NoLiMit MATLAB package v1.0

Non-Linear Bayesian partition Modeling of the Earth's Mantle Transition zone

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Preamble

This release is associated with the accepted publication Waszek L., Tauzin B., Schmerr N., Ballmer M., Afonso J.C. A poorly mixed mantle transition zone and its thermal state inferred from seismic waves. Nature Geoscience. 2021.

This version of the NoLimit software package allows prediction of synthetic seismic waveforms for SS and PP-precursors from mineral physics models, as well as their processing for reconstructing the surface of seismic boundaries associated with major mineralogical phase transitions in the Earth's mantle (the 410-km and 660-km depth discontinuities).

This version of the software is a beta version, simplified compared with the one in the publication. It applies for:

- A fixed mantle composition, which is a mechanical mixture of basalt and harzburgite with a fraction of basalt f=0.2.
- A downsampled catalog of synthetic waveforms for event depths between 0 and 80 km (enough for processing SS and PP precursors).
- Adiabatic temperature gradients with potential temperature Tpot between 1200 and 2100 K.

This version will allow any user to generate synthetic waveforms for any moment tensor, and events within the pre-defined depth interval. A demonstration of this application is obtained by editing and running the script Demo.m in the main folder.

```
>> edit Demo.m
>> Demo
```

For more advanced applications such as changing mantle composition, or generating waveforms for deeper earthquakes, please contact Benoit Tauzin (benoit.tauzin@univ-lyon1.fr) and Lauren Waszek (lauren.waszek@jcu.edu.au).

How to cite this material?

Any use of the datasets or software must also refer to the reference paper: Waszek L., Tauzin B., Schmerr N., Ballmer M., Afonso J.C. A poorly mixed mantle transition zone and its thermal state inferred from seismic waves. Nature Geoscience. 2021.

Software: NoLiMit MATLAB package v1.0. Non-Linear Bayesian partition Modeling of the Earth's Mantle Transition zone. doi: 10.5281/zenodo.5512805.

Datasets: Catalog of synthetic seismic records from mineral physics and travel-time tables from Waszek et al., 2021, Nature Geoscience. doi: 10.5281/zenodo.5512035.

1. Downloading the codes and databases

The codes are available from https://zenodo.org/record/5512805.

The database is available from https://zenodo.org/record/5512035.

2. Editing the paths on your local file system

After downloading the Matlab package and datasets, edit the **Demo.m** script for modification of the paths towards the directories for the catalog of synthetic seismograms and pre-computed tables of travel-times.

```
%% PATH FOR DATABASE
%
%   EDIT PATH_DATABASE AND PATH_TT TO ACCOUNT FOR YOUR LOCAL SYSTEM
%                               SET-UP
%
global PATH_DATABASE
global PATH_TT

% PATH TOWARDS CATALOG OF SYNTHETICS
PATH_DATABASE='/Volumes/NOLIMIT2b/Light/';

% PATH TOWARDS PRE-COMPUTED TABLES OF TRAVEL-TIMES
PATH_TT='/Volumes/NOLIMIT2b/Light/TTimes/';
```

3. What and where are the important codes?

Codes are contained into the directory "Codes" and sub-directory "./Codes/support".

```
addpath('./Codes')
addpath('./Codes/support')
addpath('./Palettes')
```

```
>> ls Codes/
AdaptiveStacking.m              DataBase_ExtractSyntModel.m     support
AdaptiveStacking_Stat.m         DataBase_readEVT.m
DataBase_ExtractSismogram.m     Param_Build.m
```

```
>> ls Codes/support/
Extract_coeff_MT.m   scaleMT.m    sort_tab.m            voronoisphere.m
myhrv2ar.m           sdr2hrv.m    vcell_solidangle.m
```

There are 3 important Matlab scripts for this tutorial:

DataBase_ExtractSismogram.m: Extract one or several seismograms for given moment tensors, event depths, distances, azimuths. In this version, the composition parameter needs to be fixed to compo=0.2 and the depth of event edep <= 80 km.

```
function [z, r, t]=DataBase_ExtractSismogram(edep,gcarc,az,MT,comp,compo,temp)
%-----------------------------------------------------------------------
%
%   [z, r, t]=DataBase_ExtractSismogram(edep,gcarc,az,MT,comp,compo,temp)
%
%   edep: depth of earthquake (km)
%   gcarc: epicentral distance (degree)
%   az: azimuth (degree)
%   MT: six component Harvard convention moment tensor
%   comp:   'a' = all three components
%           'z' = vertical
%           'r' = radial
%           't' = transverse
%   compo: composition in terms of basalt fraction between 0.0-1.0 for MM
%           OR 2.0 for EA
%
%   Extract one or several seismograms for given moment tensors, event
%       depths, distances, azimuths.
%
%
```

DataBase_ExtractSyntModel.m: Extract portions of signals for the specified seismic phase and a given list of event depths, distances, azimuths and moment tensors. The extraction can be done in the time domain or the depth domain. The composition and thermal models are given in the structure "model". See the directory ./Models for examples. In this version, the composition needs to be fixed to 0.2 and the depth of event edep <= 80 km.

```
function [trace,blat,blon,dist]=DataBase_ExtractSyntModel(model,...
    edep,gcarc,az,blat,blon,MT,is_depth)
%-----------------------------------------------------------------------
%
% [trace,blat,blon,dist]=DataBase_ExtractSyntModel(model,...
%                             edep,gcarc,az,blat,blon,MT,is_depth)
%
%   model: structure including the geographically referenced
%           thermo-chemical model (see in directory ./Models).
%          This structure also includes the phase to be considered in
%           the field model.ph.
%    edep: depth of earthquake (km)
%   gcarc: epicentral distance (degree)
%      az: azimuth (degree)
%   blat,
%    blon: latitude and longitude of piercing/reflection points
%               at discontinuities
%   MT: six component Harvard convention moment tensor
%   is_depth: time-domain (=0) or depth-domain (=1) signals
%
%
%   Extract portions of signals for the specified seismic phase and a
%       given list of event depths, distances, azimuths and moment tensors.
```

AdaptiveStacking.m: Program that runs the adaptive stacking on synthetic data requested from a user-defined list of events and for a particular type of seismic phase (e.g. S410S, S660S, P410P, P660P). These data are extracted and converted to depth from the catalog of synthetic data with function DataBase_ExtractSyntModel.m. The data is stored in a structure "net".

```
function AdaptiveStacking(model,net,nit)
%--------------------------------------------------------------------------
%   PROGRAM THAT RUNS THE ADATIVE STACKING
%
%   model:  structure with the thermo-chemical model
%   net:    time-to-depth converted data
%   nit:    maximum number of Voronoi-cell parameterization
%
```

More details on the applications of these routines are provided in next section 4. Brief explanations about other routines are given in section 5.

4. A demonstration

After update of the paths for the databases, run Demo.m at the prompt of Matlab.
>> Demo

We provide below a brief explanation of what this Demo code does.

4.1 Vertical seismogram extraction for mechanical mixture (MM)

We define the basalt fraction f (needs to be fixed to 0.2) and Tpot (between 1200 and 2100 K). We provide a 6-component moment tensor (Harvard convention).

```
%% 1.   Vertical seismogram extraction for mechanical mixture (MM),
%       basalt fraction f=0.2, potential temperature Tpot=1600, event depth
%       40 km, epicentral distance 65?


f=0.20;             % BASALT FRACTION - CANNOT BE CHANGED HERE
Tpot=1600;          % POTENTIAL TEMPERATURE BETWEEN 1200 AND 2100 K

% DEFINE A MOMENT TENSOR
mt=[0.2074    0.2026    -0.0048    -0.9711    -0.1181    -0.0321];
```

We call the function **DataBase_ExtractSismogram.m** for an event at 40 km depth, an epicentral distance of 65 degrees, a 45 degrees back-azimuth, to obtain corresponding vertical component seismogram. A band-pass filtering is applied between 5 and 50 s period.

```
% MAKE SEISMOGRAM
z=DataBase_ExtractSismogram(40,65,45,mt,'z',f,Tpot);

% FILTER SEISMOGRAMS
fn=1/(2*z.delta);                    % NYQUIST
[bf,af]=butter(2,[(1/50)/fn (1/5)/fn]);
z.trace=filtfilt(bf,af,double(z.trace));
```

The remaining instructions are for plotting the waveform. The result is shown in Figure 1.

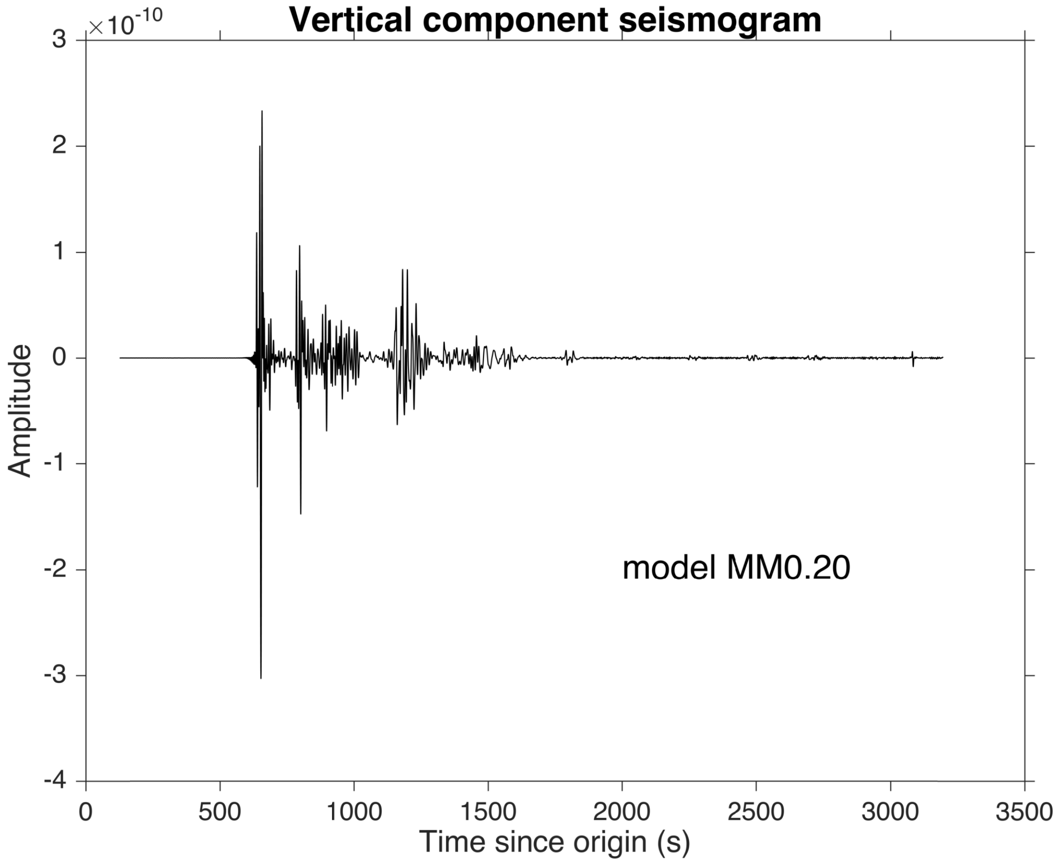

Figure 1. Vertical component seismogram extracted for a mechanical mixture (MM), a basalt fraction f=0.2, a potential temperature Tpot=1600 K, for an event depth 40 km and at 65 degree epicentral distance.

4.2 Vertical-radial-transverse seismograms extraction

A slight modification of the above instructions allows to extract the three components.

```
% MAKE SEISMOGRAM
[z,r,t]=DataBase_ExtractSismogram(40,65,45,mt,'a',f,Tpot);

% FILTER SEISMOGRAMS
```

The result is shown in Figure 2.

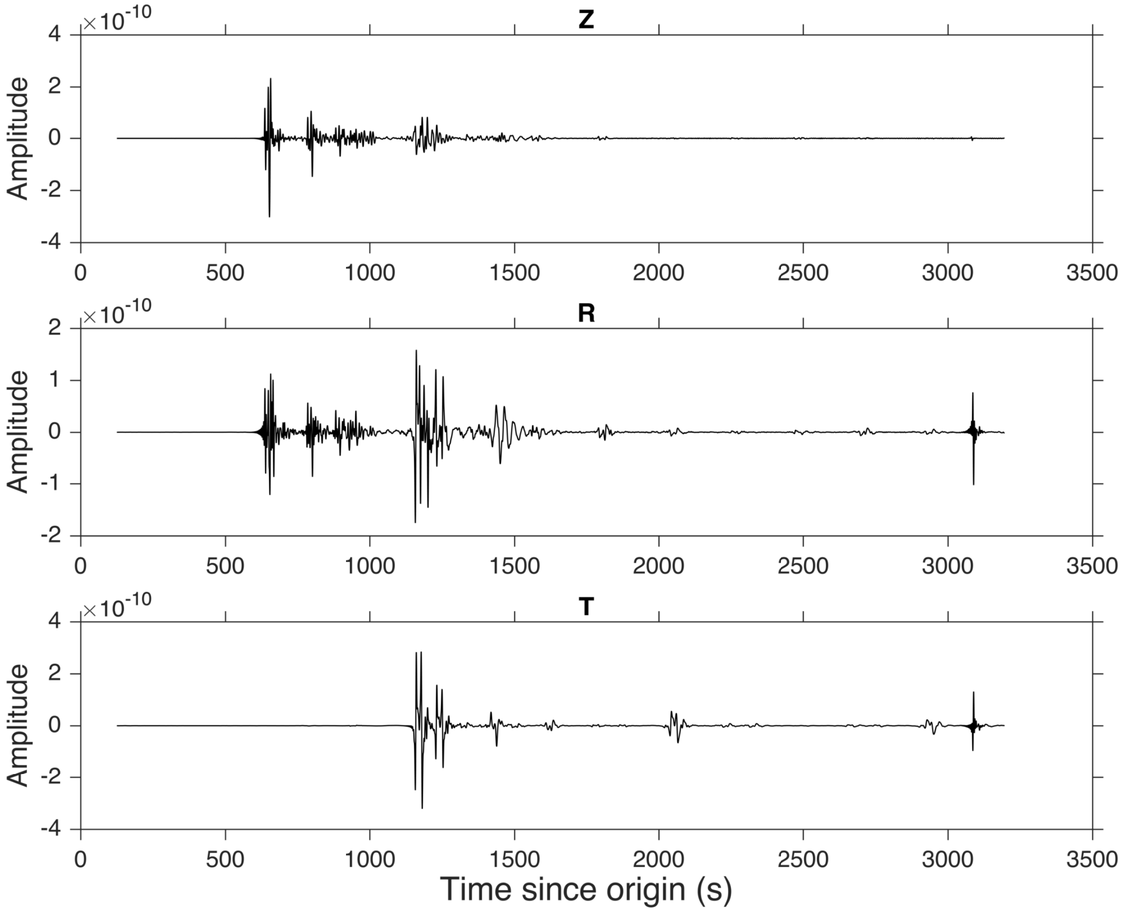

Figure 2. Vertical-radial-transverse component seismograms extracted for a mechanical mixture (MM) of basalt and harzburgite, a basalt fraction f=0.2, a potential temperature Tpot=1600 K, an event depth of 40 km, and an epicentral distance of 65 degrees.

4.3 Vertical and transverse component section extraction

We define the basalt fraction f (needs to be fixed to 0.2) and Tpot (between 1200 and 2100 K). We provide a 6-component moment tensor (Harvard convention).
We call the function **DataBase_ExtractSismogram.m** for an event at 40 km depth and a 45 degrees back-azimuth. We extract this time seismograms for epicentral distances between 80 and 180 degrees with a step of 0.5 degrees. A band-pass filtering is applied between 5 and 50 s period.

The result is shown in Figure 3.

```
%% 3. Vertical and transverse component section extraction for MM f=0.2,
% Tpot=1600, event depth 40 km, epicentral distances 30 to 90? by step of 0.5?

f=0.20;                   % BASALT FRACTION
Tpot=1600;                % POTENTIAL TEMPERATURE

compo=['MM' sprintf('%4.2f',f)];
model=[compo '_' num2str(Tpot)];

%gcarc=[30:0.5:90]';
gcarc=[80:0.5:180]';

% DEFINE A MOMENT TENSOR
mt=[0.2074    0.2026   -0.0048   -0.9711   -0.1181   -0.0321];
mt=repmat(mt,length(gcarc),1);

% MAKE SEISMOGRAM
[z,r,t]=DataBase_ExtractSismogram(40*ones(length(gcarc),1),gcarc,...
    45*ones(length(gcarc),1),mt,'a',0.2,1600);

% FILTER SEISMOGRAMS
fn=1/(2*z(1).delta);                    % NYQUIST
[bf,af]=butter(2,[(1/50)/fn (1/5)/fn]);
for i=1:length(z)
    z(i).trace=filtfilt(bf,af,double(z(i).trace));
end
```

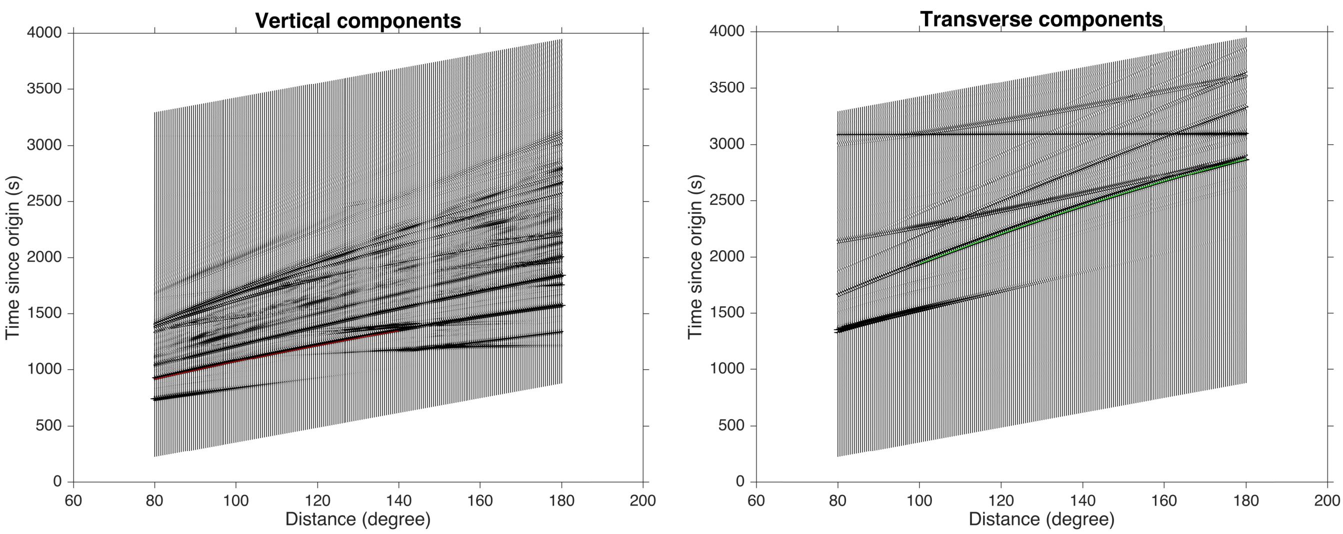

Figure 3. Seismic sections obtained for a MM with f=0.2, Tpot=1600 K, an event depth of 40 km, and epicentral distances between 30 to 90 degrees by step of 0.5 degree. (top) Vertical component. (bottom) Transverse component.

4.4 Load metadata associated with a realistic database

With the purpose of reconstructing a realistic database of SS data, we read a table of metadata from Waszek et al. (2018, 2020). The format of this table is, in column, epicentral distance, reflection point latitude and longitude, azimuth, event depth, strike, dip, slip.

We select information based on epicentral distances (110-160 degrees), and convert the source mechanism provided as fault parameters (strike, dip, slip) into a moment tensor.

```
%% 4. Extract a realistic dabase for SS-precursors

% READ EVT DATABASE
tab=DataBase_readEVT('SdS');
isort=find(tab{1} >= 110 & tab{1} <= 160);
tab=sort_tab(tab,isort);

% MOMENT TENSOR
mt=sdr2hrv(tab{6},tab{7},tab{8});
```

4.5 A thermo-chemical mantle model

The objective is to associate a couple basalt fraction-potential temperature (f, Tpot) to each data in the database. For this we need a model. Two models are provided in the directory ./Models. For the version of the software, the composition needs to be fixed to 0.2. Tpot can be varied between 1200 and 2100 K.

```
%% 5. Load a model of Tpot for the mantle transition zone
load('./Models/model_Mickey.mat');
glon=model.xmin:model.dx:model.xmax;
glat=model.ymin:model.dy:model.ymax;
```

The model is defined in a structure with fields defining the region (xmin:dx:xmax, ymin:dy:ymax), the noise level (nmin-nmax), the list of temperatures and compositions (temp1, compo1), and finally matrices giving the temperature and compositional fields (temp, compo).

An additionnel field is "ph", specifying the seismic phase that serves to reconstruct the mantle structure.

```
>> model
model =

    is_new_param: 1
              ph: 'S410S'
      model_type: 'Mickey'
              dx: 0.5000
              dy: 0.5000
            xmin: -180
            xmax: 180
            ymin: -90
            ymax: 90
            nmin: 0
            nmax: 0.3000
       cell_size: NaN
            lat1: NaN
            lon1: NaN
           temp1: [1000 1100 1200 1300 1400 1500 1600 1700 1800 1900 2000]
          compo1: [0.2000 0.2000 0.2000 0.2000 0.2000 0.2000 0.2000 0.2000 0.2000 0.2000
0.2000]
           temp2: 1000
          compo2: 0.2000
            temp: [361x721 double]
           compo: [361x721 double]
```

A plot of such a thermal model is shown in Figure 4, top left.

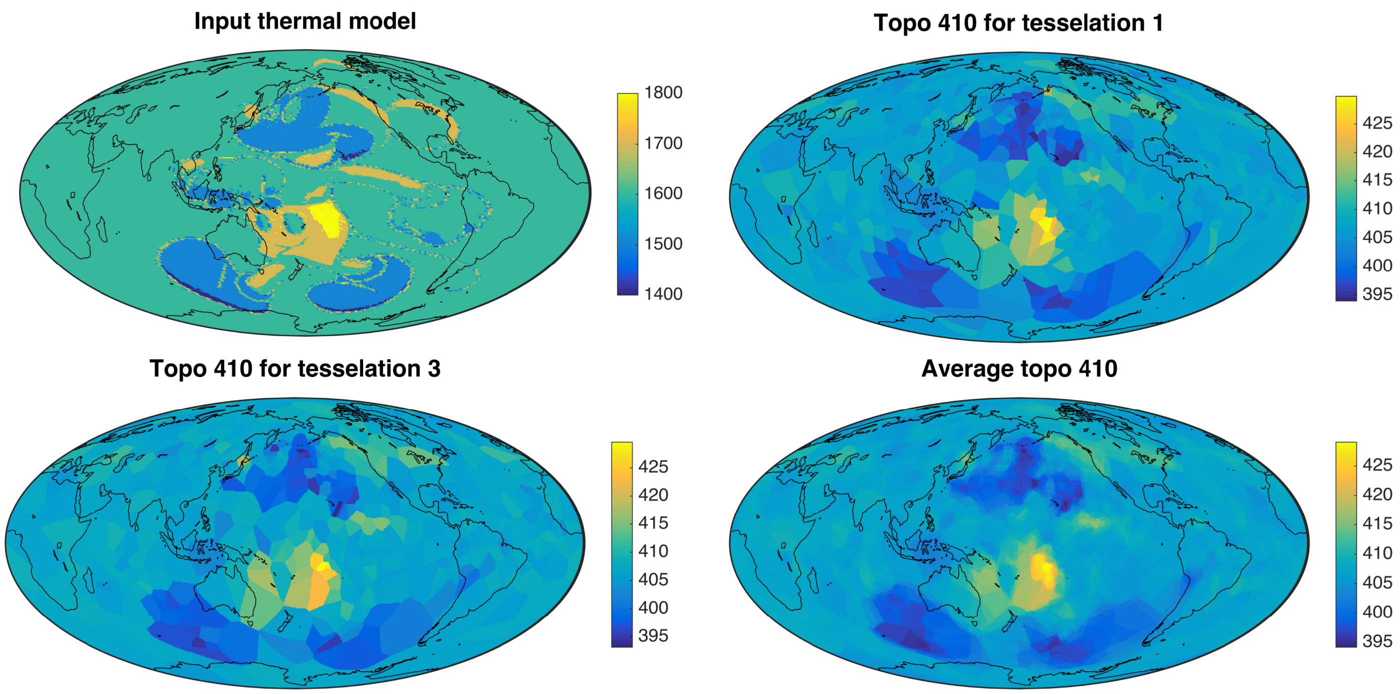

Figure 4. Result of applying the adaptive stacking over SS synthetic data computed for a Mickey Mouse thermal model. (top left) Input thermal model (in Kelvin). (top right) Result in terms of 410 topography (km) for a single parameterization of adaptive stacking (number one). (bottom left) Result for the parameterization number 3. (bottom right) Result after averaging over 5 parameterizations.

4.6 Reconstructing the waveform database

We call the function **DataBase_ExtractSyntModel.m** to reconstruct the waveforms for the data in the database. These waveforms are time-to-depth converted and returned in a structure net with fields trace (waveforms), reflection point latitude, longitude, and epicentral distance.

```
%% 6.  RECONSTRUCT FULL SdS DATABASE
[net.trace,net.plat,net.plon,net.dist]=DataBase_ExtractSyntModel(model,...
    double(tab{5}),tab{1},tab{4},tab{2},tab{3},mt,1);
```

```
>> net

net =

   trace: [1001x45236 double]
    plat: [45236x1 double]
    plon: [45236x1 double]
    dist: [45236x1 double]
```

4.7 Adaptive stacking

```
%% 7. Adaptive stacking for synthetic data
nit=5;                    % number of parameterizations for computing the
                          % statistics
AdaptiveStacking(model,net,nit);
```

We call the function **AdaptiveStacking.m**, to stack the seismograms in Voronoi cells, and implement the optimization of the Earth tessellation. This process is repeated nit times. The resulting parameterizations are saved into the directory ./Param as a Matlab file, with a name param_synt_new_' name_of_the_phase '_' name_of_the_model '.mat'.

```
>> load ./Param/param_synt_new_S410S_Mickey.mat
>> par

par =

      network: 'globe'
         n_it: 5
        n_min: 2000
        n_max: 2000
        nboot: 100
    sigma_max: 10
       z4_min: 300
       z4_max: 460
       z6_min: 600
       z6_max: 750
        x_min: -180
        x_max: 180
        y_min: -90
        y_max: 90
        n_ini: [2000 2000 2000 2000 2000]
        n_fin: [524 543 508 515 527]
            x: {[524x1 double]  [543x1 double]  [508x1 double]  [515x1 double]  [527x1 double]}
            y: {[524x1 double]  [543x1 double]  [508x1 double]  [515x1 double]  [527x1 double]}
           z4: {1x5 cell}
           a4: {1x5 cell}
           z6: {1x5 cell}
           a6: {1x5 cell}
          nss: {[524x1 double]  [543x1 double]  [508x1 double]  [515x1 double]  [527x1 double]}
            d: {[524x1 double]  [543x1 double]  [508x1 double]  [515x1 double]  [527x1 double]}
```

Coordinates of Voronoi cells for each tessellation are given in [par.x{i_it}, par.y{i_it}] with i_it the iteration number (here between 1-5).

The full distributions on the topography are provided in par.z4 for the 410-km discontinuity, and par.z6 for the 660-km discontinuity, with reflection amplitudes in par.a4 and par.a6. For instance,

```
>> par.z4

ans =

    [100x524 double]    [100x543 double]    [100x508 double]    [100x515 double]    [100x527
double]
```

There is one matrix per tessellation, e.g. the first one [100x524 double]. It can be displayed by par.z4{1}. In this case, there are 524 Voronoi cells in this particular tessellation, with for each cell 100 bootstrap samples allowing to obtain a distribution over the topography in the cell.

Topographic maps for the 410-km discontinuity for tessellations numbers 1 and 3 are displayed in Figure 4, top right and bottom left.

4.8 Produce the statistics on the model of topography and reflection amplitude

The statistics in terms of mean and standard deviations are extracted using the function **AdaptiveStacking_stat.m**., which returns a structure with fields latitude (glat), longitude (glon), mean depth of the 410 (m4), error on 410 depth (s4), reflection amplitude (a4), a count of the picked signal among the n_it tessellations, and the measurements for each individual tessellations (m4_it). Similar information is provided for the 660 discontinuity. Finally, an estimate of the average surface for Voronoi cells is provided (field s).

```
%% 8. Extract statistics on measurements from Adaptive Stacking
stat=AdaptiveStacking_Stat(model);
```

```
>> stat

stat =

     glat: [1x361 double]
     glon: [1x721 double]
       m4: [361x721 double]
       s4: [361x721 double]
       a4: [361x721 double]
       c4: [361x721 double]
    m4_it: [361x721x5 double]
       m6: [361x721 double]
       s6: [361x721 double]
       a6: [361x721 double]
       c6: [361x721 double]
    m6_it: [361x721x5 double]
        s: [361x721 double]
```

A topographic map for the 410-km discontinuity from the average over 5 Earth's tessellations is shown in Figure 4, bottom right.

5. Brief explanations about the different functions

AdaptiveStacking.m: Program that runs the adaptive stacking on synthetic data requested from a user-defined list of events and for a particular type of seismic phase.

DataBase_ExtractSyntModel.m: Extract portions of signals for the specified seismic phase and a given list of event depths, distances, azimuths and moment tensors. Extraction can be done in the time or depth domain.

AdaptiveStacking_Stat.m: Program that returns statistics over Voronoi-cell parameterizations.

DataBase_readEVT.m: Read database event file.

DataBase_ExtractSismogram.m: Extract one or several seismograms for given moment tensors, event depths, distances, azimuths.

Param_Build.m: Function that define uniformly randomly located Voronoi cells over the globe and allocate memory for all variables that are used in the adaptive stacking approach.

Extract_coeff_MT.m: Extract coefficients to apply to Green's functions given an azimuth and moment tensor. Formulation from Kikuchi and Kanamori (1991).

scaleMT.m: Scale the moment tensors to be -1 to 1. From Babak Hejrani, ANU.

sort_tab.m: Keep rows with indices in array.

voronoisphere.m: Bruno Luong (2021). Voronoi Sphere (https://www.mathworks.com/matlabcentral/fileexchange/40989-voronoi-sphere), MATLAB Central File Exchange. Retrieved September 15, 2021.

myhrv2ar.m: Convert moment tensor from Harvard from to Aki & Richards form.

sdr2hrv.m: Strike dip slip to Harvard moment tensor.

vcell_solidangle.m: Bruno Luong (2021). Voronoi Sphere (https://www.mathworks.com/matlabcentral/fileexchange/40989-voronoi-sphere), MATLAB Central File Exchange. Retrieved September 15, 2021.