User Manual for NEXD 2D

Version 0.3

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Chapter 1

Introduction

This manual describes NEXD 2D (**N**odal **D**iscontinuous **G**alerkin Finite **E**lement in **X** **D**imensions) version 0.3. NEXD is a Fortran based implementation of the nodal version of the discontinuous Galerkin approach. It is designed to simulate seismic wave propagation in complex geological structures with general physical properties and is not restricted with regard to the size of the model. The programs are currently designed to work on CPUs, only. GPUs are not supported. To run the code, no programming knowledge is required.

1.1 Supplied programs

The following programs are part of the software package NEXD 2D:

- "mesher": The pre-processor designed to read in specific files related to the mesh (see chapter 3).
- "solver": The main program to simulate the wave-propagation.
- "movie": A post-processor to generate files that show the wave-field at certain time steps.

1.2 Functionality

1.2.1 General features

As of release version v0.3 the following features are included:

- Forward simulation of wave-propagation in elastic, anelastic and poroelastic media
- Wave-propagation across fractures (elastic media only)

Since no restrictions are imposed on size and shape of the media of interest, NEXD can be used in any situation, where the propagation of elastic waves is the key information. It is able to yield the wave field at every time step of propagating waves and the output of simulated receivers. Free surface and absorbing boundary conditions (BC) are implemented. In addition, Perfectly Matched Layers (PML) (Lambrecht et al., 2018) are available to enhance the absorbing BC.

1.2.2 Source time functions

A number of pre-defined source time functions are supported:

- Gauss
- Ricker
- cubed-sine (sin^3)
- an arbitrary discrete wavelet

With sufficient programming knowledge, it is possible to add new wavelet types to the program. Appendix B.1 explains how to do that.

1.2.3 Output

As possible output, the program generates seismograms from the data recorded at the stations placed in the model. Additionally, binary files for desired fields (velocity, displacement or stress) are created according to the parameters set in the parfile (see section 3.1.1 and chapter 4 for details).

1.3 License

NEXD is designed and developed by Lasse Lambrecht, Andre Lamert, Wolfgang Friederich, Thomas Möller and Marc S. Boxberg. NEXD 2D and its components, as well as documentation and some examples, are available under terms of the GNU General Public License (version 3 or higher).

1.4 Citation

Please cite Lambrecht et al. (2018) if you use NEXD. If you use poroelasticity please cite Boxberg et al. (2017) or Boxberg (2019) and if you use the feature to simulate the effect of fractures please cite Möller and Friederich (2019).

Chapter 2

Requirements and Installation

To install and run the software, a number of requirements have to be met.

2.1 Software requirements

To install NEXD the user needs the following software installed on his system:

- GNU Make (`https://www.gnu.org/software/make/`),
- Fortran compiler (GNU Fortran or Intel Fortran). The version 0.3 of this software has been tested using the following compiler versions:
  - Intel Fortran version 19.0.0
  - GNU Fortran version 4.9.2, 6.3.0 and 7.4.0

  Version 0.2 of NEXD 2D also worked with:
  - Intel Fortran version 17.0.4
  - GNU Fortran version 5.4.0 and 7.3.0
- LAPACK libraries (`http://www.netlib.org/lapack/`,
- MPI libraries, e.g. OpenMPI,
- METIS (`http://glaros.dtc.umn.edu/gkhome/metis/metis/overview`, tested with version 4.0.3) for parallel applications,
- a Python installation.

A number of Python scripts are used during the installation of NEXD 2D and as an aid in the creation of input files. To run those, a Python version (recommended 2.7, or 3.6 or higher) is required. A good and easy way to get Python is to install it via the Anaconda distribution, which is available for Windows, Mac and Linux. It can be downloaded under `https://www.anaconda.com/download/`.

2.2 Installation

To install the software, follow these steps:

1. If not yet done, download the source code of the NEXD 2D main package by downloading it from `https://github.com/seismology-RUB/NEXD-2D`.
2. Install all software dependencies.
3. Adjust the software to your system and personal requirements by changing the Makefile appropriately (e.g., change the path to your METIS installation and set your compiler, see code listing 2.2).

4. Compile METIS.

5. Compile NEXD using the command "make all" in your console from your installation directory.

2.3 Changing the Makefile

As mentioned in step three (3) in the instruction on how to run the software, the Makefile needs to be changed at certain position. The following sections need to be adjusted by the user:

```
31 # Choose your compiler:
32 F95 = mpif90
33 #F95 = mpiifort
```

Listing 2.1: Exemplary content of the Makefile.

Change these lines to select the compiler. The default compiler flags are set for optimum performance of the user and need not be adjusted. Recommended flags for developers are given in the comments given in the Makefile. Please review the Makefile for more information.

Please adjust the path to your METIS library specified in the code listing 2.2.

```
294 #  Library paths
295 #  (specify the path to your METIS library here!)
296 #
297 la = -llapack -lblas
298 lib = metis-4.0.3/libmetis.a
```

Listing 2.2: Exemplary content of the Makefile.

2.4 Clean installation directory

Below a clean tree for the installation directory with all sub-folders is shown.

- `NEXD2D installation directory`
  - `doc` Contains all files related to the documentation, including the Latex source files
  - `simulations`
    - `2layer_pml_att`
      - `cubit` Contains the files: 2layer_pml_att.jou, cubit2dg.py and run_cubit.py
      - `data` Contains the files: parfile, source and stations
      - `ref`
        - `att` Contains reference seismograms with attenuation (66 files)
        - `no_att` Contains reference seismograms without attenuation (66 files)
    - `example_linearSlipInterface`
      - `cubit` Contains the files: lsi.jou, cubit2dg.py and run_cubit.py
      - `data` Contains the files: parfile, source, stations, interfaces and fracs
      - `ref`
        - `noPML` Contains reference seismograms with PML (60 files)
        - `withPML` Contains reference seismograms without PML (60 files)
    - `example_poro`
      - `cubit` Contains the files: example_poro.jou, matpropporo, cubit2dg.py and run_cubit.py
      - `data` Contains the files: parfile, source and stations
      - `ref` Contains reference seismograms (178 Files)
      - `tools` Contains Matlab Code to calculate velocities and required element size.
    - `lambs`
      - `cubit` Contains the files: lambs.jou, cubit2dg.py and run_cubit.py
      - `data` Contains the files: parfile, source and stations
      - `ref` Contains reference seismograms and a README (13 Files)
  - `src` Contains all fortran source files
  - `tools`
    - `python` Contains a number of python scripts
    - `scripts` Contains a number of python scripts
  - `LICENSE`
  - `Makefile`
  - `Readme.md`

For the remaining part of the manual the NEXD 2D installation directory will be referred to as `dg2d`.

Chapter 3

Input

There are at least three different parameter files that contain all parameters necessary to run the program. If fractures are to be included in the simulation, two additional files are required. These parameter files are stored in `yourSimulation/data/` and are called:

- parfile - general parameters
- source - parameters regarding the sources
- stations - parameters regarding the receivers

The contents of these files will be explained in detail in subsequent sections.

To run the simulation, a number of other files are required that are generated by the meshing program of the users choice. These files need to be stored in the directory `yourSimulation/cubit/` and are called

- absorb
- coord
- free
- mat
- matprop
- mesh

These files have a specific structure that will be explained for each file in a separate section. For the supplied examples they have been created using a python script called "cubit2dg2d.py" which uses the output from the commercial meshing software Trelis (formerly CUBIT).
If Trelis is not used, the user might have to write a script similar to "cubit2dg2d.py" that creates these files from the output of the meshing software the user uses.

General Advice Prior to discussing the contents of the parameter files some general advice is given to avoid mistakes (especially related to the input format). Parameters that appear as a certain type, e.g. integer, in the parameter files will be read in in the same way. For integers that poses no issue. For floating point numbers (floats) there are a number of formatting options that will all be accepted. For example, 0.01 will be valid if entered in this way, but also if entered 1e-2. For boolean variables, either .false./.true. or F/T are valid. If any type error is detected an error message will be raised containing the affected parameter and the simulation will not run.

3.1 Files in `data`

The first section covers all parameter files that are located in `yourSimulation/data/`.

3.1.1 parfile

This general parameter file contains all general parameters necessary to configure the programs. Here, all relevant features can be enabled/disabled. For convenience specific sections of the parameter file will be discussed separately.

General Parameters

```
1  # Parameter file for 2D NDG software
2
3  # Title of the simulation
4  title                    = Example
5
6  # Choose the way in which the flux is calculated
7  fluxtype                 = 0                  # "0" Pre-calculated flux (only
       ↪  for elastic simulations), "1" existing methods
8
9  # Convenience Parameters
10 log                      = .true.             # "true" if log should be
       ↪ displayed on screen, otherwise "false"
11 debug                    = .false.            # Parameter to enable certain
       ↪ output for debugging purposes
12
13 # Number of Processors
14 nproc                    = 40                 # depending on setup (currently
       ↪  max is 96)
15
16 # Model parameters
17 externalfilename         = cold_flach2.grd    # File containing the external
       ↪ model
18 extvel                   = .false.            # "true" if external velocity
       ↪ model should be loaded, otherwise "false"
```

Listing 3.1: General parameters

The section of the parfile displayed in listing 3.1 shows a number of general parameters.

- **title**: Currently "title" is just used to provide a name for the simulation in the output log files.
- **fluxtype**: This parameter switches between two ways to calculate the numerical fluxes. Option "0" selects the elastic fluxes calculated by Möller (2018) for the slip interface calculations. If these fluxes are selected a warning is raised, if simultaneously attenuation is set to ".true.". Option "1" selects the fluxes implemented by (Lambrecht, 2015). These fluxes do not support the calculation including fractures.
- **log**: Set "true" if the log is to be created/displayed, "false" otherwise.
- **debug**: If set to "true", additional files that are helpful to do debugging are created. This currently only includes files regarding the mesh.
- **nproc**: Defines the number of threads (processors) used in the simulation. The value is specific to the users system configuration. Single core calculations are currently not supported, thus a minimum of 2 should be entered.
- **extvel**: Select if an external velocity model is to be used.
- **externalfilename**: Set the file name of the external velocity model. Must contain the location of the file in relation to `yourSimulation`, or the absolute file path. This parameter is ignored as long as "extvel" is set to "false".

Parameters regarding seismograms

This part of the parfile is displayed in listing 3.2. There are no conflicts to other parameters.

```
20 # Parameters regarding seismograms
21 subsampling_factor      = 1                 # reduce sampling rate of
      ↪ seismograms by this factor to create smaller but less accurate files
22 autoshift               = .false.           # Corrects for the "width" of
      ↪ the used wavelet. For a Ricker or Gaussian the maximum will be at t
      ↪ =0. If set to .false plott0 is used instead.
23 plott0                  = 3e-3              # Offset for the seismogram.
      ↪ Default is 0.
24 div                     = .false.           # "true" if the radial
      ↪ component of the seimogram is to be calculated, otherwise false
25 curl                    = .false.           # "true" if the tangential
      ↪ component of the seimogram is to be calculated, otherwise false
```

Listing 3.2: Parameters regarding seismograms.

- **subsampling_factor**: Can be used to reduce the sampling rate of the seismograms, where sampling_rate = subsampling_factor · dt.
- **autoshift**: Corrects for the "width" of the used wavelet. For a Ricker or Gaussian the maximum will be at t=0. If set to .false. plott0 is used instead.
- **autodt**: Offset for the seismogram.
- **div**: "true" if the radial component of the seimogram is to be calculated, otherwise "false".
- **curl**: "true" if the tangential component of the seimogram is to be calculated, otherwise "false".

Fracture parameters

This part of the parfile is displayed in listing 3.3. These parameters influence if and how the influence of fractures is created. For a detailed description on the theory behind these calculations, the interested user is referred to Möller (2018).

```
26
27 # Fracture parameters
28 lsi                     = .false.           # "true" if the fracture
      ↪ influence is to be calculated, otherwise "false"
29 normal                  = .true.            # Jump for P-Waves
30 tangential              = .true.            # Jump for SV-Waves
```

Listing 3.3: Parameters regarding fractures.

- **lsi**: This parameter enables or disables the calculation of the influence of fractures. Enableling this feature requires the additional parameter files "fracs" and "interfaces". Currently this works not for calculation including attenuation.
- **normal**: Enables the calculation of the fracture influence normal to the fracture plane.
- **tangential**: Enables the calculation of the fracture influence parallel to the fracture plane.

```
32 # Movie parameters
33 movie                    = .true.          # if "true" the a movie is
       ↪ created, otherwise "false"
34 frame                    = 100             # Number of time steps for each
       ↪  frame of the movie
35 save_movie_trimesh       = .true.          # Create files with average in
       ↪ each element
36 save_movie_points        = .false.         # Create files with data for
       ↪ each point
37 save_movie_displacement  = .false.         # Plot displacement field
38 save_movie_velocity      = .true.          # Plot velocity field
39 save_movie_stress        = .false.         # Plot stress field
40 save_movie_p1            = .false.         # Plot pressure of the first
       ↪ fluid
41 save_movie_v1            = .false.         # Plot velocity of the first
       ↪ fluid
42 save_movie_p2            = .false.         # Plot pressure of the second
       ↪ fluid
43 save_movie_v2            = .false.         # Plot velocity of the second
       ↪ fluid
```

Listing 3.4: Movie parameters.

Movie parameters

This part of the parfile is displayed in listing 3.4. These parameters influence the creation of binary files that are used by the program `movie` to generate "vtk"-files (Visualisation Toolkit).

- **movie**: This parameter enables or disables the creation of binary files that can be used to create vtk-files.
- **frame**: This parameter needs to be between 1 and the total number of time steps in the simulation. The parameter defines the number of time steps between individual snapshots for the output.
- **save_movie_trimsh**: Create files with average values for each element. These files take significantly less space but also have a poorer resolution of the wave field.
- **save_movie_points**: Create files with data for points in the mesh. *Warning:* These files take significantly more space and slow down the simulation, but also have a much higher resolution of the wave field.
- **save_movie_displacement**: Enable to plot the displacement field.
- **save_movie_velocity**: Enable to plot the particle velocity field.
- **save_movie_stress**: Enable to plot the stress field.
- **save_movie_p1**: Enable to plot the pressure field of the first fluid (only for poroelasticity).
- **save_movie_v1**: Enable to plot the particle velocity field of the first fluid (only for poroelasticity).
- **save_movie_p2**: Enable to plot the pressure field of the second fluid (only for poroelasticity).
- **save_movie_v2**: Enable to plot the particle velocity field of the first fluid (only for poroelasticity).

```
45 # Parameters for Timeintegration
46 timeint                  = 4                  # which timeintegration?  1:
       ↪ euler 2:rk2 (TVD) 3:rk3 (TVD) 4:rk4 (LSERK)
47 autont                  = .false.            # automatic calculation of
       ↪ number of timesteps based on dt and t_total (if true t_total will be
       ↪ used, if false nt will be used)
48 nt                      = 10000              # Number of timesteps
49 t_total                 = 1.53               # Total simulated time (t_toal
       ↪ = nt*dt)
50 autodt                  = .true.             # automatic calculation of dt
51 dt                      = 0.0                # if autodt =.false. choose dt
       ↪ manually
52 cfl                     = 0.7                # cfl value for dt
53 simt0                   = 0.                 # starting time of simulation
```

Listing 3.5: Parameters regarding time integration

Parameters regarding time integration

This part of the parfile is displayed in listing 3.5. These parameters influence the selection of the method that is used for time integration, the number of time steps and the selection of the time step.

- **timeint**: This parameter selects the method for time integration. Options are:

  1. Euler,
  2. total variation diminishing (TVD) second order Runge-Kutta, rk2 (TVD),
  3. third order TVD Runge-Kutta, rk3 (TVD),
  4. low-storage five-stage fourth order Runge-Kutta, rk4 (LSERK).

  Enter the number to select the appropriate method.

- **autont**: Can be used to automatically calculate the number of timesteps to reach the time specified in t_total.
- **nt**: Select the number of time steps for the simulation. Not used if autont is true.
- **t_total**: Select the total simulated time. Not used if autont is false.
- **autodt**: Automatically calculate the time step based on the Courant-Friedrichs-Lewy (CFL) criterion.
- **dt**: Specify dt different from the automatic one. This parameter is ignored as long as autodt is set to "true".
- **cfl**: Parameter for the CFL stability criterion. Must be $0 < \text{cfl} < 1$.
- **simt0**: Specify the starting time of the simulation.

Parameters regarding PML

This part of the parfile is displayed in listing 3.6. These parameters influence the selection of the method that is used for time integration, the number of time steps and the selection of the time step.

- **set_pml**: Enable PML as absorbing boundary condition. This parameter should only be set "true" if the mesh has been designed with a PML layer (see section A for details).
- **pml_delta**: This parameter describes the thickness of the PML. This parameter assumes a uniform thickness of the PML layer throughout the model. PML layers with non-uniform thickness are currently not supported.

```
55 # pmlparameters
56 set_pml                  = .false.          # if "true" pml are set else
       ↪ absorbing boundary conditions are set
57 pml_delta                = 3.0              # pml thickness
58 pml_rc                   = 0.001            # pml reclection coff
59 pml_kmax                 = 1.0              # pml kmax
60 pml_afac                 = 1.0              # factor for amax
61 use_trigger              = .true.           # use sta_lta trigger for
       ↪ energy monitoring
62 avg_window1              = 10               # lta window
63 avg_window2              = 2                # sta window
64 sta_lta_trigger          = 0.1              # threshold
```

Listing 3.6: Parameters regarding PML

- **pml_rc**: Theoretical reflection coefficient for the PML. Default is 0.01.

The parameters below influence the dampening profile of the PML. It is advised to keep the suggested values.

- **pml_kmax**: Maximum value for the variable k. Values may range between 1 and 20.
- **pml_afac**: Factor for α_{max}.

The following parameters are not directly related to the PML layer. They serve as a control mechanism that ensures that the PML are working properly. It is designed to detect instabilities inside the PML and disables the PML, if necessary. For most cases the parameters for the length of the trigger windows can be left to the default values.

- **use_trigger**: Parameter to enable the STA-LTA trigger.
- **avg_window1**: Size of the window to determine the long term average (LTA).
- **avg_window2**: Size of the window to determine the short term average (STA).
- **sta_lta_trigger**: Threshold for the STA-LTA trigger. Values above this threshold will lead to disabling the PML.

Parameters regarding poroelasticity

This part of the parfile is displayed in listing 3.7. If this is enabeld, the materials are handled as poroelastic media. For a detailed description on the theory behind these calculations, the interested user is referred to Boxberg (2019).

- **poroelastic**: Enable poroelastic media. This requires a special choice of material properties (see section 3.2.3).
- **fluidn**: Number of immiscible fluids (1 or 2).
- **calculate_tortuosity**: If true, the material parameter tortuosity will be calculated according to $T = 1 + r\left(1 - \frac{1}{\varphi}\right)$, where φ is the porosity and r is a geometrical factor that is 0.5 for spheres (see Boxberg, 2019, for more information).
- **extmatprop**: If true, the material file specified at external_material_name will be used, else, matprop will be used.
- **extmatpropfilename**: Path and filename of the external material property file.

```
66 # Poroelasticity
67 poroelastic                = .false.           # Materials are poroelastic if
       ↪ .true. otherwise elastic
68 fluidn                     = 1                 # Number of immiscible fluids (
       ↪ either 1, i.e. saturated, or 2, i.e. unsaturated/saturated by 2
       ↪ fluids)
69 calculate_tortuosity      = .false.           # Tortuosity is calculated
       ↪ according to Berryman (1980): T = 1+r(1-1/phi) (note, that if this is
       ↪  set to .true., in the file porousmaterial r has to be specified
       ↪ instead of T!)
70 extmatprop                 = .true.            # if .true. the material file
       ↪ specified at 'external_material_name' will be used, else, matprop,
       ↪ created by e.g. 'cubit' will be used.
71 extmatpropfilename         = cubit/matpropporo # name of external material
       ↪ file
```

Listing 3.7: Parameters regarding poroelasticity

```
73 # Attenuation
74 attenuation                = .false.           # "true" to enable attenuation
       ↪ otherwise .false.
75 f0_att                     = 400               # Frequency where the model
       ↪ parameters are applied
76 f_max_att                  = 1200              # maximum of frequency band for
       ↪  anelastic modulus
77 att_factor                 = 100               # factor to define minimum
       ↪ frequency, f_min_att=f_max_att/att_factor
```

Listing 3.8: Parameters regarding attenuation

Parameters regarding attenuation

This part of the parfile is displayed in listing 3.8. If enabled, these parameters influence the calculation of the attenuation.

- **attenuation**: Enable calculation of attenuation in the medium. This requires specific values to be set in the `yourSimulation/cubit/matprop/` file (see section 3.2.3).
- **f0_att**: Attenuation is simulated by a number of Maxwell bodies (see Lambrecht (2015) for details) to introduce disperion. This parameter sets the frequency to which the model parameters are assigned.
- **f_max_att**: Defines the upper end of the frequency range for the attenuation.
- **att_factor**: Factor defining the lower end of frequency range for the attenuation by f_min_att = f_max_att / att_factor.

Global parameter for the sources

- **shift_sources**: If true, the sources will be shifted by 1.2/f0, so that the maximum is at t = simt0 + delay + 1.2/f0, otherwise the maximum of the wavelet is at t = simt0 + delay (see section 3.1.2).

Global parameter for the stations

- **rec_angle**: This parameter selects the angle by which **all** stations are rotated. For 0° the receiver points in the positive z-direction and the angle goes anti-clockwise, i.e., for 90° the receiver points in negative x-direction.

```
79 # Sources
80 shift_sources           = .true.            # if .true. then the sources
     ↪ will be shifted by 1.2/f0, otherwise the maximum of the wavelet it at
     ↪  t = simt0 + delay (see source parameter file).
```

Listing 3.9: Sources

```
82 # Receiver
83 global_rec_angle       = .true.            # If .true. the angle given
     ↪ below (rec_angle) will be used for all receivers, otherwise the angle
     ↪  has to be provided for each receiver indepentently in the receiver
     ↪ file.
84 rec_angle              = 0.0               #rotate receivers about dregree
```

Listing 3.10: Receiver angle

3.1.2 source

The example displayed in listing 3.11, shows a typical source parameter file containing one source.

- **nsrc**: This parameter specifies the total number of sources in the model.
- **source**: Number of the current source. If more than one source is in the file, these number must increase sequentially.
- **xsource**: X-coordinate of the source. Needs to be inside the boundary of the model, but not inside the PML (if activated).
- **zsource**: Z-coordinate of the source. Needs to be inside the boundary of the model, but not inside the PML (if activated).
- **delay**: Parameter to specify a time-delay for the activation of the source.
- **sourcetype**: Select what type of source is used. Options are: "0" for a single force solution and "1" for a moment-tensor.
- **stf**: Select the source time function. Currently the following wavelets are available: "1" selects a Gaussian-function, "2" selects a Ricker-wavelet, "3" a cubed-sine function and "4" enables the user to input an arbitrary discrete external wavelet.
- **extwavelet**: Path and filename of an external wavelet. Is only used if option "4" is selected for "stf".
- **f0**: Sets the central frequency of the source wavelet .
- **factor**: Variable to scale the amplitude of the source time function.
- **angle_force**: This parameter is used if a single force solution for the source is used. It sets the direction of the force action. For 0° the source points in the positive z-direction and the angle goes anti-clockwise, i.e., for 90° the source points in negative x-direction.
- **Mxx, Mzz, Mxz**: Components of the moment-tensor, $M = \begin{pmatrix} M_{xx} & M_{xz} \\ M_{xz} & M_{zz} \end{pmatrix}$. Used only for a moment-tensor source (sourcetype = 1).

If an arbitrary defined wavelet is chosen by the user, the file containing the information on the wavelet will have to be designed as follows: Two columns separated by spaces. The first column contains the time and the second column contains the amplitude of the waveform.

```
# List of Source(s)
# Sources should be added sequentially. Otherwise problems will occur when reading the file

# Number of sources
nsrc        = 1         # Total number of sources

# Source 1 - Parameters
source      = 1         # Running Number of the sources
xsource     = 25.       # x-value of the source
zsource     = 10.       # z-value of the source
delay       = 0.0       # time delay for the source
sourcetype  = 0         # Type of source: 1 = Moment tensor, 0 = single force
stf         = 2         # Type of source-time-function: 1 = gauss, 2 = ricker, 3 = sin^3, 4 = external
extwavelet  = data/1MHz0.5in_clean.txt  #file with external wavelet; required if stf = 4
f0          = 400.      # center frequency of stf
factor      = 1e6       # factor of the stf
angle_force = 00.       # angle of the force action in the media
Mxx         = 0.0       # Momenttensor Mxx
Mzz         = 0.0       # Momenttensor Mzz
Mxz         = 1.0       # Momenttensor Mxz
```

Listing 3.11: Typical source file

When selecting the central frequency (f_0) of the source(s) the user has to keep in mind that this frequency directly influences the stability of the simulation, as the maximum length of an element directly depends on f_0. Assuming that 10 grid points per wavelength are sufficient to achieve stability, the maximum edge length, l, for a given frequency is calculated according to

$$l = \frac{v_{min}}{\frac{10}{N} * f_{max}},$$

where v_{min} is the slowest velocity and N is the polynomial order (default is $N = 4$). N can be changed in `src/constants.h`. Afterwards the program has to be compiled again. f_{max} is the maximum frequency selected for the source(s).

3.1.3 stations

This example shown in listing 3.12, shows a typical stations parameter file containing ten stations. If not specificly desired by the user, stations should be placed in model space that is not part of the PML (if enabled).

- **nrec**: This parameter specifies the total number of stations in the model.
- **No xrec zrec**: The first parameter is a running number of the receiver. The other two values represent the x- and z-coordinate of the individual station.

3.1.4 fracs

This is the first parameter file that is added as part of the feature to calculate the influence of fractures on the wave-field. This parameter file specifies the location of one or more fractures and is used if the global parameter "lsi" is enabled. A sample file is displayed in listing 3.13.
The first entry after "BEGIN" gives the total number of fractures to be read in.
Each fracture is defined by the following parameters (from left to right)

```
nrec = 10
001  25.0  50.0
002  25.0  45.0
003  25.0  40.0
004  25.0  35.0
005  25.0  30.0
006  25.0  25.0
007  25.0  20.0
008  25.0  15.0
009  25.0  10.0
010  25.0  5.0
```

Listing 3.12: Typical stations file

```
# This input file defines the start and end points of crack in the medium.
# The first entry is the total number of cracks. Other values are:
# No. | Property index | Start x | Start y | End x | End y
BEGIN
1
001    1    0.0000    25.0    50.0    25.
END
```

Listing 3.13: Parameter file defining the location of fractures

- **No**: Running number of the fracture.
- **Property index**: Indicates the type of interface that creates the fracture. The interface is selected from the selection given in "interfaces". For example: If there are 4 different slip interfaces given in "interfaces" this number may be either 1, 2, 3 or 4.
- **startx, startz**: x and z coordinates of the starting point of the fracture.
- **endx, endz** x and z coordinates of the end point of the fracture.

3.1.5 interfaces

This is the second parameter file that is added as part of the feature to calculate the influence of fractures on the wave-field. This parameter file specifies the properties that can be selected for a fracture via the property index in the previous file. A sample file is displayed in listing 3.14.

```
#-------------------------------------------------------------------
#  Defines interfaces
#  First line: Number of interface types
#  Following lines: specification of interfaces from left to right
#  type (elastic [other interface-types are in development]),
#  thickness of crack [m], Elastic Modulus [GPa], C_N, C_T
#-------------------------------------------------------------------
BEGIN
1
elastic 1.e-3  84.4e9    69959    106776
END
```

Listing 3.14: Parameter file defining fracture properties

The first entry after "BEGIN" gives the total number of properties to be read in.
Each fracture property is defined by the following parameters (from left to right):

- **type**: currently only "elastic", viscoelastic interfaces are under development.
- **thickness (h)**: The thickness of the crack is given in meters, e.g., 1 mm requires something like 1.e-3 as input (0.001 would also work).
- **Elastic modulus**: The elastic modulus is given in Pascal (Pa). Usually, values are in the order of GPa. For example, a value of 45.0 GPa requires 45.e9 as input.
- $\mathbf{C_N}$, $\mathbf{C_T}$: Dimensionless constants that are needed to calculate the relaxation frequency of the interface (see Möller, 2018, for details).

3.2 Files in `cubit`

This section explains the files related to the mesh. These files are designed in a certain way that is expected by NEXD. A script is provided that creates these files from the output of Trelis. If the user does not have Trelis or Cubit installed on his/her system and uses a different meshing software, the output of the used meshing software will have to be converted to match the requirements of NEXD.

3.2.1 coord

```
1       3075
2          1          3.000000          50.000000
3          2          3.000000          25.000000
4          3          3.000000          49.000000
5          4          3.000000          48.000000
```

Listing 3.15: Excerpt from a coord file

This file contains a list that maps the number of a certain node in the mesh to its coordinates. The first entry is the total number of nodes in the mesh. All subsequent lines contain the running number of the nodes, the x-, and the z-coordinate.

Attention: Note that the coordinates referred to as z-coordinates are actually the y-coordinates in the Trelis/Cubit model. This is done with regard to the convention that in seismology the depth axis is always the z-axis.

3.2.2 absorb/free

```
1 151
2 513
3 517
4 518
5 519
```

Listing 3.16: Excerpt from a absorb/free file

These two files are set up identically. These files contain the number associated with the nodes that are used to calculate the simple absorbing BC or free surface BC. The first entry in each file is the total number of nodes contained in this file. Additional lines are added sequentially for each node. An example of the first few lines from such a file is shown in listing 3.16.

3.2.3 matprop

```
1 2
2 1 1 5800.0 3800.0 2600.0 9999.0 9999.0
3 2 1 5800.0 3800.0 2600.0 9999.0 9999.0
```

Listing 3.17: Entries for a matprop file with (visco-)elastic materials

The file in listing 3.17 lists the properties of the (visco-)elastic materials used in the model and the file in listing 3.18 lists the properties of the poroelastic materials. The first entry lists the total number of materials. The subsequent lines contain the following values for (visco-)elastic materials (from left to right):

- Block number (Cubit block)
- Index identifying the whether the material is an elastic material or not.[1]
- Compressional (P-) wave velocity (v_P).
- Shear (S-) wave velocity (v_S).
- Density (ρ).
- Quality factor regarding P-waves (Q_P).
- Quality factor regarding S-waves (Q_S).

The latter two values are related to anelastic calculations and influence attenuation. If attenuation is not selected in the parfile, these values will be irrelevant. If attenuation is selected and a quasi-elastic material is to be part of the simulation, these variables will need to have a high value ($Q = \infty$ for an elastic material). A sample file for an elastic medium is displayed in code listing 3.17.

Attention: This file contains two materials as PML are included in the mesh. If PML are included in the simulation, they are represented by an individual material. See appendix A for more details

```
1 2
2 1 1 3000.0 13560000000.0 30720000000.0 0.3 1e-17 0.7 0.74 1.33e-07 0.099
    ↪ 0.5 2080000.0 0.0 0.055 0.5 40.0 0.0 2.86 0.79 0.0 0.0
3 2 1 2350.0 20000000000.0 15000000000.0 0.3 1e-13 0.7 0.74 1.33e-11 990.0
    ↪ 0.5 20800000000.0 5.4e-5 550.0 0.5 400000.0 2.0e-4 2.86 0.79 0.00
    ↪ 0.00
```

Listing 3.18: Entries for a matprop file with poroelastic materials

The subsequent lines contain the values of material parameters, the first number defines which model is used. The used parameters are:

- Block number (Cubit block)
- rhos = density solid
- lambdaˆu = first Laméparameter (undrained)
- Kˆd = bulk modulus of skeleton (drained)
- mu = shear modulus
- phi = porosity

[1] Currently the value is always 1 as an elastic material is always used. This may change in future releases.

- kappa = permeability
- b = biot coefficient
- 1/T = inverse tortuosity (Note, that this is replaced by r, if 1/T is calculated! See 3.1.1)
- 1/N = inverse of biot modulus
- Ks = bulk modulus of solid grain material
- rho1 = density fluid 1
- S1 = saturation fluid 1
- K1 = bulk modulus fluid 1
- ny1 = viscosity fluid 1 (this is the wetting fluid)
- rho2 = density fluid 2
- S2 = saturation fluid 2
- K2 = bulk modulus fluid 2
- ny2 = viscosity fluid 2 (this is the non-wetting fluid)
- fitting_n, fitting_chi = fitting parameters for van Genuchten model n, chi (see Boxberg, 2019)
- p_b = bubbling pressure
- lambda_BC = fitting parameter for Brooks & Corey model, see (Boxberg, 2019))
- A = capillary pressure coefficient for Douglas Jr. et al. model, see (Boxberg, 2019))
- Sr1 = residual saturation fluid 1
- Sr2 = residual saturation fluid 2

The following nine different combinations are allowed:

- Block number, 1, rhos, lambdaˆu, my, phi, kappa, b, 1/T, 1/N, rho1, S1, K1, ny1, rho2, S2, K2, ny2, fitting_n, fitting_chi, Sr1, Sr2
- Block number, 2, rhos, lambdaˆu, my, phi, kappa, b, 1/T, 1/N, rho1, S1, K1, ny1, rho2, S2, K2, ny2, p_b, lambda_BC, Sr1, Sr2
- Block number, 3, rhos, Kˆd, my, phi, kappa, 0., 1/T, Ks, rho1, S1, K1, ny1, rho2, S2, K2, ny2, fitting_n, fitting_chi, Sr1, Sr2
- Block number, 4, rhos, Kˆd, my, phi, kappa, 0., 1/T, Ks, rho1, S1, K1, ny1, rho2, S2, K2, ny2, p_b, lambda_BC, Sr1, Sr2
- Block number, 5, rhos, Kˆd, my, phi, kappa, 0., 1/T, 1/N, rho1, S1, K1, ny1, rho2, S2, K2, ny2, fitting_n, fitting_chi, Sr1, Sr2
- Block number, 6, rhos, Kˆd, my, phi, kappa, 0., 1/T, 1/N, rho1, S1, K1, ny1, rho2, S2, K2, ny2, p_b, lambda_BC, Sr1, Sr2
- Block number, 7, rhos, lambdaˆu, my, phi, kappa, b, 1/T, 1/N, rho1, S1, K1, ny1, rho2, S2, K2, ny2, A, 0., Sr1, Sr2
- Block number, 8, rhos, Kˆd, my, phi, kappa, 0., 1/T, Ks, rho1, S1, K1, ny1, rho2, S2, K2, ny2, A, 0., Sr1, Sr2
- Block number, 9, rhos, Kˆd, my, phi, kappa, 0., 1/T, 1/N, rho1, S1, K1, ny1, rho2, S2, K2, ny2, A, 0., Sr1, Sr2

Instead of creating this material file, a matpropporo file can be specified (necessary for the Matlab code), which looks slightly different (see 3.19).

```
#-------------------------------------------------------------------------
# Defines porous materials:
#  First line: Number of material types
#  following lines: values of material parameters, the first number defines which model is used.
#  (rhos = density solid; lambda^u = first Lameparameter (undrained); K^d = bulk modulus of skeleton (drained); mu = shear modulus; phi = porosity;
#   kappa = permeability; b = biot coefficient; 1/T = inverse tortuosity (note, that this is replaced by r, if 1/T is calculated!);
#   1/N = inverse of biot modulus; Ks = bulk modulus of solid grain material;
#   rho1 = density fluid 1; S1 = saturation fluid 1; K1 = bulk modulus fluid 1; ny1 = viscosity fluid 1; (this is the wetting fluid)
#   rho2 = density fluid 2; S2 = saturation fluid 2; K2 = bulk modulus fluid 2; ny2 = viscosity fluid 2; (this is the non-wetting fluid)
#   fitting_n, fitting_chi = fitting parameters for van Genuchten model n, chi;
#   p_b = bubbling pressure; lambda_BC = fitting parameter for Brooks & Corey (1964) model);
#   A = capillary pressure coefficient for Douglas Jr. et al. (1993) model);
#   Sr1 = residual saturation fluid 1; Sr2 = residual saturation fluid 2:
# 1, rhos, lambda^u, my, phi, kappa, b,  1/T, 1/N, rho1, S1, K1, ny1, rho2, S2, K2, ny2, fitting_n, fitting_chi, Sr1, Sr2
# 2, rhos, lambda^u, my, phi, kappa, b,  1/T, 1/N, rho1, S1, K1, ny1, rho2, S2, K2, ny2, p_b,       lambda_BC,   Sr1, Sr2
# 3, rhos, K^d,      my, phi, kappa, 0., 1/T, Ks,  rho1, S1, K1, ny1, rho2, S2, K2, ny2, fitting_n, fitting_chi, Sr1, Sr2
# 4, rhos, K^d,      my, phi, kappa, 0., 1/T, Ks,  rho1, S1, K1, ny1, rho2, S2, K2, ny2, p_b,       lambda_BC,   Sr1, Sr2
# 5, rhos, K^d,      my, phi, kappa, 0., 1/T, 1/N, rho1, S1, K1, ny1, rho2, S2, K2, ny2, fitting_n, fitting_chi, Sr1, Sr2
# 6, rhos, K^d,      my, phi, kappa, 0., 1/T, 1/N, rho1, S1, K1, ny1, rho2, S2, K2, ny2, p_b,       lambda_BC,   Sr1, Sr2
# 7, rhos, lambda^u, my, phi, kappa, b,  1/T, 1/N, rho1, S1, K1, ny1, rho2, S2, K2, ny2, A,         0.,          Sr1, Sr2
# 8, rhos, K^d,      my, phi, kappa, 0., 1/T, Ks,  rho1, S1, K1, ny1, rho2, S2, K2, ny2, A,         0.,          Sr1, Sr2
# 9, rhos, K^d,      my, phi, kappa, 0., 1/T, 1/N, rho1, S1, K1, ny1, rho2, S2, K2, ny2, A,         0.,          Sr1, Sr2
#-------------------------------------------------------------------------
BEGIN
2
1 3000.0   13.56e9   30.720e9   0.3   1.0e-17   0.7   0.74   1.33e-7   0.099   0.5   20.8e5   0.0   0.055   0.5   4.0e1   0.0   2.86   0.79   0.00   0.00
1 2350.0   20.0e9   15.0e9   0.3   1.0e-13   0.7   0.74   1.33e-11   990.0   0.5   20.8e9   5.4e-5   550.0   0.5   4.0e5   2.0e-4   2.86   0.79   0.00   0.00
END
```

Listing 3.19: Structure of a matpropporo file

3.2.4 mat

```
1          1          2          1
2          2          2          1
3          3          2          1
4          4          2          1
5          5          2          1
```

Listing 3.20: Excerpt from the mat file

This file maps the material properties from the matprop file to the elements. Each line consists of the running element number, the ID of the block (in the "matprop" file) and an index to tell if the element is part of a PML. The latter index is either "0" if it is part of the regular medium or "1", if it is part of a PML.

3.2.5 mesh

```
1 5948
2          1          1         28          3
3          2         56        106         30
4          3          3         28         57
5          4        109         59        108
```

Listing 3.21: Excerpt from the mesh file

This file contains a mapping that relates the nodes and the material properties to the individual element. The first entry is the total number of elements in the mesh. Afterwards, each line contains the following entries (from left to right):

- Running number of the element
- The numbers of the three nodes that are used to construct the element.

A few lines from a mesh file are shown in code listing 3.21.

Chapter 4

Output

By default, the output of NEXD 2D is stored in a subdirectory to the simulation directory called "out". If the script "process.sh" is used, the parameter files used for the current simulation are copied to the "out" folder for the users convenience. That way, the user is always able to reconstruct what parameters were used to create this simulation.

4.1 Files created by `mesher`

For every simulation, files containing information of parts of the mesh called "meshVar0000001" are created. The number denotes the running number of the processor the file was created for.

If stations are placed in the model, files are created that contain the information on the location of the station, where it is located in the mesh and in which processor the receiver is located. These files are called for example "recVar000013".

If fractures are included, files that map the slip interfaces to their elements called for example "elementToLSI000032" will be created as well.

A number of visualisation files are created. They are listed in table 4.1. In addition to these vtk-files,

Table 4.1: List of vtk-files given as output.

Name	Content
mesh.vtk	triangular mesh
rec.vtk	receiver positions
src.vtk	source positions
rho_model.vtk	density model
vp_model.vtk	p-wave velocity model (if not a poroelastic simulation)
vs_model.vtk	s-wave velocity model (if not a poroelastic simulation)
vmax_model.vtk	maximum wave velocity model (if poroelastic simulation)
vmin_model.vtk	minimum wave velocity model (if poroelastic simulation)

postscript files will be created for each part of the mesh, if "debug" is set to true in the parfile.

4.2 Files created by `solver`

The output from `solver` varies with the parameters selected in the parameter files. Seismograms will be created, if stations are placed in the model and the correct parameters have been set. Binary files to generate visualisations of the wave-field are only generated if the appropriate parameters are set in the "movie" portion of the parameter file (see section 3.1.1).

4.2.1 Seismograms

Seismograms are saved as plain ASCII text files with two columns of data: The first column contains the time-axis and the second column contains the respective data. Three types of data are available: displacement, particle velocity and acceleration. Each type has its own file distinguished by the file name. The file-name is constructed in the following way:

seismo.(component).(number of the station).sd(type)

The component is "x", "z" or "p" if it is pressure data. If the parameter div and/or curl are enabled this may also be "r" or "t" respectively, where "r" is the radial and "t" the tangential component. The number of the station is a seven-digit running number starting from 0000001 the the total number of stations (cf., nrec in sec. 3.1.3) placed in the model. The file extension .sd* tells the user which kind of data is contained in the file: "a" for acceleration, "v" for (solid) particle velocity, "v1" and "v2" for fluid particle velocity, "p1" and "p2" for fluid pressure, and "u" for displacement.

Example: Given these conventions, a seismogram for the x-component of station 23 containing displacement data is named: *seismo.x.0000023.sdu*.

4.2.2 Binary file to create vtk files

The exact amount and type of binary files created by `solver` depends on the choice of parameters. First of all, the parameter "movie" needs to be enabled so that any file may be created. If that is the case, a file is created for each time-step matching the "frame" parameter per processor.

Example: If frame = 100, a file will be created for each 100th time-step.

Additionally, the user can enable the creation of binary files for acceleration, particle velocity and/or displacement. If either is selected, files will be created that contain the x-component, the z-component and the norm of the selected property, respectively. The files are named in the following way:

moviedata.(type)(component).(number of the processor)_it(time-step).bin

Here, type is "a", "v", "v1", "v2", "u", "p1", "p2", or "stress", the component is "x", "z" or "norm". In case of the norm, type and component are reversed. The number of processor is a six-digit number of the processor that created the file and time-step is a seven-digit number that describes the time-step that the file represents.

Example: Given these conventions, a movie-binary file for the x-component of the particle velocity created in processor 23 at time-step 4000 is named: *moviedata_vx_000023_it0004000.bin*. If case of the norm, but otherwise identical parameters the file is named: *moviedata_normV_000023_it0004000.bin*.

4.3 Files created by `movie`

There are two possible outputs:

- trimesh: Creates file, where the average over an element is plotted.
- point: Creates files, which contain the information on each grid point.

Both variants can be used independently and together.

4.3.1 trimesh files

This version of the wave filed output is enabled by selecting the parameter "save_movie_trimesh". The files are named in the following way:

movie_element_(type)(component)_it(framenumber).vtk

The part of the filename containing type and component follows the same pattern as above. The frame-number is a seven-digit number that increases sequentially.

Example: Given these conventions, the 4^{th} movie-vtk for the x-component of the particle velocity is called: *movie_element_vx_it0000004.vtk*. In case of the norm, but otherwise identical parameters the file is called: *movie_element_norm_v_it0000004.vtk*.

4.3.2 points files

This version of the wave-field output takes significantly more computational time as well as space on the hard-disk, but contains more detailed information. It is enabled by selecting the parameter "save_movie_points". The files are named in the following way:

movie_points_(type)(component)_it(framenumber).vtk

The part of the filename containing type and component follows the same pattern as above. The frame-number is a seven-digit number that increases sequentially.

Example: Given these conventions, the 4^{th} movie-vtk for the x-component of the particle velocity is named: *movie_points_vx_it0000004.vtk*. In case of the norm, but otherwise identical parameters the file is named: *movie_points_norm_v_it0000004.vtk*.

Chapter 5

Simulation

This chapter explains a complete simulation and suggests an efficient order of tasks, including pre- and post-processing. To follow this chapter, a successful installation of NEXD and all its requirements is necessary (see chapter 2). It is assumed that the code has been compiled without errors. To run a simulation, follow these steps:

- Prepare your simulation (see section 5.1 below for more details).
- Prepare your model, either using Trelis and the supplied routines or a meshing software of your choice.
- Check if all parameter files are present (see chapter 3 for more details).
- Run the preprocessor called `mesher` by executing the shell-script "process.sh" The present working directory of the console should be your simulation directory, e.g., `simulations/lambs`.
- Run the solver (see section 5.2 for details).
- If a visualisation apart from the seismograms is required, run `movie` by executing `./bin/movie` (see chapter 4 for details).

5.1 Preparation

After a successful installation, the directory for the first simulation has to be prepared. Follow these steps to prepare the model and parameter files:

1. Create a simulation folder according to the structure displayed in the examples and provide the relevant input files.
2. Create the model and subsequent input files for `mesher` as described in appendix A.
3. Change the appropriate files to individual specifications (see chapter 3 for details).
4. Either copy the shell script "process.sh" to the new simulation directory and run it or follow the next steps.
5. Create the folders "bin" and "out" in the simulation directory
6. Copy the executable files `mesher`, `solver` and `movie` from `dg2d/bin/` to the `yourSimulation/bin` directory in the simulation directory or create a symbolic link to these executable files.
7. run `mesher` by executing the command "./bin/mesher" in the console.

Recommendation: If "process.sh" is not used, it is advised that the parameter files from the "data" directory are copied to the "out" folder prior to running `mesher` (between steps 6 and 7). That way all information on how the simulation was created is stored with the output.

5.2 Calculation

This section is highly specialised for the individual user. Assuming that the user is able to run the program directly on his/her computer and OpenMPI is installed on the system there is only thing to do:

- run `solver` by executing `mpirun -np (nproc) bin/solver`.

The parameter "nproc" gives the number of processors as defined in the parfile. This number *must* be the same.
If desired, information on the process of the simulation are printed on screen. For select time steps the output listed in code listing 5.1 is generated. These time steps are defined by the "frame" parameter from the movie-parameter section. Each time a frame for the movie is generated, the output is printed into the file. It displays the time needed for the current interval, the estimated remaining time, the estimated total time and the mean elapsed time per time step. In addition an estimation is given on what date and time the simulation will be finished. This is particularly helpful for longer runs.

```
1  |-------------------------------------------------------------------------|
2  |       Time step number      100 (t = 6.12E-04 s) out of    10000        |
3  |       Elapsed time:                      0 h 00 m 11 s                  |
4  |       Estimated remaining time:          0 h 19 m 06 s                  |
5  |       Estimated total time:              0 h 19 m 18 s                  |
6  |       Mean elapsed time per timestep:      1.16E-01 s                   |
7  |       Current maximum norm of U     : 7.92007526E-08                    |
8  |       Current maximum norm of V     : 5.47094794E-04                    |
9  |       This run will finish on: Tue Aug 07, 2018 at 11:50                |
10 |                    1 % of the simulation completed.                     |
11 |-------------------------------------------------------------------------|
```

Listing 5.1: Output for select time steps

5.3 Evaluation

To view the seismograms, a program like GNUPLOT is sufficient. Python also offers an extended library on plotting such data.
If created, the vtk files may be viewed by a program like ParaView. According to their website "ParaView is an open-source, multi-platform data analysis and visualization application.". It can be freely downloaded from the website `https://www.paraview.org/`. Otherwise a library called "vtk" exits for Python that contains functions to process and display vtk files. It is part of the Anaconda package but may be installed separately by the user.
For the included examples, reference seismograms are provided. If one of the examples is run, they are a basis for comparison.

Chapter 6

Contact and Support

For questions, feedback, or suggestions please contact us via email (`seismology-coder@ruhr-uni-bochum.de`), or on `http://github.com/seismology-RUB`.

Chapter 7

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```
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```

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```
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```

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Appendix A

Creating a model (with Trelis)

This chapter explains very briefly how to generate a model for NEXD 2D using the Trelis software and the supplied journal (*.jou) files. Detail on how to use Trelis will not be given. If problems arise, the user is referred to the user manual of Trelis `https://www.csimsoft.com/help/trelishelp.htm`. This manual refers to Trelis 16.5. The models presented in the example were created and tested with Trelis version 15.2. A user manual of this version can be downloaded at `https://www.csimsoft.com/download?file=Documents/Trelis15UserDocumentation.pdf`.

A.1 The journal file

The journal file is a script that can be executed by Trelis to generate a pre-defined model. If the meshing process is to be done often (e.g., due to mesh refinement) it is advisable to create these files. By default, Trelis creates journal files for each run of the meshing process. If the desired model is created, it is advised to save that information in a new file related to the model.
The reset command at the beginning resets the current environment to its default condition. It is highly recommended to use this command ahead of each run. Lines 5 - 14 list the commands that are used to create the model (the geometric shape).

Warning: If the model is created using vertex points (like this example) the user has to pay attention on how the surfaces are created. The normal of all surfaces must point in the same outward direction. Otherwise an error is raised n the when "mesher" is run called ***Jacobian*** < 0. The easiest way avoid this error, is to create the surface by calling the points anticlockwise according to their coordinates (see lines 13 -14).

Lines 17 - 19 are optional and are only needed if PML are to be used. They create the PML layer by cutting it from the original volume.

Attention: If PMLs are to be included in the model, they have to be of uniform thickness. Nonuniform thickness of PMLs is currently not supported and creation of such will result in errors.

Lines 26 - 30 describe the meshing process. Usually the only portion to be adjusted here is the size of the elements. This is done in line 28 in this example. The unit of this number is meters.
Next, the materials are defined. In Lines 37 and 38 each block is assigned a number of surfaces. They are assigned by number which are given to the surfaces by Trelis. In lines 41/42 the material properties are assigned to the blocks. The properties are assigned via the blocks name and consist of the following values: v_p, v_s, ρ, Q_p, Q_s, and PML index. v_p, v_s and ρ are given in SI units. The Q-factors relate to attenuation and the last index signifies whether that block is part of the PML or not. Note, the ID for the PML changes for block 2. This indicates that all surfaces contained in this block are part of the PML.
Similar to the blocks, nodesets are created that contain the nodes on the surfaces. These nodesets are used to assign boundary conditions. Each nodeset is assigned the nodes from a number of surfaces. They my be also left empty. If, for example, no free surface is used, the nodeset can be left empty. However, it needs to be present in the file otherwise the python script will not function properly. Each nodeset

```
reset

##########################################

#model
create vertex 0 0 0
create vertex 50 0 0
create vertex 50 25 0
create vertex 50 50 0
create vertex 0 50 0
create vertex 0 25 0

create surface vertex 1 2 3 6
create surface vertex 6 3 4 5

##########################################
#pml
webcut volume all with plane normal to curve 1 distance 3 from vertex 1
webcut volume all with plane normal to curve 4 distance 3 from vertex 1
webcut volume all with plane normal to curve 10 distance 3 from vertex 2

##########################################

#meshing

imprint all
merge all
surf all size 1.0
surface all scheme TriDelaunay
mesh surface all

##########################################
# materials
# allows for elements to be part of multiple blocks
set duplicate block elements on

block 1 tri in surf 14 16
block 2 tri in surf 6 9 10 11 12 13 15

# name nr vp vs rho qp qs pml
block 1 name "elastic 1 5800 3800 2600 9999 9999 0"
block 2 name "elastic 2 5800 3800 2600 9999 9999 1"

##########################################
#edges
nodeset 1 node in curve 19 41 43
nodeset 2 node in curve 5 6 7 8 14 23 25 28 32 34 38

nodeset 1 name "free_surf"
nodeset 2 name "absorb"

save as "testtri.cub" overwrite
```

Listing A.1: Excerpt from the mat file

is assigned a name. The user is asked to use the default names, as a modification of that name would require a modification of the python script, that prepares the model for NEXD 2D.
Finally, the model is saved as a .cub file. This file will be used to create the parameter files described in section 3.2.

A.2 Prepare the input files

The relevant input files are created by running the script "run_cubit.py". This scripts loads all necessary modules and calls the script "cubit2dg2d.py". The script requires the file "cubit2dg2d.py" to be present in the folder it is executed from, or line 12 (reload command) needs to be modified with the correct path to the file.

```
1  #!python
2  #!/usr/bin/env python
3
4  import cubit
5  import cubit2dg2d
6  import os
7  import sys
8  from math import *
9  from numpy import *
10
11
12 reload(cubit2dg2d)
13
14 cubit.init([""])
15 cubit.cmd('set duplicate block elements on')
16 command = 'open "testtri.cub"'
17 cubit.cmd(command)
18
19 cubit2dg2d.mesh()
```

Listing A.2: Python script to create input file from cubit model

Modify line 16 by replacing the name "testtri.cub" by the name that has been assigned to the model (name of the .cub file).

A.3 Using a different meshing tool

Currently no other meshing tool is supported by the developers. If a user is not able to use the supported meshing software he/she is asked to create the relevant input files from the output of his/her own meshing software.

Appendix B

Adding a custom source time function

It may become necessary for certain users to add a source time function of their own. This chapter describes, which section of the source code and what entries in the parameter files need to be changed.

B.1 Source code

There are a number of portions of the source code that need to be changed. It is not simply done by adding the function itself, but also modifying the related error messages, so the new function is not rejected. First, the new source time function needs to be added as an additional function in the module "stfMod.f90". It is recommended that the basic structure of the function is similar to the already existing ones. As a basic example the function describing a Ricker-wavelet is shown in code listing B.1

```
1 (sftMod)
2 function stfRicker(t,f0,t0,factor)
3     implicit none
4     real(kind=custom_real) :: stfRicker
5     real(kind=custom_real) :: f0,t0,factor,t
6     real(kind=custom_real) :: aval
7     aval = pi*pi*f0*f0
8     stfRicker =  factor * (1.-2.*aval*(t-t0)**2.) * exp(-aval*(t-t0)**2.)
9 end function stfRicker
```

Listing B.1: Code for the Ricker wavelet.

As described in the section 3.1.2, each source time function is called by a specific number. If an additional function is added, that number increases. There are a number of sections in the code where that number influences the calculations. The first occasion is in the subroutine *initSource* in the module *sourceReceiverMod*. The relevant code is displayed in code listing B.2. Edit the call to the if-condition (line 114) to accept larger values. Edit the error-message (line 116) accordingly.
The next occasions are in the module *timeloopMod*. Here, the source code has to be changed at two locations. First between lines 498 and 548 (see code listing B.3). A new statement to the if call starting at line 503 needs to be added in the same way as the previous ones so to make the new stf available for further calculations. The number in the last segment (line 518) needs to be increased as well.
The final piece of code that needs editing is between lines 671 and 691 in *timeloopMod* (code listing B.4. In much the same way as in the previous code segment of *timeloopMod*, the if statement starting at line 672 needs to be expanded to include the new function in the same way as it is designed for the included source time functions. At this point, no error message has to be updated.

```
113 call readIntPar(this%srcstf(isrc), "stf", filename, pos, errmsg)
114 if( this%srcstf(isrc) < 1 .or. this%srcstf(isrc) > 4) then
115     !this message needs to be adjusted if new wavelets are added to the
        ↪ Program
116     call add(errmsg, 2, "Parameter to select the source time function is
        ↪ out of range. Select either 1, 2, 3 or 4.", myname, filename)
117 end if
118 if (this%srcstf(isrc) == 4) then
119     call readStringPar(this%extwavelet(isrc), "extwavelet", filename, pos,
        ↪ errmsg)
120     inquire(file=trim(this%extwavelet(isrc)), exist=file_exists)
121     if (.not. file_exists) then
122         call add(errmsg, 2, "File does not exist!", myname, filename)
123     end if
124 end if
```

Listing B.2: Code snippet from *initSource*.

```
498 ! choose source time function
499 if (mesh%has_src) then
500     do i=1,src%nsrc
501         do it=1,par%nt
502             time = (float(it)-1.)*dt
503             if (src%srcstf(i) == 1) then !GAUSS
504                 plotstf(it,1,i) = time
505                 plotDiffstf(it,1,i) = time
506                 plotstf(it,2,i) = -stfGauss(time,src%srcf0(i),t0(i)+src%
                        ↪ delay(i),src%srcfactor(i))
507                 plotDiffstf(it,2,i) = -stfDiffGauss(time,src%srcf0(i),t0(i)
                        ↪ +src%delay(i),src%srcfactor(i))
508             else if (src%srcstf(i) == 2) then !RICKER
509                 plotstf(it,1,i) = time
510                 plotDiffstf(it,1,i) = time
511                 plotstf(it,2,i) = -stfRicker(time,src%srcf0(i),t0(i)+src%
                        ↪ delay(i),src%srcfactor(i))
512                 plotDiffstf(it,2,i) = -stfDiffRicker(time,src%srcf0(i),t0(i
                        ↪ )+src%delay(i),src%srcfactor(i))
513             else if (src%srcstf(i) == 3) then !SIN^3
514                 plotstf(it,1,i) = time
515                 plotDiffstf(it,1,i) = time
516                 plotstf(it,2,i) = -stfSin3(time,src%srcf0(i),t0(i)+src%
                        ↪ delay(i),src%srcfactor(i))
517                 plotDiffstf(it,2,i) = -stfDiffSin3(time,src%srcf0(i),t0(i)+
                        ↪ src%delay(i),src%srcfactor(i))
518             else if (src%srcstf(i) > 4) then
519                 call add(errmsg, 2, "Chose a valid source time function.
                        ↪ Available functions are listed in the 'source'
                        ↪ parameter file.", myname, "data/source")
520                 call print(errmsg)
521                 call stop_mpi()
522             end if
523         end do
524         if (src%srcstf(i) == 4) then
525             filename=src%extwavelet(i)
526             call stfExternal(plotstf(:,2,i),plotstf(:,1,i),dt,par%nt,.true
                    ↪ .,6,3,trim(filename),0, errmsg)
527             call stfExternal(plotDiffstf(:,2,i),plotDiffstf(:,1,i),dt,par%
                    ↪ nt,.true.,6,3,trim(filename),1, errmsg)
528         end if
529         [...]
530     end do
531 end if
```

Listing B.3: Code snippet from *timeloopMod* (1).

```
671 do i=1, src%nsrc
672     if (src%srcstf(i) == 1) then
673         stf_val = -stfGauss(time,src%srcf0(i),t0(i)+src%delay(i),src%
                ↪ srcfactor(i))
674         stf_val_diff = -stfDiffGauss(time,src%srcf0(i),t0(i)+src%delay(i),
                ↪ src%srcfactor(i))
675     else if (src%srcstf(i) == 2) then !RICKER
676         stf_val = -stfRicker(time,src%srcf0(i),t0(i)+src%delay(i),src%
                ↪ srcfactor(i))
677         stf_val_diff = -stfDiffRicker(time,src%srcf0(i),t0(i)+src%delay(i),
                ↪ src%srcfactor(i))
678     else if (src%srcstf(i) == 3) then !Sin^3
679         stf_val = -stfSin3(time,src%srcf0(i),t0(i)+src%delay(i),src%
                ↪ srcfactor(i))
680         stf_val_diff = -stfDiffSin3(time,src%srcf0(i),t0(i)+src%delay(i),
                ↪ src%srcfactor(i))
681     end if
682     if (src%srcstf(i) == 4) then
683         if (it<par%nt) then
684             stf_val=(1.-rk_time)*plotstf(it,2,i)+rk_time*plotstf(it+1,2,i)
685             stf_val_diff=(1.-rk_time)*plotDiffstf(it,2,i)+rk_time*
                    ↪ plotDiffstf(it+1,2,i)
686         else
687             stf_val=(1.+rk_time)*plotstf(it,2,i)-rk_time*plotstf(it-1,2,i)
688             stf_val_diff=(1.+rk_time)*plotDiffstf(it,2,i)-rk_time*
                    ↪ plotDiffstf(it-1,2,i)
689         endif
690     end if
691 enddo
```

Listing B.4: Code snippet from *timeloopMod* (2).