



# *CMAQ 5.3 Parallel Performance for a 192-day Simulation*

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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 Q1+Q2 CY2016
  - 2015-12-22 to 2016-06-30 (192 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)

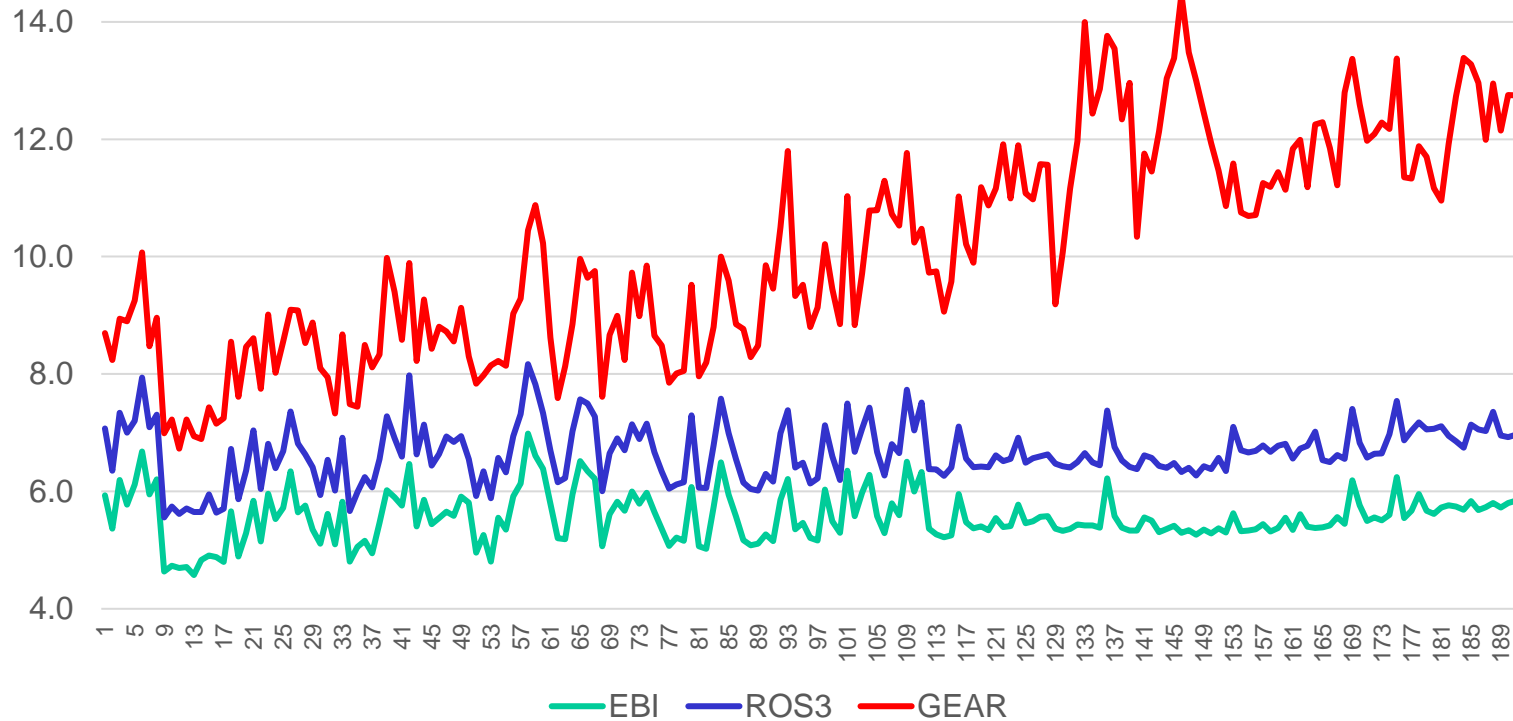
Both execute with 24 MPI processes and 8 threads each with the FSparse case

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





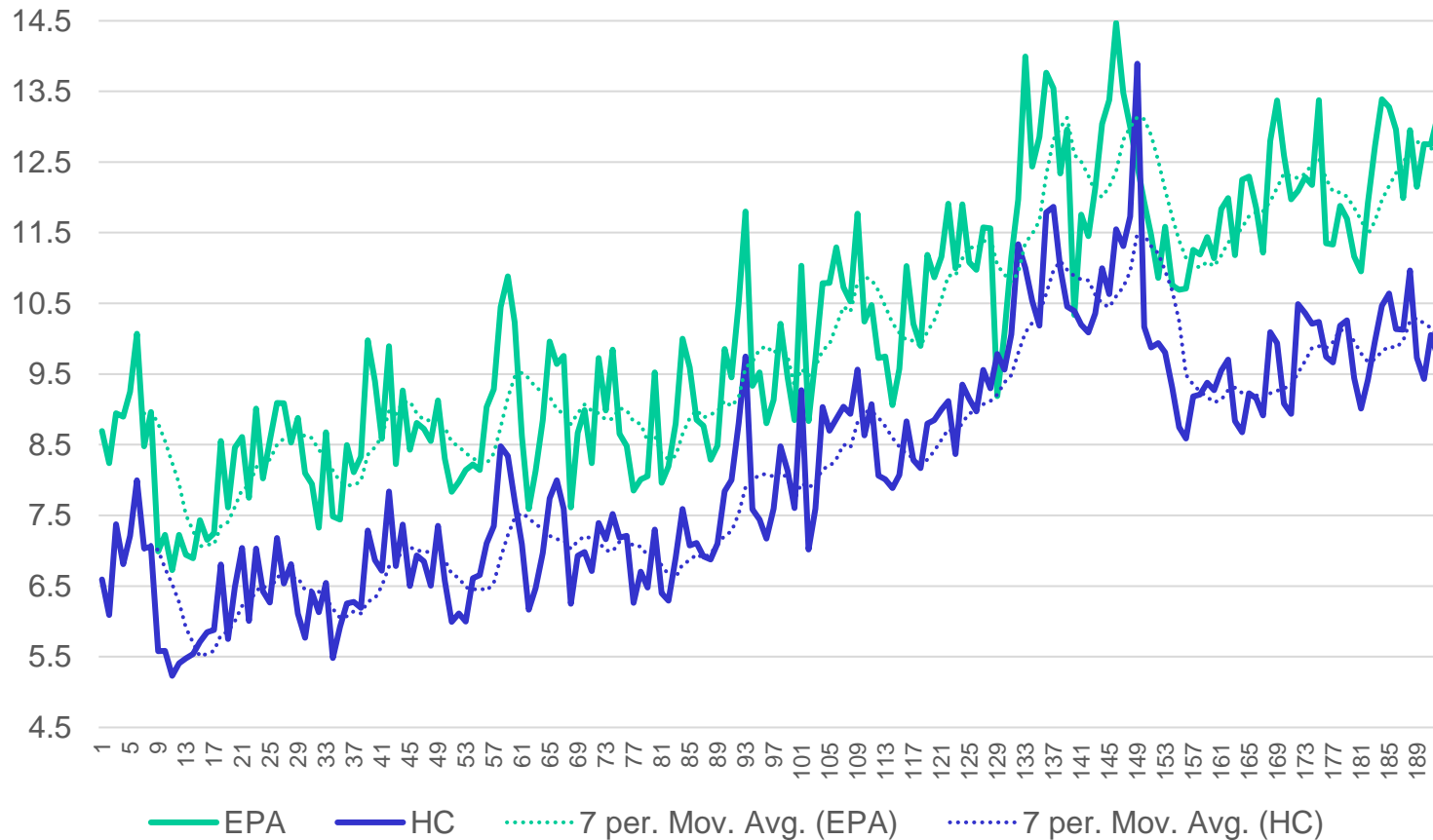
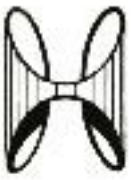
# EPA CMAQ 5.3 192-day time series in hours



Time for CMAQ 5.3 in EPA versions with these CTM solvers:

- EPA:Gear 1941 hours
- EPA: Rosenbrock (ROS3) 1279 hours
- EPA: Euler-Backward (EBI) 1068 hours

# EPA vs HC CMAQ 5.3 192-day time series in hours

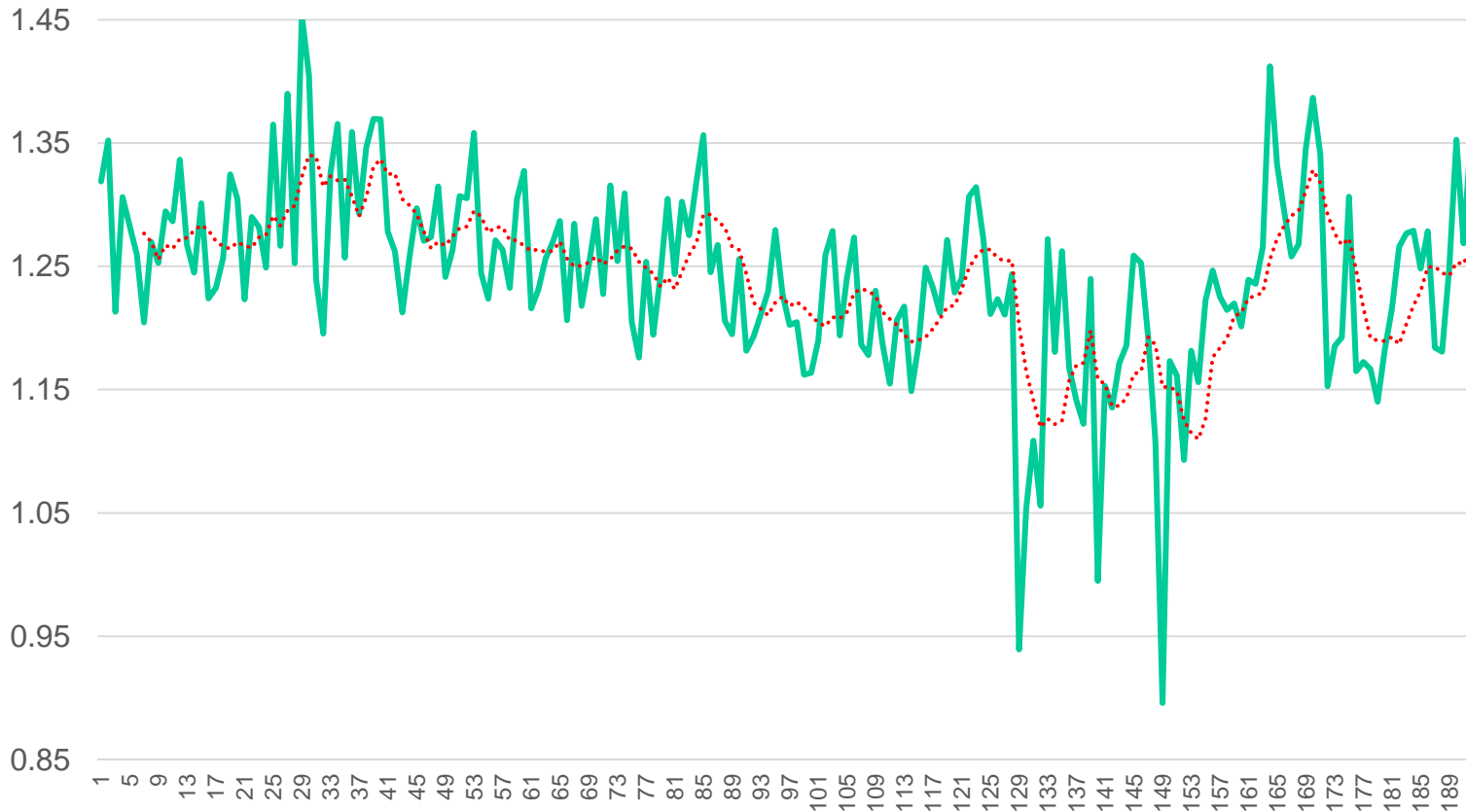


Time for CMAQ 5.3 versions with the GEAR CTM solver:

- **EPA: 1941 hours** **HC-OMP: 1572 hours**
- OpenMP **1.23 average speedup**

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# EPA vs HC CMAQ 5.3 192-day time series speedup

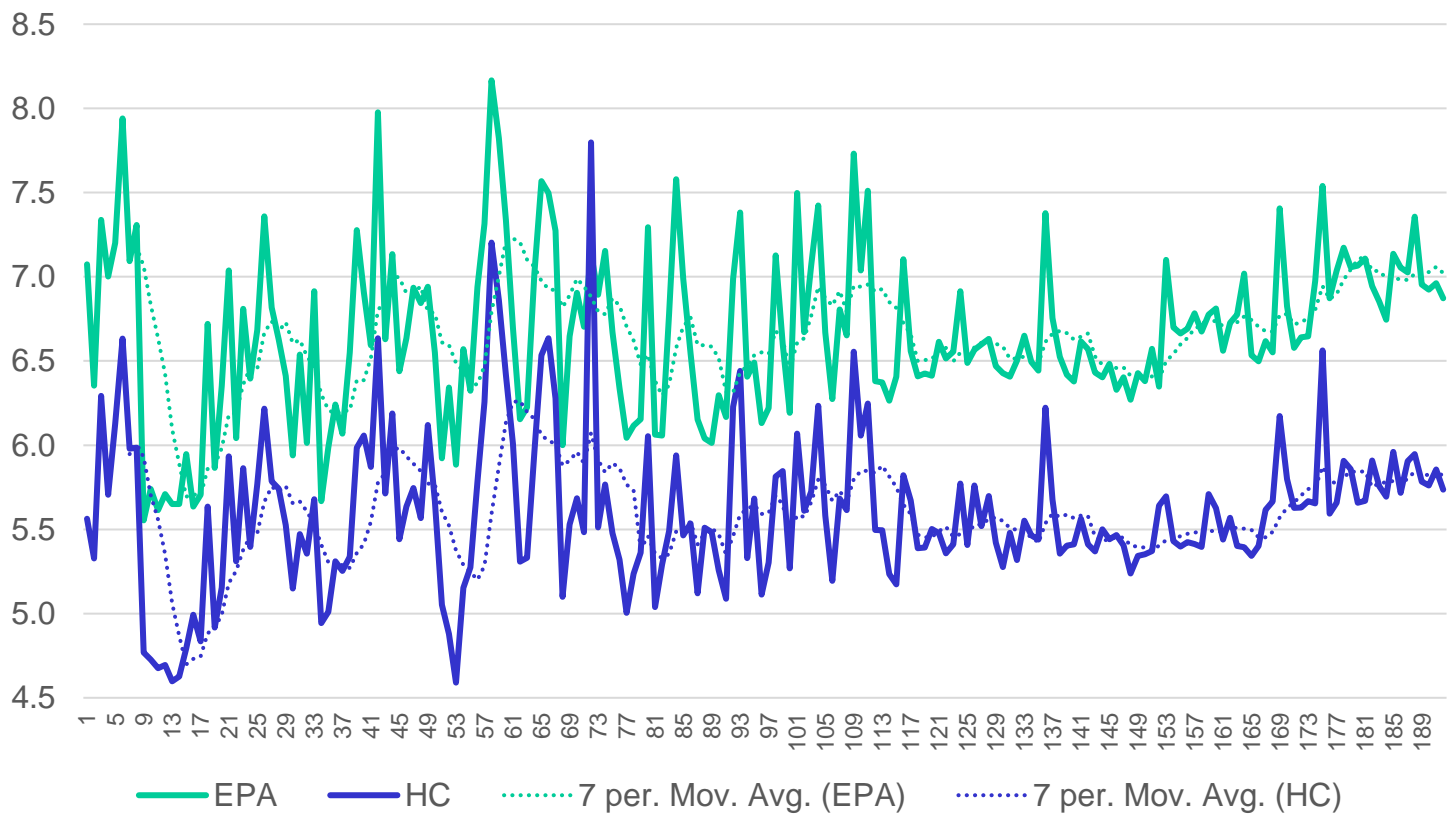


Speedup for CMAQ 5.3 parallel thread version of GEAR CTM solver:

- Speedup each day (solid line)
- Speedup with 7-day moving average (dotted line)

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# EPA vs HC CMAQ 5.3 192-day time series in hours

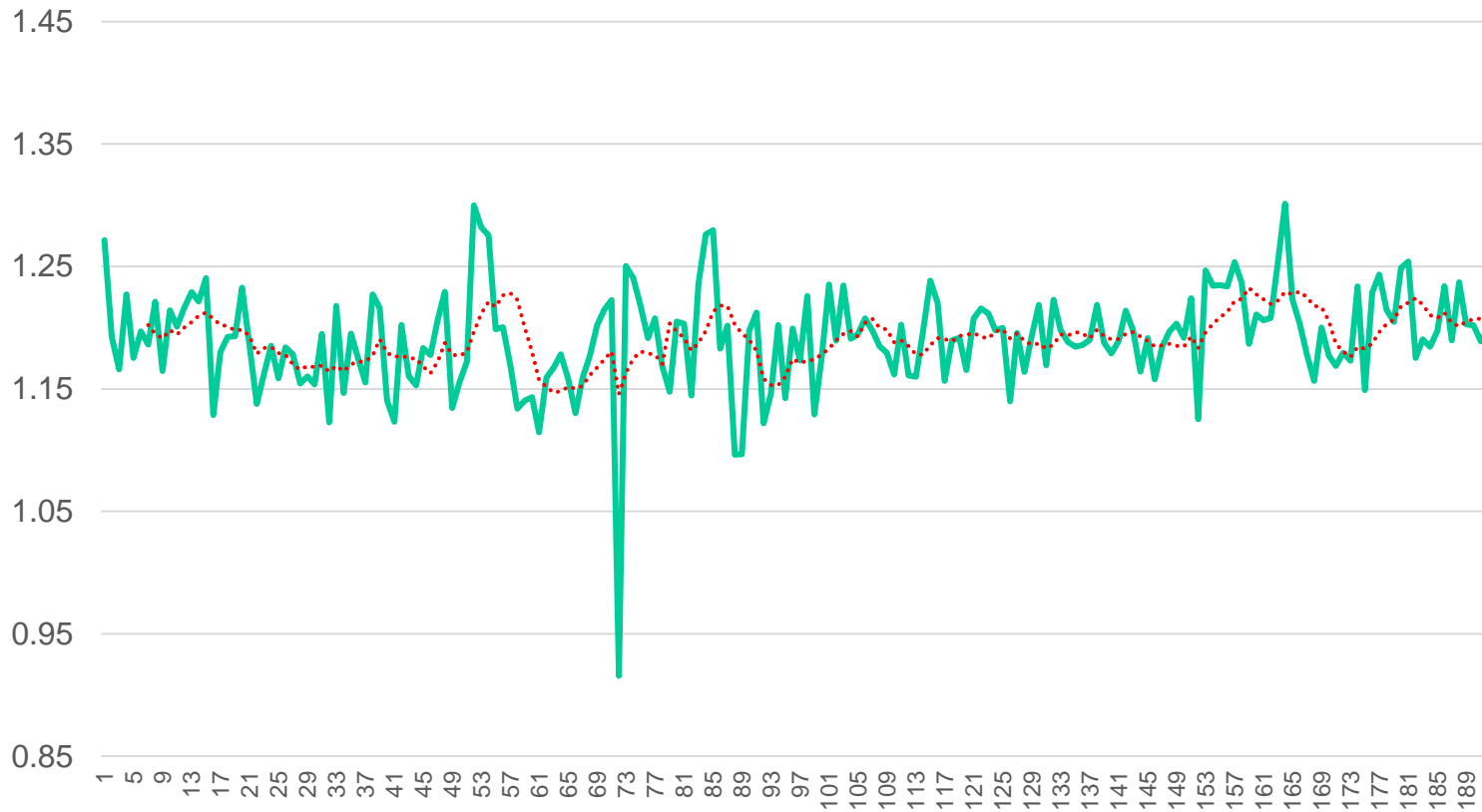


Time for CMAQ 5.3 versions with the ROS3 CTM solver:

- **EPA: 1279 hours** **HC-OMP: 1075 hours**
- OpenMP **1.19 average speedup**



# EPA vs HC CMAQ 5.3 192-day time series speedup



Speedup for CMAQ 5.3 parallel thread version of ROS3 CTM solver:

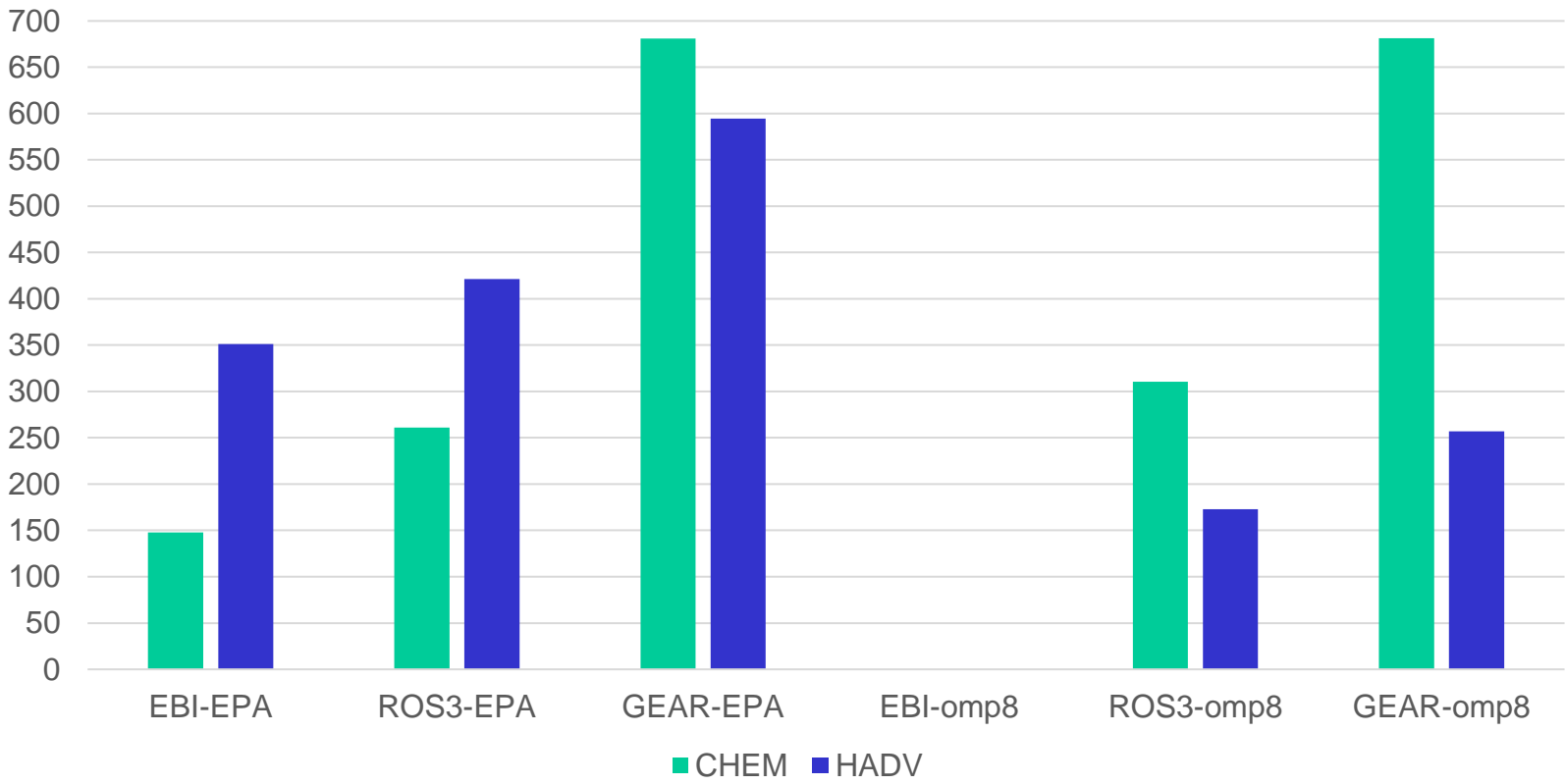
- **Speedup each day (solid line)**
- **Speedup with 7-day moving average (dotted line)**

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# 192-day performance profile (time in hours)



Time in **CHEM** and **HADV**: the left group is the EPA version, the right group the FSpase 8-thread version. All the speedup comes in HADV:

- 2.43 for ROS3
- 2.31 for GEAR

*Conclusion: The FSpase CTM needs more than 8 threads*



## Speedup in CMAQ 5.3

- FSpase OpenMP speedup vs U.S. EPA:
    - 1.19 (ROS3)
    - 1.23 (GEAR)
  - Thread speed up for the CHEM science process is in the range *1.0 to 0.84*
  - Thread speed up for the HADV science process is in the range *2.3 to 2.4*
  - Speedup is due to performance in HADV
- FSpase tests with 10 & 12 threads are pending*

## Numerical Precision in CMAQ 5.3



- The three algorithms EBI, ROS3, and GEAR can produce different precision in numerical values for species concentrations\*
- A detailed discussion is pending the conclusion of EBI version runs

\* And different predictions for some species: see the long write up at this meeting in 2020 (Section 4).

# Conclusions



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

- An average 8-thread speedup of **1.23** (GEAR) and **1.19** (Rosenbrock) cases, respectively
- The Rosenbrock (ROS3) algorithm in the FSparse version delivers a wall clock time of 1065 hours, compared to 1068 hours with the U.S. EPA Euler-backward algorithm (EBI). Since ROS3 is the superior solver, its use in the FSparse version is recommended as a replacement for EBI.
- **Results full year 2016 are pending for next year!**



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# ***Thank You For Your Attention***

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