FMTOMO

Fast Marching Tomography Package:

Instruction Manual

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Contents

1 Introduction

This document describes how to use the Fortran software package FMTOMO to perform 3-D traveltime tomography. FMTOMO uses the fast marching method (FMM) for the forward step of traveltime prediction, and a subspace inversion scheme to adjust model parameters in order to satisfy data observations. The method is iterative non-linear in that the inversion step assumes local linearity, but repeated application of FMM and subspace inversion allows the non-linear relationship between velocity and traveltime perturbations to be reconciled.

The long term goal of the FMTOMO project is to produce a comprehensive package for carrying out many different classes of traveltime tomography. In its current form (version 1.0), model structure is represented by subhorizontal layers in spherical coordinates. Within a layer, velocity is permitted to vary smoothly in all three dimensions. The geometry of layer boundaries may also vary, but all interfaces must completely span the horizontal dimensions of the model region, and cannot be multi-valued in depth (i.e. cannot fold over on itself). Although structures such as discrete bodies or salt domes cannot be accurately represented with this style of parameterization, a wide variety of other structures (e.g. a subducting slab) may nevertheless be considered.

FMTOMO uses the **fm3d** package to solve the forward problem. **fm3d** is based on the so called multi-stage Fast Marching Method (FMM), a grid based eikonal solver that implicitly tracks the evolution of wavefronts in 3-D layered media. Phases comprising any number of reflection and refraction branches may be tracked (including P-S conversions). Tests show it to be computationally efficient and robust in the presence of severe variations in both velocity and interface structure. Sources may lie at the surface, at depth, or outside the model region (i.e. teleseismic events), thus allowing many different types of traveltime datasets to be predicted, including reflection, refraction, local earthquake and teleseismic.

The subspace inversion scheme minimizes an objective function simultaneously along multiple search directions that together span a subspace of model space. Both damping and smoothing regularization can be applied in order to address the problem of solution non-uniqueness. At this stage, FMTOMO can simultaneously invert one or more classes of traveltime dataset for variations in wavespeed, interface depth and source location.

It is important to realize that a common drawback of sophisticated academic software

packages is that they are often not user friendly, and require a serious time commitment before they yield the desired results. The flexibility offered by FMTOMO to some extent necessitates a rather complex user interface, which from experience with "novice" users, takes a fair amount of time to comprehend. Therefore, if you are serious about using this package, be prepared to spend a day or two carefully reading though this instruction manual, the instructions associated with **fm3d** and journal papers that have used FMTOMO. In addition, it is strongly recommended that the three examples that come with this distribution are examined, and that the results they contain can be reproduced using your compilation of the code.

1.1 Associated documentation

- The following paper (a PDF version is included in the docs/ directory) uses FMTOMO to invert synthetic data for source location (see Example 1), and velocity and interface structure (see Example 2):
  Rawlinson, N., de Kool, M. and Sambridge, M., 2006. Seismic wavefront tracking in 3-D heterogeneous media: applications with multiple data classes. *Explor. Geophys.,* **37,** 322-330.

- The following paper (a PDF version is included in the docs/ directory) uses FMTOMO to simultaneously invert wide-angle and teleseismic data for both Moho geometry and lithospheric velocity structure beneath Tasmania, south-east Australia (see Example 3):
  Rawlinson, N. and Urvoy, M., 2006. Simultaneous inversion of active and passive source datasets for 3-D seismic structure with application to Tasmania. *Geophys. Res. Lett.,* **33 L24313,** doi:10.1029/2006GL028105.

- The following paper (a PDF version is included in the docs directory) describes the **fm3d** package in detail:
  de Kool, M., Rawlinson, N. and Sambridge, M. 2006. A practical grid based method for tracking multiple refraction and reflection phases in 3D heterogeneous media, *Geophys. J. Int.,* **167,** 253-270.

- The instructions for using **fm3d** can be found in the sub-directory fmcode/ (open the text file README_0.7). Note that in theory, you do not need a comprehensive

understanding of **fm3d** in order to use FMTOMO.

1.2 External software requirements

- The home page for the **fm3d** package can be found at:
  http://rses.anu.edu.au/seismology/fmmcode
  Note that the source code comes with the FMTOMO distribution, so there is no need to download it separately.

- The plotting routines that come with FMTOMO make use of GMT (the Generic Mapping Tool), a script-based visualization package. It is freely available to download from:
  http://gmt.soest.hawaii.edu

- **fm3d** includes an option for output files in OpenDX format. OpenDX is a sophisticated 3-D visualization package that is available for free from:
  http://www.opendx.org

1.3 Compatibility and operation

FMTOMO has been tested on several UNIX/Linux platforms. In theory, it should work with most Fortran 90 (or later) compilers. Under Linux, it has been successfully compiled and executed with Pathscale, g95 and ifort (Intel Fortran Compiler). On Sun Solaris operating systems (with both AMD and UltraSparc CPUs), it has correctly compiled and executed using the Sun Fortran 90 compiler. However, note that from our experience with Sun Blade Workstations that use UltraSparc CPUs, execution time is very slow (at least an order of magnitude slower) compared to machines that use recent Intel and AMD CPUs. Our best results have come from using Pentium 4 (or later) Intel CPUs together with Intels ifort compiler.

The memory requirements of FMTOMO vary depending on the size of the problem being solved. For most realistic scenarios (e.g. Example 3 in the distribution), a workstation with 512 Mb - 1 Gb of RAM should be sufficient.

2 Unpacking and compiling the code

FMTOMO is distributed as a tarred and gzipped archive. In order to unpack the code, type something like:

- gunzip -c fmtomov1.0.tar.gz | tar xvof -

or

- tar -xvzf fmtomov1.0.tar.gz

at the command prompt. One of the above commands will create a set of subdirectories below the current directory, which should contain:

- bin/: Contains all executable files associated with FMTOMO. Prior to compilation, the only executable file that should be present in this subdirectory is tomo3d, which is a shell script.
- compileall: A shell script for compiling all software and placing executables in bin/.
- docs/: Contains documentation associated with FMTOMO, including this instruction manual. Several journal papers which use the code are also included.
- example1/: Synthetic test example which attempts to relocate earthquake hypocenters in the presence of 3-D velocity and interface structure.
- example2/: Synthetic test example which simultaneously inverts teleseismic and wide-angle data for both velocity and interface structure.
- example3/: Inverts observed teleseismic and wide-angle traveltime data for the structure of the Tasmanian (south east Australia) lithosphere.
- fmcode/: Contains the source files for building **fm3d** and constructing the binary traveltime tables for predicting global phases in spherically symmetric Earth models (for tracking teleseismic arrivals).
- gmtfiles/: Contains several GMT shell scripts for plotting cross-sections through models produced by FMTOMO.
- source/: Contains all source files for FMTOMO, with the exception of the source files for **fm3d**.

FMTOMO is made up of a number of different Fortran programs. These include:

- arraygen: A simple program for generating rectangular arrays of receivers (latitude, longitude, depth) for performing synthetic tests.

- fm3d: Solves the forward problem of traveltime prediction by applying the so-called multi-stage Fast Marching Method. **fm3d** can also output ray paths and Fréchet derivatives, the latter of which are required by the inversion routine.

- gmtslice: A program for taking output from the tomographic inversion routine and converting it into a format suitable for use with GMT. Various types of horizontal and vertical sections can be taken through a 3-D model. Ray paths, sources and receivers may also be visualized.

- grid3dg: A program for constructing 3-D models in the format required by **fm3d**. It can be used to construct checkerboard or other synthetic test models (e.g. random structure), and initial models for tomographic inversion. In the latter case, it is best for producing models in which velocity varies with depth only, and interfaces are planar. However, it does allow more complex models to be generated using separate grid files supplied by the user.

- invert3d: This program uses the subspace inversion method to invert the traveltime data for model structure. Regularization in the form of damping and smoothing can be imposed.

- moddata: A program for generating source and receiver input files in the format required by **fm3d**. These files also contain information about path signatures, and do not have a very intuitive structure. **moddata** is best used for purely synthetic tests (e.g. Examples 1 and 2), and not cases where observational data is involved (e.g. Example 3). For these situations, **obsdata** is usually a better option.

- obsdata: A program for generating source, receiver and traveltime input files in the format required by **fm3d**. This program is best used for cases where observed data are involved. **obsdata** expects these observations to be listed in separate files which it can access. The difference between **moddata** and **obsdata** may seem confusing at this stage, but it will be made clearer later on.

- residuals: Computes summary traveltime residuals (RMS, variance and χ^2) associated with the current model.

- synthdata: A simple program for generating synthetic traveltimes. It takes output from **fm3d** (the list of arrival time predictions contained in arrivals.dat), and adds random noise (if required) and an estimate of picking error (required by **invert3d**). The output file can be used as input to the tomography routine for performing a synthetic test (e.g. a checkerboard test).

- remodl,setbrn: A pair of programs that, when run sequentially, produces the traveltime tables required for predicting the arrival times of global phases. The default setting assumes an ak135 global model, and the binary files produced are called ak135.hed and ak135.tbl. Note that if teleseismic arrival time prediction is required, these files **must** be in the same directory in which **fm3d** is executed. The source code for the two programs are contained in fmtomo/aktimes/.

All of the above programs can be compiled separately and moved to the **bin** subdirectory (except for **remodl** and **setbrn**, which only need to be executed once to produce the binary tables for the specific machine architecture that is used). However, it is much simpler to run the script **compileall**, which is the only file contained in the root directory of the distribution. This script will compile all of the above code and move the executables to bin/. It will also build and execute **remodl** and **setbrn**, and copy the output files ak135.hed and ak135.tbl to source/inputfiles.

Prior to running **compileall**, perform the following steps:

1. Open **compileall** in your favourite editor and check that the **ksh** directive on the first line points to the correct location. If you do not have **ksh**, use **zsh** instead.

2. On line 22 of **compileall**, enter the name of the Fortran 90 (or later) compiler you wish to use for compiling all the code except **fm3d**.

3. Open the **Makefile** contained in the subdirectory fmcode/. On line 7, enter the name of the the Fortran 90 (or later) compiler you wish to use for compiling **fm3d**.

4. Open the **Makefile** contained in the subdirectory fmcode/aktimes/ and enter the name of the Fortran compiler you wish to use for compiling **remodl** and **setbrn**.

Although these programs are written in Fortran 77, you should be able to use the same compiler you used for the other programs.

At this stage, you should be able to type **compileall** at the command line, hit Enter, and all the code will successfully compile (fingers crossed). On a 1.6 GHz AMD Opteron workstation running SuSe Linux 9.3, this process takes about 30 seconds when the Intel Fortran compiler (ifort) is used. There will be some screen output associated with the compilation of **fm3d** and the creation of the binary traveltime tables (a list of numbers and global phase names will appear at the end), so do not be alarmed. When **compileall** is complete, it will print the statement "compilation complete" to the screen. In order to run the executables from any directory, you will need to make sure that the path to the bin/ directory is correctly set in your startup shell script. Alternatively, you could copy the executables to a directory that you know is already specified in the path list, although this is perhaps the less desirable option. In the former case, if you use a .cshrc file, then you could add a line like:

- set path = ($path /directories/bin)

after the path is initially set. In the above example, directories refers to the directory structure above the bin directory (e.g. ∼/tomography/fmtomo).

Before using FMTOMO, open **tomo3d**, which is contained in the bin subdirectory, and make sure that the **ksh** directive on the first line points to the correct location. If you do not have **ksh**, use **zsh** instead. At this stage, you are in a position to go ahead and see if your compiled version of the code will correctly reproduce the examples provided.

3 Constructing initial and synthetic models

The first step in performing a tomographic inversion is to specify how model structure is to be represented (i.e. how the model is to be parameterized). This is a crucial choice because it immediately imposes limitations on the types of structure that can be recovered (in a sense, it represents a kind of implicit regularization of the problem). In the case of FMTOMO, velocity is represented by a regular grid of points with cubic B-splines applied to define a continuum. Interfaces are represented by a regular grid of points in latitude and longitude, the depths of which can vary, with cubic B-splines used to define a continuous surface.

Given that the underlying parameterization has already been imposed, the remaining choices for the user are: the number of layers; the density of nodes describing each velocity field and layer interface; and the values associated with these nodes. When choosing an initial or starting model for subsequent inversion, *a priori* information is often such that only a laterally homogeneous structure needs to be generated. However, when independent information on lateral structure is available, or when synthetic tests are to be performed, then it is often necessary to construct more complex models.

Details on how the interface and velocity grid files are structured can be found in the README_0.7 file under fmtomo. This information is not provided here because the format of these input files is dictated by **fm3d**, which is a separate package. However, a useful program provided as part of this distribution, called **grid3dg**, makes the task of generating initial and synthetic models much simpler than it otherwise might be. Before describing the input requirements of this program, a brief overview of the model parameterization used by FMTOMO is provided.

3.1 Model Parameterization

As mentioned previously, FMTOMO represents structure by a series of one or more subhorizontal layers which completely span the model region in latitude and longitude. Within each layer, the velocity field is defined by a regular grid of nodes. These nodes are used as the control vertices of a mosaic of cubic B-spline volume elements, which define the continuum. Layer interfaces are described by a regular mesh in latitude and longitude, which control a mosaic of cubic B-spline surface patches that describe the complete interface. Cubic B-spline functions are desirable because they exhibit local control (i.e. changing the value of a single node only affects the interface or velocity field in the vicinity of the node), continuity of the second derivative, and can be rapidly evaluated. This last property is important because in order to use the multi-stage FMM, a propagation grid must be defined over which the narrow band evolves; typically, this will involve many evaluations of the spline function.

Figure 1 demonstrates (in cross-section) the basic concept of the layered parameterization. One of the most important things to understand is that *the velocity grid within each layer is defined independently of the other layers.* This means, for example, that in the first layer $v_1(r, \theta, \phi)$ has its own grid of velocity nodes, which is separate from $v_2(r, \theta, \phi)$

in the second layer. The node spacing of these grids can be different (although in Figure 1 they are the same), and they can also spatially overlap. When interface structure is inverted for, interface nodes are perturbed in depth, which means that vertically, the layer can expand or contract. In effect, this will make some velocity nodes redundant (they will not influence traveltime), but will also activate previously redundant nodes. **fm3d** will automatically select which region of the velocity grid to use depending on the structure of the bounding interfaces.

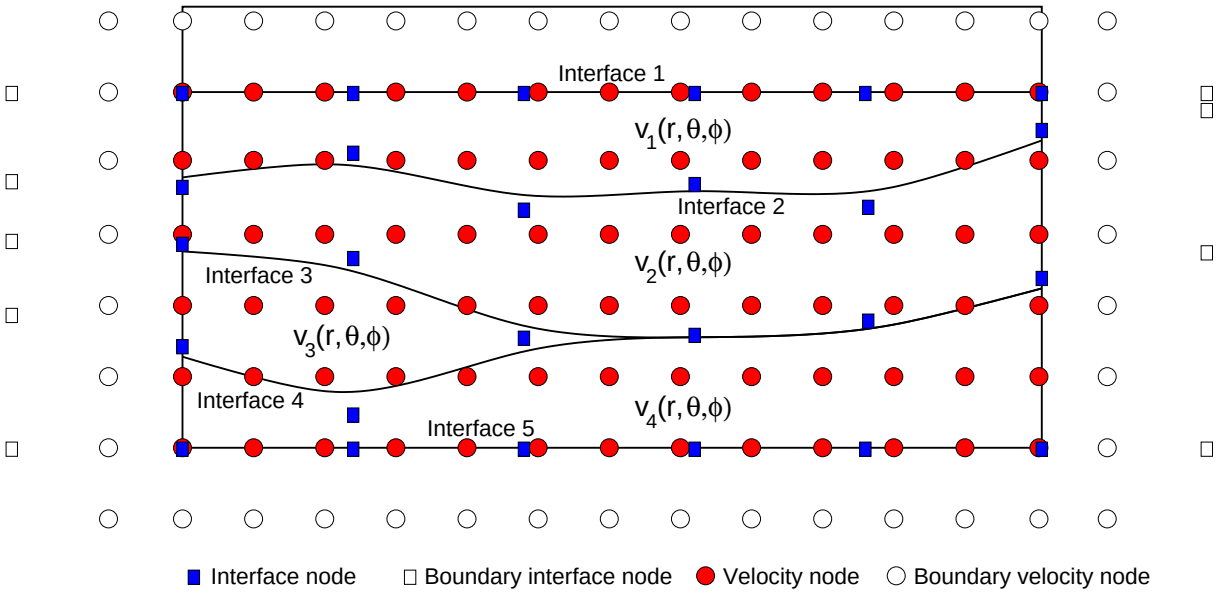


Figure 1: Schematic diagram showing in vertical cross-section the model parameterization adopted by FMTOMO. Velocity within each layer is independent of the velocity in adjacent layers. Both velocity and interface grids must have a set of boundary nodes. Note that the velocity continuum and interface surface defined by cubic B-splines need not interpolate the velocity and interface nodes.

Several other features of Figure 1 are also worth noting. First, both the interface and velocity grids are required to have a cushion of boundary nodes. The continuous velocity fields and interface surfaces **do not** extend out to these cushion nodes, but cease exactly one node inboard of the boundary. Thus, if a grid is defined by N nodes in a particular dimension, the velocity continuum or interface surface will only span $N-2$ of these nodes. A second notable feature of Figure 1 is that the surfaces do not necessarily interpolate the interface nodes. This is also true of the velocity continuum (and obviously can't be shown in Figure 1), which does not necessarily interpolate the velocity nodes.

Both of these features stem from the use cubic B-splines to define the interface surfaces and velocity fields. Cubic B-spline functions are basically piecewise cubic polynomials that are continuous in curvature where they suture together. In addition, they are locally controlled (unlike natural cubic splines) in that only four control nodes are required in order to define a single segment. Figure 2 illustrates this concept.

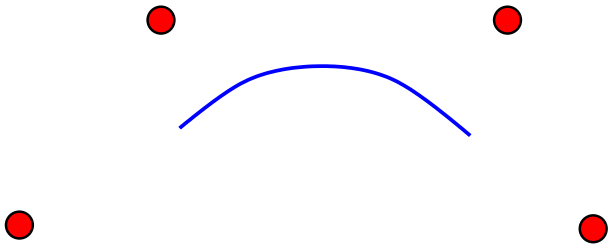


Figure 2: Segment of a cubic B-spine curve. In order to ensure local control and continuity of curvature, these splines are non-interpolating.

Figure 1 also includes a layer pinch-out, something that is permitted by FMTOMO. When this occurs, two adjacent interfaces essentially overlap, which effectively results in the layer bounded by these interfaces becoming horizontally discontinuous. In order to facilitate this feature, **fm3d** requires the horizontal node spacing of all interface grids to be identical.

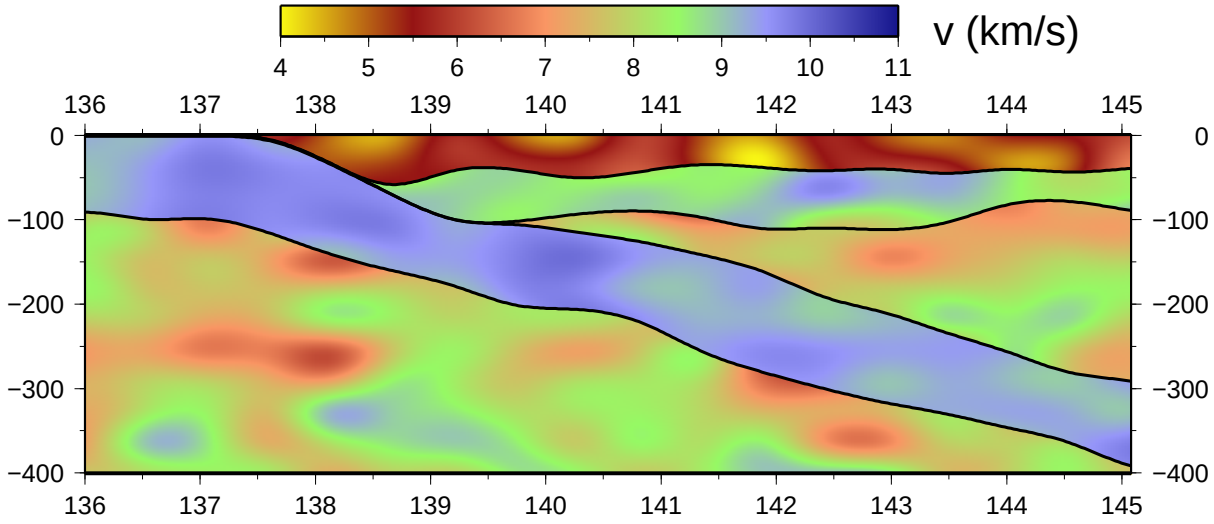


Figure 3: Cross-section through a complex layered velocity model (ostensibly showing a synthetic subduction zone) defined using the FMTOMO parameterization scheme.

An example of a cross-section through a complex synthetic velocity model that con-

forms to the above parameterization is shown in Figure 3. Note that both velocity and interface structure varies smoothly, and multiple layer pinchouts can be specified.

3.2 Using grid3dg to generate a model

A program called **grid3dg** is provided with this distribution to facilitate the generation of a range of models for use either as input starting models for a tomographic inversion, or for generating synthetic data (e.g. for a checkerboard resolution test). **grid3dg** requires an input parameter file, called grid3dg.in, in order to generate a model. A generic version of this input file can be found in source/inputfiles/.

To some extent, the format of grid3dg.in is self-explanatory, but we will nevertheless attempt to describe a selection of the more important entries. If you open the input file located in source/inputfiles, you will see that the first entry block is as follows:

```
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c Specify number of layers (= number of interfaces -1)
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
2                   c: Number of layers in model
1                   c: Number of velocity grid types (1 or 2)
0.02                c: Pinchout distance (km) (>=0.0)
vgrids.in           c: Output velocity grid file
interfaces.in       c: Output interface grid file
145678              c: Seed for random number generation (int)
```

The first line specifies the number of layers in the model. As indicated in Figure 1, the number of layers must equal the number of interfaces minus 1. The second line indicates the number of velocity grid types. **fm3d** allows both a P-wave velocity field and an S-wave velocity field to be independently defined within a single layer. This is to facilitate mode conversions (e.g. SmP). Thus, if you are only interested in a single velocity type (P or S), then set this value to 1. Note that at this stage, the ability of FMTOMO to simultaneously invert for both P and S velocities has not been properly tested. If your dataset does not include mode conversions, then there is no need to specify more than one velocity field within a single layer. The third line sets the minimum pinchout

distance between adjacent interfaces. **grid3dg** automatically checks to see whether you have specified interfaces that intersect and applies a correction if necessary. Although in some cases you may want a layer to fully pinch-out, it is usually safer to specify some small tolerance to avoid potential complications with **fm3d** (e.g. round-off error).

The next two lines specify the names of the velocity (vgrids.in) and interface (interfaces.in) files that are created by **grid3dg**. Together, these two files fully specify the model, and constitute two of the input files required by **fm3d**. As such, they have been given the appropriate filenames that are needed for **fm3d**. The final line sets the seed for random number generation. This is used to seed the generation of random noise with a Gaussian distribution, which in turn is used to superimpose random structure on a model if required by the user (e.g. for a synthetic test).

3.2.1 Setting the model dimensions

The second entry block is as follows:

```
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c Set 3-D grid size and location. Note that all layer
c velocity grids have the same spatial dimension, but can
c have different node densities. Interface grids have the
c same node distribution.
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
1.50     -80.10          c: Radial range (top-bottom) of grid (km)
-40.0    -42.0           c: Latitudinal range (N-S) of grid (degrees)
140.0    143.0           c: Longitudinal range (E-W) of grid (degrees)
6371.0                   c: Earth radius
```

These options specify the location of the model and its dimensions (in spherical coordinates). The radial range of the model is relative to the surface of the Earth, and defines how far the model extends in depth. In this case, the "top" of the model is 1.5 km above the surface of the Earth, and the "bottom" of the model is 80.1 km below the surface. When surface topography is a factor, it is usually necessary to have the top of the model above the surface of the Earth to ensure that receivers do not lie outside the bounds of

the model. When defining the N-S range of the model, note that northern hemisphere latitudes are positive, and southern hemisphere latitudes are negative. Longitudes should be defined as East of the meridian, rather than west (e.g. you should convert 115° W to 245° E). **Note: grid3dg** automatically adds a cushion of boundary nodes (see Figure 1) to the defined grid. Therefore, the 3-D model region you define will be fully spanned by all velocity fields and interface surfaces.

3.2.2 Specifying the propagation grid

The third block of parameters in grid3dg.in is:

```
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c Set up propagation grid file
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
propgrid.in                c: Name of propagation grid file
21   41   41                c: Number of points in rad lat, long
5    10                    c: Refine factor & no. of local cells
0.05                       c: Cushion factor for prop grid (<<1)
```

These parameters don't actually influence the model structure at all; instead, they define what is known as the *propagation grid* for implicitly tracking seismic wavefronts using **fm3d**. However, the reason why these parameters are defined here is that the propgrid.in file required by **fm3d** needs the origin of the propagation grid and the propagation grid spacing to be specified. Rather than try and enter this information manually in propgrid.in, it is easier to specify it at this point to avoid inconsistencies. In theory, propgrid.in can span a subset of the defined model, but **grid3dg** automatically scales the propagation grid to the boundary of the complete model. The first line above defines the name of the propagation grid file which is to be read in by **fm3d** (therefore, you should not need to change this filename). The second line specifies the number of points defining the propagation grid in depth, latitude and longitude. In this case, there are 21 propagation grid nodes spanning a depth range from 1.5 km to -80.1 km, which results in a grid spacing of 4.08 km.

It is important to understand the difference between the **inversion grid** and the **propagation grid**. The inversion grid describes the model (via vgrids.in and interfaces.in) - i.e. it represents the grid of velocity and interface control nodes (e.g. Figure 1) that describes the velocity and interface variations (in terms of cubic B-spline functions). The propagation grid, on the other hand, represents a discrete sampling of the velocity fields (and implicitly the interface surfaces) for use by **fm3d**, which is a grid-based eikonal solver. Thus, there is no relationship between these two grids. [If we were using ray tracing instead of FMM to solve the forward problem, then we would not need to define a propagation grid].

The third line in the above block of parameters defines the source grid refinement parameters that are used to improve traveltime accuracy. When energy emanates from a seismic point source, the curvature of the wavefront is very high, which means that the underlying global propagation grid does not capture its true shape very accurately. It has been shown that errors that arise from this effect in the source neighbourhood dominate the total traveltime errors of FMM. In order to mitigate this problem, **fm3d** defines a local cubic region of grid points about the source within which a much higher density of propagation grid points is defined. When the wavefront impinges on the edge of this local region, traveltimes are mapped back to the coarser global grid. This idea is illustrated in Figure 4, which shows a schematic cross-section through a locally refined grid. The *refinement factor* refers to the number of subdivisions of the global propagation grid; in Figure 4, this value is 3. The *number of local cells* refers to the number of cells outward from the source (in all three dimensions) that the refined region extends. In Figure 4, this value is also 3. In the above block of parameters from the generic input file, the refinement factor is set to 5, and the number of local cells is set to 10.

In general, care should be taken in choosing appropriate values for the refined region. The propagation grid defined above has a dimension of $21 \times 41 \times 41 = 35,301$ nodes. The refined grid is defined by a total of $(50 \times 2)^3 = 1,000,000$ nodes, which means that most of the computational effort is taken up by computing traveltimes in the source neighbourhood. In general, you will find that using a refinement factor of 5 and a cell number of 5 greatly decreases computing time (125,000 local nodes instead of 1,000,000), and does not diminish accuracy very much. The final line of the above block of parameters defines a so-called cushion factor for the propagation grid. This is a rather ad hoc parameter I have included which makes sure that the propagation grid does not extend outside the actual

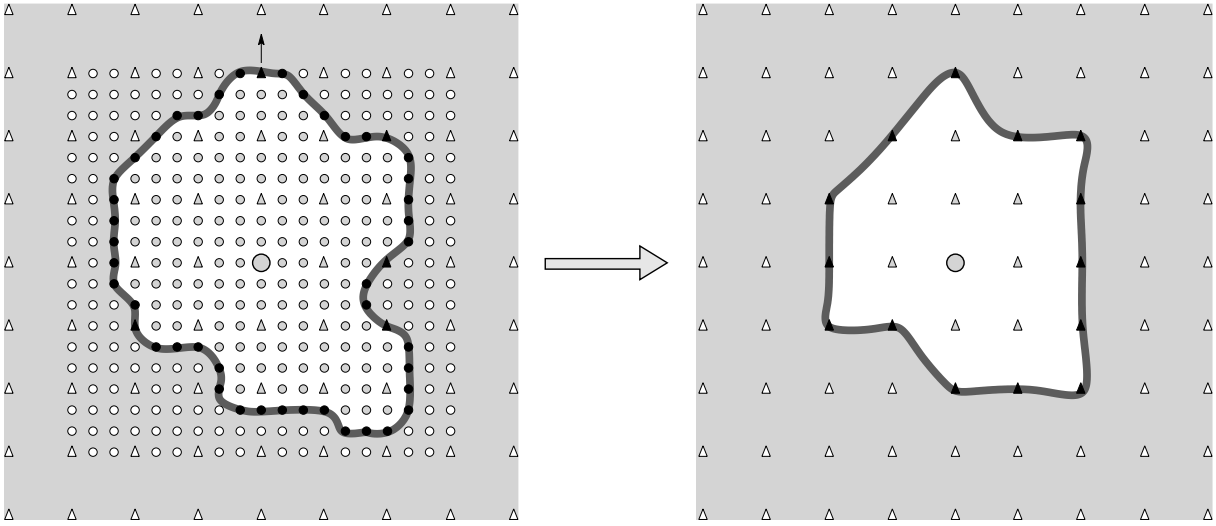


Figure 4: Schematic diagram showing the use of local grid refinement about the source in order to improve traveltime accuracy. As soon as the wavefront hits the edge of the refined grid, it is mapped back onto the coarser global propagation grid.

model bounds. I have found that **fm3d** can complain if the propagation grid extends laterally right up to the boundary of the interface surfaces. This value defines by how much the propagation grid should lie within the horizontal bounds of the model. Set it to as small a value as possible (if it is too small, **fm3d** will complain).

3.2.3 Defining the velocity grids

The next step is to set up the velocity grids which define the model. For each layer that is defined, there are four blocks of parameters that must be repeated. In the generic example, the first block is:

```
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c Set velocity grid values for layer 1
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
12          12          c: Number of radial grid points (type 1 & 2)
12          2           c: Number of grid points in theta (N-S)
12          12          c: Number of grid points in phi (E-W)
1                       c: Use model (0) or constant gradient (1)
P                       c: Use P or S velocity model
```

ak135.vel		c: Velocity model (option 0)
1		c: Dimension of velocity model (1=1-D,3=3-D)
5.4	4.0	c: Velocity at origin (km/s) (option 1)
7.0	5.0	c: Velocity at maximum depth (km/s) (option 1)

The first line specifies the number of grid points in radius. The reason why there are two entries is that, as mentioned earlier, it is possible to have both a P-wave velocity field and an S-wave velocity field independently defined in the same layer. If you specified (second parameter line in file) that there is only one velocity grid type, then you only have to deal with the left hand column of numbers. In this case, 12 grid points will span the depth range of the model volume. The higher you make this number, the greater the detail that can be described by the model (i.e. it will be able to resolve finer features). In general, it is good practice to have this number much smaller than the corresponding propagation grid number, otherwise the propagation grid will poorly represent the true velocity model, which will introduce traveltime error.

The second and third lines in the above block specify the number of grid points in latitude and longitude respectively. Note that the velocity grid for any layer actually spans the *entire* model volume. This means that there is considerable redundancy in their definition (unless the model is described by a continuous velocity field i.e. there is only one layer). However, in practice this does not detrimentally effect computation time, as only those nodes that lie within the layer are selected. The reason for defining the model in this way, apart from simplicity, is that during an inversion, interfaces can be perturbed in depth, in which case it is difficult to know in advance the actual grid extent that is required. Although 12 nodes in depth, latitude and longitude have been specified to define the velocities in layer 1, the actual number of nodes is 14, because cushion nodes are automatically added (see Figure 1). As shown in Figure 2, a minimum of four nodes in each dimension are required to define a cubic B-spline function, so you cannot specify less than two grid points. The grid spacing in depth for the above parameter block is 7.4 km.

The remaining lines in the above block are related to the velocity values that are assigned to the grid nodes. As indicated on the fourth line, there are two options; to use a specified model from an external file (option 0), or a simple constant velocity gradient

in depth (Option 1). In the former case, you can choose to use either P or S velocities (as specified on the next line). If you decide to use a velocity model defined in an external file, the the name of that external file must be entered on the 6th line. In this case it is a 1-D velocity model (ak135). An example of how this file should be formatted follows:

-100.000	5.8000	3.4600
0.000	5.8000	3.4600
20.000	5.8000	3.4600
20.000	6.5000	3.8500
35.000	6.5000	3.8500
35.000	8.0400	4.4800
77.500	8.0450	4.4900
120.000	8.0500	4.5000
165.000	8.1750	4.5090
etc.		

The first column indicates the depth below the surface, and the second and third columns indicate the corresponding P and S velocities respectively at these depths. Note that on the first row, the depth has been set to -100.0 km (i.e. 100 km above the surface); this is to ensure that cushion boundary nodes (see Figure 1) will always have a value associated with them. As long as you adhere to the above format, you can introduce whatever 1-D velocity model you like. Note that it must span the complete depth range of the 3-D model (including cushion boundary nodes).

If you would like to introduce 3-D velocity variations from an external file, then insert the file name on line six of this parameter block, and set the value in the line below to 3, to indicate that we are now dealing with a 3-D input velocity model. This file must have $(nvr + 2) \times (nvt + 2) \times (nvp + 2)$ entries, where nvr, nvt, and nvp are the number of velocity nodes in depth, latitude and longitude respectively ($nnr = nnt = nnp = 12$ in this case). Thus, your input file must in effect specify the complete velocity grid for this layer, including the boundary nodes. Unfortunately, this requires some effort by the user to properly grid their velocity field, but it would be very difficult to set up a more sophisticated input scheme. When the grid is read in by **grid3dg**, the innermost loop is

over longitude and the outmost loop is over radius. The pseudo Fortran code associated with this process is as follows:

```
DO i=0,nvr+1
   DO j=0,nvt+1
      DO k=0,nvp+1
         READ velocity value
      ENDDO
   ENDDO
ENDDO
```

which means that there is only one velocity value per line. If you choose to read in S-velocities (i.e. set line 5 to S), then you will need to append a list of S-velocities to the end of the P-velocities (in exactly the same format). The velocity value at $i = j = k = 1$ corresponds to the point at the southwest corner of the model region at the base of the box (i.e. maximum depth).

The final two lines in the above parameter block are only relevant if you chose the constant velocity gradient option (i.e. set the field in line 4 to 1). The first column represents velocities for the first velocity field, and the second column represents velocities for the second velocity field, which are used only if you set the number of velocity grid types to 2 (see entry two of the input file). The first value on the LHS (5.4 in this case) refers to the velocity at the top of the model, and the second value on the LHS (7.0 in this case) refers to the velocity at the bottom of the model. Linear interpolation between these two values is used to define the complete velocity field.

Once the basic velocity field for a particular layer has been defined, it is possible to superimpose several different types of laterally varying structures. These options are useful for performing synthetic resolution tests, for example. The first class of structure that can be superimposed is random velocity perturbations. The input parameter block that controls this option is:

```
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c Optionally apply random structure to layer 1
```

```
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
1               c: Add random structure (0=no,1=yes)
1.5             c: Standard deviation of Gaussian noise
1               c: Add a priori model covariance (0=no,1=yes)?
0.3             c: Diagonal elements of covariance matrix
```

The first option is a switch which allows the random structure to be turned off (0) or on (1). The second option specifies the standard deviation of the Gaussian noise that will be superimposed onto the velocity nodes. The third and fourth options are not actually associated with the random noise specification. Rather, they allow the diagonal elements of the *a priori* covariance matrix to be specified (only as a single constant value). Essentially, this represents the *a priori* uncertainty (in km/s) associated with each parameter value. This estimate is required by the inversion program, so should be included if you are going to use the model as a starting model for the inversion. The magnitude of this value is in itself not very significant, as it will trade off against the damping parameter. However, its value relative to what may be specified for the other layers and interfaces that are inverted for is significant.

The next parameter block allows a 3-D checkerboard pattern to be superimposed on the layer velocity field:

```
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c Optionally apply checkerboard to layer 1
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
0               c: Add checkerboard (0=no,1=yes)
1.5             c: Maximum perturbation of vertices
2               c: Checkerboard size (N×N×N)
1               c: Use spacing (0=no,1=yes)
```

The first option is a switch which toggles the checkerboard on (1) or off (0). The next parameter sets the maximum perturbation of the velocity vertices. In this case, each velocity value will be set to either $v + 1.5$ km/s or $v - 1.5$ km/s, where v is the velocity of the grid node prior to the checkerboard pattern being superimposed. The third option

sets the checkerboard size. In this case, $N = 2$, which means that along any of the three orthogonal directions, nodes will be perturbed in pairs (i.e. the first two set to $v + 1.5$ km/s, the second two to $v - 1.5$ km/s etc.). Increasing the value of N increases the size of each checkerboard element. Note that if you set $N = 1$, the amplitude of the checkerboard will appear diminished; this is due to the non-interpolating nature of cubic B-splines. The final parameter is a switch which indicates whether spacing should be used between adjacent checkerboard elements. This spacing will be of size N. Thus, rather than switching between positive and negative perturbations, there will be a gap of N points which remain unperturbed if this switch is set to 1. Again, note that the non-interpolating nature of cubic B-splines will mean that velocity field will not have exactly zero perturbation at these points. Turning this switch on results in a lower density checkerboard pattern.

The final parameter block for layer 1 introduces discrete "spikes" into the model if they are required:

```
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c Optionally, apply spikes to layer 1
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
0                          c: Apply spikes (0=no,1=yes)
1                          c: Number of spikes
2.50                       c: Amplitude of spike 1
-15.0   -41.9   141.5      c: Coordinates of spike 1 (depth, lat, long)
```

The first entry switches the spikes on (1) or off (0). The second entry specifies the number of spikes. The following pairs of lines (only one in this case as only one spike is specified) sets the amplitude of the spike (can be positive or negative) and the coordinates of the spike. If this option is turned on, **grid3dg** will find the nearest node to each specified point, and will apply the perturbation indicated. Due to the smooth behaviour of cubic B-spline functions, the resulting "spike" will not be a delta-like function; rather, it will be more like a small blob.

Once the properties of the first layer have been defined, the four parameter blocks shown above must be repeated for each subsequent layer. In the generic input file, there

are only two layers, which is why the four parameter blocks are only repeated once. For M layers, they must be specified M times (and obviously in the correct order - from the top to the bottom layer).

3.2.4 Defining the interface grids

Once the layer velocity fields have been specified, the next step is to define each of the interface grids. If M layers have been specified, then there **must** be $M+1$ interfaces. The top and bottom interfaces bound the velocity model; wavefronts may reflect from them, but they cannot penetrate or transmit through them. The first parameter block sets up the grid spacing:

```
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
12              c: Number of grid points in theta (N-S)
12              c: Number of grid points in phi (E-W)
```

The first entry is the number of grid nodes in latitude, and the second entry is the number of grid nodes in longitude. Note that **grid3dg** automatically adds cushion nodes, so the total number of nodes defining the interfaces will be $14 \times 14 = 196$. As stated earlier, one restriction of **fm3d** is that the horizontal grid node distribution for each interface must be the same. The remaining parameter blocks for each interface closely resembles the parameter blocks used for defining the layer velocities.

For interface 1, the first parameter block is:

```
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c Set up interface grid for interface 1
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
0               c: Obtain grid from external file (0=no,1=yes)
interface1.z    c: External interface grid file (option 1)
1.3             c: Height of NW grid point (option 0)
1.3             c: Height of NE grid point (option 0)
1.3             c: Height of SW grid point (option 0)
```

The first entry specifies whether the interface structure is to be obtained from an external file or not. If the switch is set to 1, then the interface grid information will be read in from an external file. As in the case of reading in a 3-D velocity grid, the interface grid file must have an entry associated with each node (196 in this case), and must include values for the cushion vertices. The pseudo Fortran code for reading in the external file is

```
DO i=0,nvt+1
   DO j=0,nvp+1
      READ interface depth value
   ENDDO
ENDDO
```

which means that there is only one interface depth entry per line. The value at $i = j = 1$ corresponds to the depth of the surface at the southwestern corner of the model.

If option 0 is chosen, then **grid3dg** will construct the interface depths from the three values provided in the third, fourth and fifth entries. These three values are used to define a plane. If they are all set equal, then the interface will not vary in depth (it won't be exactly planar, due to the curvature of the coordinate system). In the above case, the top surface is set to 1.3 km above the Earth's surface; note that this is slightly below the top of the velocity grid, which is set at 1.5 km height (the top surface should always be just slightly below the top of the velocity grid). By varying these three values, a dipping plane of arbitrary orientation can be specified. Note that if adjacent interfaces intersect each other, **grid3dg** will attempt to apply a correction.

The second, third and fourth parameter blocks have more or less exactly the same form as the corresponding blocks which define the velocity field. The only real difference is that we are now dealing with a surface rather than a volume. In this case, the random structure will be applied to the interface depths. As in the case of the velocity fields, an estimate of *a priori* model covariance is required if the model is to be used as an initial model in a tomographic inversion. Each of the four parameter blocks **must** be repeated for each interface, and if there are M layers, there must be $M + 1$ interfaces (three in this example). The bottom interface should at least lie slightly above the bottom of the model.

Once you have edited grid3dg.in to your satisfaction, you can go ahead and execute

grid3dg. It will produce three files: vgrids.in, interfaces.in and propgrid.in. These files must be placed in the same directory that you execute **fm3d** or **tomo3d** from.

4 Solving the forward problem with fm3d

fm3d is used to solve the forward problem of traveltime prediction, and also computes the Fréchet derivatives that are used in the gradient based inversion procedure. A detailed discussion of how **fm3d** works will not be given here, as it is a separate stand-alone code with its own set of instructions (see the file README_0.7 in the subdirectory fmcode/).

The input files required by **fm3d** are as follows:

- **mode_set.in:** This file sets some basic parameters for **fm3d**, including whether to save ray paths, generate OpenDX output files etc. If you look at the default mode_set.in file in source/inputfiles/, you will see that a lengthy explanation of each entry is given. For use with FMTOMO, I would recommend setting file_mode to false and no_pp_mode to true. Saving ray paths takes a lot of disk space, especially for large problems, so don't do so unless you want to visualize them. If you have access to a cluster, then you may want to turn on parallel_mode. display_mode is only useful if you would like to visualize interfaces and rays using OpenDX. The final option, save_timefields_mode, saves specified time fields to file. This may be useful if you want to perform non-linear hypocenter relocation with your own inversion code, but is not needed for FMTOMO. Note that if you set this option to true, then you will also need to provide an additional input file called gridsave.in.

- **frechet.in:** This file specifies which parameters are to be inverted for, so that **fm3d** knows which Fréchet derivatives to compute. If the first entry is set to zero, then no Fréchet derivatives will be computed. When using **fm3d** in forward mode, this file will still be read in by the code. How this file can be created for use with FMTOMO will be described in the next section.

- **interfaces.in:** Specifies the structure of all the interfaces that describe the input model. The generation of this file was discussed in the previous section.

- **proppgrid.in:** Defines the propagation grid (the sampling of the velocity model) used by **fm3d** to evolve the wavefront using finite difference solution of the eikonal

equation. The construction of this file was described in the previous section.

- **vgrids.in:** Specifies the velocity field in each layer of the input model. The generation of this file was discussed in the previous section.

- **receivers.in:** Lists all the receiver coordinates and their association with each source. How one may construct this file will be described later in this instruction manual.

- **sources.in:** Lists all the sources and their associated path signatures (the phase types produced by each source). The construction of this file will be described later.

Once all of these files are present in a given directory, then **fm3d** can be executed from the command line. As it runs, **fm3d** provides quite verbose screen output, which can be rather hard to follow in real time. If you wish, you can always redirect this output to file with the appropriate shell command (e.g. fm3d >! filename.txt). The two output files produced by **fm3d** that the inversion step requires are:

- **arrivals.dat:** This file essentially lists all of the source-receiver traveltimes that have been requested, along with some other information. Refer to the README_0.7 in the subdirectory fmcode/ for more information.

- **frechet.dat:** Contains all the Fréchet derivatives requested by frechet.in.

When you use FMTOMO to run a tomographic inversion, you do not need to run **fm3d** separately, as the **tomo3d** script will do this for you. However, if you want to construct a dataset for a synthetic resolution test (for example), then you will need to run **fm3d** by itself.

5 Solving the inverse problem with invert3d

The inverse problem involves adjusting the model parameter values (i.e. interface depth, velocity, hypocenter location) in order to try and satisfy the data observations (source-receiver traveltimes), subject to any imposed regularization. The program **invert3d** uses a subspace inversion method to solve this problem. Subspace inversion is a gradient based technique, and therefore requires Fréchet derivatives (which **fm3d** provides). The

objective function which **invert3d** minimizes in order to solve the inverse problem has the form:

$$S(\mathbf{m}) = \frac{1}{2}\left[\Psi(\mathbf{m}) + \epsilon\Phi(\mathbf{m}) + \eta\Omega(\mathbf{m})\right]$$

where ϵ is referred to as the *damping factor* and η as the *smoothing factor*. The vector $\mathbf{m}$ represents the model vector of unknowns that are adjusted during the inversion process. The first term on the RHS of the above equation is defined by:

$$\Psi(\mathbf{m}) = (\mathbf{g}(\mathbf{m}) - \mathbf{d}_{obs})^T \mathbf{C}_d^{-1} (\mathbf{g}(\mathbf{m}) - \mathbf{d}_{obs})$$

where $\mathbf{C}_d$ is a data covariance matrix. Here, $\mathbf{g}(\mathbf{m})$ represents the traveltime predictions associated with the model defined by $\mathbf{m}$. Thus, $\Psi(\mathbf{m})$ is minimized when the model traveltimes $\mathbf{g}(\mathbf{m})$ most closely resemble the observed traveltimes $\mathbf{d}_{obs}$. The data errors are assumed to be uncorrelated, in which case $\mathbf{C}_d = [\delta_{ij}(\sigma_d^j)^2]$ where σ_d^j is the uncertainty of the j^{th} data point.

A common problem with tomographic inversion is that not all model parameters will be well constrained by the data alone (i.e. the problem may be under-determined or mixed-determined). To help combat this problem, several *regularization* terms are added to the objective function. The first term $\Phi(\mathbf{m})$ is defined by

$$\Phi(\mathbf{m}) = (\mathbf{m} - \mathbf{m}_0)^T \mathbf{C}_m^{-1} (\mathbf{m} - \mathbf{m}_0)$$

where $\mathbf{C}_m$ is an *a priori* model covariance matrix. Uncertainties in the initial model are assumed to be uncorrelated, so $\mathbf{C}_m = [\delta_{ij}(\sigma_m^j)^2]$ where σ_m^j is the uncertainty associated with the j^{th} model parameter of the initial model. The effect of $\Phi(\mathbf{m})$ is to encourage solution models $\mathbf{m}$ that are near a reference model $\mathbf{m}_0$ (in this case the starting model). The values used in $\mathbf{C}_m$ are usually based on prior information.

Another approach to regularisation is the minimum structure solution which attempts to find an acceptable trade-off between satisfying the data and finding a model with the minimum amount of structural variation. This can be implemented by defining $\Omega(\mathbf{m})$ as:

$$\Omega(\mathbf{m}) = \mathbf{m}^T \mathbf{D}^T \mathbf{D}\mathbf{m}$$

where $\mathbf{Dm}$ is a finite difference estimate of a specified spatial derivative. Here, $\mathbf{D}$ is the second derivative operator, so $\Omega(\mathbf{m})$ reduces in size as the model becomes more smooth.

The two tuning parameters in the objective function, ϵ and η, govern the trade-off between how well the solution $\mathbf{m}_{est}$ will satisfy the data, how closely $\mathbf{m}_{est}$ is to $\mathbf{m}_0$, and the smoothness of $\mathbf{m}_{est}$.

The input parameter file associated with **invert3d** is invert3d.in, a generic copy of which can be found in source/inputfiles/:

```
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c This file contains all required input parameters and files for the
c inversion program "invert3d.f90"
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
vgridsref.in                    c: Reference velocity grid
vgrids.in                       c: Current velocity grid
interfacesref.in                c: Reference interface grid
interfaces.in                   c: Current interface grid
sourcesref.in                   c: Reference source coords
sources.in                      c: Current source coordinates
stimes.dat                      c: Current source time perturbations
receivers.in                    c: Receiver coordinates
otimes.dat                      c: Observed traveltimes
mtimes.dat                      c: Model traveltimes
rtimeso.dat                     c: Reference teleseismic traveltimes
frechet.in                      c: Frechet derivative parameters
frechet.dat                     c: Frechet derivatives
inviter.in                      c: File indicating current inversion step
propgrid.in                     c: File containing propagation grid parameters
0.07                            c: Minimum distance between interfaces (km)
0.5                             c: Minimum permitted velocity (km/s)
1                               c: Remove mean from predicted teleseisms (0=no,1=yes)
0    1.0    1.0                 c: Velocity inversion (0=no,1=yes),damp,smooth
1    0.1    1.0                 c: Interface inversion (0=no, 1=yes),damp,smooth
0    1.0    1.0                 c: Source inversion (0=no, 1=yes),damp1,damp2
20                              c: Subspace dimension (max=50)
1.0                             c: Global damping factor (epsilon)
1                               c: Apply second derivative smoothing (0=no,1=yes)
1.0                             c: Global smoothing factor (eta)
```

6371.0 c: Earth radius in km

The first and third entries of this file specify the initial or starting velocity (vgridsref.in) and interface grids (interfacesref.in) for the inversion. These can be constructed using **grid3dg** (you will have to rename the default output files). After **invert3d** is executed, it will write the updated interface and velocity grid files to vgrids.in and interfaces.in. Since source locations can also be inverted for, **invert3d** requires a reference source input file called (sourcesref.in). Updated source locations will be written to sources.in. Note that all three reference files are required, even if one or more of the parameter types are not inverted for (i.e. you **must** provide vgridsref.in, interfacesref.in and sourcesref.in), in which case the corresponding output file will simply be a copy of the reference input file (e.g. if you do not invert for source location, then sourcesref.in and sources.in will be identical).

The output file called stimes.dat stores the time perturbations associated with each source hypocenter that is inverted for. Thus, if **invert3d** deems that the source origin time is late by λ seconds, then λ will be written to stimes.dat for that source. This assumes that the *a priori* traveltimes are equal to the receiver arrival time minus the *a priori* origin time.

The input receivers.in file lists the receiver locations. The vector of observed traveltimes $\mathbf{d}_{obs}$ is given in the file otimes.dat. How this file can be produced from your pick files is described later. Traveltimes and their associated errors are listed in the same order as the output traveltime file produced by **fm3d** (arrivals.dat). The vector of model traveltimes $\mathbf{g}(\mathbf{m})$ is given in the file mtimes.dat. It is simply the file (arrivals.dat) produced by **fm3d** for the current model, that has been renamed to mtimes.dat.

The next file, rtimeso.dat, describes the reference model traveltimes for teleseisms. For teleseismic events, it is assumed that the traveltime information input into otimes.dat is in the form of arrival time residuals, which are equal to the arrival times minus the predicted arrival times from a global reference model. In addition, arrival time residuals associated with each source usually have their means removed, which makes them relative arrival time residuals. Since **fm3d** computes the total traveltimes from source to receiver, for teleseisms, we need a set of predicted reference traveltimes in order to compute model arrival time residuals. This is provided by rtimeso.dat. By default, **tomo3d** will produce a file called rtimes.dat, which represents the traveltimes through the reference model defined

by interfacesref.in and vgridsref.in. In many cases, it is o.k. to use this file to provide the reference model traveltimes. However, if the observed residuals includes a contribution from topography which has not been accounted for, you may want to create your own rtimes.dat file (in which case you must relabel it to rtimeso.dat or something so that it doesn't get overwritten by **tomo3d**) which is computed with all station elevations set to zero. It is acknowledged that this approach to matching observed residuals is perhaps not the most self-consistent, as it would be best to use the same reference model predictions for both the observations and the model predictions. In the end, it makes little difference, but if you want to be technically correct, you could just compute your observed residuals by using the predictions provided by rtimes.dat.

The next two input files, frechet.in and frechet.dat are the input and output Fréchet derivative files used by **fm3d**. inviter.in simply contains one integer which defines the current iteration number of **tomo3d**. This is required for housekeeping purposes (it tells **invert3d** whether we are dealing with the first or some later iteration). The final file that is listed, propgrid.in, is the propagation grid file used by **fm3d**.

Following the list of files, invert3d.in specifies the minimum allowed distance between adjacent interfaces. This is similar to the specification in grid3dg.in, and limits how close interfaces can come together. A limit can also be set on the minimum permitted velocity. Particularly in regions of low velocity (e.g. volcanic caldera or uncompacted wet sediment), uncertainties in traveltime picks and other factors may result in near zero or negative velocities, which may cause **fm3d** to fail (quite understandably so).

The next parameter indicates whether the mean should be removed from the predicted teleseismic residuals (if they are present) on a source-by-source basis. In most case, observed residuals have their means removed to account for errors in source location and broad-scale structure outside the model region. However, removing the mean from the predicted dataset can often make little difference in this case, because the average vertical variations in structure are usually preserved when teleseismic data are inverted. When combined with other classes of data, it may be more necessary to remove the mean from the model data.

The next three lines allows the user to choose whether to invert for velocity structure, interface structure and/or source location. In the first two cases, damping and smoothing factors can be specified for the velocity fields and interface surfaces. If different damping is needed for different layers and interfaces, then this should be accomplished via the *a*

priori model covariance matrix. The damp1 and damp2 factors associated with the source inversion refer to the damping of the spatial and temporal locations of the hypocenter respectively. More refinement as to which velocity, interface and source parameters are inverted for can be achieved by editing the frechgen.in file. This will be discussed shortly.

The next parameter sets the subspace dimension. Subspace inversion works by restricting the minimization of the quadratic approximation of the objective function $S(\mathbf{m})$ to an n-dimensional subspace of model space; thus, the perturbation $\delta\mathbf{m}$ is restricted to occur in the space spanned by a set of n orthogonal basis vectors. In the generic input file, the subspace dimension is set to 20. Increasing this value can potentially improve convergence, but at greater computational cost. In practice though, it is difficult to generate a large number of linearly independent search directions that significantly influence the objective function, so there is not a lot of point in making this value very large. In any case, SVD (singular value decomposition) is used to identify basis vectors that are not independent and discards them anyway. Therefore, you could set $n = 50$ (maximum allowed value) and not lose much in computational cost.

The next parameter is described as the "global damping factor", which is ϵ in our definition of the objective function. This simply pre-multiplies each of the damping factors that have been defined separately for the velocity, interface and source inversions. Likewise, one can set a global smoothing factor, which pre-multiplies the interface and velocity specific smoothing factors. A separate switch is provided for turning the second derivative smoothing off and on. Note that the specification of the Earth radius (last line) should be consistent with previous specifications (e.g. in grid3dg.in).

Although the invert3d.in file allows one to choose whether to invert for velocity structure, interface geometry, and/or source location, it does not offer the option of only inverting for a subset of, for example, source locations, or velocity layers. This can be achieved via the **frechgen** program, which constructs the frechet.in file. The input file used by **frechgen** is called frechgen.in, a generic copy of which can be found in source/inputfiles/. In determining which parameters are to be constrained in the inversion, **frechgen** actually consults both invert3d.in and frechgen.in; therefore, **frechgen** should always be executed whenever one of the three inversion parameters in invert3d.in is adjusted. The generic frechgen.in file is constructed as follows:

invert3d.in	c: Input file for invert3d
frechet.in	c: File specifying derivatives for fm3d
vgridsref.in	c: File containing reference velocity grid
sourcesref.in	c: File containing reference source locations
-1	c: Velocity derivatives (>0=subset, -1=all)
1	c: If all, type 1 (1), type 2 (2) or both (3)
2	c: Indices of velocity grids (if subset chosen)
1	c: Velocity types for inversion (1 or 2)
1	c: Interface derivatives (>0=subset, -1=all)
2	c: Indices of interface grids (if subset chosen)
-1	c: Source derivatives (>0=subset, -1=all)
sourcederivs.in	c: File specifying sources for inversion (if subset chosen)

The first entry simply specifies the default input parameter filename of **invert3d**. The second entry is the name of the output file produced by **frechgen**, which becomes the Fréchet parameter input file to **fm3d**. The third and fourth files contain the reference velocity grid and source locations. The next four lines select the velocity fields that are to be constrained in the inversion. If on line 5, the switch is set to -1, then the velocity parameters in all of the layers are selected. If a subset of m layers is to be inverted for, then m should be entered in the place of -1. On line 6, it is possible to specify which type of velocity field is used. This switch only gets activated if the switch on the line above is set to -1. If there is only one type of velocity field present (P or S), then this switch should be set to 1. If both P and S are present, then setting this switch to 1, 2 or 3 will result in the selection of P, S or both P and S velocity fields respectively.

The next two parameters are activated when only a subset of the velocity fields is chosen. For example, if for some model, the velocities in layers 2, 3, 5, 6 are to be inverted for, then $m = 4$, and line 7 should read 2 3 5 6. Line 8 then lists the velocity types associated with these four layers that are to be constrained. If there is only one velocity type present (P or S), then line 8 should read 1 1 1 1 . The specification for interfaces is similar to that of velocity; the entry on line 9 indicates whether all (-1) or some subset (m) of the interfaces are to be inverted for. In the latter case, the m interfaces are listed on the line below. For example, if interfaces 2 and 4 are to be constrained by

the inversion, then $m = 2$ and line 10 should read 2 4.

The final two lines control which sources are relocated. If the second last line is set to -1, then all sources are selected. Otherwise, a subset of sources, listed in the file sourcederivs.in will be relocated. The reason that this information is kept in an external file is that the subset of m sources may be quite large (e.g. 100s). If you do not wish to edit this file by hand, the programs **moddata** and **obsdata**, described in subsequent sections, gives you the option of generating sourcederivs.in.

The input files invert3d.in and frechgen.in provide a two-level hierarchy for determining which parameters become unknowns in the inversion. invert3d.in allows you to activate or deactivate each parameter class. For example, if you do not want to invert for velocity structure, then set the velocity inversion switch in invert3d.in to 0. This will over-rule any velocity parameter directive contained in frechgen.in. However, if the velocity inversion switch is set to 1, then frechgen.in will determine which layers are inverted for. Prior to running **invert3d**, the program **frechgen** should be executed.

Note that the **tomo3d** script automatically runs **frechgen** prior to the first iteration, so all you need to do is make sure that you have edited invert3d.in and frechgen.in to suit your requirements. In general, when using the FMTOMO package, there should be no need to run **invert3d** as a stand alone program, as the **tomo3d** script will carry out this step automatically.

When **invert3d** is executed, it produces very minimal screen output; if it works correctly, it will generate something like:

```
Due to redundancy, the subspace dimension
is being reduced from          20 to          15
Message from SVD orthogonalization algorithm
PROGRAM invert successfully completed!!
```

The first three lines may or may not be produced, depending on whether the SVD orthogonalization algorithm identifies any redundant search directions.

6 Constructing a tomographic solution model with tomo3d

tomo3d is a relatively simple shell script that sequentially executes **fm3d** and **invert3d** to iteratively minimize the objective function $S(\mathbf{m})$. Re-running **fm3d** after each inversion iteration ensures that the non-linearity of the inverse problem is taken into account. The input file used by **tomo3d** is called tomo3d.in, a generic copy of which can be found in source/inputfiles/:

```
6
0
0
```

The first entry simply sets the number of inversion iterations that are to be executed. If this number is set to some value p, then **fm3d** will be executed $p+1$ times, and **invert3d** will be executed p times. This occurs because **fm3d** will be executed first (traveltimes through initial model) and last (traveltimes through final model). If you run the inversion process for p iterations, and then decide you would like to run it for a set of additional iterations, then set the second entry to 1. If you do this, then you will need to specify (line 3) whether **tomo3d** begins by executing **invert3d** (option 0) or **fm3d** (option 1). In most cases, you should set this to 0, because **tomo3d** will have computed traveltime predictions for the previous solution model.

tomo3d can be executed from the command line like any of the other programs. All of the programs it uses will be executed in the current directory, so the relevant input files must be present. When **tomo3d** is executed with line 2 of tomo3d.in set to 0, it will start off by copying vgridsref.in to vgrids.in, interfacesref.in to interfaces.in and sourcesref.in to sources.in. It will then create the frechet.in file by executing **frechgen**. **fm3d** will then be run in order to generate traveltimes and Fréchet derivatives for the initial model. After this has completed, the output arrivals.dat file will be copied to mtimes.dat, and traveltime residuals for this model will be generated by the program **residuals**, and stored in residuals.dat. **invert3d** and **fm3d** will then be executed in sequence a total of p times, with residuals computed at the end of each iteration, and appended to residuals.dat.

The generic input file residuals.in (see sources/inputfiles/) for the program **residuals** has 5 entries:

otimes.dat	c: Observed times
mtimes.dat	c: Model times
sourcesref.in	c: Source file
rtimeso.dat	c: Reference teleseismic times
invert3d.in	c: Inversion parameters (indicates if mean is to be removed from teleseismic traveltimes)

None of these filenames should be changed, with the possible exception of the entry on the 4th line. This specifies the reference teleseismic times, which by default is rtimes.dat (**tomo3d** will automatically construct this file from the initial model traveltimes). If you want to use rtimes.dat as computed by **tomo3d**, then you should edit line 4 accordingly. When **residuals** is executed, traveltime residual information is written to screen (**tomo3d** redirects this output to residuals.dat). The three values it produces are, in order from left to right, RMS traveltime residual (in milliseconds), variance (in seconds^2), and χ^2 (which is dimensionless).

For most problems, the vast majority of computing time will be taken up running **fm3d**; even for problems with large numbers of unknowns, **invert3d** executes very rapidly. The verbose screen output generated by **fm3d** is automatically redirected by **tomo3d** to a file called fm3dlog.out. Thus, the only screen output will be generated by **invert3d**. Therefore, do not be alarmed when you do not immediately see screen output when you execute **tomo3d**; **fm3d** will have to run first with the initial model before **invert3d** is executed and produces screen output.

The input files that **must** be present in the directory from which you execute **tomo3d** are:

- frechet.in
- frechgen.in
- interfacesref.in

- invert3d.in
- mode_set.in
- otimes.dat
- propgrid.in
- receivers.in
- residuals.in
- sourcesref.in
- tomo3d.in
- vgridsref.in

Two additional files may also be needed:

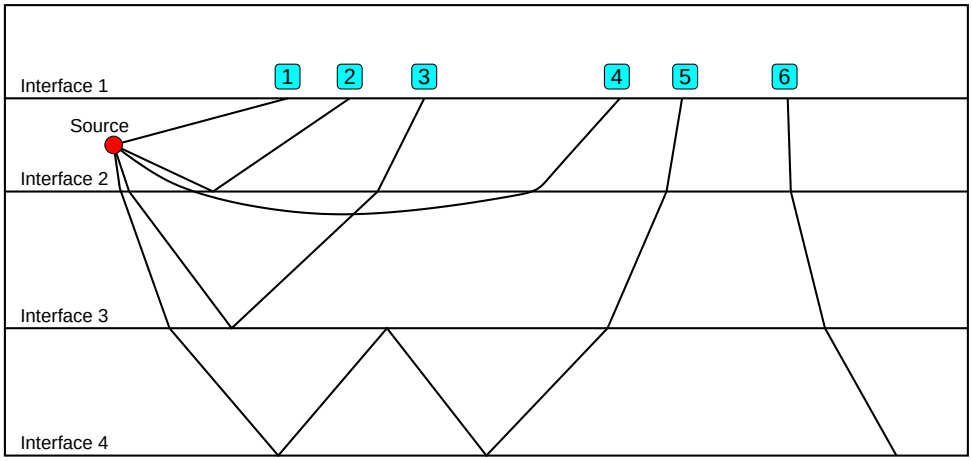
- **rtimeso.dat:** Required if reference model teleseismic traveltimes are not computed from the initial model (filename doesn't have to be rtimeso.dat in this case). If they are to be computed from the initial model, then **tomo3d** will automatically generate rtimes.dat. Obviously, rtimes.dat or rtimeso.dat are only required if teleseismic data are considered.
- **sourcederivs.in:** Required only if a subset of sources are going to be relocated.

7 Data input

The data required by the FMTOMO package in order to produce a solution model from some given initial model are the two point traveltimes and associated phase information (path signatures) for a given set of sources and receivers. All of this information is contained in the three files sourcesref.in, receivers.in and otimes.in. The format of these files is exactly that of the files sources.in, receivers.in and arrivals.dat respectively, which are used by **fm3d** (although we do add a column to sourcesref.in and otimes.in which indicates the uncertainty associated with source location and traveltime picks). As such, the exact format of these files will not be described here, as they can be found in the README_0.7 file located in fmcode/. However, before examining two programs for generating these input files, the concept of *path signatures*, as used by **fm3d**, will be explained.

7.1 Path signatures

In continuous media, the only type of phase that can be tracked by **fm3d** is the direct first arrival. However, when interfaces are present, a wide variety of other phases can be tracked. At any interface, an impinging wavefront can produce a transmission, a reflection or a mode conversion (P-S or S-P). When requesting the traveltime between any source or receiver from **fm3d**, the associated *path signature*, which describes the interaction of the wavefront with any interfaces that are present, must be specified.



Ray ID	Path signature
1	0 1
2	0 2 2 1
3	0 2 2 3 3 2 2 1
4	0 2 2 3 2 1
5	0 2 2 3 3 4 4 3 3 4 4 3 3 2 2 1
6	4 3 3 2 2 1

Figure 5: Schematic diagram demonstrating the path signature format used by **fm3d** to describe phases. In this case, all receivers lie in layer 1, but this need not be the case in general.

fm3d expects the path signature to be defined as a string of integer pairs, which describes the propagation of the wavefront between two interfaces (the multi-stage FMM tracks wavefronts from one interface to the next; at each interface, the FMM procedure is reinitialized). When beginning from a point source, the first number will be 0. To complete the first integer pair, the second number will either be the number of the top or bottom interface which bounds the layer in which the source resides. For subsequent steps,

the first number is the starting interface and the second number is the other bounding interface. Remember that interfaces are numbered starting at the surface and increase downwards.

If two equal numbers are entered as an integer pair, then **fm3d** assumes that a min-imax phase is requested (a double bounce like PP), and performs reflection matching. FMTOMO has not been tested with this type of phase. Examples of several different ray paths and their associated path signature are shown in Figure 5.

7.2 Constructing synthetic datasets with moddata

moddata is a program designed to produce sources.in and receivers.in with relatively simple input provided by the user. It does not produce an otimes.dat file, and as such, is best used for purely synthetic tests (e.g. Examples 1 and 2). The main restriction of this program is that it assumes that a path exists for **every** source-receiver pair. These limitations may make you wonder why you would want to use **moddata**, but it turns out to be a useful tool for examining what kind of path coverage and hence resolving power a particular source-receiver configuration may produce. Also, purely synthetic tests like Example 1 and 2 are interesting in their own right, as they allow one to investigate the capabilities of the package.

The input file required by **moddata** is called moddata.in. A generic copy of this program can be found in sources/inputfiles/. The first block of this input file contains the following:

```
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c Input file for generating source and receiver files
c for use by 3D FMM code. Every receiver must
c detect a traveltime from every source.
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
sources.in              c: Output source file
receivers.in            c: Output receiver file
sourcederivs.in         c: Output source derivative file
arraygen.out            c: Input receiver file
2                       c: Number of input source files
```

The first two entries specify the source (sources.in) and receiver (receivers.in) files that will be created by **moddata**. These files can then be used as input files for **fm3d**. The next entry, sourcederivs.in, is the name of the output file that identifies those sources that are to be inverted for. This file is required by **tomo3d** if a subset of sources are to be relocated. The last file on this list is the receiver input file. All this contains is the number of receivers (top line), and on each subsequent line, the latitude, longitude and depth of each receiver (negative values are above the surface). For example:

```
100
-41.70000          138.3000          -1.000000
-41.70000          138.6778          -1.000000
-41.70000          139.0556          -1.000000
-41.70000          139.4333          -1.000000
-41.70000          139.8111          -1.000000
etc.
```

The last line of the first parameter block specifies the number of input source files (in this case 2). The reason for having different source files is that it allows you to distinguish between, for example, local sources (which you may want to relocate), teleseismic sources and explosive sources. You can specify as many different source files as you like.

The second block of parameters contains the following:

```
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c First input source file and associated path information
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
sourceswa.in              c: Input source file
0                         c: Local (0) or teleseismic sources (1)
0                         c: Compute source derivatives (0=no, 1=yes)
2                         c: Number of paths from these sources
2                         c: Number of path segments for path 1
```

```
c: Path sequence information plus velocity fields below
0   2      2   1
1            1
1                                  c: Number of path segments for path 2
c: Path sequence information plus velocity fields below
0   1
1
```

The first entry is the name of the source input file. It has been named sourceswa.in to indicate that these sources generate wide-angle paths (refractions and wide-angle reflections from explosive sources). This file has exactly the same format as the receiver file, except that an additional three column of numbers must be included if the sources are going to be relocated. For example:

```
30
-41.50000        138.5000        0.000000        0.2        0.2        10.0
-41.50000        140.0000        0.000000        0.2        0.2        10.0
-41.50000        141.5000        0.000000        0.2        0.2        10.0
-40.50000        138.5000        0.000000        0.2        0.2        10.0
-40.50000        140.0000        0.000000        0.2        0.2        10.0
etc.
```

Thus, the top number is the number of sources in the file, and the first three numbers from left to right give the latitude, longitude and depth (negative is above the surface) of each source. The last three numbers of each row specify the *a priori* uncertainty associated with the latitude, longitude and depth of each source respectively. In the case of active sources which don't need to be relocated, the last three column of numbers will be ignored.

The second entry in the parameter block is a switch which indicates whether we are dealing with local (0) or teleseismic (1) sources. Local sources **must** lie within the model volume, while teleseismic sources **must** lie outside the model volume. If teleseismic sources are specified, then the input source file has a slightly different format: on the line below each source location, the phase type must be specified (e.g. P, ScP, PP, PKiKP etc.).

Note that this is not related to the path signature specification discussed above, because these phases are tracked to the edge of the model region prior to the implementation of FMM. An example of a source file for teleseisms is given below:

```
12
-33.00          80.00000          33.0000
P
-13.0           190.0000          33.0000
P
-30.0           180.0000          33.0000
PcP
10.0            100.0000          33.0000
P
etc.
```

a priori source uncertainty estimates are not required in the case of teleseismic events, because they cannot be relocated.

The third entry of the second parameter block indicates whether source derivatives should be computed. If this is set to 1, then the i.d. of all the sources in this file are written to sourcederivs.in. Thus, if only a subset of sources are relocated, then this output file can be used with frechgen.in.

The fourth entry indicates the number of paths that are to be tracked from these sources. You can use any number you like; for q path types, the four input lines following the specification of q on line 4 must be repeated q times. In this case, there are two path types, so 8 lines follow. For each path type, the number of path segments must be specified. The first path contains two segments, the path signature of which is given by 0 2 2 1, which corresponds to a simple reflection if the source lies in layer 1. For each ray segment, the velocity type must be specified in the line below. If the velocity model only specifies one type of velocity (P or S) within the relevant layer, then this should be set to 1. Mode conversions can be obtained by setting consecutive entries to different values (e.g. [1 2] gives a P-S conversion, and [2 1] gives an S-P conversion) provided two velocity fields have been defined for the corresponding layers. For p path segments,

the path sequence must contain p pairs of integers, and the velocity field specification must contain p integers. The second parameter block must be repeated for every input source file that is specified.

When moddata is executed, it will produce sources.in, receivers.in and optionally sourcederivs.in. These can then be copied to the directory from which **tomo3d** is to be run.

A very simple program called **arraygen** has been provided which generates a square grid of evenly spaced sources or receiver locations. A generic input file arraygen.in can be found in sources/inputfiles/:

```
arraygen.out                c: Output file name
-32.0       -34.0           c: N-S bounds of grid
138.5        141.5          c: W-E bounds of grid
0.0                         c: Depth of receiver grid
10        10                c: Number of receivers in lat and long
```

The first entry is the name of the output receiver (or source) file. The next two entries specifies the horizontal bounds of the square grid of points that will be generated. The fourth entry specifies the depth of the point (negative is above the surface), and the last entry specifies the number of points in latitude and longitude ($10 \times 10 = 100$ points in total). Although of limited value, **arraygen** may be of some use if you want to span a region with a rectangular array of receivers, for example.

7.3 Including observational data with obsdata

Although **moddata** is useful in some cases, generally one wants to convert their database of picked traveltimes into a format suitable for input into FMTOMO. The program **obsdata** offers one possible route for achieving this. In many ways **obsdata** is similar to **moddata**, but has some additional flexibility built in. The input file to **obsdata** is called obsdata.in, a generic version of which can be found in sources/inputfiles/. The basic format of this file is the same as moddata.in, with the exception of the first parameter block:

```
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
```

```
c Input file for generating source and receiver files
c for use by 3D FMM code. Will also generate traveltime
c file if required.
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
sources.in              c: Output source file
receivers.in            c: Output receiver file
sourcederivs.in         c: Output source derivative file
picks/                  c: Directory containing input receiver files
2                       c: Number of input source files
1                       c: Extract traveltimes (0=no, 1=yes)
otimes.dat              c: File containing extracted traveltimes
```

The fourth entry specifies a subdirectory which contains all of the receiver input files (which contain traveltimes measured from recordings at each receiver). The format of these files will be described below. The last two entries are related to constructing a list of observed traveltimes. If the traveltime extraction specification is set to 1, then all traveltimes will be read in from the files contained in picks/ and written to otimes.dat. This file can then be used as the input to **tomo3d**.

The input source files read in by **obsdata** have a very different format to those read in by **moddata**. An example of an input file containing local sources (explosions for wide-angle data) is given below:

```
16
-41.742333          145.093333          -0.200
1
1   1           pick04.9pm
-41.195666          144.818667          -0.139
3
1   1           pick05.8pm
1   1           pick05.9pm
3   2           pick05.8pg
etc.
```

The first line contains the number of sources. For each source, the coordinates are given as latitude, longitude and depth in km (negative values are above the surface). For a particular source, the number of associated pick files are then specified. In the above example, source 1 has one pick file, and source 2 has three pick files. Following this specification, the name of each pick file is listed below. These pick files **must** be located in the subdirectory picks/, which is specified in entry 4 of obsdata.in. In each row containing the name of a pick file, the filename is preceeded by two integers. The first integer specifies which path from the source these picks are associated with. This information is provided in obsdata.in (the "number of paths from these sources" entry associated with each source input file). In the above example, at least 3 path types must have been defined for this source file, because the third pick file of source 2 is associated with path type 3. In the generic obsdata.in file described above, the first path is a PmP phase, the second a Pn phase, and the third a Pg phase. You can see that the pick file name extensions given above correspond to these phases. The second integer simply indicates that, of the total number of different phase types for a particular source, where a particular pick file sits on this list. For example, source 2 has two out of a possible three phase types, and although the third pick file corresponds to path type 3, it is only the second type of phase for this source.

As pointed out in the previous section, if source relocation is to be carried out, then the input source file must contain uncertainty estimates for each source coordinate. These values are appended to each source location. For example, if a local earthquake source has an initial location at, say, (42±0.2° S, 140±0.2° W, 33±20 km depth), the source line would be entered as:

```
-42.0          220.0          33.0          0.2          0.2          20.0
```

where the last three entries represent the uncertainty in latitude (in degrees), longitude (also in degrees), and depth (in km) respectively.

The format of the traveltime pick files for local sources is relatively simple, as shown in the example below:

```
22
-42.5010778     148.304078      0.      15.6749245      0.117747625
-42.4852975     148.315989      0.      15.9046817      0.130464375
-42.4718477     148.327002      0.      16.1281673      0.141703125
-42.4550508     148.342275      0.      16.3976353      0.11687775
-42.4419621     148.354095      0.      16.599588       0.12822025
-42.4276707     148.366749      0.      16.8457135      0.119055
-42.4138321     148.379216      0.      17.0651105      0.115553
etc.
```

The first entry specifies the number of picks contained in the file. This is followed by a traveltime pick list. From left to right, each line contains the receiver coordinate corresponding to the pick (latitude, longitude, depth), the picked traveltime (in seconds), and some estimate of uncertainty associated with the pick (also in seconds).

When teleseismic sources are used instead of local sources, the format of both the input source file and the traveltime pick file is slightly different. An example input source file for teleseisms is given below:

```
110
1       1       ts0761933.ttr
1       1       ts0762143.ttr
1       1       ts0772224.ttr
1       1       ts0782214ScP.ttr
1       1       ts0782214.ttr
1       1       ts0810910.ttr
1       1       ts0810922.ttr
etc.
```

The difference between this file and the example input file for local sources given above is that the source location is not specified. This is because the teleseismic source location has been included in the associated pick file. An example pick file for teleseismic events

is given below:

```
64
-20.52          162.18          33.
P
-40.9743        145.1336        -0.166      -0.16640625     0.0754
-41.0399        145.2852        -0.276      -0.11640625     0.0616
-41.094         145.4457        -0.278      -0.06640625     0.0488
-41.1135        145.6235        -0.307      0.03359375      0.0908
-41.1899        145.7724        -0.289      0.08359375      0.0479
-41.246         145.893         -0.397      -0.01640625     0.0623
-41.3242        146.097         -0.45       -0.06640625     0.0634
etc.
```

The first line of this file specifies the number of teleseismic picks associated with this source. The second line gives the teleseismic source coordinate. Note that you **cannot** relocate teleseismic sources, so there is no need to include uncertainty estimates. The third line specifies the global phase associated with the picks. Most common phase types can be used (e.g. P, PP, ScP, PcP, PKiKP etc.). The list of entries that follow provides the pick information for each receiver in the form of the location (latitude, longitude, depth [negative values are above the surface]), the associated traveltime residual (in seconds), and an uncertainty estimate. Note that in most cases, the mean will have been removed from the traveltime residuals on a source by source basis.

7.4 Generating a synthetic traveltime dataset

In some cases, it is desirable to generate a synthetic traveltime dataset (e.g. for a checkerboard resolution test). This is relatively simple to do once all of the necessary input files for **fm3d** (i.e. mode_set.in, frechet.in, interfaces.in, propgrid.in, vgrids.in, receivers.in, sources.in) have been constructed. For a given synthetic model, executing **fm3d** in the directory containing these files will produce a file called arrivals.dat. This basically comprises the synthetic dataset, but a minimal amount of processing is required prior to it being copied to otimes.dat where it can be used to constrain a tomographic inversion. At

the very least, for local sources, some estimate of error needs to be included with each traveltime. For teleseismic sources, the two-point traveltime needs to be reduced to a teleseismic arrival time residual. It is also common practice to infect synthetic datasets with random noise in order to make them more realistic (since any observational dataset will contain noise).

A program called **synthdata** is provided with the FMTOMO distribution to help accomplish all of these tasks. A generic input file (synthdata.in) is located in source/inputfiles/, and contains the following list of parameters:

```
../syntimes.dat          c: Input observed times
0.1                      c: Data covariance (s)
otimes.dat               c: Output file
../sourcesref.in         c: Source file
../rtimes.dat            c: Reference teleseismic times
0.0                      c: DC offset to traveltimes
1                        c: Add noise to synthetic times (0=no,1=yes)
0.100                    c: Standard deviation of added noise (local)
0.077                    c: Standard deviation of added noise (teleseismic)
1                        c: Weight with standard deviation (1) or noise (2)
99827374                 c: Random seed for noise generation
```

The first entry names the file containing the synthetic traveltimes. In this example, the output arrivals.dat file from **fm3d** has simply been renamed to syntimes.dat. The second entry is a constant data covariance value that will be associated with each traveltime pick **if** random noise is **not** added to the data. The third entry is the output filename containing the synthetic "observed" traveltime dataset. This can be used as input to FMTOMO. The fourth line specifies the current sourcesref.in file, and the fifth line specifies the reference teleseismic traveltime file (only needed if teleseisms are present). This can be generated by running **fm3d** with your reference model. Currently, the mean is not removed from the residuals. The sixth line allows you to add a constant DC (positive or negative) offset to the traveltimes. This should only be set to a non-zero value if you are dealing with a synthetic local earthquake dataset, and want to test the accuracy of the hypocenter

relocation in time as well as space.

The entry on the seventh line is a switch which allows you to add Gaussian noise to the synthetic dataset. The two lines below let you set the standard deviation of the noise (in seconds) for local and teleseismic sources. On the second last line is a switch which toggles between using the standard deviation of the added noise as the uncertainty associated with each traveltime pick (option 1), or the actual noise value that is added to the pick (option 2). The last line is simply a random seed (integer) which initializes the noise generation. When **synthdata** is executed in the presence of synthdata.in, it will produce the file otimes.dat.

8 Plotting the output

An important step in analysing the results of a tomographic inversion is visualization of the solution model. When dealing with 3-D models, this is not a simple task. These days, however, there are many sophisticated software packages for performing 3-D visualization that can be used. As note earlier, **fm3d** has the option of producing files in OpenDX format. These files allow sources, receivers, rays and interfaces to be visualized, but not velocity variations. Given that OpenDX is capable of volume visualization, this could be accomplished quite readily. However, the FMTOMO package has taken the simpler route of providing a program which can take a variety of cross-sections through a 3-D model and output the result in a format that can be read in by GMT. The Generic Mapping Tool is a flexible script-based plotting program that has the dual advantage of being almost ubiquitous in the Earth Sciences community, and producing high quality PostScript output suitable for publication.

Please note that you must have at least a basic working knowledge of GMT in order to use the plotting scripts provided with this distribution.

8.1 Producing GMT output with gmtslice

gmtslice is a Fortran 90 program that is capable of taking slices through a 3-D model in **fm3d** format (as defined by the files interfaces.in and vgrids.in), and producing output in GMT format. It can also project the ray paths, sources and receivers onto the slices that are chosen. In order to run **gmtslice**, you will need an input file called gmtslice.in,

a generic copy of which can be found in sources/inputfile/. The first parameter block of this file contains the following:

```
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c Input file names
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
../vgrids.in              c: Inversion model velocity vertices
../vgridsref.in           c: Reference model velocity vertices
../interfaces.in          c: Inversion model interface vertices
../interfacesref.in       c: Reference model interface vertices
6371.0                    c: Earth radius (km)
0                         c: Generate P(0) or S(1) velocities
```

The first entry in this block specifies the inversion model velocity grid file (or any velocity model you may wish to visualize). For example, if you have executed **tomo3d** and wish to visualize the result, then the name entered here should be the vgrids.in file located in the directory from which **tomo3d** was executed. The second entry is a reference vgrids.in file; this file is only used if you specify later on in gmtslice.in that you want to visualize velocity perturbations rather than absolute velocity. The corresponding interface grid files are listed below the velocity grid files; again, it is possible to plot perturbations in interface depth rather than absolute interface depth, which is why interfacesref.in is include. The fifth entry is simply the Earth radius, and the final entry lets you choose between P or S velocity. This should only be set to 1 if both P and S velocity grids are present in vgrids.in and you wish to visualize P velocity rather than S. If only S velocities are available in vgrids.in, then this option should still be set to 0.

The second parameter block of the input file contains:

```
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c Set parameters for plotting ray paths if required
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
1                         c: Generate raypaths (0=no, 1=yes)
../rays.dat               c: File containing raypaths
```

```
raysd.xy          c: File name for depth projection
raysew.xy         c: File name for EW projection
raysns.xy         c: File name for NS projection
raysgc.xy         c: File name for GC projection
30                c: Plot every nth ray point
```

The first entry is a switch which gives you the option of generating raypaths. The second entry is the name of the raypath output file generated by **fm3d**. You will need to make sure that mode_set.in is correctly set up to generate this file if you want to visualize ray paths. The next four lines provide output file names for ray paths that are projected in one of four ways. The first projection (raysd.xy) is simply a depth projection (rays vary in longitude and latitude but not depth); the second (raysew.xy) is an east-west projection (rays vary in longitude and depth but not latitude); the third (raysns.xy) is a north-south projection (rays vary in latitude and depth but not longitude); and the final file (raysgc.xy) contains rays that have been projected onto a great circle slice. Note that in the last option, each point along the raypath is projected onto the closest point along the great circle slice. All of these files are simple ASCII text files, but list the rays in a format that GMT can interpret. The final option in the above block of parameters sets the resampling level of the ray path, which is described by a set of points. **fm3d** typically describes each ray path using a high density of points; for plotting purposes, it is often not necessary to try and interpolate every point. In the above example, **gmtslice** will simply describe the ray by taking every $n = 30^{\text{th}}$ point. When a large number of rays are present, it is a good idea to undersample the raypaths, otherwise the resulting postscript file will be very large.

The third parameter block of the input file contains:

```
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c Set parameters for plotting sources and receivers
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
1                 c: Generate sources & receivers (0=no, 1=yes)
../sources.in     c: File containing sources
../receivers.in   c: File containing receivers
```

```
sourcesd.xy          c: Output source file for depth projection
sourcesew.xy         c: Output source file for EW projection
sourcesns.xy         c: Output source file for NS projection
sourcesgc.xy         c: Output source file for GC projection
receiversd.xy        c: Output receiver file for depth projection
receiversew.xy       c: Output receiver file for EW projection
receiversns.xy       c: Output receiver file for NS projection
receiversgc.xy       c: Output receiver file for GC projection
```

The first entry sets the option of whether or not to produce source and receiver files for plotting with GMT. The second two entries correspond to the source and receiver input files used by **fm3d**, which contain all of the necessary location information. The following block of 8 files lists the output source and receiver files in GMT format for the four different projections (same as for the ray projections).

The next block of parameters set the slice parameters:

```
ccccccccccccccccccccccccccccccccccccccccccccccc
c Slice parameters
ccccccccccccccccccccccccccccccccccccccccccccccc
1                    c: Extract depth slice? (0=no, 1=yes)
-1.0                 c: Depth of slice (km)
bounddp.gmt          c: GMT plotting bounds for depth slice
contint.d            c: GMT depth contouring file
1                    c: Extract N-S slice? (0=no, 1=yes)
244.90               c: Longitude of slice (degrees)
boundns.gmt          c: GMT plotting bounds for N-S slice
1                    c: Extract E-W slice? (0=no, 1=yes)
36.25                c: Latitude of slice (degrees)
boundew.gmt          c: GMT plotting bounds for E-W slice
1                    c: Extract great circle slice? (0=no,1=yes)
36.30 244.75         c: Lat,Long of first GC point
36.10 245.15         c: Lat,Long of second GC point
boundgc.gmt          c: GMT plotting bounds for great circle slice
```

There are four separate sets of specifications relating to depth, east-west, north-south and great circle slices. The first slice option specifies whether or not to take a depth slice (i.e. a horizontal section). The depth of this slice then needs to be specified (here, negative values are below the surface). The next entry, bounddp.gmt is the name of an output file containing the plotting boundaries that are needed by GMT. These values will automatically be read into the scripts provided. The final entry for the depth slice is the name of an output contour file that contains the value of the depth slice. This will be used by GMT to contour any interface that passes through this depth.

The next set of parameters relate to taking a north-south slice (in which case the longitude of the slice is specified) and an east-west slice (in which case the latitude of the slice is specified). The final four entries specify the great circle slice, which can be taken between any two points in the model region. Thus, two sets of latitude and longitude coordinates are required. Note that if two points of common longitude are chosen, then the resulting slice will be equivalent to a north-south slice, which is also a great-circle slice. However, if two points of common latitude are chosen, then the great circle slice will not be equivalent (except at the equator) to an east-west slice, which is a slice of common latitude. It is also important to note that the manner in which ray paths and points (sources and receivers) are projected onto the great circle slice differ from the way in which they are projected onto the north-south slice. In the latter case, points are projected back along lines of constant latitude, and in the former case, points are projected back along great circle paths to the nearest point on the slice. As a result, it is not often the case that great circle slices should exactly resemble north-south or east-west slices.

Following on from setting the slice parameters, the next step is to set the resolution of the plotted velocity grid:

```
ccccccccccccccccccccccccccccccccccccccccccccccc
c Velocity grid parameters
ccccccccccccccccccccccccccccccccccccccccccccccc
1                c: 0=absolute, 1=relative velocity
10     10        c: Dicing in theta,phi
```

```
grid2dvd.z        c: GMT output file for depth slice
10      10        c: Dicing in r,theta
grid2dvns.z       c: GMT output file for N-S slice
10      10        c: Dicing in r,phi
grid2dvew.z       c: GMT output file for E-W slice
300     30        c: Total number of GC points (horizontal, vertical)
grid2dvgc.z       c: GMT output file for great circle slice
```

The first setting indicates whether or not absolute or relative velocities are to be plotted (in the latter case, a reference velocity model must be properly specified in the second entry of the file). This is followed by four sets of options, corresponding to the depth, north-south, east-west and great circle slice. In the first three cases, a dicing factor is set for the two orthogonal coordinates. When GMT plots the velocity variations, a colour contour representation is used, which is composed of a large number of constant colour pixels. Thus, the "smoothness" of the colour variation will depend on the size of the pixels. The dicing settings in the above parameter block determine how many pixels each of the velocity grid cells will be divided into. Here, a velocity grid cell is defined as the area bounded by two pairs of consecutive nodes (in two orthogonal directions) defined in vgrids.in. Thus, in the above case, each horizontal grid cell will be described by 100 pixels. For example, if a velocity model is defined using a grid of 12 by 12 nodes horizontally (not including the cushion nodes), then setting dicing factors to 10 in both θ and ϕ will result in the depth slice being described by a total of $(11 \times 10 + 1)^2 = 12,321$ pixels. Therefore, increasing the size of a dicing factor will result in an increased resolution of the plot in the corresponding direction. The obvious trade-off, however, is that the file size will increase.

For the great circle slice, the total number of pixels in the horizontal and vertical directions must instead be specified. This is because the great circle can span the region between any arbitrary pair of points that lie within the model. In the above case, the great circle slice will be described by a total of $300 \times 30 = 9,000$ pixels. In addition to the dicing factor, the name of the output GMT grid file (.z file in ASCII format) must be specified for each of the slices. These files will then be converted to binary .grd files by the GMT scripts provided.

The second last block of parameters simply specifies the output names of the interface

line files corresponding to each of the three vertical slices (north-south, east-west, and great-circle). These files enable the interfaces to be explicitly superimposed on top of the velocity cross-sections. In the generic input file, these files are names as followed:

```
ccccccccccccccccccccccccccccccccccccccccccccccc
c Interface grid parameters
ccccccccccccccccccccccccccccccccccccccccccccccc
intns.xy              c: GMT output file for N-S slice
intew.xy              c: GMT output file for E-W slice
intgc.xy              c: GMT output file for GC slice
```

The final block of parameters are related to contour plots of specific interface surfaces:

```
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c Set parameters for contour plots of interfaces
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
0                     c: 0=absolute, 1=relative depth
1                     c: Number of interfaces to plot
10      10            c: Dicing in theta,phi
boundsint.gmt         c: GMT plotting bounds for surface
2                     c: ID of first interface to plot
gridint1.z            c: GMT output file
2                     c: ID of second interface to plot
gridint2.z            c: GMT output file
```

The first entry determines whether you want to plot the absolute or relative depths of the interfaces (in the latter case, the interfacesref.in file specified near the beginning of the input file must point to the appropriate reference interface depths). The second entry indicates how many separate GMT interface files are to be generated. The plotting script

provided can only plot one interface at a time. If you decide to generate more than one of these files, then you will need to edit this script (called **plotint**) in order to select which interface to visualize. The third entry specifies the dicing factor that is used to pixelate the interface. This works in a way that is exactly analogous to the velocity case. The fourth entry is the output GMT plotting bounds file which is used by the corresponding GMT script to set the dimensions of the plotting box. The number of entries that follow depends on the number of interfaces you have decided to generate for plotting purposes. For each entry pair, you need to specify the ID of the interface to be plotted (1 = top interface, $m + 1$ = bottom interface in a model with m layers), and the corresponding GMT ASCII grid filename.

Once you have set up the gmtslice.in file, you simply need to execute **gmtslice** in the same directory to generate all of the GMT output files.

8.2 Using the GMT plotting scripts

Five generic GMT plotting scripts have been provided in gmtfiles/, and must be executed in the directory that contains all of the output files produced by **gmtslice**. **plotd** will plot a depth slice (horizontal section). Before running this script, make sure that the projection option is correctly set. By default, a Lambert conic projection is used. The output file produced by this script will be called gmtslice.ps. You will need some understanding of shell scripts and GMT to adjust this script to your liking. Note that a colour palette file is also needed as input; you will have to provide this yourself (or modify one of those included with any of the three examples provided with the distribution). By adding and removing the comment command (#) to executables in the script, you can specify which components of the output produced by **gmtslice** will be plotted.

Three of the remaining four scripts, **plotew**, **plotgc**, and **plotns** will generate east-west, great-circle, and north-south slices respectively. By default, the horizontal axis of **plotew** and **plotns** is in degrees; in the case of **plotgc**, it is in km. The final script, **plotint**, produces a contour plot showing the depth variations of a specific interface. All of these scripts have a similar structure to **plotd**, and can be edited in a similar way. Note that all of these files by default generate a postscript file called gmtslice.ps; if you find this confusing or annoying, then simply change the output file name specification in each of the scripts. In order to get a better understanding of how these plotting scripts

can be used, you are advised to closely examine each of the three examples provided.

9 Examples

A set of three examples are provided with the FMTOMO distribution. The first two examples are purely synthetic, but the final example uses observational data. Before trying to use the FMTOMO package with your own data, you are strongly advised to examine these examples and test whether your compilation of the code produces the correct output.

9.1 Example 1: Hypocenter relocation

.

All the files relating to Example 1 can be found in the subdirectory example1/. This is a relatively straightforward application of the FMTOMO package which attempts to relocate five local earthquakes in the presence of significant lateral variations in structure. Example 1 corresponds to the Earthquake relocation application presented in the following paper:

- Rawlinson, N., de Kool, M. and Sambridge, M., 2006. Seismic wavefront tracking in 3-D heterogeneous media: applications with multiple data classes. *Explor. Geophys.,* **37,** 322-330.

You should be able to recreate the plots in Figure 6 of this paper using the input files provided.

If you enter the example1/ directory, you should be able to execute **tomo3d** without needing to edit anything. With its current settings, **tomo3d** will perform six inversion iterations, and should end up correctly relocating the five sources into a cross configuration within a plane of constant latitude (see Figure 6 in this document). Note that the locations will not be *exactly* the same as in Figure 6 of the paper. This is because the propgrid.in file has been modified to make the example run faster. Originally, the last line of the the propgrid.in file was set to [5 10]; in other words, the refined grid about each source contained 10^6 grid nodes. This setting produced the result that you can see in Figure 6 of the paper. In the propgrid.in file provided, the last line now reads [5 5], which means that the refined source grid now only contains 125,000 points. Although traveltime accuracy

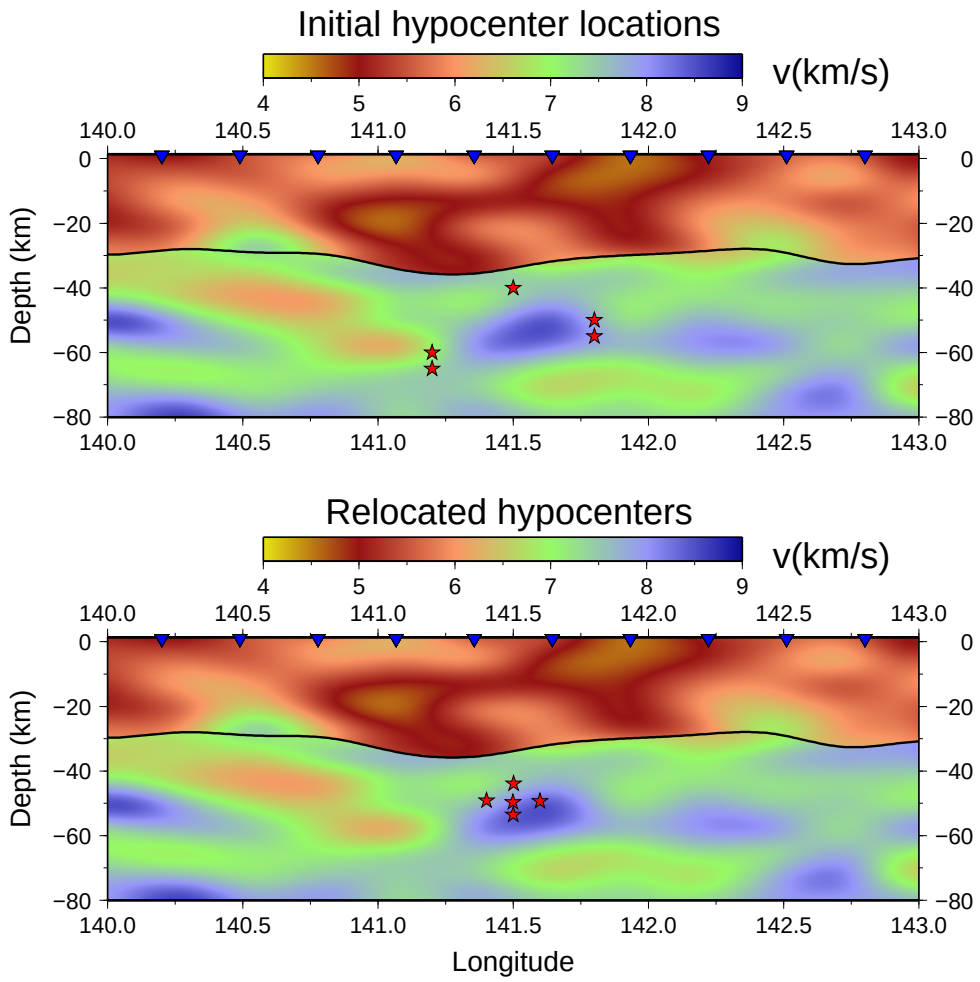


Figure 6: East-west cross-sections showing the projected locations of the five hypocenters for the initial model (top) and the final model (bottom).

will now be decreased, the computing time is much improved. With the smaller refined grid, the computing time of **tomo3d** on a Linux workstation with a 1.6 GHz AMD Opteron CPU is about 3 minutes. This compares to 15 minutes when the larger source grid is used. Comparison of Figure 6 in this document with Figure 6 of the paper shows that the increased accuracy of the relocation in the latter case is barely detectable, and does not really justify the additional computing time.

When **tomo3d** is successfully completed, you should get the following information written to screen:

```
Due to redundancy, the subspace dimension
is being reduced from          20 to          15
```

```
Message from SVD orthogonalization algorithm
PROGRAM invert successfully completed!!
Due to redundancy, the subspace dimension
is being reduced from           20 to           15
Message from SVD orthogonalization algorithm
PROGRAM invert successfully completed!!
Due to redundancy, the subspace dimension
is being reduced from           20 to           15
Message from SVD orthogonalization algorithm
PROGRAM invert successfully completed!!
Due to redundancy, the subspace dimension
is being reduced from           20 to           15
Message from SVD orthogonalization algorithm
PROGRAM invert successfully completed!!
Due to redundancy, the subspace dimension
is being reduced from           20 to           15
Message from SVD orthogonalization algorithm
PROGRAM invert successfully completed!!
Due to redundancy, the subspace dimension
is being reduced from           20 to           15
Message from SVD orthogonalization algorithm
PROGRAM invert successfully completed!!
```

The residuals.dat file should contain the following list of numbers (allow for some slight variation due to the use of different machine architecture and compilers):

```
2174.77    4.73971    472.96066
1052.36    1.10978    110.74583
378.22     0.14335    14.30517
309.36     0.09590    9.57022
312.90     0.09811    9.79057
312.92     0.09812    9.79188
```

```
311.69        0.09736        9.71515
```

Thus, the RMS traveltime residual (left column) has been reduced from 2.1 seconds to 0.3 seconds. Increasing the density of the propagation grid and the size of the refined source grid will reduce the final number, but even with no traveltime error, the residual is unlikely to reduce to zero.

The file stimes.dat contains the origin time perturbations associated with each of the five sources. This should read:

```
5
-0.2874952
-0.2921612
-0.2727162
-0.3408791
-0.3534153
```

The origin time of all sources was perturbed by +0.25 s using the program **synthdata**. Thus, if the relocation of each source was perfect in time, then each entry of stimes.dat should read −0.25 s. Again, increasing the density of the propagation grid will improve the accuracy of these times slightly.

The synthetic model and traveltime dataset used in this example was generated using the input files contained in example1/mkmodel. The 3-D heterogeneous model is based on the grid3dg.in file, and the source and receiver files are based on the moddata.in file. The array of 100 receivers was generated using **arraygen** with the arraygen.in file provided. In order to obtain the synthetic traveltime dataset, **fm3d** was run using the true source locations in the presence of the 3-D velocity model. **synthdata** was then executed using the synthdata.in file to produce otimes.dat. The sourcesle.in file specifies the true source locations. The sources.in file produced by moddata was then copied to sourcestrue.in in example1/. The sourcesref.in file was created by simply perturbing the source locations in sourcestrue.in.

The subdirectory example1/gmtplot/ contains the files needed to produce slices through the 3-D model using GMT. If you execute **gmtslice** in this directory, you will produce

all of the necessary GMT input files for plotting various sections, based on the values provided in gmtslice.in. Try editing and executing several of the plotting scripts to see if you can reproduce the plots contained in Figure 6 of the paper.

9.2 Example 2: Inversion for interface and velocity structure

All of the necessary input files relating to Example 2 can be found in the subdirectory example2/. In this application, reflection, refraction and teleseismic arrival time residuals are jointly inverted for 3-D velocity and interface structure. As in the previous example, the dataset used for the inversion is purely synthetic. Example 2 corresponds to the "Joint inversion of wide-angle and teleseismic traveltimes" example in the paper:

- Rawlinson, N., de Kool, M. and Sambridge, M., 2006. Seismic wavefront tracking in 3-D heterogeneous media: applications with multiple data classes. *Explor. Geophys.,* **37,** 322-330.

You should be able to recreate the plots in Figure 7 of this paper using the input files provided.

The format of this example is similar to Example 1, which means that you can enter example2/ and execute **tomo3d** without modifying any files. However, note that you now require the machine dependent binary files ak135.hed and ak135.tbl in this directory in order to track the teleseismic phases outside the 3-D model region. These files are produced when you execute **compileall** in the code compilation stage (see Section 2); make sure that you copy them to the example2/ directory prior to executing **tomo3d** in this case. With the tomo.in file provided, six inversion iterations will be performed. The synthetic dataset was generated using a two-layer model (nominally a crust over a mantle half-space), with a higher resolution velocity grid used in the crustal layer. The background velocity within the model varies with depth, but a checkerboard pattern of amplitude 0.8 km/s is added. The interface surface varies in depth between 33 km and 47 km. These lateral perturbations in seismic structure were created using **grid3dg** with the velocity field checkerboard option turned on for both layers, and the random structure generator turned on for interface 2 only. The starting model, described in the files vgridsref.in and interfacesref.in, was created using the same grid3dg.in file, but with the checkerboard and random interface structure options turned off. Note that when

synthdata was used to convert arrivals.in (produced by **fm3d** with the checkerboard model) into otimes.dat, random data noise was not added.

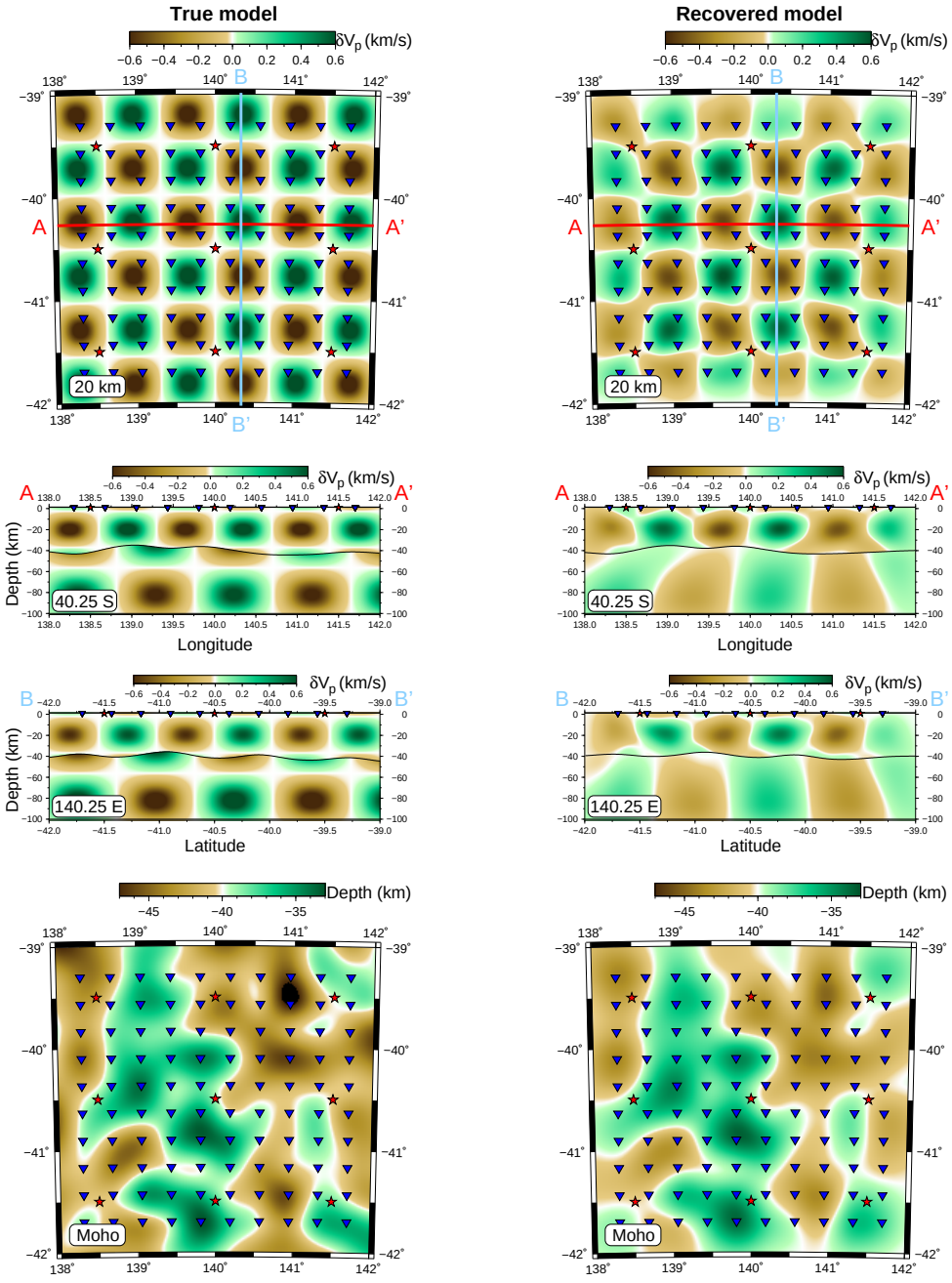


Figure 7: Velocity and interface structure of the synthetic model (left column) and the recovered model (right column), obtained after six iterations of **tomo3d**. Colour contour images of the Moho surface are shown in the bottom plots.

The execution time of **tomo3d** using the default input files provided is 24 minutes on a Linux workstation with a 1.6 GHz AMD Opteron CPU. Note that, like Example 1,

fm3d uses a refined source grid comprising 125,000 points (as defined on the last line of the propgrid.in file), rather than the 1,000,000 points used to produce the results in the paper. It turns out that the improvements in the reconstruction achieved by using the larger source grid are extremely minor, and are not justified by the significant increase in CPU time that is required. Once **tomo3d** has finished, the following output should have been written to screen:

```
PROGRAM invert successfully completed!!
PROGRAM invert successfully completed!!
PROGRAM invert successfully completed!!
PROGRAM invert successfully completed!!
PROGRAM invert successfully completed!!
PROGRAM invert successfully completed!!
```

which indicates that the six iterations have been successfully completed. Unlike Example 1, the SVD algorithm did not have to reduce the number of orthogonal search directions in this case. Three cross-sections through the synthetic and solution model are shown in Figure 7; as you can see, the recovered structure is virtually identical to that of Figure 7 in the paper, despite the use of a smaller source propagation grid. If at any time during the execution of **tomo3d** you wish to examine the progress of **fm3d**, simply open the fm3dlog.out file, which is continually updated.

The residuals.dat file should contain the following list of numbers (allow for some slight variation due to the use of different machine architecture and compilers):

```
363.85      0.13243      13.23832
134.72      0.01816      1.81503
75.96       0.00577      0.57699
53.70       0.00288      0.28837
44.81       0.00201      0.20075
39.48       0.00156      0.15589
35.97       0.00129      0.12937
```

which indicates that the RMS traveltime residual has been reduced from 364 ms to 36 ms. The vertical smearing of the checkerboard pattern that is evident in the upper mantle is unlikely to be reduced by increasing the density of the propagation grid.

Note that both the velocity and interface inversion switches in invert3d.in have been switched on (i.e. set to 1). In the frechgen.in file, the velocity derivative entry has been set to -1, indicating that all velocity parameters will be inverted for. However, the interface derivative entry has been set to 1, indicating that only one interface is to be inverted for. The entry on the line below has been set to 2, which corresponds to interface 2 (the Moho). It is important to understand how this two level hierarchy works when specifying which parameters are to be constrained by the inversion.

The synthetic model and traveltime dataset used in this example are based on the input files contained in example1/mkmodel/. The 3-D heterogeneous model is based on the grid3dg.in file, and the source and receiver files are based on the moddata.in file. **moddata** was used to generate the sources.in and receivers.in file. The input file to this program, moddata.in, reads in two source input files, sourcestele.in and sourceswa.in. The first of these files specifies the teleseismic source locations, and the second specifies the wide-angle source locations. **synthdata** was used to create otimes.dat from the arrivals.dat file produced by **fm3d** when run in forward mode with the synthetic model. The rtimes.dat file, which specifies the traveltimes through the reference model, is used to create the model arrival time residuals for the teleseisms (see invert3d.in).

The subdirectory example2/gmtplot/ contains all of the files necessary to produce slices through the 3-D model using GMT. Simply run **gmtslice** to create the GMT input files, and then execute any of the shell scripts provided (i.e. **plotd**, **plotns**, **plotew**, **plotgc** and **plotint**).

9.3 Example 3: Joint inversion of active and passive source datasets

The final example (see example3/) differs from the previous two in that observational data extracted from seismograms are used, rather than synthetic data. The active source data set comes from the 1995 TASGO project, which involved a large number of air-gun shots fired during a complete circumnavigation of Tasmania (southeast Australia). An array of land-based vertical component seismometers recorded the energy from the shots,

which arrived in the form of various phase types, including Pg, Pn, as well as PmP. The passive source dataset was recorded in 2002 during the TIGGER experiment, which involved the deployment of an array of vertical component short period seismometers in northern Tasmania for a five month period. Approximately 101 teleseismic events with sufficient signal-to-noise ratios to identify global phases such as P, PP, ScP, PKiKP etc. were identified from the continuous recordings. In total, 9692 absolute and relative traveltimes are used to simultaneously constrain the 3-D lithospheric P-wavespeed and Moho geometry beneath northern Tasmania. The full results of this study can be found in the paper (see the docs/ directory):

- Rawlinson, N. and Urvoy, M., 2006. Simultaneous inversion of active and passive source datasets for 3-D seismic structure with application to Tasmania. *Geophys. Res. Lett.,* **33 L24313,** doi:10.1029/2006GL028105.

You should be able to replicate the tomographic images contained in this paper using the input files provided.

As in the previous example, you can construct the solution model by entering example3/ and executing **tomo3d** without modifying any of the files. However, as in Example 2, note that you must copy the machine dependent binary traveltime tables ak135.hed and ak135.tbl into this directory from their default location in sources/inputfiles/ (they are placed there by **compileall**). Compared to Examples 1 and 2, this is a much larger problem, and therefore takes significantly more CPU time to compute. Six iterations on a Linux workstation with a 1.6 GHz AMD Opteron CPU took just over three hours. Note that the solution in the paper uses a refined source grid comprising 1,000,000 points; here, the refined grid only comprises 125,000 points (see the last line of the propgrid.in file). Although this only affects the active source traveltimes, the difference in computing time is still significant. The resulting solution model (see Figure 8) is virtually identical to that produced in the paper (see Figure 3 of the GRL article), so the additional computation times required by the larger source grid is not really warranted.

When **tomo3d** is executed, the full screen output that should eventually appear is as follows:

```
PROGRAM invert successfully completed!!
PROGRAM invert successfully completed!!
```

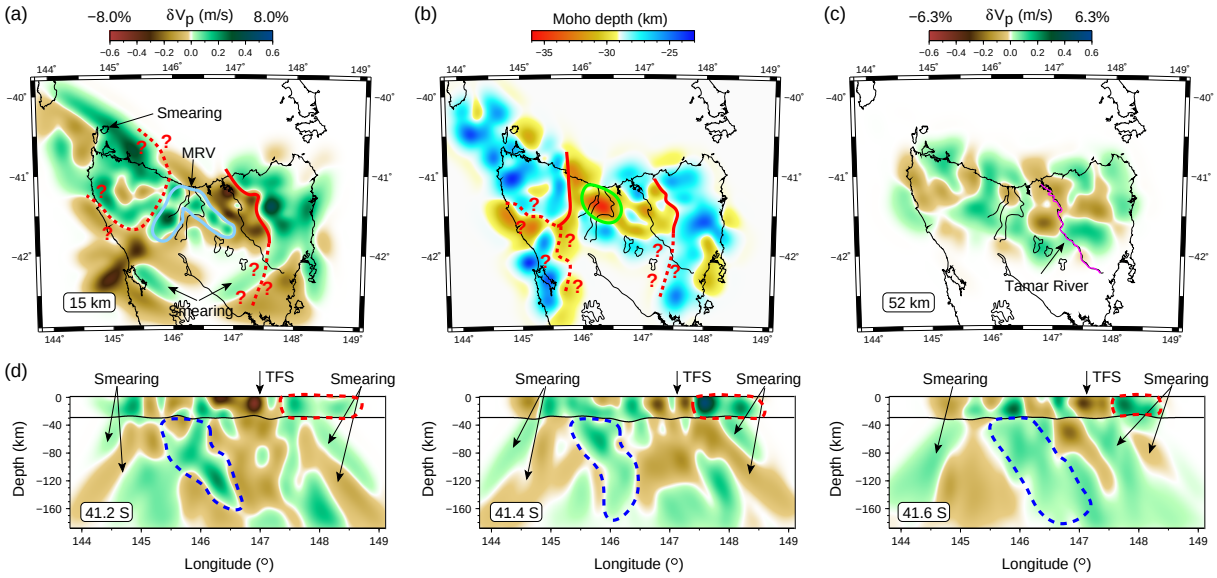


Figure 8: Summary of Tasmania tomography results. (a) Crustal section at 15 km depth; (b) Moho structure; (c) mantle section at 52 km depth; (d) three east-west cross-sections. TFS = Tamar Fracture System; MRV = Mt. Read Volcanics.

PROGRAM invert successfully completed!!
PROGRAM invert successfully completed!!
PROGRAM invert successfully completed!!
PROGRAM invert successfully completed!!

which indicates that six iterations of the inversion routine has been completed. All basis vectors used in the 20-D subspace inversion scheme are linearly independent, so the SVD orthogonalization algorithm does not need to dynamically reduce the size of the subspace (cf. Example 1). The traveltime residuals as a function of iteration number are summarized in the file residuals.dat, which should contain something like:

297.27	0.08838	13.49418
185.65	0.03447	4.53093
158.23	0.02504	3.34427
148.66	0.02210	2.99040
145.15	0.02107	2.86967
142.13	0.02020	2.78905

141.70 0.02008 2.75926

This indicates that the RMS traveltime residual has been reduced from an initial value of 297 ms to a final value of 142 ms (representing a 77% variance reduction, as computed from the second column). The final column lists the χ^2 value associated with each model. Unless you really want to visualize the ray paths, it is not advisable to switch this option on in mode_set.in, because the resulting output file is several hundred Mb in size.

Note that both the invert3d.in file and the frechgen.in file are used to specify which parameters are constrained in the inversion; in this case, both velocity layers and the Moho structure are inverted for. The "Remove mean from predicted teleseisms" option has been set to 0 in invert3d.in. To be consistent with the observed relative arrival time residuals, this switch really should be set to 1. However, for this particular problem, doing so results in the inversion diverging for some reason. It is not clear why this happens, but since the initial model essentially represents the laterally averaged solution model, this inconsistency is not serious.

Unlike Example 2, which also used teleseisms, reference teleseismic traveltimes (which are used to compute model traveltime residuals) are not computed using rtimes.dat. This is because the observed residuals in otimes.dat include a component due to elevation (i.e. the observed residuals have not been corrected for elevation). Therefore, in order to properly compare otimes.dat and mtimes.dat, the arrival time residuals in mtimes.dat must also contain a component due to elevation. This is achieved by running **fm3d** with the reference model, and setting all receiver elevations to zero (this is the file called receiversnec.dat). The arrivals.dat file that was produced has been copied to rtimesnec.dat, which then becomes the reference traveltime file. If you open invert3d.in and residuals.in, you will see that rtimesnec.dat is used in place of rtimes.dat.

The reference model used in this application was generated using the grid3dg.in file located in example3/mkmodel/. Note that an external 1-D crustal model (crust.vel) and a modified ak135 model (ak135modified.vel) are used to describe the crust and upper mantle velocities respectively. Since we are now dealing with observational data, the program **obsdata** is used to generate the sources.in, receivers.in and otimes.dat file. All of the traveltime pick files are located in the subdirectory picks. Note that the formats of the sourcestele.in and sourceswa.in file are quite different to the equivalent files in the previous

example.

The subdirectory example3/gmtplot/ contains all of the files required to produce slices through the solution model using GMT. Simply run **gmtslice** to convert FMTOMO output to GMT input, and you will be able to execute the plotting scripts provided (**plotd, plotew, plotns, plotgc** and **plotint**) to generate postscript output (i.e. the file gmtslice.ps).

10 FAQs

1. **Q.** *How can I optimize the speed of the tomographic inversion?*

   A. The key to getting the maximum performance from the code is to specify the coarsest propagation grid spacing that still produces traveltimes with sufficient accuracy. This is because the traveltime prediction step is much slower than the inversion step, and FMM scales as O(NlogN), where N is the total number of points on the computational grid. Therefore, if you halve the propagation grid spacing, the computing time will increase by a factor of at least 8. The size and density of the refined propagation grid that is used in the source neighbourhood is also a crucial consideration. The refinement level parameter (κ) and grid cell spanning parameter (τ), contained in the last line of propgrid.in, should be chosen carefully. Remember that the total number of refined grid nodes is equal to $(\kappa \times \tau \times 2)^3$. For example, if $\kappa = \tau = 5$, then the total number of refined nodes is already 125,000.

   One approach for finding the optimum size of the propagation grid is to begin by making it very coarse, and then gradually refining it until the inversion solution doesn't change significantly. At this stage, there is little point in increasing the accuracy of the traveltime predictions.

2. **Q.** *Can hypocenters be relocated into different layers?*

   A: No. This is because the path signature associated with each traveltime must be explicitly specified *a priori*. If a source is relocated to another layer by the gradient-based routine, the original path signature specification will no longer be valid. In future versions of the code, I will try and include a routine that attempts to deal with this limitation by applying some assumptions (e.g. the phase can only transmit through an interface).

3. **Q.** *Does FMTOMO include a routine for performing fully non-linear earthquake relocation?*

   A: No. However, you can edit mode_set.in so that **fm3d** generates the traveltime grid associated with all or a subset of sources. In theory, you could apply any non-linear optimization routine to search these grids and relocate the source.

4. **Q.** *Can FMTOMO be used for global tomography?*

   A: No. Although **fm3d** applies FMM in spherical coordinates, periodicity is not accounted for, nor is the degeneration of the coordinate system at the poles. In addition, no correction is made for the true ellipsoid shape of the Earth. One could make make an *a posteriori* correction for Earth flattening, however. FMTOMO is currently best used for local and regional problems.

5. **Q.** *Can FMTOMO be used to solve problems in 2-D or 2.5D?*

   A: FMTOMO requires the input model to have a finite span in all three orthogonal dimensions. Therefore, it cannot operate in 2-D space. 2.5D models, which exist in three spatial dimensions but only have structure varying in two dimensions, also cannot be inverted for. This is because cubic B-splines require at least four nodes in any dimension. However, if you only specified four nodes in one of the dimensions, then the resulting model may well be pseudo 2.5D, as the structure in this direction would probably not change very much.

6. **Q.** *I want to describe a model that is very detailed near the surface (e.g. sediment layers), but becomes coarser at greater depths (e.g. the upper mantle). Can FMTOMO deal with this kind of situation?*

   A: It can to some extent. The parameterization allows velocity grids of different resolutions to be specified for each layer; therefore, you could allow fine detail in one layer, and only coarse detail in another. However, the horizontal grid spacings of all layer boundaries must be identical, so this does not extend to interface geometry. In addition, the propagation grid must be regular, so it may be that the high resolution velocity layer gets undersampled, which will result in traveltime predictions becoming less accurate.

7. **Q.** *Will teleseismic wavefronts pass through the side of the model if necessary?*

   A: Yes, but take care with your specification of path signature to make sure that

no inconsistencies occur.

8. **Q.** *Will new features be added to the code in future?*

   A. To begin with, I will try to fix any obvious bugs. In the longer term, I hope to include the ability to jointly invert P and S traveltimes for V_p/V_s ratio or bulk sound and shear moduli. Other suggestions for additional features would be welcome.