Electromagnetic Field Computation in Strongly Heterogeneous Media – The Numerics that Models the Physics

by

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Synopsis:

- Introduction and motivation
- Description of the configuration
- EM field equations in strongly heterogeneous media
- EM field equations in the discretized geometry
- EM field expansions in the discretized geometry:
  Edge expansions, Face expansions
- The 3D Cartesian coordinate-stretched Perfectly Matched Embedding
- Equivalent system of field relations in the (truncated) embedding

A Maxwell (EM) field problem consists of the following **ingredients:**

- **Coupled system of field equations** interrelating the space-time behavior of the field quantities
- **System of constitutive relations** representative of the physical behavior of vacuum and matter (active and passive)
- **Set of initial conditions** in accordance with the property of **causality**
- **Set of conditions representing the radiation into an unbounded embedding (universe)** in accordance with the property of **causality**

such that

- **UNIQUENESS HOLDS**

Ingredients of a (uniquely solvable) Maxwell (EM) field problem

The **geometrical structure of space-time** $(\mathbb{R}^3 \times \mathbb{R})$:

- $\boldsymbol{x} = x_1\boldsymbol{i}_1 + x_2\boldsymbol{i}_2 + x_3\boldsymbol{i}_3 \in \mathbb{R}^3$ = Cartesian position vector in space
- $\{x_1, x_2, x_3\} \in \mathbb{R}^3$ = Cartesian position coordinates
- $t \in \mathbb{R}$ = time coordinate

\+ the **physics of EM phenomena** imply $\Longrightarrow$

- **Admissible EM field quantities:** Piecewise continuous, real-valued, Cartesian tensors of **Rank 1** (vectors)
- **Admissible EM source quantities (active part in the constitutive relations):** Piecewise continuous, real-valued, Cartesian tensors of **Rank 1** (vectors)
- **Admissible EM constitutive functionals (passive part in the constitutive relations):** Piecewise continuous, real-valued Cartesian tensors of **Rank 2**

Proof of **UNIQUENESS** implies [DeHoop, 2003] $\Longrightarrow$

- **Admissible constitutive behavior of matter:**
  - Linear
  - Time invariant
  - Locally reacting
  - Causally reacting
- **Causality can only be handled via the**
  TIME LAPLACE TRANSFORMATION:

•$\hat{F}(\boldsymbol{x}, s) = \int_{t=t_0}^{\infty} \exp(-st)F(\boldsymbol{x}, t)\mathrm{d}t$ analytic for $s \in \mathbb{C}, \mathrm{Re}(s) > 0$

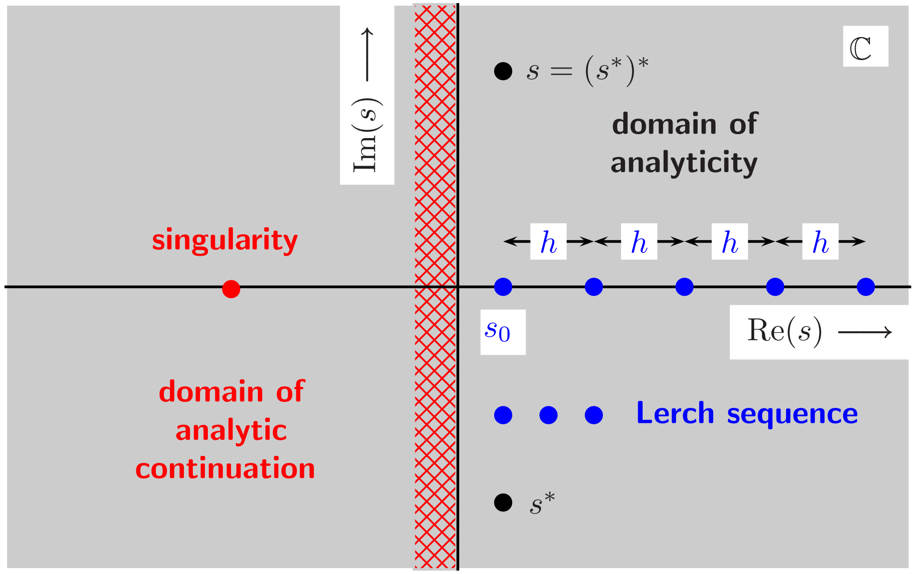
•$\hat{F}(\boldsymbol{x}, s) = o(1)$ as $|s| \to \infty$ in $s \in \mathbb{C}, \mathrm{Re}(s) \geq 0$

•$\hat{F}(\boldsymbol{x}, s^*) = \hat{F}^*(\boldsymbol{x}, s)$ (*=complex conjugate) (Schwarz' reflection principle)

Admissible constitutive behavior of matter – Time Laplace transformation

The time Laplace transformation (properties)

- $\hat{F}(\boldsymbol{x}, s) = \int_{t=t_0}^{\infty} \exp(-st) F(\boldsymbol{x}, t) \mathrm{d}t$ analytic for $s \in \mathbb{C}, \mathrm{Re}(s) > 0$



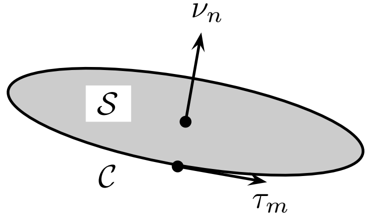
LERCH's uniqueness theorem

- $\{\hat{F}(\boldsymbol{x}, s_0 + nh); s_0 > 0, h > 0, n = 0, 1, 2, \ldots\} \Longrightarrow F(\boldsymbol{x}, t) H(t - t_0)$

The geometrical (tensorial) structure of EM fields in space-time $\mathbb{R}^3 \times \mathbb{R}$:

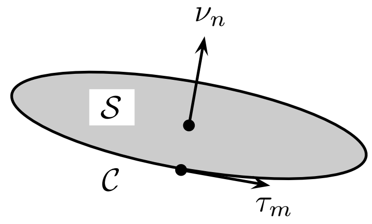
- At any time $t \in \mathbb{R}$ each EM field quantity or constitutive coefficient is a (Cartesian) **TENSOR** for $x_m \in \mathbb{R}^3$
- The (Cartesian) components of a tensor are denoted by **SUBSCRIPTED SYMBOLS** ('subscript notation')
- The number of subscripts is equal to the **RANK** of the tensor
  (tensor of rank 0 = scalar; tensor of rank 1 = vector)
- Repeated subscripts in a product indicate **SUMMATION** over the number of dimensions ('summation convention')
- **LEVI-CIVITA TENSOR** $\epsilon_{i,j,k}$ (completely anti-symmetric tensor of rank 3):
  $\epsilon_{i,j,k} = 1$ if $\{i,j,k\}$ = even permutation of $\{1,2,3\}$, $\epsilon_{i,j,k} = -1$ if $\{i,j,k\}$ = odd permutation of $\{1,2,3\}$, $\epsilon_{i,j,k} = 0$ if $\{i,j,k\}$ are not all different

EM field topology in space-time



- $\mathcal{C} \subset \mathbb{R}^3$: Bounded, oriented, closed curve with piecewise continuously turning unit vector along its tangent τ_m
  - $x_m = \xi_m(\lambda)$ for $0 \leq \lambda < L$ with $\xi_m(\lambda + L) = \xi_m(\lambda)$ ($\lambda =$ arc length)
  - $\tau_m = \partial_\lambda \xi_m(\lambda)$
- $\mathcal{S} \subset \mathbb{R}^3$: Bounded, oriented, surface with piecewise continuously turning unit vector along its normal ν_n and $\mathcal{C}$ as its boundary curve
  - $\Sigma(x_1, x_2, x_3) = 0$
  - $\nu_n = \dfrac{\pm\, \partial_n \Sigma(x_1, x_2, x_3)}{[\partial_n \Sigma(x_1, x_2, x_3) \partial_n \Sigma(x_1, x_2, x_3)]^{1/2}}$
  - $\epsilon_{n,p,m} \nu_n (\xi_p - x_p) \tau_m > 0$ **(right-handed orientation)**

Stokes' theorem:



For any piecewise continuously **differentiable** scalar field $\phi(x_1, x_2, x_3, t)$:

- $$\oint_{\mathcal{C}} \tau_m \phi \, \mathrm{d}\lambda = \epsilon_{m,n,p} \int_{\mathcal{S}} \nu_n \partial_p \phi \, \mathrm{d}A$$

For any piecewise continuously **differentiable** vector field $F_m(x_1, x_2, x_3, t)$ (take, successively: $m = 1, \phi = F_1$; $m = 2, \phi = F_2$; $m = 3, \phi = F_3$ and add the results):

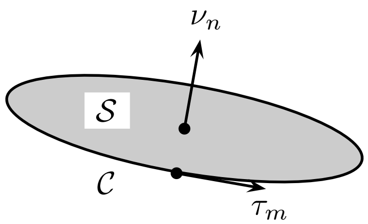
- $$\underbrace{\oint_{\mathcal{C}} \tau_m F_m \mathrm{d}\lambda}_{} = \epsilon_{m,n,p} \int_{\mathcal{S}} \nu_n \partial_p F_m \mathrm{d}A = \underbrace{\int_{\mathcal{S}} \nu_n \epsilon_{n,p,m} \partial_p F_m \mathrm{d}A}_{}$$

circulation of F_m along $\mathcal{C}$

flux of $\epsilon_{n,p,m}\partial_p F_m$ across $\mathcal{S}$

Stokes' theorem

Global EM field relations for EM field topology and time interval $\mathcal{T} \subset \mathbb{R}$ with boundary points $\partial\mathcal{T}$:

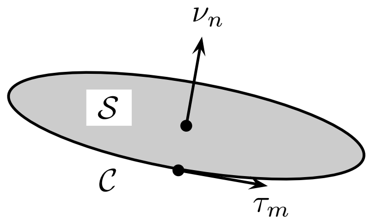


- $\int_{\mathcal{T}}$ [circulation of **magnetic field** along $\mathcal{C}$] $\mathrm{d}t =$ [**electric flux** across $\mathcal{S}$]$|_{\partial\mathcal{T}}$
  - $\int_{\mathcal{T}}$ [circulation of **electric field** along $\mathcal{C}$] $\mathrm{d}t = -$ [**magnetic flux** across $\mathcal{S}$]$|_{\partial\mathcal{T}}$

Global EM field compatibility relations:

- outward electric flux across closed surface $= 0$
- outward magnetic flux across closed surface $= 0$

The **EM field quantities:**



- circulation of **electric field** along $\mathcal{C} = \oint_{\mathcal{C}} E_r \tau_r \mathrm{d}\lambda$

  $\Longrightarrow E_r =$ electric field strength (V/m)

- circulation of **magnetic field** along $\mathcal{C} = \oint_{\mathcal{C}} H_p \tau_p \mathrm{d}\lambda$

  $\Longrightarrow H_p =$ magnetic field strength (A/m)

- **electric flux** across $\mathcal{S} = \int_{\mathcal{S}} D_i \nu_i \mathrm{d}A$

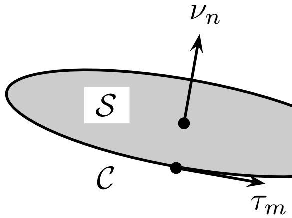
  $\Longrightarrow D_i =$ electric flux density (C/m^2)

- **magnetic flux** across $\mathcal{S} = \int_{\mathcal{S}} B_j \nu_j \mathrm{d}A$

  $\Longrightarrow B_j =$ magnetic flux density (T)

The electric and magnetic field strengths and flux densities

Global EM field equations (starting point for EM field computation in strongly heterogeneous media):



- $$\int_{\mathcal{T}} \mathrm{d}t \oint_{\mathcal{C}} H_p \tau_p \mathrm{d}\lambda = \int_{\mathcal{S}} D_i \nu_i \mathrm{d}A \Big|_{\partial \mathcal{T}}$$
- $$\int_{\mathcal{T}} \mathrm{d}t \oint_{\mathcal{C}} E_r \tau_r \mathrm{d}\lambda = -\int_{\mathcal{S}} B_j \nu_j \mathrm{d}A \Big|_{\partial \mathcal{T}}$$

Global EM compatibility relations:

- $\int_{\text{closed surface}} D_i \nu_i \mathrm{d}A = 0$ (ν_i = unit vector along outward normal)
- $\int_{\text{closed surface}} B_j \nu_j \mathrm{d}A = 0$ (ν_j = unit vector along outward normal)

The global EM field equations

Local EM field equations for differentiable fields (unsuitable for EM field computation in strongly heterogeneous media):

- $\epsilon_{i,m,p}\partial_m H_p = \partial_t D_i$ for $x_m \in \mathbb{R}^3, t \in \mathbb{R}$ **(Maxwell 1)**
- $\epsilon_{j,n,r}\partial_n E_r = -\partial_t B_j$ for $x_m \in \mathbb{R}^3, t \in \mathbb{R}$ **(Maxwell 2)**

$\Longrightarrow$ **NUMBER OF UNKNOWNS = 2 * NUMBER OF EQUATIONS**

$\Longrightarrow$ to be supplemented by **CONSTITUTIVE RELATIONS**

Local EM compatibility relations (existence conditions for Maxwell 1 & Maxwell 2):

- $\partial_i D_i = 0$ for $x_m \in \mathbb{R}^3, t \in \mathbb{R}$
- $\partial_j B_j = 0$ for $x_m \in \mathbb{R}^3, t \in \mathbb{R}$

The local EM field equations (differentiable field quantities)

Local EM constitutive relations in vacuum (SI):

- $D_i(x_m, t) = \epsilon_0 \delta_{i,r} E_r(x_m, t)$ • $B_j(x_m, t) = \mu_0 \delta_{j,p} H_p(x_m, t)$
- $\mu_0 = 4\pi * 10^{-7}$ H/m (permeability of vacuum)
- $\epsilon_0 = 1/\mu_0 c_0^2$ F/m (permittivity of vacuum)
- $c_0 = 299792458$ m/s (EM wavespeed in vacuum)
- $\delta_{i,j} = \{1, 0\}$ for $\{i = j, i \neq j\}$ (Kronecker tensor)

Macroscopic EM constitutive relations in matter: volume averaging

over $\mathcal{D}_\in$ ($\mathcal{D}_\in$ = representative elementary domain, x_m = barycenter of $\mathcal{D}_\in$) of the (causal) response of (classical or quantum) atomic models $\Longrightarrow$

$$\{E_r, H_p\}(x_m, t')|_{t' \in (-\infty < t' \leq t)} \longmapsto \{D_i, B_j\}(x_m, t) \quad \textbf{(general)}$$

$$E_r(x_m, t')|_{t' \in (-\infty < t' \leq t)} \longmapsto D_i(x_m, t) \qquad H_p(x_m, t')|_{t' \in (-\infty < t' \leq t)} \longmapsto B_j(x_m, t)$$

(most materials)

LORENTZ's theory of electrons:

- $D_i = \epsilon_0 E_i + P_i^{\rm ind} + P_i^{\rm ext}$
- $B_j = \mu_0 H_j + M_j^{\rm ind} + M_j^{\rm ext}$
- $P_i^{\rm ind}$ = (field-dependent) induced electric polarization (C/m^2)
  = atomic mechanical response to electric field excitation
  (electric force on electric charge)
- $P_i^{\rm ext}$ = (field-independent) external electric polarization (C/m^2)
- $M_j^{\rm ind}$ = (field-dependent) induced magnetization (T)
  = atomic mechanical response to magnetic field excitation
  (magnetic force on orbital electric charge and torque on magnetic spin)
- $M_j^{\rm ext}$ = (field-independent) external magnetization (T)

UNIQUENESS $\Longrightarrow$ **Admissible constitutive behavior of matter:**

- Linear
- Time invariant
- Locally reacting
- Causally reacting

$\Longrightarrow$

- $D_i(x_m,t) = \int_{t'=\mathbf{0}}^{\infty} \eta_{i,r}(x_m,t')E_r(x_m,t-t')\mathrm{d}t' + P_i^{\mathrm{ext}}$
- $B_j(x_m,t) = \int_{t'=\mathbf{0}}^{\infty} \zeta_{j,p}(x_m,t')H_p(x_m,t-t')\mathrm{d}t' + M_j^{\mathrm{ext}}$
    - $\eta_{i,r} =$ permittivity relaxation tensor (F/m*s)
    - $\zeta_{j,p} =$ permeability relaxation tensor (H/m*s)

EM constitutive relations in matter (continued)

EM constitutive relations (passive part)

($\overset{(t)}{*}$ = time convolution, $\overset{\text{LT}}{\longmapsto}$ = time Laplace transformation):

- $D_i(x_m,t) = \int_{t'=0}^{\infty} \eta_{i,r}(x_m,t')E_r(x_m,t-t')\mathrm{d}t' = \eta_{i,r}(x_m,t) \overset{(t)}{*} E_r(x_m,t)$

$\overset{\text{LT}}{\longmapsto}$ • $\hat{D}_i(x_m,s) = \hat{\eta}_{i,r}(x_m,s)\hat{E}_r(x_m,s)$

- $B_j(x_m,t) = \int_{t'=0}^{\infty} \zeta_{j,p}(x_m,t')H_p(x_m,t-t')\mathrm{d}t' = \zeta_{j,p}(x_m,t) \overset{(t)}{*} H_p(x_m,t)$

$\overset{\text{LT}}{\longmapsto}$ • $\hat{B}_j(x_m,s) = \hat{\zeta}_{j,p}(x_m,s)\hat{H}_p(x_m,s)$

Properties of $\{\hat{\eta}_{i,r}(x_m,s), \hat{\zeta}_{j,p}(x_m,s)\}$:

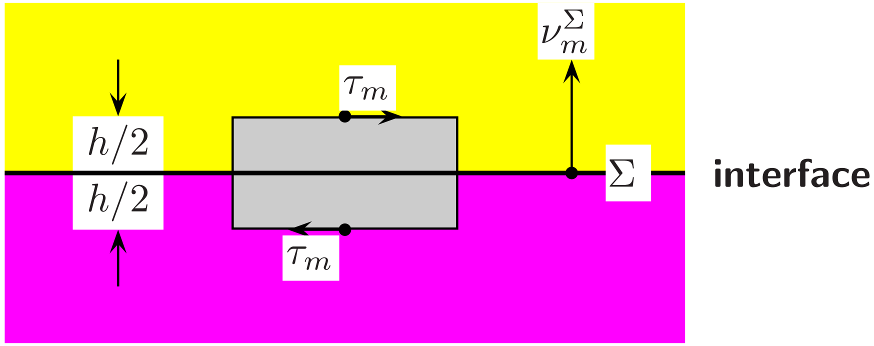
- analytic in $\mathrm{Re}(s) > 0$ • positive definite for $\mathrm{Re}(s) > 0, \mathrm{Im}(s) = 0$

Padé{n,n} representations of $\{\hat{\eta}_{i,r}(x_m,s), \hat{\zeta}_{j,p}(x_m,s)\} \Longrightarrow$

Constitutive relations: • **Local ordinary differential operators in time**

(avoids time convolutions)

Interface boundary conditions for EM field strengths (needed in uniqueness proofs):



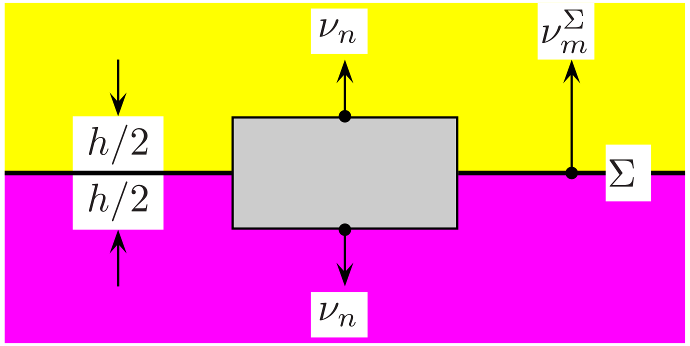
- $\oint_{\mathcal{C}} H_p \tau_p \mathrm{d}\lambda = o(1)$ as $h \downarrow 0$

  $\Longrightarrow$ $\epsilon_{i,m,p}\nu_m^\Sigma H_p$ **CONTINUOUS** across interface

- $\oint_{\mathcal{C}} E_r \tau_r \mathrm{d}\lambda = o(1)$ as $h \downarrow 0$

  $\Longrightarrow$ $\epsilon_{j,n,r}\nu_n^\Sigma E_r$ **CONTINUOUS** across interface

Interface boundary conditions for EM flux densities (needed as existence conditions):



interface

- $\int_{\mathcal{S}} D_i \nu_i \mathrm{d}A = o(1)$ as $h \downarrow 0$

  $\Longrightarrow \nu_i^\Sigma D_i$ **CONTINUOUS** across interface

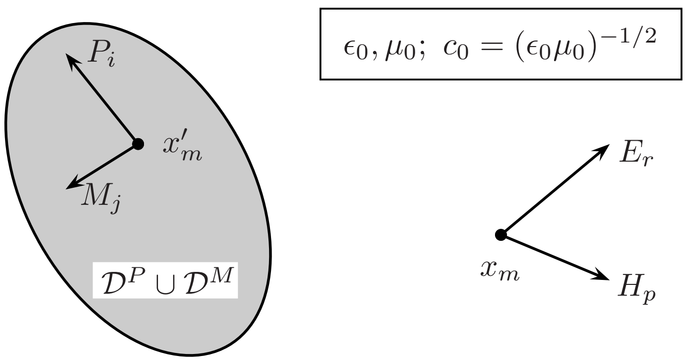
- $\oint_{\mathcal{C}} B_j \nu_j \mathrm{d}A = o(1)$ as $h \downarrow 0$

  $\Longrightarrow \nu_j^\Sigma B_j$ **CONTINUOUS** across interface

EM field interface boundary conditions (continued)

Radiation into unbounded, homogeneous, isotropic, lossless embedding (universe) via CONTRAST-SOURCE REPRESENTATION:

- $$\begin{bmatrix} E_r(x_m,t) \\ H_p(x_m,t) \end{bmatrix} = \begin{bmatrix} \mathsf{D}^{EP}_{r,i} & \mathsf{D}^{EM}_{r,j} \\ \mathsf{D}^{HP}_{p,i} & \mathsf{D}^{HM}_{p,j} \end{bmatrix} \begin{bmatrix} \int_{\mathcal{D}^P} G_0(x_m,x'_m,t) \overset{(t)}{*} P_i(x'_m,t)\mathrm{d}V(x'_m) \\ \int_{\mathcal{D}^M} G_0(x_m,x'_m,t) \overset{(t)}{*} M_j(x'_m,t)\mathrm{d}V(x'_m) \end{bmatrix}$$
  - $\mathsf{D}^{::}_{::}(\partial_m, \partial_t) =$ space-time differential operators
    - $\mathcal{D}^P = \mathrm{supp}(P_i)$
    - $\mathcal{D}^M = \mathrm{supp}(M_j)$



Green's function of the scalar wave equation:

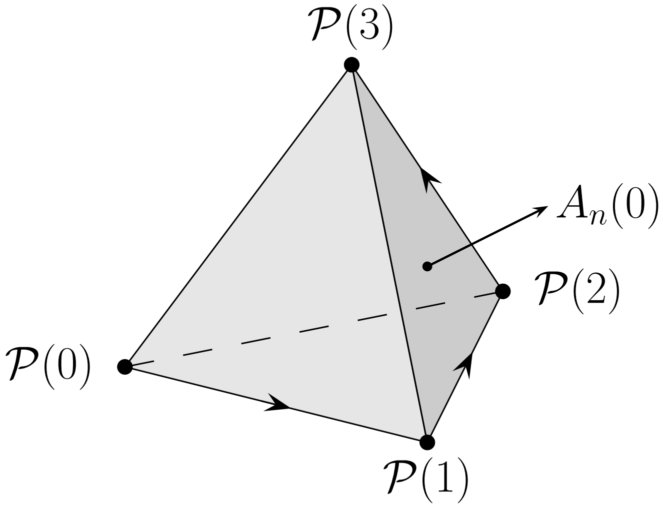
- $\partial_m \partial_m G_0 - c_0^{-2}\partial_t^2 G_0 = -\delta(x_m - x'_m, t)$
- $G_0(x_m,x'_m,t) = \dfrac{\delta(t - R/c_0)}{4\pi R}$ for $R > 0$, • $R = [(x_m - x'_m)(x_m - x'_m)]^{1/2} \geq 0$

Radiation into unbounded embedding (contrast-source representation)

Space-time differential operators in the CONTRAST-SOURCE REPRESENTATION:

- $$\begin{bmatrix} \mathsf{D}^{EP}_{r,i} & \mathsf{D}^{EM}_{r,j} \\ \mathsf{D}^{HP}_{p,i} & \mathsf{D}^{HM}_{p,j} \end{bmatrix} = \begin{bmatrix} \varepsilon_0^{-1}\partial_r\partial_i - \mu_0\partial_t^2 & -\epsilon_{r,m,j}\partial_t\partial_m \\ \epsilon_{p,n,i}\partial_t\partial_n & \mu_0^{-1}\partial_p\partial_j - \varepsilon_0\partial_t^2 \end{bmatrix}$$

The SIMPLICIAL spatial discretization:



- $\{\mathcal{P}(0), \mathcal{P}(1), \mathcal{P}(2), \mathcal{P}(3)\}$ = ordered set of points $\in \mathbb{R}^3$ **(vertices)**
- $\{x_m(0), x_m(1), x_m(2), x_m(3)\}$ = Cartesian position vectors of $\{\mathcal{P}(0), \mathcal{P}(1), \mathcal{P}(2), \mathcal{P}(3)\}$

Element = ordered 3-simplex Σ:

- **Σ = interior of the convex hull of** $\{\mathcal{P}(0), \mathcal{P}(1), \mathcal{P}(2), \mathcal{P}(3)\}$

Facets (ordered 2-faces) $\{\boldsymbol{\mathcal{F}(0), \mathcal{F}(1), \mathcal{F}(2), \mathcal{F}(3)}\}$:

- $\mathcal{F}(I) = \{\mathcal{P}(0), \ldots, \mathcal{P}(I-1), \mathcal{P}(I+1), \ldots, \mathcal{P}(3)\}, \;\; I = 0, 1, 2, 3$

Orientation of Σ ($\{\boldsymbol{x_m(J) - x_m(I); J \neq I}\}$ = edges):

$$\left\{\begin{array}{l} \bullet \text{ positive} \\ \bullet \text{ negative} \end{array}\right\} \text{ if } \det[x_m(1) - x_m(0), x_m(2) - x_m(1), x_m(3) - x_m(2)] \left\{\begin{array}{l} > 0 \\ < 0 \end{array}\right\}$$

Volume V of Σ:

- $$V = \frac{1}{3!}\ |\mathrm{det}[x_m(1) - x_m(0), x_m(2) - x_m(1), x_m(3) - x_m(2)]|$$
  $$= \frac{1}{3!}\ |\epsilon_{i,j,k}[x_i(1) - x_i(0)][x_j(2) - x_j(1)][x_k(3) - x_k(2)]|$$

Outwardly oriented vectorial areas of facets $\{A_i(I); I = 0, 1, 2, 3\}$:

- $A_i(0) = +\frac{1}{2!}\ \epsilon_{i,j,k}[x_j(2) - x_j(1)][x_k(3) - x_k(2)]$
- $A_i(1) = -\frac{1}{2!}\ \epsilon_{i,j,k}[x_j(2) - x_j(0)][x_k(3) - x_k(2)]$
- $A_i(2) = +\frac{1}{2!}\ \epsilon_{i,j,k}[x_j(1) - x_j(0)][x_k(3) - x_k(1)]$
- $A_i(3) = -\frac{1}{2!}\ \epsilon_{i,j,k}[x_j(1) - x_j(0)][x_k(2) - x_k(1)]$

Property:

- $A_i(0) + A_i(1) + A_i(2) + A_i(3) = 0$ ($\partial\Sigma$ is a closed surface)

The barycentric coordinates $\{\lambda(0), \lambda(1), \lambda(2), \lambda(3)\}$ of the position vector $x_m \in \Sigma \cup \partial\Sigma$:

- $x_m = \sum_{I=0}^{3} \lambda(I) x_m(I)$ with $0 \leq \lambda(I) \leq 1;\ I = 0, 1, 2, 3,$

  and $\sum_{I=0}^{3} \lambda(I) = 1$ for $x_m \in \Sigma \cup \partial\Sigma \implies$

- $\lambda(I) = \frac{1}{4} - \frac{1}{3V}(x_m - b_m) A_m(I)$ for $I = 0, 1, 2, 3$
- $b_m = \frac{1}{4} \sum_{I=0}^{3} x_m(I)$ **barycenter** of Σ

The local, linear, scalar, spatial expansion function $\phi(I, x_m)$ on Σ, $\mathcal{F}(I)$ and $\partial\mathcal{F}(I)$:

- $\phi(I, x_m) = \frac{1}{4} - \frac{1}{3V}(x_m - b_m) A_m(I)$ for $I = 0, 1, 2, 3 \implies \phi[I, x_m(J)] = \delta(I, J)$

The barycentric coordinates. Spatial scalar linear interpolation function on a 3-simplex

Property of edges and outwardly oriented vectorial areas of Σ:

- $[x_m(J) - x_m(I)]A_m(K) = -3V[\delta(J,K) - \delta(I,K)]$

  for $I = 0,1,2,3; J = 0,1,2,3; K = 0,1,2,3 \Longrightarrow$

- **At each vertex $\mathcal{P}(I)(I = 0,1,2,3)$ the base**

  - $\{x_m(J) - x_m(I); I = 0,1,2,3; J = 0,1,2,3; J \neq I\}$

  is RECIPROCAL to the base

  - $\{-(1/3V)A_m(K); K = 0,1,2,3; K \neq I\}$

- **At each vertex $\mathcal{P}(I)(I = 0,1,2,3)$ the base**

  - $\{A_m(K); K = 0,1,2,3; K \neq I\}$

  is RECIPROCAL to the base

  - $\{-(1/3V)[x_m(J) - x_m(I)]; I = 0,1,2,3; J = 0,1,2,3; J \neq I\}$

(cf. **CRYSTALLOGRAPHY**)

Reciprocal, affine, Cartesian base vectors at each vertex of a 3-simplex

The linear, scalar, expansion functions $\phi(I, x_m)$ on Σ:

- $\phi(I, x_m) = \frac{1}{4} - \frac{1}{3V}(x_m - b_m)A_m(I)$ for $I = 0, 1, 2, 3$

The linear, vectorial, edge expansion functions $w_r^{\text{edge}}(I, J, x_m)$ on Σ:

- $w_r^{\text{edge}}(I, J, x_m) = -(1/3V)\phi(I, x_m)A_r(J)$

  for $I = 0, 1, 2, 3; J = 0, 1, 2, 3; I \neq J$

The linear, vectorial, face expansion functions $w_i^{\text{face}}(I, J, x_m)$ on Σ:

- $w_i^{\text{face}}(I, J, x_m) = -(1/3V)\phi(I, x_m)[x_i(J) - x_i(I)]$

  for $I = 0, 1, 2, 3; J = 0, 1, 2, 3; I \neq J$

The linear, vectorial, edge and face expansion functions on a 3-simplex

The electric field strength linear edge expansion on Σ:

- $E_r(x_m,t) = \sum_{I=0}^{3}\sum_{J=0}^{3} \alpha^E(I,J,t) w_r^{\text{edge}}(I,J,x_m)$
- $\alpha^E(I,J,t) = E_r[x_m(I),t][x_r(J) - x_r(I)]$

  for $I = 0,1,2,3;\ J = 0,1,2,3;\ I \neq J$

The magnetic field strength linear edge expansion on Σ:

- $H_p(x_m,t) = \sum_{I=0}^{3}\sum_{J=0}^{3} \alpha^H(I,J,t) w_r^{\text{edge}}(I,J,x_m)$
- $\alpha^H(I,J,t) = H_p[x_m(I),t][x_p(J) - x_p(I)]$

  for $I = 0,1,2,3;\ J = 0,1,2,3;\ I \neq J$

The electric and magnetic field strengths linear edge expansions on a 3-simplex

The electric flux density linear face expansion on Σ:

- $D_i(x_m,t) = \sum_{I=0}^{3}\sum_{J=0}^{3} \alpha^D(I,J,t) w_i^{\text{face}}(I,J,x_m)$
- $\alpha^D(I,J,t) = D_i[x_m(I),t] A_i(J)$

  for $I = 0,1,2,3;\ J = 0,1,2,3;\ I \neq J$

The magnetic flux density linear face expansion on Σ:

- $B_j(x_m,t) = \sum_{I=0}^{3}\sum_{J=0}^{3} \alpha^B(I,J,t) w_j^{\text{face}}(I,J,x_m)$
- $\alpha^B(I,J,t) = B_j[x_m(I),t] A_j(J)$

  for $I = 0,1,2,3;\ J = 0,1,2,3;\ I \neq J$

The electric and magnetic flux densities linear face expansions on a 3-simplex

The computational procedure:

- Specify INPUT
- Generate SIMPLICIAL MESH that fits piecewise continuously turning interfaces up to order $\boldsymbol{o}(h)$ (h=mesh size)
- Apply FIELD EQUATIONS IN INTEGRAL FORM to all facets of each element under the application of the 'TRAPEZOIDAL' INTEGRATION RULE
- Invoke CONSTITUTIVE RELATIONS at each vertex of each element
- Invoke INTERFACE FIELD CONTINUITY CONDITIONS on the SIMPLICIAL STAR of each EDGE (E_r, H_p) and each FACET (D_i, B_j)

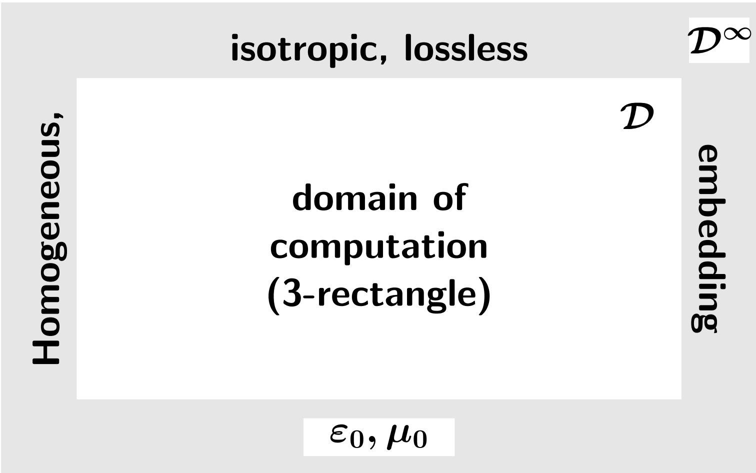
The computational procedure

The computational procedure (continued):

- Simulate radiation into unbounded embedding through CARTESIAN COORDINATE-STRETCHED PERFECTLY MATCHED EMBEDDING, with absorptive (and/or time-delaying) layers
- Truncate coordinate-stretched perfectly matched Cartesian embedding by PERIODIC BOUNDARY CONDITION (cf. QUANTUM THEORY OF SOLIDS)
- Apply TRAPEZOIDAL RULE to the TIME INTEGRATIONS
- SOLVE SYSTEM OF EQUATIONS (iteratively)
- Organize OUTPUT

The computational procedure (continued)

LT-domain contrast-source field representations with respect to unbounded, homogeneous, isotropic, lossless embedding:

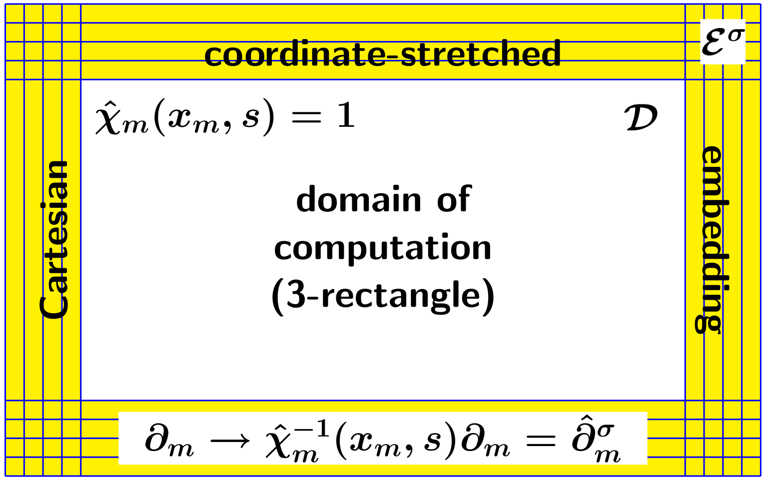


- $\hat{G}_0(x_m, x'_m, s) = \dfrac{\exp(-sR/c_0)}{4\pi R}$ for $R > 0$
- $R = [(x_m - x'_m)(x_m - x'_m)]^{1/2}$

- $$\begin{bmatrix} \hat{E}_r(x_m,s) \\ \hat{H}_p(x_m,s) \end{bmatrix} = \begin{bmatrix} \varepsilon_0^{-1}\partial_r\partial_i - \mu_0 s^2 & -\epsilon_{r,m,j} s\partial_m \\ \epsilon_{p,n,i} s\partial_n & \mu_0^{-1}\partial_p\partial_j - \varepsilon_0 s^2 \end{bmatrix} \begin{bmatrix} \int_{\mathcal{D}^P} \hat{G}_0(x_m,x'_m,s)\hat{P}_i(x'_m,s)\mathrm{d}V(x'_m) \\ \int_{\mathcal{D}^M} \hat{G}_0(x_m,x'_m,s)\hat{M}_j(x'_m,s)\mathrm{d}V(x'_m) \end{bmatrix}$$

The domain of computation and its homogeneous, isotropic, lossless embedding

The time-dependent Cartesian coordinate-stretching procedure:



Out of the homogeneous, isotropic, lossless embedding $\mathcal{D}^\infty$ a Cartesian coordinate-stretched embedding $\mathcal{E}^\sigma$ is constructed by carrying out the **LT-domain** operation:

- $\partial_m \longrightarrow [\hat{\chi}_m(x_m, s)]^{-1}\partial_m = \hat{\partial}_m^\sigma$ for $m = 1, 2, 3$ **(no summation)** with
  - $\{\hat{\chi}_1(x_1, s), \hat{\chi}_2(x_2, s), \hat{\chi}_3(x_3, s)\}$ piecewise continuous in space, analytic for $s \in \mathbb{C},\ \mathrm{Re}(s) > 0,$ and real and positive for $s \in \mathbb{R},\ s > 0$ ($\Longrightarrow$ causality in time + **UNIQUENESS**)
  - $\{\hat{\chi}_1(x_1, s), \hat{\chi}_2(x_2, s), \hat{\chi}_3(x_3, s)\} = \{1, 1, 1\}$ in domain of computation $\mathcal{D}$

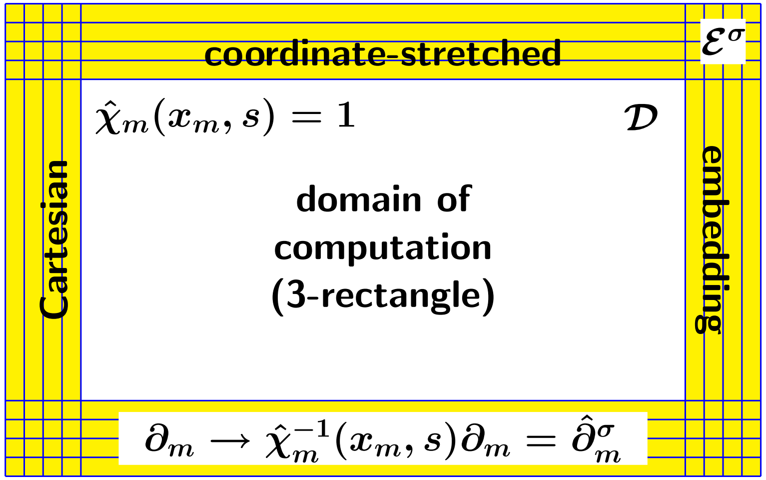
The LT-domain Green's function (propagator) $\hat{G}_0^\sigma(x_m, x'_m, s)$ of the Cartesian coordinate-stretched embedding ($\hat{\partial}_m^\sigma = [\hat{\chi}_m(x_m, s)]^{-1}\partial_m$):

- $\hat{\partial}_m^\sigma \hat{\partial}_m^\sigma \hat{G}_0^\sigma(x_m, x'_m, s) - (s^2/c_0^2)\hat{G}_0^\sigma(x_m, x'_m, s) =$
  $-[\hat{\chi}_1(x'_1, s)]^{-1}[\hat{\chi}_2(x'_2, s)]^{-1}[\hat{\chi}_3(x'_3, s)]^{-1}\delta(x_1 - x'_1, x_2 - x'_2, x_3 - x'_3)$
- $\hat{G}_0^\sigma(x_m, x'_m, s) = \dfrac{\exp(-s\hat{R}^\sigma/c_0)}{4\pi\hat{R}^\sigma}$ for $\hat{R}^\sigma \neq 0$ with
- $\hat{R}^\sigma = \left(\left[\int_{x'_1}^{x_1} \hat{\chi}_1(\xi_1, s)\mathrm{d}\xi_1\right]^2 + \left[\int_{x'_2}^{x_2} \hat{\chi}_2(\xi_2, s)\mathrm{d}\xi_2\right]^2 + \left[\int_{x'_3}^{x_3} \hat{\chi}_3(\xi_3, s)\mathrm{d}\xi_3\right]^2\right)^{1/2} \geq 0$
  for $s \in \mathbb{R}, s > 0$ **(LT-domain stretched-coordinate distance function)**

$\Longrightarrow$ **NO REFLECTIONS NOTWITHSTANDING INHOMOGENEITY**

$\Longrightarrow$ **THE CARTESIAN COORDINATE-STRETCHED EMBEDDING IS 3D REFLECTIONFREE ! (De Hoop et. al. 2005)**

LT-domain contrast-source field representations with respect to an unbounded Cartesian coordinate-stretched reflectionless embedding:



- $\hat{G}_0^\sigma(x_m, x'_m, s) = \dfrac{\exp(-s\hat{R}^\sigma/c_0)}{4\pi\hat{R}^\sigma}$

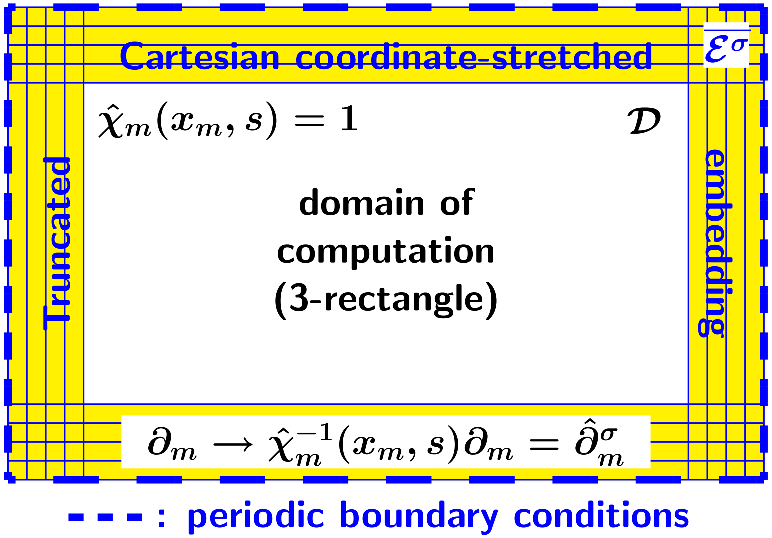
  for $\hat{R}^\sigma \neq 0$
- $\hat{R}^\sigma = \hat{R}^\sigma(x_m, x'_m, s)$

- $$\begin{bmatrix} \hat{E}_r(x_m, s) \\ \hat{H}_p(x_m, s) \end{bmatrix} = \begin{bmatrix} \varepsilon_0^{-1}\hat{\partial}_r^\sigma\hat{\partial}_i^\sigma - \mu_0 s^2 & -\epsilon_{r,m,j}s\hat{\partial}_m^\sigma \\ \epsilon_{p,n,i}s\hat{\partial}_n^\sigma & \mu_0^{-1}\hat{\partial}_p^\sigma\hat{\partial}_j^\sigma - \varepsilon_0 s^2 \end{bmatrix} \begin{bmatrix} \int_{\mathcal{D}^P} \hat{G}_0^\sigma(x_m, x'_m, s)\hat{P}_i(x'_m, s)\mathrm{d}V(x'_m) \\ \int_{\mathcal{D}^M} \hat{G}_0^\sigma(x_m, x'_m, s)\hat{M}_j(x'_m, s)\mathrm{d}V(x'_m) \end{bmatrix}$$

$\Longrightarrow$ **REPRODUCES ACTUAL FIELD IN $\mathcal{D}$**

The domain of computation and its Cartesian coordinate-stretched reflectionless embedding

LT-domain contrast-source field representations with respect to a truncated Cartesian coordinate-stretched embedding:



- $\hat{G}_0^{\sigma;\mathrm{per}}(x_m, x'_m, s) = \sum \left[\dfrac{\exp(-s\hat{R}^{\sigma;\mathrm{per}}/c_0)}{4\pi \hat{R}^{\sigma;\mathrm{per}}} \right]$
- $\hat{R}^{\sigma;\mathrm{per}}$ = distance function from periodically repeated source points

- $$\begin{bmatrix} \hat{E}_r(x_m, s) \\ \hat{H}_p(x_m, s) \end{bmatrix} = \begin{bmatrix} \varepsilon_0^{-1}\hat{\partial}^\sigma_r\hat{\partial}^\sigma_i - \mu_0 s^2 & -\epsilon_{r,m,j} s \hat{\partial}^\sigma_m \\ \epsilon_{p,n,i} s \hat{\partial}^\sigma_n & \mu_0^{-1}\hat{\partial}^\sigma_p\hat{\partial}^\sigma_j - \varepsilon_0 s^2 \end{bmatrix} \begin{bmatrix} \int_{\mathcal{D}^P} \hat{G}_0^{\sigma;\mathrm{per}}(x_m, x'_m, s)\hat{P}_i(x'_m, s)\mathrm{d}V(x'_m) \\ \int_{\mathcal{D}^M} \hat{G}_0^{\sigma;\mathrm{per}}(x_m, x'_m, s)\hat{M}_j(x'_m, s)\mathrm{d}V(x'_m) \end{bmatrix}$$

$\Longrightarrow$ **ACTUAL FIELD IN $\mathcal{D}$ + SPURIOUS CONTRIBUTIONS**

The domain of computation and its truncated Cartesian coordinate-stretched embedding

A class of coordinate-stretching functions controlling excess time delay and attenuation in the Cartesian coordinate-stretched embedding:

- $\hat{\chi}_m(x_m, s) = 1 + N_m(x_m) + s^{-1}\sigma_m(x_m)$ **(De Hoop et. al., 2005)**
  - $N_m(x_m) =$ excess time delay coefficient $[N_m(x_m) > -1]$
  - $\sigma_m(x_m) =$ absorption coefficient $[\sigma_m(x_m) \geq 0]$

for $m = 1, 2, 3$ (no summation) $\Longrightarrow$

- $$\hat{G}_0^\sigma = \frac{s}{4\pi c_0 T} \frac{\exp\{-T[(s+A)^2 + B^2]^{1/2}\}}{[(s+A)^2 + B^2]^{1/2}}$$

Abramowitz & Stegun, Formula 29.3.92, p. 1027 $\Longrightarrow$:

- $$G_0^\sigma = \frac{1}{4\pi c_0 T} \partial_t \left[\exp(-At) J_0[B(t^2 - T^2)^{1/2}] H(t-T)\right]$$

  $J_0 =$ Bessel function of the first kind and order zero

- $T =$ time delay along propagation path
- $A =$ attenuation along propagation path

The LT-domain EM field equations in the Cartesian coordinate-stretched embedding (original form):

- $\epsilon_{i,m,p}\hat{\partial}^{\sigma}_{m}\hat{H}_p = s\hat{D}_i$
- $\epsilon_{j,n,r}\hat{\partial}^{\sigma}_{n}\hat{E}_r = -s\hat{B}_j$

The LT-domain EM field constitutive relations in the Cartesian coordinate-stretched embedding (original form):

- $\hat{D}_i = \epsilon_0\delta_{i,r}\hat{E}_r$
- $\hat{B}_j = \mu_0\delta_{j,p}\hat{H}_p$

$\Longrightarrow$ **IN THE TIME DOMAIN, $\hat{\partial}^{\sigma}_{m}\hat{H}_p$ and $\hat{\partial}^{\sigma}_{n}\hat{E}_r$ $\Longrightarrow$ TIME CONVOLUTIONS (NUMERICALLY UNWANTED)**

The LT-domain EM field equations in the Cartesian coordinate-stretched embedding (equivalent form fitting the discretization stencil in $\mathcal{D}$):

- $\epsilon_{i,m,p}\partial_m \hat{H}_p^\sigma = s\hat{D}_i^\sigma$
  - $\hat{H}_1^\sigma = \hat{\chi}_1 \hat{H}_1$ • $\hat{H}_2^\sigma = \hat{\chi}_2 \hat{H}_2$ • $\hat{H}_3^\sigma = \hat{\chi}_3 \hat{H}_3$
  - $\hat{D}_1^\sigma = \hat{\chi}_2\hat{\chi}_3 \hat{D}_1$ • $\hat{D}_2^\sigma = \hat{\chi}_3\hat{\chi}_1 \hat{D}_2$ • $\hat{D}_3^\sigma = \hat{\chi}_1\hat{\chi}_2 \hat{D}_3$
- $\epsilon_{j,n,r}\partial_n \hat{E}_r^\sigma = -s\hat{B}_j^\sigma$
  - $\hat{E}_1^\sigma = \hat{\chi}_1 \hat{E}_1$ • $\hat{E}_2^\sigma = \hat{\chi}_2 \hat{E}_2$ • $\hat{E}_3^\sigma = \hat{\chi}_3 \hat{E}_3$
  - $\hat{B}_1^\sigma = \hat{\chi}_2\hat{\chi}_3 \hat{B}_1$ • $\hat{B}_2^\sigma = \hat{\chi}_3\hat{\chi}_1 \hat{B}_2$ • $\hat{B}_3^\sigma = \hat{\chi}_1\hat{\chi}_2 \hat{B}_3$

$\Longrightarrow$ **UNPHYSICAL OPERATIONS ON PHYSICAL FIELDS ARE REPLACED WITH PHYSICAL OPERATIONS ON UNPHYSICAL FIELDS (IN EMBEDDING, NOT IN $\mathcal{D}$!)**

The modified EM field equations in the Cartesian coordinate-stretched embedding

The LT-domain modified constitutive relations in the Cartesian coordinate-stretched embedding:

- $\hat{D}_1^\sigma = \dfrac{\hat{\chi}_2\hat{\chi}_3}{\hat{\chi}_1}\,\hat{E}_1^\sigma$ • $\hat{D}_2^\sigma = \dfrac{\hat{\chi}_3\hat{\chi}_1}{\hat{\chi}_2}\,\hat{E}_2^\sigma$ • $\hat{D}_3^\sigma = \dfrac{\hat{\chi}_1\hat{\chi}_2}{\hat{\chi}_3}\,\hat{E}_3^\sigma$
- $\hat{B}_1^\sigma = \dfrac{\hat{\chi}_2\hat{\chi}_3}{\hat{\chi}_1}\,\hat{H}_1^\sigma$ • $\hat{B}_2^\sigma = \dfrac{\hat{\chi}_3\hat{\chi}_1}{\hat{\chi}_2}\,\hat{H}_2^\sigma$ • $\hat{B}_3^\sigma = \dfrac{\hat{\chi}_1\hat{\chi}_2}{\hat{\chi}_3}\,\hat{H}_3^\sigma$

$\Longrightarrow$ **IN THE TIME DOMAIN, (NUMERICALLY UNWANTED) TIME CONVOLUTIONS HAVE BEEN SHIFTED TO THE CONSTITUTIVE RELATIONS $\Longrightarrow$ CAN BE CIRCUMVENTED FOR LORENTZ THEORY–OF–ELECTRONS MODEL FOR CONSTITUTIVE BEHAVIOR OF MATTER IN $\mathcal{D}$ AND ABSORPTIVE/DELAY COORDINATE-STRETCHING MODEL IN $\overline{\mathcal{E}^\sigma}$**

The modified constitutive relations in the Cartesian coordinate-stretched embedding

The time-domain EM field equations in the Cartesian coordinate-stretched embedding:

- $\epsilon_{i,m,p}\partial_m H_p^\sigma = \partial_t D_i^\sigma$
- $\epsilon_{j,n,r}\partial_n E_r^\sigma = -\partial_t B_j^\sigma$

The time-domain EM field constitutive relations in the Cartesian coordinate-stretched embedding (absorptive/delay coordinate-stretching model) follow from the inverse LT of:

- $s\ (s\hat{\chi}_1)\hat{D}_1^\sigma = (s\hat{\chi}_2)(s\hat{\chi}_3)\hat{E}_1^\sigma$
- $s\ (s\hat{\chi}_2)\hat{D}_2^\sigma = (s\hat{\chi}_3)(s\hat{\chi}_1)\hat{E}_2^\sigma$
- $s\ (s\hat{\chi}_3)\hat{D}_3^\sigma = (s\hat{\chi}_1)(s\hat{\chi}_2)\hat{E}_3^\sigma$
- $s\ (s\hat{\chi}_1)\hat{B}_1^\sigma = (s\hat{\chi}_2)(s\hat{\chi}_3)\hat{H}_1^\sigma$
- $s\ (s\hat{\chi}_2)\hat{B}_2^\sigma = (s\hat{\chi}_3)(s\hat{\chi}_1)\hat{H}_2^\sigma$
- $s\ (s\hat{\chi}_3)\hat{B}_3^\sigma = (s\hat{\chi}_1)(s\hat{\chi}_2)\hat{H}_3^\sigma$

and observing that:

- $s \longrightarrow \partial_t$
- $s\ \hat{\chi}_m(x_m, s) \longrightarrow [1 + N_m(x_m)]\partial_t + \sigma(x_m)$ for $m = 1, 2, 3$ **(no summation)**