Introduction to x3d integral equation code

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outline

- x3d theory
- Comparison with other approaches
- example

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Complex-valued conductivity

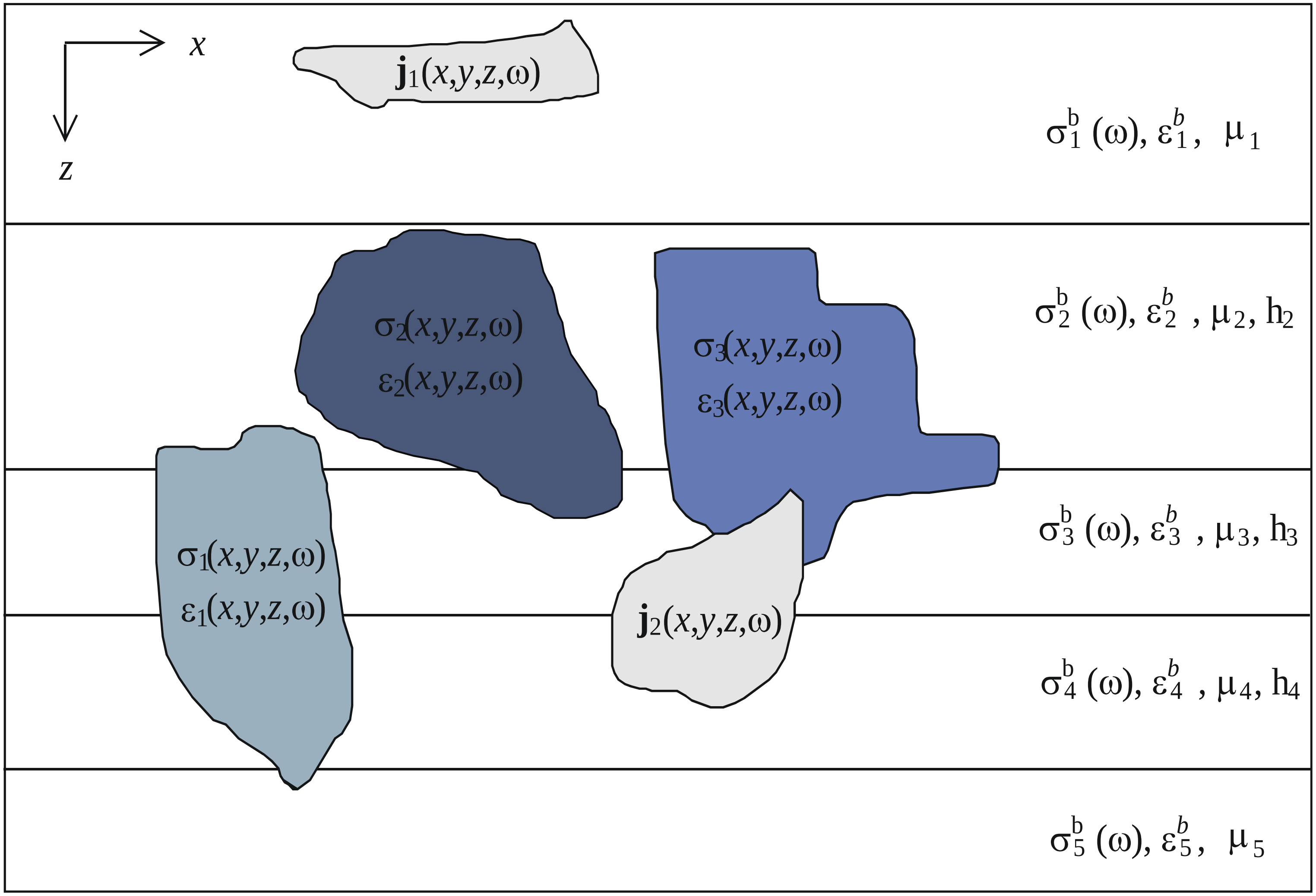

Fig. Example of a 3D model (side view) to be handled by x3d.

x3d code maths

Maxwell's equations in frequency-domain

$$\nabla\times\mathbf{H}=\underline{\underline{\zeta}}(x,y,z,\omega)\mathbf{E}+\mathbf{j}^{ext},\quad \nabla\times\mathbf{E}=i\omega\underline{\underline{\mu}}(z)\mathbf{H}.$$

$$\underline{\underline{\zeta}}(x,y,z,\omega)=\underline{\underline{\sigma}}-i\omega\underline{\underline{\varepsilon}}=\begin{pmatrix}\zeta_{xx} & 0 & 0\\ 0 & \zeta_{yy} & 0\\ 0 & 0 & \zeta_{zz}\end{pmatrix}, \qquad \underline{\underline{\mu}}(z,\omega)=\begin{pmatrix}\mu_{\tau} & 0 & 0\\ 0 & \mu_{\tau} & 0\\ 0 & 0 & \mu_{z}\end{pmatrix}.$$

Maxwell's equations for reference EM field

$$\nabla\times\mathbf{H}^{o}=\underline{\underline{\zeta}}_{o}(z,\omega)\mathbf{E}^{0}+\mathbf{j}^{ext},\quad \nabla\times\mathbf{E}^{0}=i\omega\underline{\underline{\mu}}(z)\mathbf{H}^{0}.$$

$$\underline{\underline{\zeta}}_{0}(z,\omega)=\begin{pmatrix}\zeta_{0\tau} & 0 & 0\\ 0 & \zeta_{0\tau} & 0\\ 0 & 0 & \zeta_{0z}\end{pmatrix}.$$

Maxwell's equations for scattered EM field

$$\nabla\times\mathbf{H}^{s}=\underline{\underline{\zeta}}_{o}(z,\omega)\mathbf{E}^{s}+\mathbf{j}^{q},\quad \nabla\times\mathbf{E}^{s}=i\omega\underline{\underline{\mu}}(z)\mathbf{H}^{s}.$$

$$\mathbf{j}^{q}=(\underline{\underline{\zeta}}-\underline{\underline{\zeta}}_{o})(\mathbf{E}^{s}+\mathbf{E}^{0}).$$

$$\nabla\times\frac{1}{i\omega}\underline{\underline{\mu}}^{-1}(z)\nabla\times\mathbf{E}^{s}-\underline{\underline{\zeta}}_{o}(z,\omega)\mathbf{E}^{s}=\mathbf{j}^{q} \longleftrightarrow \mathbf{E}^{s}(\mathbf{r})=\int_{V^{S}}\underline{\underline{G}}_{o}^{ee}(\mathbf{r},\mathbf{r}')\mathbf{j}^{q}(\mathbf{r}')dv'.$$

$$\mathbf{r}=(x,y,z),\quad dv'=dx'dy'dz'.$$

Conventional scattering equation (Dmitriev, 1969; Weidelt, 1975)

$$\mathbf{E}^{s}(\mathbf{r})=\mathbf{E}_{o}+Q\mathbf{E}^{s}=\mathbf{E}_{o}(\mathbf{r})+\int_{V^{S}}\underline{\underline{G}}_{o}^{ee}(\mathbf{r},\mathbf{r}')\Big(\underline{\underline{\zeta}}(\mathbf{r}')-\underline{\underline{\zeta}}_{o}(z')\Big)\mathbf{E}^{s}(\mathbf{r}')dv'. \qquad (1)$$

3x3 dyadic for the electric-to-electric Green's function of the 1D reference formation:

$$\underline{\underline{G}}_{o}^{ee}=\begin{pmatrix}G_{xx} & G_{xy} & G_{xz}\\ G_{yx} & G_{yy} & G_{yz}\\ G_{zx} & G_{zy} & G_{zz}\end{pmatrix}$$

Formal solution of eq. (1) can be expressed as an infinite Neumann series

$$\mathbf{E}^{s}(\mathbf{r})=(1-Q)^{-1}\mathbf{E}_{o}=\mathbf{E}_{o}+Q\mathbf{E}_{o}+Q^{2}\mathbf{E}_{o}+\ldots$$

As a rule, the series doesn't converge at all.

x3d code maths

Conventional scattering equation

$$\mathbf{E}^S(\mathbf{r}) = \mathbf{E}_o + Q\mathbf{E}^S = \mathbf{E}_o(\mathbf{r}) + \int_{V^S} \underline{\underline{G}}_o^{ee}(\mathbf{r},\mathbf{r}')\left(\underline{\underline{\zeta}}(\mathbf{r}') - \underline{\underline{\zeta}}_o(z')\right)\mathbf{E}^S(\mathbf{r}')dv'.$$

$$\underline{\underline{\lambda}}(z,\omega) = \begin{pmatrix} \sqrt{\mathrm{Re}\zeta_{o\tau}} & 0 & 0 \\ 0 & \sqrt{\mathrm{Re}\zeta_{o\tau}} & 0 \\ 0 & 0 & \sqrt{\mathrm{Re}\zeta_{oz}} \end{pmatrix}.$$

$\boxed{\mathbf{E}^S \to \chi:}$

$$\chi = \tfrac{1}{2}\underline{\underline{\lambda}}^{-1}\left((\underline{\underline{\zeta}} + \underline{\underline{\zeta}}_o^*)\mathbf{E}^S + (\underline{\underline{\zeta}} - \underline{\underline{\zeta}}_o)\mathbf{E}^o\right)$$

Scattering equation MIDM (Singer, 1995; Pankratov, Avdeev,Kuvshinov, 1995; Pankratov, Kuvshinov, Avdeev, 1997; Singer & Fainberg, 1995, 1997)

$$\boxed{\chi(\mathbf{r}) = \chi_o + M\chi = \chi_o(\mathbf{r}) + \int_{V^S} \underline{\underline{K}}(\mathbf{r},\mathbf{r}')\underline{\underline{R}}(\mathbf{r}')\chi(\mathbf{r}')dv'}$$

$$\underline{\underline{K}}(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}')\underline{\underline{1}} + 2\underline{\underline{\lambda}}(z)\underline{\underline{G}}_o^{ee}(\mathbf{r},\mathbf{r}')\underline{\underline{\lambda}}(z')$$

$$\underline{\underline{R}}(\mathbf{r}) = \left(\underline{\underline{\zeta}}(\mathbf{r}) - \underline{\underline{\zeta}}_o(z)\right)\left(\underline{\underline{\zeta}}(\mathbf{r}) + \underline{\underline{\zeta}}_o^*(z)\right)^{-1}$$

$$\chi = (1-M)^{-1}\chi_o = \chi_o + M\chi_o + M^2\chi_o + \ldots$$

The Neumann's series converges for any frequency and any electrical resistivity contract $\|\underline{\underline{M}}\chi\| < \|\chi\|, \ \forall\chi$

Simple iteration (MIDM; Avdeev et al., 2000)

$$\chi^{(n+1)} = \chi_o + M\chi^{(n)}, \quad n = 1,2,\ldots$$

Krylov iteration (Avdeev et al., 2002)

$$A\chi = \chi_o, \qquad A = 1 - M.$$

$$\kappa(A) = \|A\|\|A^{-1}\| \le \sqrt{C_l} \qquad \left(C_l = 10^4 \Rightarrow \kappa(A) \le 10^2\right)$$

EM field calculation

$\boxed{\chi \rightarrow \mathbf{j}^q}$

$$\mathbf{j}^q(\mathbf{r}) = 2\underline{\underline{\lambda}}\left(\underline{\underline{\zeta}} + \underline{\underline{\zeta}}_o^*\right)^{-1}\left(\underline{\underline{\zeta}} - \underline{\underline{\zeta}}_o\right)(\chi + \underline{\underline{\lambda}}\mathbf{E}^0), \quad \mathbf{r} \in V^S$$

$\boxed{\mathbf{j}^q \rightarrow \mathbf{E}^S, \mathbf{H}^S}$

$$\nabla \times \frac{1}{i\omega} \underline{\underline{\mu}}^{-1}(z) \nabla \times \mathbf{E}^S - \underline{\underline{\zeta}}_o(z,\omega)\mathbf{E}^S = \mathbf{j}^q.$$

$$\mathbf{E}^S(\mathbf{r}) = \int_{V^S} \underline{\underline{G}}_o^{ee}(\mathbf{r},\mathbf{r}')\mathbf{j}^q(\mathbf{r}')dv', \quad \mathbf{H}^S(\mathbf{r}) = \int_{V^S} \underline{\underline{G}}_o^{me}(\mathbf{r},\mathbf{r}')\mathbf{j}^q(\mathbf{r}')dv',$$

$$\mathbf{E} = \mathbf{E}^0 + \mathbf{E}^S, \quad \mathbf{H} = \mathbf{H}^0 + \mathbf{H}^S(\mathbf{r}).$$

4×9=36 Green's tensors entries (at least)

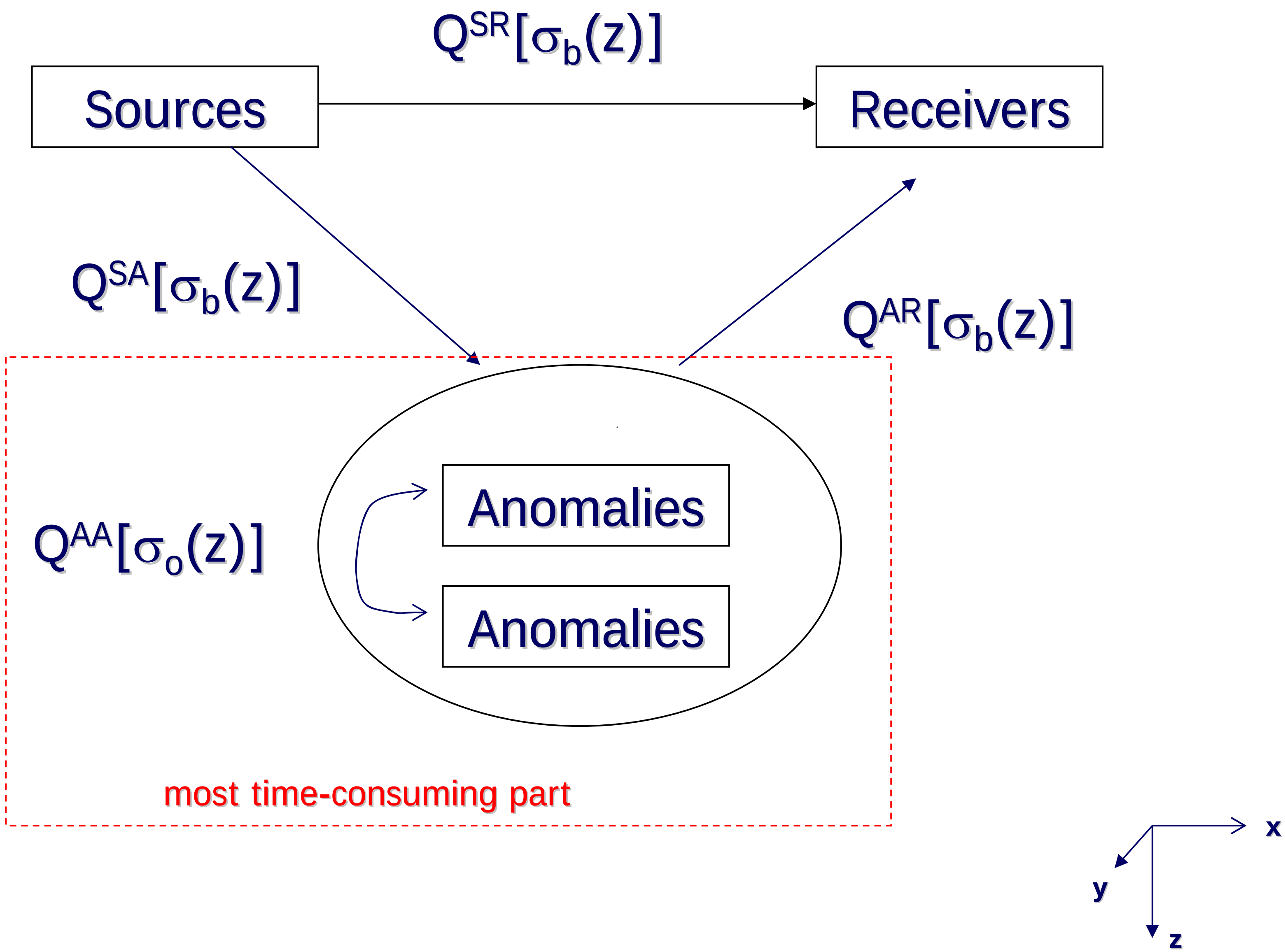

Fig. x3d Workflow

x3d code

- x3d_64x64x32_RM.exe
- x3d_125x125x16_RM.exe
- x3d_125x125x64_HD.exe
- x3d_256x256x8_RM.exe
- x3d_256x256x32_HD.exe
- x3d_350x350x16_HD.exe
- x3d_1024x1024x8_HD.exe

Fig. x3d grids available on 32-bit Windows machines.

On 64-bit computers maximum grids are far larger.


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*                                                                    *
**********************************************************************

Code requires          22 MegaBytes of disk space
     including         11 MegaBytes for Greens matrices


---------  run       #  1 of  2              polarization # 1 of 2 ---------

# Nx x Ny x Nz : 40 x 40 x 5
# model file   : "01.model"
# frequency    : 0.100000 [Hz]
#
# Computes Greens matrices (a2a)                         15.17.24.  27.10.2006
#    Computes Greens scalars                             15.17.24.  27.10.2006
#    Computes Greens matrices                            15.17.27.  27.10.2006
# Computes En (at A)                                     15.17.31.  27.10.2006
# Computes j^s=(zeta-zeta^N)*En on A                     15.17.31.  27.10.2006
# Krylov subspaces iteration (GPBi-CGZW)                 15.17.31.  27.10.2006
#    Computes free term                                  15.17.31.  27.10.2006
# free term norm = 5.00E+05                              15.17.32.  27.10.2006
# iter    residual                                       15.17.34.  27.10.2006
    1    8.009E-01                                       15.17.34.  27.10.2006
    2    4.290E-01                                       15.17.35.  27.10.2006
    3    2.954E-01                                       15.17.36.  27.10.2006
    4    2.216E-01                                       15.17.37.  27.10.2006
    5    1.422E-01                                       15.17.38.  27.10.2006
    6    1.176E-01                                       15.17.39.  27.10.2006
    7    7.474E-02                                       15.17.41.  27.10.2006
    8    6.251E-02                                       15.17.42.  27.10.2006
    9    2.904E-02                                       15.17.43.  27.10.2006
   10    2.126E-02                                       15.17.44.  27.10.2006
   11    1.936E-02                                       15.17.45.  27.10.2006
   12    1.595E-02                                       15.17.46.  27.10.2006
   13    1.359E-02                                       15.17.47.  27.10.2006
   14    1.080E-02                                       15.17.49.  27.10.2006
   15    7.777E-03                                       15.17.50.  27.10.2006
   16    6.097E-03                                       15.17.51.  27.10.2006
   17    3.702E-03                                       15.17.52.  27.10.2006
   18    2.995E-03                                       15.17.53.  27.10.2006
   19    2.834E-03                                       15.17.54.  27.10.2006
   20    2.159E-03                                       15.17.55.  27.10.2006
# iter    residual                                       15.17.57.  27.10.2006
   21    1.730E-03                                       15.17.57.  27.10.2006
   22    1.389E-03                                       15.17.58.  27.10.2006
   23    1.059E-03                                       15.17.59.  27.10.2006
   24    9.237E-04                                       15.18. 0.  27.10.2006
#    Computes Greens scalars                             15.18. 1.  27.10.2006
#    Computes Greens matrices                            15.18. 3.  27.10.2006
#    Convolutes (a2o)                                    15.18. 4.  27.10.2006
#    Computes Greens scalars                             15.18. 5.  27.10.2006
#    Computes Greens matrices                            15.18. 7.  27.10.2006
#    Convolutes (a2o)                                    15.18. 8.  27.10.2006

---------  run       #  1 of  2              polarization # 2 of 2 ---------

# Nx x Ny x Nz : 40 x 40 x 5
# model file   : "01.model"
# frequency    : 0.100000 [Hz]
#
# Computes En (at A)                                     15.18. 8.  27.10.2006
# Computes j^s=(zeta-zeta^N)*En on A                     15.18. 8.  27.10.2006
# Krylov subspaces iteration (GPBi-CGZW)                 15.18. 8.  27.10.2006
#    Computes free term                                  15.18. 8.  27.10.2006
# free term norm = 5.14E+05                              15.18. 9.  27.10.2006
```

Fig. x3d screen output example

X3d code summary

Based on the above IE approach, there have been developed 3D forward modeling solutions for various EM applications

- ✓ Induction logging in deviated boreholes
- ✓ Airborne electromagnetics
- ✓ General controlled-source EMs, MT, and CSMT
- ✓ Global induction studies

The solutions:

- give accurate results even for lateral contrast of electrical resistivity up to 100,000;
- simulate the frequency-domain responses in frequency range from DC up to 50 MHz;
- account for the induced polarization and displacement currents;
- admit an *anisotropy* of the electrical conductivity;
- allow to run large-scale models discretized to 1,000,000 cells at 32-bit machines;

- x3d theory
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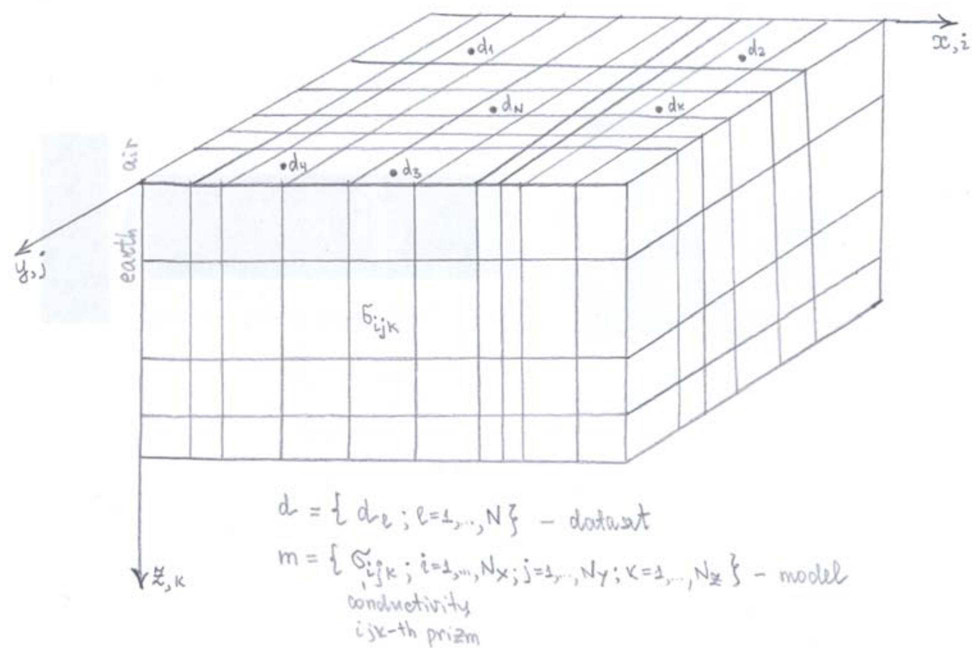
Fig. A 3-D MT model discretized with rectangular prisms.



(1) Integral equation (IE) approach

$$\chi(\mathbf{r}) = \chi_0(\mathbf{r}) + \int_{V^S} \underline{\underline{K}}(\mathbf{r},\mathbf{r}')\underline{\underline{R}}(\mathbf{r}')\chi(\mathbf{r}')dv'$$

$A_{IE} \cdot x = b$ - system of linear equations (← on a rectangular 3-D grid);

A_{IE} - complex, dense with all entries filled, non-Hermitian matrix; but much more compact than FD and FE matrices

(a) Main attraction: only the scattering volume V^s is subject to discretization;

(this reduce dramatically the size of matrix A_{IE})

(b) Drawback: most EM software developers refrain from implementation of the IE approach, since

accurate computation of the matrix A_{IE} is indeed an extremely tedious and nontrivial problem itself.

Other methods

$$\nabla\times\underline{\underline{\mu}}^{-1}\mathbf{E}-i\omega\underline{\underline{\zeta}}(x,y,z,\omega)\mathbf{E}=\mathbf{j}^{ext}$$

(2) Finite-difference (FD) approach

$A_{FD}\cdot x=b$ - system of linear equations (← on a rectangular 3D grid);

A_{FD} - large, sparse 3Mx3M symmetric, non-Hermitian matrix;
x represents the grid nodal values of electric field;
b represents the source and boundary conditions;
$M=n_x\cdot n_y\cdot n_z$ - number of model parameters.

(a) The most commonly employed
(b) Main attraction: an apparent simplicity of its numerical implementation

(3) Finite-element (FE) approach

the EM field (or its potentials) are decomposed to some basic (usually, edge and nodal) functions. The coefficients of the decomposition, a vector *x,* are sought using the Galerkin method.

$A_{FE}\cdot x=b$

A_{FE} - large, sparse, non-symmetric, non-Hermitian matrix;

(a) Main attraction: it is commonly believed to be better able than other approaches to accurately account for geometry (shapes of ore-bodies, topography, cylindrical wells, etc.)

(b) Main drawback: construction of the finite elements themselves is another nontrivial and usually time-consuming procedure.

- x3d theory
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x3d statistics: 99x99x11 prisms of 10x10x{10to2000}m^3

23 min on a serial PC for 11 frequencies & a single transmitter position;

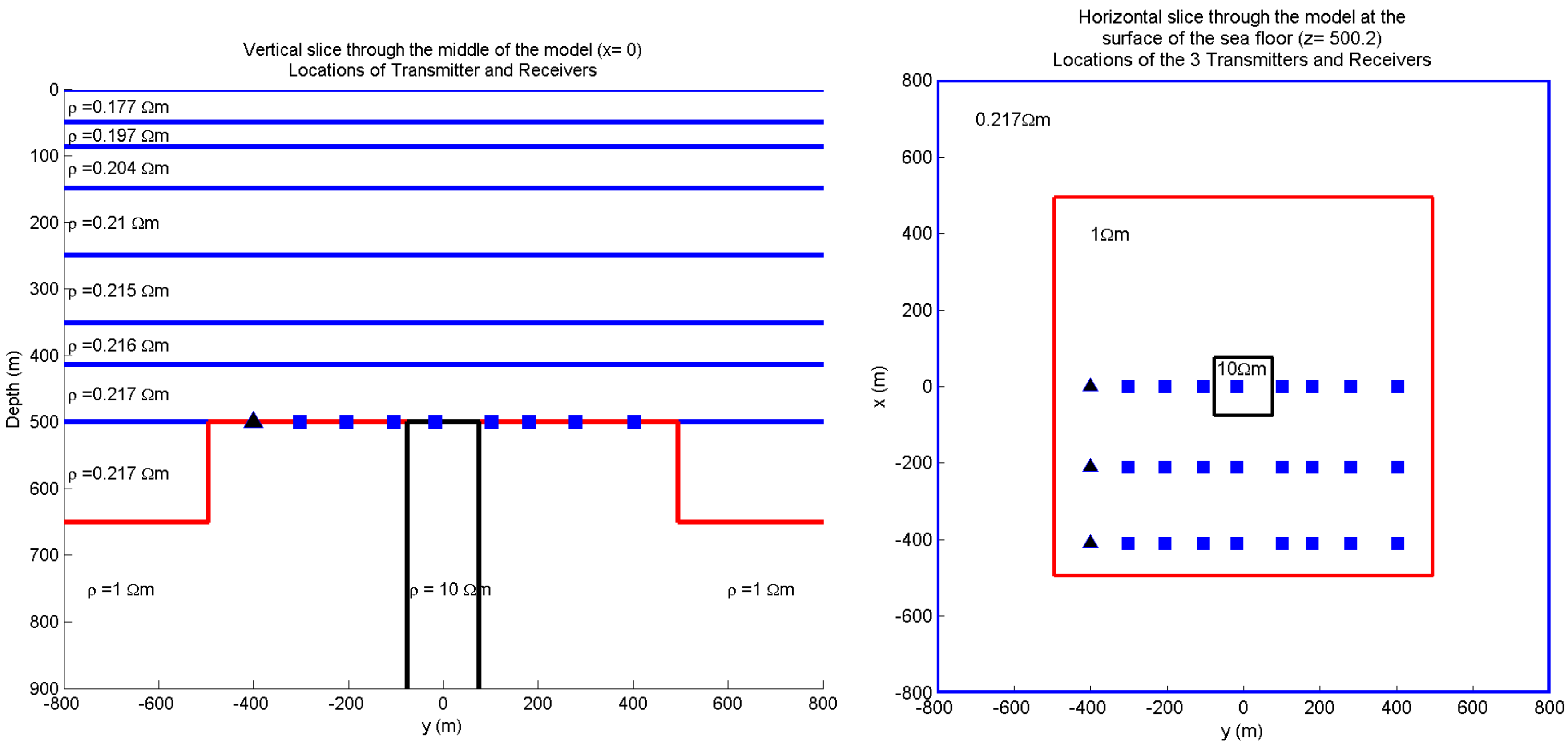

Fig. Marine CSEM model (after Anna Avdeeva)

marine csem example

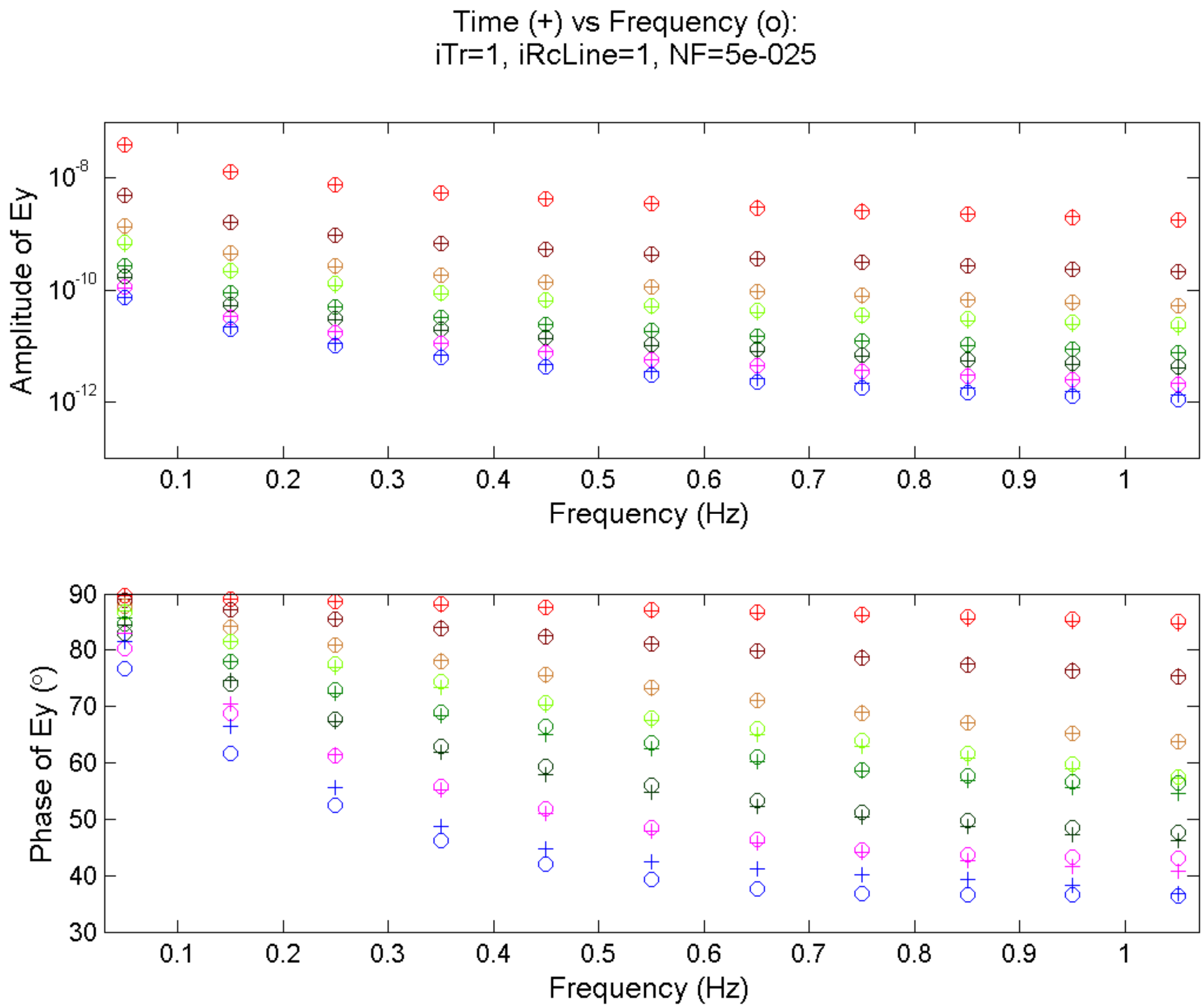

Fig. Comparison x3d code (circles) with another proprietary code (crosses). The amplitudes and phases of Ey component are color-coded for all 8 receiver's positions for profile 1 & 1st transmitter.

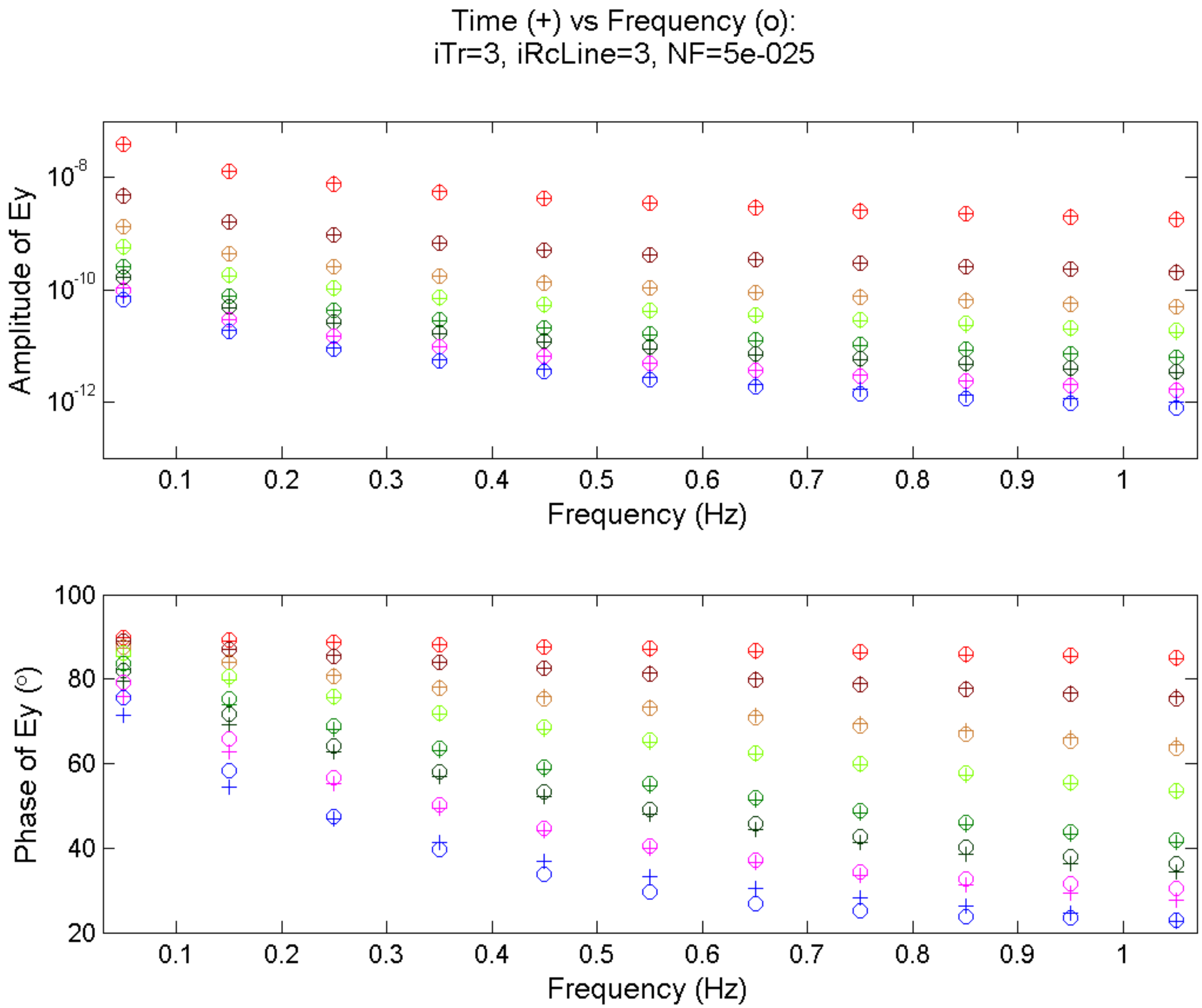

Fig. Comparison x3d code (circles) with another proprietary code (crosses) . The amplitudes and phases of Ey component are color-coded for all 8 receiver's positions for 3[rd] profile & 3rd transmitter.

marine csem example

$$\left|E_y^{3D} - E_y^{background}\right| / \left|E_y^{background}\right|$$

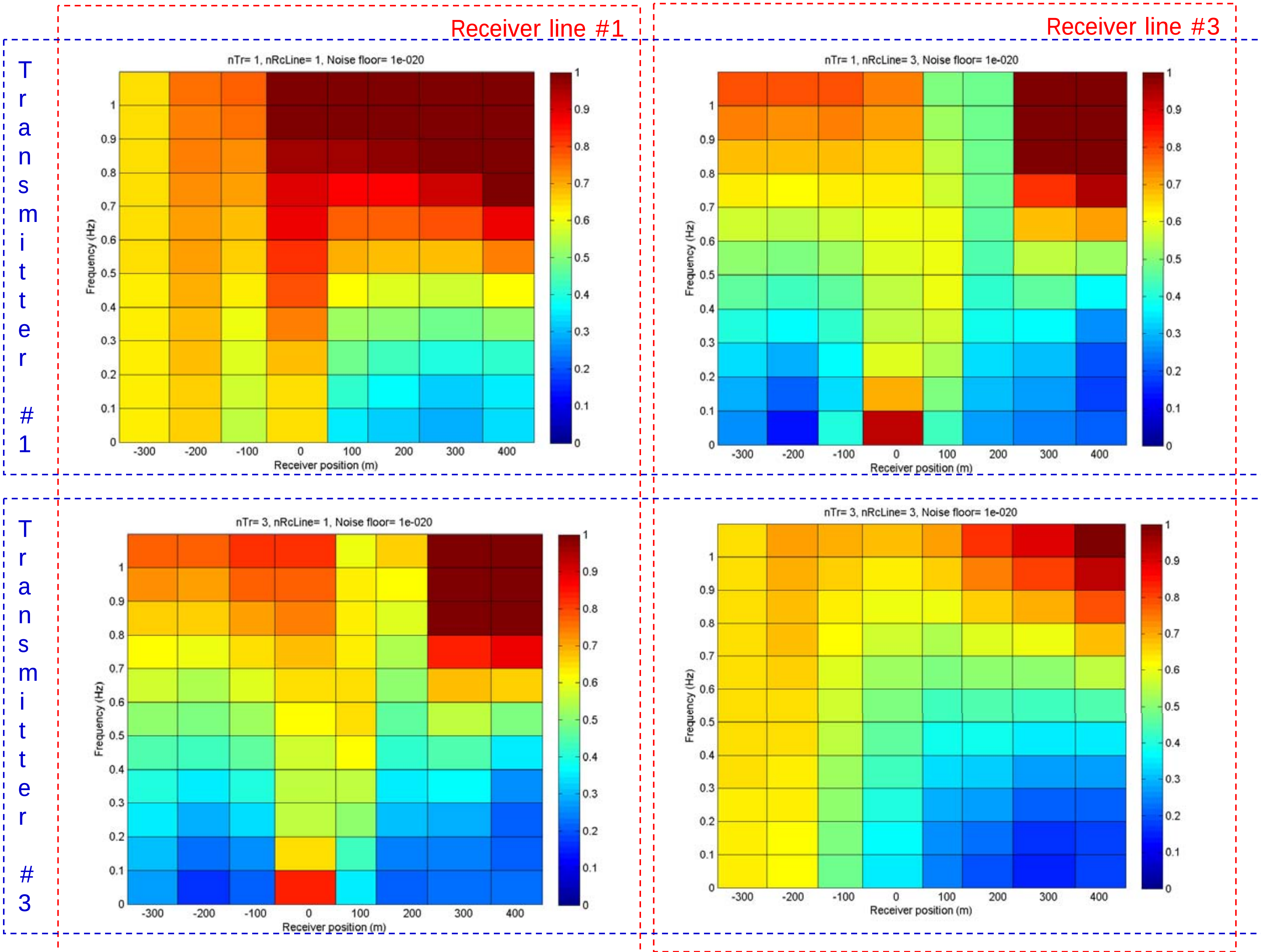

Fig. Sensitivity to the 10-ohmm resistive anomaly (i.e. /w 3-D background removed).

Thanks to ifm-geomar team (Kiel, Germany) for marine csem simulations

Thank you for your attention