Weather Research and Forecast (WRF) Scaling, Performance Assessment and Optimization

Comparison of Compilers and MPI Libraries on Cheyenne

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Outline

Background

The Weather Research and Forecast Model

"WRF is a state-of-the-art atmospheric modeling system designed for both meteorological research and numerical weather prediction. It offers a host of options for atmospheric processes and can run on a variety of computing platforms. WRF excels in a broad range of applications across scales ranging from tens of meters to thousands of kilometers, including the following."

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– Real-time NWP

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- Meteorological studies
- Real-time NWP
- Idealized simulations

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– Data assimilation

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– Idealized simulations

– Data assimilation

– Earth system model coupling

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– Real-time NWP

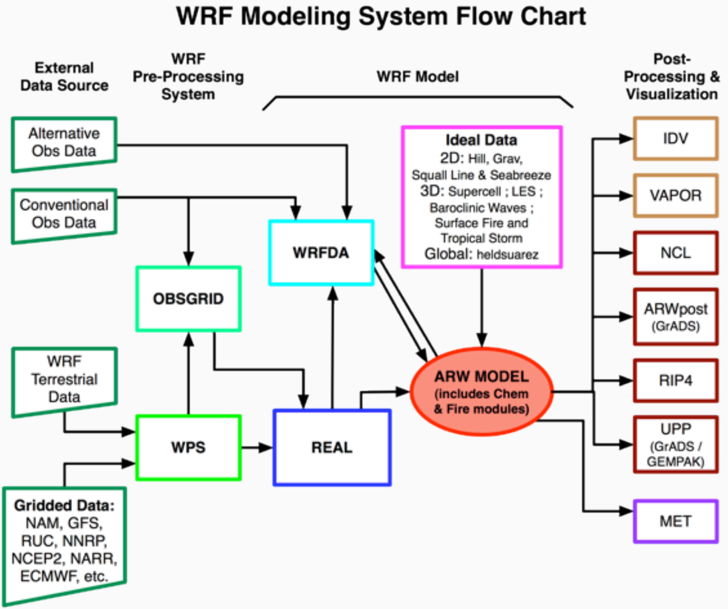
– Idealized simulations

– Data assimilation

– Earth system model coupling

– Model training and educational support

WRF Flowchart



Intro

Test cases

- conus12km
- conus2.5km
- new_conus12km
- new_conus2.5km
- katrina1km
- katrina3km
- maria1km
- maria3km

Compilers and MPI Libraries

- GNU Compiler Collection (GCC) versions 6.3.0, 8.1.0
  - WRF compiles with -O2 default
    - Tried -O3 and -mfma (enables FMA instruction set)
    - Use -ofast?
- Intel Compiler versions 17.0.1, 18.0.1
- MPT, MVAPICH

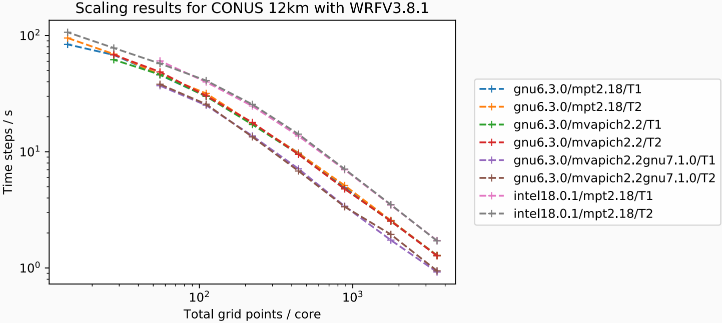
Settings

- MVAPICH

http://mvapich.cse.ohio-state.edu/static/media/mvapich/mvapich2-2.3rc2-userguide.html#x1-19100011.15

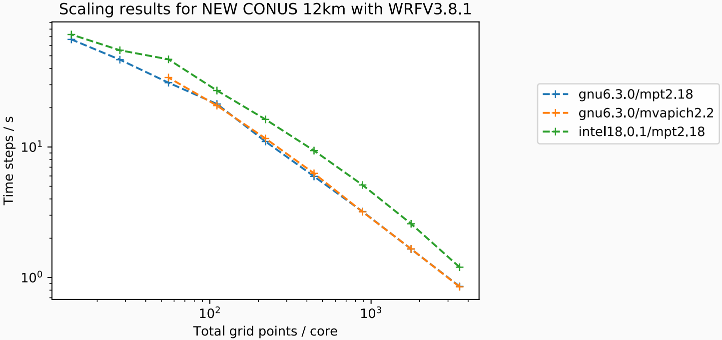
Results

CONUS 12km

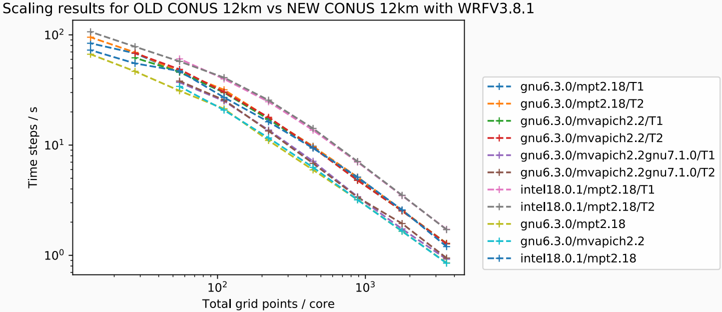


Scaling results for CONUS 12km with WRFV3.8.1
Time steps / s
Total grid points / core
10^2
10^1
10^0
10^2
10^3
gnu6.3.0/mpt2.18/T1
gnu6.3.0/mpt2.18/T2
gnu6.3.0/mvapich2.2/T1
gnu6.3.0/mvapich2.2/T2
gnu6.3.0/mvapich2.2gnu7.1.0/T1
gnu6.3.0/mvapich2.2gnu7.1.0/T2
intel18.0.1/mpt2.18/T1
intel18.0.1/mpt2.18/T2

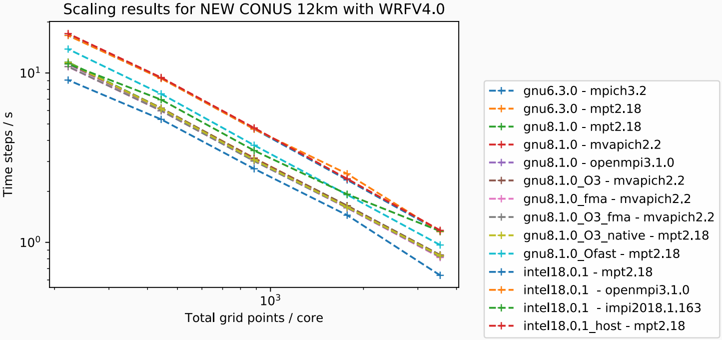
NEW CONUS 12km WRFV3.8.1



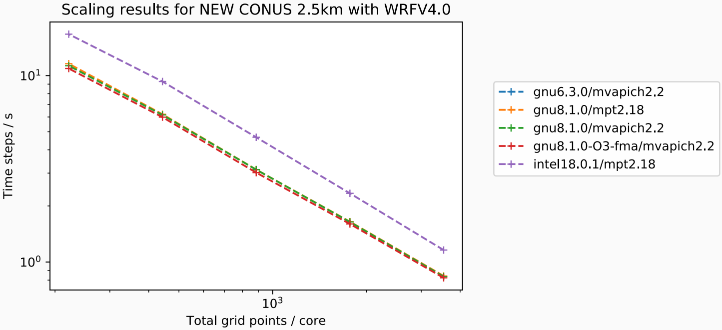
OLD CONUS 12km vs NEW CONUS 12km WRFV3.8.1



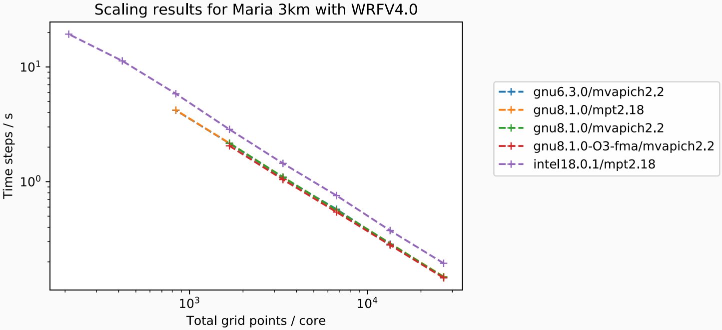
NEW CONUS 12km



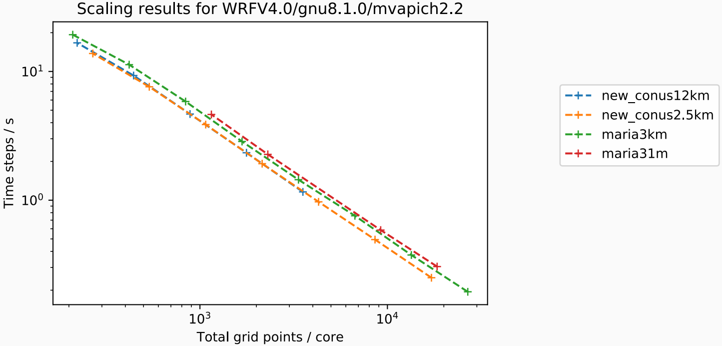
NEW CONUS 2.5km



Maria 3km

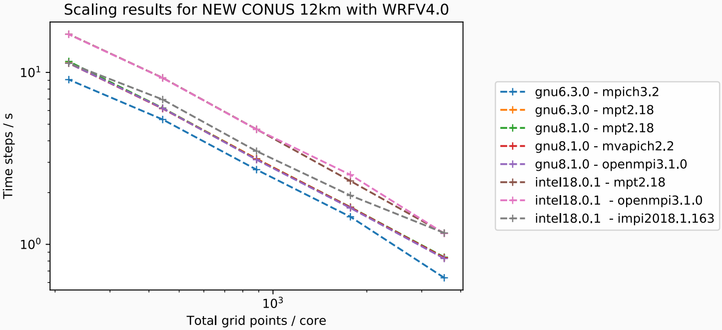

Scaling results for Maria 3km with WRFV4.0
Time steps / s
10^1
10^0
10^3
10^4
Total grid points / core
gnu6.3.0/mvapich2.2
gnu8.1.0/mpt2.18
gnu8.1.0/mvapich2.2
gnu8.1.0-O3-fma/mvapich2.2
intel18.0.1/mpt2.18

Cases

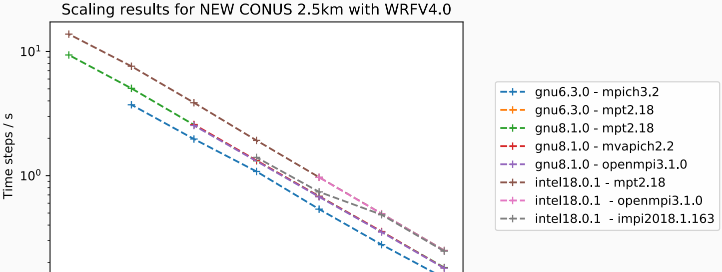


Scaling results for WRFV4.0/gnu8.1.0/mvapich2.2
Time steps / s
10^1
10^0
10^3
10^4
Total grid points / core
new_conus12km
new_conus2.5km
maria3km
maria31m

MPIs

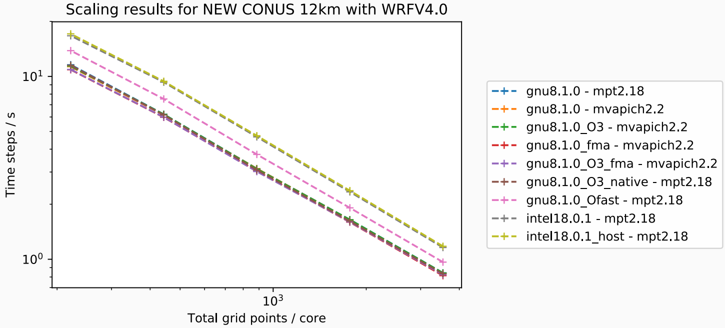


Scaling results for NEW CONUS 12km with WRFV4.0
10^1
10^0
Time steps / s
10^3
Total grid points / core
gnu6.3.0 - mpich3.2
gnu6.3.0 - mpt2.18
gnu8.1.0 - mpt2.18
gnu8.1.0 - mvapich2.2
gnu8.1.0 - openmpi3.1.0
intel18.0.1 - mpt2.18
intel18.0.1 - openmpi3.1.0
intel18.0.1 - impi2018.1.163

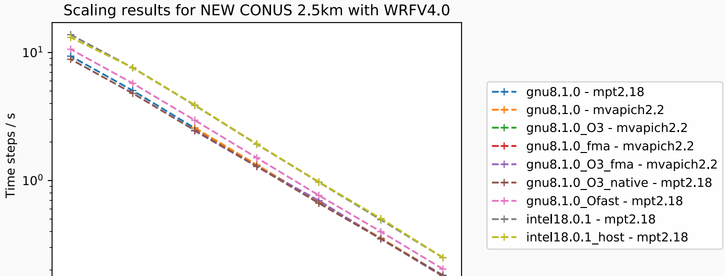


Scaling results for NEW CONUS 2.5km with WRFV4.0
10^1
10^0
Time steps / s
gnu6.3.0 - mpich3.2
gnu6.3.0 - mpt2.18
gnu8.1.0 - mpt2.18
gnu8.1.0 - mvapich2.2
gnu8.1.0 - openmpi3.1.0
intel18.0.1 - mpt2.18
intel18.0.1 - openmpi3.1.0
intel18.0.1 - impi2018.1.163

Compilers

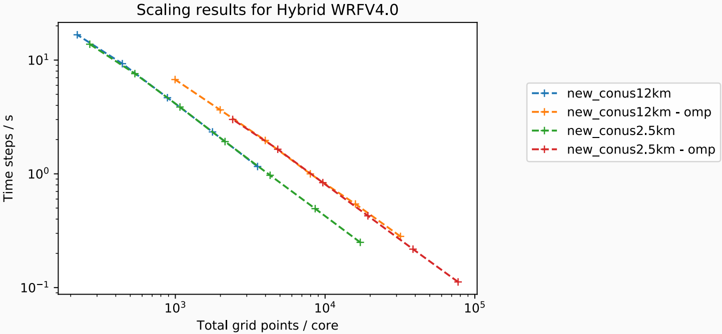


Scaling results for NEW CONUS 12km with WRFV4.0
Time steps / s
Total grid points / core
10^1
10^0
10^3
gnu8.1.0 - mpt2.18
gnu8.1.0 - mvapich2.2
gnu8.1.0_O3 - mvapich2.2
gnu8.1.0_fma - mvapich2.2
gnu8.1.0_O3_fma - mvapich2.2
gnu8.1.0_O3_native - mpt2.18
gnu8.1.0_Ofast - mpt2.18
intel18.0.1 - mpt2.18
intel18.0.1_host - mpt2.18



Scaling results for NEW CONUS 2.5km with WRFV4.0
Time steps / s
10^1
10^0
gnu8.1.0 - mpt2.18
gnu8.1.0 - mvapich2.2
gnu8.1.0_O3 - mvapich2.2
gnu8.1.0_fma - mvapich2.2
gnu8.1.0_O3_fma - mvapich2.2
gnu8.1.0_O3_native - mpt2.18
gnu8.1.0_Ofast - mpt2.18
intel18.0.1 - mpt2.18
intel18.0.1_host - mpt2.18

Hybrid



Scaling results for Hybrid WRFV4.0
Time steps / s
Total grid points / core
10^1
10^0
10^{-1}
10^3
10^4
10^5
new_conus12km
new_conus12km - omp
new_conus2.5km
new_conus2.5km - omp

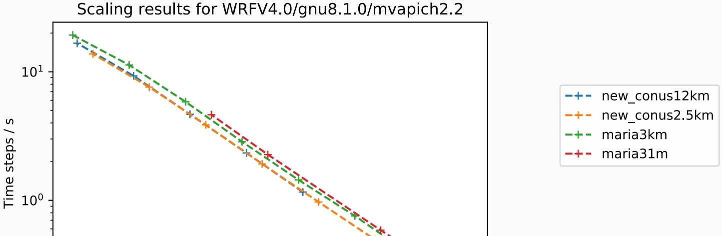
WRF scaling and timing on Cheyenne

- “Is it possible to solve a problem with such-and-such resolution in a timely manner?”
- “If I use more cores I will have the results more quickly, but with this resolution will my run be in the efficient strong-scaling regime, an intermediate one, or in the very inefficient one dominated by I/O and initialization instead of computing?”

Numbers from the figures below can help you develop some back-of-the-envelope estimates of what will happen if you increase or decrease the core counts of your runs, so that you can find one that is optimal for you both in terms of time-to-solution and in terms of your allocation.

Scaling Results

Figure 1 shows scaling results from the Katrina simulations at two different resolutions and also includes the official CONUS benchmarks from `http://www2.mmm.ucar.edu/wrf/WG2/bench/` at 12km and 2.5km resolution. For comparison, a New Zealand case with different physics parametrization and a higher number of vertical levels is also included. When expressed this way, all the cases scale similarly. Note that both axes are logarithmic, so a small distance between points corresponds to a large difference in values. Figure 1 -



Run time results

Figure 2 below shows the total run time for WRF jobs using increasing numbers of cores. Initialization time, computation time, and writing time also are shown for runs using up to 8,192 cores. Initialization and writing time rendered larger jobs impractical. Using a different output algorithm (CSG used the default) may yield better results for large jobs. Compare this to Figure 1, where only the computing time (represented in Figure 2 by the green triangles) has been taken into account to make the plot.

These results are based on simulations of Hurricane Katrina (2005) at 1km resolution.

As illustrated, initialization and writing output times may be more expensive than computing time for larger core counts. Times shown are for a single restart and single output file of the Katrina 1km case, which used a domain of about 372 million grid points. If

Summary

Conclusions?

- Brownian motion begins with a random walk
- $\langle R_N^2 \rangle = NL^2$ can be related to physical quantities through forces
  - Randomness is very helpful: it allows us to average out a terms[1]

[1] The Feynman Lectures on Physics, Vol. I