1D-3C SEM

A Spectral Element Method tool for 1D wave propagation
with three components (3C) in linear and nonlinear media

User's Guide

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Contents

Chapter 1

Introduction

The 1D-3C SEM code is a numerical tool for spectral element modeling (SEM) of one-dimensional (1D) seismic wave propagation with three components (3C) in linear and non-linear media. It is an extended version of the 1D SEM code supplied by the PhD work of Elise Delavaud (Delavaud, 2007). The additional contributions have been made by Elif Oral during her PhD thesis (Oral, 2016).

The 1D-3C SEM code offers many choices for the soil rheology in propagation medium and bottom boundary conditions. As soil constitutive model (soil rheology), it is possible to model elasticity, viscoelasticity, elastoplasticity and visco-elastoplasticity. For boundary conditions, 1D-3C SEM allows for defining rigid condition, absorbing layer condition with Perfectly Marched Layers (PML), borehole condition and free surface condition.

For viscoelastic attenuation in propagation medium, (Liu and Archuleta, 2006) model has been implemented in the code, whereas soil nonlinearity is based on MPII model of (Iwan, 1967). For nonlinearity, the code offers pressure-dependent and pressure-independent modeling possibilities. For pressure-independent models, it is possible to define soil nonlinearity with given experimental data or hyperbolic curve of (Hardin and Drnevich, 1972). Furthermore, in pressure-dependent models, effective and total stress analyses could be performed. The excess pore pressure development in effective stress analysis is modeled in 1D-3C SEM code following the front saturation model of (Iai et al., 1990). For more details on theory of these models, the user is invited to refer to (Oral, 2016).

The 1D-3C SEM code is a completely free (open) source and it is provided with several example files and Python-based scripts to be used for pre- and post-treatments. In the following, first, the compilation of the code is detailed. Second, the employment of different models into the code is explained by means of various examples. Lastly, the use of available python scripts are given.

Chapter 2

Compilation

The compilation of 1D-3C SEM code is tested for gfortran and ifort compilers. A faster computation is provided by optimization options with the compiler flags. In order to compile the code, the user should execute make command first in SRC/Modules folder, where the Makefile is available for modules. The same execution should be applied in SRC folder, where another Makefile is available for main fortran files. This procedure is written in compile.sh file. It is also possible to use directly this bash file for compilation.

For both compilers (gfortran and ifort), necessary flags are provided in Makefile. For users who prefer gfortran compiler, necessary flags are as follows:

OPT = -O2 -finline-functions -funswitch-loops -fpredictive-commoning -fpredictive-commoning -fgcse-after-reload -ftree-slp-vectorize -ftree-loop-distribute-patterns -fvect-cost-model -fipa-cp-clone -fno-math-errno -funsafe-math-optimizations -fno-rounding-math -fno-signaling-nans -fcx-limited-range -g3 -fbacktrace -fdefault-double-8 -fdefault-real-8 -fdefault-integer-8

This option is equivalent to the Ofast and avoids possible computational errors. For the use of ifort compiler, following command is suggested:

OPT= -O3 -ip -ipo -unroll

Advanced users who intend to change the content of source files are suggested to specify dependencies in Makefile.depend files in Modules directory.

Once the compilation is completed, the code creates an executable in upper directory which is named SEM1D3C. Then, the user could perform simulations in her working directory with this executable.

Chapter 3

Examples

3.1 Introduction

The 1D-3C SEM code is served to use with several examples which had been used in analyses of (Oral, 2016). First, for an elastic medium assumption, the realistic model of Volvi (Greece) is given. Second, the same model of Volvi is used with viscoelastic soil constitutive model. Afterwards, nonlinear examples are shown for different cases. One of the nonlinear cases is the pressure-independent P1 model. The soil nonlinearity in this model is considered by elastoplasticity where 50 Iwan mechanisms are defined. Another nonlinear case is the pressure-dependent model of Wildlife Refuge Liquefaction Array (WRLA) which is provided with total and effective stress analyses. Lastly, effective stress analysis of Kushiro port (KP) site model which is initially anisotropically consolidated is provided. These examples are detailed by input and output files below.

3.2 Elasticity model

For elasticity, Volvi model example is given. It can be found in EXAMPLES/VOLVI/ELASTIC directory. The model is composed of eight soil layers. In the table below, main properties of the model are shown, where ρ is soil density, V_s and V_p are shear and pressure wave velocities, Q_s and Q_p are quality factors for shear and pressure waves, respectively. For elasticity, Q_s and Q_p values are ignored.

Table 3.1: Soil properties at the Volvi model.

Layer	Thickness $[m]$	$V_s[m/s]$	$V_p[m/s]$	$\rho[kg/m^3]$	Q_s	Q_p
1	7	130	1500	2050	15	75
2	13	200	1500	2150	20	75
3	34	300	1650	2075	30	83
4	23.5	450	2050	2100	40	103
5	50	600	2450	2155	60	123
6	59	700	2550	2200	70	140
7	10	1250	3500	2500	100	200
Bedrock	103.5	2600	4500	2600	50000	50000

In this example, upper boundary is defined as free surface and at bottom of the model, PML (Perfectly Matched Layers) is used. It should be noted that 1D-3C SEM code assumes use of a single element for PML. For further changes, the user could make modifications in the code by sigeps.f90 file.

The first file that the user should provide is input.spec, which is shown in the following figure of Volvi model.

```
VOLVI            # Title of simulation
30.0             # Duration of the simulation
datamesh         # Mesh input file
material         # Material parameters file
.false.          # Source
source           # Source parameters file
stations         # Receiver parameters file
.true.           # Imposed signal
inputvolvi       # Imposed signal file
1.0              # Coefficient for input
20000            # Iteration to put on monitor
.true.           # Save traces
20               # Output factor
.true.           # Run time loop or not
.false.          # Viscoelasticity on
.false.          # Nonlinearity on
.false.          # Pressure-dependent model
1                # Water table node number
```

Figure 3.1: Input file input.spec for elastic Volvi model.

The file is self-explanatory. Title of simulation and total duration of simulation should be specified. Then, the mesh file name from which the necessary data about element and domain characteristics are to be read is needed. In pre-treatment section of this manual, an example for creating a mesh file is given.

For material properties, the code requires a file which respects the following format. The user should define total number of domains. Then , for each domain, P and S velocity values, density, PML condition (True /False), time step of simulation, GLL number, viscoelasticity quality factors for P and S waves, reference frequency and nonlinear soil type should be written. Although same time step is used all over the model, the format requires entering this data for each domain. For elastic models, even though it is not necessary viscoelastic or nonlinear parameters in computations, the user should follow the specified format for every model. For PML domain, n and A coefficients are necessary. If no PML is used, the PML data section should be left commented. Lastly, for pressure-dependent models, for each domain, the user must define whether excess pore pressure development is expected (T) or not (F) and pressure-dependent soil type. In other models such as this elastic example, this part will be ignored. However, the user should create the material file in this format.

```
# Material types
# Number of material types
9
# Type ,P and SVelocity, Density, PML ,  Delta T , Number of GLL, Viscosity Q, Reference frequency, Nonlinear Soil Number
1   1500    130     2050     F       0.00005         9          75.        15.   1.      1
2   1500    200     2150     F       0.00005         9          75.        20.   1.      1
3   1650    300     2075     F       0.00005         9          83.        30.   1.      1
4   2050    450     2100     F       0.00005         9         103.        40.   1.      1
5   2450    600     2155     F       0.00005         9         123.        60.   1.      1
6   2550    700     2200     F       0.00005         9         140.        70.   1.      1
7   3500   1250     2500     F       0.00005         9         200.       100.   1.      1
8   4500   2600     2600     F       0.00005         9       50000.    50000.   1.      1
9   4500   2600     2600     T       0.00005         9       50000.    50000.   1.      1
# For PML specify
# np-power,A-power, Left-increase
   2        10          F
# For PRESSURE-DEPENDENT condition, specify
# Domain number, Liquefiability, Overburden soil type
1           F           2
2           F           2
3           F           2
4           F           2
5           F           2
6           F           2
7           F           2
8           F           2
9           F           2
```

Figure 3.2: Material file for elastic Volvi model.

When we come back to input file, the following input data concerns sources. For cases where point source is defined as input motion, the user should set source option should be defined as .True. and specify file name in which source type and properties are given . Such a source file should contain:

1. Coordinate
2. Source kind (1 for impulse; 2 for explosion)
3. Source function (1 for Gaussian; 2 for Ricker)
4. Pulse width (Only if Gaussian type of function is given)

5. Delay time (Only if Ricker type of function is given)

6. Cut-off frequency (Only if Ricker type of function is given)

For cases where the input motion is defined by an incident wave field, the code requires a file in which time step and corresponding velocity of incident wave are included. It should be noted that time step of the input motion should not be smaller than time step of simulation. For such cases, the user should write .True. for imposed signal and file name for imposed signal file. It is also possible to define a coefficient for the given velocity field.

The receiver coordinates should be included in a file with total number of stations. An example is given below:

```
9
0.
50.
100.
150.
200.
250.
300.
310.
320.
# Stress strain hereby !
7
0.
50.
100.
150.
200.
250.
300.
```

Figure 3.3: Station (receiver) file for elastic Volvi model.

In receiver file (stations in this example), first, the receivers where acceleration, velocity time histories are desired as output are defined. In the second part of the file, different depths could be defined for saving nonlinearity and pore pressure model parameters. More details about output files are given in last chapter of this manual (See Chapter 4.2).

When the code is executed, some information are written out in terminal as below :

```
 Read input file for model parameters
 Define mesh properties
 Compute Gauss-Lobatto-Legendre weights and zeroes
 Viscoelastic Modulus Calculation
 Computing shape functions
 Computing derivatives of shape functions
 CFL     0.44891360846897516
 dxmin   0.25060501147133607
CFL greater than CFLmax = 0.3 - Press <Return> to continue.
 Receivers parameters and location
 Define Internal-External forces coefficients for Newmark scheme
 Incident wave velocity assignment
 Time step factor of input and simulation
                   2
 Entry Newmark scheme
 iter =                  20000
 elapsed time =    1.0000000000000000
 iter =                  40000
 elapsed time =    2.0000000000000000
```

Figure 3.4: Output data in terminal for 2 seconds of simulation in elastic Volvi model.

In order to control the time interval of output information concerning elapsed time, the user could change the iteration number in input.spec file by iteration to put on monitor. For the simulations where the user does not want to perform time iterations but verifies the execution of the code (useful for further modifications by advanced users), Run time loop could be chosen as .False.. Also, if the user does not want to save output files, Save traces should be chosen as False. Otherwise, at the end of simulation, the code provides output files at given receiver coordinates.

Lastly, the soil constitutive models should be defined. For elasticity, the user should set Viscoelasticity on, Nonlinearity on and Pressure-dependent model False. The other cases will be detailed in following sections. For elasticity, Water table node is not taken into consideration in computations.

3.3 Viscoelasticity model

Viscoelasticity example could be found in EXAMPLES/VOLVI/VISCOELASTIC directory. For viscoelasticity, compared to elasticity, the changes apply to input.spec and material files. In input.spec files, differently than elasticity, Viscoelasticity on should be set to True. In material file, quality factors for P and S waves with reference frequency (which will be no longer ignored by the code) should be provided for each domain.

3.4 Nonlinearity model

3.4.1 Pressure-independent nonlinearity

For pressure-independent nonlinear model, an example is given in EXAMPLES/P1 directory. The model is composed of a single layer with following properties:

Table 3.2: Soil properties at P1 model (PRENOLIN).

Layer	Thickness $[m]$	$V_s[m/s]$	$V_p[m/s]$	$\rho[kg/m^3]$	Q_s	Q_p
1	20	300	700	2000	30	70

In such a case, the user should define, first, in input.spec file, Nonlinearity on as True, so that the model follows elastoplasticity. If viscous attenuation is also demanded, then Viscoelasticity on must be set to True as well, such that the model is visco-elastoplastic.

Also, for nonlinearity, another file which should be named GoverGmax.dat is required, differently than elastic and viscoelastic cases. The format of the file is shown below:

```
# NONLINEARITY PPTS
.true.      # [Hyperbolic / Experimental model] [T/F]
50          # Spring number
# HYPERBOLIC MODEL PPTS
2         # Total nb of Nonlinearity type
0.000365  # Reference strain 1
0.000730  # Reference strain 2
#
# EXPERIMENTAL MODEL PPTS
1
1  ### PRENOLIN P1 SOIL - EXPERIMENTAL DATA ###
19
0.000010    0.9997
0.000022    0.9994
0.000046    0.9987
0.000100    0.9973
0.000215    0.9941
0.000464    0.9874
0.001000    0.9732
0.002154    0.9440
0.004642    0.8867
0.010000    0.7842
0.021544    0.6278
0.046416    0.4391
0.100000    0.2665
0.215440    0.1443
0.464160    0.0726
1.000000    0.0351
2.154400    0.0166
4.641600    0.0078
10.00000    0.0036
```

Figure 3.5: GoverGmax.dat file for P1 example.

In this latter, the choice of hyperbolic or experimental model in order to construct the backbone curve should be made. For hyperbolic models, the Equation 3.1 is used so that the user must define a reference strain.

$$\frac{G}{G_0} = \frac{1}{1 + \gamma/\gamma_{ref}} \tag{3.1}$$

In this example, two different values are available. In material file, the nonlinear soil type should be written according to the reference strain data in this file, for hyperbolic models. Otherwise, the user has the possibility of defining an experimental curve by giving strain (in percentage) and corresponding shear modulus ratio. Again, the soil type must match with the defined nonlinear soil type in material file for each domain. Lastly, in the same file, the total number of Iwan springs is obligatorily given for all nonlinear cases. In this example, it is set to 50.

3.4.2 Pressure-dependent nonlinearity

For pressure-dependent model, Wildlife Refuge Liquefaction Array site model is given. The model is composed of four layers of which only the third layer is liquefiable. In other words, only in the third layer, excess pore pressure development is expected to be developed.

Table 3.3: Soil properties at Wildlife Refuge Liquefaction Array after (Bonilla et al., 2005)

Layer	Description	Thickness $[m]$	$V_s[m/s]$	$V_p[m/s]$	$\rho[kg/m^3]$	$\phi_f[degree]$	K_0
1	Silt	1.5	99	249	1600	28	1.0
2	Silt	1.0	99	281	1928	28	1.0
3	Silty sand	4.3	116	1019	2000	32	1.0
4	Silty sand	0.7	116	1591	2000	32	1.0

For this site, the models of effective and total stress analyses are provided. First, necessary modifications for total stress analysis are detailed. Then, further changes to be made for effective stress analysis are explained.

Total stress analysis For total stress analysis, in other words, for pressure-dependent nonlinear models where no excess pore pressure develops, the first change applies to input.spec file. The user should define Nonlinearity on and Pressure-dependent model as True. The water level should be defined by the corresponding node number in mesh file. This means that if water level is present in the model, it must correspond to an elementary boundary in the model.

In addition, differently than previous cases, in pressure-dependent model, another file pressparam.dat is required. The format of the file is given below. In this file, m1 (slope of the soil failure line), cohesion and coefficient of Earth at rest are compulsory for total stress analysis. Other parameters are to be neglected in total stress analysis computations.

```
# PRESSURE-DEPENDENT MODEL PPTS (WRLA)
2           # Total domain nb
# Domain 1 [Layer 1 and 2]
0.4695   # m1   (phi=28)
0.4067   # m2
0.40     # p1
0.90     # p2
0.0100   # S1
4.0      # w1
2.0      # c1
0.0      # Cohesion [Pa]
1.0      # Coefficient of Earth at rest (K0)
# Domain 2 [Layer 3 and 4]
0.5299   # m1   (phi=32)
0.4067   # m2   (phi_p=24)
0.40     # p1
0.90     # p2
0.0100   # S1
4.0      # w1
2.0      # c1
0.0      # Cohesion [Pa]
1.0      # Coefficient of Earth at rest (K0)
```

Figure 3.6: pressparam.dat file for P1 example.

Accordingly, in the last part of the material file, the overburden soil type should match the soil number in pressparam.dat soil types. For total stress analysis, each domain is non-liquefiable such that liquefiability is specified as False.

Effective stress analysis Effective stress analysis for WRLA model can be found in EXAMPLES/WRLA/EFFECTIVE_STRESS_ANALYSIS directory. In WRLA model, the third layer is assumed to be liquefiable. This property is defined in the liquefiability part of the material file. For this example, the third layer liquefiability is True while other layers are False, as seen in Figure 3.7.

```
# Material types
# Number of material types
4
# Type ,P and SVelocity, Density, PML ,  Delta T , Number of GLL, Viscosity Q, Reference frequency, Nonlinear Soil Number
1      249        99       1600     F      0.00002          5       25.   10.          1.        1
2      281        99       1928     F      0.00002          5       28.   10.          1.        1
3     1019       116       2000     F      0.00002          5      102.   12.          1.        1
4     1591       116       2000     F      0.00002          5      160.   12.          1.        1
# For PML specify
# np-power,A-power, Left-increase
   2       10          F
# For PRESSURE-DEPENDENT condition, specify
# Domain number, Liquefiability, Overburden soil type
1          F          1
2          F          1
3          T          2
4          F          2
```

Figure 3.7: Material file for WRLA effective stress analysis model.

Compared to total stress analysis, another change is made in pressparam.dat file. The model properties necessary for pore pressure excess computation such as m_2, p_1, p_2, S_1 and w_1 (front saturation model parameters) are required for the liquefiable layer. In this example, the third layer corresponds to the overburden soil type 2. Thus, in pressparam.dat file, the code looks for the front saturation model parameters for that soil type.

Effective stress analysis - II Another example is given for effective stress analysis in Kushiro Port model (KP), which is initially consolidated in anisotropic conditions. The KP model properties are given in Table 3.4.

Table 3.4: Soil properties at Kushiro Port vertical array after (Iai et al., 1995). V_p values are calculated by assumption of Poisson ratio equal to 0.48.

Layer	Description	Thickness $[m]$	$V_s[m/s]$	$V_p[m/s]$	$\rho[kg/m^3]$	$\phi_f[degree]$	K_0
1	Fill soil	2.0	249	1270	1540	40	0.5
2	Sand	7.0	249	1270	1720	40	0.5
3	Sand	14.0	326	1662	1980	48	0.5
4	Silt	9.0	265	1351	1730	37	0.5
5	Silt	4.0	341	1739	1760	44	0.5
6	Silt	8.0	286	1458	1700	44	0.5
7	Silt	8.0	302	1540	2000	45	0.5
8	Silt	25.0	341	1739	1730	44	0.5

Since the model has a coefficient of Earth at rest equal to 0.5 for each layer, this property is defined in pressparam.dat file with K0 parameter.

Chapter 4

Prior and posterior analyses

4.1 Pre-treatment

1D-3C SEM codes provides PRE and POST folders for simple prior and posterior analyses to simulations. First, in PRE directory, a Python script create_mesh.py is provided for mesh file creation which is required for the code to define the coordinates of element nodes and boundary conditions.

The script is self-explanatory and interactive. First, the user is asked to specify the name of the mesh file to be created and its explanation. Then, total element number, total domain number and upper boundary condition should be defined. Afterwards, the script needs the set of element sizes to be used. In Figure 4.1, an example for a model of 20 meters depth which is composed of two elements is shown. Once element sizes are defined, for each domain of the model, the scripts asks total number of element for each element size. To finish, bottom boundary condition is necessary.

```
Enter the Mesh file name to be created  datamesh
Enter the Model name for information    Example mesh file
***********************************************************************************
Specify total element number please :)
Integer only 2
***
Specify total material/domain number please (PML included):
Integer only 1
***********************************************************************************
Specify upper boundary condition please :)
N for Neumann/ D for Dirichlet: N
You want Neumann condition at top, OK!
***
***********************************************************************************
Setting element size types
Please enter an element size or leave a blank line to quit: 10
You entered  10
Please enter an element size or leave a blank line to quit:
***********************************************************************************
You defined element types as:  [10.0]
***
Let's define the element type numbers for each domain...
*******************************************************************************
Domain  1  :
Element number for size : 10.0
Specify please: 2
You entered  2
***
*******************************************************************************
Domain  1
Element number:  2
Min size:  10.0
Max size:  10.0
Specify lower boundary condition please :)
N for Neumann/ D for Dirichlet/ B for Borehole: B
You want Borehole condition at bottom, OK!
***********************************************************************************
File  datamesh  is ready!
```

Figure 4.1: create _mesh.py file for 1D mesh file creation.

4.2 Post-treatment

Once the simulation terminates, the code sorts a number of output files. For all rheological models (elastic, viscoelastic, nonlinear cases), acceleration, velocity time histories in three directions of the first series of receivers are saved. Also, stress and strain parameters for the second series of receivers are written out in files.

For pressure-independent nonlinear models, such as P1 example, additionally a file with backbone curve strain and stress parameters is furnished. Depending on curve type (hyperbolic or experimental), the file name is named SOILHYPER or SOILEXP.

For pressure-dependent models, two additional files are provided. PressSoilParams00X.dat file (where X refers to receiver number) includes shear modulus, Young modulus, bulk modulus, Poisson ratio, initial shear modulus after normalization and current maximum shear modulus, for each time step. In PressEffectiveParams00X.dat, current values of principal deviatoric stress, W_s, W_n, S_0 and S parameters of the front saturation model, pore pressure excess and reference strain are given.

As posterior analyses, in POST directory, other Python-based scripts are provided to users of 1D-3C SEM code. The first file is called accel _sigeps.py which plots acceleration time histories and stress-strain curves for given files. Resultant figure for P1 model is shown in 4.2.

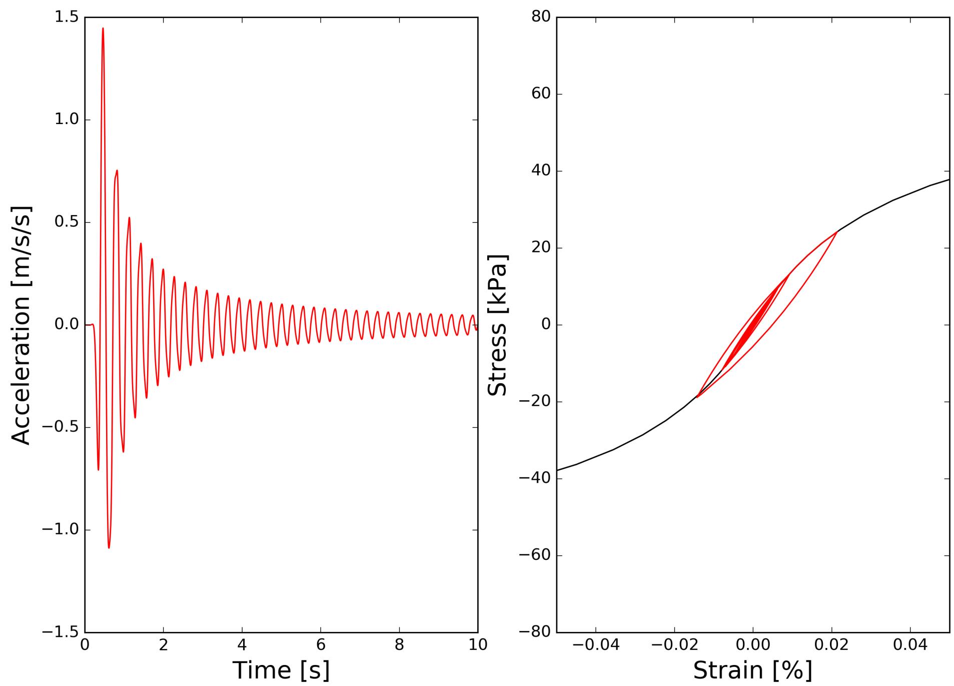

Figure 4.2: Acceleration time histories at surface (left); Stress-strain curve at mid-column of P1 model (right).

For plotting Fast Fourier transforms of a given file (acceleration or velocity time histories), fft.py file could be used. Resultant figure for WRLA model effective stress analysis is displayed in Figure 4.3.

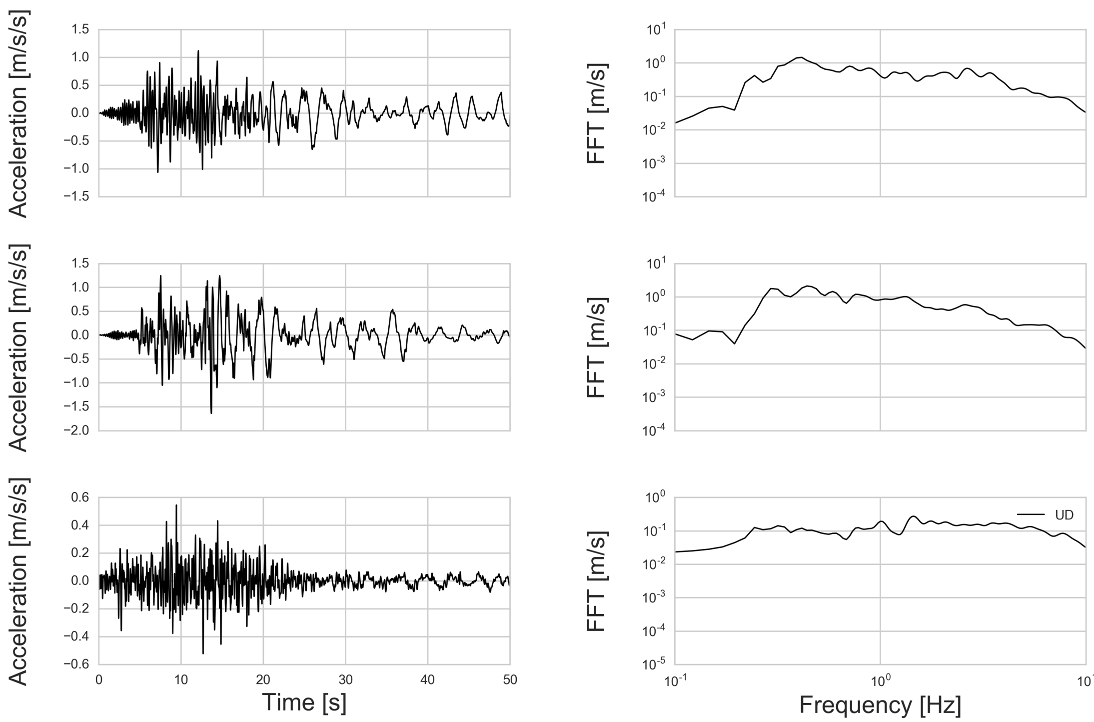

Figure 4.3: Acceleration time histories at surface (left); Fast Fourier transform (right) for three directions of WRLA model effective stress analysis.

For effective stress analyses, in order to visualize the changes in pore pressure excess, deviatoric plan, shear modulus and stress-strain curves, effective_changes.py file is ready to use. An example for WRLA model is shown in Figure 4.4.

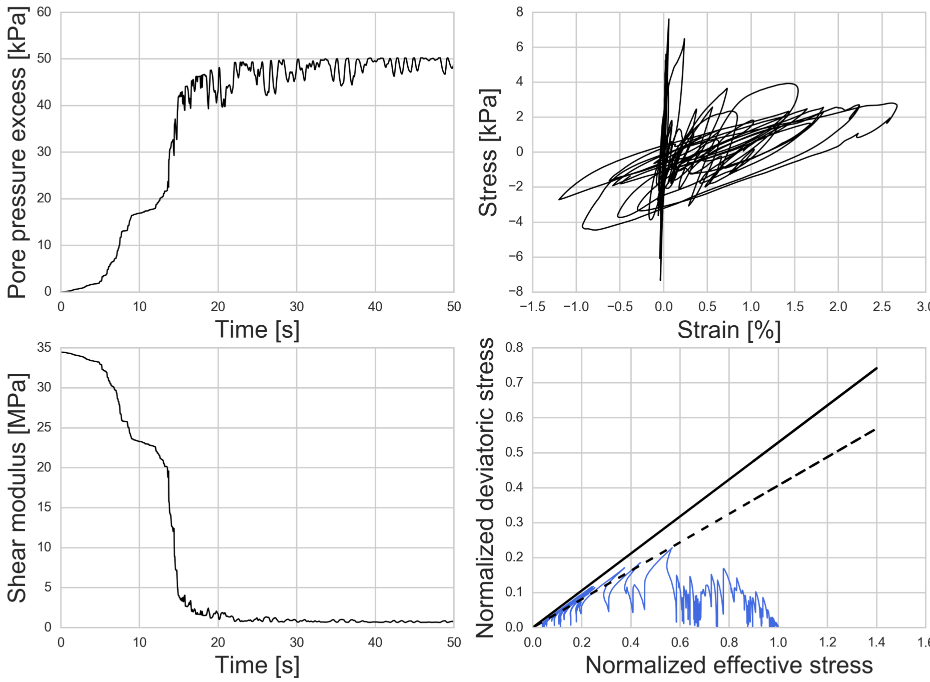

Figure 4.4: Pore pressure excess temporal change (left top); Stress-strain curve for EW-UD direction (top right); Change in shear modulus (bottom left); Deviatoric plan (bottom right) at GL-4 m for WRLA model effective stress analysis.

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