# Software Benchmarking Guidance for 3SAQS CAMx version 5.41

1. **Introduction**

The Three State Data Warehouse (3SDW) under the Three State Air Quality Study (3SAQS) developed a benchmarking modeling platform for a five-day CAMx simulation using the final 3SAQS Base 2008 configuration (3SAQS\_CAMx\_Base08a). This modeling platform is designed to benchmark the CAMxv5.41 installation before using the model to run derivative simulations from the base 3SAQS simulation. Benchmarking refers to confirming proper installation, compilation, and configuration of the model via comparison with a reference dataset. Users should follow the instructions here to build and run the 3SAQS\_CAMx\_Base08a benchmark simulation and to compare the results against the provided reference data.

The benchmark simulation is a five-day period from January 1 – January 5, 2008. Data and instructions are provided to run both the 36-km and 12-km 3SAQS modeling grids. The CAMx modeling platform distributed here is unique to the 3SAQS project and is based off of the WestJumpAQMS CAMx simulations. In particular, this version of CAMx was developed to simulate in-line plume rise for DEASCO3 fires and is not the same code base as the official CAMxv5.41 public release version.

Direct questions about the 3SAQS\_CAMx\_Base08a benchmark simulation to Zac Adelman (zac@unc.edu).

1. **Notes on the 3SAQS\_CAMx\_Base08a benchmark data provided by 3SDW**

The University of North Carolina (UNC) generated these data using the following system and compilers

Operating System: 64-bit RHEL 5.6 (Tikanga)

Hardware: Dell C6100 12-core nodes with 2.93 GHz Intel processors, 12M L3 cache (Model X5670)

Fortran Compiler: Portland Group Fortran version 11.6-0 (pgf90 11.6-0 64-bit target on x86-64 Linux -tp Nehalem)

MPI: mvapich2-1.7

CAMx: v5.41 hybrid MPI-OpenMP

Reproducing this configuration will give the best chance of exactly reproducing the 3SAQS\_CAMx\_Base08a results generated by UNC. Along with differences in compilers, hardware and processor differences will contribute to results that diverge from the UNC simulations. The differences in the CAMx results due to compiler and hardware variations should be less than 1% for both gas and aerosol species.

1. **Installation and compiling CAMx**
   1. Download the CAMx Benchmark source codes and data from the following ftp address:

[**ftp://viking.cira.colostate.edu/3SDW/3SAQS/2008/Base08a/AQ/CAMx/Benchmark**](ftp://viking.cira.colostate.edu/3SDW/3SAQS/2008/Base08a/AQ/CAMx/Benchmark)

* 1. Untar the CAMx benchmark model archive and data in a working directory:

tar xvzf 3SAQS\_CAMx\_Base08a\_Benchmark\_MODEL.tar.gz

tar xvzf 3SAQS\_CAMx\_Base08a\_Benchmark\_INPUTDATA.tar.gz

tar xvzf 3SAQS\_CAMx\_Base08a\_Benchmark\_METDATA.tar.gz

tar xvzf 3SAQS\_CAMx\_Base08a\_Benchmark\_REFDATA.tar.gz

After untarring these files you will see the following directories:

**3SAQS\_B08a\_Benchmark**

* **inputs**
  + ahomap
  + chem
  + emis
  + low
    - * 36km
* 12km
  + ptsr
  + icbc
  + landuse
  + met
  + westjump.12km.25lay
  + cr
  + kv
  + tp
  + uv
  + wv
  + zp
  + westjump.36km.25lay
  + cr
  + kv
  + tp
  + uv
  + wv
  + zp
  + tuv
* **outputs**
* **post-proc**
* m3diff
* camx2ioapi
* **ref**
* **runfiles**
* **src** 
  1. Change directories to the source code directory and build CAMx for your system configuration

cd 3SAQS\_B08a\_Benchmark/src

Set the Makefile environment variable MPI\_INST to the installation location of the MPI library and include files on you system.

Save the Makefile and run the make command to the build the CAMx executable:

make pg\_linuxomp MPI=true |& tee CAMx\_build.log

This example shows the command used to build the CAMx executable used for the 3SAQS\_CAMx\_Base08a simulation. If you use a different compiler or MPI configuration see the syntax notes in the CAMx Makefile for guidance.

1. **Configure and Run CAMx**
   1. Configure the CAMx run script run.3SAQS.3612K.25L.Base08a.Q1.job. From the CAMx home directory, change to the runfiles directory and open the CAMx run script in a text editor. Set the HOME variable to the location of the top level CAMx installation directory. Set the MPIBIN variable directory to the installation location of the MPI library and include files on your system.

**NOTE: Do not change the file input or output naming conventions in this script as the downstream post-processing programs depend on these names.**

* 1. Run CAMx for the 3SAQS benchmark simulation. The CAMx 3SAQS benchmark case is a 5-day period from January 1-5, 2008 on 36 and 12-km nested grids. The run script is configured to initialize the simulation from a CAMx restart file and to use boundary conditions for the outer domain downscaled from a MOZART GCM simulation.

The provided run script is configured for the UNC computing cluster. You will now need to configure the CAMx run script for a parallel simulation on your system. For the 3SAQS Base08a simulation, including this benchmark simulation, UNC used 24 processors in hybrid MPI-OpenMP mode. The simulation was run on 6 nodes with 4 processors per node.

1. **Post Process the CAMx Outputs and Compare to the Reference Data Files**
   1. Post-process the CAMx output data by converting it to I/O API-netCDF format.

Source code, executable, and scripts are located in:

**3SAQS\_B08a\_Benchmark/post-proc/camx2ioapi**

You should be able to use the precompiled executable for this test. If you would like to compile the program from source, configure the Makefile to point to the I/O API and netCDF installations on your system. The distributed Makefile is configured for the Portland Group Fortran compiler. This can be changed to work for other compilers. Successful compilation of the program will result in the executable file camx2ioapi\_v6.

To configure the CAMx2IOAPI run script camx2ioapi\_v6\_3SAQS.job set the CAMXDIR variable to the root directory path of the 3SAQS Benchmark installation on your system. Save and run this script to create netCDF layer 1 concentration, wet deposition, and dry deposition files.

* 1. Compare the benchmark simulation against the reference data results.

Scripts and executable are located in:

**3SAQS\_B08a\_Benchmark/post-proc/m3diff**

The precompiled executable for the I/O API utility program m3diff will be used to calculate daily max, min, and average differences between the benchmark simulation and reference data. The m3diff script compares the daily average differences and reports a message if the difference is greater than a defined threshold value.

**Note: The benchmark simulation is successful (i.e. differences less than the threshold value) if you DO NOT see the message *“Performance threshold exceeded for [CO|O3|NH3|PEC] on day [1-5] for hour [1-24].”***

By default the m3diff script uses a threshold of 0.1% (environment variable THRESH). If the daily average difference between the benchmark and reference data is > THRESH x reference data daily average, the script writes a message to the screen.

The m3diff script is configured to check average concentrations, wet deposition, and dry deposition for the pollutants CO, O3, NH3, and PEC for layer 1 only.

1. **BENCHMARKING**

This data and software package is configured to compare the CAMx outputs that you generated for the 5-day 3SAQS benchmark period to output files generated at the UNC. Only I/O API-netCDF formatted, layer 1 extractions of the CAMx outputs from UNC are available. Comparisons can be done both qualitatively, using a program like VERDI to compute spatial difference plots between two simulations and quantitatively, using the distributed m3diff scripts to compute the average differences between the simulations for each model species.

Small differences in the results are expected, due only to variations in the computing environments used to produce the results and not to differences in the model source codes, configuration, or input data.