GEOS-Chem "Classic" 12.0.0 timing results

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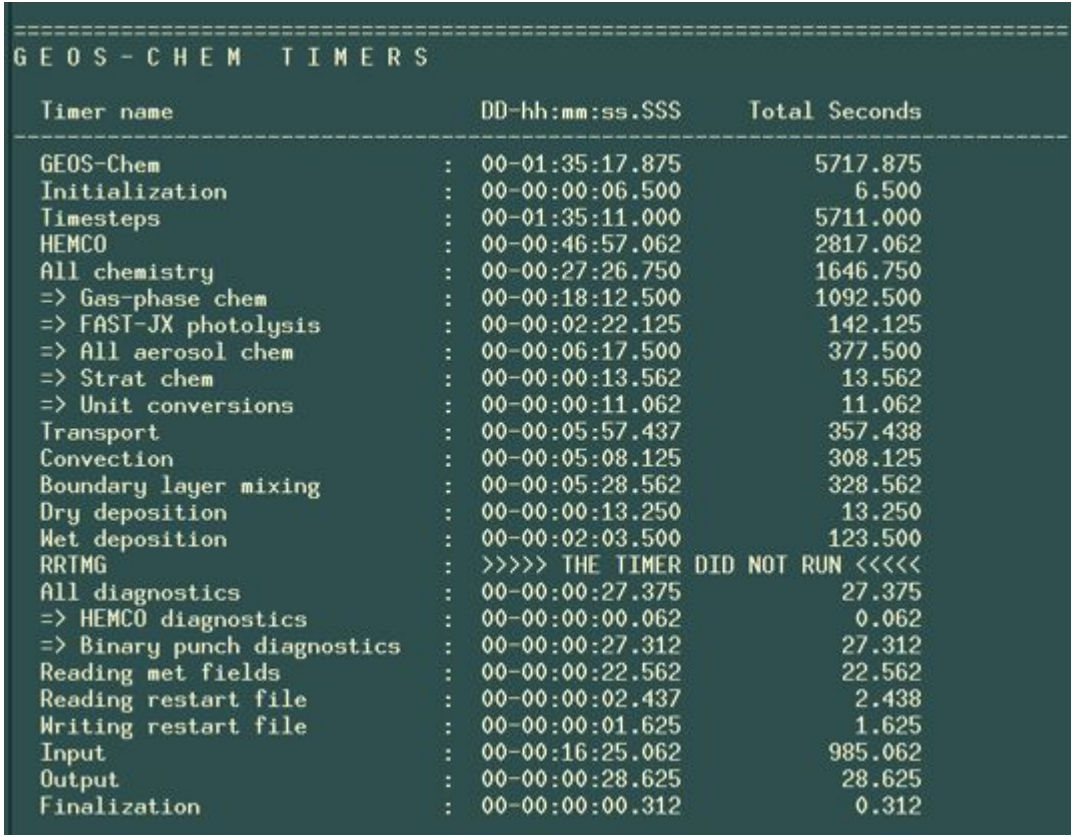
Timing test configurations

We set up 7-day timing runs with these GEOS-Chem "Classic" 12.0.0 configurations:

1. GNU Fortran v7.1 + fast-math option + bpch diagnostics
2. GNU Fortran v7.1 + fast-math option + netCDF diagnostics
3. GNU Fortran v7.1 + default build + bpch diagnostics
4. GNU Fortran v7.1 + default build + netCDF diagnostics
5. Intel Fortran 17.0.4 + default build + bpch diagnostics
6. Intel Fortran 17.0.4 + default build + netCDF diagnostics

For each configuration 1-6, we submitted jobs using 4, 8, 12, 16, 24, and 32 cores.

NOTE: "fast-math" was activated by hardcoding "-ffast-math" to the makefile.



```
================================================================================
GEOS-CHEM TIMERS

 Timer name                      DD-hh:mm:ss.SSS     Total Seconds
--------------------------------------------------------------------------------
 GEOS-Chem                  :  00-01:35:17.875          5717.875
 Initialization             :  00-00:00:06.500             6.500
 Timesteps                  :  00-01:35:11.000          5711.000
 HEMCO                      :  00-00:46:57.062          2817.062
 All chemistry              :  00-00:27:26.750          1646.750
 => Gas-phase chem          :  00-00:18:12.500          1092.500
 => FAST-JX photolysis      :  00-00:02:22.125           142.125
 => All aerosol chem        :  00-00:06:17.500           377.500
 => Strat chem              :  00-00:00:13.562            13.562
 => Unit conversions        :  00-00:00:11.062            11.062
 Transport                  :  00-00:05:57.437           357.438
 Convection                 :  00-00:05:08.125           308.125
 Boundary layer mixing      :  00-00:05:28.562           328.562
 Dry deposition             :  00-00:00:13.250            13.250
 Wet deposition             :  00-00:02:03.500           123.500
 RRTMG                      :  >>>>> THE TIMER DID NOT RUN <<<<<
 All diagnostics            :  00-00:00:27.375            27.375
 => HEMCO diagnostics       :  00-00:00:00.062             0.062
 => Binary punch diagnostics:  00-00:00:27.312            27.312
 Reading met fields         :  00-00:00:22.562            22.562
 Reading restart file       :  00-00:00:02.437             2.438
 Writing restart file       :  00-00:00:01.625             1.625
 Input                      :  00-00:16:25.062           985.062
 Output                     :  00-00:00:28.625            28.625
 Finalization               :  00-00:00:00.312             0.312
```

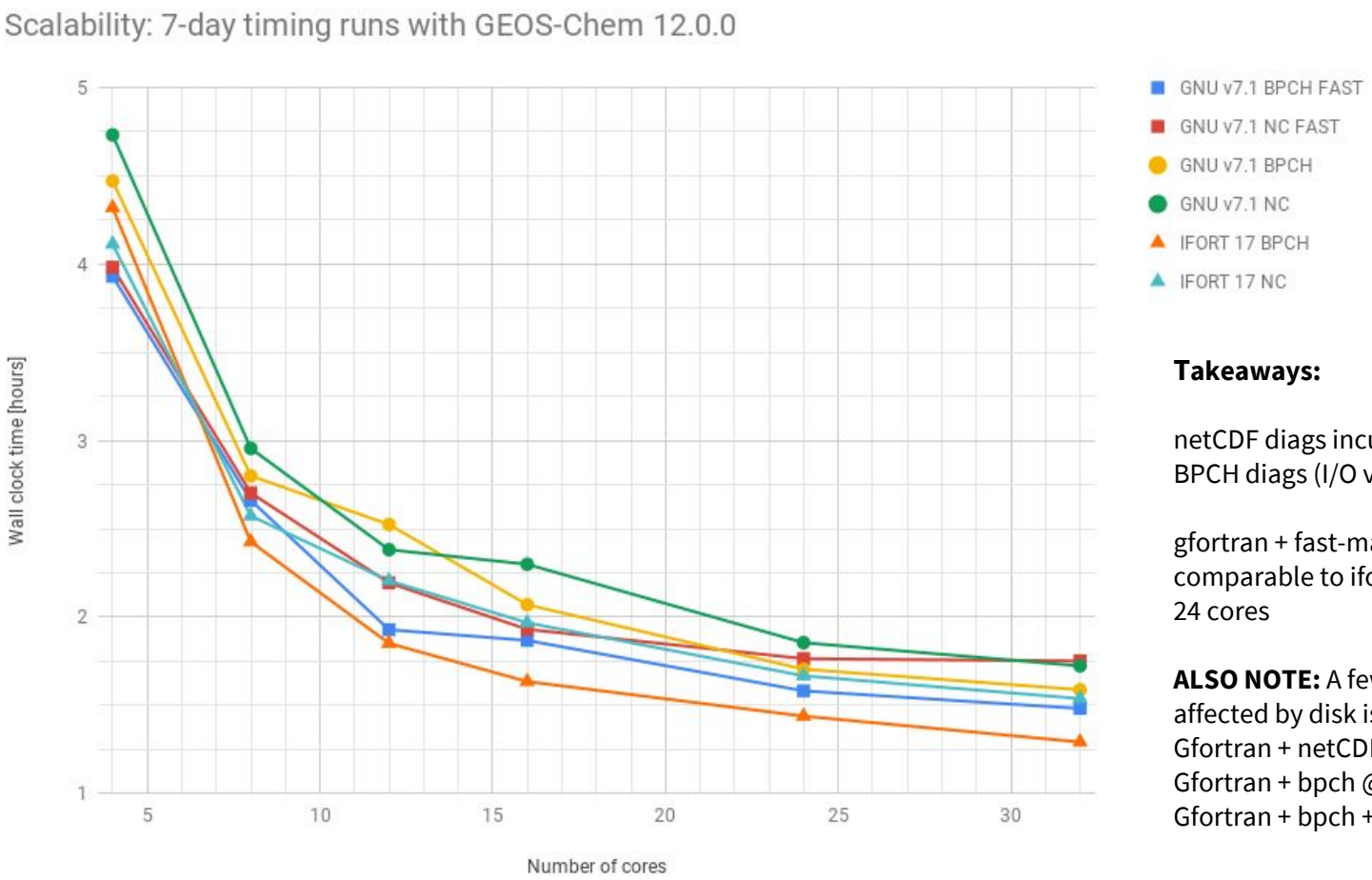
Time spent per operation

We used the output of the GEOS-Chem timers to determine the approximate amount of time that was spent in each operation.

The GEOS-Chem timers are turned on by compiling with option TIMERS=1. Results are printed at the end of the simulation log file.

Profiling with e.g. the TAU performance analyzer will always be more accurate. But the GEOS-Chem timers are sufficient to determine if there are operations that do not scale well.

Scalability across cores

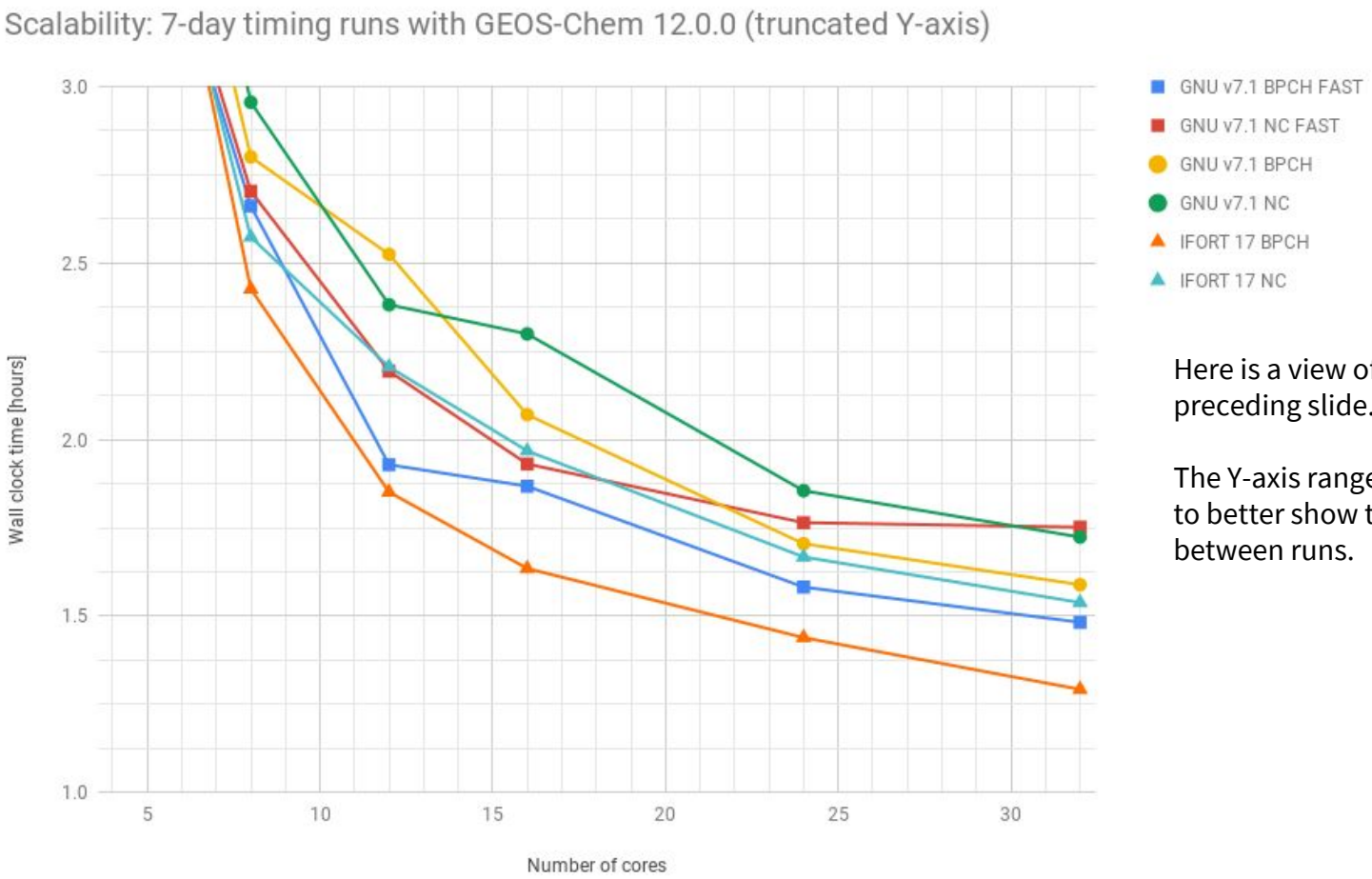


Takeaways:

netCDF diags incur more overhead than BPCH diags (I/O via library)

gfortran + fast-math + netCDF diags is comparable to ifort + netCDF up to about 24 cores

ALSO NOTE: A few runs were likely affected by disk issues on Odyssey:
Gfortran + netCDF @ 16 cores
Gfortran + bpch @ 12 cores
Gfortran + bpch + fast math @ 16 cores

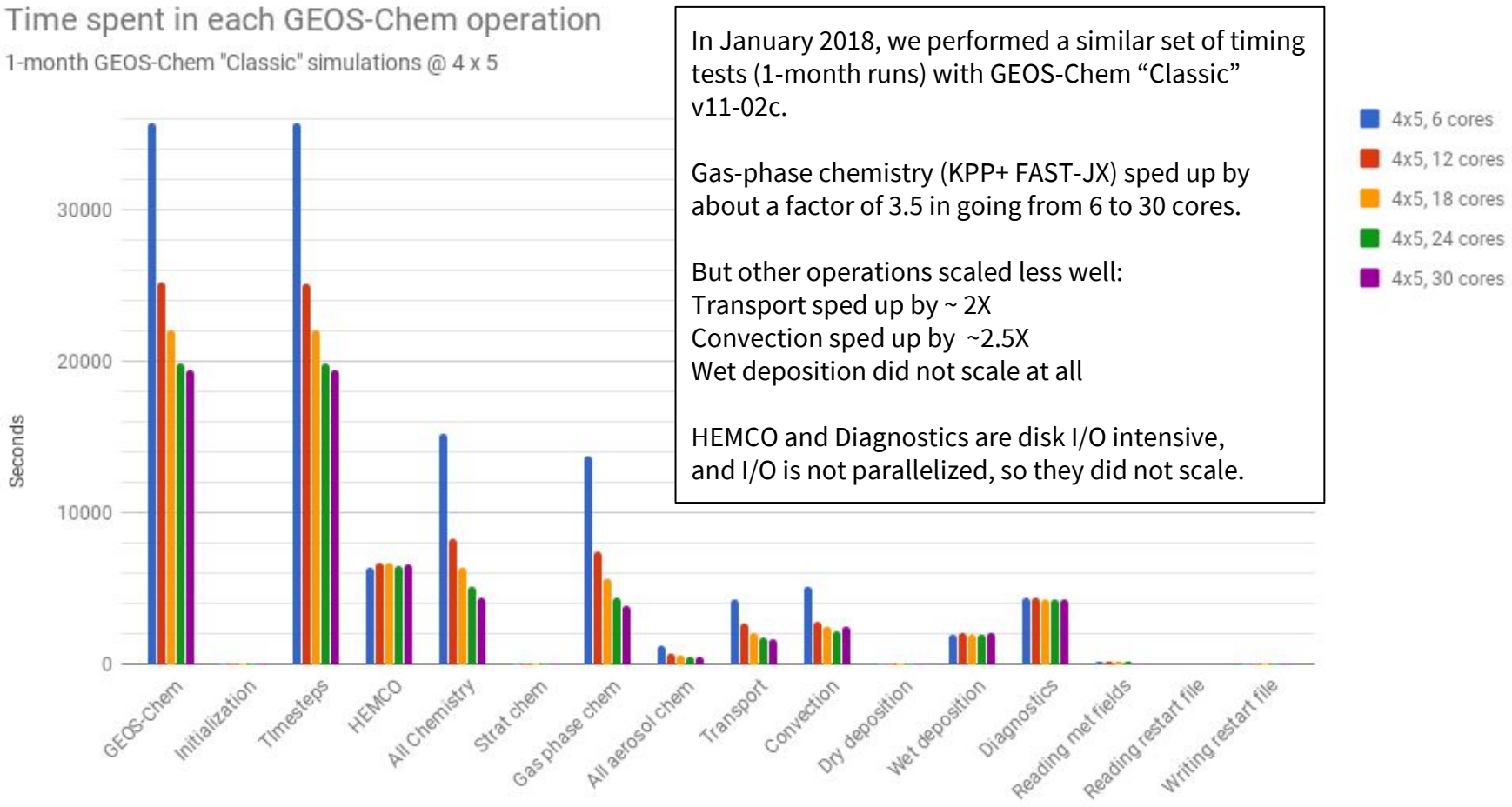


Here is a view of the same plot on the preceding slide.

The Y-axis range has been truncated to better show the differences between runs.

Time spent in each operation:

Reference run: v11-02c



In January 2018, we performed a similar set of timing tests (1-month runs) with GEOS-Chem "Classic" v11-02c.

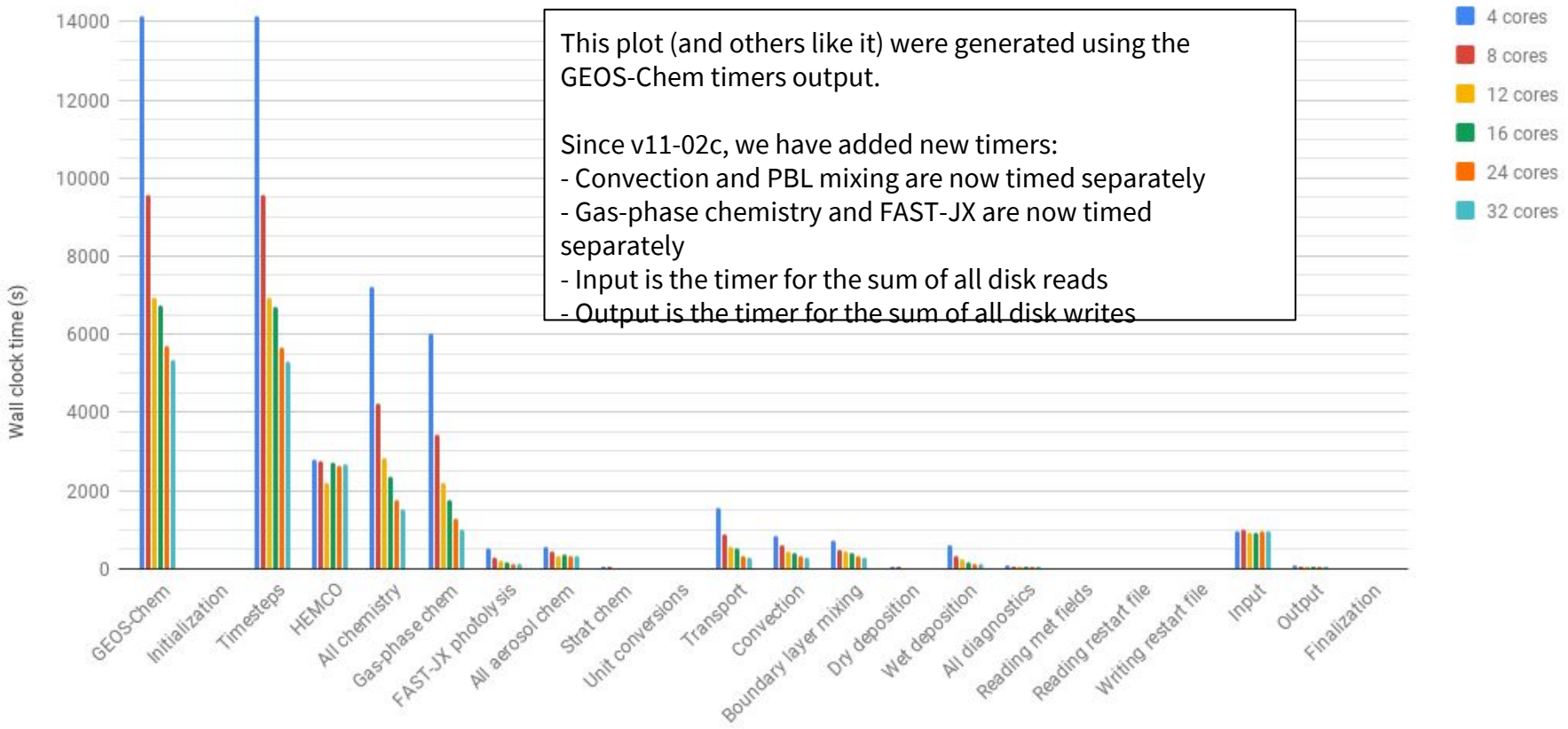
Gas-phase chemistry (KPP+ FAST-JX) sped up by about a factor of 3.5 in going from 6 to 30 cores.

But other operations scaled less well:
Transport sped up by ~ 2X
Convection sped up by ~2.5X
Wet deposition did not scale at all

HEMCO and Diagnostics are disk I/O intensive, and I/O is not parallelized, so they did not scale.

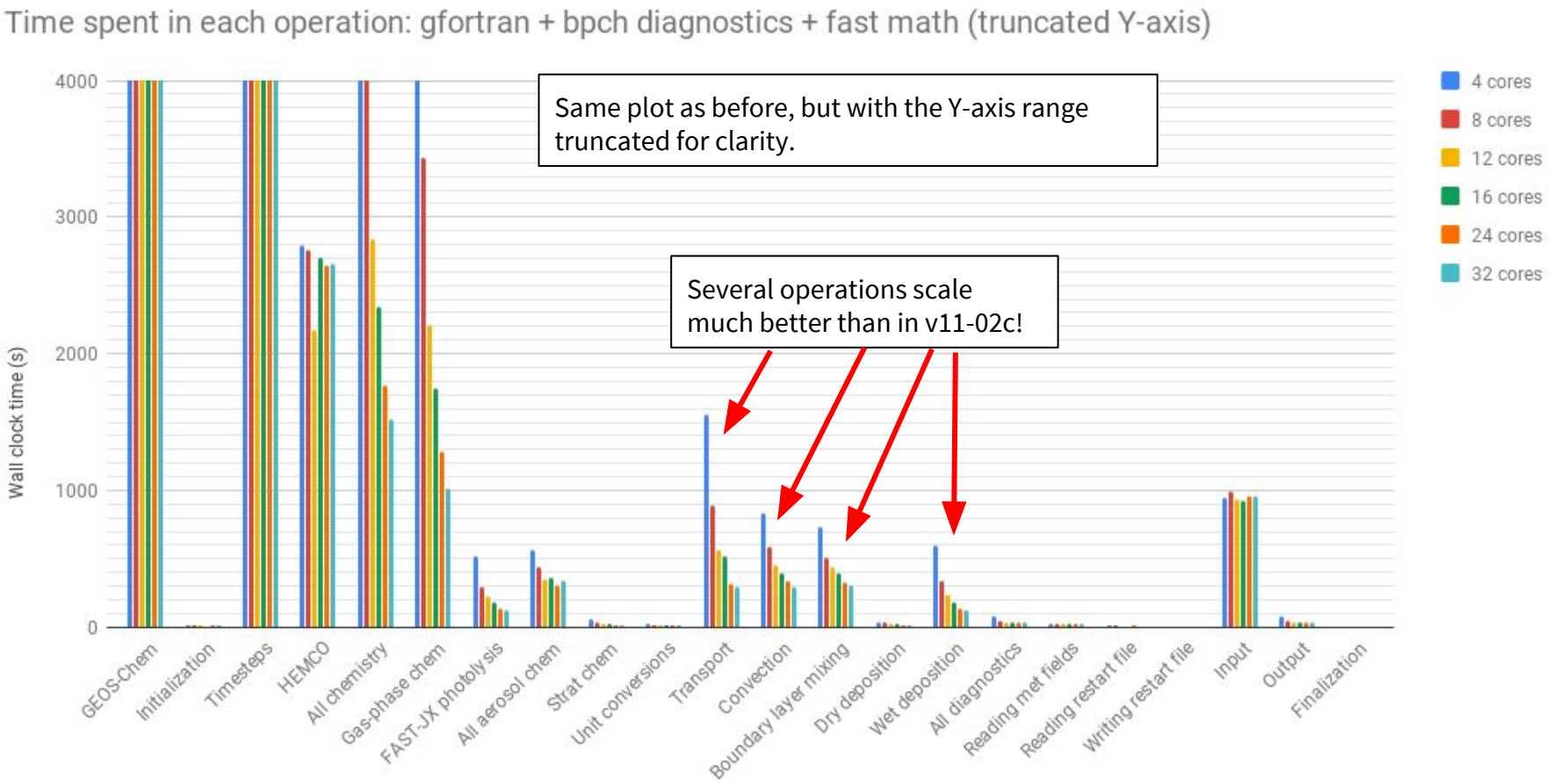
Time spent in each operation:
GNU Fortran v7.1 + fast math + bpch diagnostics

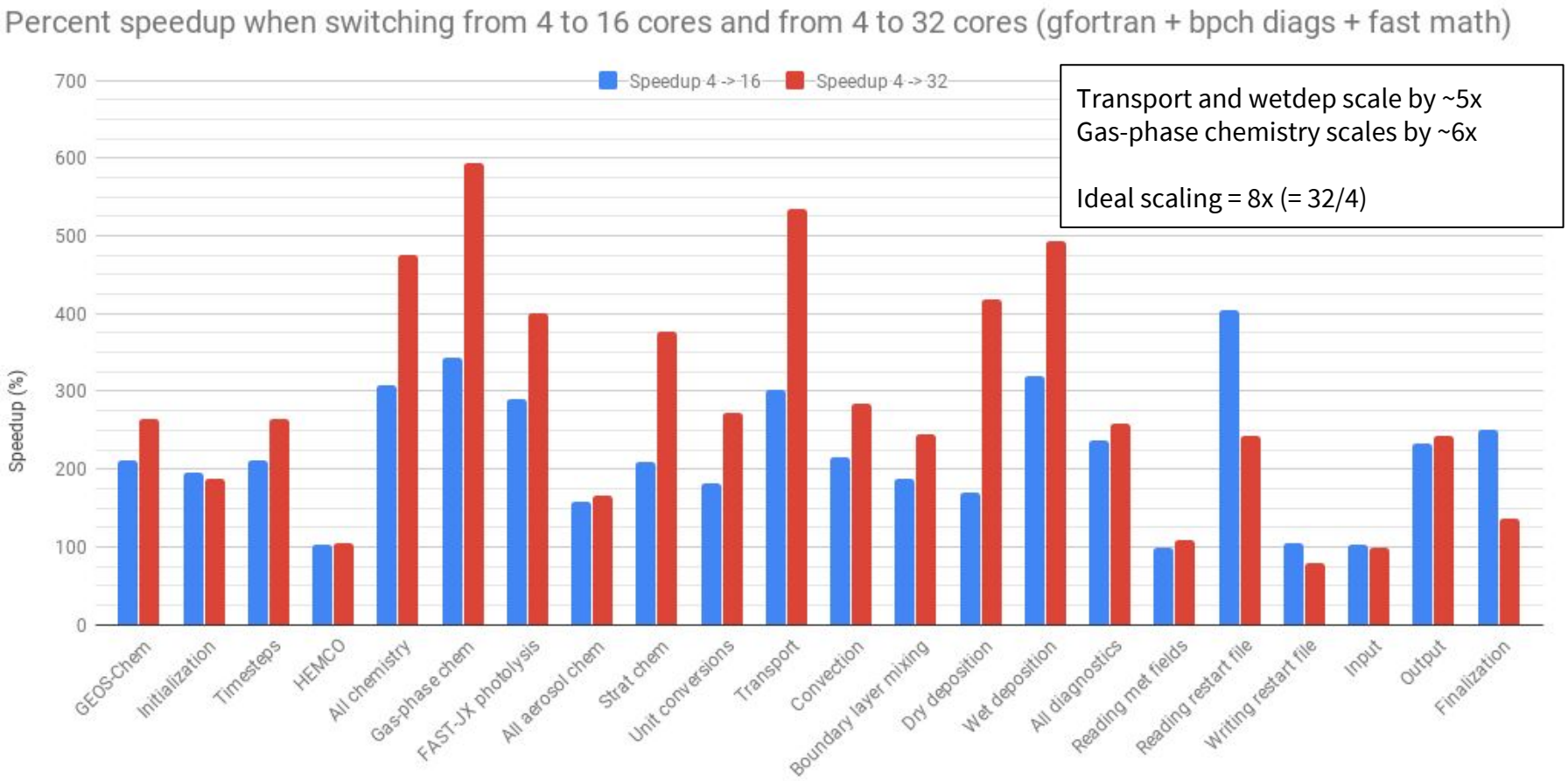
Time spent in each operation: gfortran + bpch diagnostics + fast math



This plot (and others like it) were generated using the GEOS-Chem timers output.

Since v11-02c, we have added new timers:
- Convection and PBL mixing are now timed separately
- Gas-phase chemistry and FAST-JX are now timed separately
- Input is the timer for the sum of all disk reads
- Output is the timer for the sum of all disk writes


Time spent in each operation: gfortran + bpch diagnostics + fast math (truncated Y-axis)
Same plot as before, but with the Y-axis range truncated for clarity.
Several operations scale much better than in v11-02c!
Wall clock time (s)
4000
3000
2000
1000
0
4 cores
8 cores
12 cores
16 cores
24 cores
32 cores
GEOS-Chem
Initialization
Timesteps
HEMCO
All chemistry
Gas-phase chem
FAST-JX photolysis
All aerosol chem
Strat chem
Unit conversions
Transport
Convection
Boundary layer mixing
Dry deposition
Wet deposition
All diagnostics
Reading met fields
Reading restart file
Writing restart file
Input
Output
Finalization



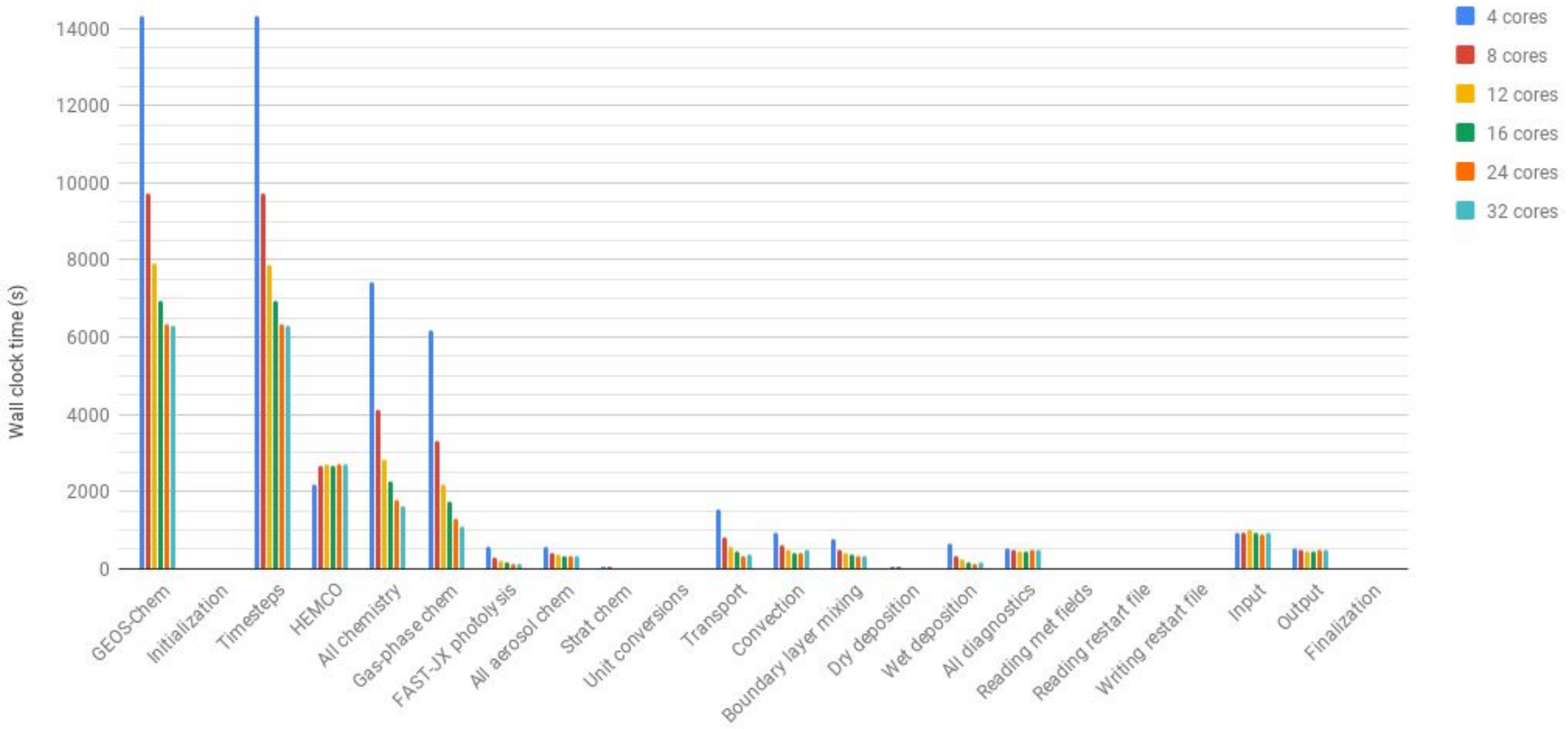
Transport and wetdep scale by ~5x
Gas-phase chemistry scales by ~6x

Ideal scaling = 8x (= 32/4)

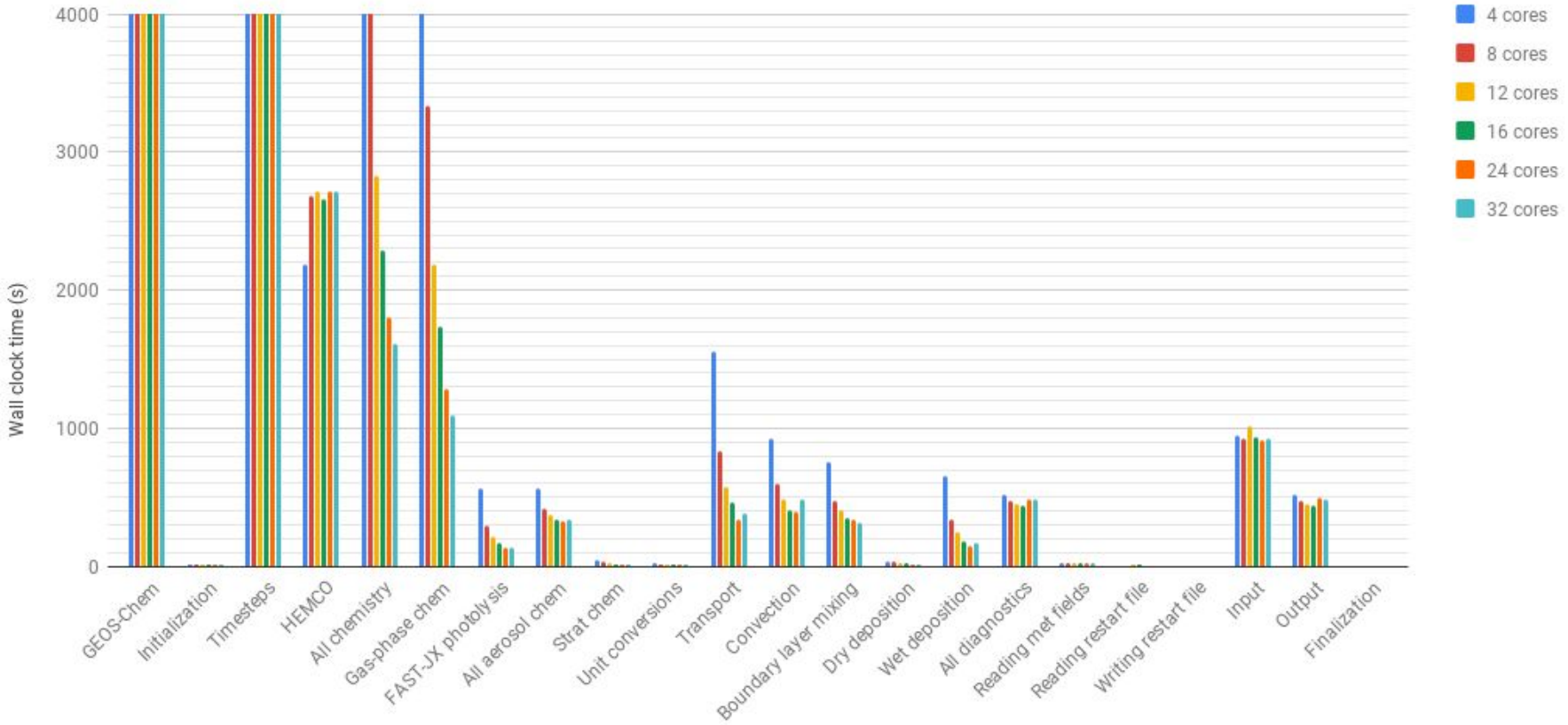
We will show the same plots for the other timing test configurations...

Time spent in each operation:
GNU Fortran v7.1 + fast math + netCDF diagnostics

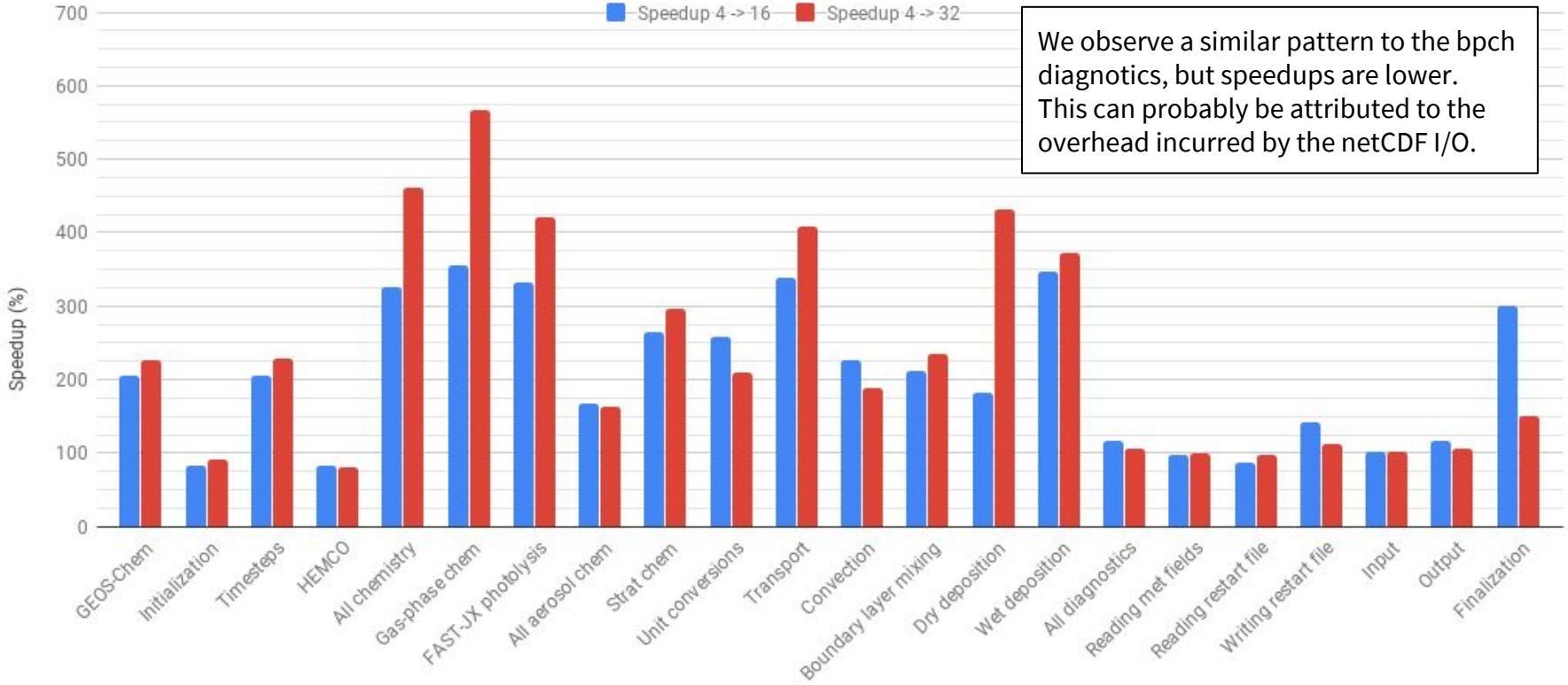
Time spent in each operation: gfortran + netCDF diagnostics + fast math



Time spent in each operation: gfortran + netCDF diagnostics + fast math (truncated Y-axis)



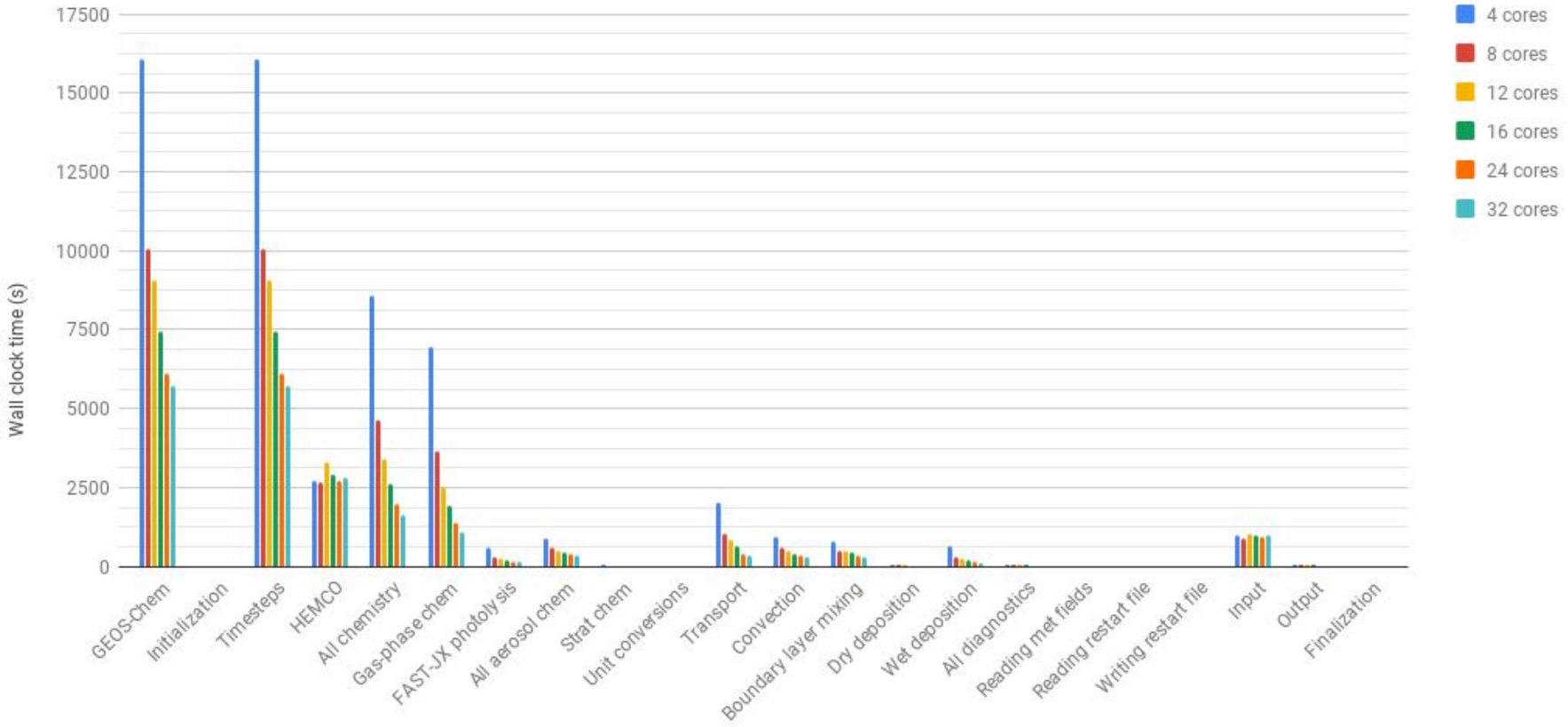
Percent speedup when switching from 4 to 16 cores and from 4 to 32 cores (gfortran + netCDF diags + fast math)

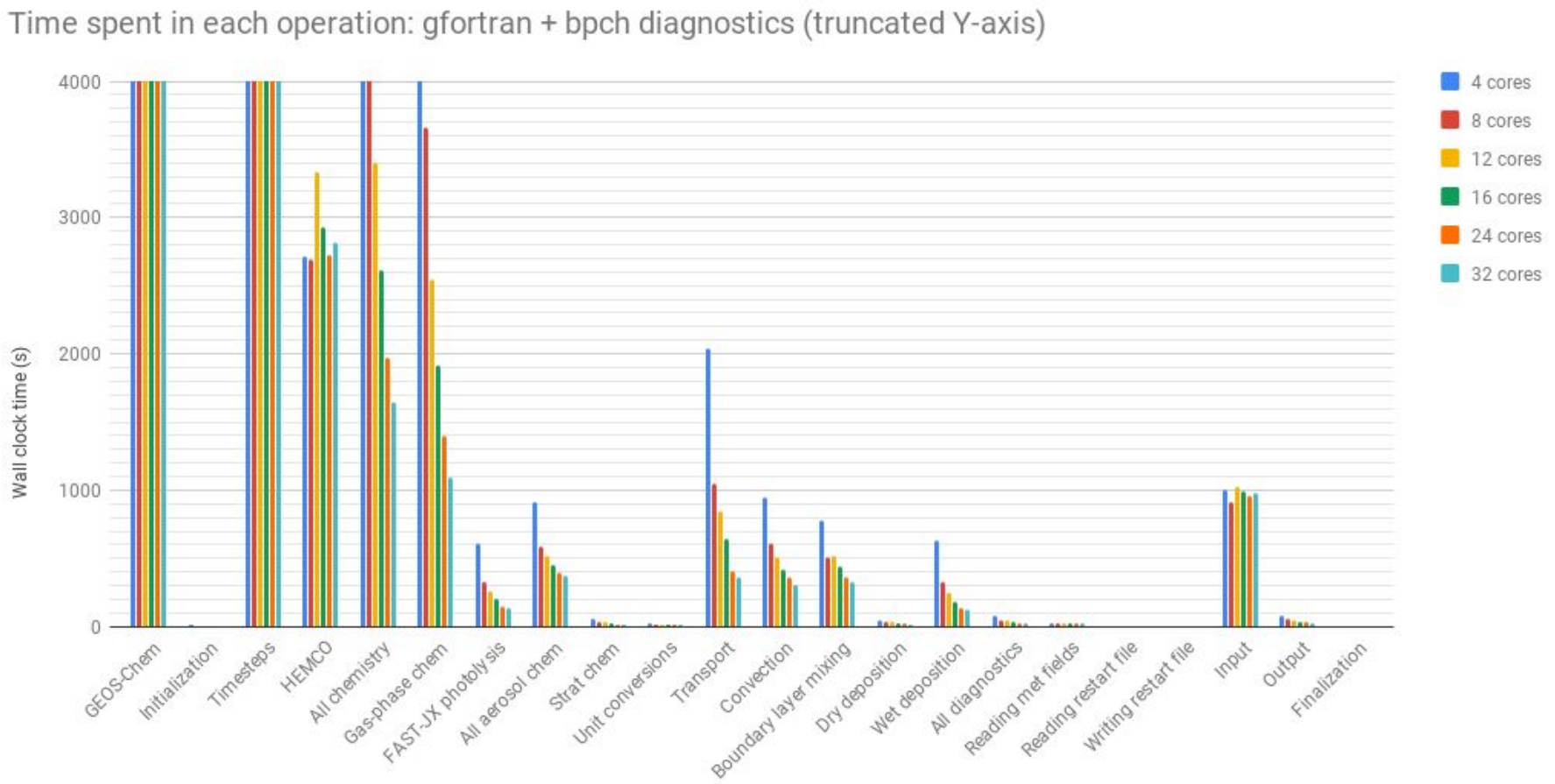


We observe a similar pattern to the bpch diagnotics, but speedups are lower. This can probably be attributed to the overhead incurred by the netCDF I/O.

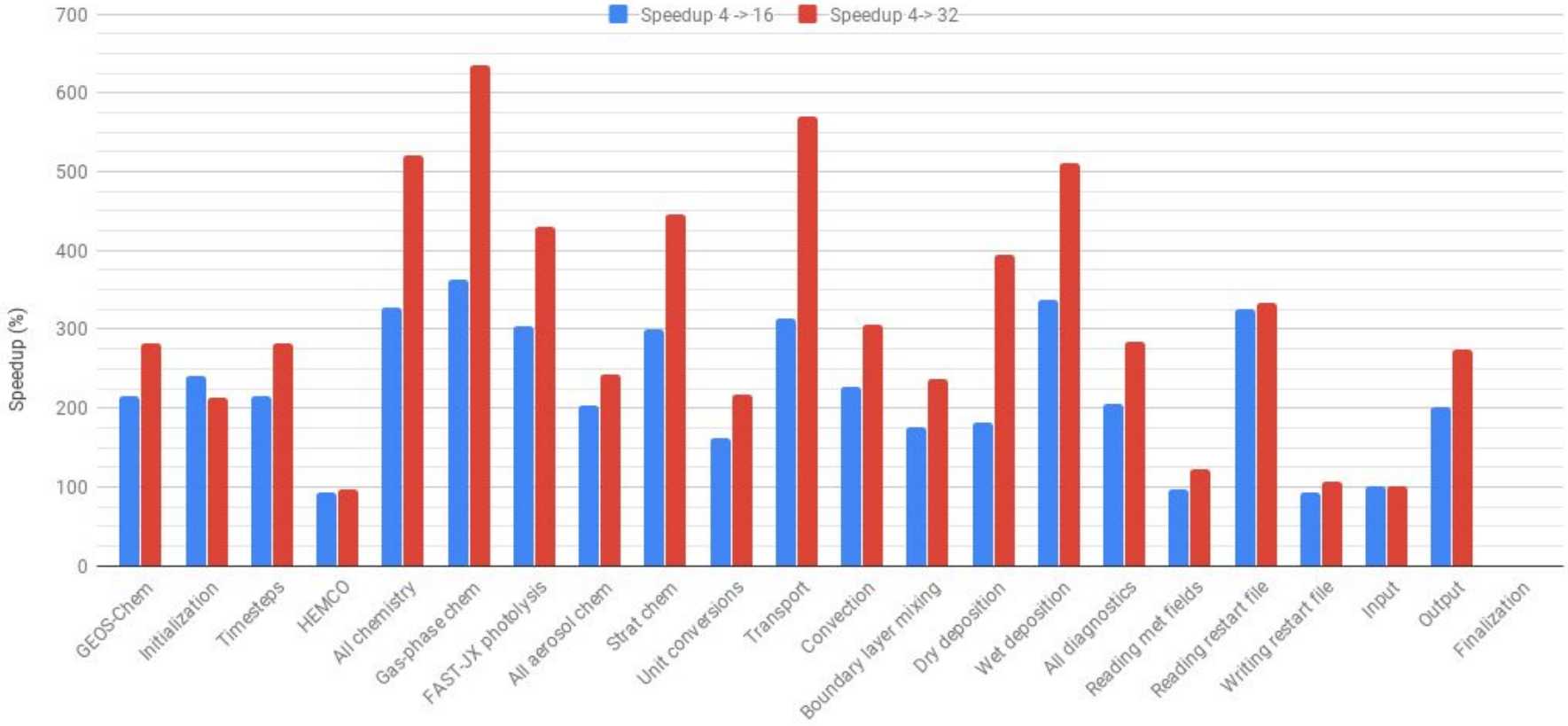
Time spent in each operation:
GNU Fortran v7.1 + default build + bpch diagnostics

Time spent in each operation: gfortran + bpch diagnostics



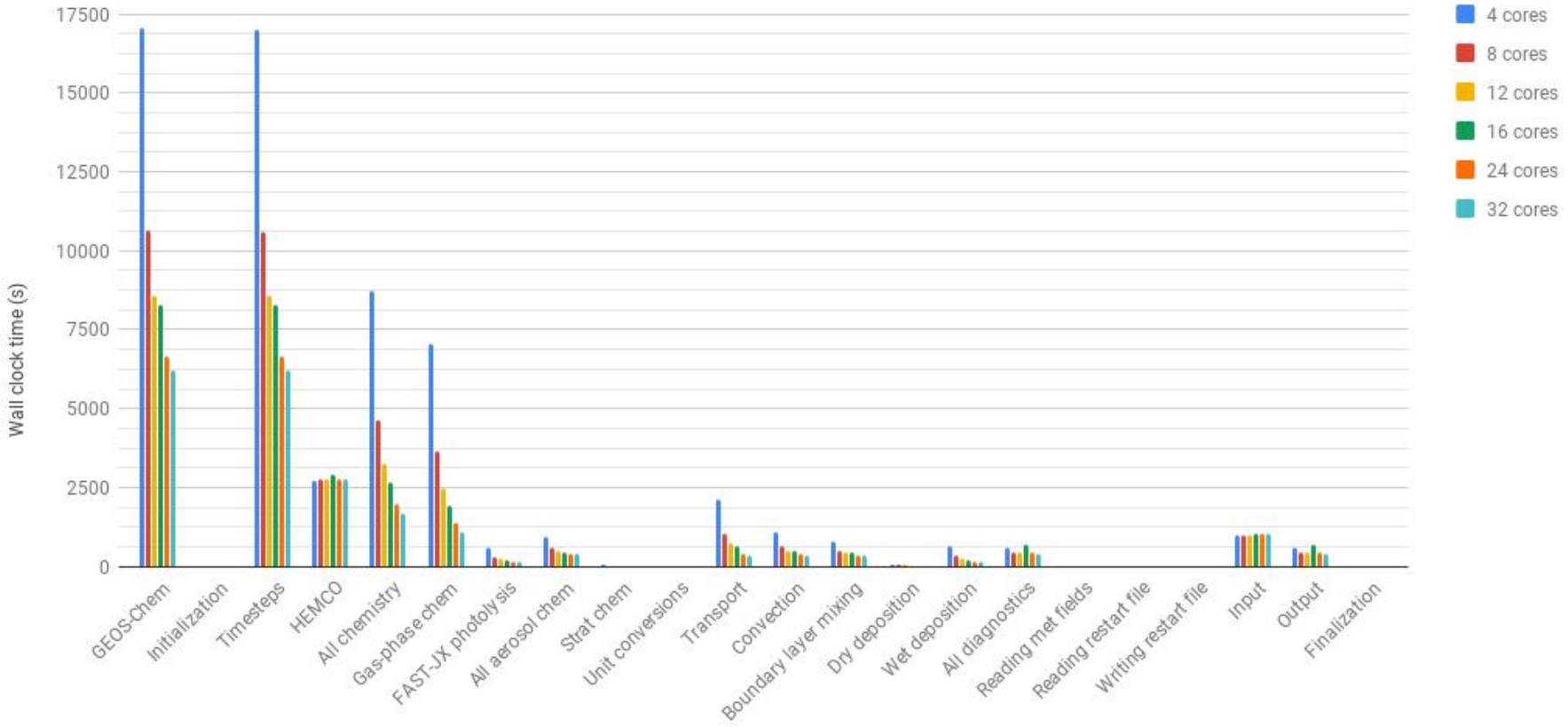

Time spent in each operation: gfortran + bpch diagnostics (truncated Y-axis)
Wall clock time (s)
4000
3000
2000
1000
0
4 cores
8 cores
12 cores
16 cores
24 cores
32 cores
GEOS-Chem
Initialization
Timesteps
HEMCO
All chemistry
Gas-phase chem
FAST-JX photolysis
All aerosol chem
Strat chem
Unit conversions
Transport
Convection
Boundary layer mixing
Dry deposition
Wet deposition
All diagnostics
Reading met fields
Reading restart file
Writing restart file
Input
Output
Finalization

Percent speedup when switching from 4 to 16 cores and from 4 to 32 cores (gfortran + bpch diagnostics)

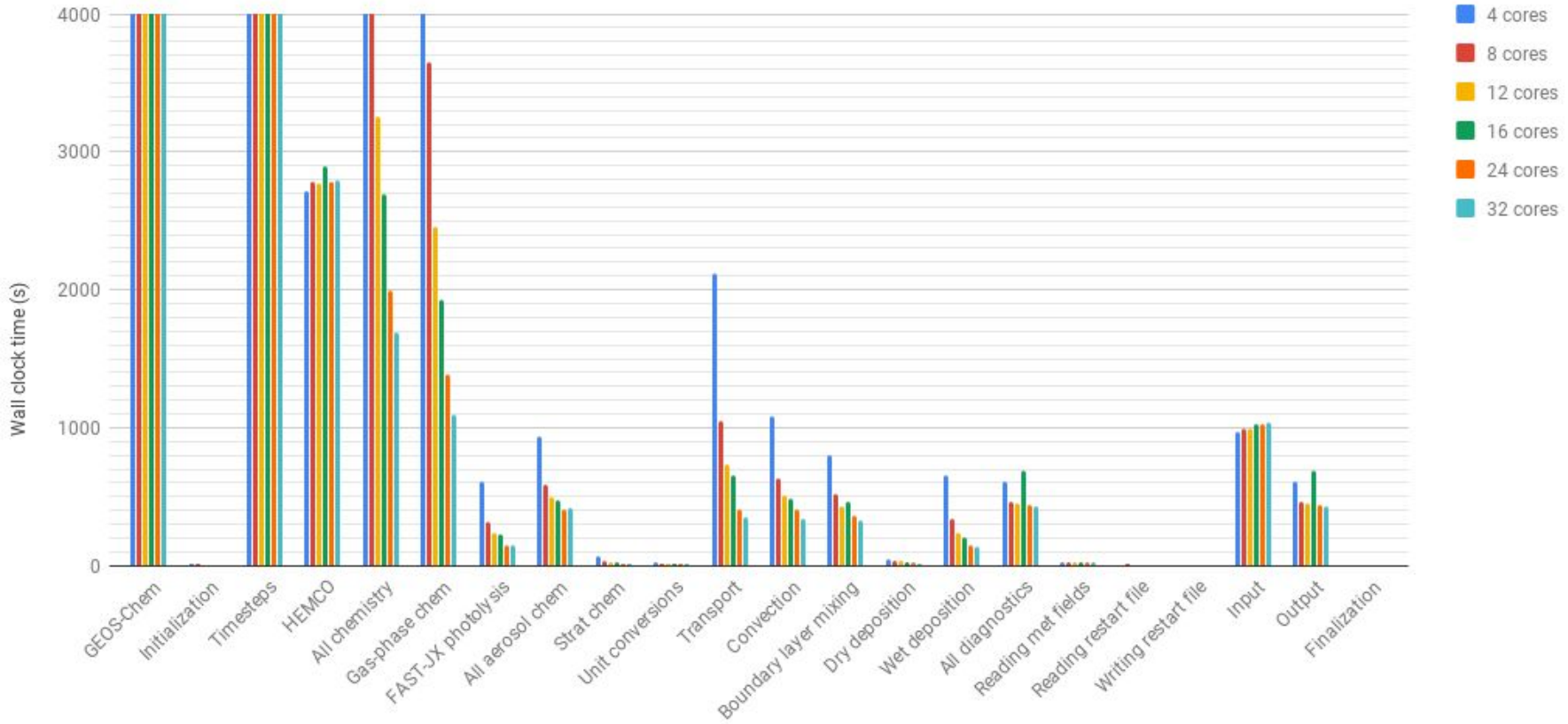


Time spent in each operation:
GNU Fortran v7.1 + default build + netCDF diagnostics

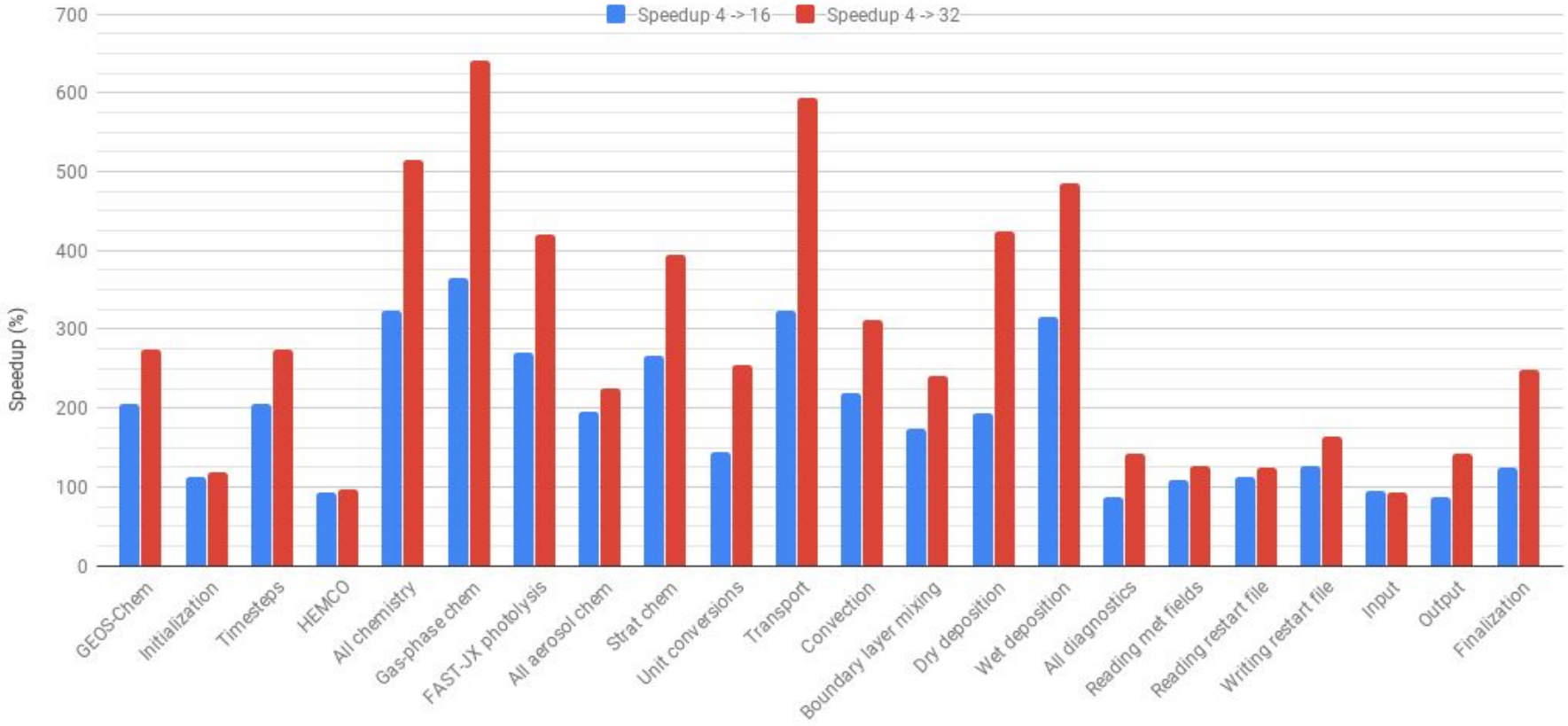
Time spent in each operation: gfortran + netCDF diagnostics



Time spent in each operation: gfortran + netCDF diagnostics (truncated Y-axis)

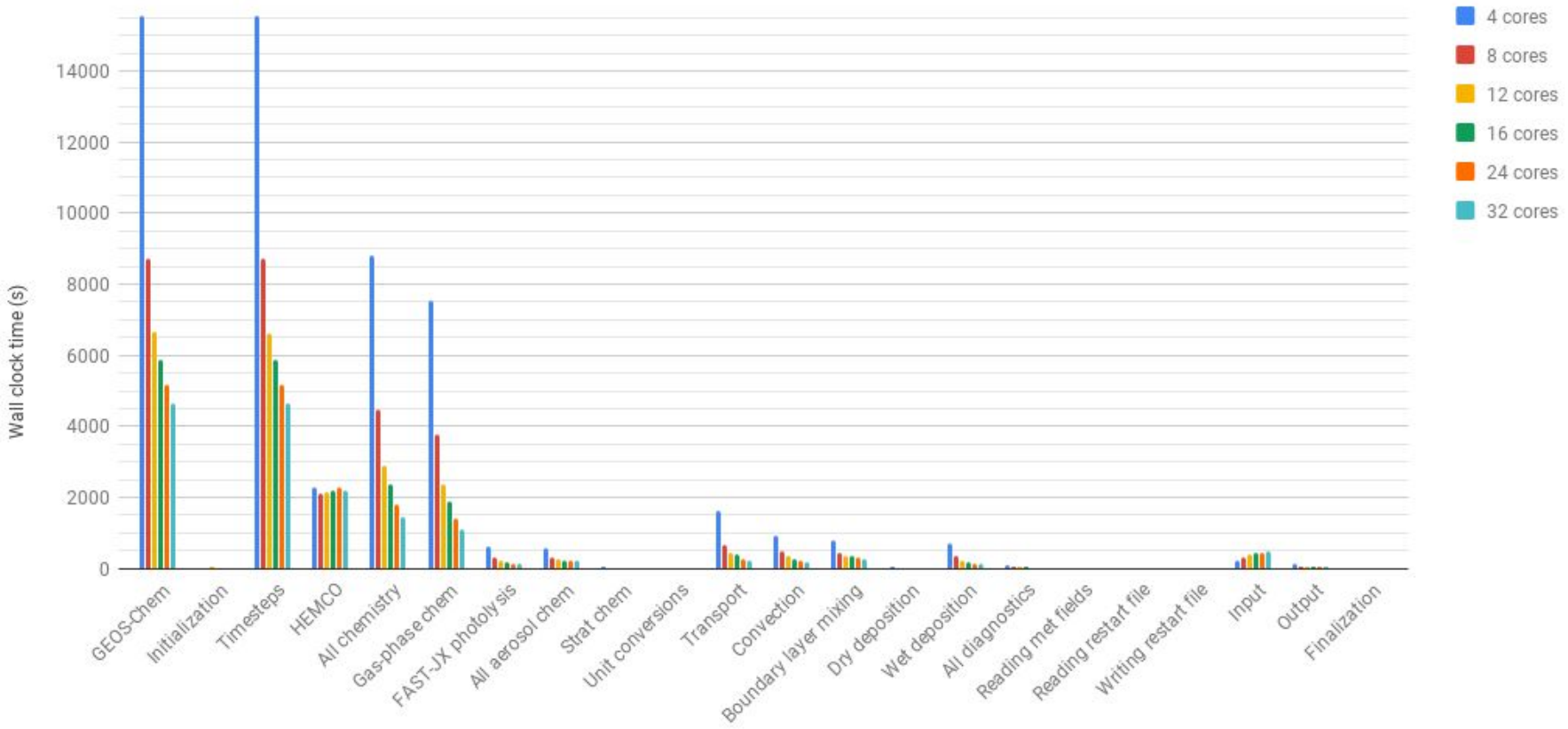


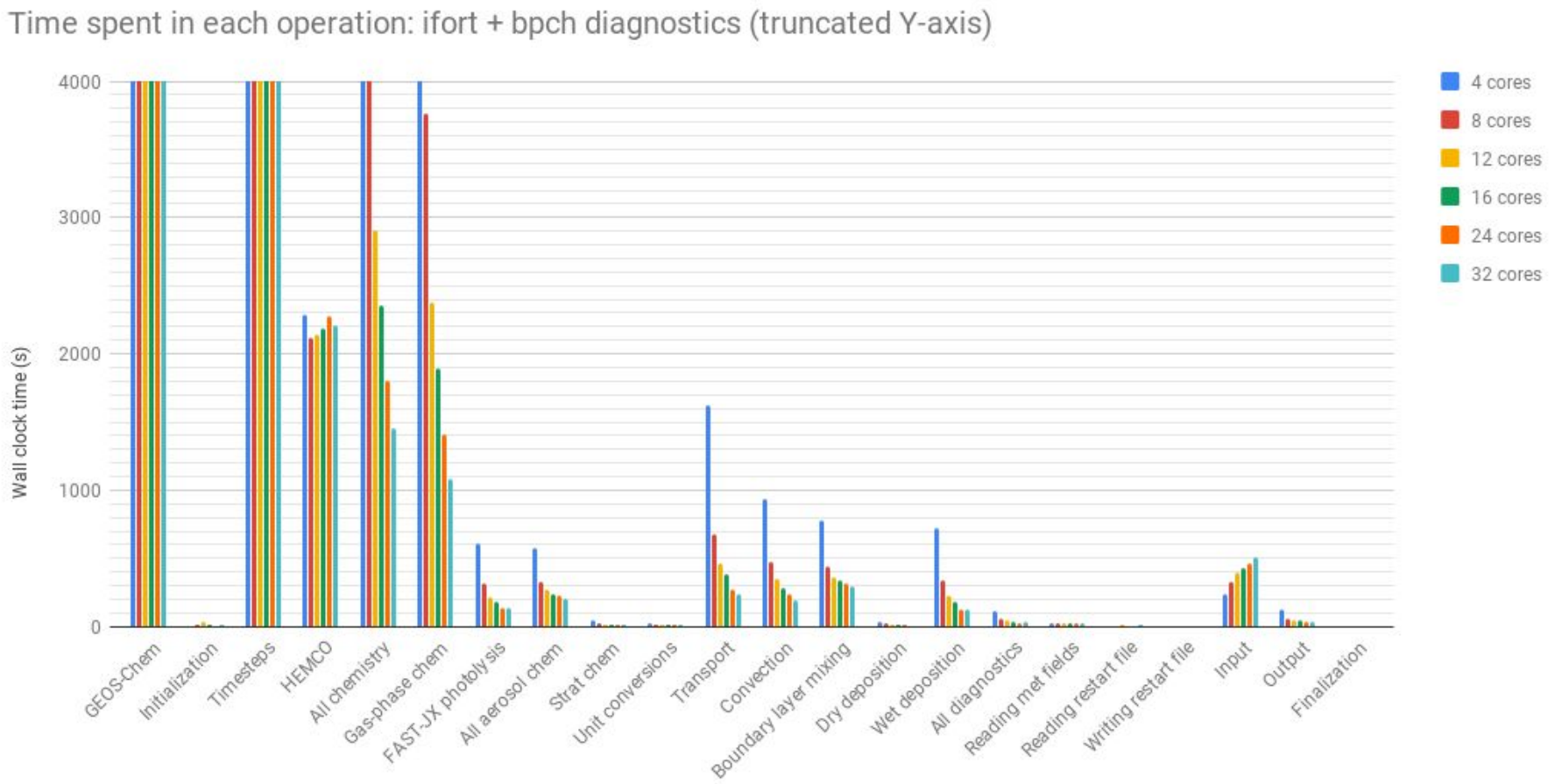
Percent speedup when switching from 4 to 16 cores and from 4 to 32 cores (gfortran + netCDF diagnostics)



Time spent in each operation:
Intel Fortran 17.0.4 + default build + bpch diagnostics

Time spent in each operation: ifort + bpch diagnostics




Time spent in each operation: ifort + bpch diagnostics (truncated Y-axis)
Wall clock time (s)
4000
3000
2000
1000
0
4 cores
8 cores
12 cores
16 cores
24 cores
32 cores
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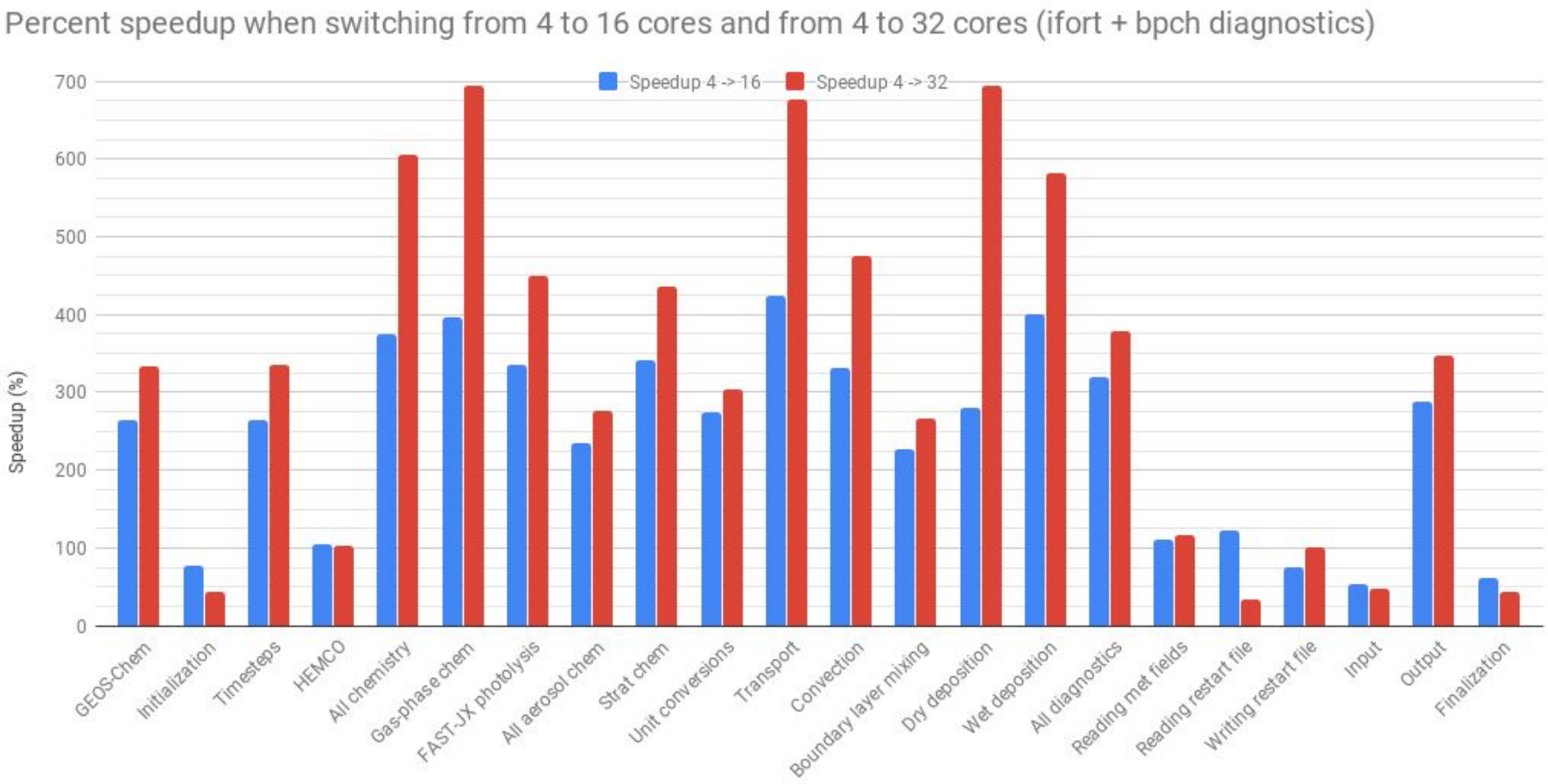
Initialization
Timesteps
HEMCO
All chemistry
Gas-phase chem
FAST-JX photolysis
All aerosol chem
Strat chem
Unit conversions
Transport
Convection
Boundary layer mixing
Dry deposition
Wet deposition
All diagnostics
Reading met fields
Reading restart file
Writing restart file
Input
Output
Finalization


Percent speedup when switching from 4 to 16 cores and from 4 to 32 cores (ifort + bpch diagnostics)
Speedup 4 -> 16
Speedup 4 -> 32
Speedup (%)
0
100
200
300
400
500
600
700
GEOS-Chem
Initialization
Timesteps
HEMCO
All chemistry
Gas-phase chem
FAST-JX photolysis
All aerosol chem
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Wet deposition
All diagnostics
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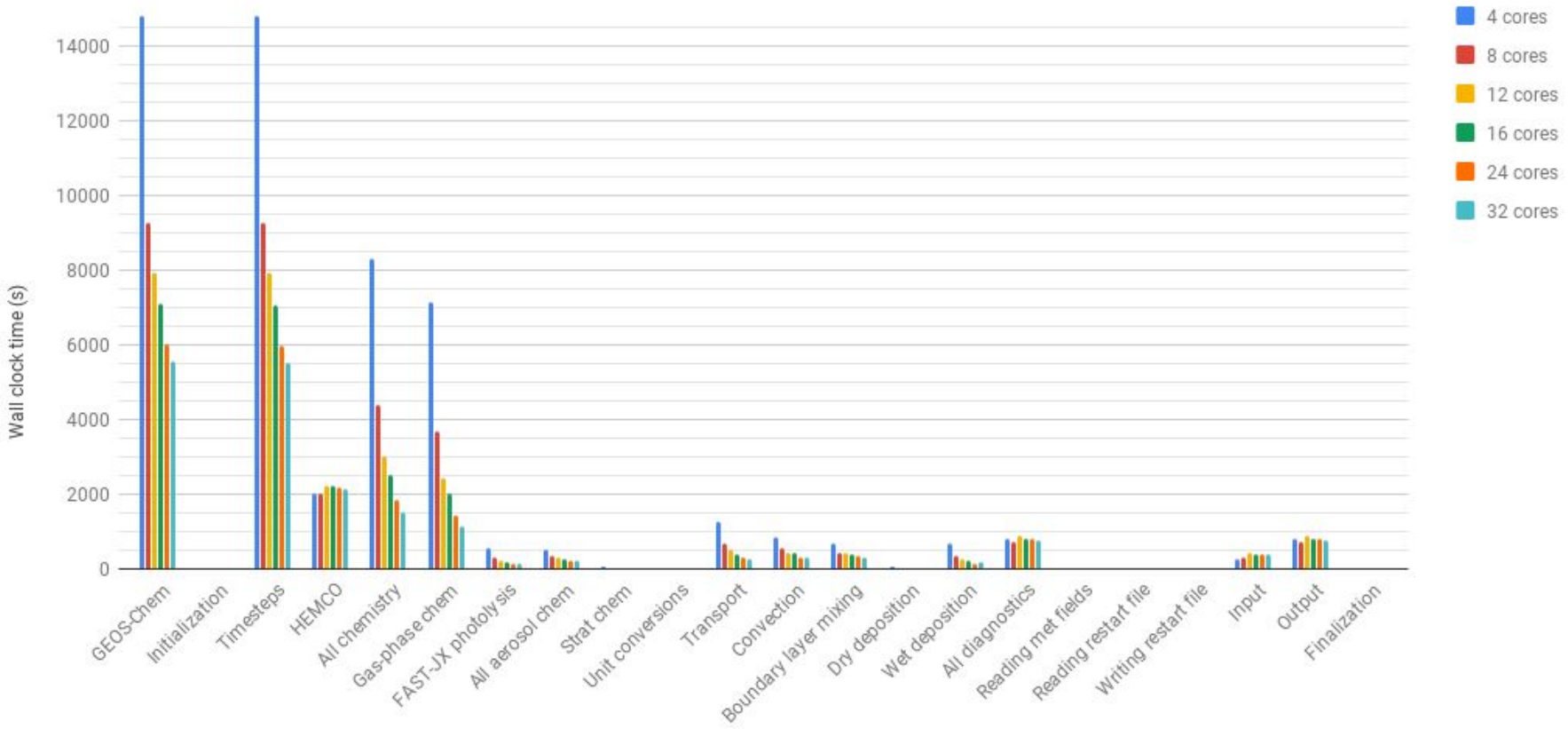
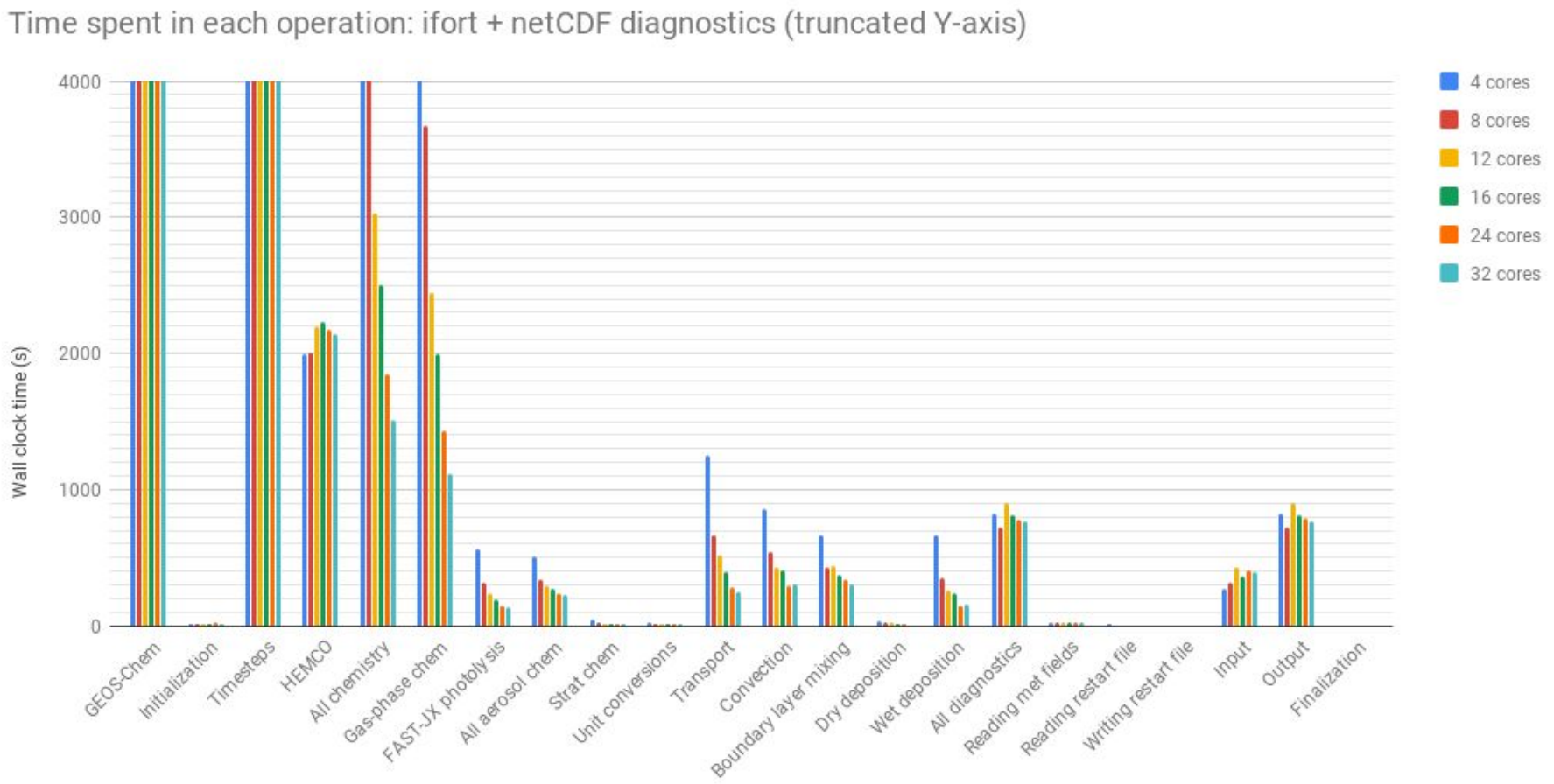
Writing restart file
Input
Output
Finalization

Time spent in each operation:
Intel Fortran 17.0.4 + default build + netCDF diagnostics

Time spent in each operation: ifort + netCDF diagnostics




Time spent in each operation: ifort + netCDF diagnostics (truncated Y-axis)
Wall clock time (s)
4000
3000
2000
1000
0
4 cores
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