CMAQ 5.3 Parallel Performance for a 101-day Simulation

George Delic
HiPERiSM Consulting, LLC
P.O. Box 569, Chapel Hill, NC 27514, USA

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2016 episode and resources

- Chemistry
  - cb6r3_ae7_aq mechanism
  - 147 active species and 329 reactions
  - day/night Jacobian has 1400/1348 non-zeros
- Date range Q1CY2016
  - 2015-12-22 to 2016-03-31 (101 days)
- Domain is 299 *x* 459 CONUS on a 12 Km grid, 35 vertical layers (4.8 million grid cells)
- Run with 24 MPI processes on 192-core heterogeneous cluster with 16 nodes

Two CMAQ 5.3 versions

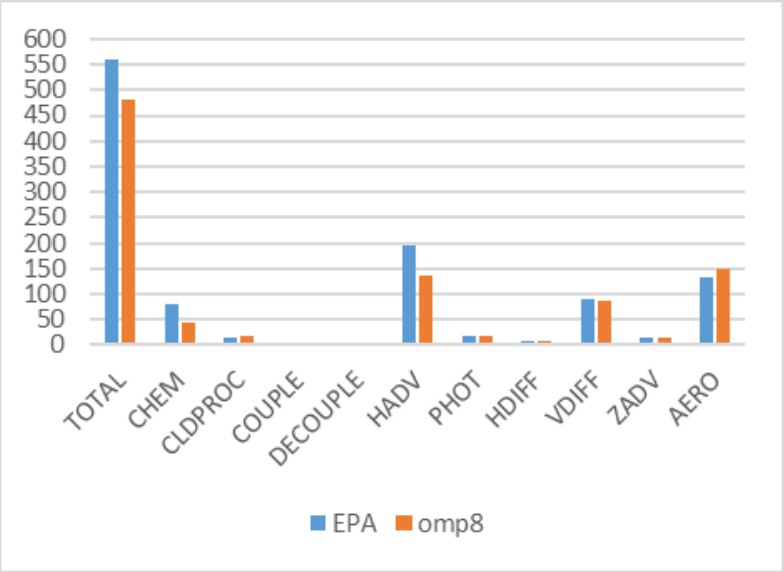
- JSparse is the standard U.S. EPA release
- FSparse is the thread parallel version with OpenMP modifications to:
  - Chemistry Transport Model (CTM)
  - Horizontal Advection Module (HADV)

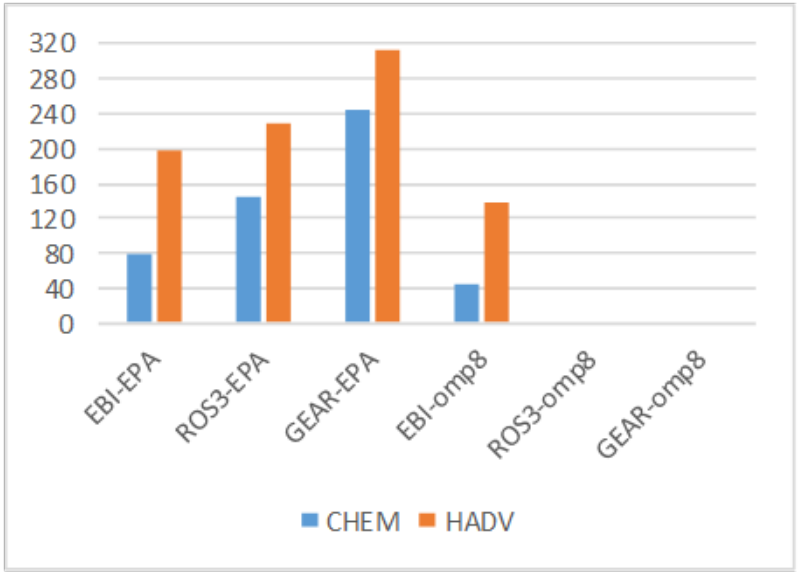
  Both execute with 24 MPI processes and 8 threads each with the FSparse case

  This report is an extension of what was published in *Modern Environmental Science and Engineering* Vol. 5, Nr.9, 2019, pp. 775-791

101-day performance profile (time in hours)

Parallel thread speedup over the standard U.S. EPA model

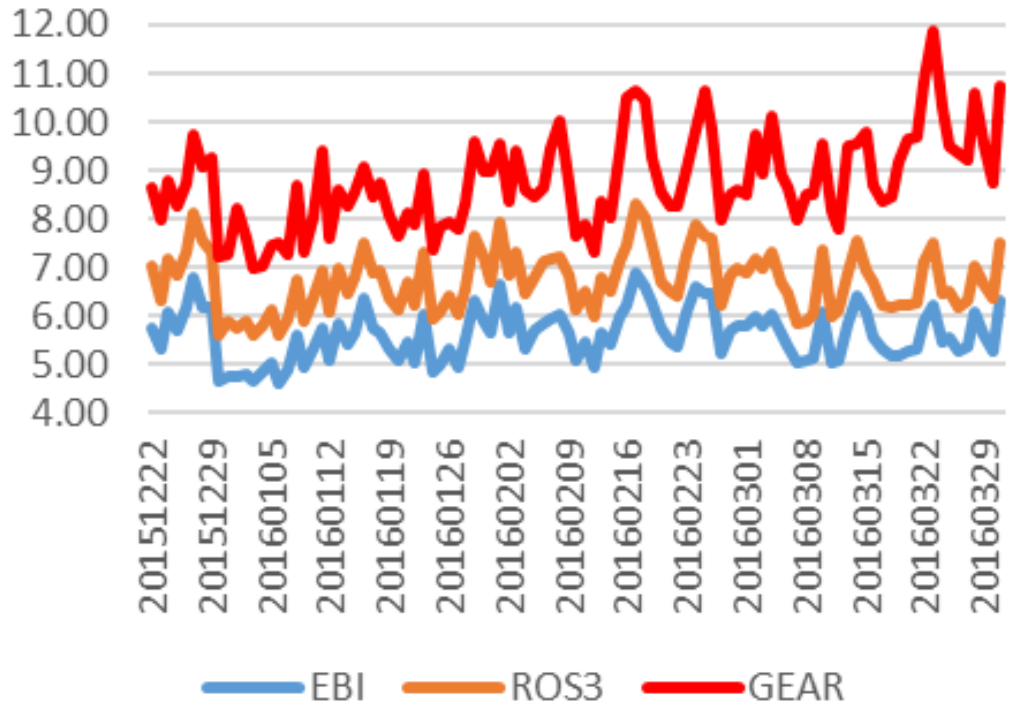




Euler-backward solver (EBI) for U.S. EPA (JSparse) and OpenMP (FSparse) versions. With FSparse the speedup over EPA is 1.8 in CHEM and 1.4 in HADV, and 1.16 for total wall clock time.

Results for Rosenbrock (ROS3) and SMV Gear (GEAR) are pending.

EPA CMAQ 5.3 101-day time series in hours



For the chart: Time for CMAQ version with three CTM solvers:

- EBI (EPA) 567 hours,
- ROS3 (EPA) 678 hours
- GEAR (EPA) 886 hours

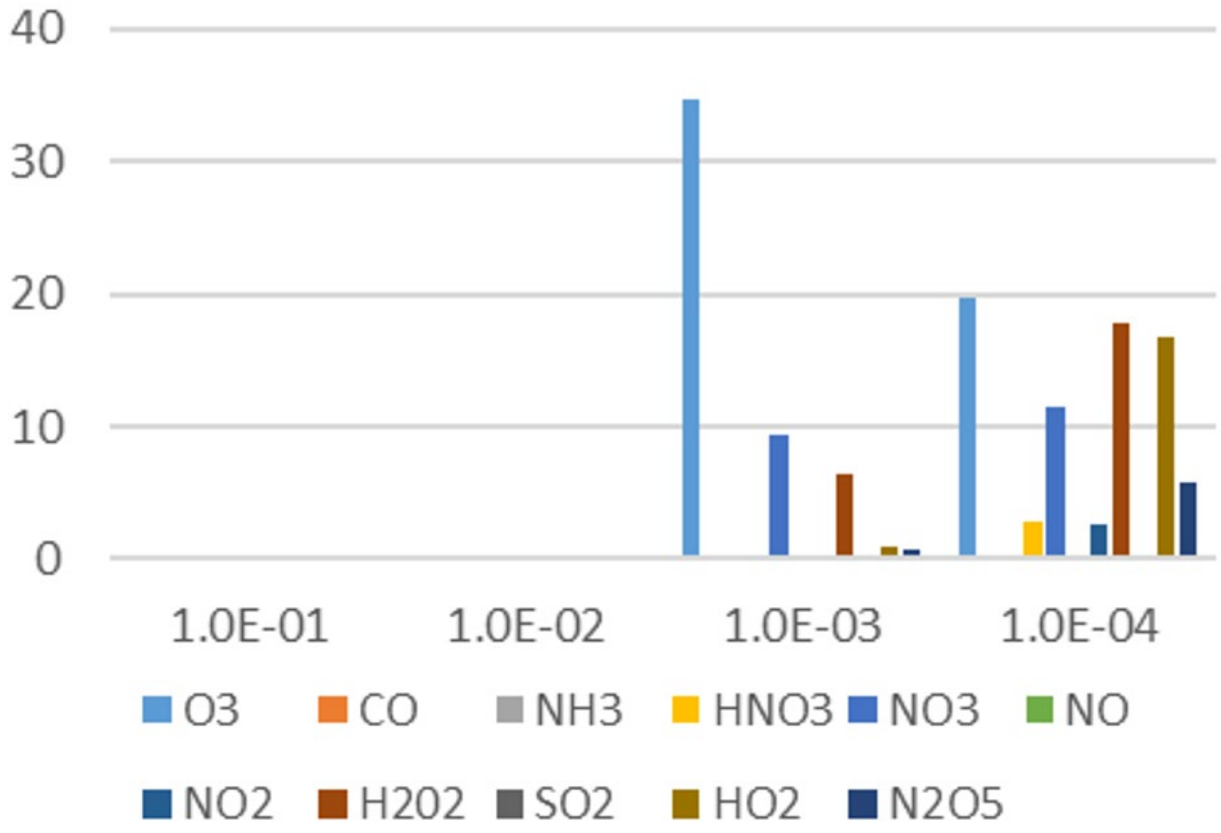
Results so far for the OpenMP FSparse version:

- EBI (omp8) 487 hours:
  A speedup of 1.16

Numerical precision: JSparse vs FSparse

Frequency data for the absolute error in comparing concentration predictions of the ROS3 solver in the EPA JSparse and FSparse versions of CMAQ for the species shown in the legend. Histogram bins are in decreasing decades from left to right. The vertical scale shows percent of total sample falling into the corresponding bin.

This demonstrates agreement to at least two decimal places.



Numerical Precision in CMAQ 5.3

- The three algorithms EBI, ROS3, and GEAR can produce different precision in numerical values for species concentrations
- The ROS3 and GEAR algorithms are superior to EBI and should be implemented in its place
- For reasons of wall clock time expense ROS3 may be preferred to GEAR in production use

For a detailed discussion see the full paper.

Speedup in CMAQ 5.3

- FSparse OpenMP speedup over the U.S. EPA version of CMAQ is in the range 1.16 (EBI) to 1.20 (ROS3)
- Thread speed up for the CHEM science process is on the order of 1.8
- Thread speed up for the HADV science process is on the order of 1.4

Other results are pending.
For a detailed discussion see the full paper.

Conclusions

Comparing runtime performance for CMAQ 5.3 in the OpenMP parallel version with the U.S. EPA release showed benefits such as:

- Thread speedup as high as 1.2 (ROS3) with 8 threads
- Numerical values of predicted species concentration that are within the error tolerance inherent in the algorithms
- The CTM with the Rosenbrock algorithm in the FSparse version delivers wall clock times similar to (or less than) the Euler-backward algorithm in the standard U.S. EPA release of CMAQ

Thank You For Your Attention

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