

# **SPECFEMX 1.0 Beta**

## **User Manual**

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July 27, 2018

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# Acknowledgments

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# Chapter 1

## Introduction

### 1.1 Background

SPECFEMX is a free and open-source command-driven software for 3D slope stability analysis (for more details see Gharti et al., 2011) and simulation of 3D multistage excavation (for more details see Gharti et al., 2011) based on the spectral-element method (e.g., Patera, 1984; Canuto et al., 1988; Seriani, 1994; Faccioli et al., 1997; Komatitsch and Vilotte, 1998; Komatitsch and Tromp, 1999; Peter et al., 2011). The software can run on a single processor as well as multi-core machines or large clusters. It is written mainly in FORTRAN 90, and parallelized using MPI (Gropp et al., 1994; Pacheco, 1997) based on domain decomposition. For the domain decomposition, the open-source graph partitioning library SCOTCH (Pellegrini and Roman, 1996) is used. The element-by-element preconditioned conjugate-gradient method (e.g., Hughes et al., 1983; Law, 1986; King and Sonnad, 1987; Barragy and Carey, 1988) is implemented to solve the linear equations. For elastoplastic failure, a Mohr-coulomb failure criterion is used with a viscoplastic strain method (Zienkiewicz and Cormeau, 1974).

This program does not automatically determine the factor of safety of slope stability. Simulations can be performed for a series of safety factors. After plotting the safety factor verses maximum displacement curve, one can determine the factor of safety of the given slope. Although the software is optimized for slope stability analysis and multistage excavation, other relevant simulations of quasistatic problems in solid (geo)mechanics can also be performed with this software.

The software currently does not include an inbuilt mesher. Existing tools, such as Gmsh (Geuzaine and Remacle, 2009), CUBIT (CUBIT, 2011), TrueGrid (Rainsberger, 2006), etc., can be used for hexahedral meshing, and the resulting mesh file can be converted to the input files required by SPECFEMX. Output data can be visualized and processed using the open-source visualization application ParaView ([www.paraview.org](http://www.paraview.org)).

### 1.2 Status summary

Slope stability analysis	: Yes
Multistage excavation	: Yes

Gravity loading	: Yes
Surface loading	: Yes (point load, uniformly distributed load, linearly distributed load) [Experimental]
Water table	: Yes [Experimental]
Pseudo-static earthquake loading	: Yes [Experimental]
Automatic factor of safety	: No

## Revisions

HNG, Jan 12, 2012; HNG, Sep 08, 2011; HNG, Jul 12, 2011; HNG, May 20, 2011; HNG, Jan 17, 2011

# Chapter 2

## Getting started

### 2.1 Package structure

The original SPEC-FEMX package comes in a single compressed file `SPEC-FEMX.tar.gz`, which can be extracted using `tar` command:

```
tar -zxvf SPEC-FEMX.tar.gz
```

or using, for example, 7-zip ([www.7-zip.org](http://www.7-zip.org)) under WINDOWS. The package has the following structure:

`SPEC-FEMX/`

<code>COPYING</code>	: License.
<code>README</code>	: brief description of the package.
<code>CMakeLists.txt</code>	: CMake configuration file.
<code>bin/</code>	: all object files and executables are stored in this folder.
<code>doc/</code>	: documentation files for the SPEC-FEMX package. If built this file is created.
<code>input/</code>	: contains input files.
<code>partition/</code>	: contains partition files for parallel processing.
<code>output/</code>	: default output folder. All output files are stored in this folder unless the different output path is defined in the main input file.
<code>src/</code>	: contains all source files.
<code>util/</code>	: contains all utilities source files.

### 2.2 Prerequisites

- CMake build system. The CMake version  $\geq 2.8.4$  is necessary to configure the software. It is free and open-source, and can be downloaded from [www.cmake.org](http://www.cmake.org).



- Make utility. The make utility is necessary to build the software using Makefile. This utility is usually installed by default in most LINUX systems. Under WINDOWS, one can use Cygwin ([www.cygwin.com](http://www.cygwin.com)) or MinGW ([www.mingw.org](http://www.mingw.org)) to install the make utility.
- A recent FORTRAN compiler. The software is written mainly in FORTRAN 90, but it also uses a few FORTRAN 2003 features (e.g., streaming IO). These features are already available in most of the FORTRAN compilers, e.g., gfortran version  $\geq 4.2$  ([gcc.gnu.org/wiki/GFortran](http://gcc.gnu.org/wiki/GFortran)) and g95 ([www.g95.org](http://www.g95.org)).

Following libraries are necessary for parallel processing.

- A recent MPI library. It should be built with the same FORTRAN compiler used to compile the software. Please see [www.open-mpi.org](http://www.open-mpi.org) or [www.mcs.anl.gov/research/projects/mpich2](http://www.mcs.anl.gov/research/projects/mpich2) for details on how to install MPI library and how to run MPI programs.
- SCOTCH graph partitioning library. This library should be compiled with the same FORTRAN compiler used to compile the software. Please see [www.labri.fr/perso/pelegrin/scotch](http://www.labri.fr/perso/pelegrin/scotch) for details on how to install SCOTCH.

Finally, the following compiler is necessary to build the documentation (this file):

- L<sup>A</sup>T<sub>E</sub>X compiler. This is necessary to compile the documentation files.

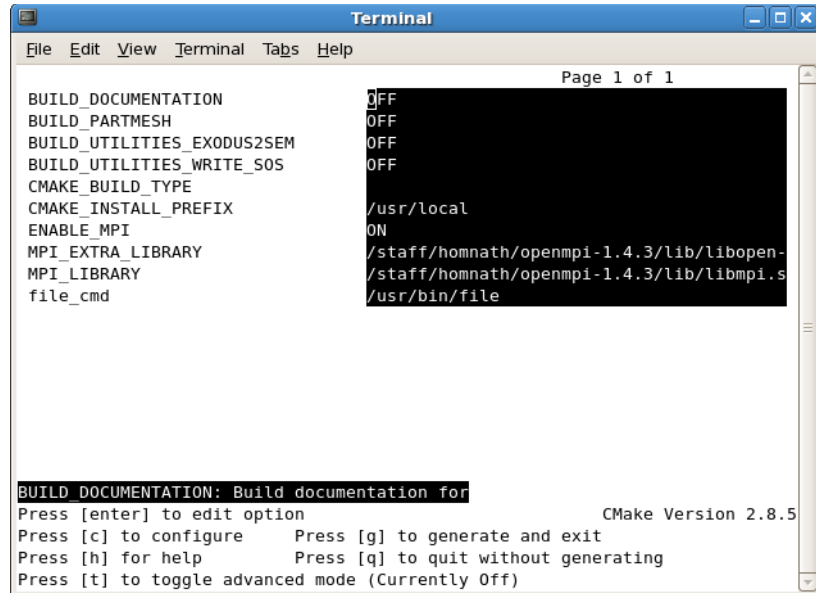
## 2.3 Configure

Software package SPECFEMX is configured using CMake, and the package uses an out-of-source build. Hence, DO NOT build in the same source directory. Let's say the full path to the package (source directory) is `$HOME/download/SPECFEMX`.

- Create a separate build directory, e.g.,  
`mkdir $HOME/work/SPECFEMX`
- Go to the build directory  
`cd $HOME/work/SPECFEMX`
- Type the cmake command  
`ccmake $HOME/projects/SPECFEMX`

CMake configuration is an iterative process (See Figure 2.1):

- Configure (c key or Configure button)
- Change variables' values if necessary
- Configure (c key or Configure button)

A screenshot of a terminal window titled "Terminal" showing the CMake configuration process for SPECfemX. The window has a menu bar with "File", "Edit", "View", "Terminal", "Tabs", and "Help". The main content area displays a list of CMake variables and their values. A black rectangular box highlights the values for several variables. At the bottom, there are instructions for navigating the CMake configuration interface, including pressing keys like 'enter', 'c', 'h', 't', 'g', and 'q'. The CMake version is 2.8.5.

```
Page 1 of 1
BUILD_DOCUMENTATION      OFF
BUILD_PARTMESH           OFF
BUILD_UTILITIES_EXODUS2SEM OFF
BUILD_UTILITIES_WRITE_SOS OFF
CMAKE_BUILD_TYPE
CMAKE_INSTALL_PREFIX     /usr/local
ENABLE_MPI               ON
MPI_EXTRA_LIBRARY         /staff/homnath/openmpi-1.4.3/lib/libopen-
MPI_LIBRARY              /staff/homnath/openmpi-1.4.3/lib/libmpi.s
file_cmd                 /usr/bin/file

BUILD DOCUMENTATION: Build documentation for
Press [enter] to edit option
Press [c] to configure    Press [g] to generate and exit
Press [h] for help        Press [q] to quit without generating
Press [t] to toggle advanced mode (Currently Off)

CMake Version 2.8.5
```

Figure 2.1: CMake configuration of SPECfemX .

If WARNINGS or ERRORS occur, press the e key (or the OK button) to return to configuration. These steps have to be repeated until successful configuration. Then, press the g key (or the Generate button) to generate build files. Check carefully that all necessary variables are set properly. Unless configuration is successful, generate is not enabled. Sometimes, the c key (or Configure button) has to be pressed repeatedly until generate is enabled. Initially, all variables may not be visible. To see all variables, toggle advanced mode by pressing the t key (or the Advanced button). To set or change a variable, move the cursor to the variable and press Enter key. If the variable is a boolean (ON/OFF), it will flip the value on pressing the Enter key. If the variable is a string or a file, it can be edited. For more details, please see the CMake documentation ([www.cmake.org](http://www.cmake.org)).

Following are the main CMake variables for the SPECfemX (See Figure 2.1)

<code>BUILD_DOCUMENTATION</code>	: If ON, the user manual (this file) is created. The default is OFF.
<code>BUILD_PARTMESH</code>	: If ON, the <code>partmesh</code> program is built. The default is OFF. The <code>partmesh</code> program is necessary to partition the mesh for parallel processing.
<code>BUILD_UTILITIES_EXODUS2SEM</code>	: If ON, the <code>exodus2sem</code> program is built. The default is OFF. The <code>exodus2sem</code> program convert exodus mesh file to input files required by the SPECFEMX package (see also Chapter 5).
<code>BUILD_UTILITIES_WRITE_SOS</code>	: If ON, the <code>write_sos</code> program is built. The default is OFF. The <code>write_sos</code> program writes a EnSight SOS file necessary for the parallel visualization (see also Chapter 5).
<code>ENABLE_MPI</code>	: If ON, the main parallel program <code>psemgeotech</code> is built otherwise main serial program <code>semgeotech</code> is built. The default is OFF.
<code>SCOTCH_LIBRARY_PATH</code>	: This is required if <code>BUILD_PARTMESH</code> is ON. If not found automatically, it can be set manually.
<code>CMAKE_Fortran_COMPILER</code>	: This defines the Fortran compiler. If not found automatically or the automatically found compiler is not correct, it can be set manually.

*Note 1: If `CMAKE_Fortran_COMPILER` has to be changed, first change this and configure, and then change other variables if necessary and configure.*

*Note 2: Even if some of the above variables are set ON, if appropriate working compilers are not found, corresponding variables are internally set OFF with WARNING messages.*

## 2.4 Compile

Once configuration and generation are successful, the necessary build files are created. Now to build the main program, type:

```
make
```

On multi-processor systems (let's say eight processors), type:

```
make -j 8
```

To clean, type

```
make clean
```

*Note: If reconfiguration is necessary, it is better to delete all Cache files of the build directory.*

## 2.5 Run

### Serial run

- To run the serial program, type  
`./bin/semgeotech input_file_name`

Example:

```
./bin/semgeotech ./input/validation1.sem
```

### Parallel run

- To partition the mesh, type  
`./bin/partmesh input_file_name`

Example:

```
./bin/partmesh ./input/validation1.psem
```

- To run the parallel program, type  
`mpirun -n number_of_nodes ./bin/psemgeotech input_file_name`

OR

```
mpirun -n number_of_nodes --hostfile host_file ./bin/psemgeotech input_file_name
```

Example:

```
mpirun -n 8 ./bin/psemgeotech ./input/validation1.psem
```

*Note: see Chapter 3 for details on input and input files. Try to run one or more examples included in `input/`. By default, example files included in the package are not copied to build directory during build process. If necessary, copy files within `input/` folder of source directory to the `input/` folder of build directory.*

# Chapter 3

## Input

### 3.1 Main input file

The main input file structure is motivated by the “E3D” (Larsen and Schultz, 1995) software package. The main input file consists of legitimate input lines defined in the specified formats. Any number of blank lines or comment lines can be placed for user friendly input structure. The blank lines contain no or only white-space characters, and the comment lines contain “#” as the first character.

Each legitimate input line consists of a line type, and list of arguments and corresponding values. All argument-value pair are separated by comma (.). If necessary, any legitimate input line can be continued to next line using FORTRAN 90 continuation character “&” as an absolute last character of a line to be continued. Repetition of same line type is not allowed.

Legitimate input lines have the format

*line\_type* *arg*<sub>1</sub> = *val*<sub>1</sub>, *arg*<sub>2</sub> = *val*<sub>2</sub>, ....., *arg*<sub>*n*</sub> = *val*<sub>*n*</sub>

Example:

```
preinfo:  nproc=8, ngllx=3, nglly=3, ngllz=3, nenod=8, ngnod=8, &  
inp_path='../input', part_path='../partition', out_path='../output/'
```

All legitimate input lines should be written in lower case. Line type and argument-value pairs must be separated by a space. Each argument-value pair must be separated by a comma(,) and a space/s. No space/s are recommended before line type and in between argument name and “=” or “=” and argument value. If argument value is a string, the FORTRAN 90 string (i.e., enclosed within single quotes) should be used, for example, `inp_path='../input'`. If the argument value is a vector (i.e., multi-valued), a list of values separated by space (no comma!) should be used, e.g, `srf=1.0 1.2 1.3 1.4`.

#### 3.1.1 Line types

Only the following line types are permitted.

```
preinfo:  preliminary information of the simulation  
mesh:      mesh information
```

**bc:** boundary conditions information  
**traction:** traction information [optional]  
**eqsource:** earthquake source information [optional]  
**stress0:** initial stress information [optional]. It is generally necessary for multistage excavation.  
**benchmark:** benchmark information [Optional]. This is necessary to compute benchmark results. Benchmark results are not available for all cases.  
**material:** material properties  
**eqload:** pseudo-static earthquake loading [optional]  
**water:** water table information [optional]  
**control:** control of the simulation  
**save:** options to save data  
**devel:** development parameters for experimental features [optional]

### 3.1.2 Arguments

Only the following arguments under the specified line types are permitted.

#### preinfo:

**nproc** : number of processors to be used for the parallel processing [integer > 1]. Only required for parallel processing.  
**ngllx** : number of Gauss-Lobatto-Legendre (GLL) points along  $x$ -axis [integer > 1].  
**nglly** : number of GLL points along  $y$ -axis [integer > 1].  
**ngllz** : number of GLL points along  $z$ -axis [integer > 1].

*Note: Although the program can use different values of **ngllx**, **nglly**, and **ngllz**, it is recommended to use same number of GLL points along all axes.*

**inp\_path** : input path where the input data are located [string, optional, default  $\Rightarrow$  '../input'].  
**part\_path** : partition path where the partitioned data will be or are located [string, optional, default  $\Rightarrow$  '../partition']. Only required for parallel processing.  
**out\_path** : output path where the output data will be stored [string, optional, default  $\Rightarrow$  '../output'].  
**disp\_dof** : switch to activate displacement degree of freedom [integer, optional, 0 = OFF, 1 = ON, default  $\Rightarrow$  1].

`grav_dof` : switch to activate gravity potential degree of freedom [integer, optional, 0 = OFF, 1 = ON, default  $\Rightarrow$  0].

`magnetic` : switch gravity potential to magnetic potential degree of freedom [integer, optional, 0 = OFF, 1 = ON, default  $\Rightarrow$  0].

`mesh:`

`xfile` : file name of  $x$ -coordinates [string].

`yfile` : file name of  $y$ -coordinates [string].

`zfile` : file name of  $z$ -coordinates [string].

`confile` : file name of mesh connectivity [string].

`idfile` : file name of element IDs [string].

`gfile` : file name of ghost interfaces, i.e., partition interfaces [string]. Only required for parallel processing.

`bc:`

`ubc` : switch to apply primary/essential boundary condition [integer, optional, 0 = OFF, 1 = ON, default  $\Rightarrow$  1].

`uxfile` : file name of displacement boundary conditions along  $x$ -axis [string].

`uyfile` : file name of displacement boundary conditions along  $y$ -axis [string].

`uzfile` : file name of displacement boundary conditions along  $z$ -axis [string].

`infbc` : switch to apply infinite boundary condition [integer, optional, 0 = OFF, 1 = ON, default  $\Rightarrow$  0].

`add_infmesh` : switch to add infinite mesh layer [integer, optional, 0 = OFF, 1 = ON, default  $\Rightarrow$  0].

`infrfile` : surface file on which the infinite elements are created [string].

`mat_type` : type of material block for infinite elements [string, 'define' = Define specific material block IDs for transition infinite and infinite regions, 'inherit' = Inherit material block IDs of the parent elements].

`imat_trinf` : material block ID for transition-infinite elements [integer, optional].

`imat_inf` : material block ID for infinite elements [integer, optional but must be defined if `mat_type`='define'].

`pole0` : initial pole for the infinite element layer [string, optional, 'origin' = Origin of the model, 'center' = Center of the model, 'user' = User-defined, default  $\Rightarrow$  'origin'].

**pole\_type** : pole type for the infinite element layer [string, optional, 'point' = A point, 'axis' = Multipoles on the axis, 'pointaxis' = Single pole and multipoles on the axis, 'plane' = Multipoles on the plane, default  $\Rightarrow$  'point'].

**coord0** : user defined coordinates for the pole [real vector].

**coord1** : user defined coordinates for the end pole [real vector, optional]. It is necessary only if the **pole\_type**='pointaxis'.

**pole\_axis** : pole axis [integer, 1 = X-axis, 2 = Y-axis, 3 = Z-axis]. This must be defined for 'pole\_type' = 'axis' or 'pointaxis'.

**axis\_range** : range of the pole coordinates along the pole axis [real two-component vector, optional]. This must be defined for 'pole\_type' = 'pointaxis'.

**rinf** : reference radius for infinite elements [real].  $rinf >$  largest corner distance from the pole.

**valinf** : value of the primary variable at the infinity [real, default  $\Rightarrow$  0.0].

**infquad** : quadrature type in the infinite elements [string, optional, 'radau' = Radau quadrature, 'gauss' = Gauss quadrature, default  $\Rightarrow$  'radau'].

**traction:**

**trfile** : file name of traction specification [string].

**eqsource:**

**type** : type of earthquake source [integer, optional, 0 = slip source, 1 = CMT source, 2 = Finite fault, 3 = Slip with split node, default  $\Rightarrow$  0].

**slipfile** : file name of slip information [string].

**cmtfile** : file name of CMT information [string].

**faultslipfile\_plus** : file name of fault slip information for plus side [string].

**faultslipfile\_minus** : file name of fault slip information for minus side [string].

**shalf** : switch to use equal, i.e., half of the slip on each side of the fault [integer, optional, 0 = No, 1 = Yes, default  $\Rightarrow$  0]. Only required for slip with split node.

**taper** : switch to taper the slip on the fault edge [integer, optional, 0 = No, 1 = Yes, default  $\Rightarrow$  1]. Only required for slip with split node.

**stress0:**

**type** : type of initial stress [integer, optional, 0 = compute using SEM itself, 1 = compute using simple vertical lithostatic relation, default  $\Rightarrow$  0].



**z0** : datum (free surface) coordinate [real, m]. Only required if **type**=1.  
**s0** : datum (free surface) vertical stress [real, kN/m<sup>2</sup>]. Only required if **type**=1.  
**k0** : lateral earth pressure coefficient [real].

#### benchmark:

**okada** : compute Okada benchmark results [integer, optional, 0 = NO, 1 = YES, default  $\Rightarrow$  0].

**error** : compute error norm with benchmark result [integer, optional, 0 = NO, 1 = YES, default  $\Rightarrow$  0].

#### material:

**matfile** : file name of material list [string].

**ispart** : flag to indicate whether the material file is partitioned [integer, optional, 0 = No, 1 = Yes, default  $\Rightarrow$  0]. Only required for parallel processing.

**matpath** : path to material file [string, optional, default  $\Rightarrow$  '../input' for serial or unpartitioned material file in parallel and '../partition' for partitioned material file in parallel].

**allelastic** : assume all entire domain as elastic [integer, optional, 0 = No, 1 = Yes, default  $\Rightarrow$  0].

**density** : flag to indicate that unit weight column is density [integer, optional, 0 = No, 1 = Yes, default  $\Rightarrow$  0].

#### eqload:

**eqkx** : pseudo-static earthquake loading coefficient along  $x$ -axis [real,  $0 \leq \text{eqkx} \leq 1.0$ , default  $\Rightarrow$  0.0].

**eqky** : pseudo-static earthquake loading coefficient along  $y$ -axis [real,  $0 \leq \text{eqky} \leq 1.0$ , default  $\Rightarrow$  0.0].

**eqkz** : pseudo-static earthquake loading coefficient along  $z$ -axis [real,  $0 \leq \text{eqkz} \leq 1.0$ , default  $\Rightarrow$  0.0].

*Note: For the stability analysis purpose, these coefficients should be chosen carefully. For example, if the slope face is pointing towards the negative  $x$ -axis, value of **eqkx** is taken negative.*

#### water:

**wsfile** : file name of water surface file.

control:

`ksp_tol` : tolerance for conjugate gradient method [real].

`ksp_maxiter` : maximum iterations for conjugate gradient method [integer > 0].

`nl_tol` : tolerance for nonlinear iterations [real].

`nl_maxiter` : maximum iterations for nonlinear iterations [integer > 0].

`ninc` : number of load increments for the plastic iterations [integer>0 default  $\Rightarrow$  1]. This is currently not used for slope stability analysis.

Arguments specific to slope stability analysis:

`nsrf` : number of strength reduction factors to try [integer > 0, optional, default  $\Rightarrow$  1].

`srf` : values of strength reduction factors [real vector, optional, default  $\Rightarrow$  1.0]. Number of `srf`s must be equal to `nsrf`.

`phinu` : force  $\phi - \nu$  (Friction angle - Poisson's ratio) inequality:  $\sin \phi \geq 1 - 2\nu$  (see Zheng et al., 2005) [integer, 0 = No, 1 = Yes, default  $\Rightarrow$  0]. Only for TESTING purpose.

Arguments specific to multistage excavation:

`nexcav` : number of excavation stages [integer > 0, optional, default  $\Rightarrow$  1].

`nexcavid` : number of excavation IDs in each excavation stage [integer vector, default  $\Rightarrow$  1].

`excavid` : IDs of blocks/regions in the mesh to be excavated in each stage [integer vector, default  $\Rightarrow$  1].

*Note: Do not mix arguments for slope stability and excavation.*

save:

`disp` : displacement field [integer, optional, 0 = No, 1 = Yes, default  $\Rightarrow$  0].

`model` : model properties [integer, optional, 0 = No, 1 = Yes, default  $\Rightarrow$  0].

`porep` : pore water pressure [integer, optional, 0 = No, 1 = Yes, default  $\Rightarrow$  0].

`gpot` : gravitational or magnetic potential [integer, optional, 0 = No, 1 = Yes, default  $\Rightarrow$  0].

`agrav` : gradient of potential, e.g., acceleration due to gravity [integer, optional, 0 = No, 1 = Yes, default  $\Rightarrow$  0].

devel:

`nondim` : nondimensionalize model [integer, optional, 0 = No, 1 = Yes, default  $\Rightarrow$  1].

`example` : simulate particular example [string, optional, default  $\Rightarrow$  None].

### 3.1.3 Examples of main input file

#### Input file for a simple elastic simulation

```
#-----  
#input file elastic.sem  
#pre information  
preinfo:  ngllx=3, nglly=3, ngllz=3, nenod=8, ngnod=8, &  
inp_path='../input', out_path='../output/'  
  
#mesh information  
mesh:  xfile='validation1_coord_x', yfile='validation1_coord_y', &  
zfile='validation1_coord_z', confile='validation1_connectivity', &  
idfile='validation1_material_id'  
  
#boundary conditions  
bc:  uxfile='validation1_ssbcux', uyfile='validation1_ssbcuy', &  
uzfile='validation1_ssbcuz'  
  
#material list  
material:  matfile='validation1_material_list', allelastic=1  
  
#control parameters  
control:  ksp_tol=1e-8, ksp_maxiter=5000  
#-----
```

## Serial input file for slope stability

```
#-----
#input file validation1.sem
#pre information
preinfo:  ngllx=3, nglly=3, ngllz=3, nenod=8, ngnod=8, &
inp_path='../input', out_path='../output/'

#mesh information
mesh:  xfile='validation1_coord_x', yfile='validation1_coord_y', &
zfile='validation1_coord_z', confile='validation1_connectivity', &
idfile='validation1_material_id'

#boundary conditions
bc:  uxfile='validation1_ssbcux', uyfile='validation1_ssbcuy', &
uzfile='validation1_ssbcuz'

#material list
material:  matfile='validation1_material_list'

#control parameters
control:  ksp_tol=1e-8, ksp_maxiter=5000, nl_tol=0.0005, nl_maxiter=3000,
&
nsrf=9, srf=1.0 1.5 2.0 2.15 2.16 2.17 2.18 2.19 2.20
#-----
```

## Parallel input file for slope stability

```
#-----
#input file validation1.psem
#pre information
preinfo: nproc=8, ngllx=3, nglly=3, ngllz=3, nenod=8, &
ngnod=8, inp_path='../input', out_path='../output/'

#mesh information
mesh: xfile='validation1_coord_x', yfile='validation1_coord_y', &
zfile='validation1_coord_z', confile='validation1_connectivity', &
idfile='validation1_material_id', gfile='validation1_ghost'

#boundary conditions
bc: uxfile='validation1_ssbcux', uyfile='validation1_ssbcuy', &
uzfile='validation1_ssbcuz'

#material list
material: matfile='validation1_material_list'

#control parameters
control: ksp_tol=1e-8, ksp_maxiter=5000, nl_tol=0.0005, nl_maxiter=3000,
&
nsrf=9, srf=1.0 1.5 2.0 2.15 2.16 2.17 2.18 2.19 2.20
#-----
```

## Serial input file for excavation

```
#-----  
#input file excavation_3d.sem  
#pre information  
preinfo:  ngllx=3, nglly=3, ngllz=3, nenod=8, ngnod=8, &  
inp_path='../input', out_path='../output/'  
  
#mesh information  
mesh:  xfile='excavation_3d_coord_x', yfile='excavation_3d_coord_y', &  
zfile='excavation_3d_coord_z', confile='excavation_3d_connectivity', &  
idfile='excavation_3d_material_id'  
  
#boundary conditions  
bc:  uxfile='excavation_3d_ssbcux', uyfile='excavation_3d_ssbcuy', &  
uzfile='excavation_3d_ssbcuz'  
  
#initial stress stress0:  type=0, z0=0, s0=0, k0=0.5, usek0=1  
  
#material list  
material:  matfile='excavation_3d_material_list'  
  
#control parameters  
control:  ksp_tol=1e-8, ksp_maxiter=5000, nl_tol=0.0005, nl_maxiter=3000,  
&  
nexcav=3, excavid=2 3 4, ninc=10  
#-----
```

## Parallel input file for excavation

```
#-----
#input file excavation_3d.psem
#pre information
preinfo: nproc=8, ngllx=3, nglly=3, ngllz=3, nenod=8, &
ngnod=8, inp_path='../input', out_path='../output/'

#mesh information
mesh: xfile='excavation_3d_coord_x', yfile='excavation_3d_coord_y', &
zfile='excavation_3d_coord_z', confile='excavation_3d_connectivity', &
idfile='excavation_3d_material_id', gfile='excavation_3d_ghost'

#boundary conditions
bc: uxfile='excavation_3d_ssbucx', uyfile='excavation_3d_ssbucy', &
uzfile='excavation_3d_ssbucz'

#initial stress stress0: type=0, z0=0, s0=0, k0=0.5, usek0=1

#material list
material: matfile='excavation_3d_material_list'

#control parameters
control: ksp_tol=1e-8, ksp_maxiter=5000, nl_tol=0.0005, nl_maxiter=3000,
&
nexcav=3, excavid=2 3 4, ninc=10
#-----
```

There are only two additional pieces of information, i.e., number of processors '**nproc**' in line '**preinfo**' and file name for ghost partition interfaces '**gfile**' in line '**mesh**' in parallel input file.

## 3.2 Input files detail

All local element/face/edge/node numbering follows the EXODUS II convention.

### 3.2.1 Coordinates files: xfile, yfile, zfile

Each of the coordinates files contains a list of corresponding coordinates in the following format:

```
number of points
coordinate of point 1
coordinate of point 2
coordinate of point 3
..
..
```

..

Example:

```
2354
40.230394465164999
40.759090909090901
42.700000000000003
40.957142857142898
40.230394465164999
40.759090909090901
42.700000000000003
40.957142857142898
...
...
```

### 3.2.2 Connectivity file: confile

The connectivity file contains the connectivity lists of elements in the following format:

```
number of elements
n1 n2 n3 n4 n5 n6 n7 n8 of element 1
n1 n2 n3 n4 n5 n6 n7 n8 of element 2
n1 n2 n3 n4 n5 n6 n7 n8 of element 3
n1 n2 n3 n4 n5 n6 n7 n8 of element 4
..
..
```

Example:

```
1800
1 2 3 4 5 6 7 8
9 10 2 1 11 12 6 5
9 1 4 13 11 5 8 14
15 16 10 9 17 18 12 11
15 9 13 19 17 11 14 20
21 22 16 15 23 24 18 17
21 15 19 25 23 17 20 26
27 28 22 21 29 30 24 23
27 21 25 31 29 23 26 32
33 34 28 27 35 36 30 29
33 27 31 37 35 29 32 38
34 33 39 40 36 35 41 42
33 37 43 39 35 38 44 41
...
...
```



### 3.2.3 Element IDs (or Material IDs) file: idfile

This file contains the IDs of elements. This ID will be used in the program mainly to identify the material regions. This file has the following format:

```
number of elements
ID of element 1
ID of element 2
ID of element 3
ID of element 4
...
...
```

Example:

```
1800
1
1
1
1
1
1
1
1
1
1
1
...
...
```

### 3.2.4 Ghost partition interfaces file: gfile

This file will be generated automatically by a program `partmesh`.

### 3.2.5 Displacement boundary conditions files: uxfile, uyfile, uzfile

This file contains information on the displacement boundary conditions (currently only the zero-displacement is implemented), and has the following format:

```
number of element faces
elementID faceID
elementID faceID
elementID faceID
...
...
```

Example:

```
849
2 2
3 4
5 1
6 1
7 1
8 1
9 1
...
...
```

### 3.2.6 Traction file: trfile

This file contains the traction information on the model in the following format:

```
traction type (integer, 0 = point, 1 = uniformly distributed, 2 = linearly distributed)
if traction type = 0
qx qy qz (load vector in kN)
if traction type = 1
qx qy qz (load vector in kN/m2)
if traction type = 2
relevant-axis x1 x2 qx1 qy1 qz1 qx2 qy2 qz2
number of entities (points for point load or faces for distributed load)
elementID entityID
elementID entityID
elementID entityID
...
...
```

This can be repeated as many times as there are tractions.

The *relevant-axis* denotes the axis along which the load is varying, and is represented by an integer as 1 = *x*-axis, 2 = *y*-axis, and 3 = *z*-axis. The variables *x<sub>1</sub>* and *x<sub>2</sub>* denote the coordinates (only the *relevant-axis*) of two points between which the linearly distributed load is applied. Similarly, *q<sub>x1</sub>*, *q<sub>y1</sub>* and *q<sub>z1</sub>*, and *q<sub>x2</sub>*, *q<sub>y2</sub>* and *q<sub>z2</sub>* denote the load vectors in kN/m<sup>2</sup> at the point 1 and 2, respectively.

Example:

The following data specify the two tractions: a uniformly distributed traction and a linearly distributed traction.

```
1
0.0 0.0 -167.751
363
```

```

56 1
57 1
58 1
59 1
60 1
61 1
62 1
...
...
2
3 7.3 24.4 51.8379 0.0 -159.5407 0.0 0.0 0.0
594
38 1
39 1
40 1
41 1
42 1
43 1
44 1
45 1
46 1
...
...

```

### 3.2.7 Material list file: matfile

This file contains material properties of each material regions. Material properties must be listed in a sequential order of the unique material IDs. In addition, this data file optionally contains the information on the water condition of material regions. Material regions or material IDs must be consistent with the Material IDs (Element IDs) defined in `idfile`. The `matfile` has the following format:

```

comment line
number of material regions (unique material IDs)
materialID, domainID, type,  $\gamma$ ,  $E$ ,  $\nu$ ,  $\phi$ ,  $c$ ,  $\psi$ 
materialID, domainID, type, file
materialID, domainID, type,  $\gamma$ ,  $E$ ,  $\nu$ ,  $\phi$ ,  $c$ ,  $\psi$ 
...
...
number of submerged material regions
submerged materialID
submerged materialID
...
...

```

The *materialID* must be in a sequential order starting from 1. The *domainID* represents

the material domain (e.g., 1 = elastic or 11 = viscoelastic), and *type* represents the type of material properties input (0 = Homogeneous material block  $\Rightarrow$  define  $\gamma$ ,  $E$ ,  $\nu$ ,  $\phi$ ,  $c$ , and  $\psi$ ; -1 = Tomographic model input defined on the structured grid  $\Rightarrow$  define file name). Similarly,  $\gamma$  represents the unit weight in kN/m<sup>3</sup>,  $E$  the Young's modulus of elasticity in kN/m<sup>2</sup>,  $\phi$  the angle of internal friction in degrees,  $c$  the cohesion in kN/m<sup>2</sup>, and  $\psi$  the angle of dilation in degrees. Finally, *file* is the file name of the tomographic structured grid input.

Example:

The following data defines four material regions. No region is submerged in water.

```
# material properties (id, domain, type, gamma, ym, nu, phi, coh, psi)
4
1 1 0 18.8 1e5 0.3 20.0 29.0 0.0
2 1 0 19.0 1e5 0.3 20.0 27.0 0.0
3 1 0 18.1 1e5 0.3 20.0 20.0 0.0
4 1 0 18.5 1e5 0.3 20.0 29.0 0.0
```

The following data defines four material regions with two of them submerged.

```
# material properties (id, domain, type, gamma, ym, nu, phi, coh, psi)
4
1 1 0 18.8 1e5 0.3 20.0 0.0 0.0
2 1 0 19.0 1e5 0.3 20.0 27.0 0.0
3 1 0 18.1 1e5 0.3 20.0 0.0 0.0
4 1 0 18.5 1e5 0.3 20.0 29.0 0.0
2
1
3
```

The following data defines 1 material region with tomographic structured grid input.

```
# material properties (id, domain, type, gamma, ym, nu, phi, coh, psi)
1
1 1 -1 Groningen_DH_1500mstart.txt
```

Tomographic structured grid file has the following format:

```
 $x_0$   $y_0$   $z_0$   $x_{\text{end}}$   $y_{\text{end}}$   $z_{\text{end}}$ 
 $dx$   $dy$   $dz$ 
 $n_x$   $n_y$   $n_z$ 
 $v_p$  min  $v_p$  max  $v_s$  min  $v_s$  max  $\rho$  min  $\rho$  max
 $x_1$   $y_1$   $z_1$   $v_{p1}$   $v_{s1}$   $\rho_1$ 
 $x_2$   $y_2$   $z_2$   $v_{p2}$   $v_{s2}$   $\rho_2$ 
```

```

 $x_3$   $y_3$   $z_3$   $v_{p3}$   $v_{s3}$   $\rho_3$ 
...
...
 $x_n$   $y_n$   $z_n$   $v_{pn}$   $v_{sn}$   $\rho_n$ 

```

where,  $n = n_x \times n_y \times n_z$  is the total number of grid points.

### 3.2.8 Water surface file: wsfile

This file contains the water table information on the model in the format as

*number of water surfaces*

*water surface type* (integer, 0 = horizontal surface, 1 = inclined surface, 2 = meshed surface)

if *wstype*=0 (can be reconstructed by sweeping a horizontal line)

*relevant-axis*  $x_1$   $x_2$   $z$

if *wstype*=1 (can be reconstructed by sweeping a inclined line)

*relevant-axis*  $x_1$   $x_2$   $z_1$   $z_2$

if *wstype*=2 (meshed surface attached to the model)

*number of faces*

*elemetID, faceID*

*elemetID, faceID*

*elemetID, faceID*

...

...

The *relevant-axis* denotes the axis along which the line is defined, and it is taken as 1 =  $x$ -axis, 2 =  $y$ -axis, and 3 =  $z$ -axis. The variables  $x_1$  and  $x_2$  denote the coordinates (only *relevant-axis*) of point 1 and 2 that define the line. Similarly,  $z$  denotes a  $z$ -coordinate of a horizontal water surface, and  $z_1$  and  $z_2$  denote the  $z$ -coordinates of the two points (that define the line) on the water surface.

Example:

Following data specify the two water surfaces: a horizontal surface and an inclined surface.

```

2
0
1 42.7 50.0 6.1
1
1 0.0 42.7 12.2 6.1

```

# Chapter 4

## Output and Visualization

### 4.1 Output files

#### 4.1.1 Summary file

This file is self explanatory and it contains a summary of the results including control parameters, maximum displacement at each step, and elapsed time. The file is written in ASCII format and its name follows the convention *input\_file\_name\_header\_summary* for serial run and *input\_file\_name\_header\_summary\_procprocessor\_ID* for parallel run.

#### 4.1.2 Mesh files

This file contains the mesh information of the model including coordinates, connectivity, element types, etc., in EnSight Gold binary format (see EnSight, 2008). The file name follows the format *input\_file\_name\_header\_summary* for serial run and *input\_file\_name\_header\_summary\_procprocessor\_ID* for parallel run.

#### 4.1.3 Displacement field file

This file contains the nodal displacement field in the model written in EnSight Gold binary format. The file name follows the format *input\_file\_name\_header\_stepstep.dis* for serial run and *input\_file\_name\_header\_stepstep\_procprocessor\_ID.dis* for parallel runs.

#### 4.1.4 Pore pressure file

This file contains the hydrostatic pore pressure field in the model written in EnSight Gold binary format. The file name follows the format *input\_file\_name\_header\_stepstep.por* for serial run and *input\_file\_name\_header\_stepstep\_procprocessor\_ID.por* for parallel run.

#### 4.1.5 CASE file

This is an EnSight Gold CASE file written in ASCII format. This file contain the information on the mesh files, other files, time steps etc. The file name follows the format *input\_file\_name\_header.case* for serial run and *input\_file\_name\_header\_procprocessor\_ID.case* for parallel run.

### 4.1.6 SOS file

This is an EnSight Gold server-of-server file for parallel visualization. The `write_sos.f90` program provided in the `/utilities/` may be used to generate this file. See Chapter ??, Section 5.2 for more detail.

All above EnSight Gold files correspond to the model with spectral-element mesh. Additionally, the CASE file/s and mesh file/s are written for the original model. These file names follow the similar conventions and they have the tag '`original`' in the file name headers.

## 4.2 Visualization

### 4.2.1 Serial visualization

Requirement: ParaView version later than 3.7. Precompiled binaries available from ParaView web ([www.paraview.org](http://www.paraview.org)) may be installed directly or it can be build from the source.

- open a session
- open paraview client  
`paraview`
- In ParaView client:  $\Rightarrow$  File  $\Rightarrow$  Open  
select appropriate serial CASE file (.case file)  
see ParaView wiki [paraview.org/Wiki/ParaView](http://paraview.org/Wiki/ParaView) for more detail.

### 4.2.2 Parallel visualization

Requirement: ParaView version later than 3.7. It should be built enabling MPI. An appropriate MPI library is necessary.

- open a session
- open paraview client  
`paraview`
- start ParaView server  
`mpirun -np 8 pvserver -display :0`
- In ParaView client:  $\Rightarrow$  File  $\Rightarrow$  Connect and connect to the appropriate server
- In ParaView client:  $\Rightarrow$  Open  
select appropriate SOS file (.sos file)  
see ParaView wiki ([paraview.org/Wiki/ParaView](http://paraview.org/Wiki/ParaView)) for more detail.

*Note: Each CASE file obtained from the parallel processing can also be visualized in a serial.*

# Chapter 5

## Utilities

### 5.1 Convert EXODUS mesh into SEM files

The program `exodus2sem.c` contained in the `util` directory can be used to convert the mesh file in EXODUS II format to input files required by the SPEC FEMX .

#### Compile

```
gcc -o exodus2sem exodus2sem.c
```

#### Run

```
exodus2sem EXODUS_mesh_file OPTIONS
```

For more details, see `util/README_exodus2sem`. It can also be compiled automatically during the build process of main package SPEC FEMX (see Section 2.3).

### 5.2 Generate SOS file

The program `write_sos.f90` contained in the `util` directory can be used to write EnSight Gold server-of-server file (.sos file, see (EnSight, 2008)) to visualize the multi-processors data in parallel. This file does not contain the actual data, but only information on the data location and parallel processing.

#### Compile

```
gfortran -o write_sos write_sos.f90
```

#### Run

```
exodus2sem input_file
```

For more details, see `util/README_write_sos`. It can also be compiled automatically during the build process of main package SPEC FEMX (see Section 2.3).



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