

COUPLING AXISEM AND SPECFEM3D

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NOTE : We have to finally choose which AxiSEM version we add and definitely use for coupling with SPECFEM3D.

The paths present here are from specfem3d home directory.

Here, 'run' is an alias for Curie defined as : `run='ccc_msub -q standard'`.

1 STEP 1 : meshfem3D

- Go in 'EXAMPLES/coupling_with_EXTERNAL_CODES/with_AxiSEM/example_1st_for_validation', (OR, create another subdirectory in '[...]/with_AxiSEM', copy files from '[...]/example_1st_for_validation' and modify them if you need)
- **CAUTION!!** : Check the file 'paths_for_coupling_SPECFEM3D_AxiSEM.sh' and modify the variable 'HOME_SPECFEM3D' \implies this is the only path you have to modify for specfem3d
- Type :

```
./clean_this_example_dir.sh
```

```
run ./batch_coupling_step1_create_dir_and_paths+_meshfem3d_for_AxiSEM.sh
```

It generates mesh files (on 1 proc on Curie), and copies files 'list_gll_boundary_spherical.txt' and 'list_gll_boundary_cartesian.txt' in AxiSEM solver dir.

Also, check Meshfem3D with parameters \implies In the directory MESH/ :

- 'ParFileMeshChunk' : parameters for the chunk meshing
- 'iasp91_dsm' or 'prem_dsm' : background model used in both AxiSEM and Specfem3D

In the Directory DATA/ :

- 'CMTSOLUTION' : with 0 in order to not use source inside
- 'coeff_poly_deg12' : to generate smooth initial solution
- 'STATIONS' : stations files
- Set the file 'Par_file' with these parameters :
 - SIMULATION_TYPE=1
 - SAVE_FORWARD = .false.
 - COUPLE_WITH_EXTERNAL_CODE = .true
 - EXTERNAL_CODE_TYPE = 2

2 STEP 2 : AxiSEM mesher

Go in : 'utils/EXTERNAL_CODES_coupled_with_SPECFEM3D/AxiSEM_for_SPECFEM3D/AxiSEM_modif_for_coupling_with_specfem/MESHER'.

Check the file 'inparam_mesh'

Type : ./submit.csh

It run the mesher in serial : check file OUTPUT (wait for "....DONE WITH MESHER" to appear in OUTPUT)

Type : ./movemesh.csh NAME_OF_DESTINATION_MESH_DIR

It moves mesh files to ../SOLVER/MESHES/NAME_OF_DESTINATION_MESH_DIR

For more details, see Axisem manual.

3 STEP 3 : AxiSEM solver

2 files produced by meshfem3D (input_box.txt and input_box_sem_cart.txt) were copied (and the first line indicating the number of line to be read were add at the beginning of the files too) during the STEP 1 in the AxiSEM SOLVER dir.

Go in 'utils/EXTERNAL_CODES_coupled_with_SPECFEM3D/AxiSEM_for_SPECFEM3D/AxiSEM_modif_for_coupling_with_specfem/SOLVER'

Check 'inparam_basic' (set the value for MESHNAME to the meshname from above, among others), and also (differences with *.TEMPLATES provided by AxiSEM) :

- ATTENUATION false
- SAVE_SNAPSHOTS true

Check 'inparam_advanced' :

- KERNEL_WAVEFIELDS true
- KERNEL_IBEG 0
- KERNEL_IEND 4

Type : ./sub_launch_script_for_run_AxiSEM_Curie_CD.csh NAME_OF_RESULTS_DIR

!! CAUTION : don't forget "NAME_OF_RESULTS_DIR" (it will be your results folder, and a sub-folder of SOLVER/)

It run, on N procs in batch on Curie, the compilation and the execution of AxiSEM solver. Among others, this script calls :

./add_line_number_in_points_lists.sh (rename files 'list_gll_boundary_spherical.txt' & 'list_gll_boundary_cartesian.txt', and add number of lines)

run ./sub_called_batch_for_AxiSEM_Curie_CD.sh (submit the job on Curie)

4 STEP 4 : Specfem Partitionning & STEP 5 : Specfem Generate data-base

Go back in 'EXAMPLES/coupling_with_EXTERNAL_CODES/with_AxiSEM/example_1st_for_validation'

Type : `run ./batch_coupling_step4_and_step5_scoth_part_and_generdata_for_AxiSEM.sh`

!! CAUTION : the number of procs in DATA/Par_file, have to be the same as in the 'inparam_mesh' (cf STEP 2) of AxiSEM!!

5 Interface \implies STEP 6 : expand 2D to 3D & STEP 7 : reformat

Go in 'utils/EXTERNAL_CODES_coupled_with_SPECFEM3D/AxiSEM_for_SPECFEM3D/AxiSEM_modif_for_coupling_with_specfem/SOLVER'

- Check the file 'expand_2D_3D.par', cf THE PATHS IN THE 3 LAST LINES (normally, these are the only paths you to modify in the AxiSEM dir)!! \implies Caution : for the tractions path (for example : `/[...]/AxiSEM_tractions/1/`), the directory need to be created!!!! \implies the script 'sub_launch_script_for_make+_run_expand2D3D_and_reformat_Curie_CD.sh' create a traction directory here :

'EXAMPLES/coupling_with_EXTERNAL_CODES/with_AxiSEM/example_1st_for_validation/DATA/AxiSEM_tractions/1/'

BUT, if you don't use this script or if you want to create another tractions dir, you have to create the directory yourself.

Example :

```
input_box.txt
input_box_sem_cart.txt
32                # number of AxiSEM mpi processes used in solver
90. 0.            # source position (lat lon)
0. 60.           # chunk center (lat lon)
1                # number of axisem simus depends on moment tensor used
32               # number of Specfem3D MPI processes
/[...]/example_1st_for_validation/MESH                # Specfem MESH dir
/[...]/example_1st_for_validation/OUTPUT_FILES/DATABASES_MPI # Specfem databases dir
/[...]/example_1st_for_validation/DATA/AxiSEM_tractions/1  # AxiSEM tractions dir
```

- Check the file 'reformat.par'

Example :

```
10.              # = 1/DT, i.e. output sampling in Hz (time step that will use in Specfem3D simu)
710. 1800.       # begin time and end time (s.)
```

You can launch the compilation (of expand_2D_3D and reformat) AND the execution of this two programs with the single script :

`./sub_launch_script_for_make+_run_expand2D3D_and_reformat_Curie_CD.sh NAME_OF_RESULTS_DIR`

!! CAUTION : don't forget "NAME_OF_RESULTS_DIR"!!

It will do the compilation, launch `./sub_called_batch_for_expand2D3D_Curie_CD.sh`, and at the end, launch `./sub_called_batch_for_reformat_Curie_CD.sh` \Leftarrow IMPORTANT : for the expand_2D_3D part, the number processes is arbitrary, BUT for the reformat part you have to configure the batch with the ****SAME**** number of processes that Specfem3D will use. One file is created by one process for one Specfem3D partion of domain.

All the results will be in 'NAME_OF_RESULTS_DIR'.

If you prefer you do this step by step :

- Go in 'utils/EXTERNAL_CODES_coupled_with_SPECFEM3D/AxiSEM_for_SPECFEM3D/UTILS_COUPLING_SpecFEM' to make the compilation.
- Go in NAME_OF_RESULTS_DIR and type : `run ../sub_called_batch_for_expand2D3D_Curie_CD.sh` to submit expand_2D_3D
- Go in NAME_OF_RESULTS_DIR and type : `run ../sub_called_batch_for_reformat_Curie_CD.sh` to submit reformat

6 STEP 8 : Running specfem3D

Go in 'EXAMPLES/coupling_with_EXTERNAL_CODES/with_AxiSEM/example_1st_for_validation'

Check in 'DATA/Par_file', the lines after the comment "# time step parameters", these parameters must coincide with the parameters in 'reformat.par' (cf STEP 7) :

- `NSTEP = 10900` # \Rightarrow cf the two values in the second line of 'reformat.par'. This value equals to :

$$\frac{\text{second value} - \text{the first}}{DT} \left(= \frac{\text{duration of physical time}}{DT} \right)$$

So here, it is : $\frac{1800 - 710}{0.1} = 10900$

- `DT = 0.1` # \Rightarrow the inverse of the first line in 'reformat.par' (which is 1/DT)

Also check in 'DATA/Par_file', the lines after the comment "# to couple with an external code (such as DSM, AxiSEM, or FK)" :

- `COUPLE_WITH_EXTERNAL_CODE = .true.` # \Rightarrow always set it to '.true.' in this case
- `EXTERNAL_CODE_TYPE = 2` # 1 = DSM, 2 = AxiSEM, 3 = FK \Rightarrow always set it to '2' for AxiSEM
- `TRACTION_PATH = ./DATA/AxiSEM_tractions/1/` # \Rightarrow This is where there are the tractions from AxiSEM (from steps 6 and 7)!! CAUTION : verify that they are in this dir, in the form of files 'proc0000*_sol_axisem', etc.!!
- `MESH_A_CHUNK_OF_THE_EARTH = .true.` # \Rightarrow always set it to '.true.' in this case

And finally, type : `run ./batch_coupling_step8_xspecfem3d.sh`

7 STEP ? : Set up scripts