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'`.

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 (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 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_genderdata_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/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 (Tractions/1/), the directory need to be created !! ==>

  it is created in the script 'sub_launch_script_for_make_+_run_expand2D3D_and_reformat_Curie_CD.sh', but if you don't use this script, 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. Onefile is created by one process for one Spefem3D 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 # $\Longrightarrow$ 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

7 STEP ? : Set up scripts