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EE 5337

Computational Electromagnetics

Lecture #18

Maxwell's Equations in Fourier Space

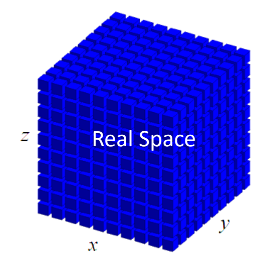
Outline

- 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

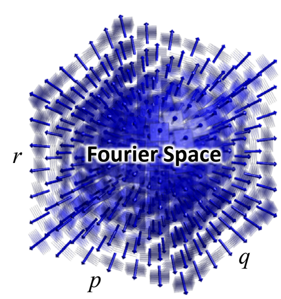
Maxwell's Equations in Fourier Space

What is Fourier Space?

Real Space
So far, we have been representing fields and devices on an x-y-z grid where field values are known at discrete points.



Fourier Space
In Fourier-space, we represent fields as a sum of plane waves at different angles and wavelengths called *spatial harmonics*. We will represent devices as the sum of sinusoidal gratings at different angles and periods.



Fourier-Space Vs. Frequency-Domain

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

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

We Fourier transform t to ω.

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

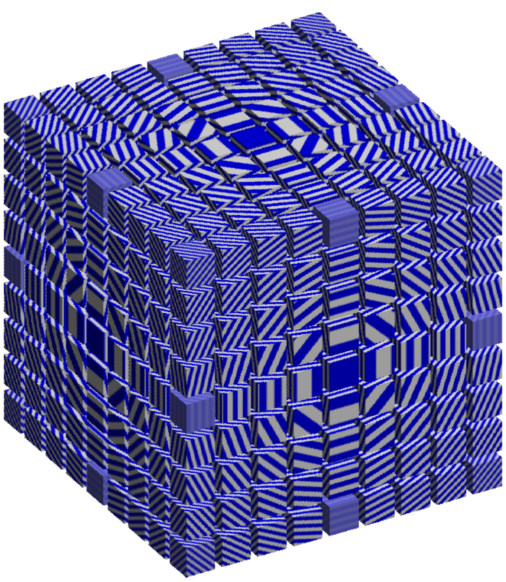
Fourier Space

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

Frequency Domain

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

Visualizing the Spatial Harmonics



$$\vec{k}(p,q,r) = k_x(p)\hat{x} + k_y(q)\hat{y} + k_z(r)\hat{z}$$

$$k_x(p) = \frac{2\pi p}{\Lambda_x} \qquad p \equiv \text{integer}$$

$$k_y(q) = \frac{2\pi q}{\Lambda_y} \qquad q \equiv \text{integer}$$

$$k_z(r) = \frac{2\pi r}{\Lambda_z} \qquad r \equiv \text{integer}$$

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

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

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

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

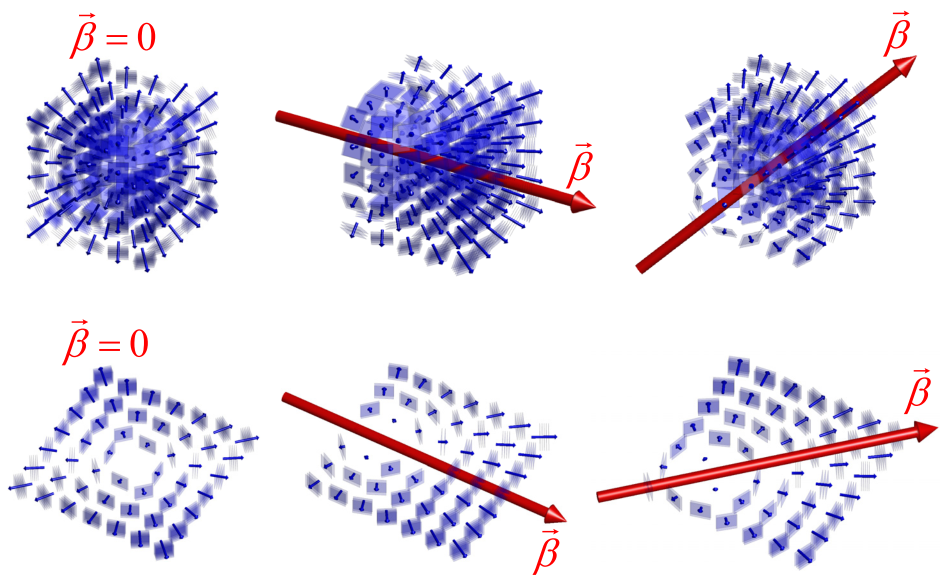
For 3D periodic functions, this is

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

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

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

Visualizing Expansions with Different $\vec{\beta}$s



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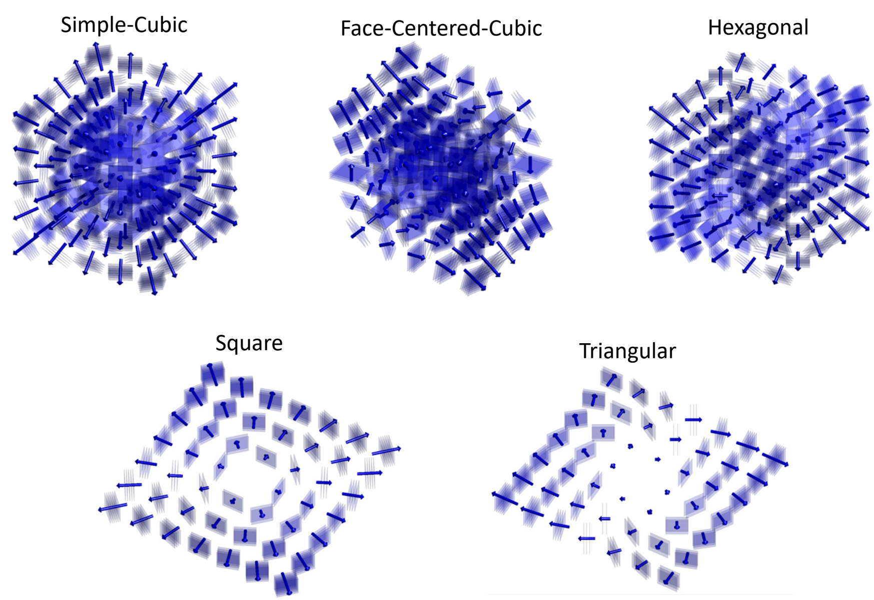
Visualizing Expansions with Different Symmetries



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Starting Point

We 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 we normalized the magnetic field according to

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

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Fourier Expansion of the Materials

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

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

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

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Fourier Expansion of the Fields (1 of 2)

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 $\vec{k}_{\text{inc}}$

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

Let this be $\vec{k}(p,q,r)$

$e^{-j\vec{\beta}\bullet\vec{r}}$ 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 $\vec{k}(p,q,r)$.

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

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

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

Fourier Expansion of the Fields (2 of 2)

For cubic, tetragonal, and orthorhombic symmetry, the expansions reduce to

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

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

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

$$\boxed{k_x(p,q,r)} = \boxed{k_x(p)} = \beta_x - \frac{2\pi p}{\Lambda_x} \qquad p = -\infty,\cdots,-2,-1,0,1,2,\cdots,\infty$$

$$\boxed{k_y(p,q,r)} = \boxed{k_y(q)} = \beta_y - \frac{2\pi q}{\Lambda_y} \qquad q = -\infty,\cdots,-2,-1,0,1,2,\cdots,\infty$$

$$\boxed{k_z(p,q,r)} = \boxed{k_z(r)} = \beta_z - \frac{2\pi r}{\Lambda_z} \qquad r = -\infty,\cdots,-2,-1,0,1,2,\cdots,\infty$$

The wave vectors k_x, k_y, and k_z are still distributed over all possible values of p, q, and r. However, their values only change in one direction, which is conveyed by the argument in parentheses.

Think this way for size of arrays.

Think this way for dependence.

Substitute Expansions into Maxwell's Equations

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

$$\varepsilon_r(\vec{r}) = \sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty} a(p,q,r)e^{j\left(\frac{2\pi p}{\Lambda_x}x+\frac{2\pi q}{\Lambda_y}y+\frac{2\pi r}{\Lambda_z}z\right)}$$

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

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

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

$$\frac{\partial}{\partial y}\left[\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty} U_z(p,q,r)e^{-j[k_x(p)x+k_y(q)y+k_z(r)z]}\right] - \frac{\partial}{\partial z}\left[\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty} U_y(p,q,r)e^{-j[k_x(p)x+k_y(q)y+k_z(r)z]}\right]$$
$$= k_0\left[\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty} a(p,q,r)e^{j\left(\frac{2\pi p}{\Lambda_x}x+\frac{2\pi q}{\Lambda_y}y+\frac{2\pi r}{\Lambda_z}z\right)}\right]\left[\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty} S_x(p,q,r)e^{-j[k_x(p)x+k_y(q)y+k_z(r)z]}\right]$$

Algebra for the Left Side Terms

First ugly term…

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

Second ugly term…

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

Algebra for the Right Side Term

Third ugly term…

Here we have the product of two triple summations.

$$\left[\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty} a(p,q,r)e^{j\left(\frac{2\pi p}{\Lambda_x}x+\frac{2\pi q}{\Lambda_y}y+\frac{2\pi r}{\Lambda_z}z\right)}\right]\left[\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty} S_x(p,q,r)e^{-j\left[k_x(p)x+k_y(q)y+k_z(r)z\right]}\right]$$

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, we get

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

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Combine the Terms Inside Summation

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

$$=k_0\left[\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}a(p,q,r)e^{j\left(\frac{2\pi p}{\Lambda_x}x+\frac{2\pi q}{\Lambda_y}y+\frac{2\pi r}{\Lambda_z}z\right)}\right]\left[\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}S_x(p,q,r)e^{-j\left[k_x(p)x+k_y(q)y+k_z(r)z\right]}\right]$$

$$\Downarrow$$

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

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

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

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

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

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

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

$$-jU_z(p,q,r)k_y(q)e^{-j[k_x(p)x+k_y(q)y+k_z(r)z]}+jU_y(p,q,r)k_z(r)e^{-j[k_x(p)x+k_y(q)y+k_z(r)z]}$$
$$=k_0e^{-j[k_x(p)x+k_y(q)y+k_z(r)z]}\sum_{p'=-\infty}^{\infty}\sum_{q'=-\infty}^{\infty}\sum_{r'=-\infty}^{\infty}a(p-p',q-q',r-r')S_x(p',q',r')$$

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

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

Alternate Derivation

We start with

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

Point-by-point multiplication in real-space…

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

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

Our point-by-point multiplication becomes a convolution.

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

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

We now realized that the strange triple summation remaining in our equation is actually 3D convolution in Fourier space!

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

Maxwell's Equations in Fourier Space

Real-Space

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

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

Fourier-Space

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

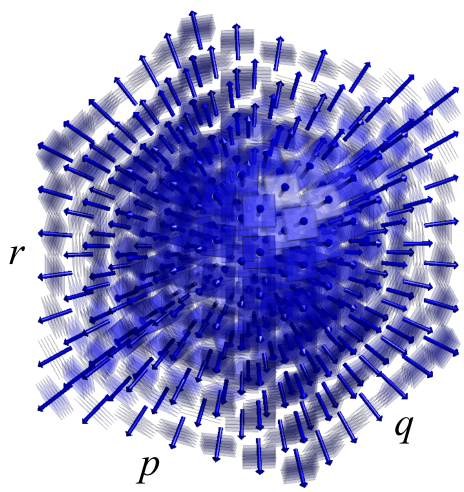
$$k_x(p) = \beta_x - \frac{2\pi p}{\Lambda_x} \qquad p = -\infty, \cdots, -2, -1, 0, 1, 2, \cdots, \infty$$
$$k_y(q) = \beta_y - \frac{2\pi q}{\Lambda_y} \qquad q = -\infty, \cdots, -2, -1, 0, 1, 2, \cdots, \infty$$
$$k_z(r) = \beta_z - \frac{2\pi r}{\Lambda_z} \qquad r = -\infty, \cdots, -2, -1, 0, 1, 2, \cdots, \infty$$

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

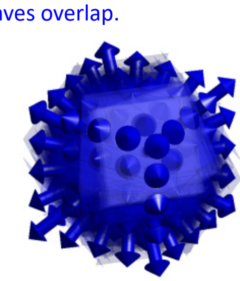
Lecture 18 — Slide 21

Visualizing Maxwell's Equations in Fourier Space

In real-space, we know the field values at discrete points.
In Fourier-space, we know the amplitudes of discrete plane waves.



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



Lecture 18 — Slide 22

Matrix Form of Maxwell's Equations in Fourier Space

Conversion to Matrix Form

The following equation is written once for each spatial harmonic.

$$k_y(q)U_z(p,q,r) - k_z(r)U_y(p,q,r) = jk_0 \sum_{p'=-P/2}^{P/2} \sum_{q'=-Q/2}^{Q/2} \sum_{r'=-R/2}^{R/2} a(p-p',q-q',r-r')S_x(p',q',r')$$

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

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

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

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

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

Only Toeplitz for 1D

$$[\![\varepsilon_r]\!] = \begin{bmatrix} \text{Toeplitz} \end{bmatrix}$$

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.

Matrix Form of Maxwell's Equations in Fourier Space

Analytical Equations

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

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

Numerical Equations

$$\mathbf{K}_y\mathbf{u}_z-\mathbf{K}_z\mathbf{u}_y=jk_0\left[\!\left[\varepsilon_r\right]\!\right]\mathbf{s}_x$$
$$\mathbf{K}_z\mathbf{u}_x-\mathbf{K}_x\mathbf{u}_z=jk_0\left[\!\left[\varepsilon_r\right]\!\right]\mathbf{s}_y$$
$$\mathbf{K}_x\mathbf{u}_y-\mathbf{K}_y\mathbf{u}_x=jk_0\left[\!\left[\varepsilon_r\right]\!\right]\mathbf{s}_z$$

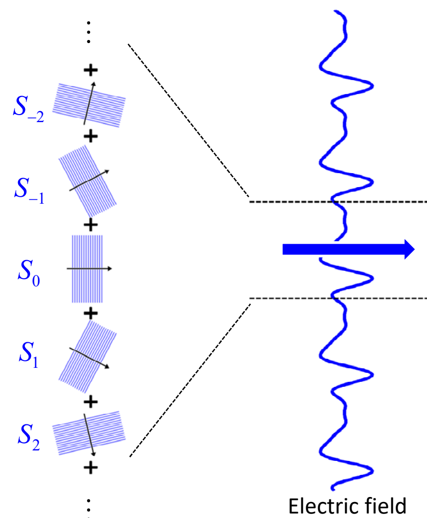
$$\mathbf{K}_y\mathbf{s}_z-\mathbf{K}_z\mathbf{s}_y=jk_0\left[\!\left[\mu_r\right]\!\right]\mathbf{u}_x$$
$$\mathbf{K}_z\mathbf{s}_x-\mathbf{K}_x\mathbf{s}_z=jk_0\left[\!\left[\mu_r\right]\!\right]\mathbf{u}_y$$
$$\mathbf{K}_x\mathbf{s}_y-\mathbf{K}_y\mathbf{s}_x=jk_0\left[\!\left[\mu_r\right]\!\right]\mathbf{u}_z$$

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



Spatial harmonics

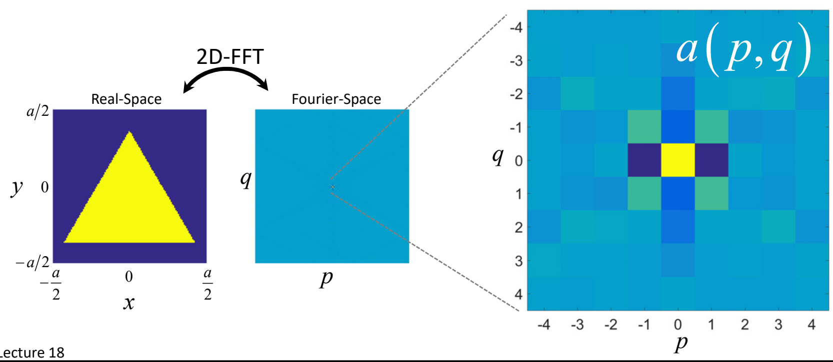
Constructing the Convolution Matrices

Calculating the Fourier Coefficients

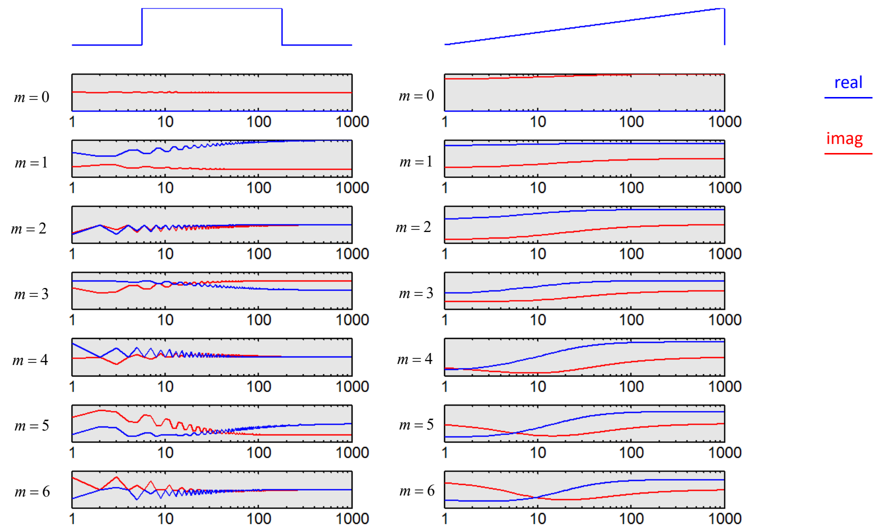
The Fourier coefficients are calculated by solving the following equation for every combination of values of p, q, and r.

$$a(p,q,r)=\frac{1}{V}\iiint_V \varepsilon_r(\vec{r})\,e^{j\left(\frac{2\pi p}{\Lambda_x}x+\frac{2\pi q}{\Lambda_y}y+\frac{2\pi r}{\Lambda_z}z\right)}dV$$

For cubic, tetragonal, and orthorhombic symmetries, these are easily calculated using a multi-dimensional Fast Fourier Transform (FFT).

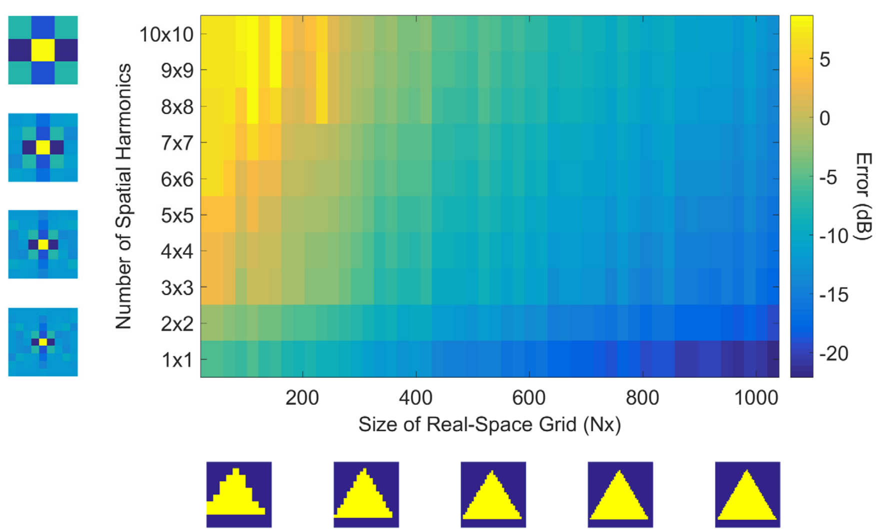


How Many Points Are Needed on the Real-Space Grid?



Several hundred in order to accurately calculate the coefficients of the Fourier series.

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.

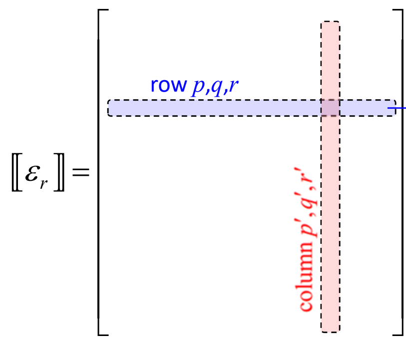
The Convolution Matrix

There are two matrices that we must construct that perform a 3D convolution in Fourier space.

$$[\![\mu_r]\!] \text{ and } [\![\varepsilon_r]\!]$$

Don't confuse these for μ_r and ε_r used in FDFD that were diagonal matrices. These will be full convolution matrices.

We construct these matrices with the following picture in mind.



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

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

Constructing the convolution matrices is as simple as placing the Fourier coefficients in the proper order in each row in the matrix.

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…

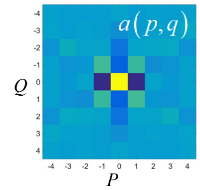
```
function C = convmat(A,P,Q,R)
% CONVMAT       Rectangular Convolution Matrix
%
% C = convmat(A,P);              for 1D problems
% C = convmat(A,P,Q);            for 2D problems
% C = convmat(A,P,Q,R);          for 3D problems
%
% This MATLAB function constructs convolution matrices
% from a real-space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

Step 1: Calculate the Fourier Coefficients

We begin by calculating 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 x
q  = [-floor(Q/2):+floor(Q/2)];       %indices along y
r  = [-floor(R/2):+floor(R/2)];       %indices along z
```



$P \equiv$ number of spatial harmonics along x
$Q \equiv$ number of spatial harmonics along y
$R \equiv$ number of spatial harmonics along z

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

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

We need to 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

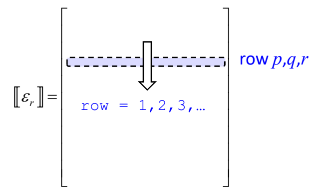
The `convmat()` function will run very slow if the convolution matrix is not first initialized.

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

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

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.



$P \equiv$ number of spatial harmonics along x

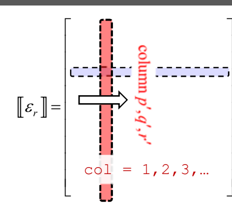
$Q \equiv$ number of spatial harmonics along y

$R \equiv$ number of spatial harmonics along z

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



    •
    •
    •



end
end
end
```


Step 4: Loop Through the Columns

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



$P \equiv$ number of spatial harmonics along x

$Q \equiv$ number of spatial harmonics along y

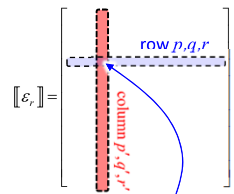
$R \equiv$ number of spatial harmonics along z

```
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
```

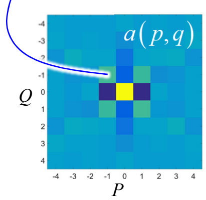
Step 5: Calculate Where to Get Value from FFT

CEM

We need to know which Fourier coefficient to place into C(row,col). To determine this, we refer to the original summation that defined the convolution.



$P \equiv$ number of spatial harmonics along x
$Q \equiv$ number of spatial harmonics along y
$R \equiv$ number of spatial harmonics along z




```
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
```

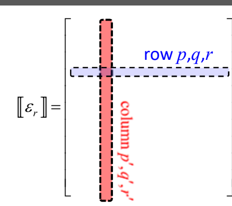
$\rightarrow a_{\text{pfft},\text{qfft},\text{rfft},}$

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

Step 6: Fill in Element of Convolution Matrix

CEM

Last, we copy the Fourier coefficient from the n-FFT into the convolution matrix at element (row,col).



$P \equiv$ number of spatial harmonics along x
$Q \equiv$ number of spatial harmonics along y
$R \equiv$ number of spatial harmonics along z

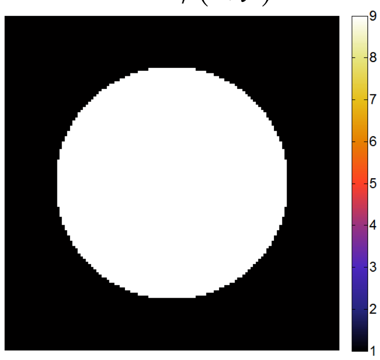
```
for rrow = 1 : R
for qrow = 1 : Q
for prow = 1 : P
    row = (rrow-1)*Q*P + (qrow-1)*P + prow;
    for rcol = 1 : R
    for qcol = 1 : Q
    for pcol = 1 : P
        col = (rcol-1)*Q*P + (qcol-1)*P + pcol;
        pfft = p(prow) - p(pcol);
        qfft = q(qrow) - q(qcol);
        rfft = r(rrow)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

We have included the offsets to the zero-order harmonic.

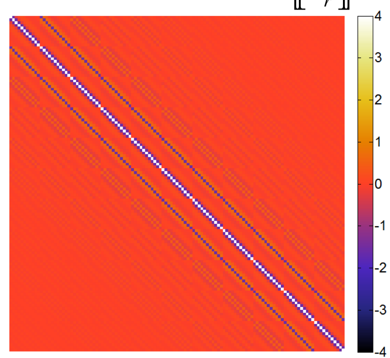
`pfft = qfft = rfft = 0` needs to access the zero-order harmonic located at `p0`, `q0`, `r0`.

What Does a Convolution Matrix Look Like?

Device $\varepsilon_r(x,y)$



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



High Resolution Grid

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

Convolution Matrix

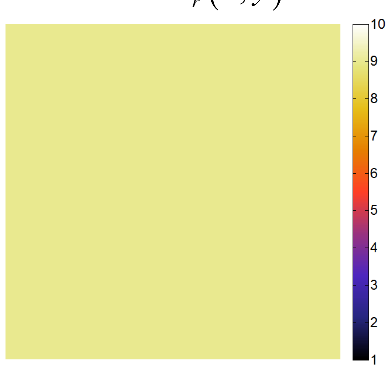
- Full matrix
- Numbers tend smaller with distance from the center diagonal.

Lecture 18 Slide 39

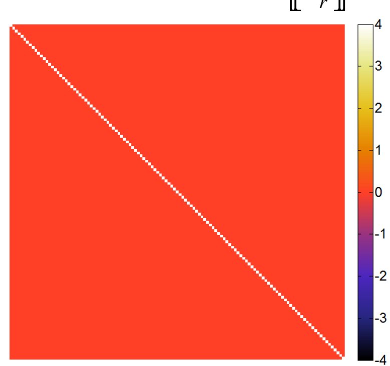
Convolution Matrices for Homogeneous Media

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

Device $\varepsilon_r(x,y)$



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



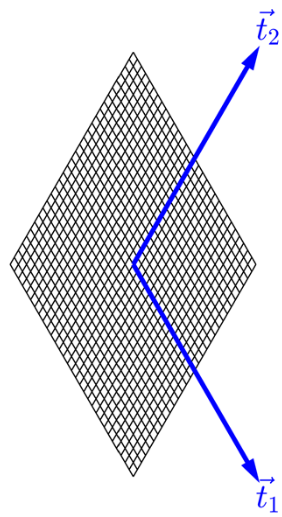
$$[\![\varepsilon_r]\!] = \varepsilon_r \mathbf{I}$$

Lecture 18 Slide 40

Oblique Symmetry (1 of 3)

Step 1 – Create Oblique Meshgrid

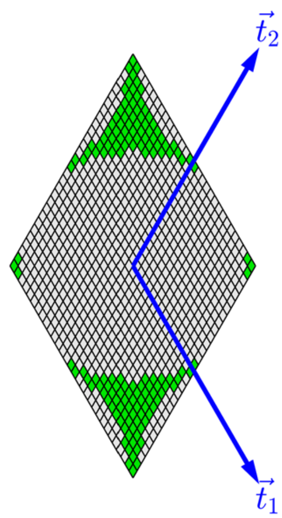
```
% OBLIQUE MESHGRID
p = linspace(-0.5,0.5,Nx);
q = linspace(-0.5,0.5,Nx);
[Q,P] = meshgrid(q,p);
XO = P*t1(1) + Q*t2(1);
YO = P*t1(2) + Q*t2(2);
```



Oblique Symmetry (2 of 3)

Step 2 – Build Unit Cell

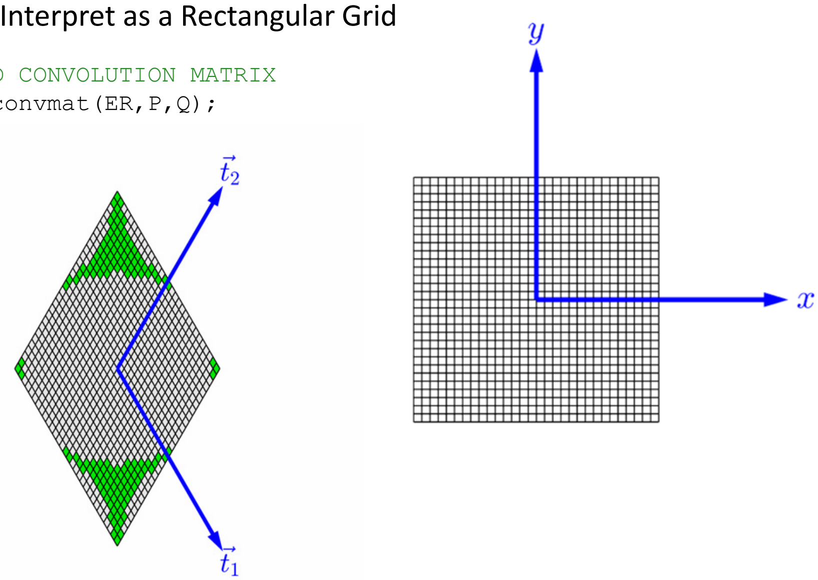
```
% BUILD HEXAGONAL UNIT CELL
RSQ = XO.^2 + YO.^2;
ER  = (RSQ <= rhole^2);
RSQ = (XO - a/2).^2 ...
    + (YO - sqrt(3)*a/2).^2;
ER  = ER | (RSQ <= rhole^2);
RSQ = (XO - a/2).^2 ...
    + (YO + sqrt(3)*a/2).^2;
ER  = ER | (RSQ <= rhole^2);
RSQ = (XO + a/2).^2 ...
    + (YO - sqrt(3)*a/2).^2;
ER  = ER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

% CONVERT TO REAL MATERIALS
ER = erfill + (erhole - erfill)*ER;
```



Oblique Symmetry (3 of 3)

Step 3 – Interpret as a Rectangular Grid

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



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: $P \geq 1$, $Q \geq 1$, $R \geq 1$
- This code can only be used for any photonic crystal symmetry.
- Convolution matrices for homogeneous materials are diagonal with the form $[\![\varepsilon_r]\!] = \varepsilon_r \mathbf{I}$.
- Uniform directions require only one harmonic.

Fast Fourier Factorization (FFF)

Product of Two Functions

Suppose we have the product of two periodic functions that have the same period:

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

Then we 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.

Finite Number of Terms

To describe devices on a computer, we can retain only a finite number of terms

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

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

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

Cases 1–2: No problem

Case 3: Problem is fixable

Case 4: Problem is NOT fixable

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

The Fix for Case 3

We can write our product of two functions 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, we bring $f(x)$ to the right-hand side of the equation.

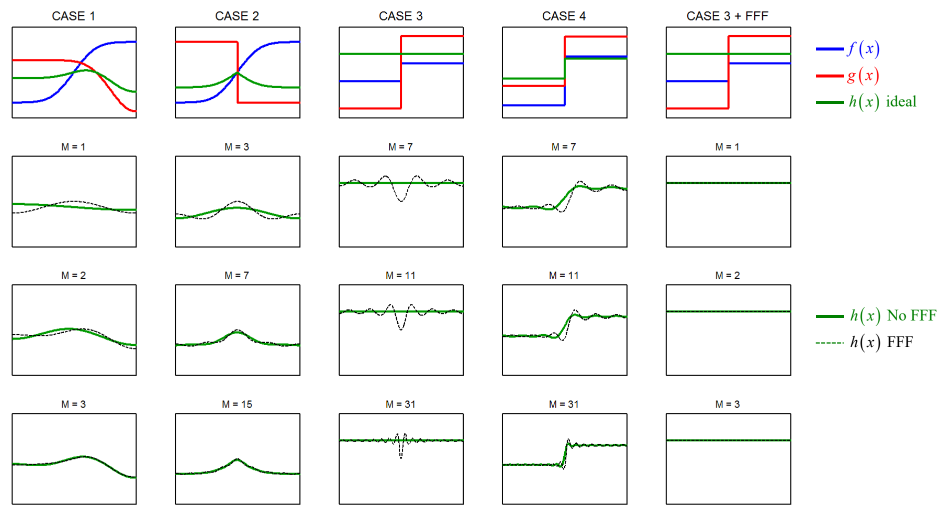
$$g=\frac{1}{f}\cdot h \quad \rightarrow \quad [G]=\left[\!\left[\frac{1}{F}\right]\!\right][H]$$

Now, there are no problems with this new equation because both sides of the equation are Case 2. We bring the convolution matrix 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!

Convergence Problem with Finite Terms



Fast convergence

Slow convergence

Fast convergence again!

FFF and Maxwell's Equations

In Maxwell's equations, we have the product of two functions…

$$\varepsilon_r(\vec{r}) \cdot \vec{E}(\vec{r})$$

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

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

Tangential component is continuous across the interface

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

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

We conclude that we must handle the convolution matrix differently for the tangential and normal components. This implies that the final convolution matrix will be a tensor.

FFF for Maxwell's Equations

First, we decompose the electric field into tangential and normal components at all interfaces.

$$\left[\!\left[\varepsilon_r\right]\!\right]\mathbf{s}=\left[\!\left[\varepsilon_r\right]\!\right]\left[\mathbf{s}_{\parallel}+\mathbf{s}_{\perp}\right]=\left[\!\left[\varepsilon_r\right]\!\right]\mathbf{s}_{\parallel}+\left[\!\left[\varepsilon_r\right]\!\right]\mathbf{s}_{\perp}$$

We now have the opportunity to associate different convolution matrices with the different field components.

$$\left[\!\left[\varepsilon_r\right]\!\right]\mathbf{s}\rightarrow\underbrace{\left[\!\left[\varepsilon_{r,\parallel}\right]\!\right]\mathbf{s}_{\parallel}}_{\text{Case 2. No problems.}}+\underbrace{\left[\!\left[\varepsilon_{r,\perp}\right]\!\right]\mathbf{s}_{\perp}}_{\text{Case 3. Fixable with FFF.}}$$

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

Normal Vector Field

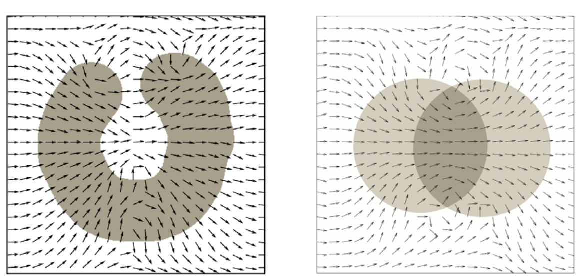
To implement FFF, we must determine what directions are parallel and perpendicular at each point in space.

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

We must construct a vector function 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).

Incorporating Normal Vector Function

Recall the FFF fix

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

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

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

Substituting these into the FFF equation yields

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

This defines a new convolution matrix that incorporates FFF.

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Revised Convolution Matrix

The convolution matrix incorporating FFF is then

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

This is often written as

$$[\![\varepsilon_r]\!]_{\text{FFF}} = [\![\varepsilon_r]\!] + \underbrace{[\![\Delta\varepsilon_r]\!]}_{}\mathbf{N} \qquad [\![\Delta\varepsilon_r]\!] = [\![1/\varepsilon_r]\!]^{-1} - [\![\varepsilon_r]\!]$$

This is interpreted as a correction term that incorporates FFF.

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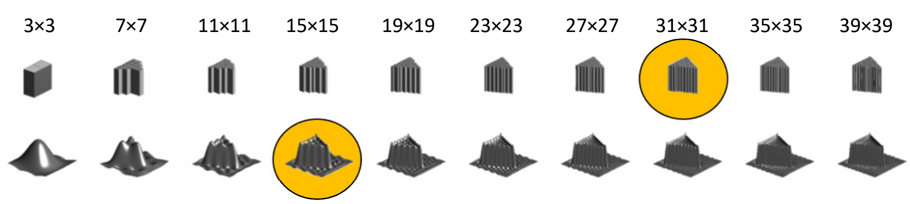
Consequences of Fourier-Space

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.



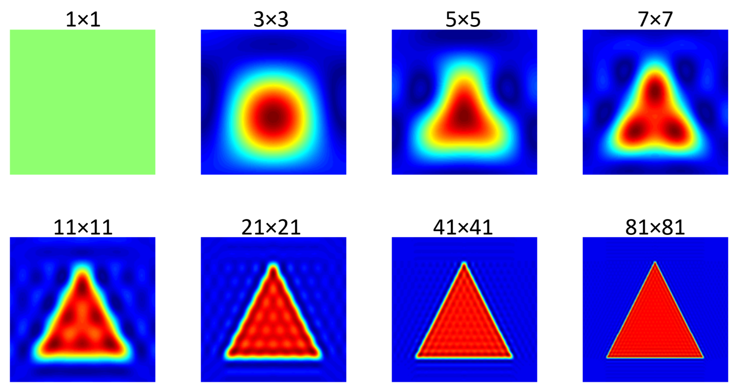
For 2D problems in real space, 4× more terms are needed making the matrices 16× larger.

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.

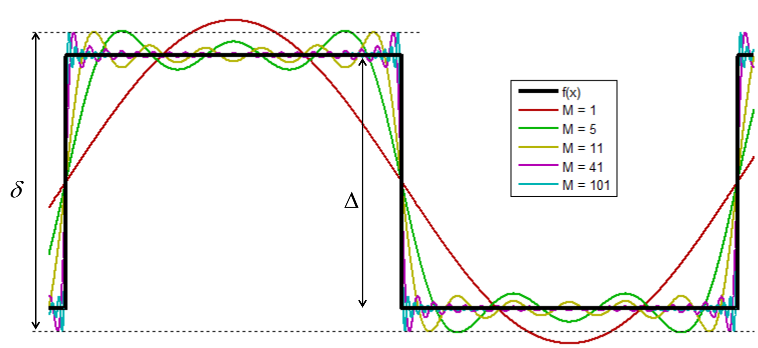
- Boundaries are artificially blurred.
- Reflections at boundaries are artificially reduced.
- It is difficult or impossible to resolve fine features or rapidly varying fields.



Rule of Thumb: # harmonics = 10 per λ

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.



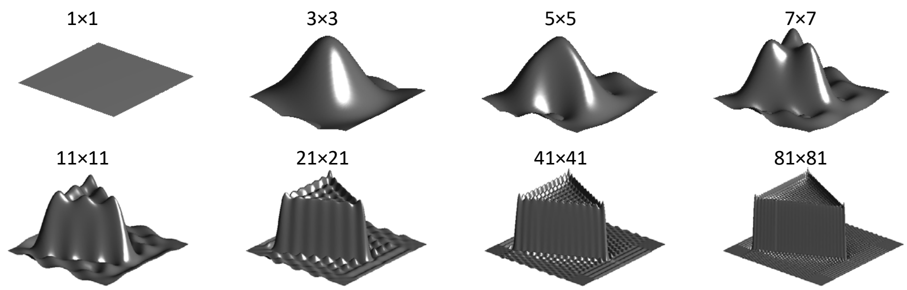
http://mathworld.wolfram.com/GibbsPhenomenon.html

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

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.