CEMAC Documentation: UNRESP August 2018

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Contents

1 Python scripts

1.1 3dNicaragua.py

1.1.1 Purpose

Used to generate a 3D topographic plot of the area around Masaya from DEM data.

1.1.2 Usage

The script should be run from a UNIX command line as follows:

```
$ python3 <py-path>/3dNicaragua.py <demFile>
```

where:

- `<py-path>` is the path (either relative to the current directory, or full) to the directory in which the python script is located (replace with "./" if it is in the current directory).
- `<demFile>` is the path (relative or full) to the DEM data file. This should be a tab delimited ASCII file with the 6 lines of metadata (ncols, nrows, xllcorner, yllcorner, cellsize, NODATA_value) followed by a matrix of topographic heights (m) where the top-left/bottom-right heights correspond to the North-West/South-East corners of the area covered by the DEM data.

1.1.3 Dependencies

The script requires a number of external python packages to be imported. CEMAC periodically asks faculty (FoE) IT suppurt at the University of Leeds to add any required packaes to the loadable python/python-libs modules. Any faculty member should therefore be able to access the required packages by typing the following into the UNIX command line:

```
$ module load python3
$ module load python-libs
```

If the user still experiences any import errors when running the script, they should install the missing python packages themselves.

This is no longer the standard setup: Moved to anaconda for portability!

1.1.4 Output

Running the script successfully will launch the 3D plot in a separate window. The left and right mouse buttons can be used to rotate and zoom in/out of the plot, respectively.

1.1.5 Algorithm details

The python script works as follows:

- The DEM metadata is read in, and the lower left x and y coordinates, along with the cell size, is used to calculate the projected coordinates of each data point. These are then converted to lat/lon using the utm package, assuming a UTM zone P16 projected coordinate system (appropriate for the Masaya area of Nicaragua).
- The DEM height data are also read in, and any 'NODATA' values (measurements taken over water) are replaced with zeros.
- The Basemap and matplotlib packages are used to plot the 3D data.
- The 'stride' parameter is hard-coded to 100 but can be reduced to increase the resolution of the plot (takes longer to execute).

2 CALPUFF: Installation guide

2.1 General compiler settings

The intel compilers are preferred

To use the pgi compilers:

- Switch out the gnu compilers for the pgi compilers using: `$ module switch gnu/native pgi/16.9`
- Compile using: `$ pgf90 -O0 -Kieee -Ktrap=fp -Msave <mainFortranFile>.f -o <mainFortranFile>_pgi.exe`. These compiler flags are based on the ones given here: `http://www.src.com/calpuff/FAQ-answers.htm#1.1.13`. Note that the -tp flag has been removed, as the default is to build as appropriate for the current system, and the pgi library path has also been removed, since this is added to LD_LIBRARY_PATH by default when loading the pgi module (can confirm using '`$ module show pgi`'. The remaining flags do the following:
  - `-O0` – Don't perform any optimisation (compilation will be fast, executable will be slow)
  - `-Kieee` – Perform floating-point operations in strict conformance with the IEEE 754 standard.
  - `-Ktrap=fp` – Controls the behaviour of the processor when exceptions occur. fp traps on floating point exceptions (divide by zeros, invalid operations, floating-point overflows), otherwise they would be masked and the processor would recover from the exception and continue).
  - `-Msave` – Assume that all local variables are subject to the Fortran SAVE statement. (Note: this flag can greatly reduce performance, so might consider adding explicit statements only where needed in the source code to achieve speed-up?)

To use the Intel compilers:

- Switch out the gnu compilers for the Intel compilers using: `$ module switch gnu/native intel/17.0.0`
- Compile using: `$ ifort -O0 -fltconsistency <mainFortranFile>.f -o <mainFortranFile>_intel.exe`. It appears that the Intel compilers don't have an equivalent flag for Ktrap=fp or Msave (I think Msave behaviour is done by default through the default -auto-scalar flag).

2.2 TERREL

2.2.1 Build

To build the original source code:

- Download and unzip version 7.0.0 (L141010) from `http://www.src.com/calpuff/download/mod7_codes.htm`.
- Convert all filenames to lowercase using: `$ ls | while read upName; do loName=‘echo "$upName" | tr '[:upper:]' '[:lower:]'‘; mv "$upName" "$loName"; done`.
- In terrel.for, delete the 'flen' argument in the line "inquire(file=datafil(k),exist=lexist,flen=isize)". This is a Lahey-specific argument.
- To get the pgi compilers to work, make the following additional changes:
  - In terrel.for, replace the instance of '\' with '/'.
- To get the Intel compilers to work, make the following additional changes:
  - In params.trl, comment out the 'Lahey F95 Compiler' block and uncomment the 'Compaq DF Compiler' block.
  - In setsrtm() (terrel.for), remove 'access=caccess' from the open statement (otherwise TERREL crashes when trying to read in the first line of an SRTM3 data file with a "sequential-access I/O to unit open for direct access" error)
- Compile using preferred compiler, as described above.

2.2.2 Setup

To set up TERREL:

- Make a subdirectory called 'data' and put the following files inside it:
  - w100n40.dem – (If using 1km resolution data) The DEM data file for Central America from the GTOPO30 dataset (downloaded via `http://www.src.com/calpuff/data/terrain.html`). Make sure to rename this file to the name given here if necessary.
  - n11w086.bil, n12w086.bil, n11w087.bil, n12w087.bil – (If using 90m resolution data) The DEM data files the Masaya region from the SRTM 3-sec dataset (downloaded via `https://earthexplorer.usgs.gov/` – choose 'SRTM Void Filled' and 'BIL' format). Make sure to rename the files to the names given here if necessary.

- (optional) xy_masaya.dat – This is a 2-column text file containing the x and y coordinates (in km, in the same projection as used for the main grid) of receptor points at which the terrain height will be calculated in addition to the gridded points in the main output file (only output if LXY = T in the input file).

- Open the input file (terrel.inp) and make the following changes:
  - NTDF – Change to '1' if using GTOPO30 data (as we only have one input DEM file) or '4' if using SRTM3 data
  - OUTFIL – Change to e.g. 'masaya.dat'. This is main output file that will contain the gridded processed terrain data.
  - LSTFIL – Change to e.g. 'masaya.lst'. This is essentially the log file.
  - PLTFIL – Change to e.g. 'masaya.grd'. This is an output file that can be plotted with e.g. the Surfer software package.
  - RAWECHO – Change to e.g. 'raw_masaya.dat'. This is an output file that simply echoes the raw input DEM data but in ASCII format.
  - SAVEFIL – Change to e.g. 'masaya.sav'. This is an output binary save file that can later be used for a continuation run of TERREL (we probably don't need this).
  - XYINP – (if LXY = T is set below) Change to 'data/xy_masaya.dat'. This is the path to the input receptor points file.
  - XYOUT – (if LXY = T is set below) Change to e.g. 'xyoutput_masaya.rec'. This is output (elevation heights) at the receptor points.
  - LCFILES – Set to T (true). This is a bit annoying, but all files have to have names in either full uppercase or lowercase, and I find lowercase nicer.
  - Subgroup (0b) – At the end of this section, ensure that there are as many lines as input data files. If using GTOPO30 data, there should be one line that reads "1 !GTOPO30 = data/w100n40.dem ! !END!". If using SRTM3 data, there should be 4 lines that read "1 !SRTM3 = data/n11w086.bil ! !END!", "2 !SRTM3 = data/n11w087.bil ! !END!", etc
  - LINTXY – Set to F (false). Receptor point elevations will not be interpolated but be be the peak heights.
  - XYRADKM – Set to 5.0. Search radius (km) for locating the peak heights at the receptor points.
  - LCOAST – Set to F. We don't have coastline data to process.
  - LBLNREAD – Set to F. We don't have coastline data to process.
  - LVOIDFIL – Set to F. Don't interpolate to fill void cells. This should ensure the same behaviour as used by Sara.
  - MSHEET – Set to 0 for now. This will ensure the same coordinate mapping as used by Sara. Consider switching back to 1 at a later date.
  - IUTMZN – Set to 16. This is the UTM zone for Nicaragua.

- XREFKM – Set to 525.09417. This is the x-coordinate of the reference point (lower left corner) of the intended output grid. I think this is an easting (km) relative to the lower left corner of the UTM zone being used.
- YREFKM – Set to 1294.23926. This is the corresponding y-coordinate (northing).
- NX – For a 1km resolution, set to 91; for a 100m resolution, set to 901. This is the intended number of grid cells in x.
- NY – For a 1km resolution, set to 55; for a 100m resolution, set to 541. This is the intended number of grid cells in y.
- DGRIDKM – For a 1km resolution, set to 1.0; for a 100m resolution, set to 0.1. This is the intended grid spacing (in x and y) in km.

2.2.3 Run

To run TERREL, type:

```
$ ./terrel_<compiler>.exe
```

2.3 CTGPROC

2.3.1 Build

To build the original source code:

- Download and unzip version 7.0.0 (L150211) from `http://www.src.com/calpuff/download/mod7_codes.htm`.
- Convert all filenames to lowercase using: `$ ls | while read upName; do loName=‘echo "$upName" | tr ’[:upper:]’ ’[:lower:]’‘; mv "$upName" "$loName"; done`.
- If using a 100m resolution, increase mxnx and mxny to 901 and 541 respectively in params.ctg
- To get the pgi compilers to work, make the following changes:
  - In ctgproc.for, replace the instance of ‘\’ with ‘/’.
- To get the Intel compilers to work, make the following changes:
  - In params.ctg, comment out the ‘Lahey F95 Compiler’ block and uncomment the ‘INTEL Compiler’ block.
  - In control.ctg, add the missing variable ‘lll’ to the /CONTROL/ common block.
- Compile using preferred compiler, as described above, but add -mcmodel=medium (or equivalent of if not using ifort) to avoid memory overflow errors.

2.3.2 Setup

To set up CTGPROC:

- Make a subdirectory called 'data' and put the following file inside it: nalulcl20.bil – The 'USGS Land Use/Land Cover' BIL format file for North America (Global Lambert Azimuthal), downloaded via `http://www.src.com/calpuff/data/land_use.html`. Note that the TIFF-format version of this data file does not work properly (alignment issues).
- Open the input file (ctgproc.inp) and make the following changes:
  - NDBF – Set to 1 (we only have one input land-use file).
  - LUDAT – Set to e.g. lulc1km_masaya.dat. This is the main output file containing the land-use categories on the intended CALPUFF grid.
  - RUNLST – Set to e.g. ctgproc_masaya.lst.
  - Subgroup (0b) – At the end of this section, ensure that there is only one line that reads "! GLAZNA = data/nalulcl20.bil ! !END!". This is the path to the land-use data file.
  - MESHGLAZ – Set to 2 (1km res) or 11 (100m res). This will e.g. split each 1km input grid cell into 2x2 grid cells (each assigned the same land-use category). This ensures that there will be no 1km-res CALPUFF grid cells with missing data in them.
  - PMAP – Set to 'UTM'
  - IUTMZN – Set to 16
  - DATUM – Set to 'WGS-84'
  - XREFKM – Set to 525.09417
  - YREFKM – Set to 1294.23926
  - NX – Set to 91 (1km res) or 901 (100m res)
  - NY – Set to 55 (1km res) or 541 (100m res)
  - DGRIDKM – Set to 1.0 (1km res) or 0.1 (100m res)

2.3.3 Run

To run CTGPROC, type:

```
$ ./ctgproc_<compiler>.exe
```

****NOTE**** PGI compiler claims that it can't find the data file, even though it is there. Can therefore only use Intel compilers at present.

2.4 MAKEGEO

2.4.1 Build

To build the original source code:

- Download and unzip version 3.2 (L110401) from `http://www.src.com/calpuff/download/mod7_codes.htm`.
- Convert all filenames to lowercase using: `$ ls | while read upName; do loName=‘echo "$upName" | tr ’[:upper:]’ ’[:lower:]’‘; mv "$upName" "$loName"; done`.
- If using a 100m resolution, increase mxnx and mxny to 901 and 541 respectively in params.geo
- In subroutine ‘comline’ (calutils.for), comment out the call to ‘getcl’ and uncomment the Sun compiler block (this seems to work for both the intel and pgi compilers).
- Compile using preferred compiler, as described above, but add -mcmodel=medium (or equivalent of if not using ifort) to avoid
- ***Note*** There are a lot of warning messages with the intel compiler regarding a common block in snow.geo, however, the executable is still generated.

2.4.2 Setup

To set up MAKEGEO:

- Make a subdirectory called ‘data’ and put the following file inside it:
  - masaya.dat – The terrain output file from running TERREL.
  - lulc1km_masaya.dat – The land-use output file from running CTGPROC.
- Open the input file (makegeo.inp) and make the following changes:
  - LUDAT – Set to data/lulc1km_masaya.dat (or whatever the path to the land-use input data file is).
  - TERRDAT – Set to data/masaya.dat (or whatever the path to the terrain input data file is).
  - GEODAT – Set to e.g. geo_masaya.dat. This is the main output file that will serve as input to CALMET for the geophysical data.
  - RUNLST – Set to e.g. geo_masaya.lst
  - LCFILES – Set to T to keep all filenames lowercase.
  - LSNOW – Set to F (we don’t have any snow data)
  - IUTMZN – Set to 16
  - XREFKM – Set to 525.09417
  - YREFKM – Set to 1294.23926
  - NX – Set to 91 (1km res) or 901 (100m res)
  - NY – Set to 55 (1km res) or 541 (100m res)
  - DGRIDKM – Set to 1.0 (1km res) or 0.1 (100m res)
  - Comment out (i.e. replace all occurrences of ‘!’ with ‘*’) the entries in subgroup 4c and 4e

2.4.3 Run

To run MAKEGEO, type:

```
$ ./makegeo_<compiler>.exe
```

2.5 CALETA

We now use open-source NAM data (the ECMWF data is only free to academic institutions, and so INETER would not be able to acquire this data going forward). However, for completeness, below is information on how to build, setup and run CALETA for using the ECMWF GRIB files

2.5.1 Build

To build the original source code:

- Download version 3.2 (100727) from `http://www.src.com/calpuff/download/mod7_codes.htm` and unzip
- To get the pgi compilers to work, open caleta.f in a text editor, navigate to subroutines 'getfile_fst' and 'getfile_ana' in turn, and replace the '/' with a '\' in the 101 format statement.
- Compile using preferred compiler, as described above.

****NOTE, the original caleta.f and the one supplied by IMO are markedly different (see, for example, differences in subroutine lists using `'$ fgrep 'subroutine' <path/to/orig/caleta.f -i > Orig_caleta.txt'`, then `'$ fgrep 'subroutine' <path/to/IMO/caleta.f -i > IMO_caleta.txt'`, then `'$ tkdiff Orig_caleta.txt IMO_caleta.txt`.

To build the IMO version:

- Copy the files caleta.f, eta2m3d.blk and eta2m3d.cm1 from Mark's Caleta directory, and eta2m3d.par from Mark's RUN directory, into a clean directory and run the appropriate compilation command as above (ifort is preferred).

2.5.2 Setup

Sara's input file for Caleta (eta2m3d.inp) contains the following 8 lines:

```
M3D file Created from ETA AWIPS 212 Grid for Falconbridge CALMET
3  ! Flag to indicate ECMWF input data
/path/to/GRIB/files/directory/
/path/to/output/directory/
eta2m3d.lst  ! list file name
10.5,12.5  ! Range Lat
272,275  ! Range Long
1, 25  ! Vertical levels
```

2.5.3 Run

To run the self-built IMO version:

- From Mark's RUN directory, copy the files grid.dat, timestmp.dat and eta2m3d.inp into the directory. timestmp.dat contains the start date of the simulation in the format ddmmyyyy and is created after running launch_long_run.sh.
- Run caleta using:

```
$ ./caleta_<compiler>.exe
```

***NOTE: This gives an output file (out_caleta.m3d) that is different to the one in Mark's RUN directory. Specifically, the new file has non-zero terrain heights where Mark has all zeros, and also some zeros for sea-level-pressure and bad output (*****) for precipitation. This causes issues in the next step (CALMET). Running the IMO-built version (the "caleta_masaya" executable in the EXEC directory) on the same input files produces a valid out_caleta.m3d file; this suggests that the code in Mark's Caleta directory is somehow different to the code used to build the Caleta executable in the EXEC directory.

2.6 CALMET

2.6.1 Build

To build the original source code:

- Download version 6.5.0 (150223) from `http://www.src.com/calpuff/download/mod7_codes.htm` and unzip. Create a temporary directory, cd into it, and unzip the second file inside. Copy CALMET.INP from this temporary directory into the main unzipped directory, and then delete the temporary directory.
- Convert all filenames to lowercase using: `$ ls | while read upName; do loName=‘echo "$upName" | tr ’[:upper:]’ ’[:lower:]’‘; mv "$upName" "$loName"; done`.
- If using a 100m resolution, increase mxnx and mxny to 901 and 541 respectively in params.met
- In params.met, change mxnz from 12 to 27 and mxnzi from 12 to 50.
- Compile using preferred compiler, as described above.

2.6.2 Setup

To set up CALMET:

- Make a subdirectory called ‘data’ and put the following file inside it:
  - geo_masaya.dat – The output file from running MAKEGEO.
  - out_caleta.m3d – The output file from running CALETA.

- Fix the apparent issue in the out_caleta.m3d file – In the first surface data-block, replace the latitudes and longitudes of the first few points in the extraction subdomain to match all the other surface data-blocks.
- Open the input file (calmet.inp) and make the following changes:
  - GEODAT – Set to data/geo_masaya.dat.
  - LCFILES – Set to T
  - NUSTA – Set to 0 (we don't have any upper-air stations)
  - NOWSTA – Set to 0 (we don't have any overwater stations)
  - UPDAT – Comment out all three lines (we don't have upper air data)
  - SEADAT – Comment out (we don't have overwater stations data)
  - M3DDAT – Set to data/out_caleta.m3d
  - IBYR, IBMO, IBDY, IBHR – Set to required simulation start date/-time (e.g. 2017, 12, 04, 0)
  - IEYR, IEMO, IEDY, IEHR – Set to required simulation end date/-time (e.g. 2017, 12, 06, 0)
  - ABTZ – Set to UTC+0000 (we want times in UTC)
  - LCALGRD – Set to F (don't compute special data fields)
  - IUTMZN – Set to 16
  - DATUM – Set to WGS-84
  - NX – Set to 91 (1km res) or 901 (100m res)
  - NY – Set to 55 (1km res) or 541 (100m res)
  - DGRIDKM – Set to 1.0 (1km res) or 0.1 (100m res)
  - XORIGKM – Set to 525.09417
  - YORIGKM – Set to 1294.23926
  - NZ – Set to 24
  - ZFACE – Set to "0, 20, 60, 140, 260, 540, 1000, 2000, 3000, 4000, 5000, 6000, 7000, 8000, 9000, 10000, 11000, 12000, 13000, 14000, 15000, 16000, 17000, 18000, 19000". These are the heights of the output grid
  - NOOBS – Set to 2 (use 3D data for surface, overwater and upper air data)
  - NSSTA – Set to 0 (no surface stations)
  - NPSTA – Set to -1 (flag to use 3D precip data)
  - MCLOUD – Set to 4 (use prognostic 3D RH fields to get gridded cloud cover at all levels)
  - BIAS – Set to 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 (i.e. zero bias at each Z level)
  - IPROG – Set to 14 (i.e. use 3D winds as initial guess field)
  - ISTEPPGS – Set to 10800 (timestep of the prognostic met model) ***This was set to 3 in Mark's input file, but this caused an error for me, plus 10800 seems correct.***

- RMAX1-RMAX3 – Set all to 5.0 (radii of influence in km for stations)
- RPROG – Set to 1.0 (weighting parameter of the 3D data).
- NSMTH – Set to 2, 4, 4, 4, 4, 4, 4, 4, 4, 4, 4, 4, 4, 4, 4, 4, 4, 4, 4, 4, 4, 4 ,4 (number of passes in the smoothing procedure for each Z level)
- NINTR2 – (not needed?) Set to 5,5,5,5,5,5,5,5,5,5,5,5,5,5,5,5,5,5,5,5,5,5,5,5 (max stations used per Z level for interpolation)
- FEXTR2 – (not needed?) Set to 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 (not used but need NZ values)
- ISURFT – Set to -2 (use domain-average prognostic lapse rate)
- IUPT – Set to -2 (use domain-average prognostic lapse rate)
- ZUPT – Set to 100. (depth through which the domain-scale lapse rate is computed)
- IMIXH – Set to 2 (Batchvarova and Gryning mixing height method used over all surfaces)
- DZZI – Set to 300. (depth, m, of layer above current convective mixing height through which lapse rate is computed)
- ZIMIN – Set to 250. (minimum overland mixing height)
- ITPROG – Set to 1 (use prognostic RH)
- ITPROG – Set to 2 (no surface or upper-air temperature observations; use 3D data).

2.6.3 Run

To run CALMET, type:

```
$ ./calmet_<compiler>.exe
```

2.7 CALPUFF

2.7.1 Build

To build the original source code:

- Download version 7.2.1 (150618) from `http://www.src.com/calpuff/download/mod7_codes.htm` and unzip
- Convert all filenames to lowercase using: `$ ls | while read upName; do loName=‘echo "$upName" | tr ’[:upper:]’ ’[:lower:]’‘; mv "$upName" "$loName"; done`.
- If using a 100m resolution, increase mxnx and mxny to 901 and 541 respectively in params.puf
- In params.puf, change mxnz from 12 to 27 and mxrec from 10000 to 20000.
- In calpuff.for, near the end of subroutine ‘comp’ (e.g. just after the call to FOGOUT), insert the following lines of code to write out the hourly concentrations to individual files:

```
      do ispec=1,nspec
      write(infile,10000) ispec, nn
10000 format('concrec',I2.2,I4.4,'.dat')
      open(50,file=infile)
       do i=1,nrec
       write(50,*) chirec(i,ispec)
       end do
      end do
      close(50)
```

Also add 'character*150 infile' to the declarations of this subroutine.

- Build in two stages. For intel compilers:
  ```
  $ ifort -c modules.for
  $ ifort -O0 -fltconsistency calpuff.for modules.o -o calpuff.exe
  ```
  (Add the flag -mcmodel=medium if running with 100m resolution)

2.7.2 Setup

To set up CALPUFF:

- Make a subdirectory called 'data' and put calmet.dat (the output file from CALMET) inside it
- Rename the input file from calpuff_v7.inp to calpuff.inp, open it, and make the following changes:
  - METDAT – Change to data/calmet.dat
  - RSTARTE – Uncomment and set to restart_so2_e.dat. This is the name given to the generated restart file at simulation end.
  - OZDAT – Comment out
  - DEBUG – Uncomment and set to debug.dat (we want an output debug file)
  - BALDAT – Uncomment and set to massbal.dat (we want an output mass balance file)
  - LCFILES – Set to T
  - IBYR, IBMO, IBDY, IBHR – Set to required simulation start date/-time (e.g. 2017, 12, 04, 0)
  - IEYR, IEMO, IEDY, IEHR – Set to required simulation end date/-time (e.g. 2017, 12, 06, 0)
  - ABTZ – Set to UTC+0000 (we want times in UTC)
  - NSPEC – Set to 2 (we have SO2 and SO4)
  - NSE – Set to 1 (only one species actually emitted; SO4 is created in the atmosphere)
  - MRESTART – Set to 2 for main run (i.e. write a restart file at the end of the run)
  - MTRANS – Set to 0 (don't model transitional plume rise)
  - MTIP – Set to 0 (don't model stack downwash)

- MBDW – (not needed?) Set to 2 (use PRIME building downwash method)
- MSHEAR – Set to 1 (vertical wind shear modelled)
- MCHEM – Set to 1 (use MESOPUFF II cheical scheme)
- MWET – Set to 0 (don't model wet removal)
- MPARTL – Set to 0 (don't model partial plume penetration)
- MPARTLBA – Set to 0 (don't model partial plume penetration)
- CSPEC – Delete all but SO2 and SO4 from both the list and the table
- IUTMZN – Set to 16
- DATUM – Set to WGS-84
- NX – Set to 91 (1km res) or 901 (100m res)
- NY – Set to 55 (1km res) or 541 (100m res)
- DGRIDKM – Set to 1.0 (1km res) or 0.1 (100m res)
- NZ – Set to 24
- ZFACE – Set to "0,20,60,140,260,540,1000,2000,3000,4000,5000,6000,7000, 8000,9000,10000,11000,12000,13000,14000,15000,16000,17000,18000,19000"
- XORIGKM – Set to 525.09417
- YORIGKM – Set to 1294.23926
- IECOMP – Set to 91 (1km res) or 901 (100m res) (X index of UR corner)
- JECOMP – Set to 55 (1km res) or 541 (100m res) (J index of UR corner)
- LSAMP – Set to F (no gridded receptors)
- IDRY – Set to 0 (no dry fluxes output)
- IWET – Set to 0 (no wet fluxes output)
- IVIS – Set to 0 (no RH output)
- LCOMPRS – Set to F (no compression to output file)
- IPFTRAK – Set to 0 (no puff-tracking output)
- INRISE – Set to 1 (create plume properties output file rise.dat)
- ICFRQ – Set to 24 (concentration print interval in timesteps)
- IPRTU – Set to 1 (use g/m3 for printing)
- SPECIES LIST – Delete all but SO2 and SO4, and set both to "1, 1, 0, 0, 0, 0, 0" (just print and save concentrations)
- LDEBUG – Set to T (debug output wanted) ***NOTE: Set this to F to dramatically reduce .lst file size***
- NPFDEB – Set to 1044 (track this many puffs in debug)
- NN2 – Set to 24 (stop debug output after this number of timesteps)
- XHILL2M – (not needed?) Set to 0 (factor to convert horizontal dimensions to meters if MHILL is 1)

- ZHILL2M – (not needed?) Set to 0 (factor to convert vertical dimensions to meters if MHILL is 1)
- INPUT GROUP 7 – (not needed?) Delete all but SO2 line
- INPUT GROUP 8 – (not needed?) Delete all but SO4 line
- INPUT GROUP 10 – (not needed?) Delete all but SO2 line, and change liquid precip to 2.61E-05 and frozen precip to 3.0E-05
- MOZ – Set to 0 (use monthly background ozone value)
- BCKO3 – Set all values to 30 (monthly background ozone)
- BCKNH3 – Set all values to 1.0 (monthly background ammonia)
- XMXLEN – Set to 0.5 (maximum length of a slug)
- NCOUNT – Set to 5 (number of iterations when computing transport wind)
- SZCAP_M – Set to -1.0 (disable)
- WSCALM – Set to 0.01 (minimum wind speed for non-calm conditions)
- XMINZI – Set to 20.0 (minimum mixing height)
- SL2PF – Set to 5.0 (slug-to-puff transition criterion factor)
- SYSPLITH – Set to 0.8 (min sig-y before split)
- SHSPLITH – Set to 1.0 (min puff elongation rate before split)
- RSAMPBC – Set to 15.0 (search radius for sampling nearest BC puff)
- MDEPBC – Set to 0 (no adjustment for depletion)
- NPT1 – Set to 0 (no point sources to follow)
- NSPT1 – Set to 0 (no variable emissions factors)
- Subgroup 13b – Delete all sources
- Subgroup 13d – Delete all sources
- NAR1 – Set to 1 (one area source to follow)
- Subgroup 14b – Add following lines (source parameters):
  ! SRCNAM = MASAYA2 !
  ! X = 0, 520, 50, 0.004 !
  !END!
- Subgroup 14c – Add following lines (source coordinates):
  1 ! SRCNAM = MASAYA2 !
  1 ! XVERT = 590.495, 590.740, 590.702, 590.435!
  1 ! YVERT = 1324.876, 1324.831, 1325.058, 1325.078!
  !END!
- NREC – Set to 18000 (number of non-gridded receptor points to follow)
- NRGRP – Set to 0 (no groups of receptors)
- Subgroup 20b – Delete all groups
- Subgroup 20c – Paste in 18000 non-gridded receptor points from Sara's input file.

2.7.3 Run

To run CALMET, type:

```
$ ./calpuff_<compiler>.exe
```

Modify calpuff.inp so the the restart flag (RESTARTB) is set to 0 and run again.