IM Calculation Refactor

Please read the readme @ https://github.com/ucgmsim/IM_calculation/blob/master/README.md for instructions on how to run the code.

DONE

- IM calculations have been separated from the "old post-processing" repository, extracting the relevant functions and classes.
- IM values validated on Hypocentre and Kupe against "old post-processing" on the same data.
- Two types of workflows: text based (most likely observations) and binary based (simulations once the binary workflow is in place).
    - If binary workflow does not happen soon, the text based option will be used in both cases.
- Outputs match the formats requested in File Formats Used In Ground Motion Simulation and should therefore be usable on the upcoming Non-ergodic codes.
- Tested on very simple multi-process on Kupe with good speed-up using 40 and 80 cores. For the sample, 2228 stations were used

Machine	Cores	Time
Hypocentre	1	132m
Hypocentre	8	8.7m
Kupe	40	27m
Kupe	80	

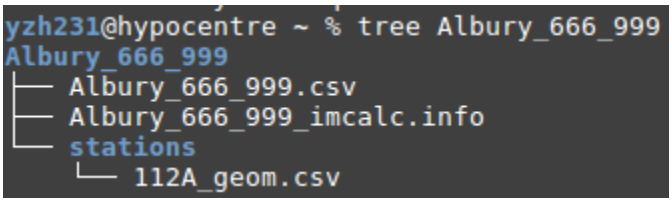
OUTPUT STRUCTURE

With command : python calculate_ims.py ../BB.bin b -o /home/yzh231/ -i Albury_666_999 -r Albury -t s -v 18p3 -n 112A -m PGV pSA -p 0.02 0.03 -e -c geom -np 2

- **input file path**: **../BB.bin**
- **b**: input file type is **binary**
- **-o**: output result csvs location is **/home/yzh231,** default is /home/$user
- **-i**: unique identifier/runname of the simrun and output folder name are **Albury_666_999,** default is 'all_station_ims'. This attribute will be stored in the meta data file.
- **-r**: rupture name is **Albury,** default is unknown. This attribute will be stored in the meta data file.
- **-t**: type of simrun is **simulated,** default is unknown. This attribute will be stored in the meta data file.
- **-v**: version of simrun is **v18p3, default is XXpY.** This attribute will be stored in the meta data file.
- **-n**: station names used to perform im claculation are **112A,** default is all the stations in the binary file
- **-m**: measures used to perform im calculation are **PGV and pSA,** default is all the measures
- **-p**: period of pSA used to perform im calculation are **0.02 0.03,** default is Karim's 15 periods
- **-e**: In addition to the period specified by -p option, **use extended 100 period of pSA,** default not using
- **-c**: component of waveform acceleration used to perform im calculation is **geom,** default is '090, 000, ver'
- **-np**: number of processors used to perform im calculation is **2,** default is 2

The result is outputted to the following location, where:

- 'Albury_666_999' is the folder that contains all outputs. The folder name 'Albury_666_999' is made of the string specified by the '-i' argument. Default is 'all_station_ims' if not specified.
- 'Albury_666_999.csv' is the summary csv file that contains all stations' im calculations. The summary file name is made of the string specified by the '-i' argument.
- 'Albury_666_999_imcalc.info' is the meta data file. The meta data file name is made of the string specified by the '-i' argument.
- 'station' is the folder that contains all individual station's im_calculations. The folder name is defaulted and cannnot be specified by the user.
- '112A_geom.csv' is the individual csv file that contains geom component im calculation for station 112A. Each name of the individual station csv file name is made of station_name + component



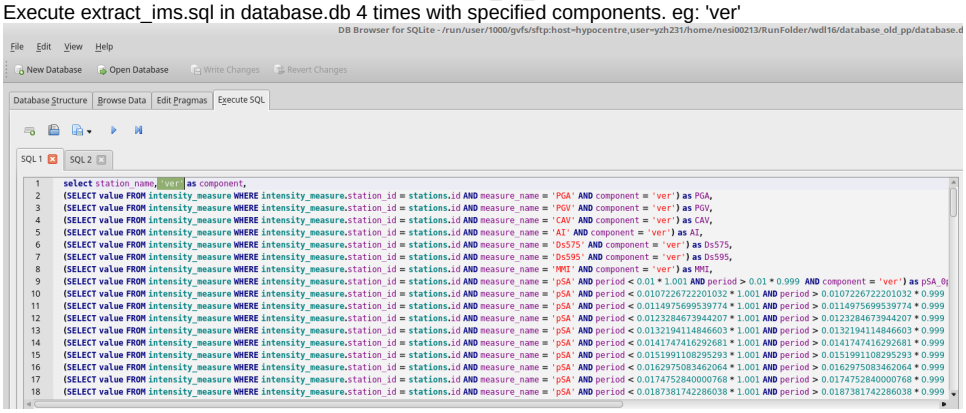
TEST FOR CALCUALTE_IMS.PY

All the steps below are to be carried out in hypocentre

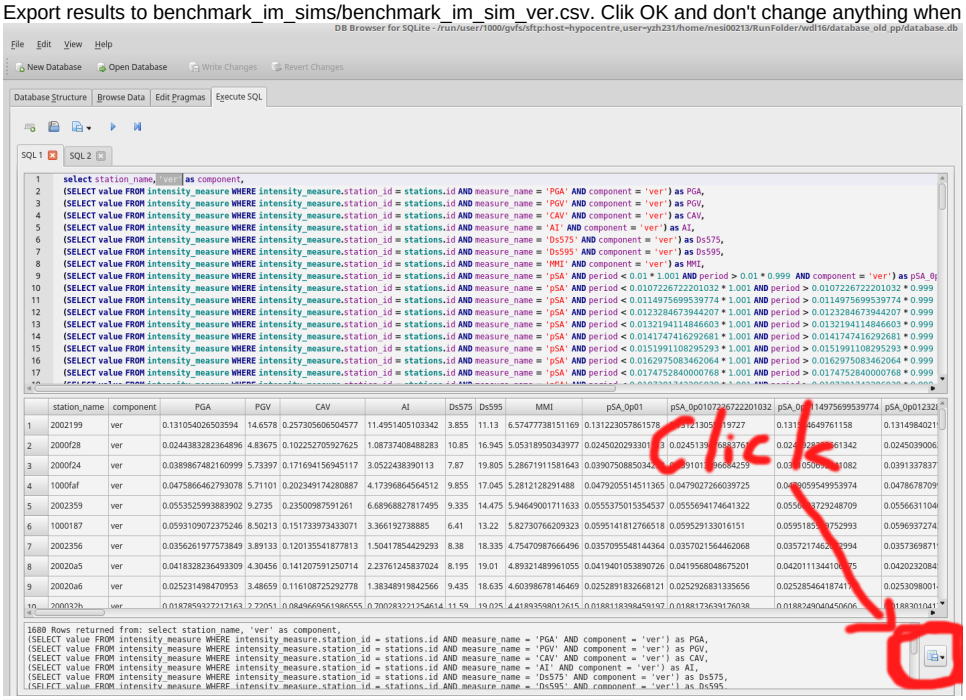
1.Generate summary benchmark:

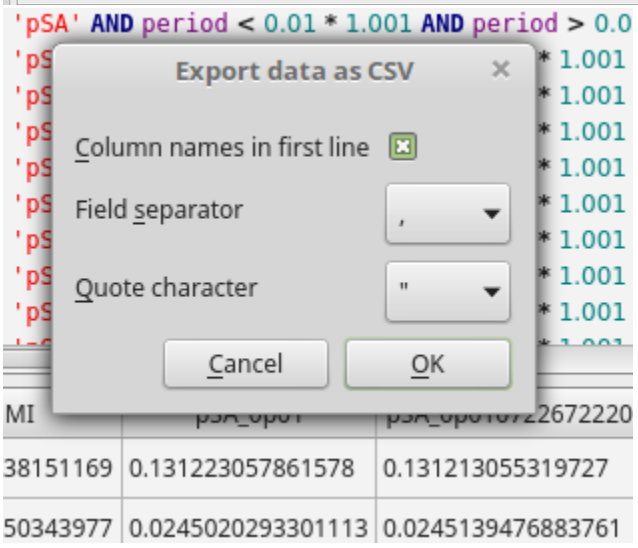
The following steps should only be performed once for each selected binary file

1. Select a source binary file: **/nesi/transit/nesi00213/RunFolder/daniel.lagrava/Kelly_VMSI_Kelly-h0p4_EMODv3p0p4_180531/BB/Cant1D_v2-midQ_leer_hfnp2mm+_rvf0p8_sd50_k0p045/Kelly_HYP01-03_S1244/Acc/BB_with_siteamp.bin**
2. Identify corresponding databse for the selected source binary file: **/home/nesi00213/RunFolder/wdl16/database_old_pp/database.db**
3. Find the script to extract benchmark im value files from the database in step 2: **/nesi/projects/nesi00213/dev/impp_datasets/extract_ims.sql**
4. Create a folder to store benchmark files. eg benchmark_im_sims
5. Execute extract_ims.sql in database.db 4 times with specified components. eg: 'ver'



6. Export results to benchmark_im_sims/benchmark_im_sim_ver.csv. Clik OK and don't change anything when 'Export data as csv' window prompts





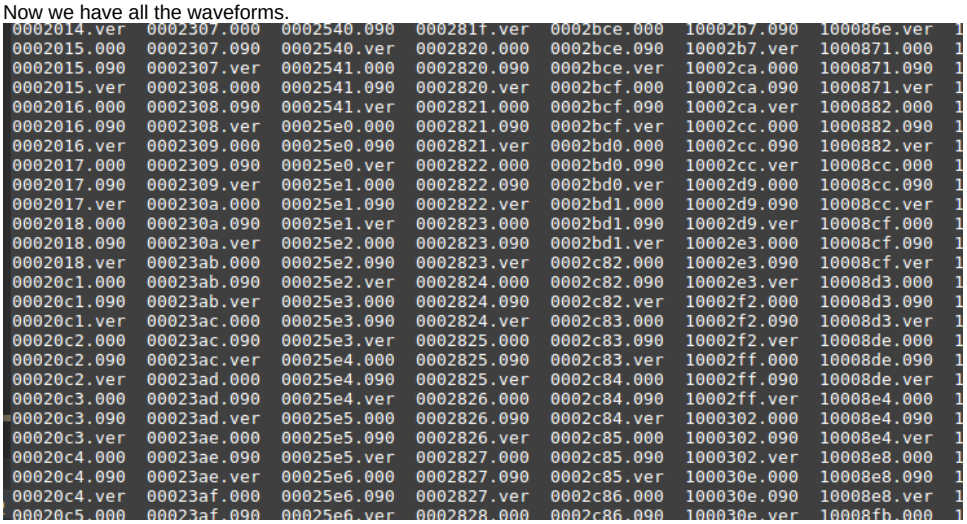
7. Repeat step 4 and 5 with different components: '090', '000', 'geom'
8. Now you have 4 summary benchmark files benchmark_im_sim_090/000/ver/geom.csv

2.Generate test input files

1. Follow the instruction in Binary Workflow FAQ, we can generate single waveform files. These waveforms are intended for the testing of ascii functionality of calculate_ims.py. Open a python cell

```
from qcore.timeseries import BBSeis
bb = BBSeis('/nesi/transit/nesi00213/RunFolder/daniel.lagrava/Kelly_VMSI_Kelly-h0p4_EMODv3p0p4_180531/BB
/Cant1D_v2-midQ_leer_hfnp2mm+_rvf0p8_sd50_k0p045/Kelly_HYP01-03_S1244/Acc/BB_with_siteamp.bin')
bb.all2txt(self, prefix='/home/$user/benchmark_im_sim_waveforms/', f='acc'):
```

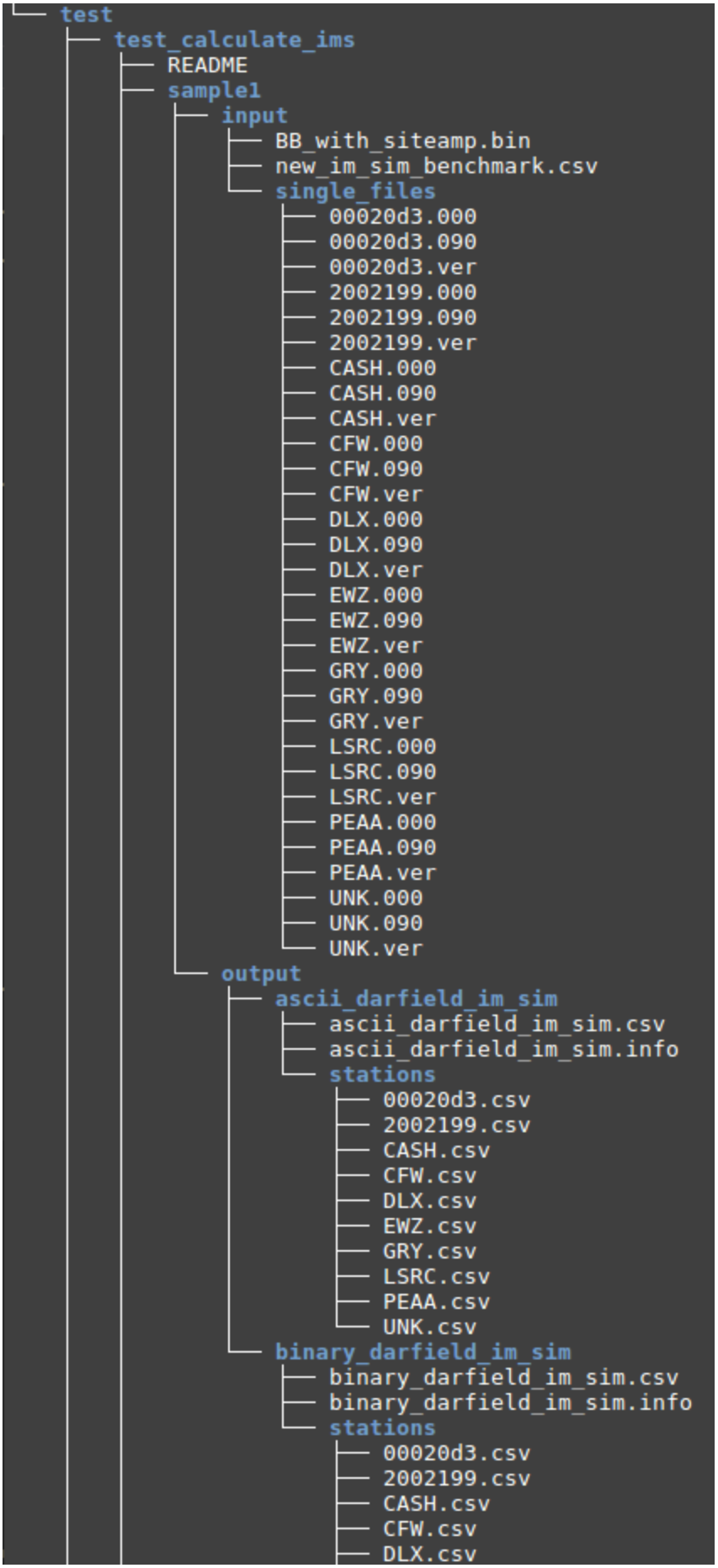
Now we have all the waveforms.

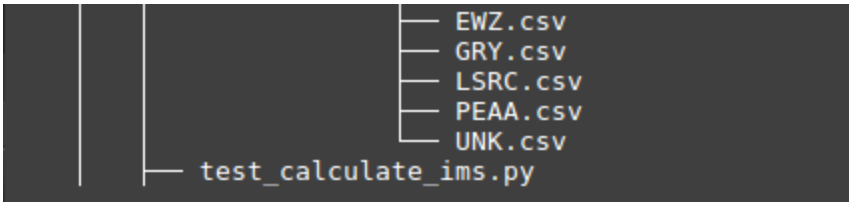


3. Create Test Folder

1. Create The test folder structure follows Testing Standards for ucgmsim Git repositories
2. Select 10 stations you want to test and cp corresponding waveforms files to the singel_files directory as below
3. Copy the source binary file 'BB_with_siteamp.bin' to the input folder
4. Run 'write_benchmark_csv(sample_bench_path)' function inside test_calculate_ims.py to generate 'new_im_sim_benchmark.csv', where 'sample_bench_path' is the folder we created in 1.4 Generate summary_benchmark: benchmark_im_sims. This function should only be run once for each binary file.

NOW you have all the input files ready


test
test_calculate_ims
README
sample1
input
BB_with_siteamp.bin
new_im_sim_benchmark.csv
single_files
00020d3.000
00020d3.090
00020d3.ver
2002199.000
2002199.090
2002199.ver
CASH.000
CASH.090
CASH.ver
CFW.000
CFW.090
CFW.ver
DLX.000
DLX.090
DLX.ver
EWZ.000
EWZ.090
EWZ.ver
GRY.000
GRY.090
GRY.ver
LSRC.000
LSRC.090
LSRC.ver
PEAA.000
PEAA.090
PEAA.ver
UNK.000
UNK.090
UNK.ver
output
ascii_darfield_im_sim
ascii_darfield_im_sim.csv
ascii_darfield_im_sim.info
stations
00020d3.csv
2002199.csv
CASH.csv
CFW.csv
DLX.csv
EWZ.csv
GRY.csv
LSRC.csv
PEAA.csv
UNK.csv
binary_darfield_im_sim
binary_darfield_im_sim.csv
binary_darfield_im_sim.info
stations
00020d3.csv
2002199.csv
CASH.csv
CFW.csv
DLX.csv



4. Run Pytest

Make sure you are currently under the test_calculate_ims folder, run:

```
$ pytest -v -s test_calculate_ims.py
```

```
yzh231@hypocentre ~/IM_calculation/test/test_calculate_ims (git)-[test] % pytest -v -s test_calculate_ims.py
============================================================================================================ test session starts ==
platform linux2 -- Python 2.7.14, pytest-3.2.2, py-1.4.34, pluggy-0.4.0 -- /usr/bin/python2.7
cachedir: ../../.cache
rootdir: /home/yzh231/IM_calculation, inifile:
plugins: cov-2.3.1
collecting 0 items
/home/yzh231/IM_calculation/calculate_ims.py
collected 6 items

test_calculate_ims.py::test_binary_script_calculate_ims python /home/yzh231/IM_calculation/calculate_ims.py /home/yzh231/IM_calcula
alculate_ims/sample1/output -i binary_darfield_im_sim -t s -n 2002199 GRY 00020d3 UNK CASH CFW DLX LSRC EWZ PEAA -p 0.01 0.2 0.5 1.
/home/yzh231/IM_calculation/test/test_calculate_ims/sample1/output/binary_darfield_im_sim/binary_darfield_im_sim.csv
Calculations are outputted to /home/yzh231/IM_calculation/test/test_calculate_ims/sample1/output/binary_darfield_im_sim

PASSED
test_calculate_ims.py::test_ascii_script_calculate_ims python /home/yzh231/IM_calculation/calculate_ims.py /home/yzh231/IM_calculat
_ims/sample1/output -i ascii_darfield_im_sim -t s -n 2002199 GRY 00020d3 UNK CASH CFW DLX LSRC EWZ PEAA -p 0.01 0.2 0.5 1.0 3.0 4.0
```

CHECKPOINTING & SPLITTING A BIG SLURM

Responsible scripts

1. slurn header template: https://github.com/ucgmsim/slurm_gm_workflow/blob/master/templates/slurm_header.cfg
2. im_calc_slurm template: https://github.com/ucgmsim/slurm_gm_workflow/blob/master/templates/im_calc_sl.template
3. submit_hf.py that generates the slurm files: https://github.com/ucgmsim/slurm_gm_workflow/blob/master/scripts/submit_hf.py
4. checkpointing functions: https://github.com/ucgmsim/slurm_gm_workflow/blob/master/scripts/checkpoint.py

Checkpointing

Checkpointing is needed for IM_calculation due to large job size and limited running time on Kupe. Therefore, we implemented checkpointing to track the current progress of an im_calculation job, and carry on from where the job was interrupted by slurm.

Note, the checkpointing code relies on the input/output directory structure specified in the im_calc_al.template in the checkpoint branch. Failure to match the dir structure will result in runtime error. A quick fix would be modifying the template to suit your own dir structure.

Example:

(1) Simulation

Input/output structure defined in im_calc_al.template

```
echo ___calculating simulations___
{% for sim_dir, sim_name, fault_name in sim_dirs %}
    time python2 $IMPATH/calculate_ims.py {{sim_dir}}/Acc/BB.bin b -o {{sim_dir}}/../../../IM_calc/ -np 40 -i {{sim_name}} -r {{fault_name}} -t s -s
{% endfor %}
```

Actual input data structure:

```
melody.zhu@kupe01:/nesi/nobackup/nesi00213/RunFolder/Cybershake/v18p6_batched/v18p6_1k_under2p0G_ab/Runs> ls
Aratiatia  ArielBank  ArielEast  Astrolabe01  Astrolabe02  Astrolabe03  Astrolabe05  Astrolabe07  Awakeri  Barefell  Bidwill  Billys  BlueLk  BlueMtn  BooBooEAST
```

The input binary file is under:

```
/nesi/nobackup/nesi00213/RunFolder/Cybershake/v18p6_batched/v18p6_1k_under2p0G_ab/Runs/BlueMtn/BB/Cant1D_v3-midQ_OneRay_hfnp2mm+_rvf0p8_sd50_k0p045/BlueMtn_HYP28-31_S1514/Acc/BB.bin
```

The output **IM_calc** folder is under:

```
melody.zhu@kupe01:/nesi/nobackup/nesi00213/RunFolder/Cybershake/v18p6_batched/v18p6_1k_under2p0G_ab/Runs> ls ./BlueLk/IM_calc
BlueLk_HYP01-29_S1244  BlueLk_HYP03-29_S1264  BlueLk_HYP06-29_S1294  BlueLk_HYP09-29_S1324  BlueLk_HYP11-29_S1344  BlueLk_HYP15-29_S1384  BlueLk_HYP19-29_S1424  BlueLk_HYP22-29_S1454  BlueLk_HYP26-29_S1494  BlueLk_HYP29-29_S1524
BlueLk_HYP02-29_S1254  BlueLk_HYP04-29_S1274  BlueLk_HYP07-29_S1304  BlueLk_HYP10-29_S1334  BlueLk_HYP13-29_S1364  BlueLk_HYP18-29_S1414  BlueLk_HYP20-29_S1434  BlueLk_HYP23-29_S1464  BlueLk_HYP27-29_S1504
```

(2) Observed

Input/output structure defined in im_calc_al.template

```
echo ___calculating observed____
{% for obs_dir, obs_name, fault_name in obs_dirs %}
        time python2 $IMPATH/calculate_ims.py {{obs_dir}}/*/*/accBB a -o {{obs_dir}}/../IM_calc/ -np {{np}} -i {{obs_name}} -r {{fault_name}} -t o -s
{% endfor %}
```

Actual input data structure:

```
melody.zhu@kupe01:~> ls test_obs/IMCalcExample/
2012p713691  2012p764736  2012p801609  2013p049577  2013p368016  2013p653606  2013p708602  2013p817946  2013p868761  2014p237547  2014p933966  2014p965622  2016p119534  2016p158394  2016p355041  2122842  3631755
```

The output **IM_calc** folder is under:

```
melody.zhu@kupe01:~> ls test_obs/IMCalcExample/IM_calc/
2012p713691  2012p764736  2012p801609  2013p049577  2013p368016  2013p653606  2013p708602  2013p817946  2013p868761
```

Splitting a big slurm

Splitting a big slurm script into several smaller slurms is needed due to the maximum number of lines allowed in a slurm script on Kupe.

Inside **submit_imcalc.py** The **-ml** argument specifies the maximum number of lines of python call to calculate_ims.py/caculate_rrups.py. **Header** and **foot er** like '#SBATCH --time=15:30:00', 'date' etc are **NOT** included.

Say if the max number of lines allowed in a slurm script is 1000, and your (header + footer) is 30 lines, then the number **n** that you pass to **-ml** should be 0 < **n** <=967. eg. **-ml 967**.

Example:

We have 250 simulation dirs to run, by specifying -ml 100 (100 python calls to calculate_ims.py per slurm script), we expect 3 sim slurm scripts to be outputted.(1-100, 100-200, 200-250)

We have 3 observed dirs to run, by specifying -ml 100 (100 python calls to calculate_ims.py per slurm script), we expect 1 sim slurm scripts to be outputted.

We have 61 rrup files to run, by specifying -ml 100 (100 python calls to calcualte_rrups.py per slurm script), we expect 1 sim slurm scripts to be outputted.

Command to run checkpointing and splitting:

```
 python submit_imcalc.py -obs ~/test_obs/IMCalcExample/ -sim runs/Runs -srf /nesi/nobackup/nesi00213/RunFolder
/Cybershake/v18p6_batched/v18p6_exclude_1k_batch_6/Data/Sources -ll /scale_akl_nobackup/filesets/transit
/nesi00213/StationInfo/non_uniform_whole_nz_with_real_stations-hh400_v18p6.ll -o ~/rrup_out -ml 1000 -e -s -i
OtaraWest02_HYP01-21_S1244 Pahiatua_HYP01-26_S1244 -t 24:00:00
```

Output:

```
-rw-r--r-- 1 melody.zhu melody.zhu  48890 Jul  1 03:47 sim_im_calc_0.sl
-rw-r--r-- 1 melody.zhu melody.zhu  48674 Jul  1 03:47 sim_im_calc_100.sl
-rw-r--r-- 1 melody.zhu melody.zhu  31922 Jul  1 03:47 sim_im_calc_200.sl
-rw-r--r-- 1 melody.zhu melody.zhu   1329 Jul  1 03:47 obs_im_calc_0.sl
-rw-r--r-- 1 melody.zhu melody.zhu  23246 Jul  1 03:47 rrup_im_calc_0.sl
```

To submit the slurm script:

```
$cp test.sl /nesi/nobackup/nesi00213/tmp/auto_preproc
$sbatch test.sl
```

The reason that we have to run 'test.sl' under '/nesi/nobackup/nesi00213/tmp/auto_preproc' is otherwise slurm cannot find machine.env specified by the test.sl script:

```
source machine_env.sh
```

TODO

- Creation of semi-automatic slurm generation that will have all the calls to produce the results as needed.
- Progress printing statements
- Rrup calculation on a smaller station list - currently when generating the slurm script it does the full grid even for stations outside the domain

Notes

- Extensive re-writing of code needs to have smaller deliverables in the future, as this simplifies the integration.