# MANUAL

# SES3D version 1.0

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## 1. INTRODUCTION

## 2. DIRECTORY AND FILE STRUCTURE

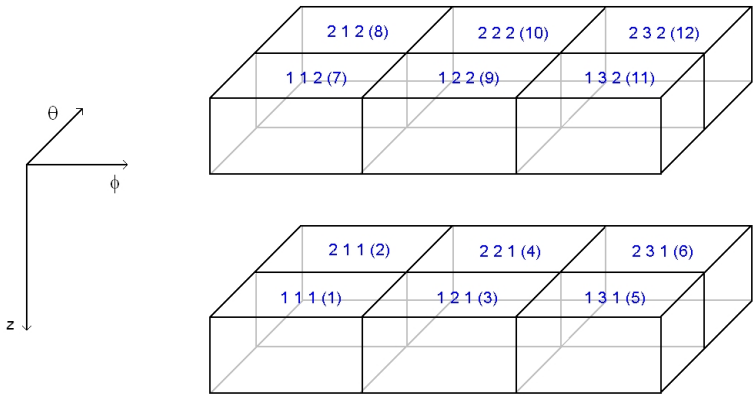
The following table summarises the directory and file structure of the ses3d package. Details on the meaning and functionality of the various files are given in the text. Files that are part of the package itself are underlined and files that are generate by the code are *italic*.

| Directory | Directory | Directory | Files |
|---|---|---|---|
| SES3D_1.0 | MAIN | | |
| | MODELS | | generate_models.f90<br>modules.f90<br>model_parameters<br>stf<br>s_make<br>s_mpirun<br><br>*mu0, mu1, …*<br>*lambda0, lambda1, …*<br>*rhoinv0, rhoinv1, …*<br>*…*<br><br>*logfile0, logfile1, …* |
| | DATA | OUTPUT | |
| | | LOGFILES | |
| | | COORDINATES | |
| | MATLAB | | |

## 3. PARALLELISATION

SES3D is designed to run on parallel computers with several processors. The computational domain, i.e., the spherical section, is subdivided into smaller spherical subsections, as illustrated in the figure below. A single index and an index triplet are used to address each subsection.

During the computation one subsection is assigned to one processor. In each iteration a processor propagates the wave field in its own subsection. Then, the wave field along the boundary between adjacent subsections is interchanged and the next iteration starts.



## 4. MODEL GENERATION

SES3D is a tool for modelling elastic wave propagation through 3D heterogeneous Earth models. The values of the parameters describing the model have to be known at each point of the numerical grid. In an isotropic, non-dissipative medium the model parameters are density (ρ) and the two Lame parameters λ and μ. In a model with viscous dissipation also a set of relaxation times are required. In the case of anisotropy additional elastic parameters are needed as well.

### Programs

The model parameters for each subsection of the spherical section are generated with the program *generate_models*. The source code for *generate_models* is contained in the files *modules.f90* and *generate_models.f90*. Both can be found in the directory *MODELS*. In order to build *generate_models* you need to compile the *.f90 source files. This can be done, for example with the script file *s_make* or with a makefile. You may need to modify *s_make* depending on the available compilers and the setup of your system. Note that *generate_models* already needs to run on the number of processors that you later want to use for the actual wave field propagation. Therefore, a machinefile has to be provided!

You can run *generate_models* by executing the script file *s_mpirun*. Again, *s_mpirun* may need to be adapted depending on your system, the number of processors you wish to use, ... .

### Input

The file *model_parameters* is the only input needed for the model generation. It has the following structure:

```
!- geometrical model parameters for spherical sem ----------------
56                          ! global number of elements in theta (colatitude) direction
42                          ! global number of elements in phi (longitude) direction
14                          ! global number of elements in r direction
6                           ! LAGRANGE polynomial degree
85.0                        ! global minimum theta (colatitude) value [deg]
125.0                       ! global maximum theta (colatitude) value [deg]
135.0                       ! global minimum phi (longitude) values [deg]
165.0                       ! global maximum phi (longitude) value [deg]
5371000                     ! global minimum r value [m]
6371000                     ! global maximum r value [m]
!- physical model parameters -----------------------------------
7                           ! model type (1=homogeneous)
8.0e10                      ! homogeneous mu
1.19e11                     ! homogeneous lambda
3543.25                     ! homogeneous rho
0.0                         ! homogeneous A
0.0                         ! homogeneous B
0.0                         ! homogeneous C
0                           ! is_aniso
0                           ! is_formatted
!- parallelisation ----------------------------------------------
8                           ! processors in theta (latitude) direction
6                           ! processors in phi (longitude) direction
2                           ! processors in r direction
```

The first part of *model_parameters* describes the geometric setup of the model. The total number of elements in each of the coordinate directions is followed by the degree of the Lagrange polynomials used to represent the dynamic fields (displacements and stresses).

Then, the extension of the model is specified. Note that the spherical section must not be close to the poles or the center of the Earth because SES3D uses the natural spherical coordinates. Hence, you may need to rotate your model towards the equator in order to achieve the optimal numerical efficiency.

The second part of *model_parameters* starts with the *model_type*. This variable refers determines the actual Earth model of which we want to generate a discrete version. Currently, there are three Earth models hard wired in *generate_models.f90*:

m*odel_type=1* → homogeneous model with parameters given in *model_parameters*
*model_type=3* → PREM
*model_type=7* → AK135

If you wish to have more complicated Earth models, then you need to modify *generate_models.f90*. Currently, *generate_models* produces only the isotropic and non-dissipative versions of PREM and AK135.

Finally, in the last section of *model_parameters*, the number of subsections (or processors) in each coordinate direction is specified. The product of the three numbers equals the total number of processors – 96 in the example given above.

**Output**

The principal output of *generate_models* are - in the case that we work with an isotropic model without dissipation - the files *rhoinvXX, muXX* and *lambdaXX*, where *XX* denotes the index of a subsection. Each of those files contains the model information for the subsection with the index *XX*.

Information about the geometries of the different subsections is written into the file *boxfile*, which is also a necessary input for the actual wave propagation. Moreover, a logfile is generated for each subsection. The logfiles summarise the work of *generate_models* and may be useful for debugging.

## 5. RUNNING SES3D

The main code of ses3d is located in the directory MAIN. It comprises the following source files:

| **source file** | **description** |
|---|---|
| *ses3d_main.f90* | main program |
| *ses3d_init.f90* | initialise dynamic fields, mass matrix, collocations points and geometry |
| *ses3d_input.f90* | read input: physical model parameters, source and receiver locations |
| *ses3d_evolution.f90* | forward propagation of the wave field, executed once per iteration |
| *ses3d_output* | write output to files |
| *ses3d_comm.f90* | communication between the processors |
| *ses3d_modules.f90* | definitions of parameters and variables |
| *lgll.f90* | evaluation of Lagrange polynomials |

The source files can be compiled using the script *s_make* or a variant of *s_make* that has been adapted to your system. This should generate the executable *main.exe*.

**INPUT**

The most important input file is *Par*, an example of which is given below

```
Simulation parameters
=============================================================
5000                                    ! nt, number of time steps
0.2                                     ! dt in sec, time increment
Source ----------------------------------------------------------------
95.45                                   ! xxs, theta-coord. center of source in
deg
152.26                                  ! yys, phi-coord. center of source in
deg
23400.0                                 ! zzs, source depth in (m)
10                                      ! srctype, 1:f_x, 2:f_y, 3:f_z,
4:expl., 10:M_ij
2.436e18                                ! M_theta_theta
-0.207e18                               ! M_phi_phi
2.643e18                                ! M_r_r
-1.011e18                               ! M_theta_phi
3.293e18                                ! M_theta_r
1.371e18                                ! M_phi_r
MISC------------------------------------------------------------------
100000                                  ! ssamp, snapshot sampling
14                                      ! iplanex, ix for snaps
10                                      ! iplaney, iy for snaps
37                                      ! iplanez, iz for snaps,=izfree for
surface
85.0                                    ! theta_min deg
125.0                                   ! theta_max deg
135.0                                   ! phi_min deg
165.0                                   ! phi_max deg
5371000.0                               ! z_min (m)
6371000.0                               ! z_max (m)
0                                       ! is_aniso
0                                       ! is_diss
0                                       ! is_formatted
OUTPUT DIRECTORY ------------------------------------------------------
../DATA/OUTPUT/
```

The first section of *Par* determines the length of the simulation (*nt*=5000 time steps, in this example) and the length of one time step (*dt*=0.2 s).
In the second section of *Par* the seismic source is specified. The source location is followed by the source type: 1, 2 and 3 are single forces and 10 is a moment tensor source with the moment tensor components specified below.
The third section starts with the parameter *ssamp, iplanex, iplaney* and *iplanex*. Their funcionality is currently disabled. Do not change them. They will become important in future version of ses3d. As in the file *model_parameters*, the geometry of the spherical section must be specified. Make sure that the values are identical to those in *model_parameters*. The parameters *is_aniso* and *is_diss* indicate whether anisotropy and dissipation are included. If you set them to 1 then you need to provide the appropriate input files in the folder MODELS. The functionality of the parameter *is_formatted* is also currently disabled.
Finally, the the output directory has to be specified in the last line of the *Par* file.

Some of the parameters of ses3d are hardwired in the source file *ses3d_modules.f90*. An example for the first lines of *ses3d_modules.f90* is given below. The parameters *nx_max, ny_max, nz_max* specify the maximum number of elements per sub-section (processor) in each of the corrdinate directions. This is followed by the degree of the Lagrange polynomials (*lpd*), the maximum number of iterations (*maxnt*), the maximum number of receivers (*maxnr*) and the width of the perfectly matched layers in elements (*pml*).

The parameter *nrdiss* determines the number of relaxation mechanisms in the case that visco-elastic dissipation is included.

```
module parameters
implicit none

        integer, parameter :: nx_max=7              ! maximum number of elements
in x direction
        integer, parameter :: ny_max=7              ! maximum number of elements
in y direction
        integer, parameter :: nz_max=7              ! maximum number of elements
in z direction

        integer, parameter :: lpd=6           ! LAGRANGE polynomial degree

        integer, parameter :: maxnt=15000         ! maximum number of time
steps
        integer, parameter :: maxnr=20        ! maximum number of receivers
        integer, parameter :: pml=3                 ! number of elements occupied
by the pml

        integer, parameter :: nrdiss=2        ! number of relaxation mechanisms

        real, parameter :: pi=3.1415926535898

end module parameters
```

The file *Par_ad* is important only when ses3d is run is ‘adjoint mode’. You can leave it unchanged if you only do forward modelling.

The positions and the total number of receivers are specified in the *recfile*.

Another important input is the source time function. It can be found in the file *stf* which is located in the folder MODELS.

**OUTPUT**

The most important output are the seismograms recorded at the receivers given in the *recfile*. They can be found in the folder DATA/OUTPUT. There is one file for each sub-section (processor) given that it contains at least one receiver.

Files containing the coordinate lines of each sub-section are written to DATA/COORDINATES.

In the directory DATA/LOGFILES you can can find a logfile for each processor. It documents the execution of ses3d and may be useful for debugging.

The part of the source code responsible for the output is contained in *ses3d_output.f90*. Modify it as you wish in order to output whatever you are interested in.