
26

Calculating the Fourier Coefficients

The Fourier coefficients are calculated by solving the following equation for every combination of values of p, q, and r.

$$a(p,q,r)=\frac{1}{V}\iiint_{V}\varepsilon_{\mathrm{r}}(\vec{r})\,e^{-j\left(p\vec{T}_1+q\vec{T}_2+r\vec{T}_3\right)\bullet\vec{r}}\,dV$$

Instead of using the above equation, the Fourier coefficients are easily calculated using a multi-dimensional Fast Fourier Transform (FFT).



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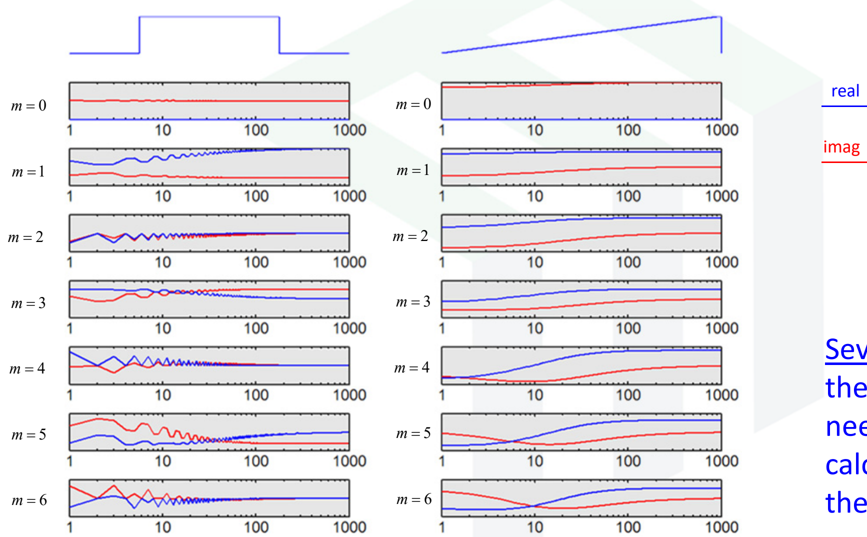
Slide 27

27

How Many Points Are Needed on the Real-Space Grid?



Several hundred points on the real-space grid are needed n order to accurately calculate the coefficients of the Fourier series.

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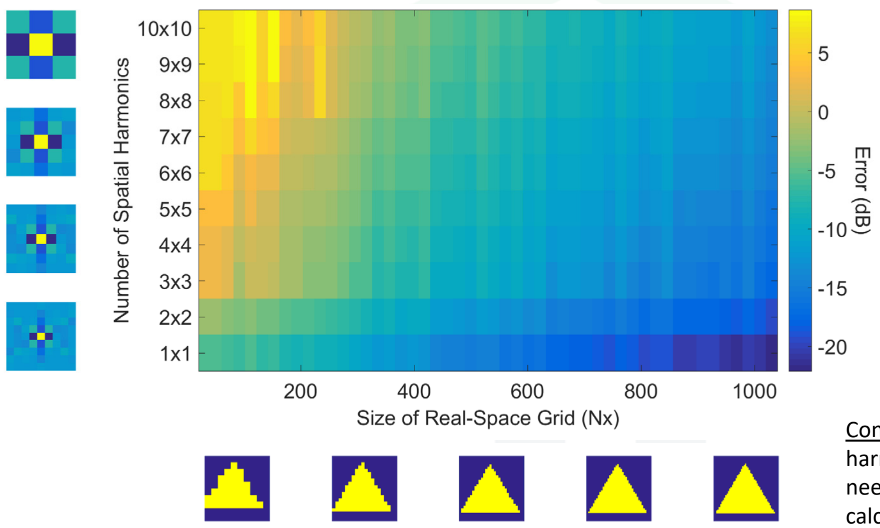
Slide 28

28

Convergence of Fourier Coefficients for 2D Functions



Conclusion: when using more spatial harmonics, even more points are needed on the high-resolution grid to calculate accurate Fourier coefficients.

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29

The Convolution Matrix

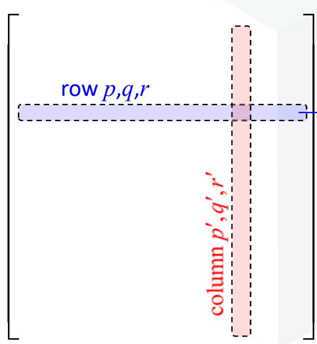
There are two matrices that must be constructed that perform a 3D convolution in Fourier space.

$$[\![\mu_{\mathrm{r}}]\!] \text{ and } [\![\varepsilon_{\mathrm{r}}]\!]$$

Don't confuse these for μ_r and ε_r used in FDFD that were diagonal point-by-point multiplication matrices. $[\![\mu_r]\!]$ and $[\![\varepsilon_r]\!]$ are full convolution matrices.

The convolution matrices are constructed with the following picture in mind.

$$[\![\varepsilon_{\mathrm{r}}]\!] =$$



$$\sum_{p'=-\infty}^{\infty} \sum_{q'=-\infty}^{\infty} \sum_{r'=-\infty}^{\infty} a(p-p',q-q',r-r') S_x(p',q',r')$$

$$m_{\mathrm{row}} = (r'-1)PQ + (q'-1)P + p'$$

Constructing a convolution matrix is as simple as placing the Fourier coefficients in the proper location in each row in the matrix.

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30

Header for MATLAB Code to Construct Convolution Matrices

The following slides will step you through the procedure to write a MATLAB code that calculates convolution matrices for 1D, 2D, or 3D problems. To handle an arbitrary number of dimensions, the header should look like…

```
function C = convmat(A,P,Q,R)
% CONVMAT       Rectangular Convolution Matrix
%
% C = convmat(A,P);              for 1D problems
% C = convmat(A,P,Q);            for 2D problems
% C = convmat(A,P,Q,R);          for 3D problems
%
% This MATLAB function constructs convolution matrices
% from a real-space grid.

%% HANDLE INPUT AND OUTPUT ARGUMENTS

% DETERMINE SIZE OF A
[Nx,Ny,Nz] = size(A);

% HANDLE NUMBER OF HARMONICS FOR ALL DIMENSIONS
if nargin==2
    Q = 1;
    R = 1;
elseif nargin==3
    R = 1;
end
```

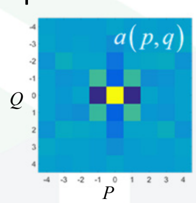
This lets us treat all cases as if they were 3D.

P is the number of spatial harmonics along $\vec{T}_1$.
Q is the number of spatial harmonics along $\vec{T}_2$.
R is the number of spatial harmonics along $\vec{T}_3$.

Step 1: Calculate the Fourier Coefficients

Begin by calculating 1D arrays of the indices of the spatial harmonics, centered at 0.

```
% COMPUTE INDICES OF SPATIAL HARMONICS
NH = P*Q*R;                         %total number
p  = [-floor(P/2):+floor(P/2)];     %indices along T1
q  = [-floor(Q/2):+floor(Q/2)];     %indices along T2
r  = [-floor(R/2):+floor(R/2)];     %indices along T3
```



$P \equiv$ number of spatial harmonics along $\vec{T}_1$
$Q \equiv$ number of spatial harmonics along $\vec{T}_2$
$R \equiv$ number of spatial harmonics along $\vec{T}_3$

Then the Fourier coefficients are calculated using an n-dimensional FFT.

```
% COMPUTE FOURIER COEFFICIENTS OF A
A = fftshift(fftn(A)) / (Nx*Ny*Nz);
```

Calculate the position of the zero-order harmonic in the array `A`. Knowing this, all others can be found because they are centered around the zero-order harmonic.

```
% COMPUTE ARRAY INDICES OF CENTER HARMONIC
p0 = 1 + floor(Nx/2);
q0 = 1 + floor(Ny/2);
r0 = 1 + floor(Nz/2);
```

These equations are valid for both odd and even values of `Nx`, `Ny`, and `Nz`.

Step 2: Initialize Convolution Matrix

The `convmat()` function will run very slow if the convolution matrix is not first initialized.

```
% INITIALIZE CONVOLUTION MATRIX
C = zeros(NH,NH);
```

$$[\![\varepsilon_{\mathrm{r}}]\!] = \begin{bmatrix} 0 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{bmatrix}$$

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Slide 33

33

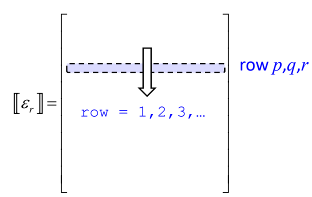
Step 3: Loop Through the Rows

With the picture in mind of filling in rows, it makes sense to start by creating a loop that steps through each row of the convolution matrix.

```
for rrow = 1 : R
for qrow = 1 : Q
for prow = 1 : P
    row = (rrow-1)*Q*P + (qrow-1)*P + prow;

•
•
•

end
end
end
```



$P \equiv$ number of spatial harmonics along $\vec{T}_1$

$Q \equiv$ number of spatial harmonics along $\vec{T}_2$

$R \equiv$ number of spatial harmonics along $\vec{T}_3$

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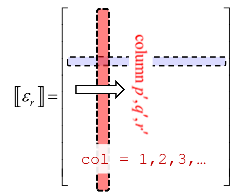
Slide 34

34

Step 4: Loop Through the Columns

Now step from left to right within the current row by looping through the columns.



$P \equiv$ number of spatial harmonics along $\vec{T}_1$

$Q \equiv$ number of spatial harmonics along $\vec{T}_2$

$R \equiv$ number of spatial harmonics along $\vec{T}_3$

```
for rrow = 1 : R
for qrow = 1 : Q
for prow = 1 : P
    row = (rrow-1)*Q*P + (qrow-1)*P + prow;
    for rcol = 1 : R
    for qcol = 1 : Q
    for pcol = 1 : P
        col = (rcol-1)*Q*P + (qcol-1)*P + pcol;
        •
        •
        •

    end
    end
    end
end
end
end
```

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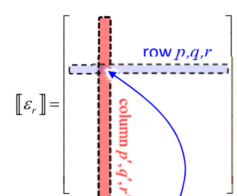
35

Step 5: Calculate Where to Get Value from FFT

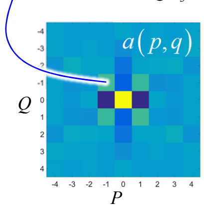
Determine which Fourier coefficient to place into `C(row,col)`. To figure this out, refer to the triple summation that defines the convolution.



$P \equiv$ number of spatial harmonics along $\vec{T}_1$

$Q \equiv$ number of spatial harmonics along $\vec{T}_2$

$R \equiv$ number of spatial harmonics along $\vec{T}_3$




```
for rrow = 1 : R
for qrow = 1 : Q
for prow = 1 : P
    row = (rrow-1)*Q*P + (qrow-1)*P + prow;
    for rcol = 1 : R
    for qcol = 1 : Q
    for pcol = 1 : P
        col = (rcol-1)*Q*P + (qcol-1)*P + pcol;
        pfft = p(prow) - p(pcol);
        qfft = q(qrow) - q(qcol);
        rfft = r(rrow) - r(rcol);
        •
    end
    end
    end
end
end
end
```

$\rightarrow a_{\text{pfft},\text{qfft},\text{rfft},}$

$$\sum_{p'=-P/2}^{P/2}\sum_{q'=-Q/2}^{Q/2}\sum_{r'=-R/2}^{R/2} a(p-p',q-q',r-r')S_x(p',q',r')$$

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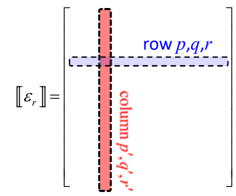
36

Step 6: Fill in Element of Convolution Matrix

Last, the Fourier coefficient from the n-FFT is copied into the convolution matrix at element (`row,col`).



$P \equiv$ number of spatial harmonics along $\vec{T}_1$

$Q \equiv$ number of spatial harmonics along $\vec{T}_2$

$R \equiv$ number of spatial harmonics along $\vec{T}_3$

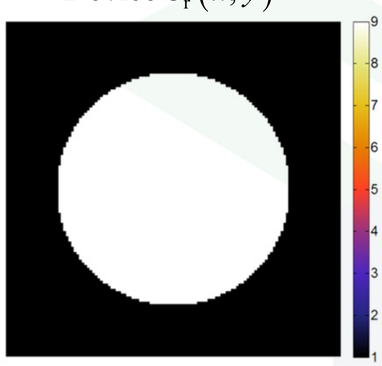
```
for rrow = 1 : R
for qrow = 1 : Q
for prow = 1 : P
    row = (rrow-1)*Q*P + (qrow-1)*P + prow;
    for rcol = 1 : R
    for qcol = 1 : Q
    for pcol = 1 : P
        col = (rcol-1)*Q*P + (qcol-1)*P + pcol;
        pfft = p(prow) - p(pcol);
        qfft = q(qrow) - q(qcol);
        rfft = r(rrow) - r(rcol);
        C(row,col) = A(p0+pfft,q0+qfft,r0+rfft);
    end
    end
    end
end
end
end
```

The offsets to the zero-order harmonic have been included here.

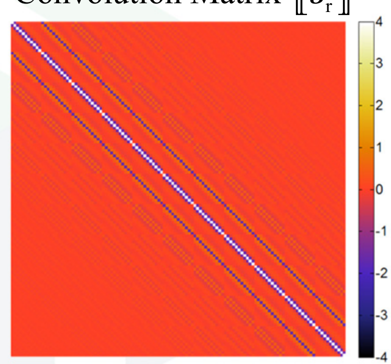
`pfft = qfft = rfft = 0` needs to access the zero-order harmonic located at `p0`, `q0`, `r0`.

What Does a Convolution Matrix Look Like?

Device $\varepsilon_{\mathrm{r}}(x,y)$



Convolution Matrix $[\![\varepsilon_{\mathrm{r}}]\!]$



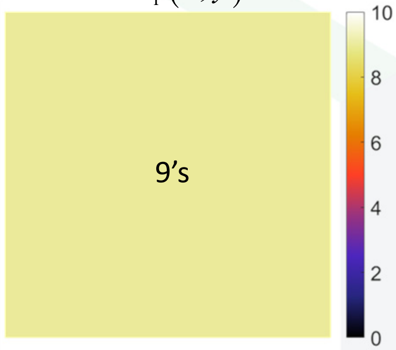
High Resolution Grid
- Must be on a very high resolution grid to calculate accurate Fourier coefficients.

Convolution Matrix
- Full matrix
- Numbers tend smaller with distance from the center diagonal.

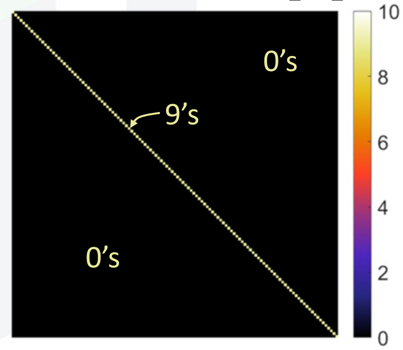
Convolution Matrices for Homogeneous Media

The convolution matrix for a homogeneous material is simply a diagonal matrix with the diagonals all set to ε_r.

Device $\varepsilon_r(x,y) = 9.0$



Convolution Matrix $[\![\varepsilon_r]\!]$



$$[\![\varepsilon_r]\!] = \varepsilon_r \mathbf{I}$$

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Slide 39

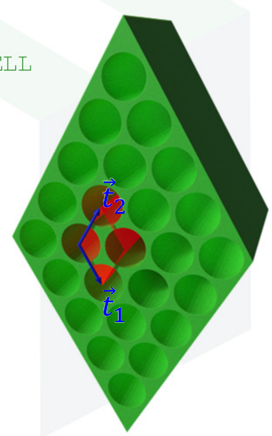
39

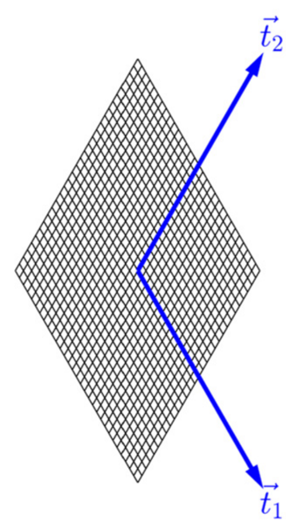
Oblique Symmetry (1 of 3)

Step 1 – Create Oblique Meshgrid

```
% LATTICE VECTORS FOR HEXAGONAL UNIT CELL
t1 = [ a/2 ; -a*sqrt(3)/2 ];
t2 = [ a/2 ; +a*sqrt(3)/2 ];

% BUILD OBLIQUE MESHGRID
p = linspace(-0.5,0.5,N1);
q = linspace(-0.5,0.5,N2);
[Q,P] = meshgrid(q,p);
XO = P*t1(1) + Q*t2(1);
YO = P*t1(2) + Q*t2(2);
```





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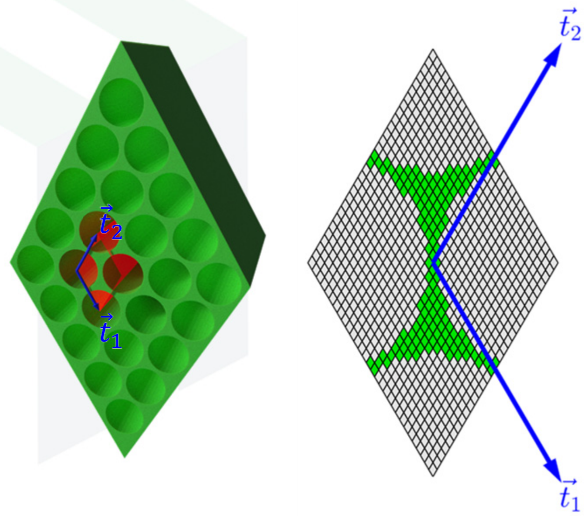
Slide 40

40

Oblique Symmetry (2 of 3)

Step 2 – Build Unit Cell

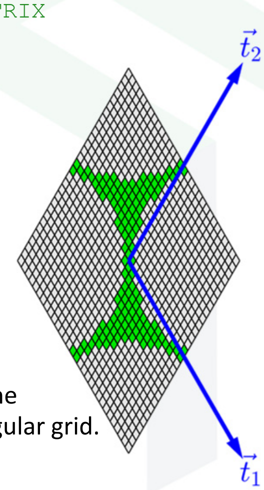
```
% BUILD HEXAGONAL UNIT CELL
b   = sqrt(3)*a;
RSQ = XO.^2 + (YO - b/2).^2;
ER  = (RSQ <= r^2);
RSQ = XO.^2 + (YO + b/2).^2;
ER  = ER | (RSQ <= r^2);
RSQ = (XO - a/2).^2 + YO.^2;
ER  = ER | (RSQ <= r^2);
RSQ = (XO + a/2).^2 + YO.^2;
ER  = ER | (RSQ <= r^2);

% CONVERT TO REAL MATERIALS
ER = 1 - ER;
ER = 1 + (er - 1)*ER;
```



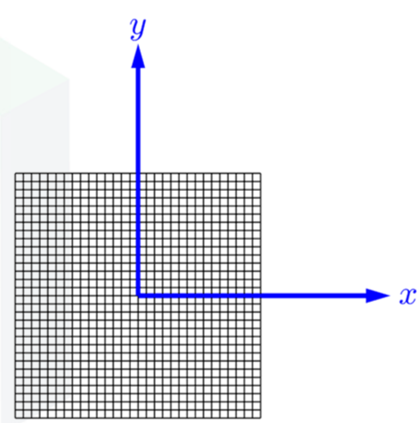
Oblique Symmetry (3 of 3)

Step 3 – Call `convmat()`

```
% BUILD CONVOLUTION MATRIX
ERC = convmat(ER,P,Q);
```



The FFT “sort of” sees the oblique grid as a rectangular grid.



Notes

- You now have a very powerful code!
- Most of the tediousness of Fourier space methods are absorbed into the convolution matrices.
- It is able to construct 1D, 2D, and 3D convolution matrices without changing anything.
  - For 1D devices: $P \geq 1$, $Q=1$, $R=1$
  - For 2D devices: $P \geq 1$, $Q \geq 1$, $R=1$
  - For 3D devices: $P \geq 1$, $Q \geq 1$, $R \geq 1$
- The `convmat()` function can be used for any photonic crystal symmetry without modification.
- Convolution matrices for homogeneous materials are diagonal with the form $[\![\varepsilon_{\mathrm{r}}]\!] = \varepsilon_{\mathrm{r}}\mathbf{I}$.
- Uniform directions require only one spatial harmonic.

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Slide 43

43

Fast Fourier Factorization (FFF)

Slide 44

44

Product of Two Functions

Consider the product of two periodic functions that have the same period:

$$f(x) \cdot g(x) = h(x)$$

Expand each function into its own Fourier series.

$$\left(\sum_{m=-\infty}^{\infty} a_m e^{j\frac{2\pi mx}{\Lambda}} \right) \left(\sum_{m=-\infty}^{\infty} b_m e^{j\frac{2\pi mx}{\Lambda}} \right) = \sum_{m=-\infty}^{\infty} c_m e^{j\frac{2\pi mx}{\Lambda}}$$

This is exact, as long as an infinite number of terms is used.

Obviously, only a finite number of terms can be retained in the expansion if it is to be solved on a computer.

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Slide 45

45

Finite Number of Terms

To describe devices on a computer, only a finite number of terms can be retained in the expansions.

$$\left(\sum_{m=-M}^{M} a_m e^{j\frac{2\pi mx}{\Lambda}} \right) \left(\sum_{m=-M}^{M} b_m e^{j\frac{2\pi mx}{\Lambda}} \right) = \sum_{m=-M}^{M} c_m e^{j\frac{2\pi mx}{\Lambda}}$$

Problem: In certain circumstances, the left side of the equation converges slower than the right. That is, more terms are needed for a given level of "accuracy."

There are four special cases for $f(x) \cdot g(x) = h(x)$:

1. $f(x)$ and $g(x)$ are continuous everywhere.
2. Either $f(x)$ or $g(x)$ has a step discontinuity, but not both at the same point.

No problem

3. Both $f(x)$ and $g(x)$ have a step discontinuity at the same point, but their product is continuous.

Problem is fixable

4. Both $f(x)$ and $g(x)$ have a step discontinuity at the same point and their product is also discontinuous.

Problem is NOT fixable

When only a finite-number of terms are retained, cases 3 and 4 exhibit slow convergence. Only case 3 is fixable.

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Slide 46

46

The Fix for Case 3

The product of two functions can be written in Fourier space.

$$f \cdot g = h \quad \rightarrow \quad [\![F]\!][G] = [H]$$

For Case 3, both $f(x)$ and $g(x)$ are have a step discontinuity at the same point, but their product $f(x)g(x)=h(x)$ is continuous. To handle this case, $f(x)$ is brought to the right-hand side of the equation.

$$g = \frac{1}{f} \cdot h \quad \rightarrow \quad [G] = \left[\!\!\left[\frac{1}{F}\right]\!\!\right][H]$$

Now, there are no problems with this new equation because both sides of the equation are Case 2. Now the convolution matrix is brought back to left side of the equation.

$$\left(\frac{1}{f}\right)^{-1} \cdot g = h \quad \rightarrow \quad \left[\!\!\left[\frac{1}{F}\right]\!\!\right]^{-1} [G] = [H]$$

This is FFF!

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Slide 47

47

FFF and Maxwell's Equations

In Maxwell's equations, there exists a product of two functions…

$$\varepsilon_{\mathrm{r}}(\vec{r}) \cdot \vec{E}(\vec{r})$$

The dielectric function is discontinuous at the interface between two materials. Boundary conditions require that

$$E_{1,\|} = E_{2,\|}$$

Tangential component is continuous across the interface

$$\varepsilon_1 E_{1,\perp} = \varepsilon_2 E_{2,\perp}$$

Normal component is continuous across the interface, but the product of $\varepsilon E_{\perp}$ is continuous.

In conclusion, the convolution matrix must be handled differently for the tangential and normal components. This implies that the final convolution matrix will be a tensor.

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Slide 48

48

FFF for Maxwell's Equations

First, the electric field is decomposed into tangential and normal components at all interfaces.

$$[\![\varepsilon_{\mathrm{r}}]\!]\mathbf{s} = [\![\varepsilon_{\mathrm{r}}]\!]\left[\mathbf{s}_{\|} + \mathbf{s}_{\perp}\right] = [\![\varepsilon_{\mathrm{r}}]\!]\mathbf{s}_{\|} + [\![\varepsilon_{\mathrm{r}}]\!]\mathbf{s}_{\perp}$$

This creates the opportunity to associate different convolution matrices with the different field components.

$$[\![\varepsilon_{\mathrm{r}}]\!]\mathbf{s} \rightarrow \underbrace{[\![\varepsilon_{\mathrm{r},\|}]\!]\mathbf{s}_{\|}}_{\substack{\text{Case 2.}\\ \text{No problems.}}} + \underbrace{[\![\varepsilon_{\mathrm{r},\perp}]\!]\mathbf{s}_{\perp}}_{\substack{\text{Case 3.}\\ \text{Fixable with FFF.}}}$$

$$[\![\varepsilon_{\mathrm{r}}]\!]_{\mathrm{FFF}}\,\mathbf{s} = [\![\varepsilon_{\mathrm{r},\|}]\!]\mathbf{s}_{\|} + [\![1/\varepsilon_{\mathrm{r},\perp}]\!]^{-1}\mathbf{s}_{\perp}$$

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Slide 49

49

Normal Vector Field

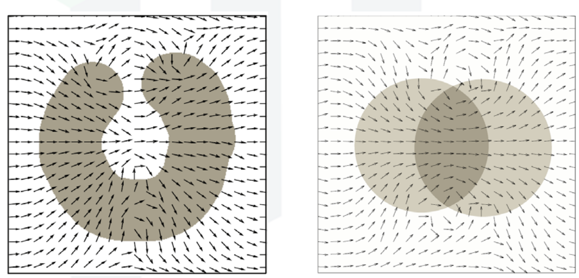
To implement FFF, which directions are parallel and perpendicular must be determined at each point in space.

For arbitrarily shaped devices, this comes from knowledge of the materials within the layer.

A vector function must be constructed throughout the grid that is normal to all the interfaces. This called the "normal vector" field.

$$\hat{n}(x, y, z)$$

This can be very difficult to calculate!!



P. Gotz, T. Schuster, K. Frenner, S. Rafler, W. Osten, "Normal vector method for the RCWA with automated vector field generation," Opt. Express 16(22), 17295-17301 (2008).

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Slide 50

50

Incorporating Normal Vector Function

Recall the FFF fix

$$[\![\varepsilon_{\mathrm{r}}]\!]_{\mathrm{FFF}}\,\mathbf{s} = [\![\varepsilon_{\mathrm{r}}]\!]\mathbf{s}_{\parallel} + [\![1/\varepsilon_{\mathrm{r}}]\!]^{-1}\mathbf{s}_{\perp}$$

The parallel and perpendicular components of $\mathbf{s}$ can be calculated using the normal vector matrix $\mathbf{N}$.

$$\mathbf{s}_{\perp} = \mathbf{N}\mathbf{s}$$

$$\mathbf{s}_{\parallel} = \mathbf{s} - \mathbf{N}\mathbf{s} = (\mathbf{I}-\mathbf{N})\mathbf{s}$$

Substituting these into the FFF equation yields

$$\begin{aligned}
[\![\varepsilon_{\mathrm{r}}]\!]_{\mathrm{FFF}}\,\mathbf{s} &= [\![\varepsilon_{\mathrm{r}}]\!](\mathbf{I}-\mathbf{N})\mathbf{s} + [\![1/\varepsilon_{\mathrm{r}}]\!]^{-1}\mathbf{N}\mathbf{s} \\
&= [\![\varepsilon_{\mathrm{r}}]\!]\mathbf{s} - [\![\varepsilon_{\mathrm{r}}]\!]\mathbf{N}\mathbf{s} + [\![1/\varepsilon_{\mathrm{r}}]\!]^{-1}\mathbf{N}\mathbf{s} \\
&= \underbrace{\left([\![\varepsilon_{\mathrm{r}}]\!] - [\![\varepsilon_{\mathrm{r}}]\!]\mathbf{N} + [\![1/\varepsilon_{\mathrm{r}}]\!]^{-1}\mathbf{N}\right)}\mathbf{s}
\end{aligned}$$

This defines a new convolution matrix that incorporates FFF.

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Slide 51

51

Revised Convolution Matrix

The convolution matrix incorporating FFF is then

$$\begin{aligned}
[\![\varepsilon_{\mathrm{r}}]\!]_{\mathrm{FFF}} &= [\![\varepsilon_{\mathrm{r}}]\!] - [\![\varepsilon_{\mathrm{r}}]\!]\mathbf{N} + [\![1/\varepsilon_{\mathrm{r}}]\!]^{-1}\mathbf{N} \\
&= [\![\varepsilon_{\mathrm{r}}]\!] + \left([\![1/\varepsilon_{\mathrm{r}}]\!]^{-1} - [\![\varepsilon_{\mathrm{r}}]\!]\right)\mathbf{N}
\end{aligned}$$

This is often written as

$$[\![\varepsilon_{\mathrm{r}}]\!]_{\mathrm{FFF}} = [\![\varepsilon_{\mathrm{r}}]\!] + \underbrace{[\![\Delta\varepsilon_{\mathrm{r}}]\!]\mathbf{N}}_{\text{This is interpreted as a correction term that incorporates FFF.}} \qquad [\![\Delta\varepsilon_{\mathrm{r}}]\!] = [\![1/\varepsilon_{\mathrm{r}}]\!]^{-1} - [\![\varepsilon_{\mathrm{r}}]\!]$$

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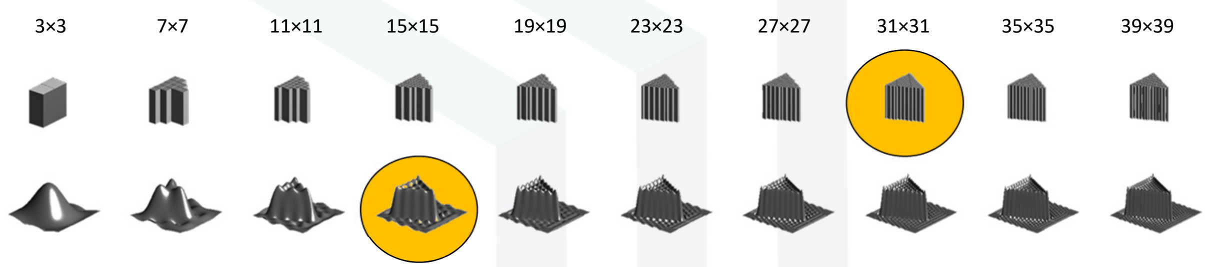
Slide 52

52

Consequences of Fourier-Space

Efficient Representation of Devices

Along a given direction, approximately half the number of the terms are needed in Fourier space than would be needed in real space.



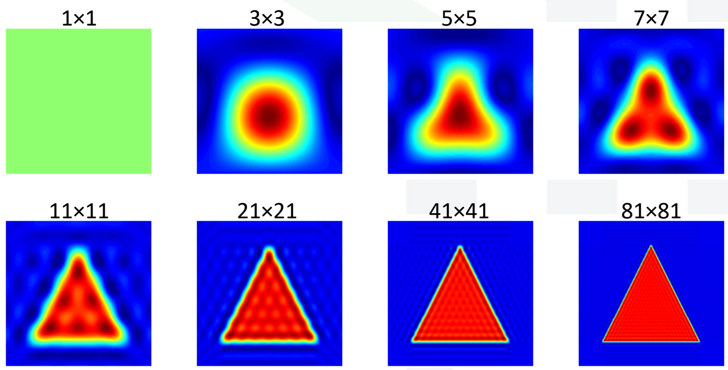
For 2D problems in real space, 4× more terms are needed making the matrices 16× larger.

For 3D problems in real space, 8× more terms are needed making the matrices 64× larger.

Blurring from Too Few Harmonics

If too few harmonics are used, the geometry of the device is blurred.

- Boundaries are artificially blurred.
- Reflections at boundaries are artificially reduced.
- It is difficult or impossible to resolve fine features or rapidly varying fields.



Rule of Thumb: # harmonics = 10 per λ

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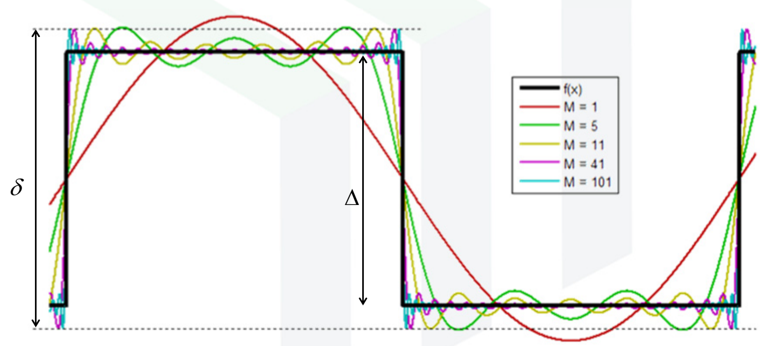
Slide 55

55

Gibb's Phenomena

A problem occurs when a discontinuous function (material interface) is represented by continuous basis functions (sin's and cos's). When the Fourier transform is used, "spikes" appear around each discontinuity. Fourier space methods act is if those spikes are actually present.



http://mathworld.wolfram.com/GibbsPhenomenon.html

$$\frac{\delta}{\Delta} = \frac{2}{\pi}\int_0^{\pi} \frac{\sin x}{x}\,dx \cong 1.1789797445$$

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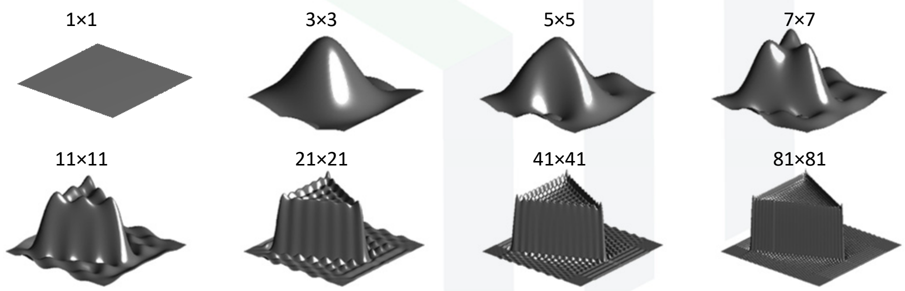
Slide 56

56

Gibb’s Phenomena in Maxwell’s Equations

A Fourier-space numerical method treats the spikes as if they are real.

- The magnitude of the spikes remains constant no matter how many harmonics are used.
- The magnitude of the spikes is proportional to the severity of the discontinuity.
- The width of the spikes becomes more narrow with increasing number of harmonics.
- In Fourier-space, Maxwell’s equations really think the spikes are there.



Due to Gibb’s phenomenon, Fourier-space analysis is most efficient for structures with low to moderate index contrast, but many people have modeled metals effectively.

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Slide 57

57