CMAQ 5.1 PERFORMANCE WITH PORTLAND AND INTEL COMPILERS

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Introduction

This presentation reports on implementation of the parallel sparse matrix solver, FSparse, in the Chemistry Transport Model (CTM) in CMAQ [1]. This release is v6.2 and is a major redesign. It is applicable in the CMAQ version that uses either the Rosenbrock (ROS3) or SMV Gear (GEAR) [2] algorithms in the CTM..

Test Bed Environment

The hardware systems chosen were the platforms at HiPERiSM Consulting, LLC, where each of two nodes host two Intel E5v3 CPUs with 16 cores each. In addition, each node has four 1st generation Intel Phi co-processor many integrated cores (MIC) cards with 60 and 59 cores for the respective models. With four MIC cards per node, and 4 threads per MIC core, the total available thread count is 960 and 944, for the respective nodes. This report implemented the Intel Parallel Studio® suite (release 17.0) using options for either host CPU or Phi coprocessor with the same episode as in the previous report [1]

Profile of the original CMAQ version

The totals of wall clock time for ROS3 and GEAR CTM solvers, with various values of NP, is shown in Figure 1. The combination of MPI processes, NP = NPROW x NPCOL, is in the range 1 to 64, with doubling of row and column processes. MPI parallel efficiency declines to ~67% when NP=16, and ~36% when NP=64.

FSparse CMAQ on the host CPU

For NP=1 (one MPI process) Figure 2 shows speedup versus thread count on the host CPU of the OpenMP parallel FSparse version over the standard U.S. EPA release of CMAQ. With 4 to 16 threads the speedup over the standard EPA version ranges from 1.1 to 1.38 for ROS3 and 1.3 to 1.75 for GEAR. The enhancement for the GEAR algorithm is due to more work per thread when compared to ROS3. The diminution of performance gain with higher thread counts is due to the smaller partitions of work per thread calculated from 5040 blocks of cells divided amongst the number of available threads. Grid cells are partitioned into blocks of size 50 and these blocks are distributed to threads in a thread team in the OpenMP version.

FSparse CMAQ on the Intel Phi

Figure 3 shows speedup versus thread count on the Intel Phi processor of the OpenMP parallel FSparse version over the standard U.S. EPA release of CMAQ. With two vector processing units (VPU) per core on the Intel Phi 7120, there is a saturation visible with more than 120 threads. An additional consideration is that 5040 blocks are partitioned over a larger thread team: e.g. 5040/120, 5040/180, and 5040/240, thereby reducing the workload per thread.

Comparing host and Intel Phi results

For host CPU and Phi cases the speedup of the thread parallel version FSparse over the standard release of CMAQ increases monotonically with thread count. However, there are differences between ROS3 and GEAR results. Possible reasons include different data movement patterns, especially for the offload to the Phi. Another contributing factor is the difference in iteration patterns and their number.

Results

Figure 1: Wall clock time (in seconds) versus MPI process count on host CPUs for the original U.S. EPA version of CMAQ 5.1 for ROS3 and GEAR CTM solvers.

Figure 2: For one MPI process this shows the speedup versus thread count (1-16) of the FSparse versions of ROS3 and GEAR CTM solvers of CMAQ 5.1 on host CPUs

Figure 3: For one MPI process this shows the speedup versus thread count (60-240) of the FSparse versions of ROS3 and GEAR CTM solvers of CMAQ 5.1 when off-loaded to the Intel Phi 7120.

Fig. 1

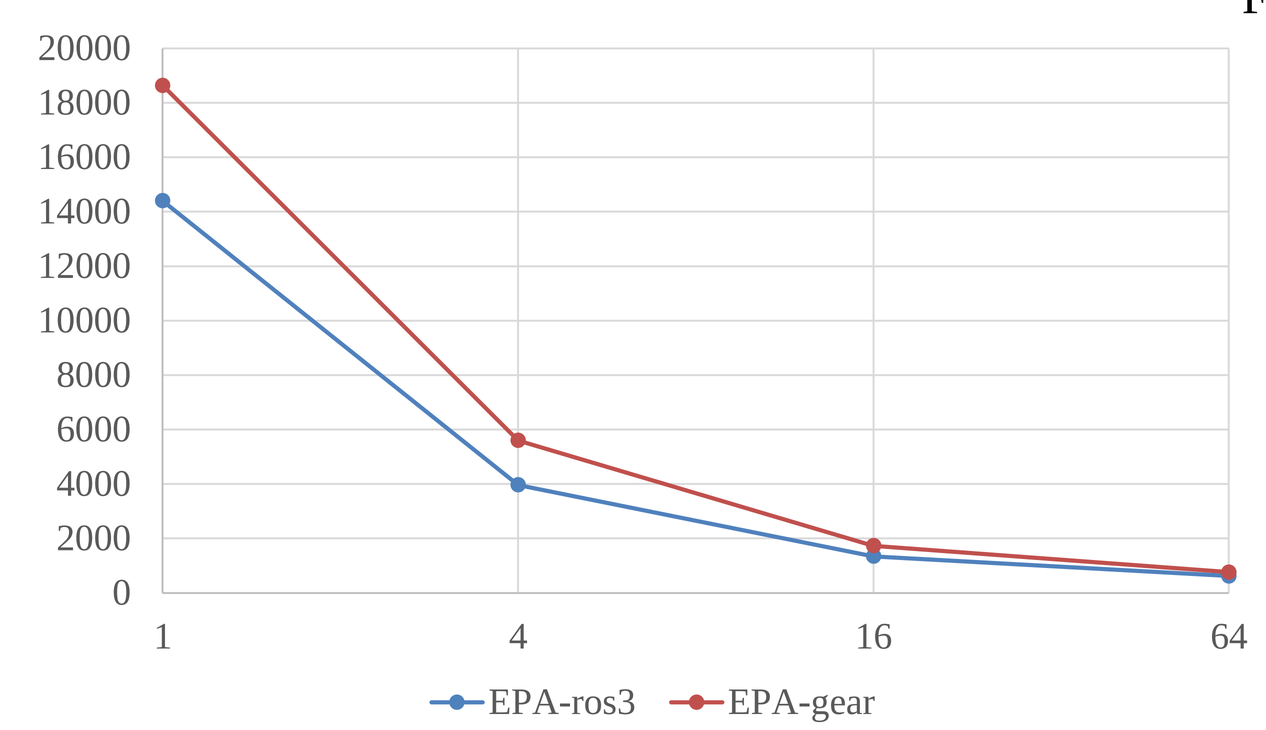


Fig. 2

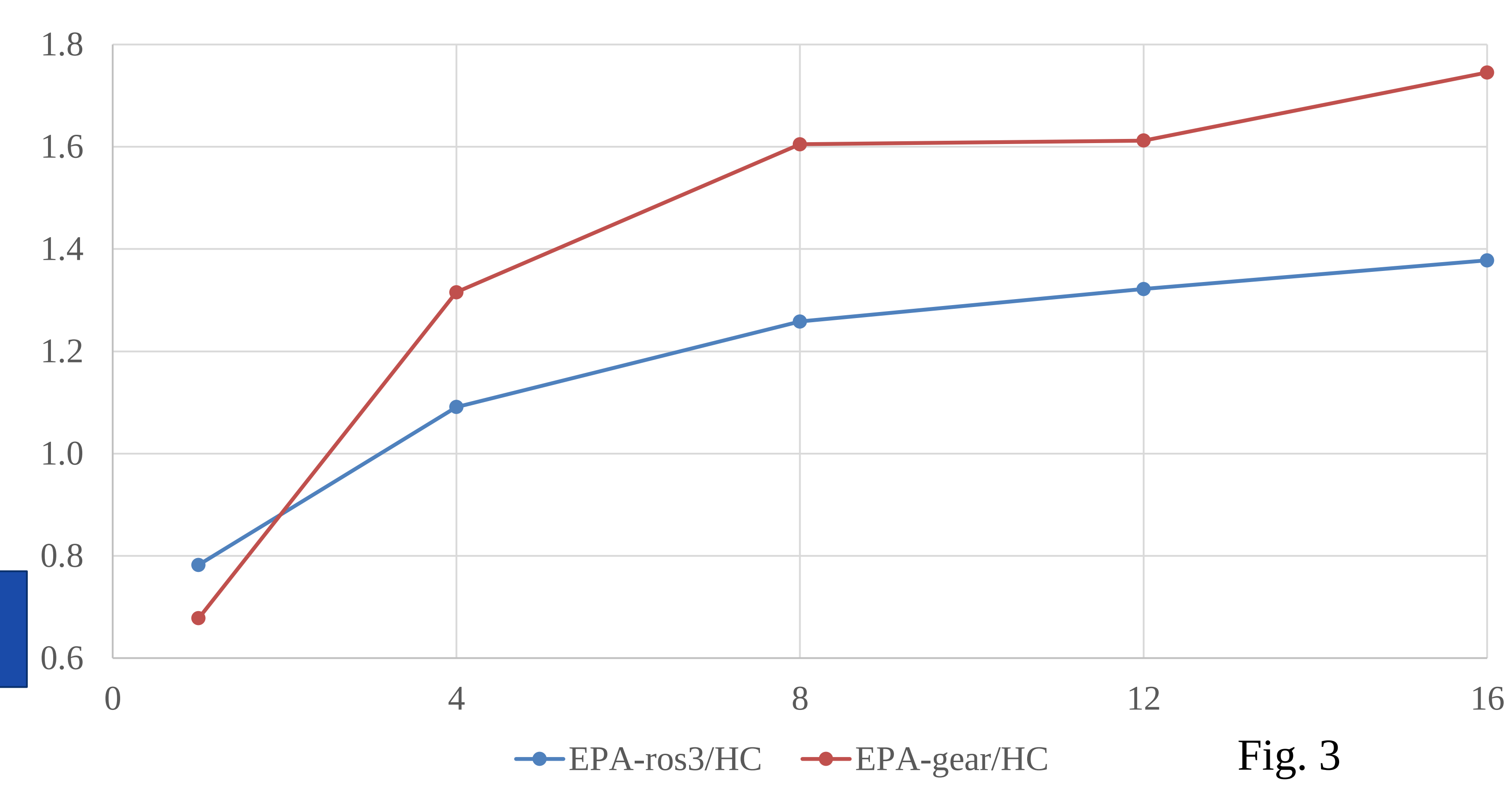
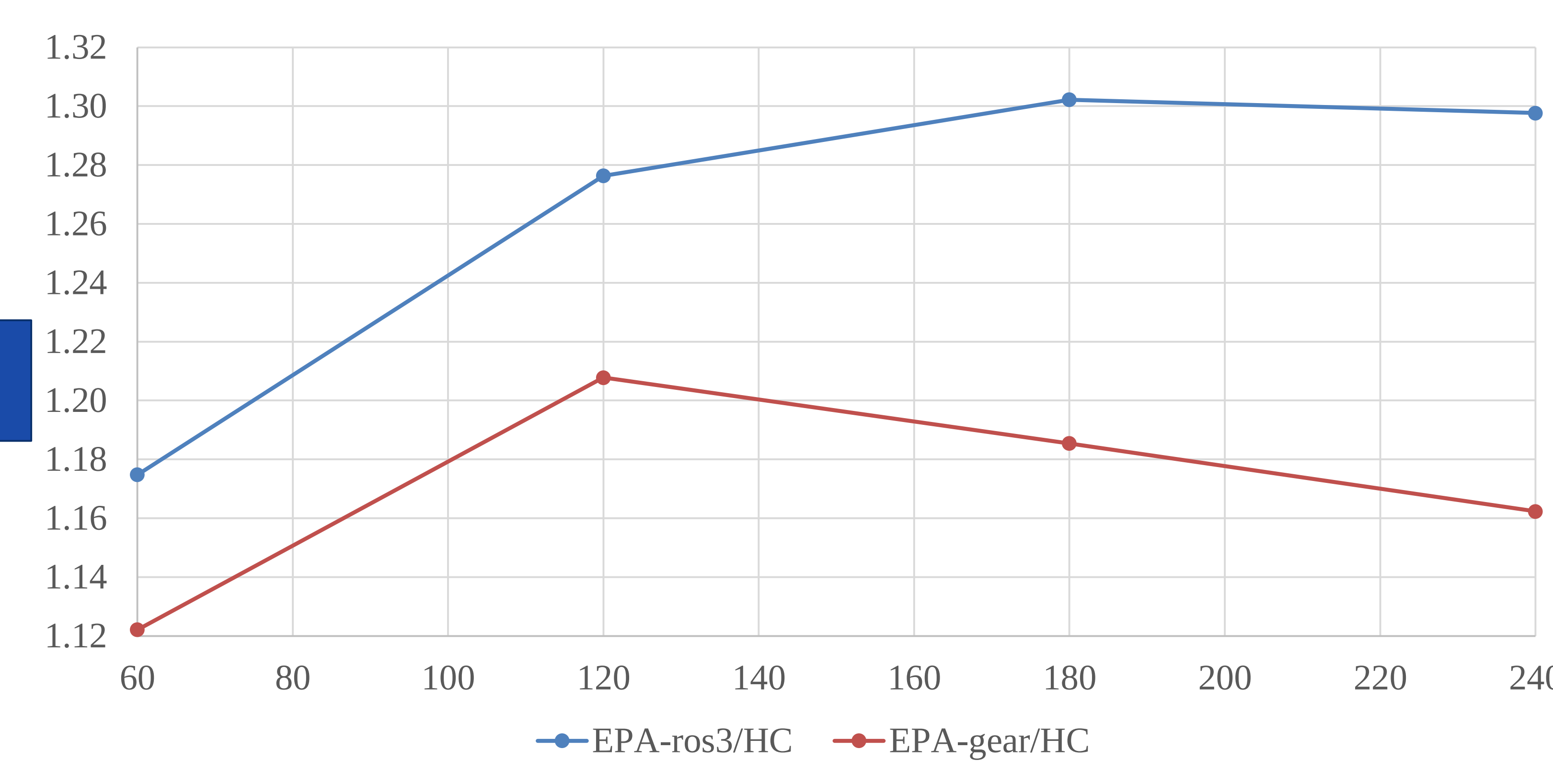


Fig. 3



Benefits of the FSparse method

Speedup

- ~1.2 to 1.75 depending on the solver algorithm and thread count.

Source Code

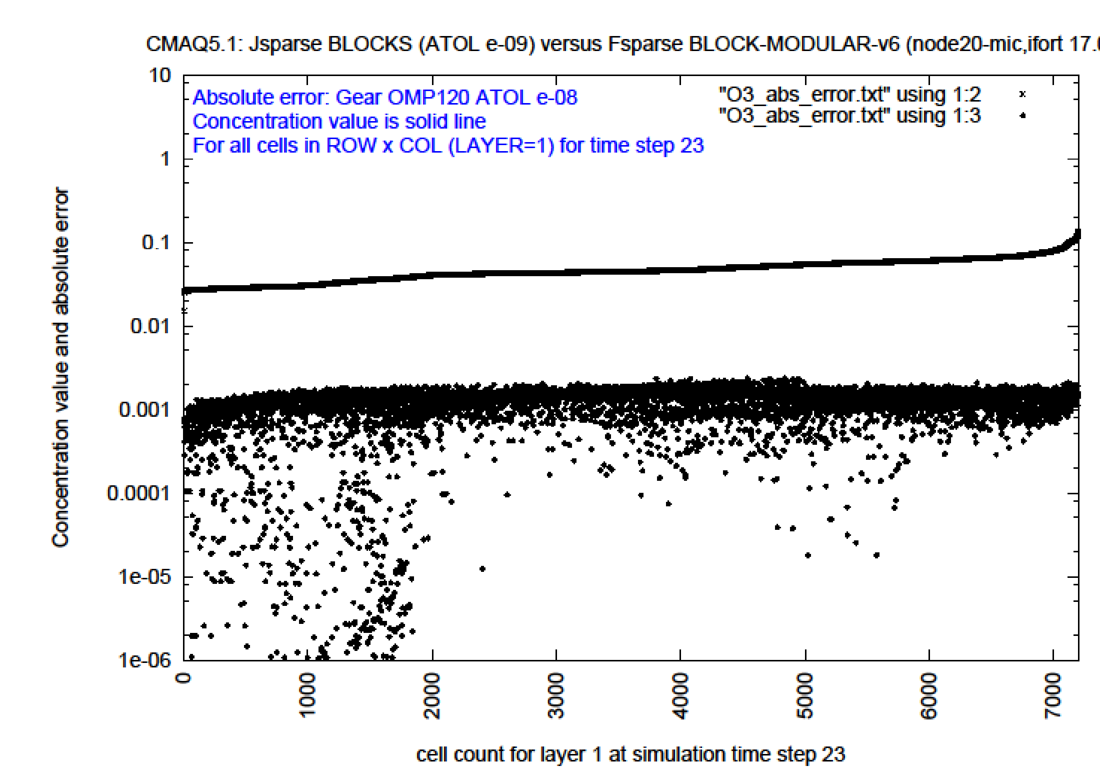
- A single source code version of the CTM suitable for either host CPU or offload to the Phi co-processor.

Hybrid parallel algorithm

- Hybrid MPI+OpenMP algorithms that offer more on-node compute intensity as the number of available threads rises to 100's and beyond.

Numerical results

For the FSparse GEAR solver of CMAQ on the Intel Phi (with 120 OpenMP threads and ATOL=10.0e-08) the figure below shows the O3 species concentration absolute error (scattered points) and concentration value (solid line) for 7200 values in layer 1 of the domain. The error is the difference in predicted concentration between original and FSparse versions of CMAQ. The ranking is in increasing concentration value from left to right



Conclusions

This report has described an analysis of CMAQ 5.1 behavior in the standard U.S. EPA release and a new thread parallel version of CMAQ for the Rosenbrock and Gear solvers. In this version (v6.2) subroutines common to both algorithms have been successfully developed for applications on host CPUs or Intel Phi processors. The new FSparse version of CMAQ offers layers of parallelism not available in the standard U.S. EPA release and is portable across multi- and many-core hardware and compilers that support thread parallelism.

References

[1] Delic, G., 2016: see presentation at the Annual CMAS meeting (http://www.cmasecenter.org).

[2] Jacobson, M. and Turco, R.P., (1994), Atmos. Environ. 28, 273-284.