

**Numerical Methods of
Electromagnetic Field Theory II (NFT II)
Numerische Methoden der
Elektromagnetischen Feldtheorie II (NFT II) /**

7th Lecture / 7. Vorlesung

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CG Method – Conjugate Gradient Method – References / KG-Methode – Konjugierte Gradientenmethode

Jonathan Richard Shewchuk:
An Introduction to the Conjugate Gradient Method
Without the Agonizing Pain, p. , August 1994.

An Introduction to
the Conjugate Gradient Method
Without the Agonizing Pain
Edition 1 $\frac{1}{4}$
Jonathan Richard Shewchuk
August 4, 1994

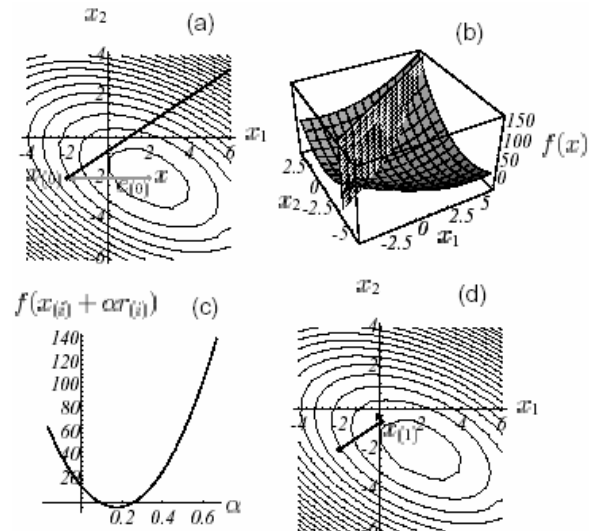
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Abstract

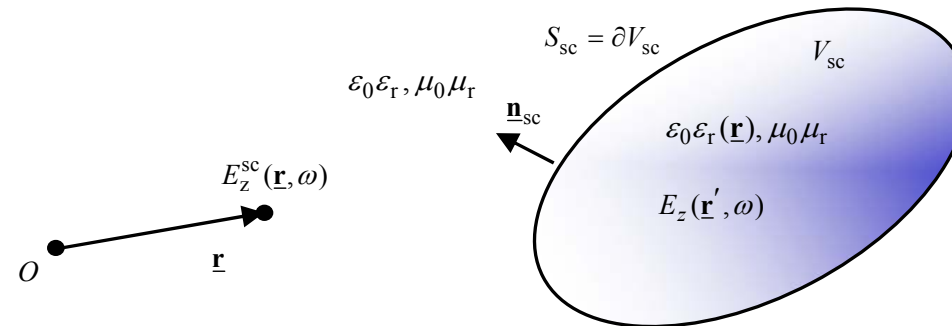
The Conjugate Gradient Method is the most prominent iterative method for solving sparse systems of linear equations. Unfortunately, many textbook treatments of the topic are written with neither illustrations nor intuition, and their victims can be found to this day babbling senselessly in the corners of dusty libraries. For this reason, a deep, geometric understanding of the method has been reserved for the elite brilliant few who have painstakingly decoded the mumblings of their forebears. Nevertheless, the Conjugate Gradient Method is a composite of simple, elegant ideas that almost anyone can understand. Of course, a reader as intelligent as yourself will learn them almost effortlessly.

The idea of quadratic forms is introduced and used to derive the methods of Steepest Descent, Conjugate Directions, and Conjugate Gradients. Eigenvectors are explained and used to examine the convergence of the Jacobi Method, Steepest Descent, and Conjugate Gradients. Other topics include preconditioning and the nonlinear Conjugate Gradient Method. I have taken pains to make this article easy to read. Sixty-six illustrations are provided. Dense prose is avoided. Concepts are explained in several different ways. Most equations are coupled with an intuitive interpretation.

Supported in part by the Natural Sciences and Engineering Research Council of Canada under a 1987 Science and Engineering Scholarship and by the National Science Foundation under Grant ASC-9318163. The views and conclusions contained in this document are those of the author and should not be interpreted as representing the official policies, either express or implied, of NSERC, NSF, or the U.S. Government.



**Penetrable Scatterer: Data Equation and Lippmann-Schwinger Equation – 2-D TM Case/
Penetrable Streuer: Datengleichung und Lippmann-Schwinger Gleichung – 2D-TM-Fall**

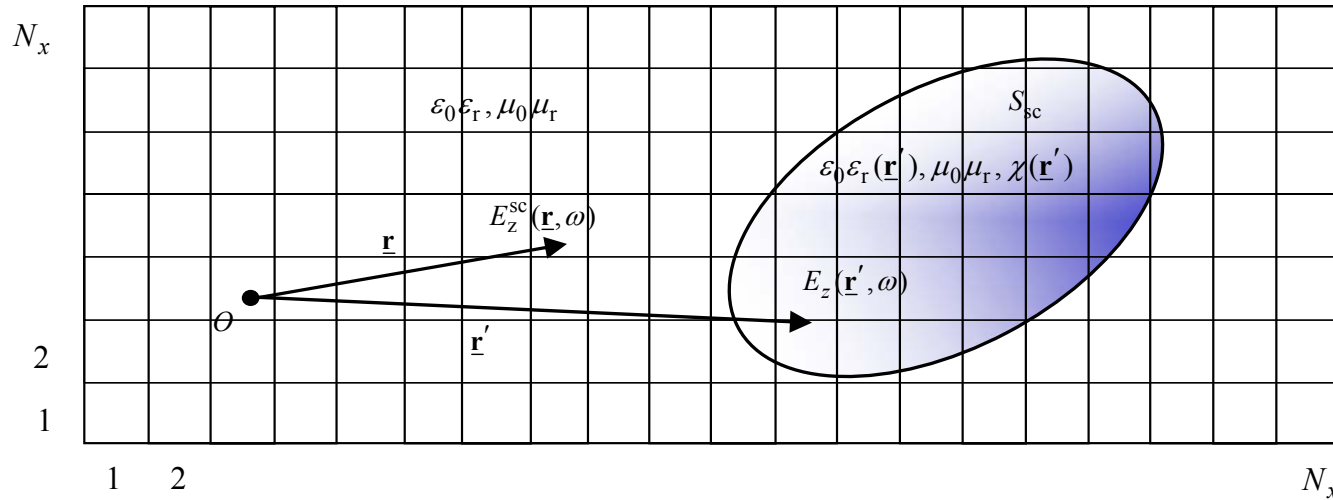


$$E_z^{\text{sc}}(\underline{\mathbf{r}}, \omega) = k^2 \iint_{\underline{\mathbf{r}}' \in S} G(\underline{\mathbf{r}} - \underline{\mathbf{r}}', \omega) \chi(\underline{\mathbf{r}}') E_z(\underline{\mathbf{r}}', \omega) d^2 \underline{\mathbf{r}}'$$

$$\{E_z^{\text{sc}}\} = [\mathbf{G}][\chi]\{E_z\}$$

$$[\mathbf{G}] \rightarrow G_{mn} = \begin{cases} j \frac{\pi}{2} ka J_1(ka) H_0^{(1)}(k|\underline{\mathbf{r}}_m - \underline{\mathbf{r}}_n|) & m \neq n \\ -1 + j \frac{\pi}{2} ka H_1^{(1)}(ka) & m = n \end{cases}$$

**PEN Scatterer: Discretization of the Domain Integral Equation – Richmond Method /
PEN-Streuer: Diskretisierung der Bereichsintegralgleichung – Richmod-Methode**



$$E_z^{\text{sc}}(\underline{\mathbf{r}}, \omega) = k^2 \iint_{\underline{\mathbf{r}}' \in S_{\text{sc}}} G(\underline{\mathbf{r}} - \underline{\mathbf{r}}', \omega) \chi(\underline{\mathbf{r}}') E_z(\underline{\mathbf{r}}', \omega) d^2 \underline{\mathbf{r}}'$$

$$\{E_z^{\text{sc}}\}_N = [\mathbf{G}]_{N \times N} \{\chi E_z\}_N \quad N = N_x \times N_y$$

$$[\mathbf{G}] \rightarrow G_{mn} = \begin{cases} j \frac{\pi}{2} ka J_1(ka) H_0^{(1)}(k|\underline{\mathbf{r}}_m - \underline{\mathbf{r}}_n|) & m \neq n & n, m = 1, 2, \dots, N = N_x N_y \\ -1 + j \frac{\pi}{2} ka H_1^{(1)}(ka) & m = n & n, m = 1, 2, \dots, N = N_x N_y \end{cases}$$

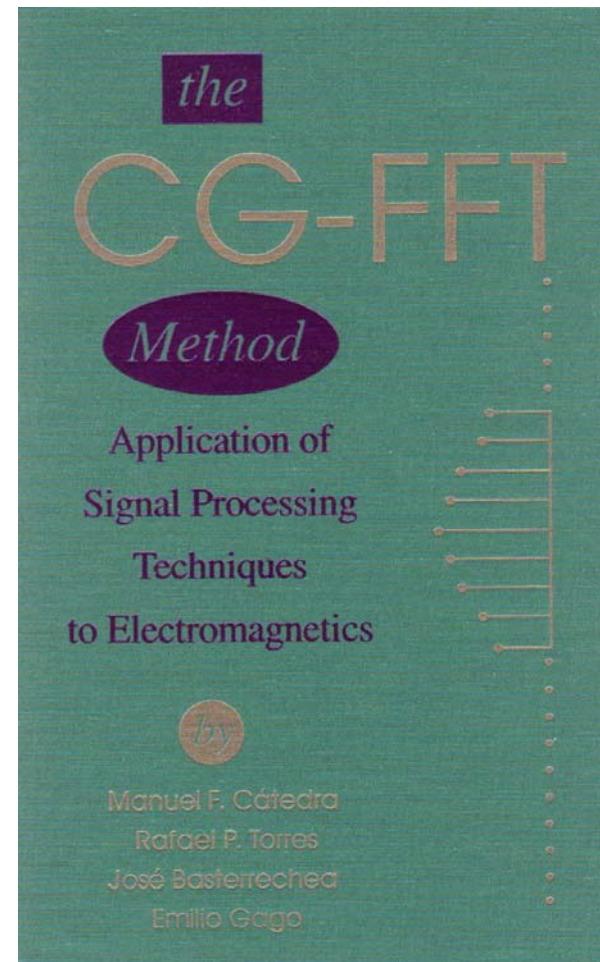
CG-FFT: Conjugate Gradient – Fast Fourier Transform / KG-SFT: Konjugierte Gradienten – Schnelle Fourier-Transformation

The Numerical Solution of a Linear Matrix Equation Requires the Storage of the Full $N \times N$ Matrix in the Computer Main Memory. This is the Main Bottleneck in the Solution of a **Large Set of Linear Equations.** /

Die numerische Lösung einer linearen Matrixgleichung erfordert die Speicherung der vollen $N \times N$ -Matrix im Hauptspeicher des Computers. Dies stellt den wesentlichsten **Flaschenhals** bei der **numerischen Lösung von großen linearen Gleichungssystemen** dar.



CG-FFT
Conjugate Gradient – Fast Fourier Transform /
KG-SFT
Konjugierte Gradienten – Schnelle Fourier-Transformation



CG-FFT: Conjugate Gradient – Fast Fourier Transform / KG-SFT: Konjugierte Gradienten – Schnelle Fourier-Transformation

Two-Dimensional Convolution Integral /
Zweidimensionales Faltungsintegral

$$E_z^{\text{sc}}(\underline{\mathbf{r}}, \omega) = k^2 \iint_{\underline{\mathbf{r}}' \in S} G(\underline{\mathbf{r}} - \underline{\mathbf{r}}', \omega) \chi(\underline{\mathbf{r}}') E_z(\underline{\mathbf{r}}', \omega) d^2 \underline{\mathbf{r}}'$$

$$\underbrace{E_z^{\text{sc}}(\underline{\mathbf{r}}, \omega)}_{=E(\underline{\mathbf{r}}, \omega)} = \iint_{\underline{\mathbf{r}}' \in S} G(\underline{\mathbf{r}} - \underline{\mathbf{r}}', \omega) \underbrace{k^2 \chi(\underline{\mathbf{r}}') E_z(\underline{\mathbf{r}}', \omega)}_{=J(\underline{\mathbf{r}}', \omega)} d^2 \underline{\mathbf{r}}'$$

$$E(\underline{\mathbf{r}}, \omega) = \iint_{\underline{\mathbf{r}}' \in S} G(\underline{\mathbf{r}} - \underline{\mathbf{r}}', \omega) J(\underline{\mathbf{r}}', \omega) d^2 \underline{\mathbf{r}}'$$

2-D Convolution Integral in Cartesian Coordinates /
2D-Faltungsintegral in Kartesische Koordinaten

$$E(x, y, \omega) = \int_{x'=-\infty}^{\infty} \int_{y'=-\infty}^{\infty} G(x-x', y-y', \omega) J(x', y', \omega) dx' dy'$$

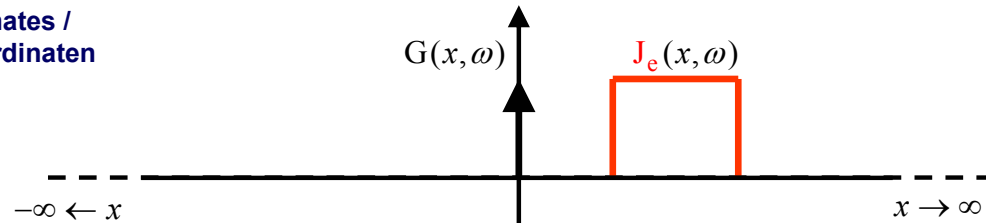
1-D Convolution Integral in Cartesian Coordinates /
1D-Faltungsintegral in Kartesischen Koordinaten

$$E(x, \omega) = \int_{x'=-\infty}^{\infty} G(x-x', \omega) J(x', \omega) dx'$$

CG-FFT: Conjugate Gradient – Fast Fourier Transform / KG-SFT: Konjugierte Gradienten – Schnelle Fourier-Transformation

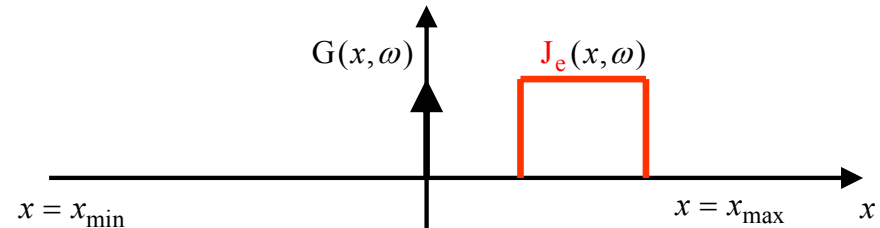
**Infinite 1-D Convolution Integral in Cartesian Coordinates /
Unendliches 1D-Faltungsintegral in Kartesischen Koordinaten**

$$E(x, \omega) = \int_{x'=-\infty}^{\infty} G(x-x', \omega) J(x', \omega) dx'$$



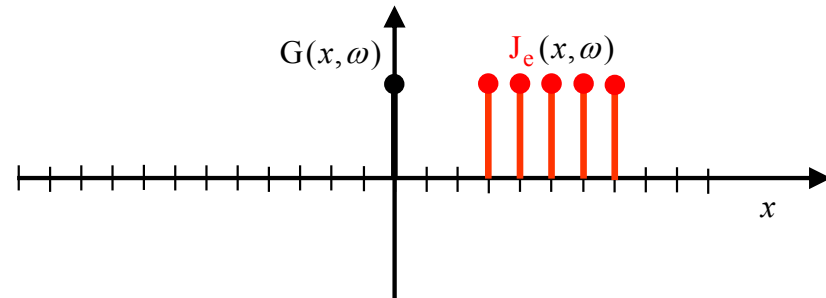
**Finite 1-D Convolution Integral in Cartesian Coordinates /
Endliches 1D-Faltungsintegral in Kartesischen Koordinaten**

$$E(x, \omega) = \int_{x'=x_{\min}}^{x_{\max}} G(x-x', \omega) J(x', \omega) dx'$$



**Discrete Convolution /
Diskrete Faltung**

$$E_m = \Delta x \sum_{n=0}^{N-1} G_{m-n} J_n \quad m = 0, 1, 2, \dots, N-1$$



CG-FFT: Conjugate Gradient – Fast Fourier Transform / KG-SFT: Konjugierte Gradienten – Schnelle Fourier-Transformation

Discrete Convolution /
Diskrete Faltung

$$E_m = \Delta x \sum_{n=0}^{N-1} G_{m-n} J_n \quad m = 0, 1, 2, \dots, N-1$$

Discrete Convolution in Matrix Form /
Diskrete Faltung in Matrixform

$$\{\mathbf{E}\}_N = \Delta x [\mathbf{G}]_{N \times N} \{\mathbf{J}\}_N$$

Example: $N = M = 4$ / Beispiel: $N = M = 4$

$$m = 0: \quad E_{m=0} = \Delta x \sum_{n=0}^{4-1=3} G_{m-n} J_n$$

$$= \Delta x [G_{0-0=0} J_0 + G_{0-1=-1} J_1 + G_{0-2=-2} J_2 + G_{0-3=-3} J_3] \quad \rightarrow \quad E_0 = \Delta x [G_0 J_0 + G_{-1} J_1 + G_{-2} J_2 + G_{-3} J_3]$$

$$m = 1: \quad E_{m=1} = \Delta x \sum_{n=0}^{4-1=3} G_{m-n} J_n$$

$$= \Delta x [G_{1-0=1} J_0 + G_{1-1=0} J_1 + G_{1-2=-1} J_2 + G_{1-3=-2} J_3] \quad \rightarrow \quad E_1 = \Delta x [G_1 J_0 + G_0 J_1 + G_{-1} J_2 + G_{-2} J_3]$$

$$m = 2: \quad E_{m=2} = \Delta x \sum_{n=0}^{4-1=3} G_{m-n} J_n$$

$$= \Delta x [G_{2-0=2} J_0 + G_{2-1=1} J_1 + G_{2-2=0} J_2 + G_{2-3=-1} J_3] \quad \rightarrow \quad E_2 = \Delta x [G_2 J_0 + G_1 J_1 + G_0 J_2 + G_{-1} J_3]$$

$$m = 3: \quad E_{m=3} = \Delta x \sum_{n=0}^{4-1=3} G_{m-n} J_n$$

$$= \Delta x [G_{3-0=3} J_0 + G_{3-1=2} J_1 + G_{3-2=1} J_2 + G_{3-3=0} J_3] \quad \rightarrow \quad E_3 = \Delta x [G_3 J_0 + G_2 J_1 + G_1 J_2 + G_0 J_3]$$

CG-FFT: Conjugate Gradient – Fast Fourier Transform / KG-SFT: Konjugierte Gradienten – Schnelle Fourier-Transformation

Discrete Convolution / Diskrete Faltung $E_m = \Delta x \sum_{n=0}^{N-1} G_{m-n} J_n \quad m = 0, 1, 2, \dots, N-1$

Example: $N = M = 4$ / Beispiel: $N = M = 4$

$$\begin{aligned} G_0 J_0 + G_{-1} J_1 + G_{-2} J_2 + G_{1-N} J_{N-1} &= \frac{1}{\Delta x} E_0 \\ G_1 J_0 + G_0 J_1 + G_{-1} J_2 + G_{2-N} J_{N-1} &= \frac{1}{\Delta x} E_1 \\ G_2 J_0 + G_1 J_1 + G_0 J_2 + G_{3-N} J_{N-1} &= \frac{1}{\Delta x} E_2 \\ G_{N-1} J_0 + G_{N-2} J_1 + G_{N-3} J_2 + G_0 J_{N-1} &= \frac{1}{\Delta x} E_{N-1} \end{aligned}$$

**Discrete Convolution in Matrix Form /
Diskrete Faltung in Matrixform**

$$\begin{bmatrix} G_0 & G_{-1} & G_{-2} & \cdots & G_{1-N} \\ G_1 & G_0 & G_{-1} & \cdots & G_{2-N} \\ G_2 & G_1 & G_0 & \cdots & G_{3-N} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ G_{N-1} & G_{N-2} & G_{N-3} & \cdots & G_0 \end{bmatrix}_{N \times N} \begin{Bmatrix} J_0 \\ J_1 \\ J_2 \\ \vdots \\ J_{N-1} \end{Bmatrix}_N = \frac{1}{\Delta x} \begin{Bmatrix} E_0 \\ E_1 \\ E_2 \\ \vdots \\ E_{N-1} \end{Bmatrix}_N$$

$$[\mathbf{G}]\{\mathbf{J}\} = \frac{1}{\Delta x} \{\mathbf{E}\}$$

CG-FFT: Conjugate Gradient – Fast Fourier Transform / KG-SFT: Konjugierte Gradienten – Schnelle Fourier-Transformation

Discrete Convolution in Matrix Form /
Diskrete Faltung in Matrixform

$$\begin{bmatrix} G_0 & G_{-1} & G_{-2} & \cdots & G_{1-N} \\ G_1 & G_0 & G_{-1} & \cdots & G_{2-N} \\ G_2 & G_1 & G_0 & \cdots & G_{3-N} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ G_{N-1} & G_{N-2} & G_{N-3} & \cdots & G_0 \end{bmatrix}_{N \times N} \begin{Bmatrix} J_0 \\ J_1 \\ J_2 \\ \vdots \\ J_{N-1} \end{Bmatrix}_N = \frac{1}{\Delta x} \begin{Bmatrix} E_0 \\ E_1 \\ E_2 \\ \vdots \\ E_{N-1} \end{Bmatrix}_N$$

$$[\mathbf{G}]\{\mathbf{J}\} = \frac{1}{\Delta x} \{\mathbf{E}\}$$

The Matrix $[\mathbf{G}]$ is a $N \times N$ Matrix and is a General Toeplitz Matrix /
Die Matrix $[\mathbf{G}]$ ist eine $N \times N$ -Matrix und ist eine allgemeine Toeplitz-Matrix

All Different Elements of the Matrix $[\mathbf{G}]$ are given by the $2N - 1$ Entries of the 1st Row and 1st Column /
Alle unterschiedlichen Elemente der Matrix $[\mathbf{G}]$ sind durch die $2N - 1$ Einträge der 1. Zeile und 1. Spalte gegeben

$$G_{1-N}, \dots, G_{-2}, G_{-1}, G_0, G_1, G_2, \dots, G_{N-1}$$

$2N - 1$ Elements /
Elemente

CG-FFT: Conjugate Gradient – Fast Fourier Transform / KG-SFT: Konjugierte Gradienten – Schnelle Fourier-Transformation

Discrete Convolution in Matrix Form /
Diskrete Faltung in Matrixform

$$\begin{bmatrix} G_0 & G_{-1} & G_{-2} & \cdots & G_{1-N} \\ G_1 & G_0 & G_{-1} & \cdots & G_{2-N} \\ G_2 & G_1 & G_0 & \cdots & G_{3-N} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ G_{N-1} & G_{N-2} & G_{N-3} & \cdots & G_0 \end{bmatrix}_{N \times N} \begin{Bmatrix} J_0 \\ J_1 \\ J_2 \\ \vdots \\ J_{N-1} \end{Bmatrix}_N = \frac{1}{\Delta x} \begin{Bmatrix} E_0 \\ E_1 \\ E_2 \\ \vdots \\ E_{N-1} \end{Bmatrix}_N$$

$$[\mathbf{G}]\{\mathbf{J}\} = \frac{1}{\Delta x}\{\mathbf{E}\}$$

The Sequenz of the Elements of the Matrix $[\mathbf{G}]$ are Periodic after N Elements /
Die Sequenz der Elemente der Matrix $[\mathbf{G}]$ sind periodisch nach N Elementen

$$G_{n-N} = G_n \quad n = 0, 1, 2, \dots, N-1$$

Then, the Discrete Convolution is a **Circular Discrete Convolution** of the Length $2N-1$ and
the Matrix $[\mathbf{G}]$ is a **Circular Matrix**. Otherwise the Discrete Convolution is a **Linear Discrete Convolution**. /
Dann ist die diskrete Faltung eine zirkulare diskrete Faltung der Länge $2N-1$ und
die Matrix $[\mathbf{G}]$ ist eine zirkulierende Matrix. Anderenfalls ist die diskrete Faltung eine lineare diskrete Faltung.

CG-FFT: Conjugate Gradient – Fast Fourier Transform / KG-SFT: Konjugierte Gradienten – Schnelle Fourier-Transformation

$$\begin{bmatrix} G_0 & G_{-1} & G_{-2} & \cdots & G_{1-N} \\ G_1 & G_0 & G_{-1} & \cdots & G_{2-N} \\ G_2 & G_1 & G_0 & \cdots & G_{3-N} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ G_{N-1} & G_{N-2} & G_{N-3} & \cdots & G_0 \end{bmatrix}_{N \times N} \begin{Bmatrix} J_0 \\ J_1 \\ J_2 \\ \vdots \\ J_{N-1} \end{Bmatrix}_N = \frac{1}{\Delta x} \begin{Bmatrix} E_0 \\ E_1 \\ E_2 \\ \vdots \\ E_{N-1} \end{Bmatrix}_N$$

$$G_{n-N} = G_n \quad n = 0, 1, 2, \dots, N-1$$

Periodic / Periodisch

$$\begin{bmatrix} G_{N-1} & \cdots & G_2 & G_1 & G_0 & G_{-1} & G_{-2} & \cdots & G_{1-N} \\ G_{1-N} & G_{N-1} & \cdots & G_2 & G_1 & G_0 & G_{-1} & \cdots & G_{2-N} \\ G_{2-N} & G_{1-N} & G_{N-1} & \cdots & G_2 & G_1 & G_0 & \cdots & G_{3-N} \\ \vdots & G_{2-N} & G_{1-N} & G_{N-1} & \cdots & \vdots & \vdots & \ddots & \vdots \\ G_{-1} & \cdots & G_{2-N} & G_{1-N} & G_{N-1} & G_{N-2} & G_{N-3} & \cdots & G_0 \end{bmatrix}_{2N-1 \times 2N-1} \begin{Bmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ J_0 \\ J_1 \\ J_2 \\ \vdots \\ J_{N-1} \end{Bmatrix}_{2N-1} = \frac{1}{\Delta x} \begin{Bmatrix} E_0 \\ E_1 \\ E_2 \\ \vdots \\ E_{N-1} \end{Bmatrix}_N$$

CG-FFT: Conjugate Gradient – Fast Fourier Transform / KG-SFT: Konjugierte Gradienten – Schnelle Fourier-Transformation

$$\underbrace{\begin{bmatrix} G_{N-1} & \cdots & G_2 & G_1 & G_0 & G_{-1} & G_{-2} & \cdots & G_{1-N} \\ G_{1-N} & G_{N-1} & \cdots & G_2 & G_1 & G_0 & G_{-1} & \cdots & G_{2-N} \\ G_{2-N} & G_{1-N} & G_{N-1} & \cdots & G_2 & G_1 & G_0 & \cdots & G_{3-N} \\ \vdots & G_{2-N} & G_{1-N} & G_{N-1} & \cdots & \vdots & \vdots & \ddots & \vdots \\ G_{-1} & \cdots & G_{2-N} & G_{1-N} & G_{N-1} & G_{N-2} & G_{N-3} & \cdots & G_0 \end{bmatrix}}_{2N-1 \times 2N-1} \begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ J_0 \\ J_1 \\ J_2 \\ \vdots \\ J_{N-1} \end{bmatrix}_{2N-1} = \frac{1}{\Delta x} \begin{bmatrix} E_0 \\ E_1 \\ E_2 \\ \vdots \\ E_{N-1} \end{bmatrix}_N$$

Periodic / Periodisch

$$\underbrace{\begin{bmatrix} G_0 & G_{-1} & G_{-2} & \cdots & G_{1-N} & G_{N-1} & \cdots & G_2 & G_1 \\ G_1 & G_0 & G_{-1} & \cdots & G_{2-N} & G_{1-N} & G_{N-1} & \cdots & G_2 \\ G_2 & G_1 & G_0 & \cdots & G_{3-N} & G_{2-N} & G_{1-N} & G_{N-1} & \cdots \\ \cdots & \vdots & \vdots & \ddots & \vdots & \vdots & G_{2-N} & G_{1-N} & G_{N-1} \\ G_{N-1} & G_{N-2} & G_{N-3} & \cdots & G_0 & G_{-1} & \cdots & G_{2-N} & G_{1-N} \end{bmatrix}}_{2N-1 \times 2N-1} \begin{bmatrix} J_0 \\ J_1 \\ J_2 \\ \vdots \\ J_{N-1} \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}_{2N-1} = \frac{1}{\Delta x} \begin{bmatrix} E_0 \\ E_1 \\ E_2 \\ \vdots \\ E_{N-1} \end{bmatrix}_N$$

CG-FFT: Conjugate Gradient – Fast Fourier Transform / KG-SFT: Konjugierte Gradienten – Schnelle Fourier-Transformation

Discrete Convolution / Diskrete Faltung $E_m = \Delta x \sum_{n=0}^{N-1} G_{m-n} J_n \quad m = 0, 1, 2, \dots, N-1$

Comment: Every **Linear Discrete Convolution** of the Length N can be formulated in a **Circular Discrete Convolution** of the Length $2N-1$ by Expanding the Sequence G to a Periodic Sequence of the Length $2N-1$. And the Sequence J will be Filled with Zeros up to a Length of $2N-1$: **Zero Padding /**
 Anmerkung: Jede lineare diskrete Faltung der Länge N kann in eine zirkulierende diskrete Faltung der Länge $2N-1$ gebracht werden. Dazu wird die Sequenz G in eine periodische Sequenz der Länge $2N-1$ umgewandelt. Und die Sequenz J wird mit Nullen aufgefüllt: Nullen-Auffüllung

$$\{\mathbf{J}\} = \left\{ \begin{array}{c} J_0 \\ J_1 \\ J_2 \\ \vdots \\ J_{N-1} \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \end{array} \right\}_{2N-1}$$

$\left. \begin{array}{c} \vdots \\ \vdots \\ \vdots \end{array} \right\} N$

$\left. \begin{array}{c} \vdots \\ \vdots \\ \vdots \end{array} \right\} N-1$

**Original Sequence /
Originalsequenz**

**Zero Padding /
Nullen-Auffüllung**

CG-FFT: Conjugate Gradient – Fast Fourier Transform / KG-SFT: Konjugierte Gradienten – Schnelle Fourier-Transformation

$$E_m = \Delta x \sum_{n=0}^{N-1} G_{m-n} J_n \quad m = 0, 1, 2, \dots, N-1 \quad \mathcal{O}(N^2)$$

**The Fast Fourier Transform (FFT) is an Efficient Way of Implementation the Discrete Fourier Transform (DFT) /
Die schnelle Fourier-Transformation (SFT) ist ein effizienter Weg der Implementierung der diskreten Fourier-Transformation (DFT)**

$$\tilde{G}_n = \sum_{k=0}^{N-1} G_k e^{-j2\pi nk/N} \quad n = 0, 1, 2, \dots, N-1$$

$$G_k = \frac{1}{N} \sum_{n=0}^{N-1} \tilde{G}_n e^{j2\pi nk/N} \quad k = 0, 1, 2, \dots, N-1$$

N is a Power of /
ist eine Potenz von $2 \rightarrow N = 2^p, p = 0, 1, 2, 3, \dots$

$$\{\tilde{\mathbf{G}}\} = \mathcal{FFT}_N \{\mathbf{G}\}$$

$$\{\mathbf{G}\} = \mathcal{FFT}_N^{-1} \{\tilde{\mathbf{G}}\}$$

$$\mathcal{FFT}_N \{\mathbf{E}\} = \Delta x \mathcal{FFT}_N \{\mathbf{G}\} \mathcal{FFT}_N \{\mathbf{J}\} \quad n = 0, 1, 2, \dots, N-1$$

$$\{\mathbf{E}\} = \Delta x \mathcal{FFT}_N^{-1} \{ \mathcal{FFT}_N \{\mathbf{G}\} \mathcal{FFT}_N \{\mathbf{J}\} \} \quad n = 0, 1, 2, \dots, N-1 \quad \mathcal{O}(N \log N)$$

**End of 7th Lecture /
Ende der 7. Vorlesung**