Hexagonal Grids for solving PDEs

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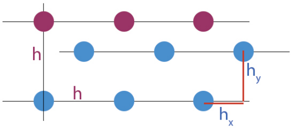
Objectives

1. Construction of Spatial Grid
2. Staggered Grids
3. Triangular and Hexagonal Nets
4. Grid functions for solving PDEs
5. Finite Difference Operators
6. Stability Conditions
7. Numerical Dispersion
8. Example: Use of Staggered Grids in Computational Optics/Electro-magnetics

Introduction to Spatial Grid



A regular 2-D spatial grid is a collection of points defined as:

$$\mathbf{G}_h = \left\{ \mathbf{r}_{m_1,m_2} = h(m_1\mathbf{x_1} + m_2\mathbf{x_2}) | (m_1, m_2) \in \mathbb{Z}^2 \right\}$$

A hexagonal grid is obtained when we displace each layer of points by $(h_x, h_y) = (\frac{h}{2}, \frac{h\sqrt{3}}{2})$.

Spatial Grids

For each regular lattice, a suitable coordinate axis may be chosen for facilitating analysis. For the Rectilinear Grid, we have $(\mathbf{x_1}, \mathbf{x_2}) = ([1,0]^T, [0,1]^T)$.

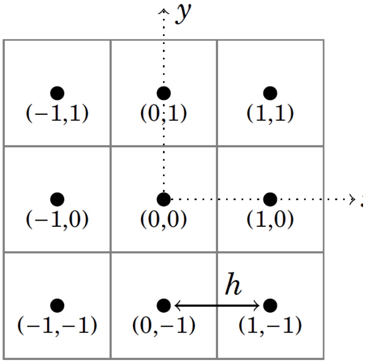


Figure: Rectilinear Grid

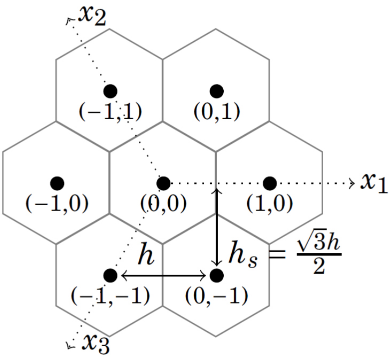


Figure: Hexagonal Grid

For the Hexagonal Grid, we have $(\mathbf{x_1}, \mathbf{x_2}) = ([1,0]^T, [\frac{-1}{2}, \frac{\sqrt{3}}{2}]^T)$.

Staggered Grids

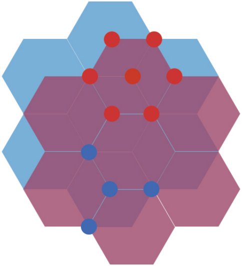


Figure: Staggered Colocated Hexagonal Grids

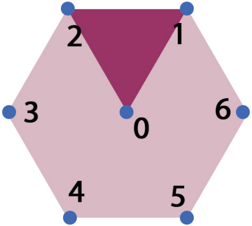


Figure: Hexagonal Grid Structure

Triangular and Hexagonal Nets

Triangular Net

$$
\begin{aligned}
u_1 - u_0 &= u(x+h, y) - u(x,y) \\
&= h(\frac{\partial}{\partial x})u + \frac{h^2}{2!}(\frac{\partial^2}{\partial^2 x})u + \frac{h^3}{3!}(\frac{\partial^3}{\partial^3 x})u + \cdots \\
u_2 - u_0 &= u(x+\frac{h}{2}, y + \frac{\sqrt{3}h}{2}) - u(x,y) \\
&= h\left(\frac{1}{2}\frac{\partial}{\partial x} + \frac{\sqrt{3}}{2}\frac{\partial}{\partial y}\right)u \\
&+ \frac{h^2}{2!}\left(\frac{1}{2}\frac{\partial}{\partial x} + \frac{\sqrt{3}}{2}\frac{\partial}{\partial y}\right)^2 u \\
&+ \frac{h^3}{3!}\left(\frac{1}{2}\frac{\partial}{\partial x} + \frac{\sqrt{3}}{2}\frac{\partial}{\partial y}\right)^3 u + \cdots \\
u_3 - u_0 &= u(x-\frac{h}{2}, y + \frac{\sqrt{3}h}{2}) - u(x,y) \\
&= h\left(\frac{-1}{2}\frac{\partial}{\partial x} + \frac{\sqrt{3}}{2}\frac{\partial}{\partial y}\right)u \\
&+ \frac{h^2}{2!}\left(\frac{-1}{2}\frac{\partial}{\partial x} + \frac{\sqrt{3}}{2}\frac{\partial}{\partial y}\right)^2 u \\
&+ \frac{h^3}{3!}\left(\frac{-1}{2}\frac{\partial}{\partial x} + \frac{\sqrt{3}}{2}\frac{\partial}{\partial y}\right)^3 u + \cdots
\end{aligned}
$$

$\cdots (u_4 - u_0), (u_5 - u_0), (u_6 - u_0)$

Hexagonal Net

$$
\begin{aligned}
u_1 - u_0 &= u(x+\frac{h}{2}, y + \frac{\sqrt{3}h}{2}) - u(x,y) \\
&= h\left(\frac{1}{2}\frac{\partial}{\partial x} + \frac{\sqrt{3}}{2}\frac{\partial}{\partial y}\right)u \\
&+ \frac{h^2}{2!}\left(\frac{1}{2}\frac{\partial}{\partial x} + \frac{\sqrt{3}}{2}\frac{\partial}{\partial y}\right)^2 u \\
&+ \frac{h^3}{3!}\left(\frac{1}{2}\frac{\partial}{\partial x} + \frac{\sqrt{3}}{2}\frac{\partial}{\partial y}\right)^3 u + \cdots \\
u_2 - u_0 &= u(x-h, y) - u(x,y) \\
&= -h(\frac{\partial}{\partial x})u + \frac{h^2}{2!}(\frac{\partial^2}{\partial^2 x})u + \frac{-h^3}{3!}(\frac{\partial^3}{\partial^3 x})u + \cdots \\
u_3 - u_0 &= u(x+\frac{h}{2}, y - \frac{\sqrt{3}h}{2}) - u(x,y) \\
&= h\left(\frac{1}{2}\frac{\partial}{\partial x} + \frac{-\sqrt{3}}{2}\frac{\partial}{\partial y}\right)u \\
&+ \frac{h^2}{2!}\left(\frac{1}{2}\frac{\partial}{\partial x} + \frac{-\sqrt{3}}{2}\frac{\partial}{\partial y}\right)^2 u \\
&+ \frac{h^3}{3!}\left(\frac{1}{2}\frac{\partial}{\partial x} + \frac{-\sqrt{3}}{2}\frac{\partial}{\partial y}\right)^3 u + \cdots
\end{aligned}
$$

Triangular and Hexagonal Nets

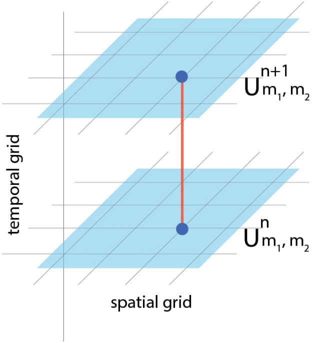
Triangular Net

$$\frac{2}{3h^2}(\sum u_i - 6u_0) = \Delta u + \frac{h^2}{16}\Delta^2 u + R_0\left(O(h^4)O(\frac{\partial^6}{\partial^k x \partial^{6-k} y})\right) \tag{1}$$

Hexagonal Net

$$\frac{4}{3h^2}\left(\sum_{i=1}^{3} u_i - 3u_0\right) = \Delta u + R_0\left(O(h)O(\frac{\partial^3}{\partial^k x \partial^{3-k} y})\right) \tag{2}$$

Grid-functions for solving PDEs



We define a grid function $u^n_{m_1,m_2}$ as a time series at each point on the spatial grid which approximates the continuous functions $u(t, x, y)$ at time $t = nk$, where k is the time-step and at the spatial position $(x, y) = \mathbf{r}_{m_1,m_2}$.

Finite Difference Operators

In the FDTD method, differential operators are approximated by finite difference operators.
First, we define the Unit-Shift operators as follows:

$$S_{t\pm}\left(u^n_{m_1,m_2}\right) = \left(u^{n+1}_{m_1,m_2}\right) \tag{3}$$

$$S_{x_1\pm}\left(u^n_{m_1,m_2}\right) = \left(u^n_{m_1\pm 1,m_2}\right) \tag{4}$$

$$S_{x_2\pm}\left(u^n_{m_1,m_2}\right) = \left(u^n_{m_1,m_2\pm 1}\right) \tag{5}$$

$$S_{x_3\pm} = S_{x_2\mp} \cdot S_{x_2\mp} \tag{6}$$

Next, we proceed to build second-order finite difference operators as:

$$\delta_{tt} = \frac{1}{k^2}\left(S_{t-} + S_{t+} - 2\right) \tag{7}$$

$$\delta_{x_i x_i} = \frac{1}{h^2}\left(S_{x_i-} + S_{x_i+} - 2\right) \tag{8}$$

$$\tag{9}$$

Finite Difference Operators

On the hexagonal grid we employ seven-points to build a second-order accurate approximation to the Laplacian:

$$\begin{aligned}\delta_{\Delta \mathrm{HEX}} &= \frac{2}{3}\left(\delta_{x_1 x_1} + \delta_{x_2 x_2} + \delta_{x_3 x_3}\right) \\ &= \Delta + \frac{h^2}{16}\Delta^2 + O(h^4) \qquad (10)\end{aligned}$$

where $\Delta = \frac{2}{3}\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2}\right)$ is the 2-D Laplacian operator for the 2-D Wave Equation

$$\left(\frac{\partial^2}{\partial t^2} - c^2 \Delta\right) u = 0 \qquad (11)$$

Finite Difference Operators

Using the finite-difference operators, we solve the approximate finite-difference 2-D Wave Equation

$$\left(\frac{\partial^2}{\partial t^2} - c^2\Delta\right)u^n_{m_1,m_2} = 0 \tag{12}$$

using the explicit update equation

$$u^{n+1}_{m_1,m_2} = \frac{2\mu^2}{3}\left(u^n_{m_1+1,m_2} + u^n_{m_1-1,m_2} + u^n_{m_1,m_2+1}\right. \tag{13}$$

$$\left. + u^n_{m_1,m_2-1} + u^n_{m_1+1,m_2+1} + u^n_{m_1-1,m_2-1}\right) \tag{14}$$

$$+ (2-4\mu^2)u^n_{m_1,m_2} - u^{n-1}_{m_1,m_2} \tag{15}$$

where,

$$\mu = ck/h \tag{16}$$

μ is the Courant Number, which is the ratio between the time step and the grid spacing for a given wave speed.

Stability Conditions

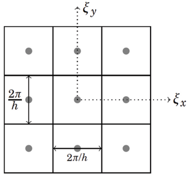


Figure: Dual-Rectilinear Grid

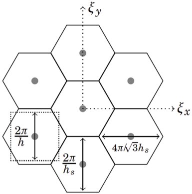


Figure: Dual-Hexagonal Grid

Determine the maximum value of Courant Number, $\mu = ck/h$ such that no exponentially growing plane-wave solutions of the form

$$u^n_{m_1,m_2} = e^{jkn\omega} e^{jh(\xi_x,\xi_y)\cdot(m_1\mathbf{x_1}+m_2\mathbf{x_2})}$$

where $(\omega, \xi_x, \xi_y) \in \mathbb{C}^3$ are the wave-numbers in complex frequency domain, $(h, k) \in \mathbb{R}^2$ grid spacing and the integral grid locations $(n, m_1, m_2) \in \mathbb{Z}^3$.

Stability Conditions

Stability Conditions:

1. $\omega \in [0, \pi]$
2. $(\xi_x, \xi_y) \in \{$ One Wave-Number Cell $\}$ of the Grid.

For the Hexagonal Grid, the maximum Courant number is determined to be

$$\mu \leq \sqrt{\frac{2}{3}} \tag{17}$$

which, is achieved at the corners of the hexagon.
By searching over $\xi_x, \xi_y \in [-\frac{\pi}{h}, \frac{\pi}{h}]$ is in-sufficient to cover the entire the hexagonal wave-number cell, due to issues with aliasing associated with Fourier analysis. The way the frequency ranges is handled not a trivial issue.

Numerical Dispersion

The condition for the plane waves of the form $u = e^{j\omega t}e^{j(\xi_x x + \xi_y y)}$ are solutions to the 2-D wave equation is given by the well-known dispersion relation

$$\omega^2 = c^2|\xi|^2 = c^2(\xi_x^2 + \xi_y^2) \tag{18}$$

The Phase Velocity(Wave Speed) for $|\xi| > 0$ is $\omega/|\xi| = c$.
The finite difference scheme approximates (18) as

$$\mathcal{D}_{tt}(\omega) = \mathcal{D}_{\Delta}(\xi) \tag{19}$$

for some $\mathcal{D}_{tt} : \mathbb{C} \to \mathbb{C}$ and $\mathcal{D}_{\Delta} : \mathbb{C}^2 \to \mathbb{C}$, which are Fourier symbols of the Finite-Difference Operators of the scheme.

$$\mathcal{D}_{tt}(\omega) = -\frac{4}{k^2} sin^2(\omega \frac{k}{2}) \tag{20}$$

$$\mathcal{D}_{\Delta}(\xi) = -\frac{8}{3h^2} \sum_{i=1}^{3} sin^2((\xi \cdot \mathbf{x_i})\frac{h}{2}) \tag{21}$$

Numerical Dispersion

For all practical considerations, we consider Real-valued Frequencies and Wave-numbers.

To make $\mathcal{D}_{tt}$ injective, we consider the positive real wave-numbers $\xi \in \mathbb{B}$, where $\mathbb{B}$ is any Wave-Number Grid Cell.

If stability conditions are satisfied, we have

$$\mathcal{D}_{tt}^{-1}\left(c^2\mathcal{D}_{\Delta}(\xi)\right) : \mathbb{B} \to \left[0, \frac{\pi}{k}\right] \tag{22}$$

Numerical Phase Velocity of as a function of wave-number:

$$v(\xi) = \frac{\omega(\xi)}{|\xi|}, \omega(\xi) = \mathcal{D}_{tt}^{-1}\left(c^2\mathcal{D}_{\Delta}(\xi)\right). \tag{23}$$

Polar Plots:

- Polar Radius: Temporal frequency ω
- Polar Angle: Angle of Propagation θ for $\xi = (|\xi|, \theta)$.

Numerical Phase Velocity(Wave-Speed) as a function of wave-number and temporal-frequency:

$$v\left(\omega(|\xi|, \theta), \theta\right) = \frac{\omega(\xi)}{|\xi|}, \text{ where}$$

$$\xi = |\xi|e^{j\theta}, \omega(\xi) = \mathcal{D}_{tt}^{-1}\left(c^2\mathcal{D}_{\Delta}(\xi)\right)$$

Numerical Dispersion

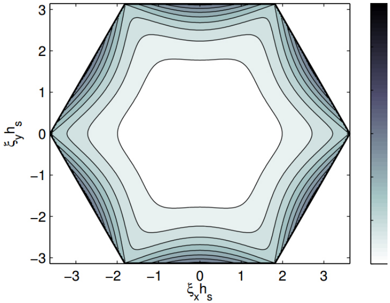


Figure: Numerical Dispersion: Wave-number tiling

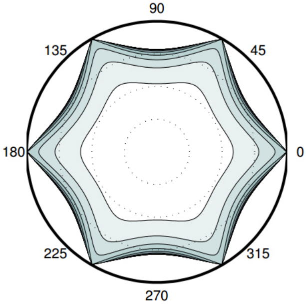
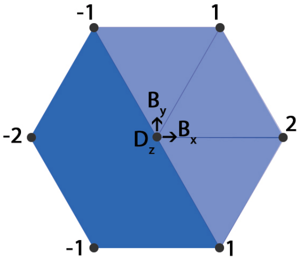
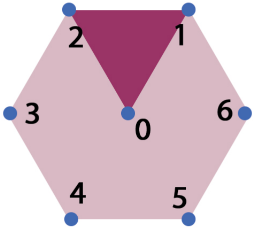


Figure: Numerical Phase Velocity: Polar plot

Application of Staggered Spatial Grids in Optics/Electro-magnetics



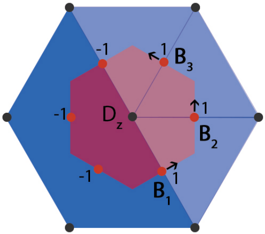


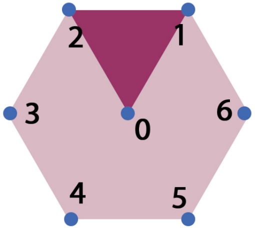
$$\frac{dD_{z0}}{dt} = \frac{1}{6h}\Big[(2H_{y6} - 2H_{y3} + H_{y1} - H_{y4} + H_{x5} - H_{x2}) - \sqrt{3}(H_{x1} - H_{x5} + H_{x2} - H_{x4})\Big]$$

$$\frac{dB_{x0}}{dt} = \frac{-\sqrt{3}}{6h}(E_{z1} - E_{z4} + E_{z2} - E_{z5})$$

$$\frac{dB_{y0}}{dt} = \frac{1}{6h}(2E_{z6} - 2E_{z3} + E_{z1} - E_{z4} + E_{z2} - E_{z5})$$

Application of Staggered Spatial Grids in Optics/Electro-magnetics





$$\frac{dD_{z0}}{dt} = \frac{2}{3h}\left(H_1^a - H_1^d + H_2^b - H_2^e + H_3^c - H_3^f\right)$$
$$\frac{dB_1^a}{dt} = \frac{1}{k}\left(E_{z5} - E_{z0}\right)$$

$$\frac{dB_2^b}{dt} = \frac{1}{k}\left(E_{z6} - E_{z0}\right)$$
$$\frac{dB_3^c}{dt} = \frac{1}{k}\left(E_{z1} - E_{z0}\right)$$

References

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