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 form specfem3d home directory.

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

We show the process of the coupling, for the example : 'EXAMPLES/coupling_with_EXTERNAL_CODES/with_AxiSEM/example_1st_for_validation', see the file 'README_example_details' for some particulars of this example.

There are other examples in 'EXAMPLES/coupling_with_EXTERNAL_CODES/with_AxiSEM/' with other set of parameters.

In Axisem directory, there are all the parameter files, scripts, stations, etc., to put in Axisem mesher and solver directories, for each example, here : 'utils/EXTERNAL_CODES_coupled_with_SPECFEM3D/AxiSEM_for_SPECFEM3D/Parfiles_and_scripts_for_examples' Cf 'README' in this directory for more details.

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' $\Longrightarrow$ 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 $\Longrightarrow$ 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 intitial 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 ('list_gll_boundary_spherical.txt' and 'list_gll_boundary_cartesian.txt') were copied 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) :

- MESHNAME NAME_OF_DESTINATION_MESH_DIR
- ATTENUATION false
- SAVE_SNAPSHOTS true

Check 'inparam_advanced' :

- KERNEL_WAVEFIELDS true
- KERNEL_IBEG 0
- KERNEL_IEND 4

- KERNEL_DUMPTYPE coupling_box

Type : ./sub_launch_script_for_run_AxiSEM_Curie_CD.csh NAME_OF_RESULTS_DIR

(or 'sub_launch_script_for_run_AxiSEM_Curie_CD_VM.csh', it depends on examples)

!! 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' and 'list_gll_boundary_cartesian.txt' to 'input_box.txt' and 'input_box_sem_cart.txt', resp. and add number of lines at the beginning of the two files too.

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

4 STEP 4 : Specfem Partitionning & STEP 5 : Specfem Generate database

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

Type : run ./batch_coupling_step4_and_step5_scotch_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 $\Longrightarrow$ STEP 6 : expand 2D to 3D & STEP 7 : reformat

Go in 'utils/EXTERNAL_CODES_coupled_with_SPECFEM3D/AxiSEM_for_SPECFEM3D/UTILS_COUPLING_SpecFEM' and make the compilation (make clean ; make all).

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) !! ==> Caution : for the tractions path (for example : /[...]/AxiSEM_tractions/1/), the directory need to be created !!!

  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.  0.                 # chunk center (lat lon azi_rot)
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
```

- Go in NAME_OF_RESULTS_DIR and type : run ../sub_called_batch_for_expand2D3D_Curie_CD.sh to submit expand_2D_3D (the number processes is here arbitrary)
- At the end of expand_2D_3D, check the file 'StaLta.txt' to see at what time, the seismos begin to be non-zero. With this information, you can configure begin time (corresponding to a little before the time when the values in 'StaLta.txt' begin to be non-zero) in the file 'reformat.par' :

  Example :

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

- Stay in NAME_OF_RESULTS_DIR and type : run ../sub_called_batch_for_reformat_Curie_CD.sh to submit reformat. IMPORTANT : 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 Spefem3D partition of domain.

NOTE : If you already know the value of the begin time and if it is already configured in 'reformat.par', you can launch the compilation of expand_2D_3D and reformat, AND the execution of this two programs with the single script (AND uncomment the LAST LINE of the script 'sub_called_batch_for_expand2D3D_Curie_CD.sh' BEFORE that) :

./sub_launch_script_for_make_+_run_expand2D3D_and_reformat_Curie_CD.sh NAME_OF_RESULTS_DIR

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

!! CAUTION : don't forget to UNCOMMENT the last line
(####ccc_msub -q standard ../sub_called_batch_for_reformat_Curie_CD.sh)
of 'sub_called_batch_for_expand2D3D_Curie_CD.sh', which will launch the reformat script at the end !!

It will do the compilation, create a traction directory here :
'EXAMPLES/coupling_with_EXTERNAL_CODES/with_AxiSEM/example_1st_for_validation/DATA/AxiSEM_tractions/1/',
AND launch ./sub_called_batch_for_expand2D3D_Curie_CD.sh, AND at the end, launch
./sub_called_batch_for_reformat_Curie_CD.sh

BUT, if you don't use this script or if you want to create another tractions dir, you have to create the directory yourself and launch the complication and the two run separately.

All the results will be in 'NAME_OF_RESULTS_DIR'.

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 # $\Longrightarrow$ cf the two values in the second line of 'reformat.par'. This value equals to :

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

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

- DT = 0.1 # $\Longrightarrow$ 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. # $\Longrightarrow$ always set it to '.true.' in this case
- EXTERNAL_CODE_TYPE = 2 # 1 = DSM, 2 = AxiSEM, 3 = FK $\Longrightarrow$ always set it to '2' for AxiSEM
- TRACTION_PATH = ./DATA/AxiSEM_tractions/1/ # $\Longrightarrow$ 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. # $\Longrightarrow$ always set it to '.true.' in this case

And finally, type : run ./batch_coupling_step8_xspecfem3d.sh