A Thread Parallel Sparse Matrix Chemistry Algorithm for the Community Multiscale Air Quality Model

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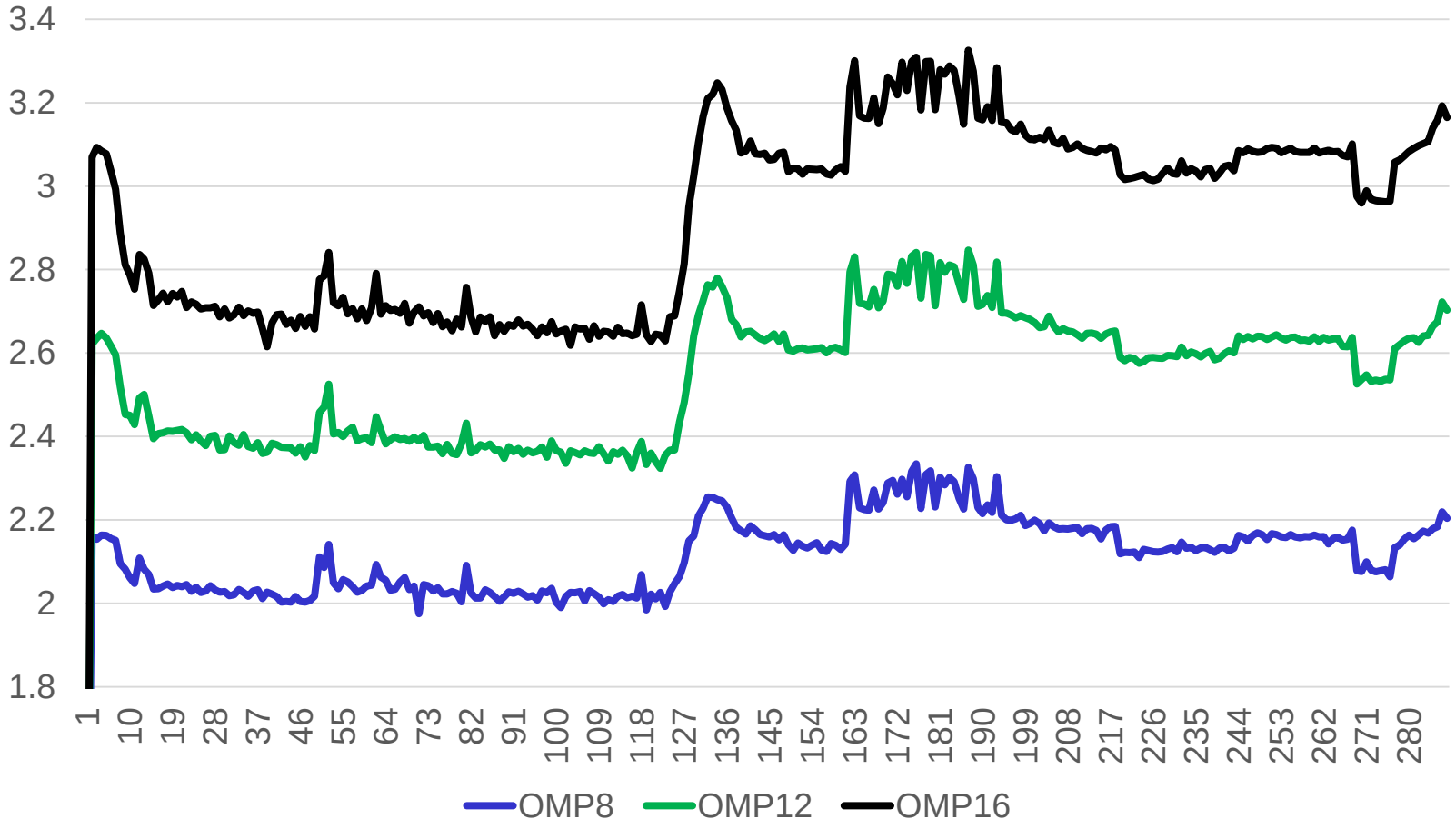
Two 24 hour episodes

- CMAQ 5.3.b
  - July 1st, 2011 cb6r3_ae6_aq mechanism
  - 154 active species and 338 reactions
  - day/night Jacobian has 1338/1290 non-zeros
- CMAQ 5.3
  - July 1st, 2011 cb6r3_ae7_aq mechanism
  - 147 active species and 343 reactions
  - day/night Jacobian has 1400/1348 non-zeros
- 80 *x* 100 California domain at 12 Km grid, 35 vertical layers (280,000 grid cells=small case)

Speedup: HC vs EPA CMAQ 5.3.b (8, 12, 16 threads)

Parallel thread speedup over the standard U.S. EPA model in 288 calls to CHEM with the Gear algorithm for 8, 12 and 16 threads (OMP8 to OMP16), for NP=1 MPI process.



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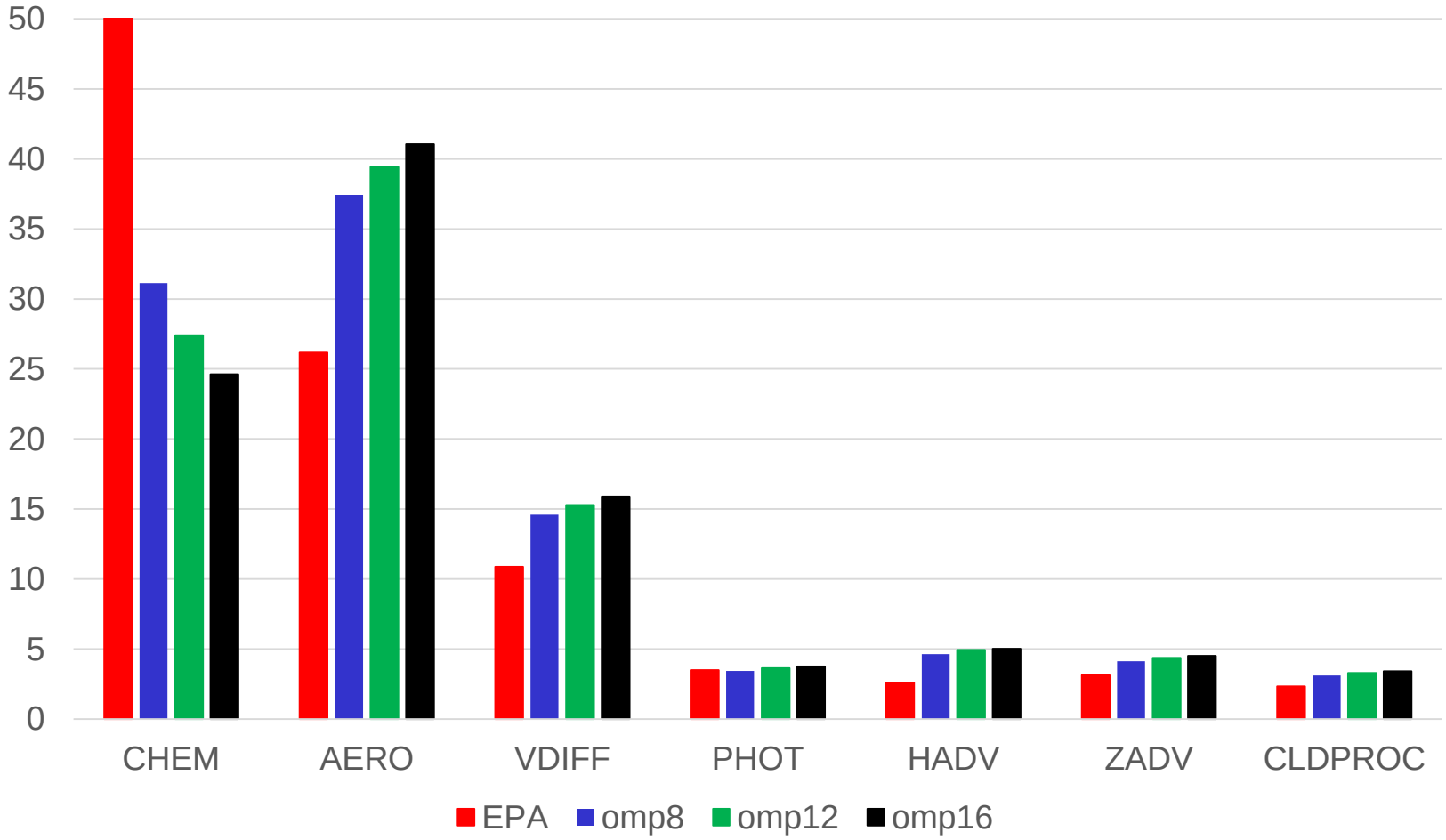
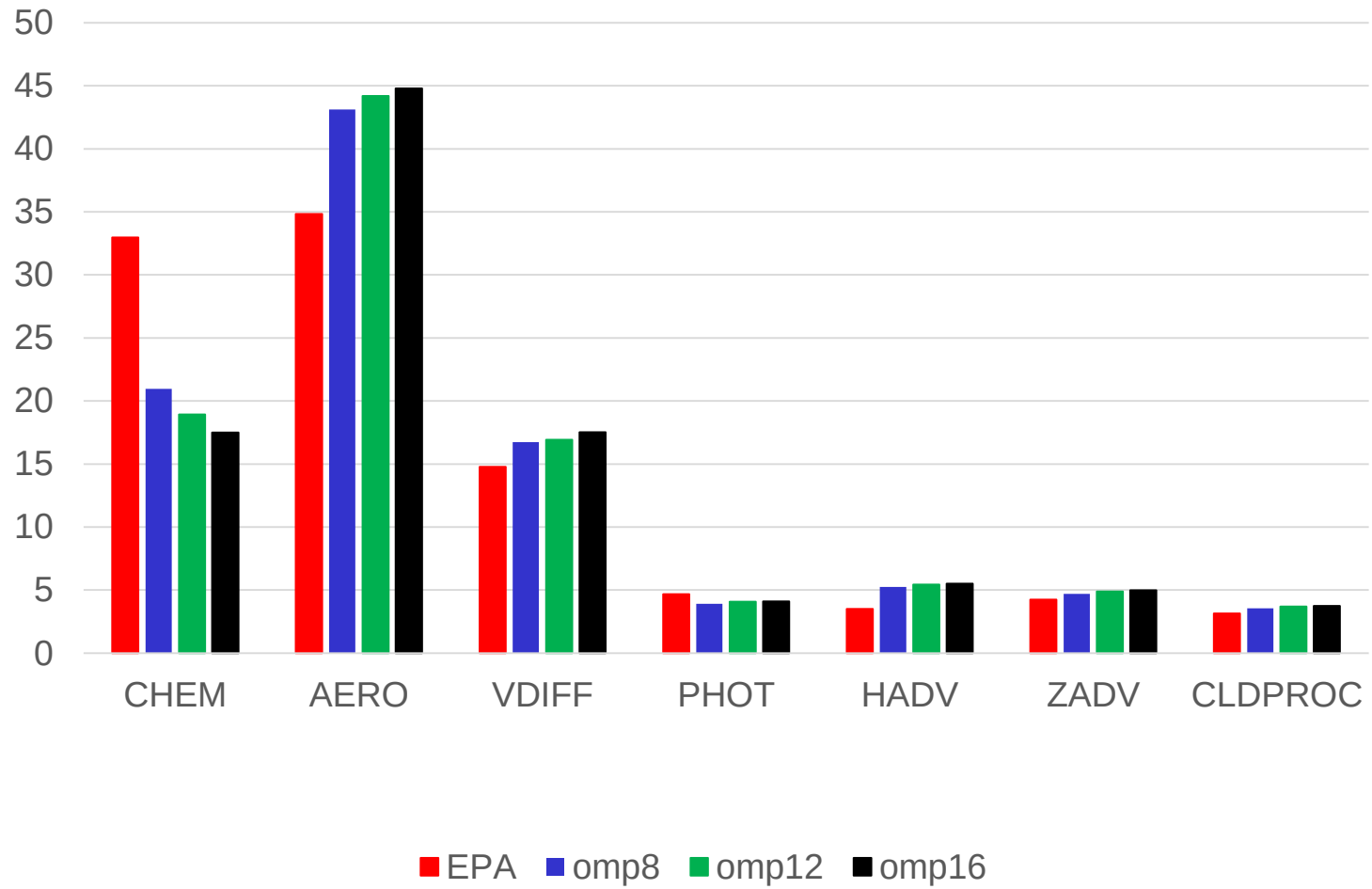
Fraction of time by process (NP=1): EPA CMAQ 5.3.b vs HC (8, 12,16 threads)

Fraction of wall clock time (percent) by science process in CMAQ for the FSparse Gear algorithm compared to JSPARSE (EPA) for NP=1 MPI process and OpenMP thread counts of 8, 12, and 16.



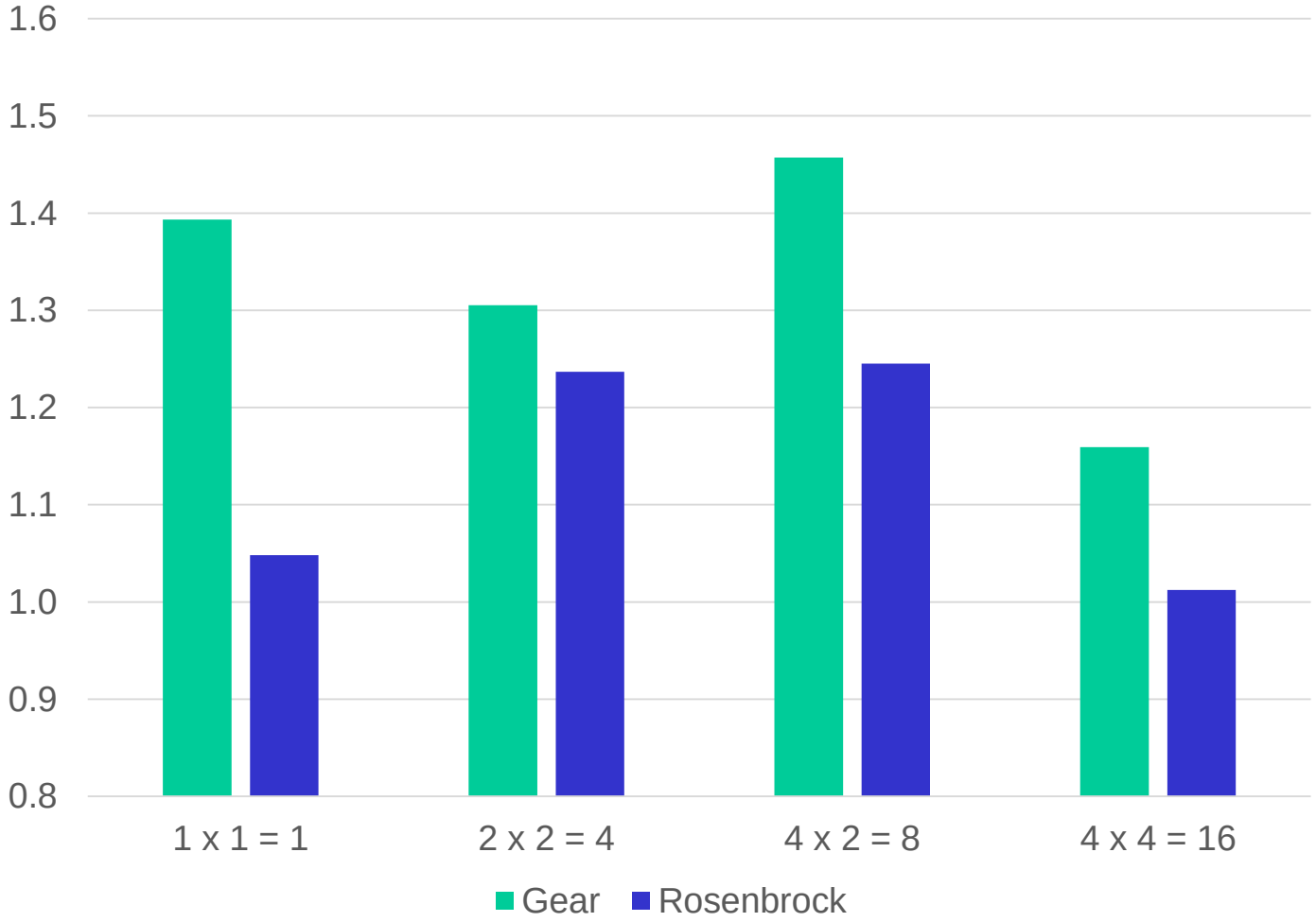
Fraction of time by process (NP=1): EPA CMAQ 5.3.b vs HC (8, 12,16 threads)

Fraction of wall clock time (percent) by science process in CMAQ for the FSparse Rosenbrock algorithm compared to JSPARSE (EPA) for NP=1 MPI process and OpenMP thread counts of 8, 12, and 16.



Speedup: HC vs EPA (8 threads)

Parallel thread speedup over the standard U.S. EPA model for the Gear and Rosenbrock algorithms with 8 threads, for NP=1 to 16 MPI processes (assigned row *x* column) on the heterogeneous cluster



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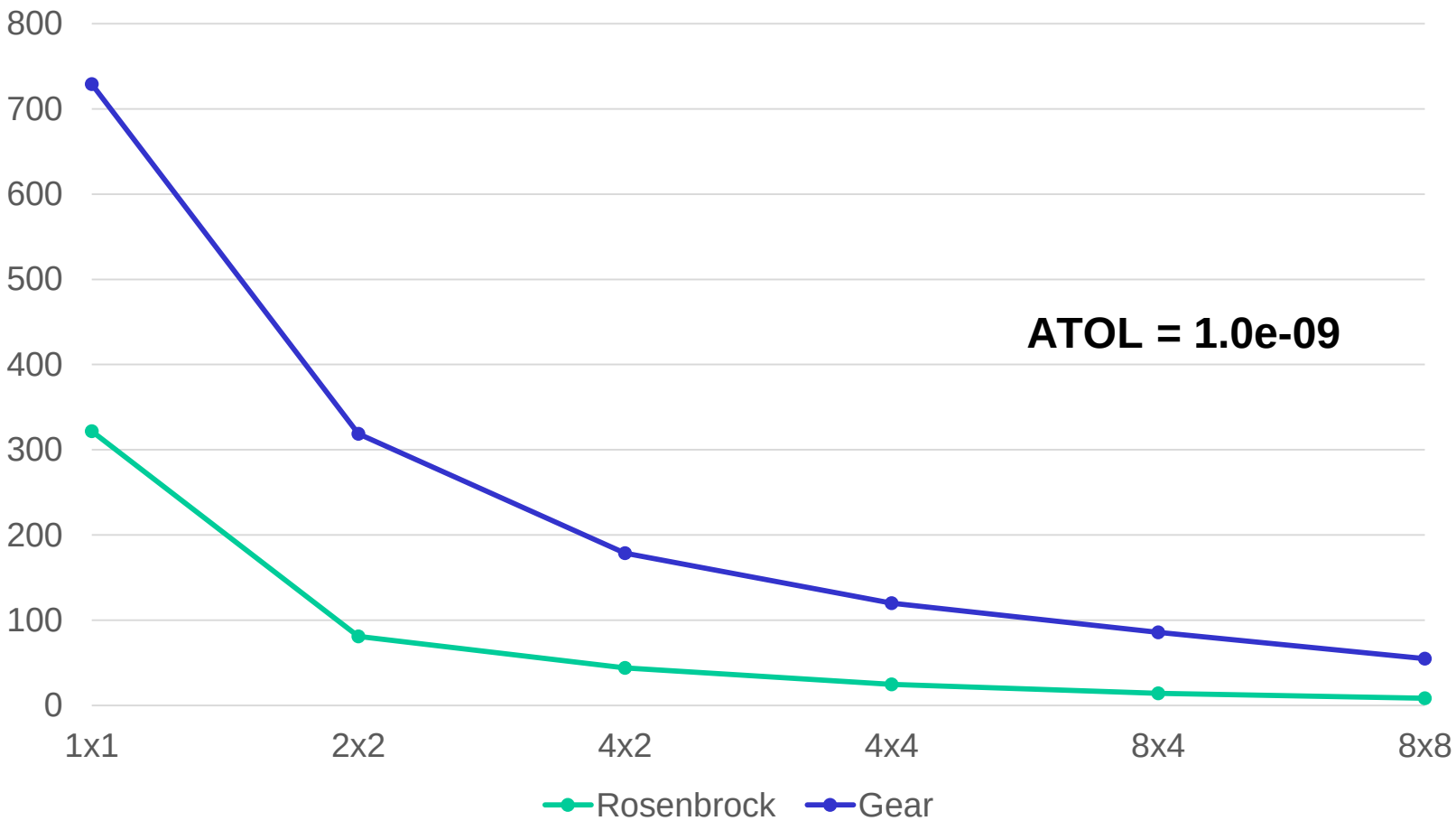
EPA CMAQ 5.3 Gear wall clock time

- MPI communication time exceeds compute time when ATOL = 1.0e-09
- There are numerical precision issues
- Compare results when:

  ATOL = 1.0e-09 versus ATOL = 1.0e-08

EPA CMAQ 5.3 Gear and Rosenbrock

Wall clock time (minutes) versus MPI process count



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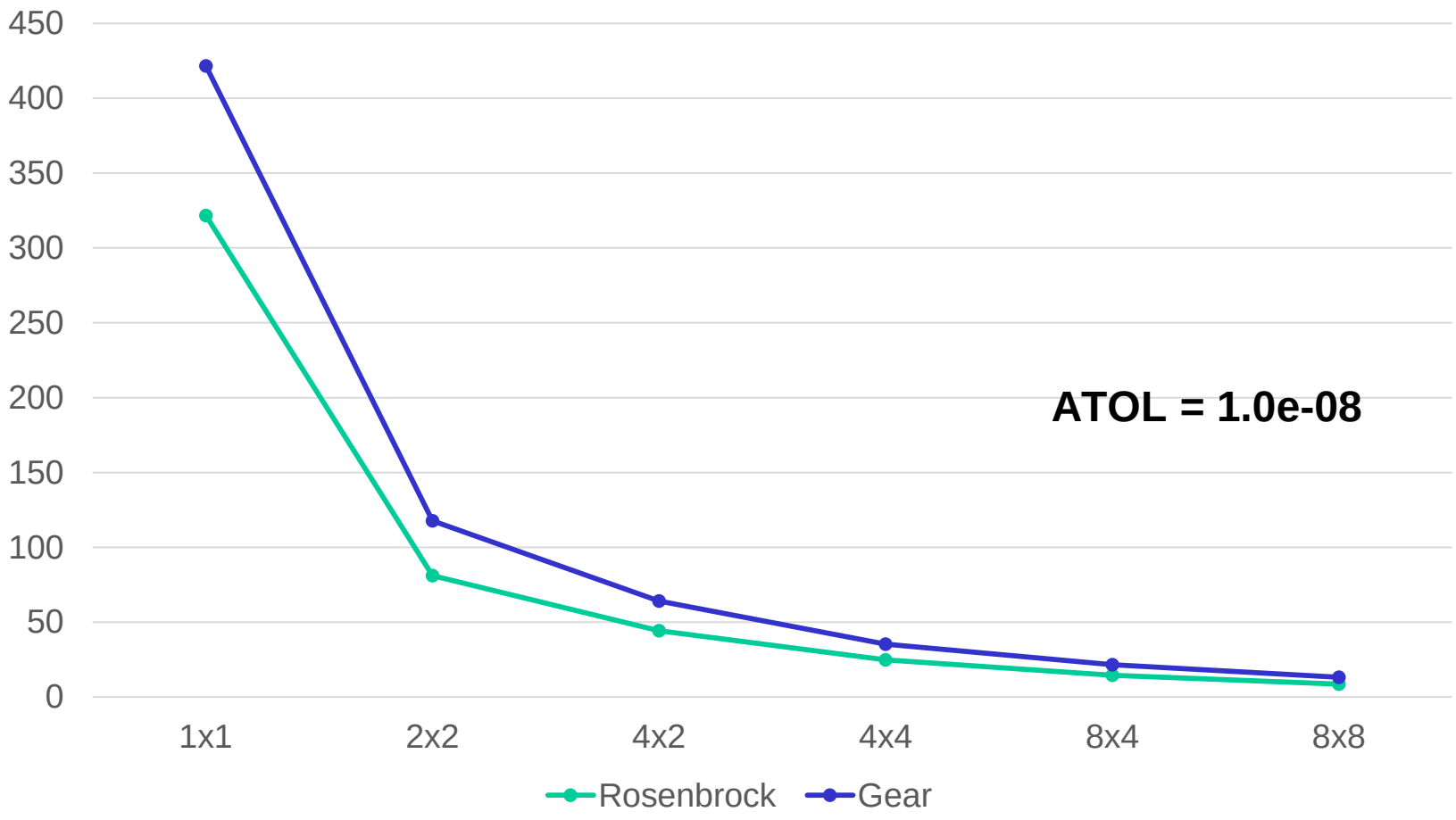

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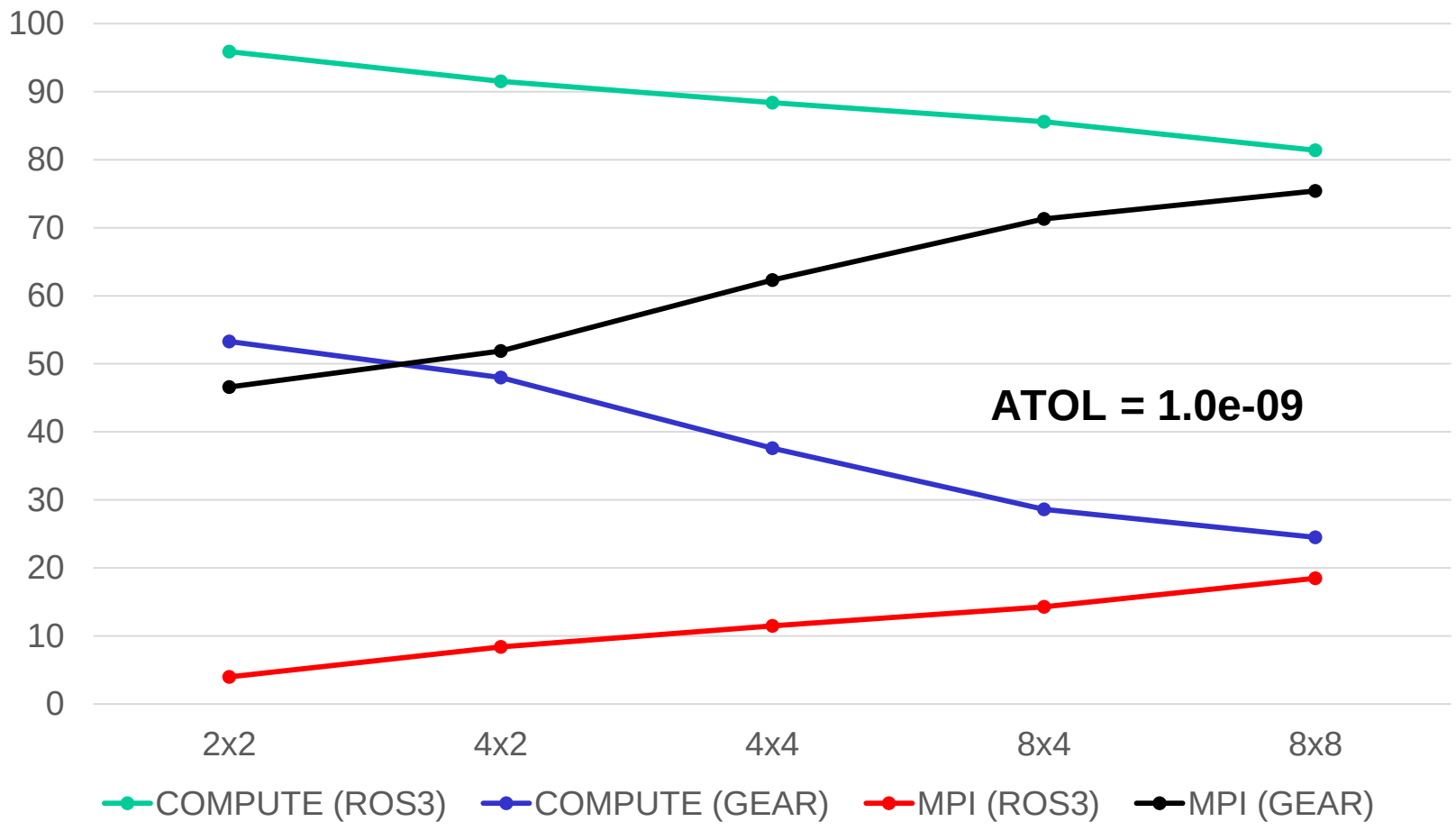
EPA CMAQ 5.3 Gear and Rosenbrock (ROS3)

Fraction of COMPUTE vs MPI COMMUNICATION time (percent)



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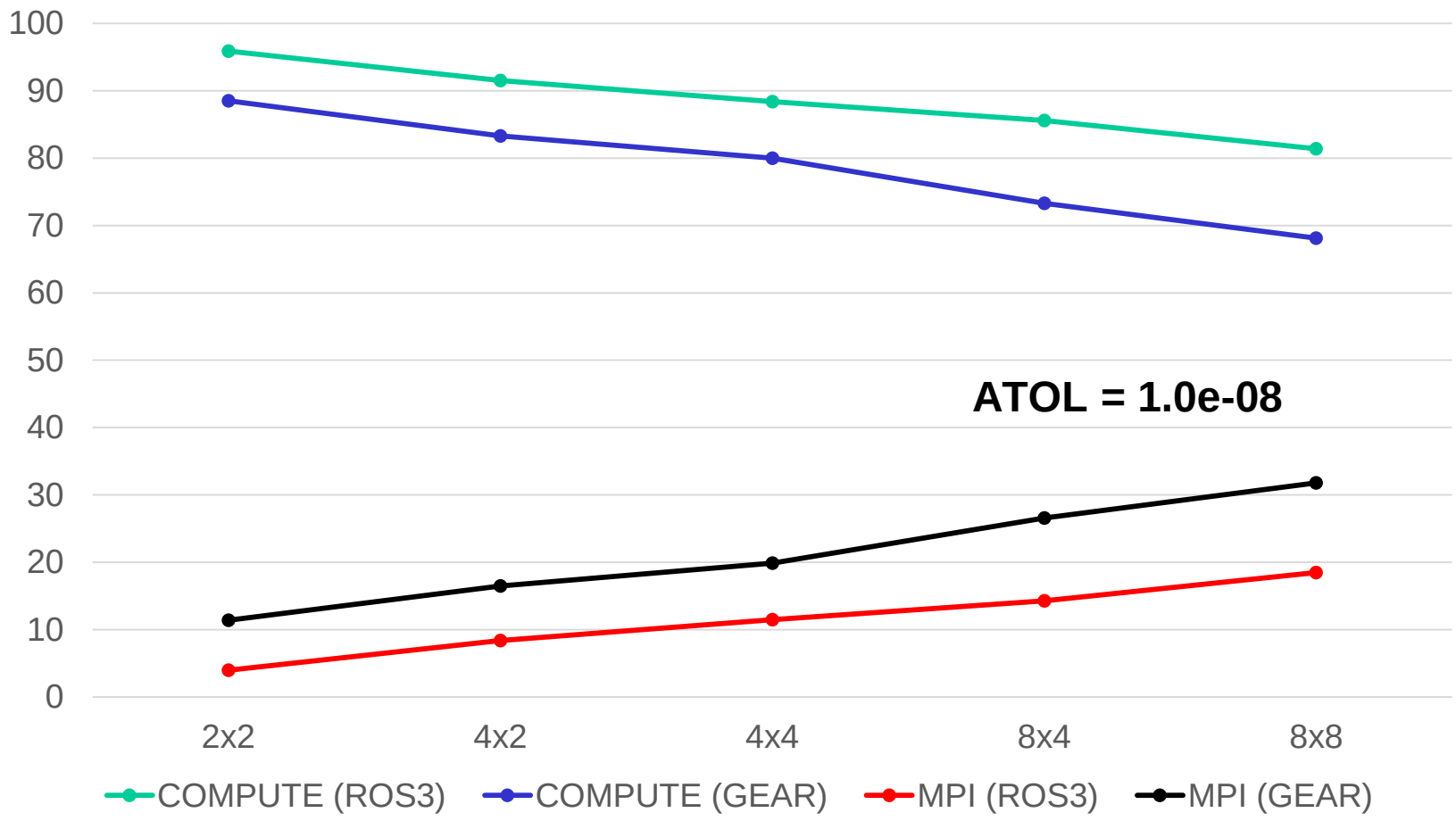

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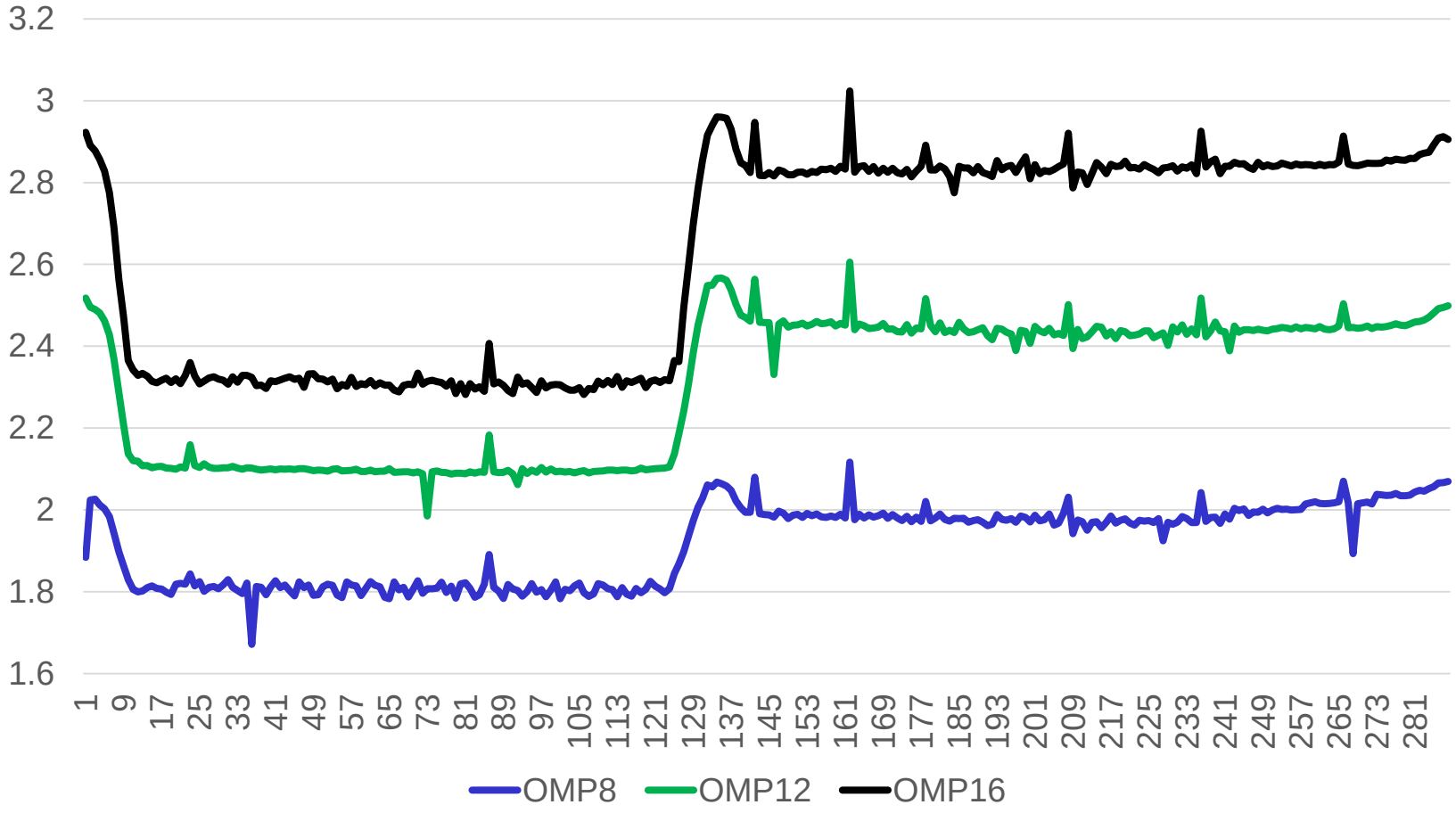

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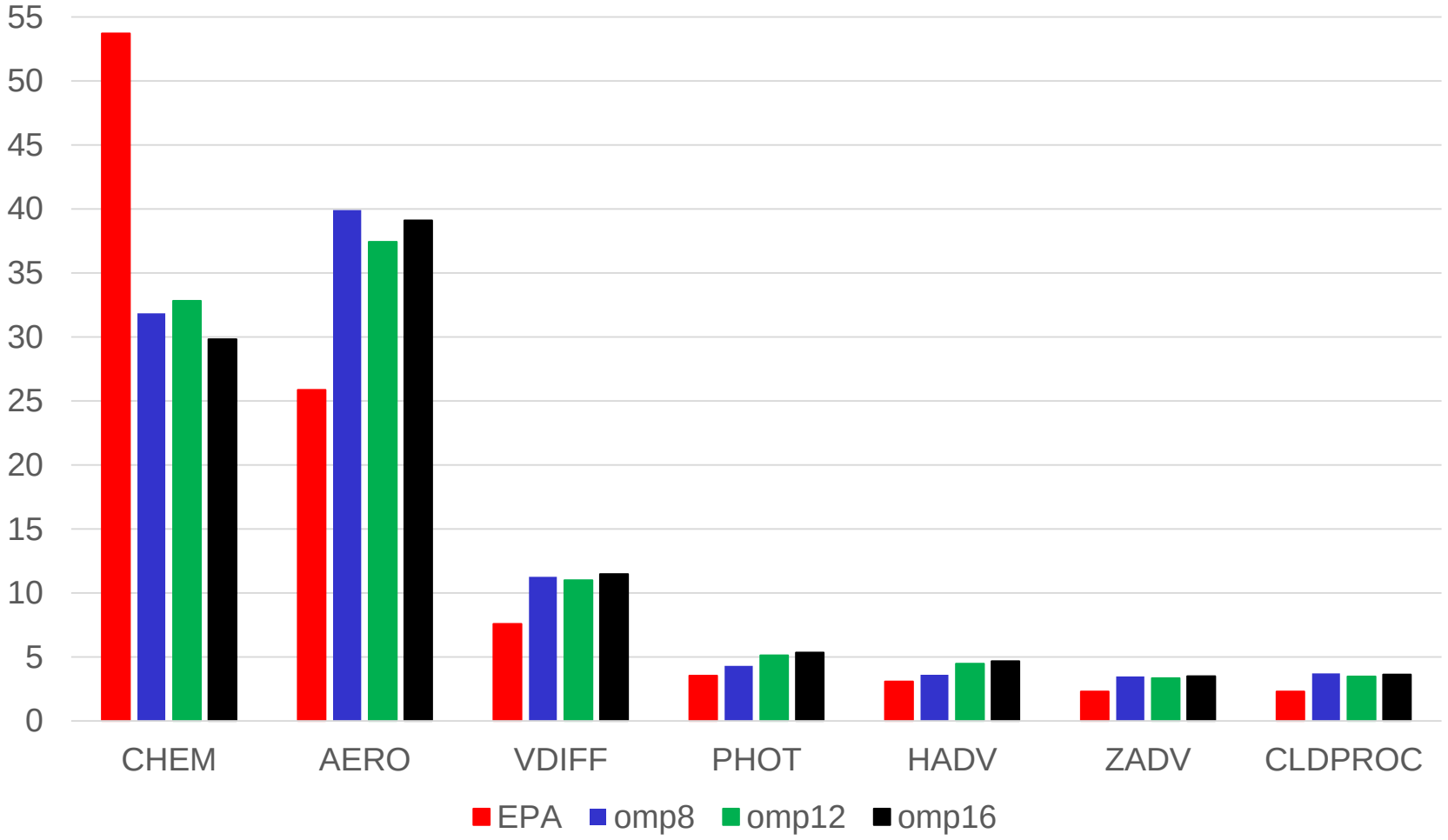

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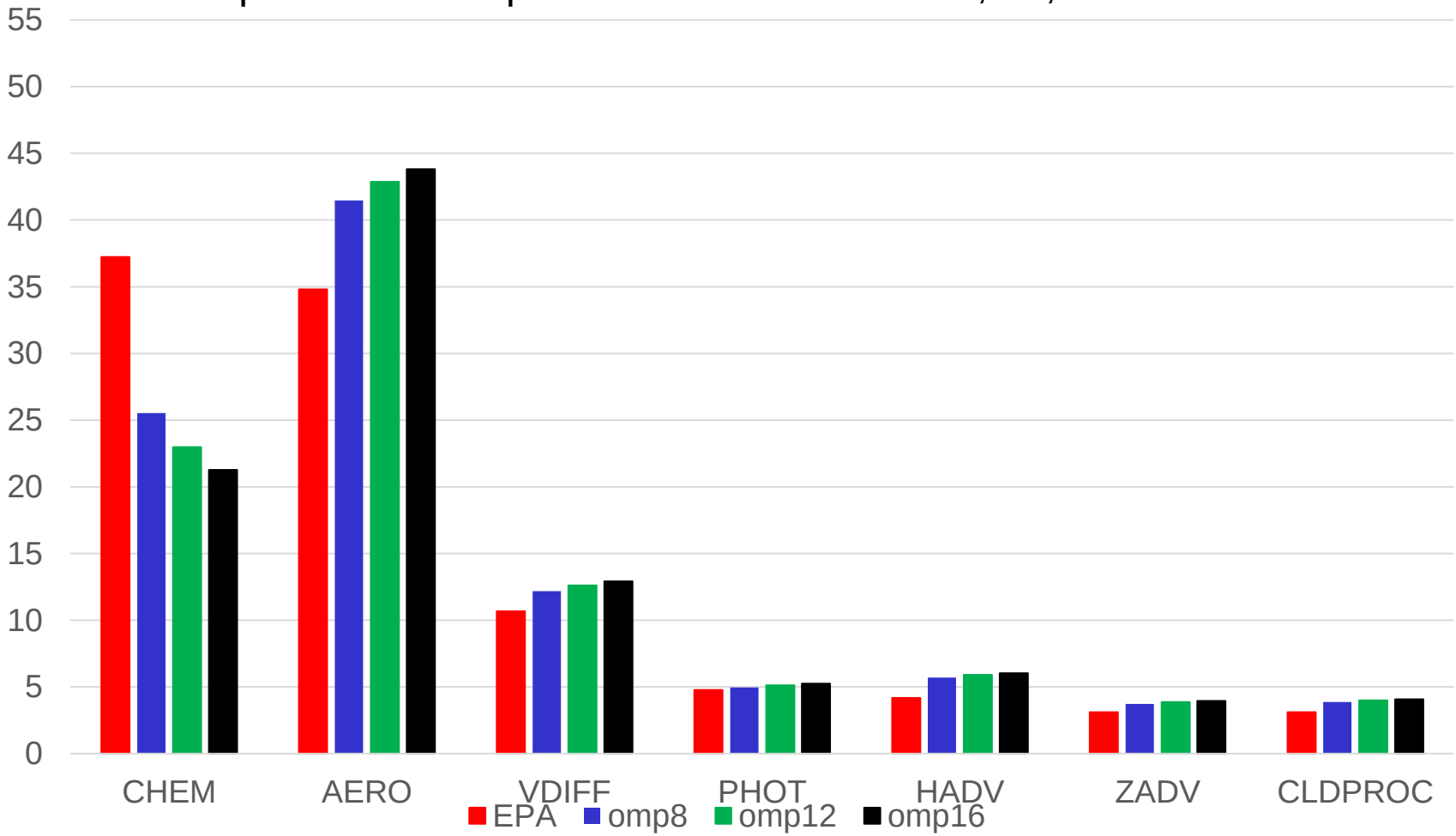

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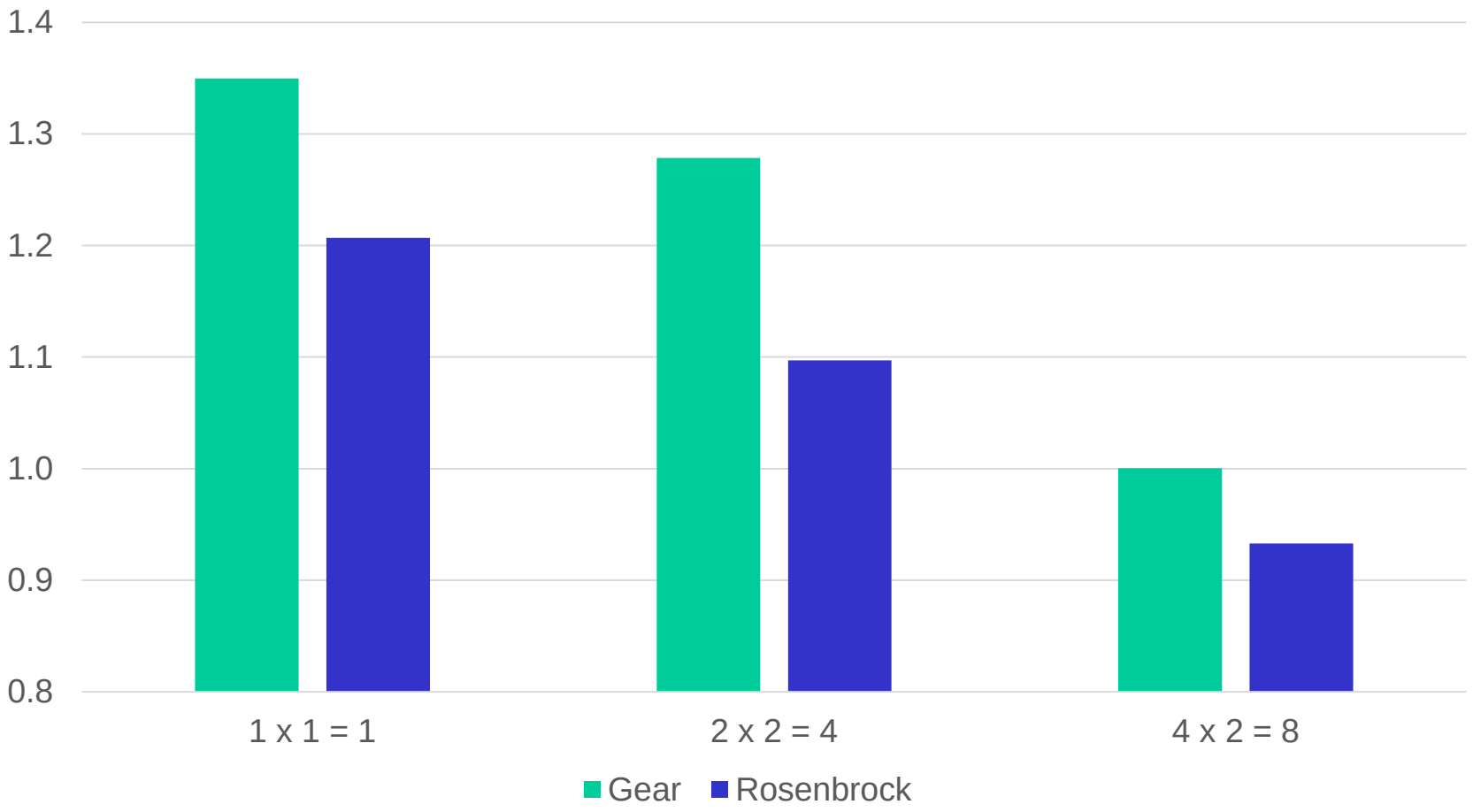

Conclusions

- FSparse computational performance compared to serial EPA version often better
- The FSparse algorithm offers performance gains that are portable across platforms
- Recommend thread parallel version included as an option in EPA CMAQ releases

Next steps:

1. **14 day runs for SE-USA and CONUS**
2. **Thread parallelism for AEROPROC**