H3DTDinv – MUMPS

A Program Library for Forward Modelling of Multi-Transmitter, Time-Domain Electromagnetic Data over 3D structures.

Version 1.0

Developed under the MITEM consortium Research Project
Multi-Source Inversion of Time Domain Electromagnetic Data

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`http://www.eos.ubc.ca/research/ubcgif/`

Introduction

H3DTDinv is a flexible program library for inversion of geophysical time domain electromagnetic survey data resulting from a wide range of sources and source waveforms. The objective of H3DTDinv is to recover a 3D model of the earth's electrical conductivity structure, discretized using a mesh of rectangular cells. This recovery of geo-electrical parameters is achieved through an iterative process, which includes 3D forward simulation at each step and minimization of the objective function (Φ), which, in turn is controlled by data misfit (Φ_d) and the model norm (Φ_m). The forward simulation is solving Maxwell's equations in the time domain. The equations are discretized in time using backward Euler method and discretized in space by using a finite volume technique on a staggered grid. The sources can be grounded dipoles or loop currents that reside in the air, on the surface, or inside the earth. The responses can be any combination of components of E, H, or dB/dt. The transmitter waveform is user-defined and there are no restrictions on the length or shape of the waveform. The Earth model is an arbitrary 3D conductivity distribution, defined on a structured rectangular mesh.

From the user's viewpoint, the software operates much like EH3DTDinv, a previous GIF code developed to carry out time domain inversion. The principal difference is that H3DTDinv inherently works with many transmitters. To facilitate this multi-transmitter capability, the forward modelling matrix is first decomposed using Cholesky decomposition, such that the solution for different transmitters is easily carried out. The solutions are achieved by factorizing the forward modelling matrix. H3DTDinv, although it requires significant computing resources, under certain conditions can be run on single modern laptop or desktop computer. Factorization of the forward modelling matrix is facilitated via the MUMPS software for which documentation and downloads can be found at the following website: `http://graal.ens-lyon.fr/MUMPS/ .` Unlike the forward modelling code, H3DTD, where only one factorization is stored at one time, in H3DTDinv, all factorizations must be stored at the same time, which requires a lot more RAM.

The MUMPS routines are built-in to H3DTDinv and do not need to be installed separately. However, since the forward modelling matrix is large and its decomposition is computationally intensive, H3DTDinv is most efficiently run on an array of computers, or on a single multi-core computer with lots of RAM (~ 16GB). The parallel implementation is carried out using the Message Passing Interface standard (MPI), discussed further in this document.

List of the input files and Graphical User Interface utilities (GUI's)

Programs and GUI's	**Input files**	**File names**
H3DTDinv.exe	Input control file	h3dtdinv.inp (fixed name)
	Conductivity model files (initial, reference)	model_ini.txt (user defined) model_ref.txt (user defined)
	Data file	data.dat (user-defined)
	Topography file	topo.dat (user-defined)
	Weighting file	weight.txt (user-defined)
Mesh_builder.exe GUI	Mesh file	mesh.txt (user defined)
Wave_builder.exe GUI	Wave file	wave.txt (user defined)

Table 1. List of H3DTDinv components and control files (green color indicates that these files are not mandatory to run the inversion).

Setting up the control files

"H3DTDinv.exe" is the executable for the 3D time domain inversion. It has to be run in a separate folder (further "workdir"), which also contains the input file *"h3dtdinv.inp"*. The remainder of the input files do not have any strict naming convention and can be located in any hard drive or network location under any name, as long as they are properly referenced in the *"h3dtdinv.inp"* file. However for convenience we recommend keeping all files relevant to a single inversion in your "workdir".

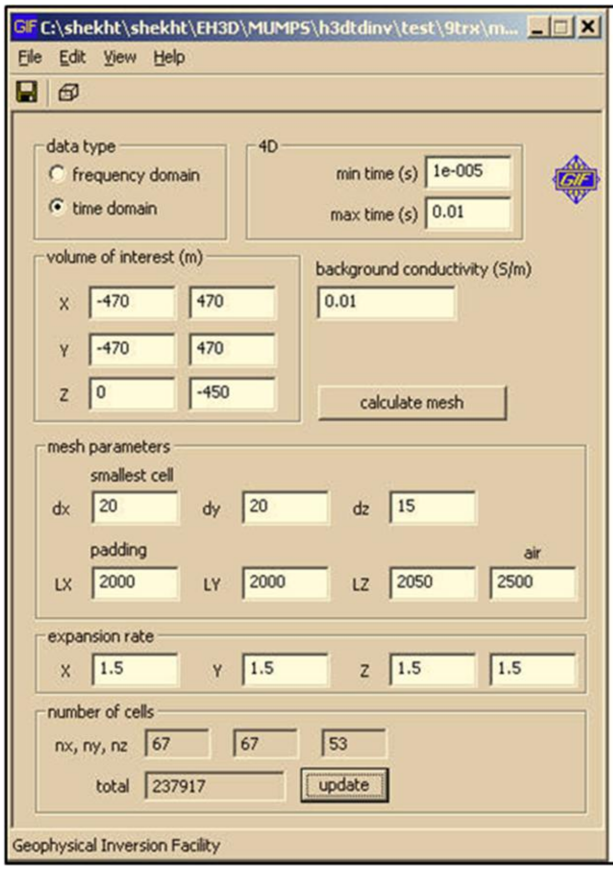
H3DTDinv requires a number of input files and parameters. The control file *"h3dtdinv.inp"* contains references to all necessary files in the 15-line format (see an example below):

```
mesh.txt  ! mesh file
VALUE 0.01 | FILE model_ini.con ! initial conductivity file
VALUE 0.01 | FILE model_ref.con ! reference conductivity file
data_H.txt  ! data file
wave.txt  ! wave file
TOPO_CONST 0. | TOPO_FILE topo.dat
```

```
ignore
BOUNDS_NONE           ! BOUNDS_NONE | BOUNDS_CONST bl bu | BOUNDS_FILE file
NONE                  ! weight file
1.e+2  1.e-9  0.2  ! beta_max  beta_min  beta_factor
1.e-4  1. 1. 1.       ! alpha
CHANGE_MREF           ! CHANGE_MREF | NOT_CHANGE_MREF
SMOOTH_MOD_DIF        ! SMOOTH_MOD | SMOOTH_MOD_DIF
1.                    ! chifact
3  10  1.e-3          ! max_iter_beta  max_iter_ipcg  tol_ipcg
```

In this example there are several other supplementary input files listed, which are described below:

The ***mesh file*** listed in **line 1**, can be located in any folder and can have arbitrary name, as long as it is in ASCII format. The design of the mesh can be handled by the GUI utility *"Meshbuilder.exe".* Selection of mesh parameters is very important and it will be discussed further in this document. In figure 1 there is a screenshot of Meshbuilder GUI with explanations



data type
frequency domain
time domain [✓]

4D
min time (s) 1e-005
max time (s) 0.01

volume of interest (m)
X -470 470
Y -470 470
Z 0 -450

background conductivity (S/m) 0.01

calculate mesh

mesh parameters
smallest cell
dx 20 dy 20 dz 15
padding
LX 2000 LY 2000 LZ 2050 air 2500

expansion rate
X 1.5 Y 1.5 Z 1.5 1.5

number of cells
nx, ny, nz 67 67 53
total 237917
update

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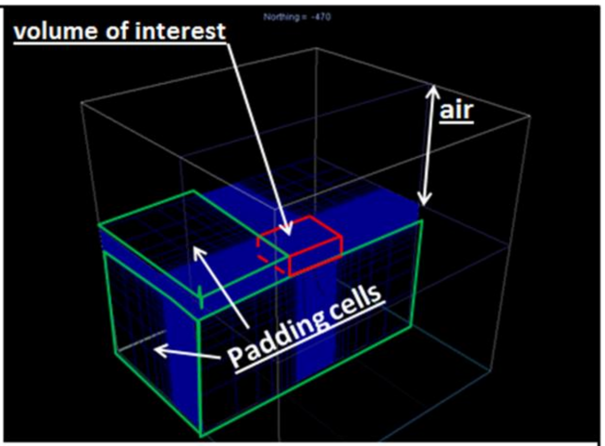


- Data type = "time domain"
- Min time = your first time gate (seconds)
- Max time = your last time gate (seconds)
- Volume of interest = the bounds of area you are modeling (X,Y and Z)
- Background conductivity = half-space conductivity for calculating the mesh parameters

Figure 1. Mesh file builder GUI parameters setup and graphical representation.

of described parameters”. In setting the mesh parameters, the cell size of “volume of interest” (“smallest cell” in the menu) should depend on the actual geometry of the survey (primarily on density of stations defined by line spacing and sampling rate). The user has to maintain a balance between saving computing time (by coarsening the mesh) and getting more accurate solution of the forward simulation by making the mesh finer. The padding distance, depends on the latest data acquisition time gate and is calculated automatically to diffusion distance defined by equation (1):

$$\textbf{(1)} \qquad \mathbf{D(t) = 1250^*}\sqrt{t/\sigma} \qquad \text{(meters)}$$

In this equation *t* is the latest time gate and σ – is the conductivity of the background half-space in Siemens per meter (S/m).

The background conductivity in meshbuilder is only used to calculate the diffusion radius and is not being further assigned for the forward starting model. The expansion rate is the geometric progression coefficient used for building the padding cells. Generally values between 1.3 and 1.6 are reasonable choices for the expansion rate.

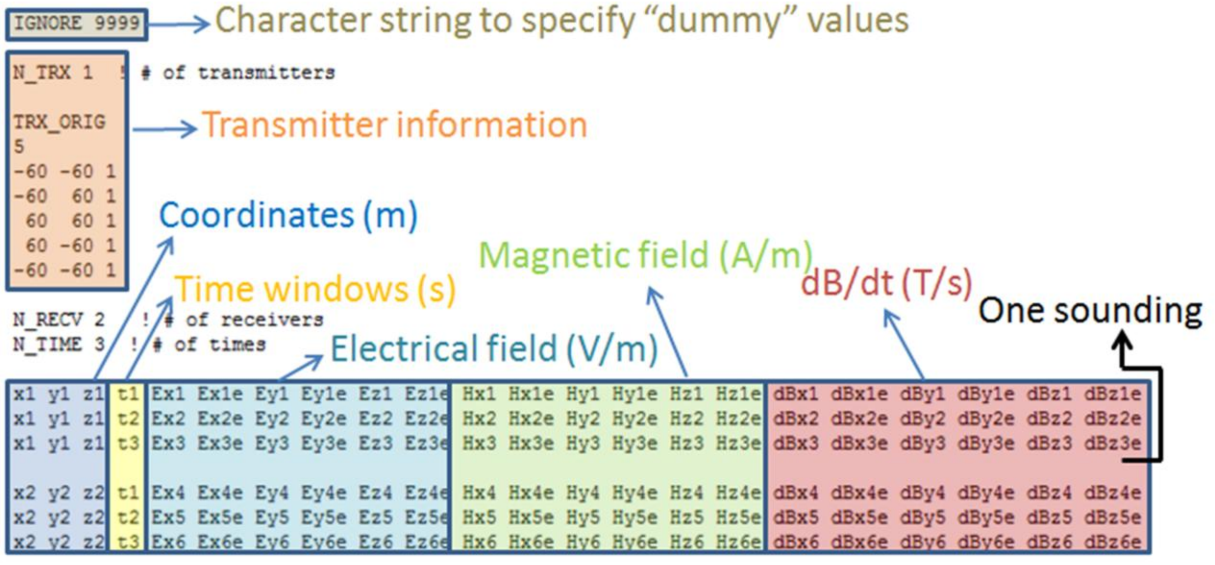
The format of the mesh file is:

`nx ny nz`	(number of cells in the X, Y, and Z directions)
`x0 y0 z0`	(coordinates of the top south west corner of the mesh)
`dx_1 dx_2 ... dx_nx`	(cell widths in X)
`dy_1 dy_2 ... dy_ny`	(cell widths in Y)
`dz_1 dz_2 ... dz_nz`	(cell widths in Z)

The ***initial model file*** is the starting model for the initial forward simulation. It is referenced in **line 2** of the input control file, and is defined in the standard UBC format, as a single column of values, one value for each cell. The first value corresponds to the top south-western cell. The values are ordered such that Z (depth) changes the fastest, followed by X (easting), followed by Y (northing). For constant half-space model parameters, a single value entered in the input control file can be used as a substitute to the model files. When a file is entered, the line in the input file should start with “FILE”, and when a constant value is entered, the line should start with VALUE. The model is updated after every iterative step and used to calculate data misfit. Each updated model is written in the workdir with a new name “inv_*.con”, containing the iteration number.

The ***reference model file*** is specified in **line 3** of the input control file. It may or may not be updated throughout the inversion process, depending on a user-defined optional parameter. The file has identical format to that of the initial model and can be also produced using the “Modelbuilder v1.0” package. This file is used to calculate the model norm (Φ_m). The reference model may as well be the same as the starting model if no specific geological constraints are known.

The ***data file*** is specified in **line 4** of the input control file. This file contains information about transmitter and receiver locations, acquisition time windows, the measured data and the standard deviations. In figure 2 the format of the data file is shown.



```
IGNORE 9999
N_TRX 1    ! # of transmitters

TRX_ORIG
5
-60 -60 1
-60  60 1
 60  60 1
 60 -60 1
-60 -60 1
N_RECV 2   ! # of receivers
N_TIME 3   ! # of times
x1 y1 z1 t1 Ex1 Ex1e Ey1 Ey1e Ez1 Ez1e Hx1 Hx1e Hy1 Hy1e Hz1 Hz1e dBx1 dBx1e dBy1 dBy1e dBz1 dBz1e
x1 y1 z1 t2 Ex2 Ex2e Ey2 Ey2e Ez2 Ez2e Hx2 Hx2e Hy2 Hy2e Hz2 Hz2e dBx2 dBx2e dBy2 dBy2e dBz2 dBz2e
x1 y1 z1 t3 Ex3 Ex3e Ey3 Ey3e Ez3 Ez3e Hx3 Hx3e Hy3 Hy3e Hz3 Hz3e dBx3 dBx3e dBy3 dBy3e dBz3 dBz3e

x2 y2 z2 t1 Ex4 Ex4e Ey4 Ey4e Ez4 Ez4e Hx4 Hx4e Hy4 Hy4e Hz4 Hz4e dBx4 dBx4e dBy4 dBy4e dBz4 dBz4e
x2 y2 z2 t2 Ex5 Ex5e Ey5 Ey5e Ez5 Ez5e Hx5 Hx5e Hy5 Hy5e Hz5 Hz5e dBx5 dBx5e dBy5 dBy5e dBz5 dBz5e
x2 y2 z2 t3 Ex6 Ex6e Ey6 Ey6e Ez6 Ez6e Hx6 Hx6e Hy6 Hy6e Hz6 Hz6e dBx6 dBx6e dBy6 dBy6e dBz6 dBz6e
```

Figure 2. Format of *data.dat* file for H3DTDinv program.

The format of this file allows complete freedom of using any combination of electric and/or magnetic field components or magnetic induction derivative components (dB/dt) defined in Cartesian metric coordinate system (XYZ) and specified in SI units. Each data value must be followed by its standard deviation. Unfortunately there is no actual time domain system, which is able to acquire all of these data and most common time domain data comes in units of magnetic induction time derivative (dB/dt). Therefore a character string is included (Figure 2), which would specify the dummy values to be ignored in the data file. For example if only dBz/dt measurements are provided in a particular data set then all other E, H and dBx/dt or dBy/dt components in the file should be set to this “dummy” value.

One of the most important features of the H3DTDinv is the ability to invert data from multiple transmitters. This feature makes it possible to invert airborne time domain data in 3D, as well as multiple source ground EM soundings. The number of transmitters is specified in the second line of data file (N_TRX). The transmitter label (i.e., “TRX_ORIG”) is specified in the third line of the file and indicates the type of transmitter. There are four options for describing the transmitter source (Figure 3):

- TRX_ORIG (Figure 3A,B): connecting individual wire segments to form a grounded or inductive source
- TRX_LINES (Figure 3A): primary field is generated from analytic expressions for wires in free space
- TRX_LOOP (Figure 3C): circular loop with arbitrary orientation
- TRX_MAGNETIC_DIPOLE (Figure 3D): magnetic dipole

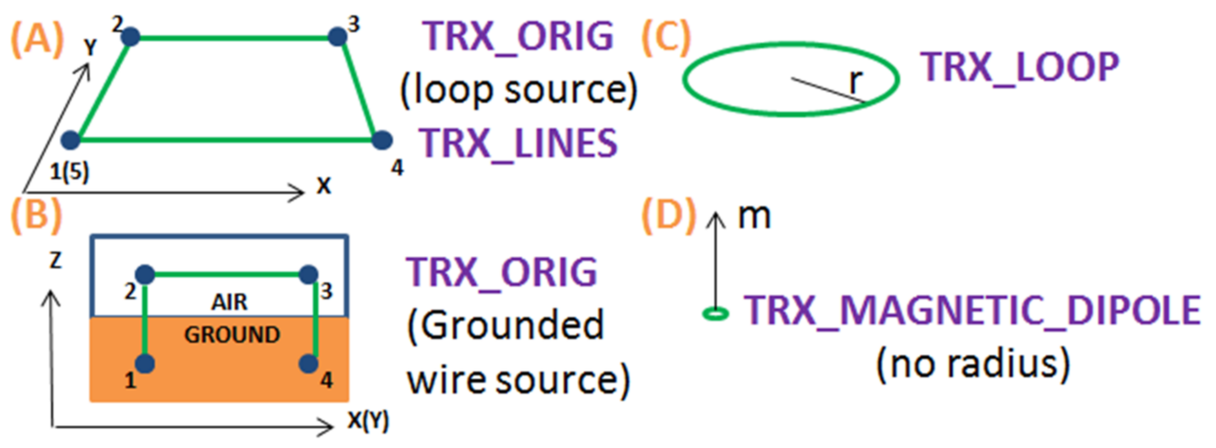


Figure 3. (A) Original or TRX_LINES transmitter type configuration using closed loop source geometry; (B) Original transmitter configuration based on grounded wire source geometry (C) Loop transmitter type (D) Magnetic dipole transmitter type.

TRX_ORIG : the “original” distributed current source (closed loops or grounded wires). This type is a good approximation of any conventional large square loop system (ground and airborne), including, Crone, Geonics (EM47, 57, 67), Zonge, GeoTEM, MegaTEM, MegaTEM II, SkyTEM, etc. The source in this case is described by number of nodes `“N”` (4 for grounded wire or n>4 for closed loop) and `xi yi zi` coordinates for each node (see example below).

```
TRX_ORIG
N                                   (number of nodes)
x1 y1 z1                            (node coordinates)
x2 y2 z2
:
xn yn zn
```

Conceptually the source involves a uniform current density within the cells where the source current flows. The grounded wire (Figure 3B) is strictly defined over the air/ground boundary, with nodes 1 and 4 being in the ground domain and 2, 3, in the air. For a closed loop (Figure 3A), the first and last nodes must be identical (i.e., a square loop is specified with 5 nodes). Current in the transmitter is assumed to be 1 Ampere.

TRX_LOOP: an analytical circular loop (Figure 3C). This type is described by X, Y, Z location, circular loop radius. This type is a good approximation for large airborne transmitters (VTEM, HeliGeotem, AeroTEM II and IV, HoisTEM, NewTEM, etc). The following is an example of the TRX_LOOP source description format:

```
TRX_LOOP
x y z  radius theta alpha
```

Here `x`, `y` and `z` are the coordinates, `“radius”` is the loop radius, `“theta”` is the vertical angle from positive Z (up) axis and `“alpha”` is the vertical angle from positive Y (North) axis. For a loop parallel to XY plane use alpha = theta = 0.

TRX_MAGNETIC_DIPOLE: an analytical magnetic dipole. This is a good approximation of small radius airborne TDEM systems (AeroTEM I, II) and small loop ground TDEM systems (Geonics EM61, EM63, etc). The following is an example of the TRX_MAGNETIC_DIPOLE source description format:

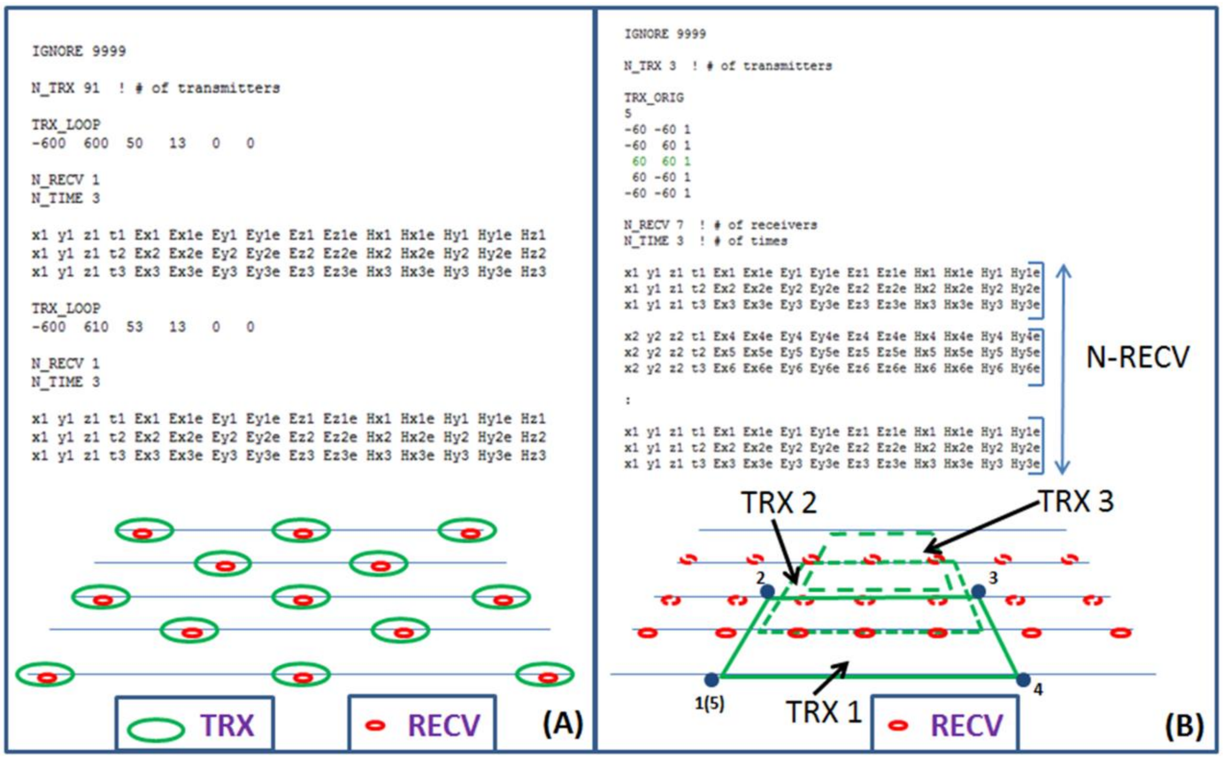
```
TRX_MAGNETIC_DIPOLE
```

```
    x y z theta alpha  m
```

In this file format, `x`, `y` and `z` are the coordinates, `"theta"` is the vertical angle from positive Z (up) axis, `"alpha"` is the vertical angle from positive Y (North) axis and `"m"` is the dipole moment of the transmitter, which should be listed in SI units. Similar to previous example, for a loop parallel to XY plane use alpha = theta = 0.

TRX_LINES: an analytical general closed loop of line currents. It is designed to handle arbitrary complex transmitters with user defined number of nodes. The format for this source type is same as for the TRX_ORIG. The number of nodes has to be greater than 4. The main difference is in numerical algorithms, simulating transmitter currents.

The structure of the data file is transmitter oriented, which means that each transmitter is followed by data from all receiver locations, associated with this transmitter. For instance, in figure 4, examples are shown illustrating the data file structure suitable for airborne TDEM survey (Figure 4A), where each transmitter location is associated with a single receiver location and with a multiple source ground EM survey, where each loop location is associated with multiple transmitters.



```
IGNORE 9999

N_TRX 91  ! # of transmitters

TRX_LOOP
-600  600  50   13   0   0

N_RECV 1
N_TIME 3

x1 y1 z1 t1 Ex1 Ex1e Ey1 Ey1e Ez1 Ez1e Hx1 Hx1e Hy1 Hy1e Hz1
x1 y1 z1 t2 Ex2 Ex2e Ey2 Ey2e Ez2 Ez2e Hx2 Hx2e Hy2 Hy2e Hz2
x1 y1 z1 t3 Ex3 Ex3e Ey3 Ey3e Ez3 Ez3e Hx3 Hx3e Hy3 Hy3e Hz3

TRX_LOOP
-600  610  53   13   0   0

N_RECV 1
N_TIME 3

x1 y1 z1 t1 Ex1 Ex1e Ey1 Ey1e Ez1 Ez1e Hx1 Hx1e Hy1 Hy1e Hz1
x1 y1 z1 t2 Ex2 Ex2e Ey2 Ey2e Ez2 Ez2e Hx2 Hx2e Hy2 Hy2e Hz2
x1 y1 z1 t3 Ex3 Ex3e Ey3 Ey3e Ez3 Ez3e Hx3 Hx3e Hy3 Hy3e Hz3
```

```
IGNORE 9999

N_TRX 3  ! # of transmitters

TRX_ORIG
5
-60 -60 1
-60  60 1
 60  60 1
 60 -60 1
-60 -60 1

N_RECV 7  ! # of receivers
N_TIME 3  ! # of times

x1 y1 z1 t1 Ex1 Ex1e Ey1 Ey1e Ez1 Ez1e Hx1 Hx1e Hy1 Hy1e
x1 y1 z1 t2 Ex2 Ex2e Ey2 Ey2e Ez2 Ez2e Hx2 Hx2e Hy2 Hy2e
x1 y1 z1 t3 Ex3 Ex3e Ey3 Ey3e Ez3 Ez3e Hx3 Hx3e Hy3 Hy3e

x2 y2 z2 t1 Ex4 Ex4e Ey4 Ey4e Ez4 Ez4e Hx4 Hx4e Hy4 Hy4e
x2 y2 z2 t2 Ex5 Ex5e Ey5 Ey5e Ez5 Ez5e Hx5 Hx5e Hy5 Hy5e
x2 y2 z2 t3 Ex6 Ex6e Ey6 Ey6e Ez6 Ez6e Hx6 Hx6e Hy6 Hy6e

:

x1 y1 z1 t1 Ex1 Ex1e Ey1 Ey1e Ez1 Ez1e Hx1 Hx1e Hy1 Hy1e
x1 y1 z1 t2 Ex2 Ex2e Ey2 Ey2e Ez2 Ez2e Hx2 Hx2e Hy2 Hy2e
x1 y1 z1 t3 Ex3 Ex3e Ey3 Ey3e Ez3 Ez3e Hx3 Hx3e Hy3 Hy3e
```

Figure 4. Building data file for multiple transmitters: (A) Airborne; (B) Ground multiple loop survey

The ***wave file*** is specified in **line 5** of the input control file. Its format is similar to previous UBC-GIF codes (EH3DTD). The same wave file is used for all transmitters. Users will likely have their own wave file for their transmitter. The wave file has control over the discretization of the actual waveform in both on-time and off-time. This discretization is carried out by defining time stepping “Δt”, used to solve Maxwell’s equations in time domain. This time stepping is used for factorization of the modeling matrix. A new factorization of the modelling matrix is required whenever the stepping time “Δt” is changed. Maxwell's equations are most efficiently solved for a constant time step or a few time intervals each with a constant time step. Since the inversion needs to store all factorizations in memory, having many different “Δt” would require a lot of RAM.

The most computationally efficient discretization is when a single value of Δt can be used for the full time range of interest. Most systems consist of an “on-time” portion (exponential, half-sign, ramp, etc) followed by an “off-time”. The on-time portion of the waveform may be modelled using a large value of Δt. Data acquired in the off-time often spans a few decades of time (Figure 5).

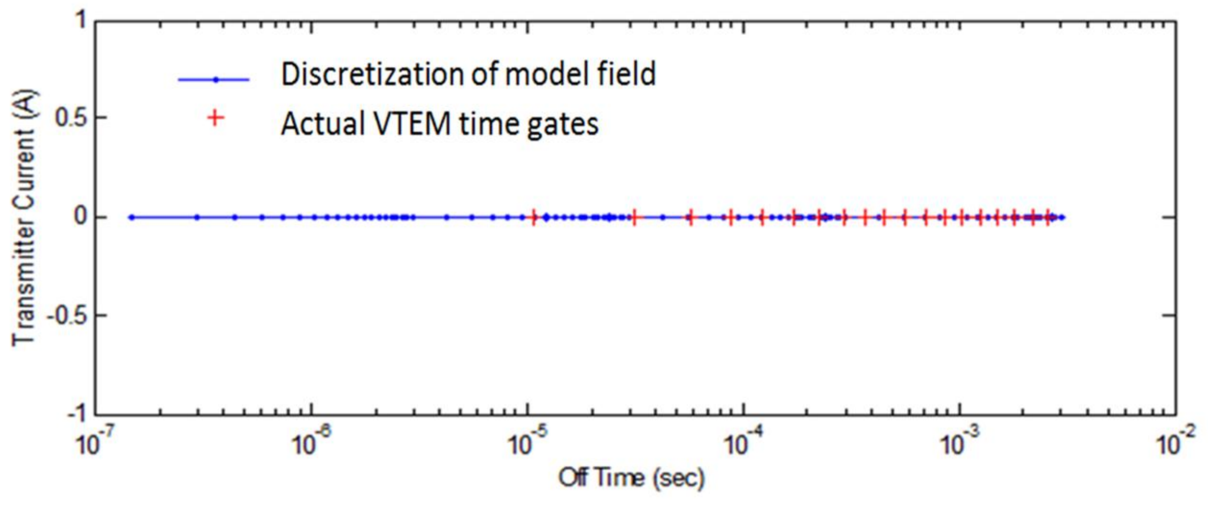


Figure 5. Example: off-time steps (blue) shown versus actual off-time data acquisition time gates for VTEM system (red).

The stepping time region begins one decade prior to the user-defined earliest time, and extends until the latest data time is defined. It is divided into logarithmic segments, usually a decade in length. Each segment is time stepped with a uniform Δt (linearly spaced). Generally 10-20 time steps are adequate for each decade in time. The total computation time depends upon the number of factorizations, the number of time steps, and the number of transmitters. Please note, that if time stepping does not match the actual data acquisition time windows, interpolated values of the fields are assigned to the predicted data at times specified in the data file.

A *"Wavebuilde.exe"* GUI has been provided with the inversion code to assist the user in generating the wave files. Figures 6, 7 and 8 show the user interface for generating different types of waveforms. Among the GUI settings there are some general parameters, which are applicable to any waveform and other parameters specific to each waveform type in particular. Among the general parameters are the following:

Max/min: "min" and "max" values denote the beginning and end values of the time window through which equations are time-stepped. "min" should be smaller (typically about a decade) smaller than the first datum time. "max" can correspond to the last datum time.

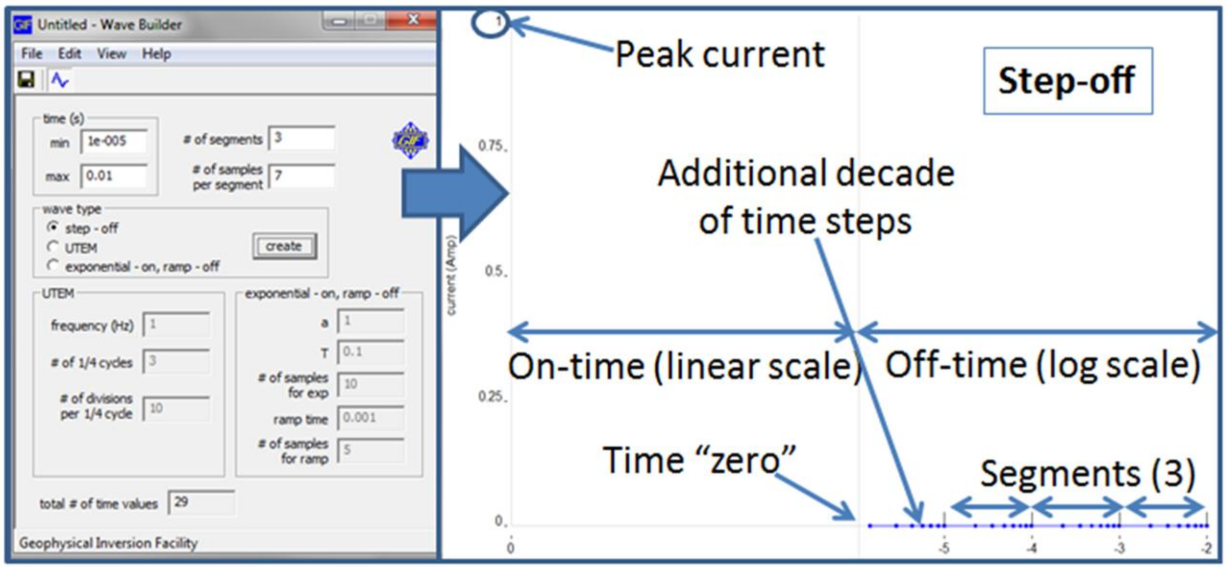
# of segments and *# of samples per segment* are the number of logarithmically spaced segments and linearly spaced samples per each segment

There are three wave type options included in the present GUI.

- Step off (Figure 6)
- UTEM (Figure 7)
- Exponential plus a ramp (Figure 8)

Each of these are described in further detail below, accompanied by explanations of the parameters of the interface that are of relevance, and also plots of the times at which the equations are solved. For each waveform type all time values are referenced to the "time zero", which is the beginning of both: factorization time steps and data acquisition time gates.

Step-off (Figure 6). The current prior to t=0 is assumed to be uniform and solution of the steady state fields are generated by the program. This reverse Heaviside function is the simplest waveform to model. No actual geophysical system uses this exact waveform; however recorded signals can often be deconvolved to conform to this waveform type. Peak current (maximum current) data are generally sampled only in the log domain.


Untitled - Wave Builder

File Edit View Help

time (s)
min 1e-005
max 0.01
# of segments 3
# of samples per segment 7

wave type
(●) step - off
( ) UTEM
( ) exponential - on, ramp - off

UTEM
frequency (Hz) 1
# of 1/4 cycles 3
# of divisions per 1/4 cycle 10

exponential - on, ramp - off
a 1
T 0.1
# of samples for exp 10
ramp time 0.001
# of samples for ramp 5

total # of time values 29

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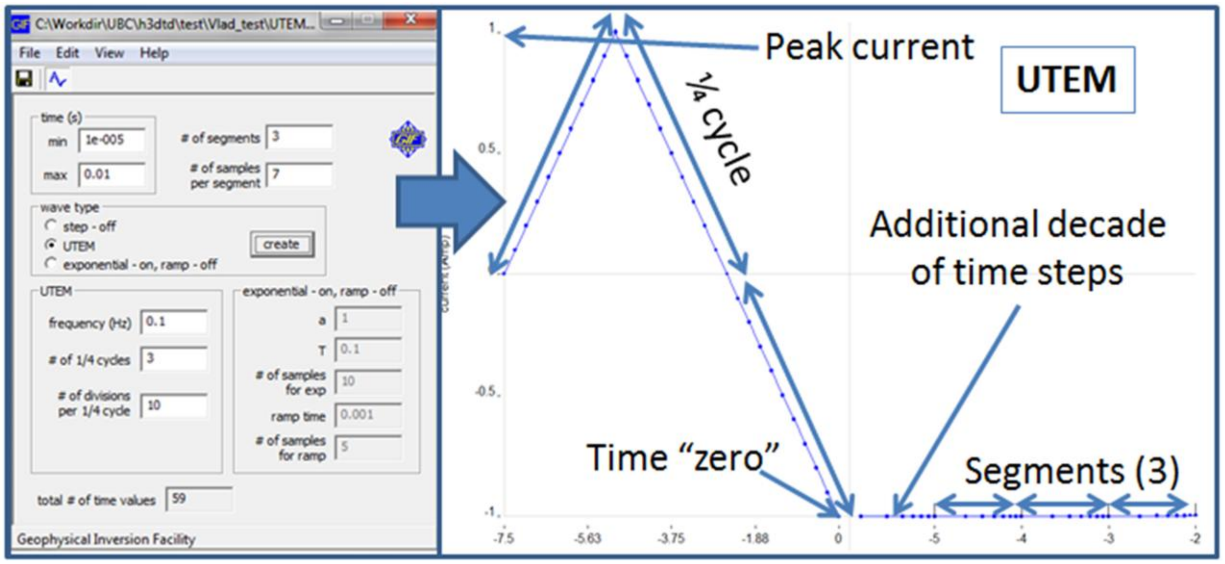
Figure 6. An example of "Step-off" waveform.

UTEM (Figure 7). Also often referred to as "sawtooth". This is another simple waveform, which is periodic defined by the frequency and the amplitude. For UTEM waveform there is no off-time, all measurements acquired in the on-time. The forward modelling begins with all field values set to zero and hence ¾ of a cycle is usually modelled prior to data collection times. The ¾ cycle can be modelled in linear time steps and following data times in logarithmic steps. The number of quarter cycles to be modelled prior to data collection is governed by a user-defined parameter which has to be an odd number.


C:\Workdir\UBC\h3dtd\test\Vlad_test\UTEM...

File Edit View Help

time (s)
min 1e-005
max 0.01
# of segments 3
# of samples per segment 7

wave type
( ) step - off
(●) UTEM
( ) exponential - on, ramp - off

UTEM
frequency (Hz) 0.1
# of 1/4 cycles 3
# of divisions per 1/4 cycle 10

exponential - on, ramp - off
a 1
T 0.1
# of samples for exp 10
ramp time 0.001
# of samples for ramp 5

total # of time values 59

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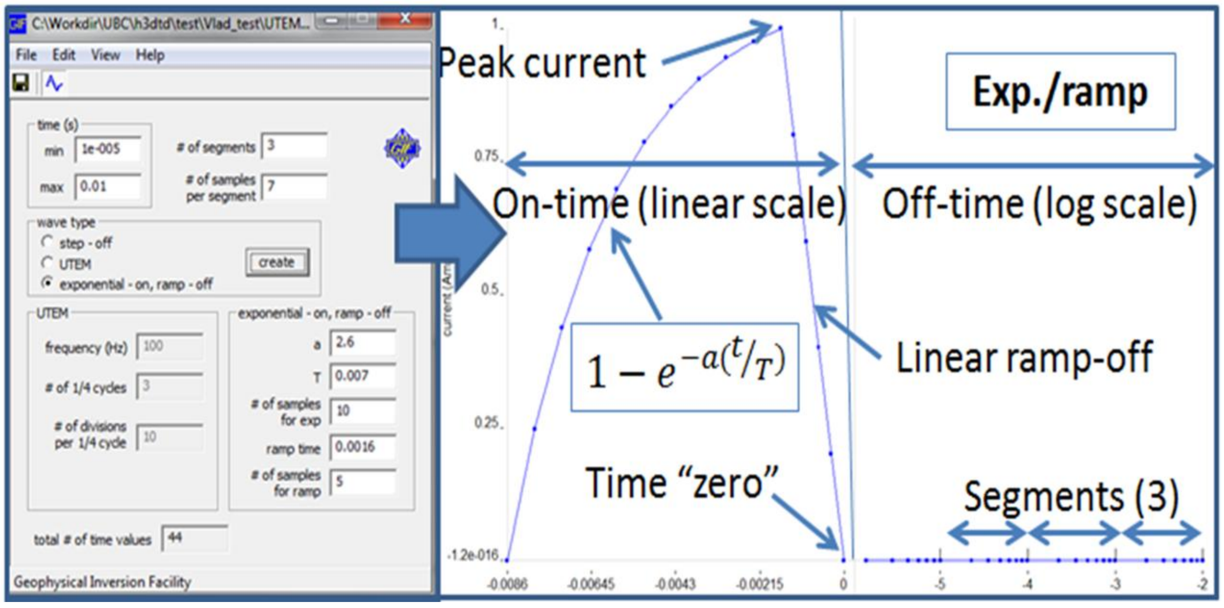
Figure 7. An example of "UTEM" waveform.

It is convenient to have the data times begin at t=0 and so the UTEM waveform will begin at some negative time. The time stepping for the data channel portion of the waveform is controlled by the "max-min" values on the interface.

Exponential-on/ramp-off (Figure 8) This is a general expression that can approximate the waveform from many systems. This is an exponential rise in current followed by a ramp off. The ramp-on is defined by the equation (2):

(2) $\mathbf{I = 1 -} \; e^{-a(t/T)}$, where I is the current, **a** is the exponential decay coefficient, **T** is a user defined parameter equal to the desired length of the exponential ramp-on. Thus the exponential ramp is defined for 0<t<T. For later times the waveform is a ramp-off and its length is designated in the box "ramp time" in the interface. The end of the ramp is adjusted so that it corresponds to "t=0" and subsequent times are logarithmically generated by the "max-min" portion of the interface.


C:\Workdir\UBC\h3dtd\test\Vlad_test\UTEM...

File Edit View Help

time (s)
min 1e-005
max 0.01
# of segments 3
# of samples per segment 7

wave type
step - off
UTEM
[✓ exponential - on, ramp - off]
create

UTEM
frequency (Hz) 100
# of 1/4 cycles 3
# of divisions per 1/4 cycle 10

exponential - on, ramp - off
a 2.6
T 0.007
# of samples for exp 10
ramp time 0.0016
# of samples for ramp 5

total # of time values 44

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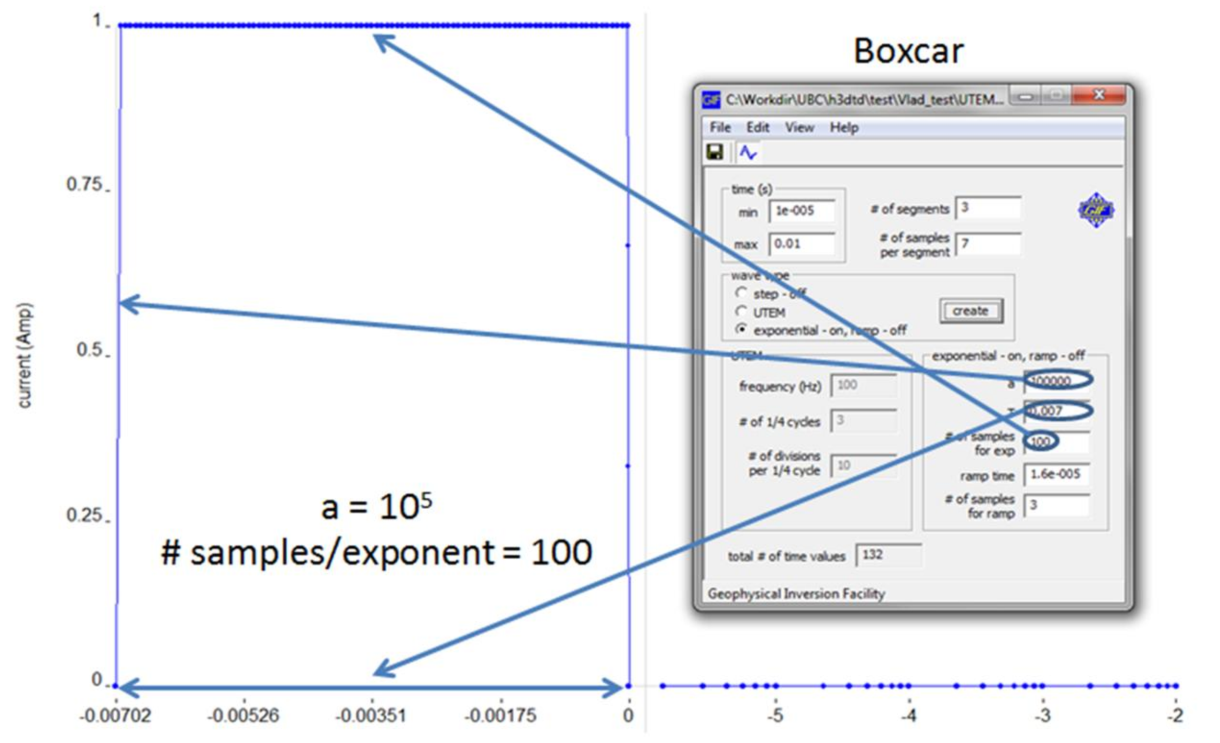
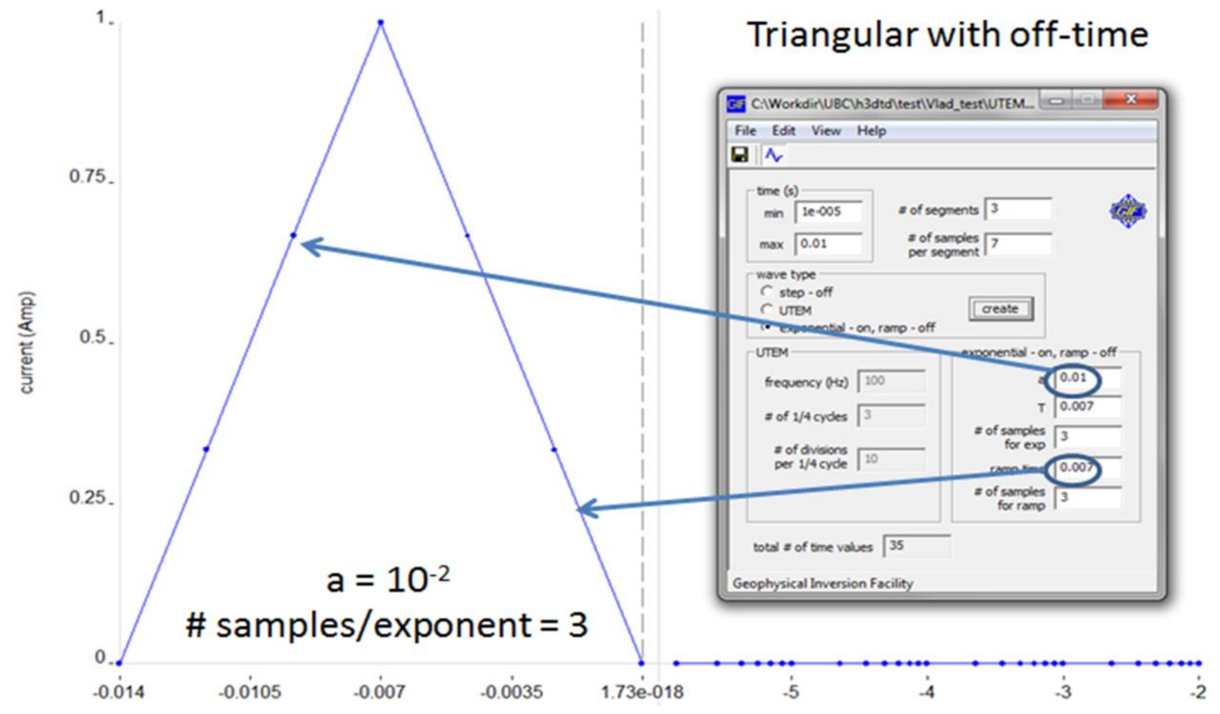
Figure 8. An example of "Exponential rise/ramp-off" waveform.

Figures 9 and 10 show examples of how to approximate boxcar pulse and triangular pulse with off-time, using "exponential ramp-on/linear ramp-off" waveform type by changing the exponential rise **"a"** coefficient and number of samples per exponent.



time (s) min 1e-005
max 0.01
# of segments 3
# of samples per segment 7
wave type
step - off
UTEM
[✓ exponential - on, ramp - off]
UTEM
frequency (Hz) 100
# of 1/4 cycles 3
# of divisions per 1/4 cycle 10
exponential - on, ramp - off
a 100000
T 0.007
# of samples for exp 100
ramp time 1.6e-005
# of samples for ramp 3
total # of time values 132

Figure 9. An example of simulating a boxcar waveform using the exponential ramp-on/linear ramp-off approximation.



time (s) min 1e-005
max 0.01
# of segments 3
# of samples per segment 7
wave type
step - off
UTEM
[✓ exponential - on, ramp - off]
UTEM
frequency (Hz) 100
# of 1/4 cycles 3
# of divisions per 1/4 cycle 10
exponential - on, ramp - off
a 0.01
T 0.007
# of samples for exp 3
ramp time 0.007
# of samples for ramp 3
total # of time values 35

Figure 10. An example of simulating a triangular pulse with off-time, using the exponential ramp-on/linear ramp-off approximation.

By default, the "*Wavebuilder"* GUI assigns a peak current value of 1 A. In the *"edit"* menu, under *"advanced"* features it is possible to include user-defined peak current value. The user should be especially careful, when dealing with the dipole transmitter types, which contain peak current values in the dipole moment and ensure that current in the waveform is de-normalized by the peak value.

The waveform file can be saved under user-defined name with arbitrary extension. The format is shown below.

```
0.0000000e+000  1.0000000e+000
1.0000000e-005  0.0000000e+000  15
1.0000000e-004  0.0000000e+000  15
1.0000000e-003  0.0000000e+000  15
1.0000000e-002  0.0000000e+000  15
1.0000000e-001  0.0000000e+000  15
```

This is the example of a step-off current. The first column is the time (in seconds) and the second column is the current (in amperes). The optional third column indicates the number of equal time steps to use. The first time value in the wave file does not necessarily have to be 0. In fact, zero-time should be defined relative to the acquisition time gates, rather than beginning of the pulse in the waveform. The on-time pulse can be in the negative domain. In this particular example there will be 15 equal time steps between 0 and 10^{-5} s. The time steps will therefore be 10^{-5} / 15 = 6.67*10^{-7} s. Between 10^{-4} and 10^{-5} s, there will also be another 15 equal time steps equal to (10^{-4} - 10^{-5}) / 15 = 6.0*10^{-6} s.

A ***<u>topography file</u>*** is specified in **<u>line 6</u>** of the input control file. If no topography is available, a constant value can be used for the inversion, in which case the line should be set to

```
TOPO_CONST value,
```

where `"value"` corresponds to where the earth-air interface is in the mesh. All cells above with Z coordinates, exceeding `"value"` will be air, which is assigned a conductivity of 10^{-8} S/m. When inverting data sets, collected in rugged terrains, the topography will play an increasingly important role in the accuracy of forward model calculation. If not set to a constant, the topography can be specified in two different ways:

1. UBC-GIF standard 3 column topographic file format, specified in line 6 of the *H3DTDinv.inp* as: `TOPO_FILE topo.dat`

   ```
   n
   x1 y1 elev1
   x2 y2 elev2
     :
   xn yn elevn
   ```

   If topo file is used, all model conductivity values with $Z>Z_{topo}$ are fixed at 10^{-8} S/m
2. Using cell masking on a model file. In order to activate this capability, a parameter `MNZ  mask_file.dat` should be specified in line 6 of the *H3DTDinv.inp*. of the *"mask_file.dat"* file is stored in identical format as the model file and it should contain values of either 1 or 0, with "1" meaning that this cell will be used for the inversion (actrive) and "0" meaning that this value is fixed to the corresponding value of the reference model (inactive).

   This masking capability can be potentially used for assigning topography by setting the reference model cells, corresponding to zeroes in the *mask_file.dat* to 10^{-8} S/m.

Line 7 is currently obsolete and is not used by the inversion.

A ***bounds file*** may be specified in **line 8** of *H3DTDinv.inp,* with a particular conductivity model. The bounds are used to put constraints on the inversion. There are three options to set up the conductivity bounds

`BOUNDS_NONE`	(No bounds are imposed on the conductivity values)
`BOUNDS_CONST bl bu`	(Same bounds for all cells: `bl` – lower bound, `bu` – upper bound)
`BOUNDS_FILE`	(A bounds file to be used)

The bounds file has the same number of lines as the model file. It consists of 2 columns, containing the lower bounds in the first column and the upper bounds in the second column.

Weighting coefficients file is specified in **line 9** of the *"H3DTDinv.inp"* file. User-defined weights, which are applied to the model norm, are in the same format the model file. A single column is composed of values greater or equal to one. Each cell's weight is equal to "1" by default. It is not recommended to use numbers smaller than "1" as the latter may destabilize the inversion. By increasing the weighting coefficient of a particular cell, the user is suppressing the recovery of electrical conductivity for this cell. Weights of inactive cells are ignored.

`file.txt` is entered for referencing a weighting coefficient file
If `NONE` is entered, no weighting will be used.

The ***trade-off parameter*** is the coefficient used to scale the model norm. The inversion convergence and stability are in many ways dependant on the correct selection of this parameter. In **line 10** of the control file, the range of trade-off parameter is specified along with the step used at each iteration. In the inversion we use a cooling algorithm, in accordance with equation **(3)**, in order to achieve the target misfit.

(3) $\beta_{k+1} = \beta_{factor} * \beta_k$, where β_{factor} is the cooling parameter and β_i are the values of trade-off parameter at consequent iteration steps. The range of trade-off parameters may be entered into *H3DTDinv.inp* as following:

`beta_max   beta_min   beta_factor`, or else set to `DEFAULT`

During the inversion the trafe-off parameter will start at `beta_max` and at each iteration it will be reduced by the factor `beta_factor` until it reaches `beta_min`. In case `DEFAULT` is entered the trade-off parameter range will be calculated as follows:

$$\boxed{\beta_{max} = 1000\frac{\| Jr \|^2}{\| Wr \|^2}; \quad \beta_{min} = 10^{-7}\beta_{max}; \quad \beta_{factor} = 0.16681}$$

Here, r is a random vector, **J** is the sensitivity matrix and **W** is the model weighting matrix.

The ***smoothing parameters*** may be entered into **line 11** of the input control file. These are model objective function parameters used in an identical manner to other UBC-GIF codes. They should be entered as follows:

```
alpha_s alpha_x alpha_y alpha_z
```

Here `alpha_s` is the coefficient for the smallest model component.
`alpha_x` is the coefficient for the derivative in the easting direction.
`alpha_y` is the coefficient for the derivative in the northing direction.
`alpha_z` is the coefficient for the derivative in the vertical direction.

None of the alpha's can be negative and they cannot be all equal to 0 at the same time. There are no default values, the smoothing parameters must be user-defined. They are chosen in an identical manner to other UBC-GIF codes. Here are some tips:

Consider the ratios: $\frac{\alpha_x}{\alpha_s}$ and $\frac{\alpha_z}{\alpha_s}$. Larger ratios result in smoother models. As a rule of thumb, keep the following relationships in mind:

$\boldsymbol{\frac{\alpha_x}{\alpha_s}, \frac{\alpha_z}{\alpha_s} \gg 1}$ The "smoothness" terms dominate in the equation being minimized and the structure is penalized. Models tend to be as "smooth" as possible. The reference model is less important.

$\boldsymbol{\frac{\alpha_x}{\alpha_s}, \frac{\alpha_z}{\alpha_s} \Rightarrow 0}$ The "close to the reference" term dominates in the equation being minimized, so models may be "rough". The process tries to make a model that looks like the reference, with smoothness being less important.

To estimate values for the α's for a specific case, start by defining two length scale terms as follows:

$$\boldsymbol{L_z = \sqrt{\frac{\alpha_z}{\alpha_s}}} \text{ and } \boldsymbol{L_x = \sqrt{\frac{\alpha_x}{\alpha_s}}}$$

Then consider these rules of thumb to help choose the α's:
- In general, keep Lx approximately the same as the smallest diffusion radius for the latest time

window and Keep Lx approximately equal to Lz. Also, the following relations are useful:

Lx > mesh cell width

Lz > mesh cell thickness

Lx < total width of the mesh

Lz < total depth of the mesh

Line 12

`CHANGE_MREF` the reference model will be changed to the recovered model after each beta iteration.

`NOT_CHANGE_MREF` the reference model will never be changed.

Line 13

`SMOOTH_MOD` model norm does not contain the reference model.

`SMOOTH_MOD_DIF` model norm contains the reference model.

Chifact is specified in **Line 14**

Target misfit is reached when: *data misfit <= chifact * N,* where "*N"* is the total number of data. This value should usually be equal to 1.

Line 15

`max_iter_beta` is the user-defined number of iterations to perform for each trade-off parameter. A good value is about 3 (see "Inversion flowchart" for details).

`max_iter_ipcg` is the maximum number of IPCG iterations to perform. A good value is between 10 and 15 (See "inversion flowchart" for details).

`tol_ipcg` is the stopping tolerance for IPCG iterations. This value should be about 10^{-3} (see "inversion flowchart" for details).

Verification of the mesh

In setting the mesh parameters, the user has to maintain a balance between saving computing time (by coarsening the mesh) and getting more accurate solution of the forward simulation by making the mesh finer. In order to verify the validity of a particular mesh, it is suggested to compare the 3D simulated decay curves to the 1D simulated decay curve. Changing the time discretization can also affect the accuracy.

The first step is building a mesh. The importance of the correct mesh design is the key to recovery of meaningful geo-electrical parameters; however a reasonable balance has to be maintained in terms of keeping the mesh discretization at balance with the computing capabilities of the workstation. For mesh validation *"Data_viewer.exe"* GUI can be used. Figure 11 shows how finer discretization of the mesh plays role in the modeling accuracy. In this particular example the computing time differs between fine mesh and coarse mesh by a factor of 10.

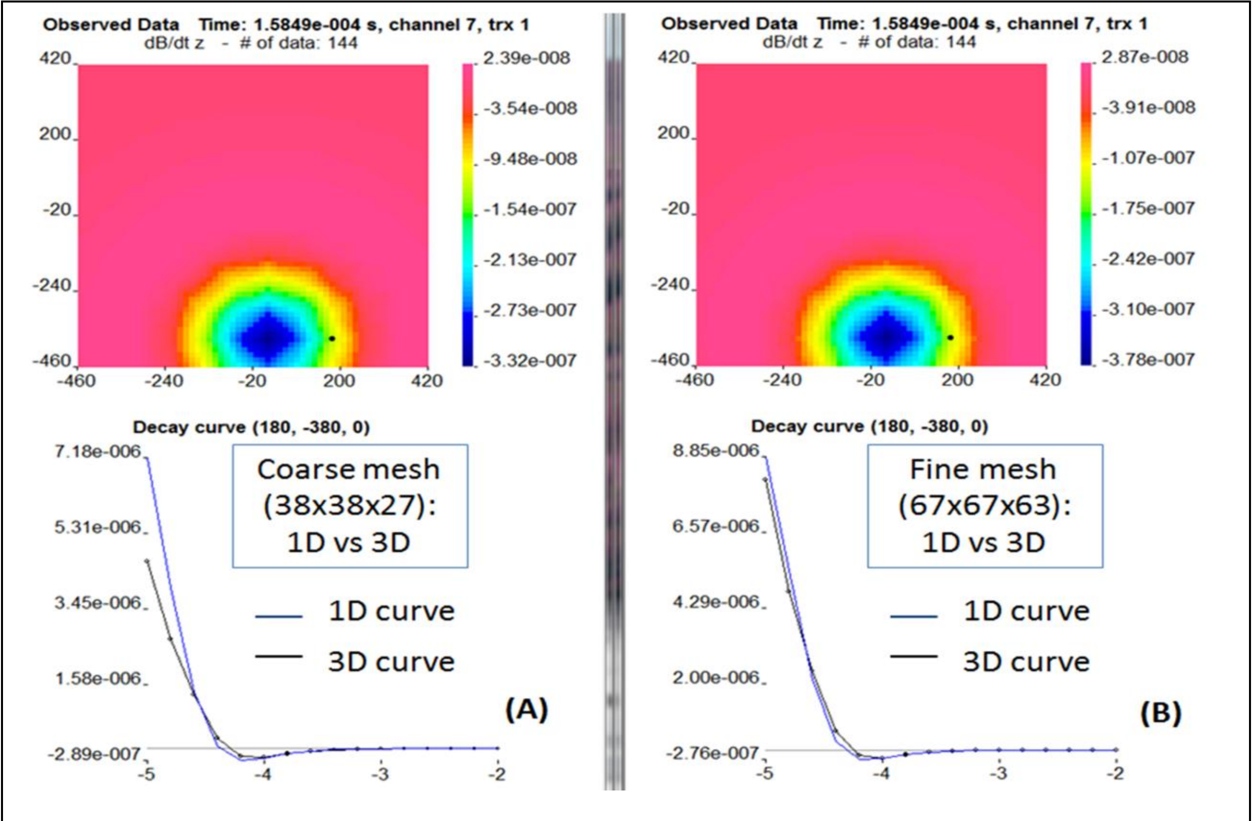


Figure 11. (A) Comparison between dBz/dt decay curves simulated for a one loop source 100 Ohm m half-space using 1D forward modeling and 3D forward modeling and a 38x38x27 mesh; (B) similar comparison for a 67x67x63 mesh.

Running the inversion

It is recommended that for every inversion, a separate folder should be created where all the control files are stored. This folder should be your working directory (further referred to as "*workdir*"). Every time any of the inversion parameters are changed, a new "workdir" should be created specifically for the new inversion control and output files. Separate from the working directory, a shared executable directory (*"execdir"*) should exist on the workstation. It is not recommended to keep executable files in the same directory as the control files. The following table is showing, which files should be kept in which directory (please note that not all files listed in the *"workdir"* may be necessarily needed for running the code, the bare minimum is having the "*h3dtdinv.inp"; "data.dat"; "mesh.txt"; "model_ini.con" and, "wave.txt"* the rest of the files are optional):

Execdir	**Workdir**
H3DTDinv.exe	h3dtdinv.inp
mkl_mc3.dll	data.dat
mkl_intel_thread.dll	mesh.txt
mkl_def.dll	wave.txt
mkl_core.dll	model_ini.con
mkl_blacs_msmpi_lp64.dll	model_ref.con
mkl_blacs_mpich2_lp64.dll	topo.dat
mkl_blacs_lp64.dll	weight.txt
mkl_blacs_intelmpi_lp64.dll	machinefile.txt
libiomp5md.dll	

Table 2. List of files specific for *"workdir"* and *"execdir".*

For optimal performance of the inversion (H3DTDinv) it is best to use the Message Passing Interface (MPI), which allows running multiple computational devices in parallel, including commodity clusters, hi-speed networks and multi-core processors on local computers. In order to install the MPI application library, download it from http://www.mcs.anl.gov/research/projects/mpich2/

Linux:

For commodity clusters operated under Linux system, the code can be run on any number of processors listed in a description ASCII file. The following is an example of such description file:

```
Compname01:nProc
Compname02:nProc
Compname03:nProc
```

The description file name is completely arbitrary. `“Compname”` is the network name of the computer to be used and `“nProc”` is the number of processors to be employed for the procedure. If the computer is on the local network and can be directly accessed, then no path is needed to be specified. The following is an example of a command line to be used under Linux operating system in order to start the forward simulation:

```
mpiexec -machinefile machines.txt -n 20 ./h3dtdinv_mumps
```

In this command line `“-machinefile”` calls for a description file *“machines.txt”* and “–n 20” indicates a total amount of processors to be used on all the machines listed in the description file.

Windows:

For single multi-core computer usage, under Windows operating system, the command line will look like this:

```
"C:\Program Files\MPICH2\bin\mpiexec.exe" -localonly 4 h3dtdinv
```

In this line `“-localonly`” limits the computation to only one machine, from which the command line is launched and `“4”` specifies the number of processors to be used..

For running the code on several computers or a network:

- Make sure each computer has the same version of MPI installed.
- The user running the program should have the same “UserID” and “password” on each

computer (the user does not have to be logged on to every computer, but has to have a network account set up on each computer with same identification).

- Make your *"workdir"* and *"execdir"* folders shareable, and make sure that *"workdir"* provides full sharing (read and write).
- Make sure your shared folders are visible on each computer then place the input files and executables in sharable folders, as per Table 2.
- The firewall in each computer (except for the host) should be turned off, or else the h3dtd program should be added to the exceptions list.

The command line to start the MPI job is:

```
mpiexec.exe -machinefile machines.txt -n 8 -priority 1 -dir
\\MYCOMP\share \\MYCOMP\share\exe\h3dtdinv.exe
```

In the above example:

`machines.txt` - file containing the names of the computers to use. Each computer name can be followed be `:p` which indicates the number of processes to start on that machine.

`-n 8` - total number of processes to start.

`-priority 1` - (optional) indicates that all jobs should be started at low priority.

`-dir \\MYCOMP\share` - sharable folder that should be visible on all computers.

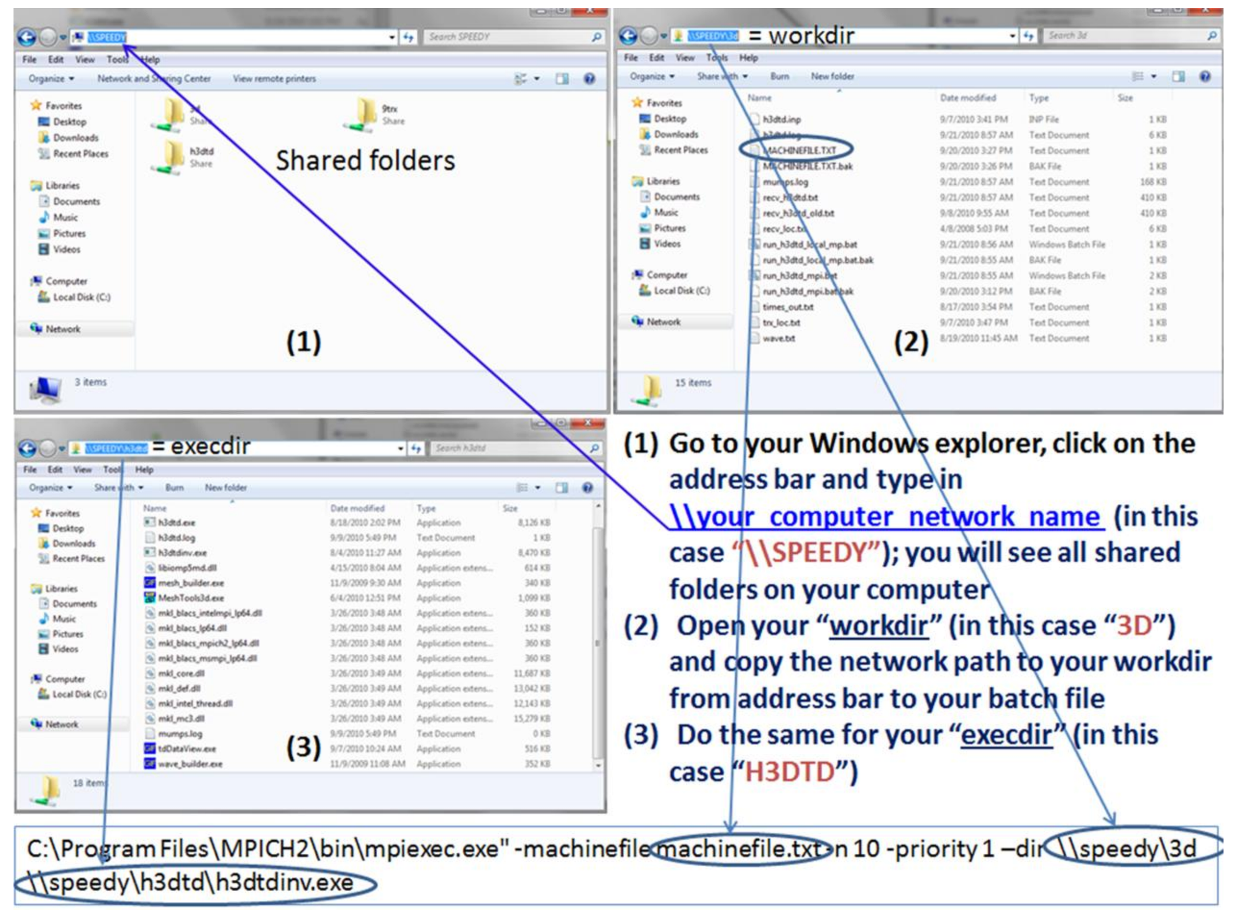
`\\MYCOMP\share\exe\h3dtdinv.exe` - full path of the executable. Other computers must be able to see it.

For convenience, it is recommended to set up batch files (*.bat) for running H3DTD.exe on a local network. Two examples of such batch files are provided with the documentation. The file *"run_h3dtdinv_local_mpi.bat"* is to be used for running H3DTD on local workstation alone and the file *"run_h3dtdinv_mpi.bat*" is to be used for running the code on the local network.

In editing the file: *"run_h3dtdinv_local_mpi.bat"* the editable text includes the path to the h3dtdinv.exe file, which should be set to your "execdir" location. The editable parts of the *"run_h3dtdinv_mpi.bat"* are listed in Figure 12 and include the following:

- machinefile.txt

- number of processors
- path to “workdir”
- path to “execdir”



Name	Date modified	Type	Size
h3dtd.inp	9/7/2010 3:41 PM	INP File	1 KB
h3dtd.log	9/21/2010 8:57 AM	Text Document	6 KB
MACHINEFILE.TXT	9/20/2010 3:27 PM	Text Document	1 KB
MACHINEFILE.TXT.bak	9/20/2010 3:26 PM	BAK File	1 KB
mumps.log	9/21/2010 8:57 AM	Text Document	168 KB
recv_h3dtd.txt	9/21/2010 8:57 AM	Text Document	410 KB
recv_h3dtd_old.txt	9/8/2010 9:55 AM	Text Document	410 KB
recv_loc.txt	4/8/2008 5:03 PM	Text Document	6 KB
run_h3dtd_local_mp.bat	9/21/2010 8:56 AM	Windows Batch File	1 KB
run_h3dtd_local_mp.bat.bak	9/21/2010 8:55 AM	BAK File	1 KB
run_h3dtd_mpi.bat	9/21/2010 8:55 AM	Windows Batch File	2 KB
run_h3dtd_mpi.bat.bak	9/20/2010 3:12 PM	BAK File	2 KB
times_out.txt	8/17/2010 3:54 PM	Text Document	1 KB
trx_loc.txt	9/7/2010 3:47 PM	Text Document	1 KB
wave.txt	8/19/2010 11:45 AM	Text Document	1 KB

Name	Date modified	Type	Size
h3dtd.exe	8/18/2010 2:02 PM	Application	8,126 KB
h3dtd.log	9/9/2010 5:49 PM	Text Document	1 KB
h3dtdinv.exe	8/4/2010 11:27 AM	Application	8,470 KB
libiomp5md.dll	4/15/2010 8:04 AM	Application extens...	614 KB
mesh_builder.exe	11/9/2009 9:30 AM	Application	340 KB
MeshTools3d.exe	6/4/2010 12:51 PM	Application	1,099 KB
mkl_blacs_intelmpi_lp64.dll	3/26/2010 3:48 AM	Application extens...	360 KB
mkl_blacs_lp64.dll	3/26/2010 3:48 AM	Application extens...	152 KB
mkl_blacs_mpich2_lp64.dll	3/26/2010 3:48 AM	Application extens...	360 KB
mkl_blacs_msmpi_lp64.dll	3/26/2010 3:48 AM	Application extens...	360 KB
mkl_core.dll	3/26/2010 3:49 AM	Application extens...	11,687 KB
mkl_def.dll	3/26/2010 3:49 AM	Application extens...	13,042 KB
mkl_intel_thread.dll	3/26/2010 3:49 AM	Application extens...	12,143 KB
mkl_mc3.dll	3/26/2010 3:49 AM	Application extens...	15,279 KB
mumps.log	9/9/2010 5:49 PM	Text Document	0 KB
tdDataView.exe	9/7/2010 10:24 AM	Application	516 KB
wave_builder.exe	11/9/2009 11:08 AM	Application	352 KB

(1) Go to your Windows explorer, click on the address bar and type in \\your_computer_network_name (in this case “\\SPEEDY”); you will see all shared folders on your computer

(2) Open your “workdir” (in this case “3D”) and copy the network path to your workdir from address bar to your batch file

(3) Do the same for your “execdir” (in this case “H3DTD”)

```
C:\Program Files\MPICH2\bin\mpiexec.exe" -machinefile machinefile.txt -n 10 -priority 1 –dir \\speedy\3d
\\speedy\h3dtd\h3dtdinv.exe
```

Figure 12. Block diagram for editing batch file in order to run the code on the network.

In figure 12, the file *“machinefile.txt”* used for executing the code under local network has the same format as the example shown above for Linux environment and should be located in the *“workdir”.* Please note that for running the code on multiple network computers, the total number of processors should be specified, equal to the sum of all processors on all computers listed in *machinefile.txt*.

Inversion flowchart

The inversion flowchart is very similar to the inversion flowcharts for other UBC-GIF inversion codes. The objective of the inversion is to minimize the objective function $\Phi = \Phi_d + \beta * \Phi_m$, which is a combination of data misfit Φ_d and model norm Φ_m . $\Phi_d = \mathbf{W_d}||\mathbf{d_{pred}} - \mathbf{d_{obs}}||^2$ and should be in the range of the target misfit, equal to N***chifact**, where N is the total number of data from the *data.dat* file (excluding the dummy values) and **chifact** is 1 by default and can be weighted to increase or decrease the desired target misfit. In the equation for Φ_d, $\mathbf{W_d}$ is the standard deviation matrix ($\mathbf{W_d}$ = diag(1/SD$_i$)), which is taken from the data.dat file and $\mathbf{d_{pred}}$ is the forward model field matrix, updated at every iteration step.

Φ_m is the model norm, which is used to regularize the objective function and is scaled to Φ_d using the trade-off parameter $\boldsymbol{\beta}$. The model norm is a combination of model perturbation functions $\mathbf{\Delta m = (m_i - m_{ref})}$, scaled using model weighting matrices $\mathbf{W_{s,x,y,z}}$, which in turn, are dependent on the user-defined smoothing parameters (α's). The inversion is driven by 3 levels of iterative processes: the outer loop (minimizing the objective function), the beta-loop (minimizing the trade-off parameter) and the IPCG loop, solving for the model perturbation Δm. This model perturbation is used to calculate the forward model to get updated predicted data ($\boldsymbol{d_{pred}}$). Other parameters and abbreviations listed in Figure 13 include:

J and $\mathbf{J^T}$ – are the sensitivity matrix and the transposed sensitivity matrix respectively (**J** is a measure of how sensitive is the model field to changes in electrical conductivities of the mesh cells)

IPCG – Inexact Preconditioned Conjugate Gradient (a numerical method used to solve minimization problems

g – gradient, calculated from the sensitivity matrix and used to solve for Δm

p, q, v – arbitrary vectors

The inversion is terminated if either the trade-off parameter becomes smaller that bmin, or the objective function is minimized below the target misfit, or else if the maximum number of iterations has been reached

```
observed data $d_{obs}$
standard deviations $W_d$
initial model$m = m_0$
target misfit $chifactN$
**Forward model** $(m)$to get predicted data $d_{pred}$

initial tradeoff parameter$\beta = \beta_{max}$

start $\beta$ loop

    start inner loop 1 to max_iter_beta

        gradient$g = J^T(d_{pred} - d_{obs}) + \beta W^T W(m - m_{ref})$(***)

        solve for model perturbation using IPCG:$(J^T J + \beta W^T W)\Delta m = -g$
        start IPCG iterations 1 to max_iter_ipcg
            during each iteration need to calculate $q = (J^T J)v$
                $p = Jv$(***)
                $q = J^T p$(***)
            quit if tolerance < tol_ipcg
        end IPCG iterations

        update the model: $m = m + \Delta m$
        **Forward model** $(m)$to get predicted data $d_{pred}$

        $\varphi_d = 0.5 \parallel W_d(d_{pred} - d_{obs}) \parallel^2$
        model norm$\varphi_m = 0.5 \parallel W(m - m_{ref}) \parallel^2$
        objective function$\varphi = \varphi_d + \beta\varphi_m$
        data misfit $2\varphi_d$
        quit inversion if  *data misfit < target misfit*

    end inner loop

    update tradeoff parameter $\beta = \beta\beta_{factor}$
    if $\beta < \beta_{min}$quit inversion

end $\beta$ loop
```

Figure 13. Flowchart for H3DTDinv 3D time domain inversion; (***) is computationally intensive step.

```
**Forward model** $(m)$
    factor the matrices $A(m, \Delta t)$(***)

    solve $A(m, \Delta t)u = rhs$(***)
    predicted data $d_{pred} = Qu$
end **Forward model**
```

Output files

h3dtdinv.log - a log file showing the progress of the inversion.

h3dtdinv.out - a file containing similar information as the log file, but arranged in a table.

h3dtdinv_stat.txt - a file showing the factorizations and cpu time.

inv_*.con - recovered model for each beta iteration.

dpred_*.txt - predicted data for each beta iteration.