ELECTROMAGNETIC WAVEFIELD COMPUTATION - A RECIPROCITY-BASED STRUCTURED APPROACH

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The **objective** is to construct a **computational discretization** of the (forward) electromagnetic wave problem that is

- as **coherent** and **internally consistent** as possible
- as **close** as possible to the **physics of the problem**

Type of **configuration**:

- arbitrary piecewise continuous distribution of constitutive parameters
- arbitrary piecewise continuous volume source distributions

Computational (discretization) procedure:

- We **want** $\Longrightarrow$ **approximate solution** to **exact problem**
- We **get** $\Longrightarrow$ **exact solution** to **approximate problem**

Questions:

- **Exact solution** to **approximate problem** $\stackrel{?}{\simeq}$ **approximate solution** to **exact problem**
- What do we mean by $\simeq$?

Computational procedure (general)

The **exact problem** involves **pointwise (= local) satisfaction** of:

- **Space/time partial differential equations (Maxwell's equations)**
- **compatibility relations** (existence conditions)
- **interface boundary conditions** (uniqueness conditions in space)
- **causality conditions** (uniqueness conditions in time)
- **embedding procedure for unbounded domains** (embedding has analytically known Green's functions)

Exact problem (mapping physics on to mathematics)

A computational procedure **replaces** the **exact problem** by an **equivalent weak formulation**, where

- **weak formulation = global (integral) formulation (on domain of computation) that meets the conditions that**
  - **invoking it for any field necessarily leads to the exact (local) problem**

  and
  - **delta distributions are avoided**

Computational procedure (weak formulation of the problem)

Appropriate **weak formulations** of the **electromagnetic space/time partial differential equations are:**

- **Lorentz's time-convolution reciprocity relation**
- **space-time integrated Maxwell equations***

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* These are a special case of the time-convolution Lorentz reciprocity relation

The **weak formulation of the electromagnetic wavefield problem** involves **satisfaction** of:

- **LORENTZ'S TIME-CONVOLUTION RECIPROCITY RELATION** over the **domain of computation**
- **compatibility relations**
- **interface boundary conditions**
- **causality conditions**
- **embedding procedure for unbounded domains** (embedding has analytically known Green's functions)

Spatial-temporal discretization procedure of a **time-invariant** configuration:

- the configuration is **spatially discretized** into **subdomains**
  - where the **medium properties** vary **continuously differentiably with position**
  - the **boundaries of which** fit interfaces up to $o(h)$ as $h \to 0$
- the **wavefield quantities** are replaced by **expansions** that **approximate** them up to $o(h)$ as $h \to 0$
- h = **mesh size** of the spatial discretization (maximum diameter of the **"geometrical elements"**)

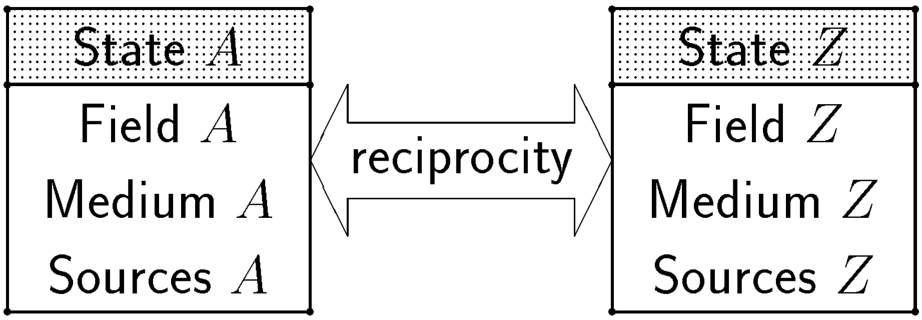
The physical **wavefield constituents** that characterize an **electromagnetic STATE** are:

- the **sources** that generate the field (**excitation**)
- the **medium** in which the field is present (**propagation**)
- the **wavefield state quantities** through which the field is accessible to measurement (**reception**)

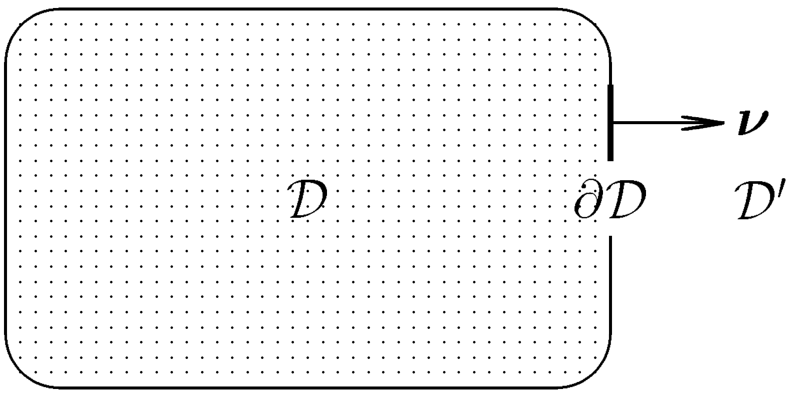
LORENTZ RECIPROCITY = TIME-CONVOLVED INTERACTION OF TWO STATES OVER BOUNDED DOMAIN IN SPACE

Wavefield constituents and reciprocity

- **The two States A and Z:**



- **Domain of application:**



In the reciprocity theorem of the time-convolution type, applied to the domain of computation, we substitute

- **State A = global expansions of field and source quantities**
- **State Z = sequence of suitable "computational" States C**

Depending on the **choice of State C**, the

- **finite-element method**
- **integral-equation method**
- **domain integration method**

result

To generate the **system of equations in the expansion coefficients** of the discretized wave-field problem

- **Satisfy EXACTLY** all physical conditions that can be satisfied exactly
- Subject each physical condition that cannot be satisfied exactly to a **MINIMIZATION PROCEDURE** operating on a suitable **ERROR CRITERION**

Generation procedure of discretized system of equations

Solution procedure of the discretized system of equations in the expansion coefficients:

- Subject the (overdetermized) system of equations to a **MINIMIZATION PROCEDURE** operating on a suitable **ERROR CRITERION**
- Apply an **ITERATIVE SOLUTION PROCEDURE** with a **guaranteed decrease** in the **norm of the misfit**

Solution procedure of discretized system of equations

Wave phenomena are phenomena in

- **(three-dimensional) space** ($\boldsymbol{x} \in \boldsymbol{\mathcal{R}}^3$)

and

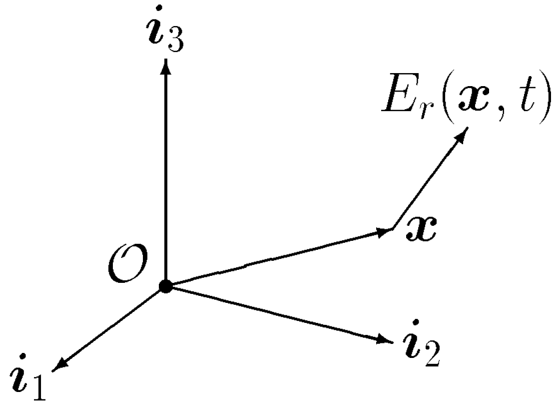
- **time** ($t \in \mathcal{R}$)

They

- are **causally related to the action of their sources**
- **transfer energy from source to receiver**
- **SHARE** the property of **RECIPROCITY**

Wave phenomena (some general characteristics)

Reference frame in $\mathcal{R}^3$:



Position vector:

- $\boldsymbol{x} = x_1\boldsymbol{i}_1 + x_2\boldsymbol{i}_2 + x_3\boldsymbol{i}_3$

Subscript notation, summation convention:

- $\epsilon_{k,r}E_r = \Sigma_{r=1}^{3}\,\epsilon_{k,r}E_r$ for $k = 1, 2, 3$
- ∂_m = derivative with respect to x_m

Cartesian reference frame, subscript notation

- **Electromagnetic wave quantities**:

$$E_r = \text{electric field strength (V/m)}$$
$$H_p = \text{magnetic field strength (A/m)}$$
$$D_k = \text{electric flux density (C/m}^2\text{)}$$
$$B_j = \text{magnetic flux density (T)}$$

- **Electromagnetic source quantities**:

$$J_k = \text{volume source density of electric current (A/m}^2\text{)}$$
$$K_j = \text{volume source density of magnetic current (V/m}^2\text{)}$$

Electromagnetic wave and source quantities

- **Electromagnetic medium parameters for an inhomogeneous, anisotropic medium with relaxation**:

$$\kappa^{\mathrm{e}}_{k,r} = \text{electric relaxation function (F/m·s)}$$
$$\kappa^{\mathrm{m}}_{j,p} = \text{magnetic relaxation function (H/m·s)}$$

- **Electromagnetic constitutive relations**:

$$D_k = \kappa^{\mathrm{e}}_{k,r} \overset{(t)}{*} E_r$$
$$B_j = \kappa^{\mathrm{m}}_{j,p} \overset{(t)}{*} H_p$$

where

$$\overset{(t)}{*} = \text{time convolution}$$

- **Electromagnetic constitutive relations for a simple inhomogeneous, anisotropic medium**:

$$\partial_t D_k = \sigma_{k,r} E_r + \epsilon_{k,r} \partial_t E_r$$
$$\partial_t B_j = \chi_{j,p} H_p + \mu_{j,p} \partial_t H_p$$

where

$\sigma_{k,r}$ = conductivity (S/m)

$\epsilon_{k,r}$ = permittivity (F/m)

$\chi_{j,p}$ = linear magnetic hysteresis loss coefficient (H·s/m)

$\mu_{j,p}$ = permeability (H/m)

Electromagnetic medium properties (continued)

- **Electromagnetic field equations**:

$$-\epsilon_{k,m,p}\partial_m H_p + \partial_t D_k = -J_k$$
$$\epsilon_{j,n,r}\partial_n E_r + \partial_t B_j = -K_j$$

- **Electromagnetic compatibility relations**:

$$\int_{\mathcal{S}} \nu_k \partial_t D_k \mathrm{d}A = -\int_{\mathcal{S}} \nu_k J_k \mathrm{d}A$$
$$\int_{\mathcal{S}} \nu_j \partial_t B_j \mathrm{d}A = -\int_{\mathcal{S}} \nu_j K_j \mathrm{d}A$$

for any closed surface $\mathcal{S}$ ($\nu_m =$ unit vector along outward normal to $\mathcal{S}$)

- **Levi-Civita tensor**:

$\epsilon_{k,m,p} = \{+1, -1, 0\}$ if $\{k, m, p\}$ is {even, odd, no} permutation of $\{1, 2, 3\}$

Electromagnetic field equations, compatibility relations

- **Interface boundary conditions**: across any surface of discontinuity in medium properties

$$\begin{aligned} \boldsymbol{\epsilon}_{k,m,p}\nu_m H_p &= \text{continuous} \\ \boldsymbol{\epsilon}_{j,n,r}\nu_n E_r &= \text{continuous} \end{aligned}$$

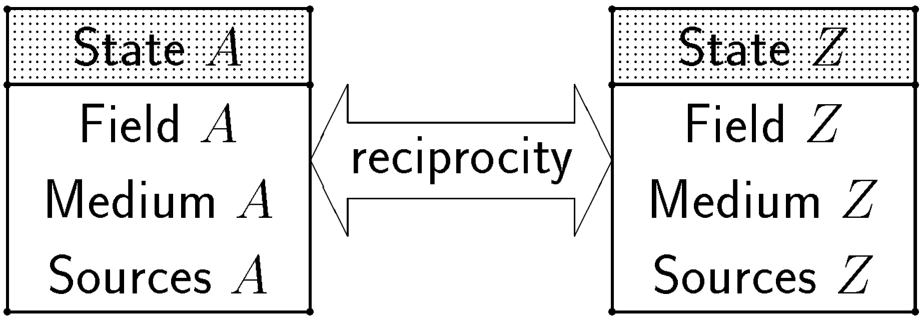
$\nu_m =$ unit vector along the normal to the interface

- **Compatibility boundary conditions**: across any surface of discontinuity in medium properties and/or volume source distributions

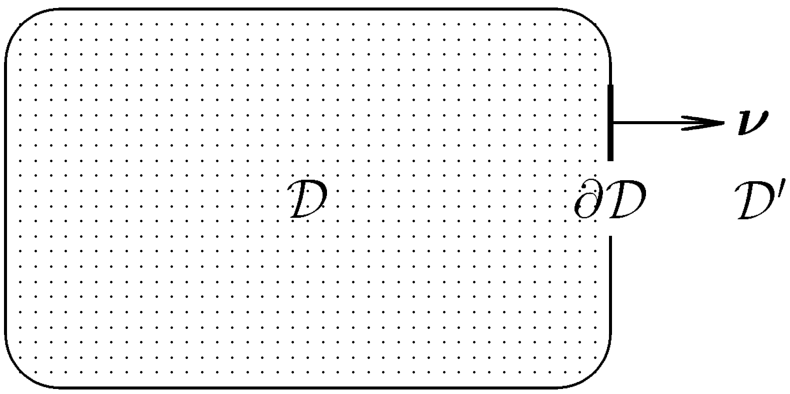
$$\begin{aligned} \nu_k(\partial_t D_k + J_k) &= \text{continuous} \\ \nu_j(\partial_t B_j + K_j) &= \text{continuous} \end{aligned}$$

$\nu_k =$ unit vector along the normal to the surface of discontinuity

- **The two States A and Z:**



- **Domain of application:**



- **Electromagnetic reciprocity theorem of the time-convolution type**:

$$\epsilon_{m,r,p} \int_{\partial\mathcal{D}} \nu_m [E_r^A \overset{(t)}{*} H_p^Z - E_r^Z \overset{(t)}{*} H_p^A] \mathrm{d}A$$

$$= \int_{\mathcal{D}} [\partial_t D_k^A \overset{(t)}{*} E_k^Z - \partial_t D_r^Z \overset{(t)}{*} E_r^A$$

$$-\partial_t B_j^A \overset{(t)}{*} H_j^Z + \partial_t B_p^Z \overset{(t)}{*} H_p^A] \mathrm{d}V$$

$$+ \int_{\mathcal{D}} [J_k^A \overset{(t)}{*} E_k^Z - K_j^A \overset{(t)}{*} H_j^Z$$

$$-J_r^Z \overset{(t)}{*} E_r^A + K_p^Z \overset{(t)}{*} H_p^A] \mathrm{d}V$$

- **The reciprocity relation is a "weak" formulation of the field problem: for the theorem to hold for arbitrary States Z, State A must satisfy the field equations**

Reciprocity theorem of the time-convolution type

- **Reciprocity theorem**

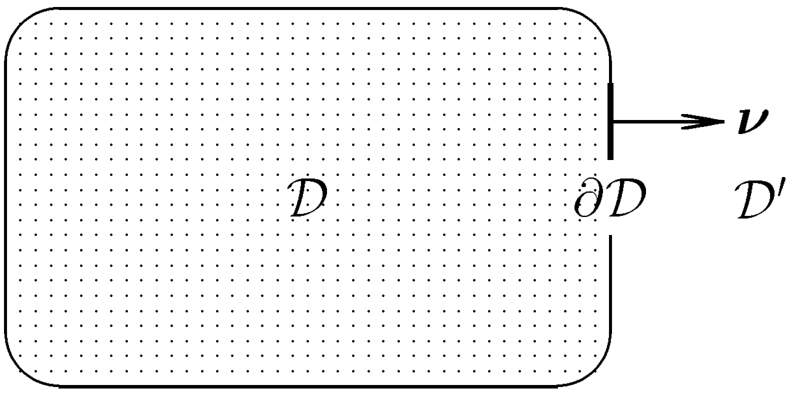
$$\int_{\partial\mathcal{D}} \text{[surface interaction term]}_m \nu_m \mathrm{d}A$$
$$= \int_{\mathcal{D}} \text{[domain interaction terms]} \mathrm{d}V$$

  - [domain interaction terms]

    $= \text{[contrast in media terms]}$

    $+\text{[source/field interaction terms]}$

- **Domain of application:**



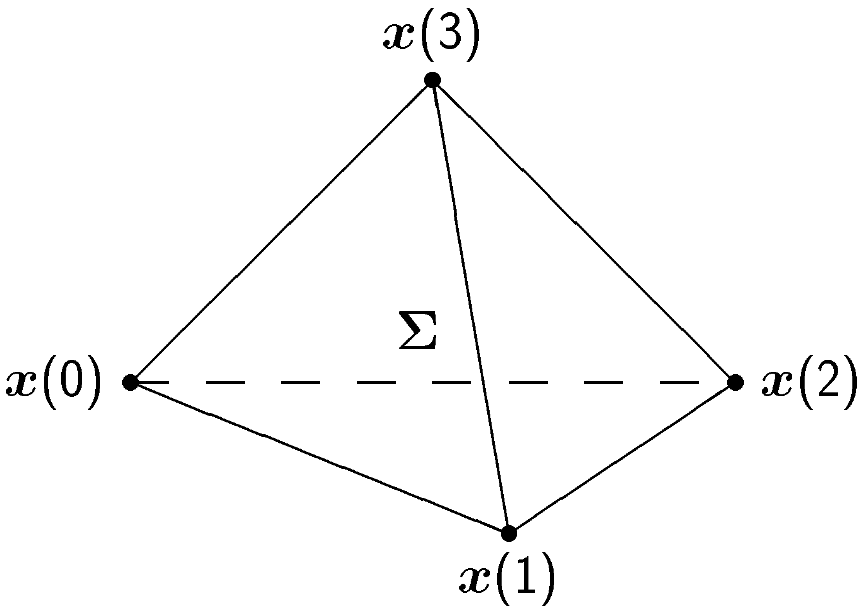
Reciprocity theorem (general structure)

Consistently linear, local expansions can be defined on a

- **simplicial mesh**, i.e., a mesh consisting of **simplices** (tetrahedra in $\mathcal{R}^3$), all having **vertices, edges** and **faces** in common

The mesh enables one to:

- **Represent space-time quantities as expansions up to $o(h)$ as $h \to 0$**
- **Approximate interfaces up to $o(h)$ as $h \to 0$**



Oriented **simplex** $\boldsymbol{\Sigma}$ in $\mathcal{R}^3$ with

ordered set of vertices

$$\{\boldsymbol{x}(0), \boldsymbol{x}(1), \boldsymbol{x}(2), \boldsymbol{x}(3)\}$$

Simplex in $\mathcal{R}^3$ (tetrahedron)

• **Vectorial edges** leaving the vertex $\boldsymbol{x}(I)$:

$$\{\boldsymbol{x}(J) - \boldsymbol{x}(I)\} \text{ for } I = 0,1,2,3; J = 0,1,2,3; \\ I \neq J$$

• Outwardly oriented **vectorial faces** meeting at the vertex $\boldsymbol{x}(I)$:

$$\{\boldsymbol{A}(J)\} \text{ for } I = 0,1,2,3; J = 0,1,2,3; I \neq J$$

where

• $\boldsymbol{A}(I) =$ outwardly oriented **face opposite the vertex** $\boldsymbol{x}(I)$

Vectorial edges and faces of a simplex in $\mathcal{R}^3$

- **Property:**

  $$[x_m(J) - x_m(I)]A_m(K)$$
  $$-3V_\Sigma[\delta(J,K) - \delta(I,K)]$$
  for $I = 0,1,2,3;\ J = 0,1,2,3;\ K = 0,1,2,3$

where

- V_Σ is the **volume** of Σ

$\Longrightarrow$ **At the vertex $\boldsymbol{x}(I)$, the set of base vectors $\{\boldsymbol{x}(J) - \boldsymbol{x}(I); I \neq J\}$ is reciprocal to the set of base vectors $\{-(3V_\Sigma)^{-1}\boldsymbol{A}(K); K \neq I\}$**

Base vectors at the vertex of a simplex Σ

All field quantities, medium parameters and source quantities are locally (i.e. in each tetrahedron Σ) represented as

• **spatially linear interpolations**

of their values at the vertices of Σ

Vertex-based local representation

• A **vertex-based** representation is a local, spatially linear representation of a scalar, vector or tensor quantity whose vertex values are **decomposed along the axes of the background Cartesian reference frame**

Local, spatially linear (vertex-based) representation

Edge-based local vector representation

• An **edge-based** representation is a local, spatially linear representation of a vector quantity whose vertex "components" are **the projections of that vector on the vectorial edges leaving that vertex**

Face-based local vector representation

• A **face-based** representation is a local, spatially linear representation of a vector quantity whose vertex "components" are **the projections of that vector on the vectorial faces meeting at that vertex**

Edge- and face-based local vector representation

The **number of local expansion coefficients of a vector quantity** in a tetrahedron is:

- *Vertex-based representation*:

  4 (vertices) $\times$ 3 (components)

- *Edge-based representation*:

  6 (edges) $\times$ 2 (projections)

- *Face-based representation*:

  4 (faces) $\times$ 3 (projections)

Number of local expansion coefficients (vector quantity)

The **global representations of the field quantities** $\{E_r, H_p, D_k, B_j\}$ on the discretized geometry are constructed out of their

- **local representations**

plus the application of the

- **interface boundary conditions** to the **edge-based** expansion coefficients of $\{E_r, H_p\}$
- **compatibility boundary conditions** to the **face-based** expansion coefficients of $\{D_k, B_j\}$

The **global representations** of the

- **medium parameters** $\{\kappa^{\mathrm{e}}_{k,r}, \kappa^{\mathrm{m}}_{j,p}\}$

and the

- **source quantities** $\{J_k, K_j\}$

on the discretized geometry are constructed out of their

- **local vertex-based representations**

Global representations (medium parameters, sources)

To accomodate **radiation problems** without explicit boundary conditions on the boundary of the domain of computation, an **embedding procedure** is applied; the **embedding** has:

- $\mathcal{R}^3$ as support
- **medium parameters** $\{\kappa^{\mathrm{e;b}}_{k,r}, \kappa^{\mathrm{m;b}}_{j,p}\}$, such that the **Green's functions (point-source solutions)** are **analytically known**

$\Longrightarrow$ Field computation problem can be reformulated as a **scattering problem** with **contrast source distributions** that have the contrasting domain of computation as their support

Computational steps:

- Substitute **Global expansions** of **flux densities & volume source densities** in the **compatibility relations** applied to **each geometrical element** of the discretized configuration
- Substitute **Global expansions** of **flux densities, field strengths & constitutive parameters** in the **constitutive relations** and subject these to the **minimization** of an appropriate **error criterion**
- Take **Global expansions** of **flux densities, field strengths & volume source densities** as **State A** in the **reciprocity relation**

Computational steps

Computational state:

- Substitute for **State** Z in the reciprocity relation a **sequence of computational States** C, with the **property** that they **formally are 'electromagnetic fields'**. The **choice** of the **sequence** $\{$**States** $C\}$ determines the **type of computational algorithm**, for example,
  - **finite-element method**
  - **integral-equation method**
  - **domain integration method**

The **finite-element method** is characterized by the **computational state:**

- **medium parameters**$^{C} = 0$
  $\Longrightarrow$ • **flux densities**$^{C} = 0$
- $\{$**field strengths**$\}^{C} \in \delta(t)\{$**edge-based global expansion functions**$\}$
  $\Longrightarrow$ • **corresponding** $\{$**volume source densities**$\}^{C}$

Finite-element method (computational state)

The **passive, causal radiation into the embedding** is modeled by ('aborbing boundary condition')

- **interrelating** the **field strengths & flux densities** of the **scattered field** at the **vertices** on the **boundary of the domain of computation** to their **contrast volume source densities** via the (analytically known) **Green's functions of the embedding**

The **integral-equation method** is characterized by the **computational state:**

- **medium parameters**^{C} = **adjoint medium parameters of embedding**
- $\{$**volume source densities**$\}^{C}$ $\in$ $\delta(t)\{$**vertex-based local expansion functions**$\}$
  $\Longrightarrow$ • **corresponding** $\{$**field strengths, flux densities of scattered field**$\}^{C}$ through **Green's functions of the embedding**

Integral equation method (computational state)

Integral-equation method (final step)

- **minimize the discrepancy in the two resulting expressions for the contrast volume source densities** over the **domain of computation**

The **domain integration method** is characterized by the **computational state:**

- **medium parameters**$^C = 0$

  $\Longrightarrow$ • **flux densities**$^C = 0$

- $\{$**field strengths**$\}^C \in \delta(t)\{$**global constant**$\}$

  $\Longrightarrow$ • $\{$**volume source densities**$\}^C = \mathbf{0}$

Domain integration method (computational state)

The **passive, causal radiation into the embedding** is modeled by ('aborbing boundary condition')

- **interrelating** the **field strengths & flux densities** of the **scattered field** at the **vertices** on the **boundary of the domain of computation** to their **contrast volume source densities** via the (analytically known) **Green's functions of the embedding**

Note:

In the substitution of the computational states in the reciprocity theorem of the time-convolution type, the value of the chosen constant drops out and the resulting equations are the same as when the field equations are integrated over the domain of computation and Gauss' integral theorem is applied. The latter **domain integration method** can therefore also be approached directly.

Operator equation to be "solved":

- $\mathsf{L}u \simeq q$

Inner product:

- $< v, u >$ with
- $< v, u > = < u, v >^*$
- $< v, \mathsf{L}u > = < \mathsf{L}^{\mathsf{H}} v, u >$

  ($\mathsf{L}^{\mathsf{H}} =$ **Hermitean conjugate** of L)

Associated norm:

- $||u|| = < u, u >^{1/2}$

Residual:

- $r = q - \mathsf{L}u$

Operator equation, inner product, norm, residual

Iterative solution procedure:

- $u^{[n+1]} = u^{[n]} + \delta u^{[n]}$ for $n = 0, 1, 2, \ldots$

Residual after n steps:

- $r^{[n]} = q - \mathsf{L}u^{[n]}$ for $n = 0, 1, 2, \ldots$

  $\Longrightarrow r^{[n+1]} = r^{[n]} - \mathsf{L}\delta u^{[n]}$

"Improvement condition":

- $||r^{[n]}||^2 > ||r^{[n+1]}||^2$ for $n = 0, 1, 2, \ldots$

Sufficient condition for improvement:

- $< r^{[n+1]}, \mathsf{L}\delta u^{[n]} > + < \mathsf{L}\delta u^{[n]}, r^{[n+1]} >= 0$

which is satisfied by*

- $\delta u^{[n]} = \alpha^{[n]}\mathsf{L}^{\mathsf{H}} r^{[n]}$ with • $\alpha^{[n]} = \frac{||\mathsf{L}^{\mathsf{H}} r^{[n]}||^2}{||\mathsf{L}\mathsf{L}^{\mathsf{H}} r^{[n]}||^2}$

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*More sophisticated choices for $\delta u^{[n]}$ exist

Iterative solution procedure, "improvement condition"

CONCLUSION:

The RECIPROCITY THEOREM of the TIME-CONVOLUTION TYPE yields the BASIS for a STRUCTURED APPROACH to the problems of WAVEFIELD COMPUTATION

Mapping of **causal time functions** to the **complex frequency domain** takes place via the **Laplace transformation**:

- $\hat{u}(\boldsymbol{x}, s) = \int_{t_0}^{\infty} \exp(-st) u(\boldsymbol{x}, t) \mathrm{d}t$
  for $\{s \in \mathcal{C}, \mathrm{Re}(s) > s_0\}$

Properties:

- $\partial_t \to s$
- $u(\boldsymbol{x}, t) \overset{(t)}{*} v(\boldsymbol{x}, t) \to \hat{u}(\boldsymbol{x}, s)\hat{v}(\boldsymbol{x}, s)$
- **Real frequences:** $s = \mathrm{j}\omega$ with $\omega \in \mathcal{R}$

- The spatial discretization parts run parallel to the ones for the time-domain analysis