Module 3 – Spatially-Variant Lattices

Course Website:
http://emlab.utep.edu/scSVL.htm

EM Lab Website:
http://emlab.utep.edu/

Lecture Outline

• Fourier decomposition of lattices
• Rotation matrices
• Algorithm for synthesis of spatially-variant lattices
• Improving efficiency of the algorithm
• Implementation tips and tricks
Recall Complex Fourier Series

Periodic functions can be expanded into a Fourier series.

For 1D periodic functions, this is

\[
f(x) = \sum_{p=-\infty}^{\infty} a_p e^{\frac{2\pi px}{\Lambda}}, \quad a_p = \frac{1}{\Lambda} \int_{-\Lambda/2}^{\Lambda/2} f(x) e^{-\frac{2\pi px}{\Lambda}} \, dx
\]

For 2D periodic functions, this is

\[
f(x,y) = \sum_{p=-\infty}^{\infty} \sum_{q=-\infty}^{\infty} a_{p,q} e^{\frac{2\pi px}{\Lambda_x} + \frac{2\pi qy}{\Lambda_y}}, \quad a_{p,q} = \frac{1}{A} \iint_{A} f(x,y) e^{-\frac{2\pi px}{\Lambda_x} - \frac{2\pi qy}{\Lambda_y}} \, dA
\]

For 3D periodic functions, this is

\[
f(x,y,z) = \sum_{p=-\infty}^{\infty} \sum_{q=-\infty}^{\infty} \sum_{r=-\infty}^{\infty} a_{p,q,r} e^{\frac{2\pi px}{\Lambda_x} + \frac{2\pi qy}{\Lambda_y} + \frac{2\pi rz}{\Lambda_z}}, \quad a_{p,q,r} = \frac{1}{V} \iiint_{V} f(x,y,z) e^{-\frac{2\pi px}{\Lambda_x} - \frac{2\pi qy}{\Lambda_y} - \frac{2\pi rz}{\Lambda_z}} \, dV
\]
### Fourier Expansion in Terms of Grating Vectors

\[
f(x, y) = \sum_{p=-\infty}^{\infty} \sum_{q=-\infty}^{\infty} a_{p,q} e^{i \left[ \frac{2\pi px}{\Lambda_x} + \frac{2\pi qy}{\Lambda_y} \right]}
\]

\[
K_x(p, q) = \frac{2\pi p}{\Lambda_x}
\]

\[
K_y(p, q) = \frac{2\pi q}{\Lambda_y}
\]

\[
f(x, y) = \sum_{p=-\infty}^{\infty} \sum_{q=-\infty}^{\infty} a_{p,q} e^{i [K_x(p, q)x + K_y(p, q)y]} = \sum_{p=-\infty}^{\infty} \sum_{q=-\infty}^{\infty} a(p, q) e^{i \vec{K}(p, q) \cdot \vec{r}}
\]

### Visualize the Terms

\[
f(x, y) = \sum_{p=-\infty}^{\infty} \sum_{q=-\infty}^{\infty} a(p, q) e^{i \vec{K}(p, q) \cdot \vec{r}}
\]
Lattices Can be Decomposed into a Set of Planar Gratings

Using the concept of the complex Fourier series, we decompose the unit cell into a set of planar gratings. Each planar grating is described by a grating vector $\mathbf{k}_{pq}$ and a complex amplitude $a_{pq}$.

$$
\sum_{p} \sum_{q} a_{pq} e^{i\mathbf{k}_{pq} \cdot \mathbf{r}}
$$

Two Parts to the Decomposition

$$f(x, y) = \sum_{p=-\infty}^{\infty} \sum_{q=-\infty}^{\infty} a_{pq} e^{i\mathbf{k}_{pq} \cdot \mathbf{r}}$$

- Calculated using FFT.
- Calculated analytically.

Input

Fourier Coefficients

Grating Vectors

\begin{align*}
a(p,q) &= \text{FFT}_{xy}[f(x,y)] \\
\mathbf{k}_{pq} &= \frac{2\pi p}{\Lambda_x} \hat{x} + \frac{2\pi q}{\Lambda_y} \hat{y}
\end{align*}
**The Grating Amplitudes**

Short Course

Image of 2D-FFT with amplitudes represented in a 2D space.

**Impact of Number of Planar Gratings**

Short Course

Images showing the impact of different numbers of planar gratings on the distribution of grating amplitudes.
3D Decomposition

\[
\tilde{K} = K_x \hat{x} + K_y \hat{y} + K_z \hat{z}
\]

\[
K_x = \frac{2\pi p}{\Lambda_x}, \quad p = \text{integer}
\]

\[
K_y = \frac{2\pi q}{\Lambda_y}, \quad q = \text{integer}
\]

\[
K_z = \frac{2\pi r}{\Lambda_z}, \quad r = \text{integer}
\]

Rotation Matrices
Definition of a Rotation Matrix

Rotation matrix \([R]\) is defined as

\[
\begin{bmatrix}
\vec{b}
\end{bmatrix} = \left[ R(\phi) \right] \begin{bmatrix}
\vec{a}
\end{bmatrix}
\]

The rotation matrix should not change the amplitude. This implies that \([R]\) is unitary.

\[
|\vec{b}| = |\vec{a}|
\]

\[
[R]^H = [R]^{-1}
\]

\[
[R][R]^H = [R]^H[R] = I
\]

2D Rotation Matrix

\[
\begin{bmatrix}
|b_x| \\
|b_y|
\end{bmatrix} = \begin{bmatrix}
\cos \phi & -\sin \phi \\
\sin \phi & \cos \phi
\end{bmatrix} \begin{bmatrix}
|a_x| \\
|a_y|
\end{bmatrix}
\]

\[
[R(\phi)]
\]
3D Rotation Matrices

Rotation matrices for 3D coordinates can be written directly from the previous result.

Rotation matrices for 3D coordinates can be written directly from the previous result.

\[
\begin{bmatrix}
1 & 0 & 0 \\
0 & \cos\phi & -\sin\phi \\
0 & \sin\phi & \cos\phi
\end{bmatrix}
\]

\[
\begin{bmatrix}
\cos\phi & 0 & \sin\phi \\
0 & 1 & 0 \\
-\sin\phi & 0 & \cos\phi
\end{bmatrix}
\]

\[
\begin{bmatrix}
\cos\phi & -\sin\phi & 0 \\
\sin\phi & \cos\phi & 0 \\
0 & 0 & 1
\end{bmatrix}
\]

Composite Rotation Matrix

We can combine multiple rotation matrices into a single composite rotation matrix \([R]\).

\[
\begin{bmatrix}
R
\end{bmatrix} = \begin{bmatrix}
R_z
\end{bmatrix} \begin{bmatrix}
R_y
\end{bmatrix} \begin{bmatrix}
R_x
\end{bmatrix}
\]

Vector rotation using the composite rotation matrix is

\[
\vec{b} = [R] \vec{a}
\]
Algorithm for Synthesis of Spatially-Variant Lattices

Step 1 – Generate Input to Algorithm

A grayscale unit cell allows easier adjustment of fill fraction.
Step 2 – Build a Grayscale Unit Cell

A grayscale unit cell allows for better control of fill fraction in the end.

Step 3 – Decompose Unit Cell Into a Set of Planar Gratings

A grayscale unit cell allows for better control of fill fraction in the end.
**Step 4 – Truncate the Set of Planar Gratings**

We must retain only a minimum number of spatial harmonics.

\[
% \text{COMPUTE 2D-FFT}
\text{ERF} = \text{fftshift}(\text{fft2(ER)})/(\text{Nx} \times \text{Ny});
\]

\[
% \text{TRUNCATE SPATIAL HARMONICS}
\text{p0} = 1 + \text{floor}(\text{Nx}/2); \quad \% \text{p position of zero-order harmonic}
\text{q0} = 1 + \text{floor}(\text{Ny}/2); \quad \% \text{q position of zero-order harmonic}
\text{p1} = \text{p0} - \text{floor}(\text{P}/2); \quad \% \text{start of p range}
\text{p2} = \text{p0} + \text{floor}(\text{P}/2); \quad \% \text{end of p range}
\text{q1} = \text{q0} - \text{floor}(\text{Q}/2); \quad \% \text{start of q range}
\text{q2} = \text{q0} + \text{floor}(\text{Q}/2); \quad \% \text{end of q range}
\text{ERF} = \text{ERF}(\text{p1}:\text{p2},\text{q1}:\text{q2}); \quad \% \text{truncate harmonics}
\]

**Step 5 – Spatially Vary Each Planar Grating Individually and Sum the Results**

For each spatial harmonic...

- **Construct spatially variant K-function**
- **Compute grating phase on low resolution grid**
- **Interpolate grating phase into high resolution grid**
- **Compute spatially variant planar grating**
- **Add planar grating to overall lattice**
Step 5 – For Each Grating

a) Construct K-Function

- Uniform $K_{pq}$ Function
- Unit Cell Orientation $\theta(x,y)$
- Intermediate $K_{pq}$

\[ K_{pq} = \sum \left( \text{Intermediate } K_{pq} \right) \]

- Lattice Spacing $a(x,y)$
- $K$-Function

b) Solve for the Grating Phase

Construct Matrix Equation

\[
\begin{bmatrix}
D_x \\
D_y \\
\end{bmatrix}
\begin{bmatrix}
k_{x,pq} \\
k_{y,pq} \\
\end{bmatrix} = b
\]

Solve Using Least Squares

\[
A' = A'A \quad b' = A'b
\]

\[
\Phi_{pq} = (A')^{-1} b'
\]

Reshape Back to a 2D Grid

\[
\Phi_{pq} \rightarrow \Phi_{pq}(x,y)
\]

Interpolate to a Higher Resolution Grid Using \texttt{interp2()}

\[
\Phi_{pq}(x,y) \rightarrow \Phi_{pq}(x_2,y_2)
\]

All of this is performed by \texttt{svlsolve(Kx,Ky,dx,dy)}

or

\texttt{svlsolve(Kx,Ky,Kz,dx,dy,dz)}
Step 5 – For Each Grating

c) Sum All of the Spatially-Variant Gratings

Generate the $pq^{th}$ spatially variant grating

$$e_{pq}(\vec{r}) = a_{pq} \exp\left[j\Phi_{2,pq}(\vec{r})\right]$$

Add this analog planar grating to the overall analog lattice

$$e_{\text{analog}}(\vec{r}) = e_{\text{analog}}(\vec{r}) + e_{pq}(\vec{r})$$

\[\sum\]

Step 6 – Incorporate Spatially-Variant Fill Fraction

At this point, we have the analog lattice. Set any imaginary components to zero.

$$e_{\text{analog}}(\vec{r}) = \Re\left[e_{\text{analog}}(\vec{r})\right]$$

From the analog lattice, we calculate the binary lattice with a spatially-variant fill fraction.

$$e_{\text{binary}}(\vec{r}) = \begin{cases} e_1 & e_{\text{analog}}(\vec{r}) \leq \gamma(\vec{r}) \\ e_2 & e_{\text{analog}}(\vec{r}) > \gamma(\vec{r}) \end{cases}$$

From analog lattices that have a smooth cosine looking profile, the threshold can be estimated as

$$\gamma(\vec{r}) \approx \cos\left[\pi f(\vec{r})\right]$$
Summary of Spatially Variant Algorithm

1. Define the spatial variance: orientation, lattice spacing, fill fraction, ...
2. Build the baseline unit cell.
3. Decompose unit cell into a set of planar gratings.
4. Truncate the set of planar gratings to a minimal set.
5. Loop over each spatial harmonic
   a. Construct $K$-function that is uniform across the grid according to the grating vector of the spatial harmonic.
   b. Solve for grating phase $\Phi$ from the $K$-function.
   c. Add the planar grating to the overall lattice.
6. Incorporate spatially-variant fill fraction.

Improving Efficiency of the Algorithm
Collinear Spatial Harmonics

If a spatial harmonic is collinear to another (i.e. their grating vectors are parallel), we can calculate its grating phase by scaling the grating phase of the other. Therefore, we only have to solve for one of them.

\[ \vec{K}_1 \]
\[ \vec{K}_2 = a\vec{K}_1 \]
\[ \vec{K}_3 = b\vec{K}_1 \]

\[ \nabla \Phi_1 = \vec{K}_1 \]
\[ \nabla \Phi_2 = \vec{K}_2 = \left( a\vec{K}_1 \right) \]
\[ \nabla \left( \frac{\Phi_2}{a} \right) = \vec{K}_1 \rightarrow \frac{\Phi_2}{a} = \Phi_1 \]
\[ \Phi_2 = a\Phi_1 \]

We solve this numerically.

Identifying Collinear Planar Gratings

121 spatial harmonics

40 “unique” spatial harmonics. The rest are collinear.
Performance Gain by Eliminating Collinear Gratings

\[ \sim 69\% \text{ for 2D} \]

\[ \sim 59\% \text{ for 3D} \]

Eliminating Gratings According to Their Amplitude

We neglect all planar gratings with amplitude \( a_{pq} \) less than some threshold.

\[ |a_{pq}| < a_{\text{threshold}} \quad a_{\text{threshold}} \approx 0.02 \max |a_{pq}| \]

A threshold that works in many cases is one that is around 2% of the maximum \( a_{pq} \) in the expansion.
Overall Efficiency Improvement

Implementation Tips and Tricks
Grid Strategy

- High Resolution Unit Cell Grid
  - Need enough points for the FFT to converge.
  \[ \Delta_{\text{FFT}} < a/(N \cdot P) \]

- Low Resolution Lattice Grid
  - Need enough resolution to resolve the spatial variance. Usually this is \( N > 10 \) grid cells per unit cell.
  \[ \Delta_{\text{coarse}} < a/N \]

- High Resolution Lattice Grid
  - Need enough resolution to resolve the shortest period planar grating.
  \[ \Delta_{\text{fine}} < \frac{a_{\text{min}}}{N} \]
  \[ a_{\text{min}} = \frac{2\pi}{\max[K_{pq}]} \]
When the lattice is composed of an array of discontinuous metallic elements, it is not efficient to decompose the unit cells into planar gratings.
Arrays of Metallic Elements Over Curved Surfaces

(a) Surface Mesh
(b) Curved Metasurface
(c) Grating 1
(d) Grating 2
(e) Superimposed

3D view