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EXCELENCIA SEVERO OCHOA

XIOS Integration for ~~Open~~IFS: Computational Aspects and Performance Evaluation

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1. Introduction

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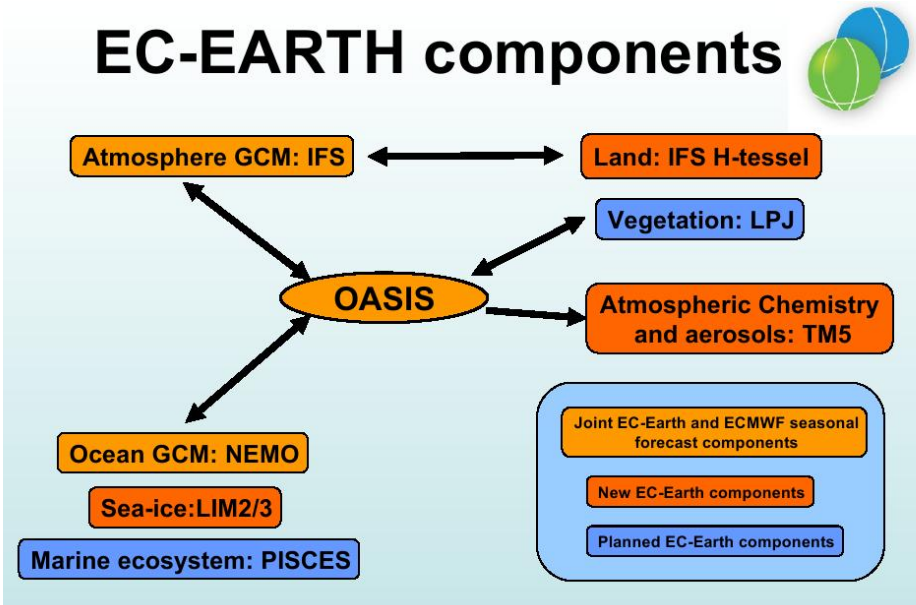
Introduction

- IFS is a global forecasting system developed by ECMWF
- It has two different output schemes:
  - The Météo-France (MF) I/O server (ECMWF only)
  - An inefficient sequential I/O scheme (the rest of users)
- The sequential I/O scheme requires a serial process:
  - Gather all data in the master process of the model
  - Then, the master process sequentially writes all data
- This is not scalable for higher grid resolutions, and even less, for future exascale machines
- IFS is also used in some Earth system models, such as EC-Earth

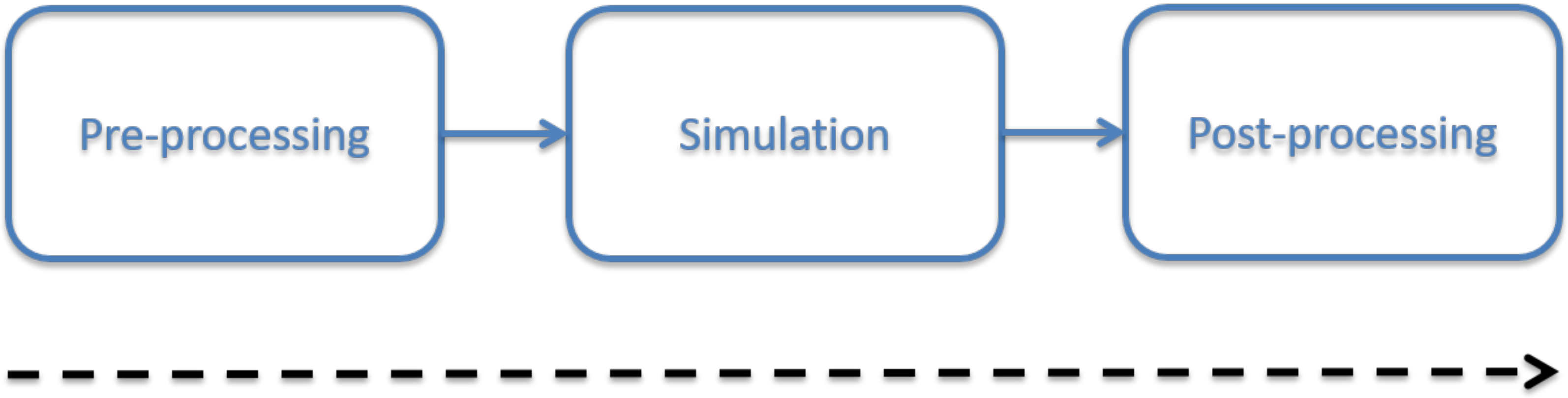
Introduction

- EC-Earth is a global coupled climate model, which integrates a number of component models in order to simulate the Earth system
- The two main components are **IFS as the atmospheric model** and NEMO as the ocean model



Introduction

- In addition, Earth system models such as EC-Earth, run experiments that have other tasks in their workflow
- Post-processing task can perform data format conversion, compression, diagnostics, etc.



Critical path = Pre-processing + Simulation + Post-processing

Introduction

- When IFS is used in EC-Earth for climate modeling, post-processing is needed to:
  - Convert GRIB to netCDF files
  - Transform data to be CMIP-compliant
  - Compute diagnostics
- Post-processing turns into an expensive process

Motivation

- In particular, we are experiencing an I/O bottleneck in the IFS version of EC-Earth
- EC-Earth has been recently used to run ultra-high resolution experiments under the H2020 PRIMAVERA project
- However, it suffers a considerable slowdown, where the I/O in IFS represents about 30% of the total execution time

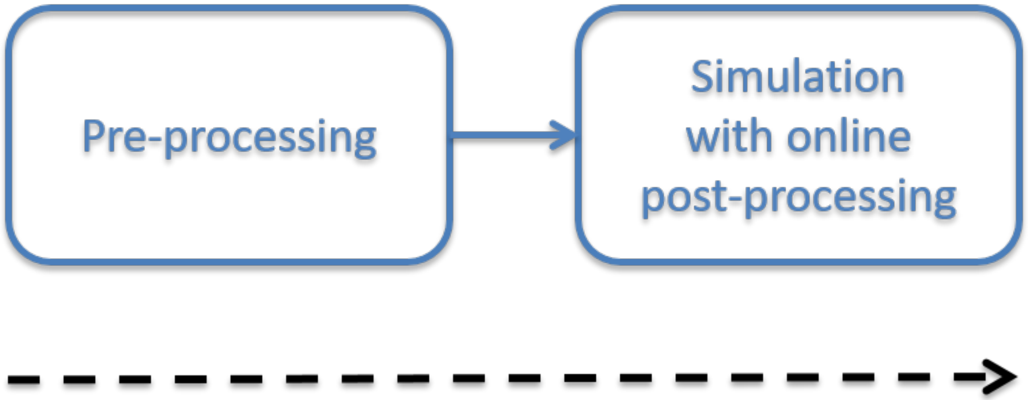
Motivation

- In order to address the I/O issue, we have to select a suitable tool that fulfills a series of needs:
  1. It must be a parallel, efficient and scalable I/O tool
  2. Data must be written using netCDF format (standard in climate modelling) and must follow the CMIP standard
  3. It must perform online post-processing along with the simulation, such as interpolations or data compression
- There is a tool designed to that end: XIOS
- XIOS is an I/O server

Motivation

The use of a tool such as XIOS has a twofold effect:

- Improve the computational performance and efficiency of a model, and thus, reduce the execution time
- Reduce the critical path of its workflow by avoiding the post-processing task



Critical path = Pre-processing + Simulation

European collaboration

- European Centre for Medium-Range Weather Forecasts (ECMWF)
  - Help in decisions: design, setups, etc.
  - Support with ECMWF enviroment
  - XIOS as an optional I/O scheme of OpenIFS
- Netherlands eScience Center (NLeSC)/Koninklijk Nederlands Meteorologisch Instituut (KNMI)
  - Help in decisions: design, setups, etc.
  - Add FullPos features
  - Ensure a user-friendly output

2. State-of-the-art overview

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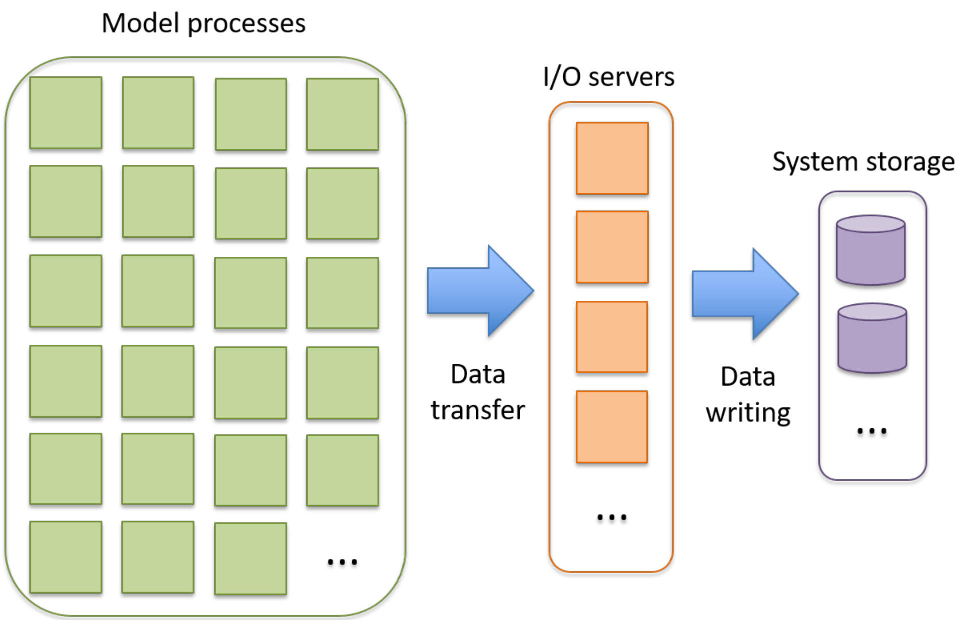
State-of-the-art overview

- Sequential I/O
- Parallel I/O libraries: MPI-IO, HDF5 and netCDF
- I/O servers:
  - ADIOS
  - CDI-pio
  - CFIO
  - XIOS



4. IFS-XIOS integration

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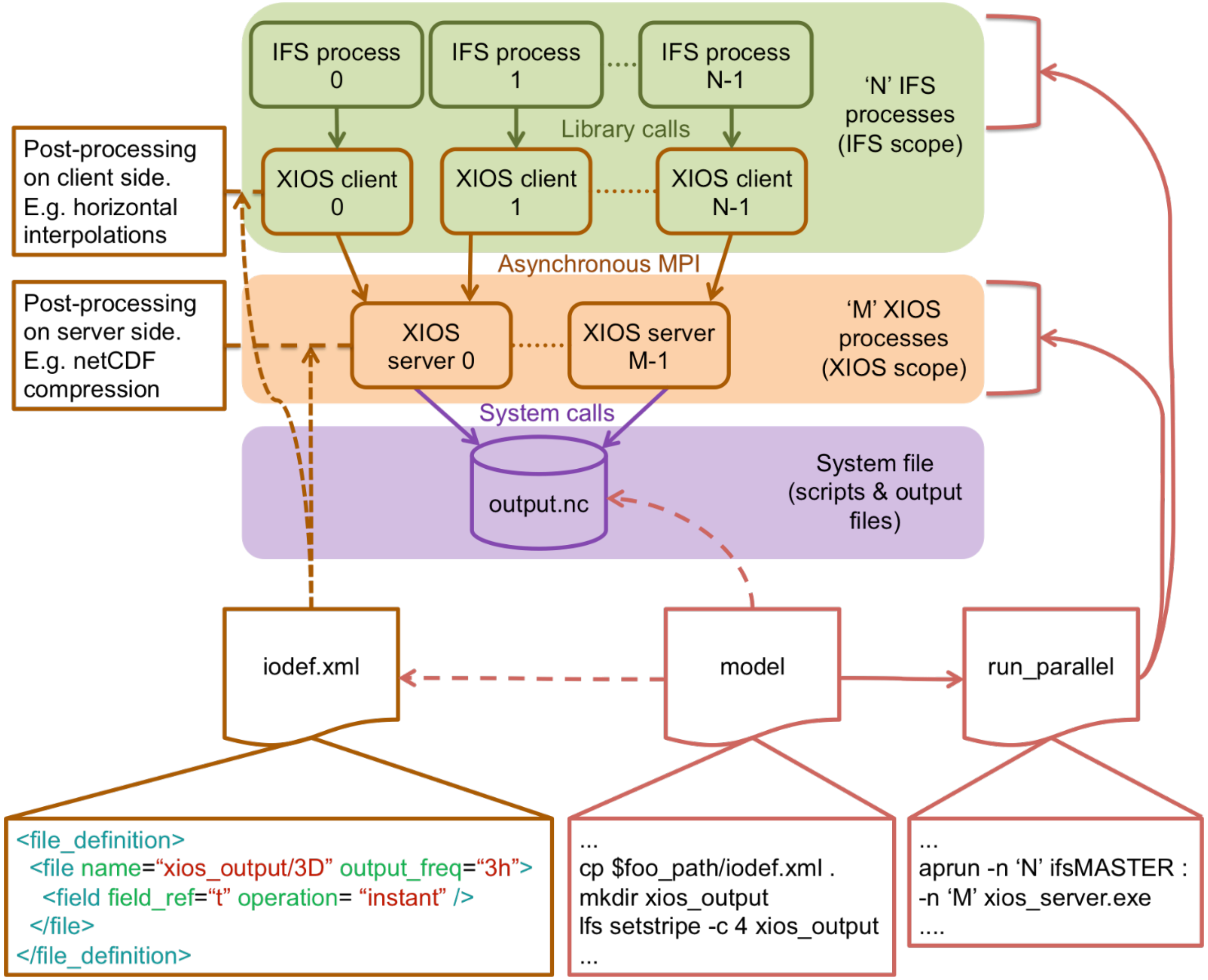
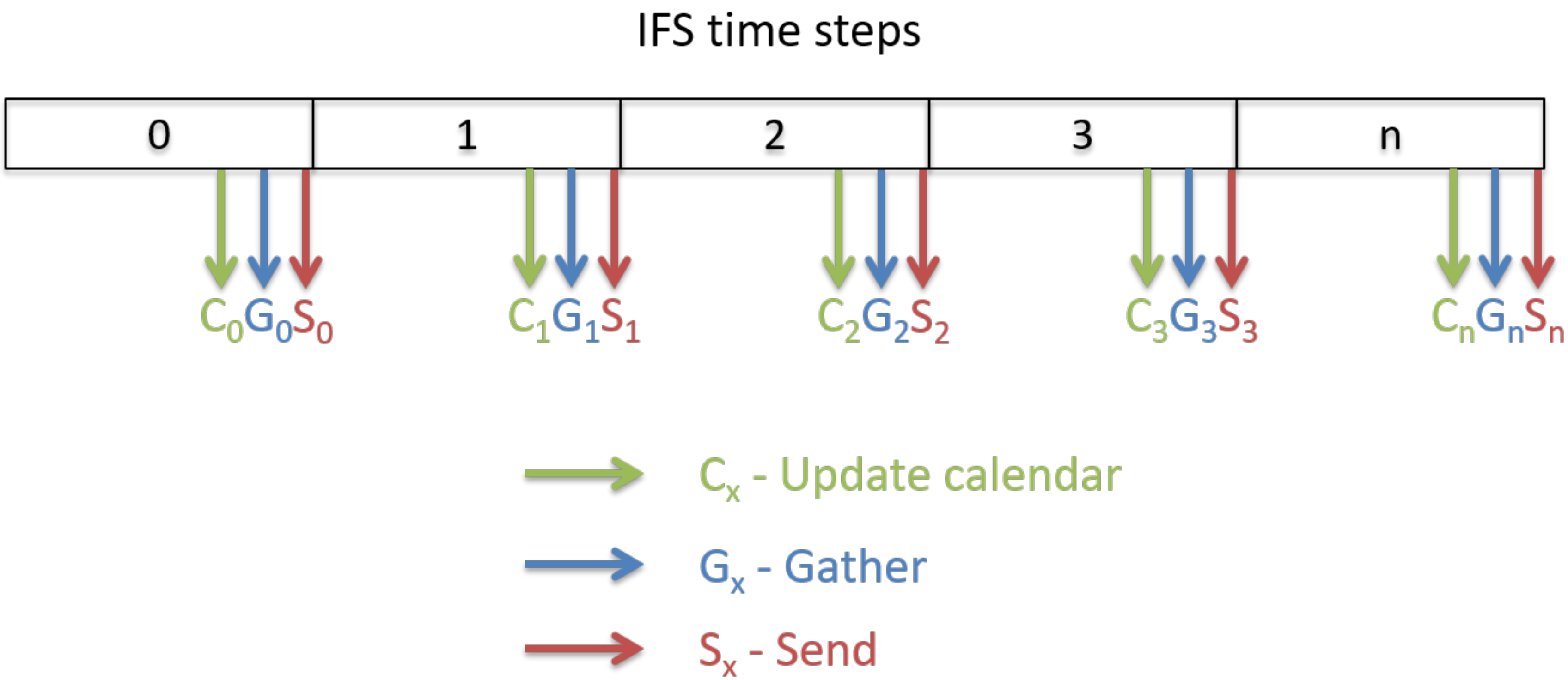
Scheme of IFS-XIOS integration



Output scheme approach

- If it is an output time step, at the end of it IFS sequentially executes three steps
- Otherwise, IFS only executes the update calendar step



Development steps

- XIOS setup
  - Initialization
  - Finalization
  - Context
    - Calendar
    - Geometry (axis, domain and grid)
  - *Iodef.xml* file
- Grid-point fields transfer
  - NPROMA blocks gather
  - Send fields
- Environment setup
  - XIOS compilation
  - Include and link XIOS, netCDF and HDF5
  - Model script
  - Supporting MPMD mode

Development steps

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  - Initialization
  - Finalization
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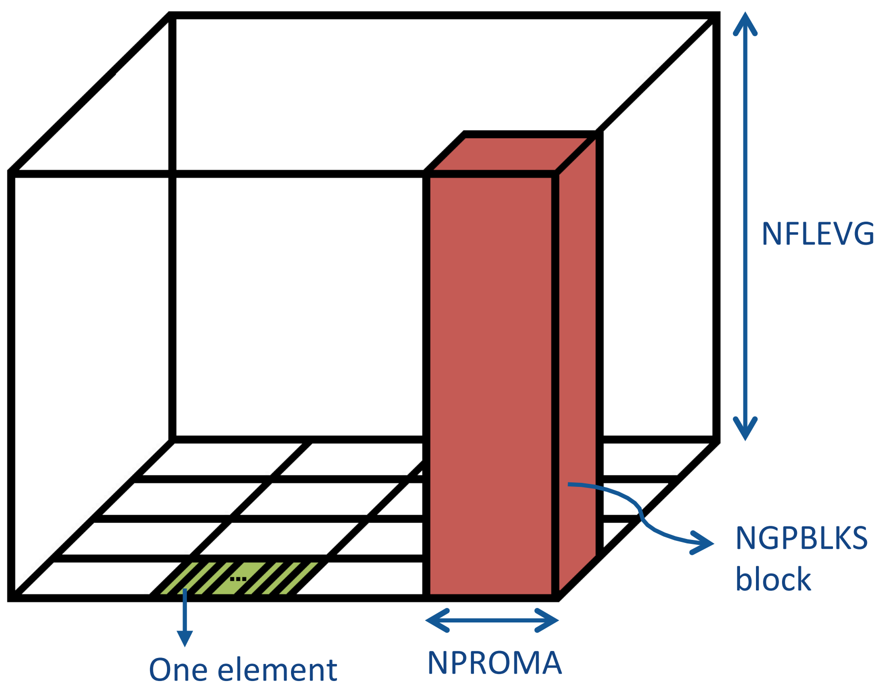
NPROMA blocks gather

- The IFS data arrays do not match with the XIOS ones:
  - IFS_data_array(NPROMA, NFLEVG, NFIELDS, NGPBLKS)
  - XIOS_data_array(unidimensional 2D domain, NFLEVG)
- We have to re-shuffle fields data before sending them
- According to the blocking strategy used in IFS, we have to build an XIOS-style array by gathering NPROMA blocks

Subdomain decomposition in IFS

- IFS uses a blocking strategy to efficiently parallelize the manipulation of data arrays using OpenMP
- IFS_data_array(NPROMA, NFLEVG, NFIELDS, NGPBLKS)



5. Performance analysis and optimization

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Execution overview

- 702 MPI processes, each with 6 OpenMP threads
- 10 days of forecast with a time step of 600 seconds
- Output size of netCDF files: 3.2 TB
- Execution times:
  - Sequential output: 9054 seconds
  - MF I/O server: 7535 seconds
  - IFS-XIOS integration: 7773 seconds
  - No output: 7356 seconds

Threading with OpenMP

- Using GSTATS timers, we profiled the NPROMA blocks gather. For instance, the gather of the ciwc field:

ROUTINE	CALLS	SUM(s)	AVE(ms)	STDDEV(ms)	MAX(ms)	SUMB(s)	FRAC(%)
ciwc_GATHER	80	0.5	5.8	0.9	6.5	0.0	0.01

- It does not take too much time. However, it only works the master thread, while the rest are idle
- This is not efficient and could become a bottleneck

Threading with OpenMP

- We used OpenMP to parallelize the NPROMA blocks gather
- In addition, we overlap the send of one field with the gather of the next one

Threading with OpenMP

```
!$OMP PARALLEL PRIVATE(jstglo,icend,ibl,jlev)

! GFL – Specific humidity
IF (q) THEN
  !$OMP DO SCHEDULE(DYNAMIC)
  DO jstglo = 1, YDGEOMETRY%YRGEM%NGPTOT, YDGEOMETRY%YRDIM%
      ↪ NPROMA
    icend = MIN(YDGEOMETRY%YRDIM%NPROMA,YDGEOMETRY%YRGEM%
        ↪ NGPTOT−jstglo+1)
    ibl = (jstglo−1)/YDGEOMETRY%YRDIM%NPROMA + 1
    DO jlev = 1, YDGEOMETRY%YRDIMV%NFLEVG
      xios_gfl(jstglo:jstglo+icend−1,jlev) = YDFIELDS%YRGFL%GFL(1:icend,jlev,
          ↪ YGFL%YQ%MP,ibl)
    END DO
  END DO
  !$OMP END DO
  !$OMP SINGLE
  CALL xios_send_field("q",xios_gfl)
  !$OMP END SINGLE NOWAIT
END IF

! GMV – Temperature
IF (t) THEN
  !$OMP DO SCHEDULE(DYNAMIC)
  DO jstglo = 1, YDGEOMETRY%YRGEM%NGPTOT, YDGEOMETRY%YRDIM%
      ↪ NPROMA
```

Gather

Send

Gather and send overlap among two fields

Threading with OpenMP

- The profiling shows an improvement:

ROUTINE	CALLS	SUM(s)	AVE(ms)	STDDEV(ms)	MAX(ms)	SUMB(s)	FRAC(%)
ciwc_GATHER	80	0.1	1.2	0.2	2.3	0.0	0.00

- The execution time is reduced 68 seconds, from 7773 seconds to 7705 seconds

Optimized compilation of XIOS

- We had a lot of issues to optimally compile XIOS
- For this reason, we used a conservative option: *-O1*
- XIOS reports too much time for just outputting data:

Client

```
-> report :  Performance report : Whole time from XIOS init and
   ↪ finalize: 7681.68 s
-> report :  Performance report : total time spent for XIOS :
   ↪ 132.715 s
-> report :  Performance report : time spent for waiting free
   ↪ buffer : 3.80519 s
-> report :  Performance report : Ratio : 0.0495359 %
```

Server

```
-> report : Performance report : Time spent for XIOS : 7681.68
-> report : Performance report : Time spent in processing events :
   ↪ 3196.4
-> report : Performance report : Ratio : 41.6107%
```

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Optimized compilation of XIOS

- A bug was previously reported in the compilation of XIOS using *-O2* and *-O3* for Cray compilers
- However, it was reported using older Cray compilers, so it might be solved in newer versions
- Certainly, XIOS compiled and tests successfully passed

Optimized compilation of XIOS

- The execution time in both client and server sides is reduced

Client

```
-> report :  Performance report : Whole time from XIOS init and
   ↪ finalize: 7562.36 s
-> report :  Performance report : total time spent for XIOS :
   ↪ 40.3018 s
-> report :  Performance report : time spent for waiting free
   ↪ buffer : 0.463693 s
-> report :  Performance report : Ratio : 0.00613159 %
```

Server

```
-> report : Performance report : Time spent for XIOS : 7562.37
-> report : Performance report : Time spent in processing events :
   ↪  1382.16
-> report : Performance report : Ratio : 18.2768%
```

- The execution time is reduced 76 seconds, from 7705 seconds to 7629 seconds

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Overlapping computation and communication

In an output time step, there is a slight increase in the execution time of the three following time steps

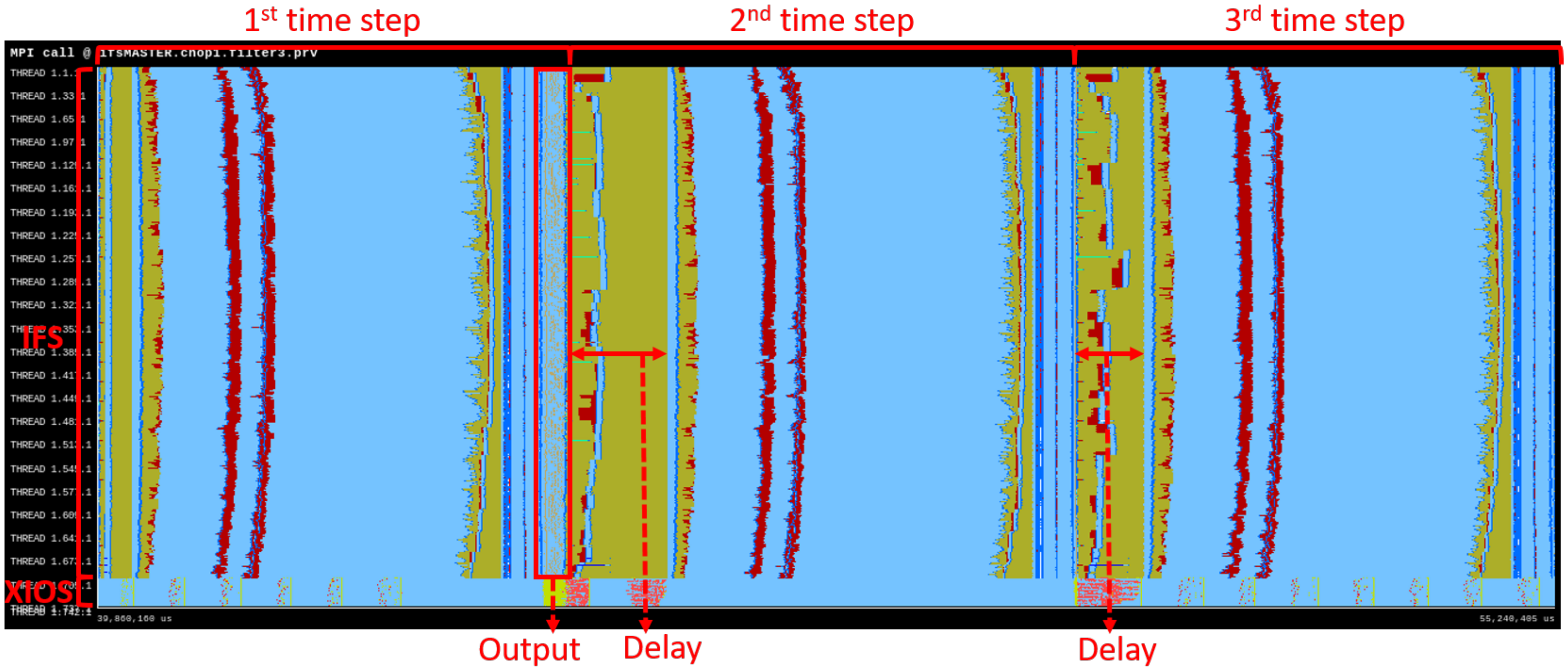
Non-output

Output

12:24:55	0AAA00AAA	STEPO	318	27.370	27.370	4.592	167:53
12:25:02	0AAA00AAA	STEPO	319	39.994	39.994	6.708	168:33
12:25:07	0AAA00AAA	STEPO	320	28.826	28.826	4.826	169:02
12:25:12	0AAA00AAA	STEPO	321	28.034	28.034	4.701	169:30
12:25:16	0AAA00AAA	STEPO	322	27.770	27.770	4.655	169:58
12:25:21	0AAA00AAA	STEPO	323	27.690	27.690	4.654	170:26
12:25:26	0AAA00AAA	STEPO	324	27.854	27.854	4.679	170:53
12:25:33	0AAA00AAA	STEPO	325	42.771	42.771	7.158	171:36
12:25:38	0AAA00AAA	STEPO	326	30.114	30.114	5.044	172:06
12:25:43	0AAA00AAA	STEPO	327	30.870	30.870	5.181	172:37
12:25:48	0AAA00AAA	STEPO	328	27.874	27.874	4.682	173:05

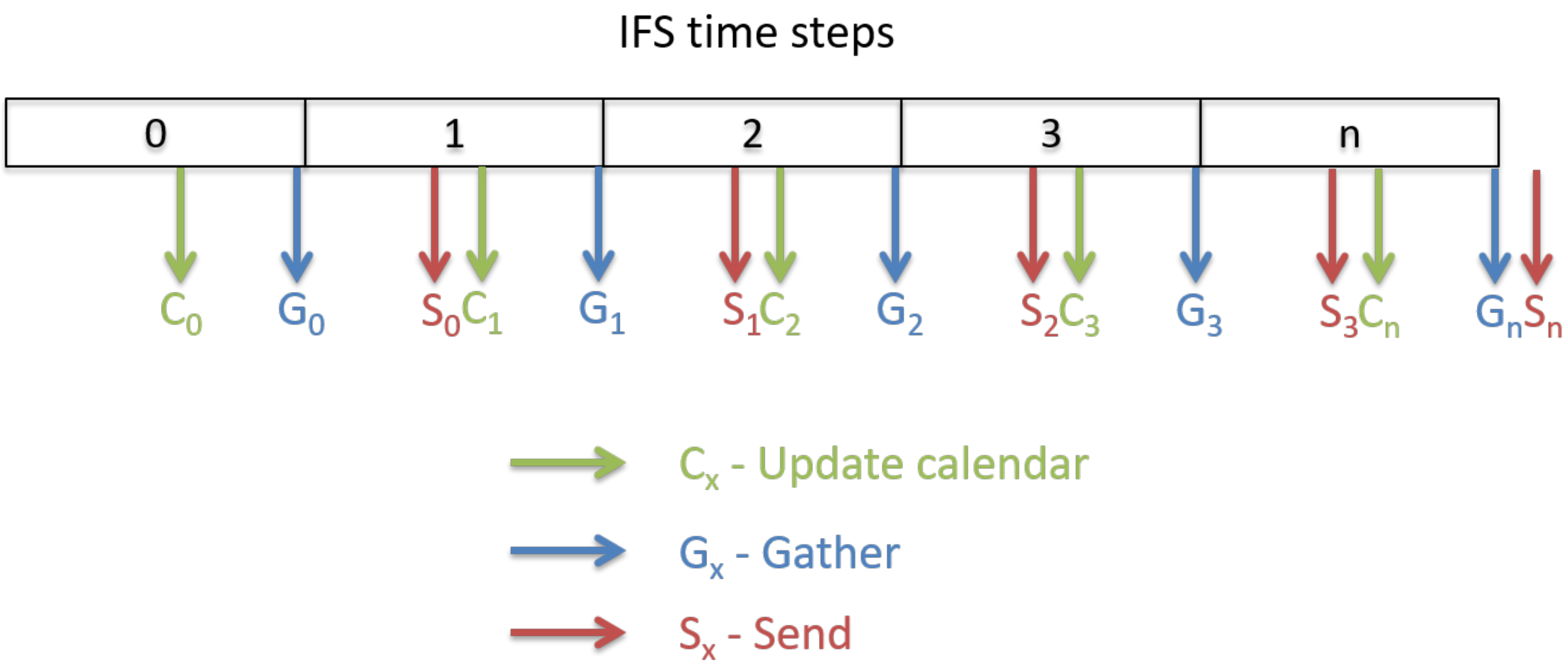
Overlapping computation and communication

- The trace shows that after an output time step, there is a delay in the communication of the next two time steps (*MPI_Waitany* and *MPI_Alltoallv*)
- There is a conflict between intra IFS communication and IFS to XIOS communication



Overlapping computation and communication

- We used a new output scheme to truly overlap XIOS communication with IFS computation
- It splits the three needed steps to output data through XIOS:



Overlapping computation and communication

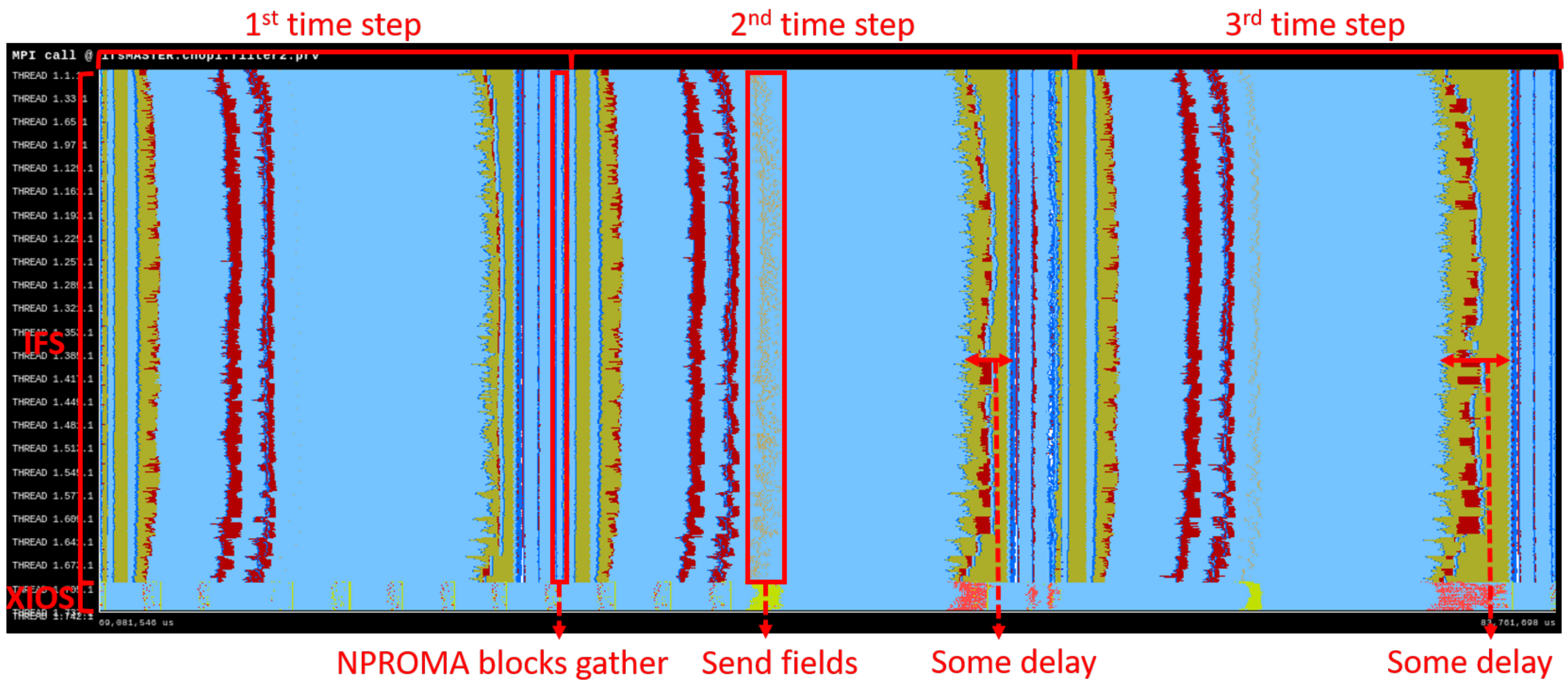
- This new scheme improves the execution time of the three time steps that follow an output time step:

Non-output	12:27:45	0AAA00AAA	STEP0	318	26.926	26.926	4.514	162:23
	12:27:52	0AAA00AAA	STEP0	319	38.414	38.414	6.441	163:01
	12:27:56	0AAA00AAA	STEP0	320	27.054	27.054	4.535	163:28
	12:28:01	0AAA00AAA	STEP0	321	27.030	27.030	4.534	163:55
	12:28:05	0AAA00AAA	STEP0	322	26.882	26.882	4.502	164:22
	12:28:10	0AAA00AAA	STEP0	323	27.394	27.394	4.607	164:50
Output	12:28:15	0AAA00AAA	STEP0	324	27.142	27.142	4.549	165:17
	12:28:21	0AAA00AAA	STEP0	325	39.310	39.310	6.579	165:56
	12:28:26	0AAA00AAA	STEP0	326	28.318	28.318	4.755	166:24
	12:28:31	0AAA00AAA	STEP0	327	28.686	28.686	4.813	166:53
	12:28:35	0AAA00AAA	STEP0	328	26.990	26.990	4.527	167:20

- The execution time is reduced 122 seconds, from 7629 seconds to 7507 seconds

Overlapping computation and communication

- The trace shows that there is no delay at the beginning of the 2nd and 3rd time steps
- However, there is some delay at the end, but it is less significant



6. Evaluation

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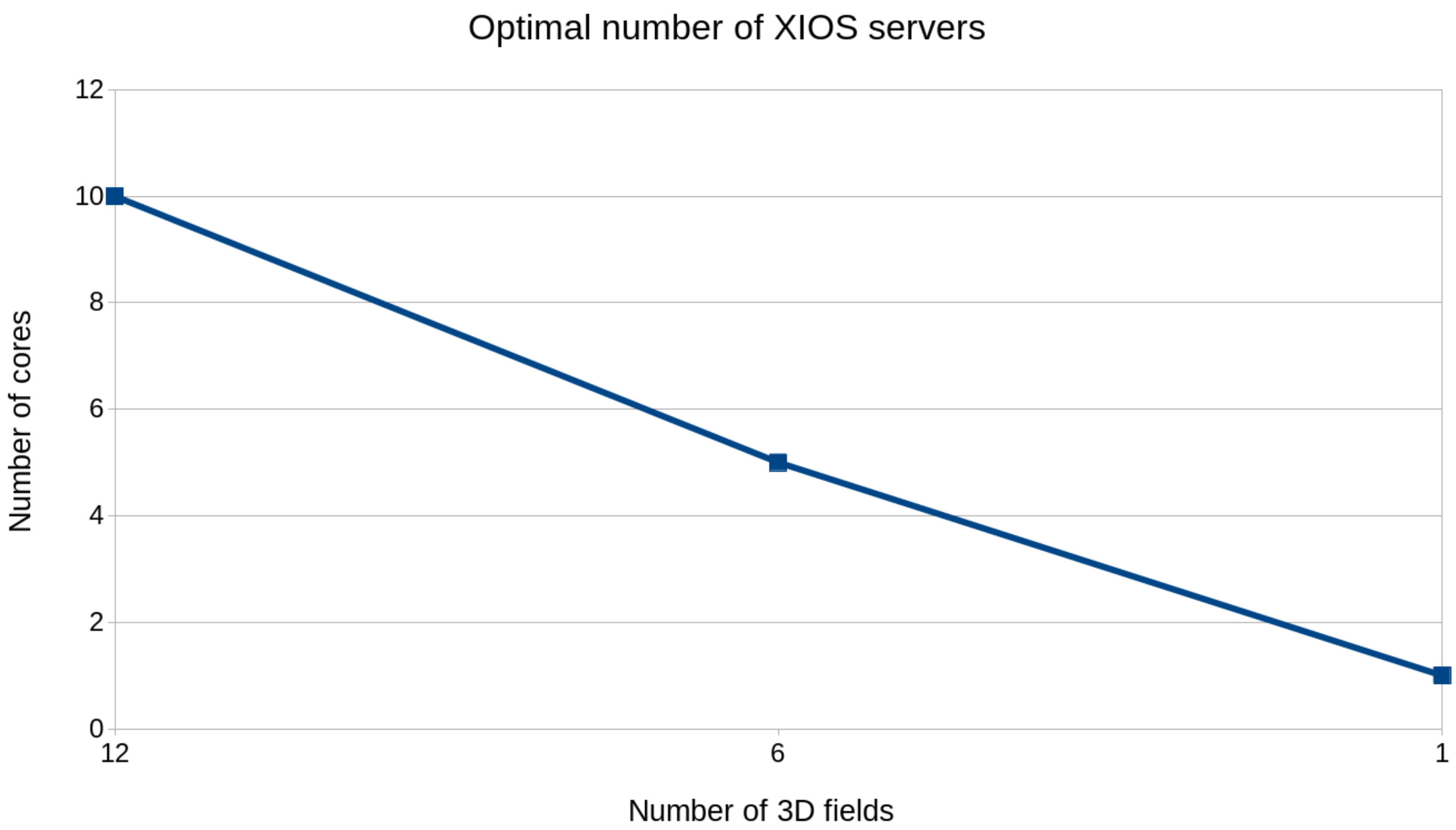
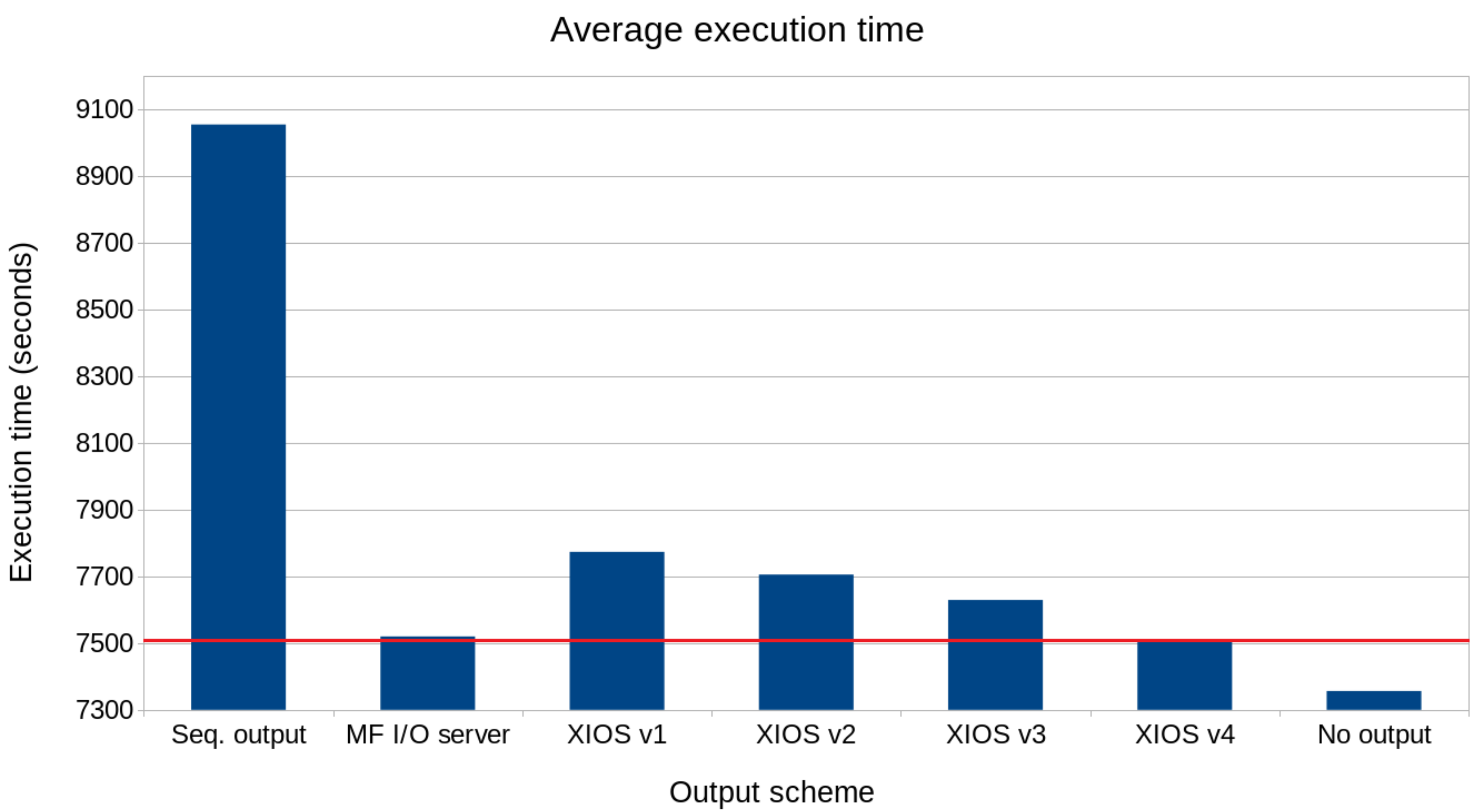
Optimal number of XIOS servers

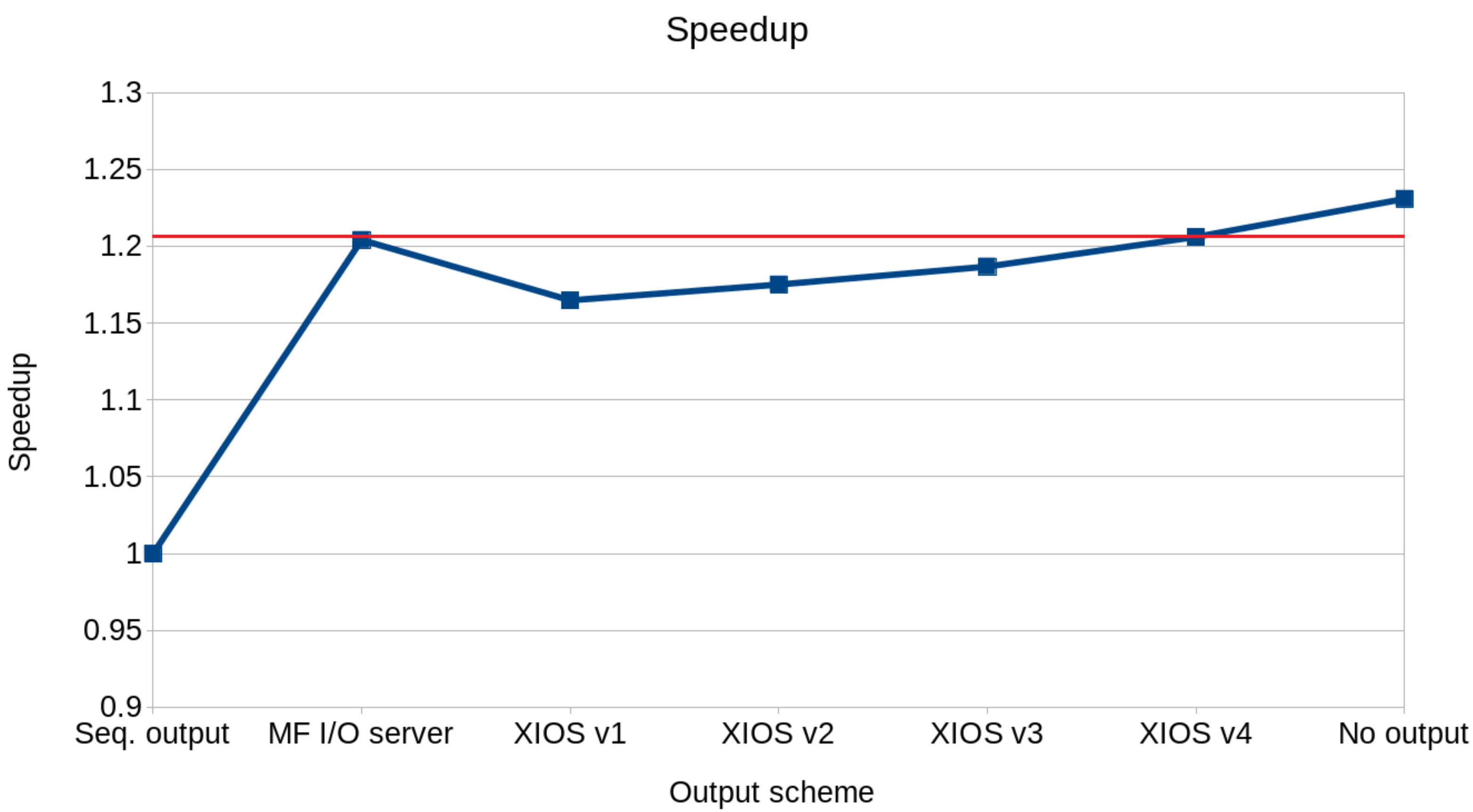


Comparison test



*MF I/O server includes FullPos calls

Comparison test



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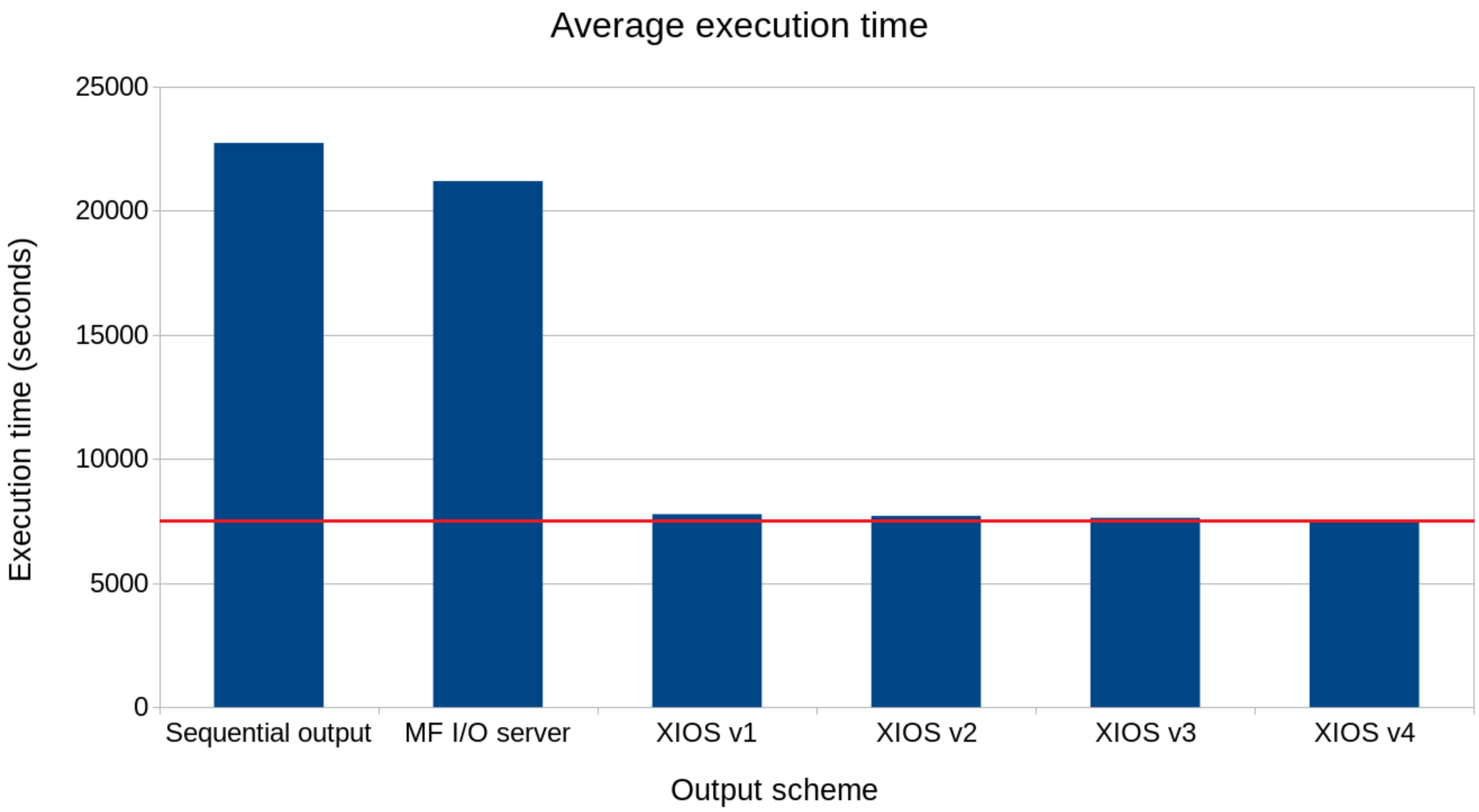
Comparison test adding GRIB to netCDF post-processing



*MF I/O server includes FullPos calls

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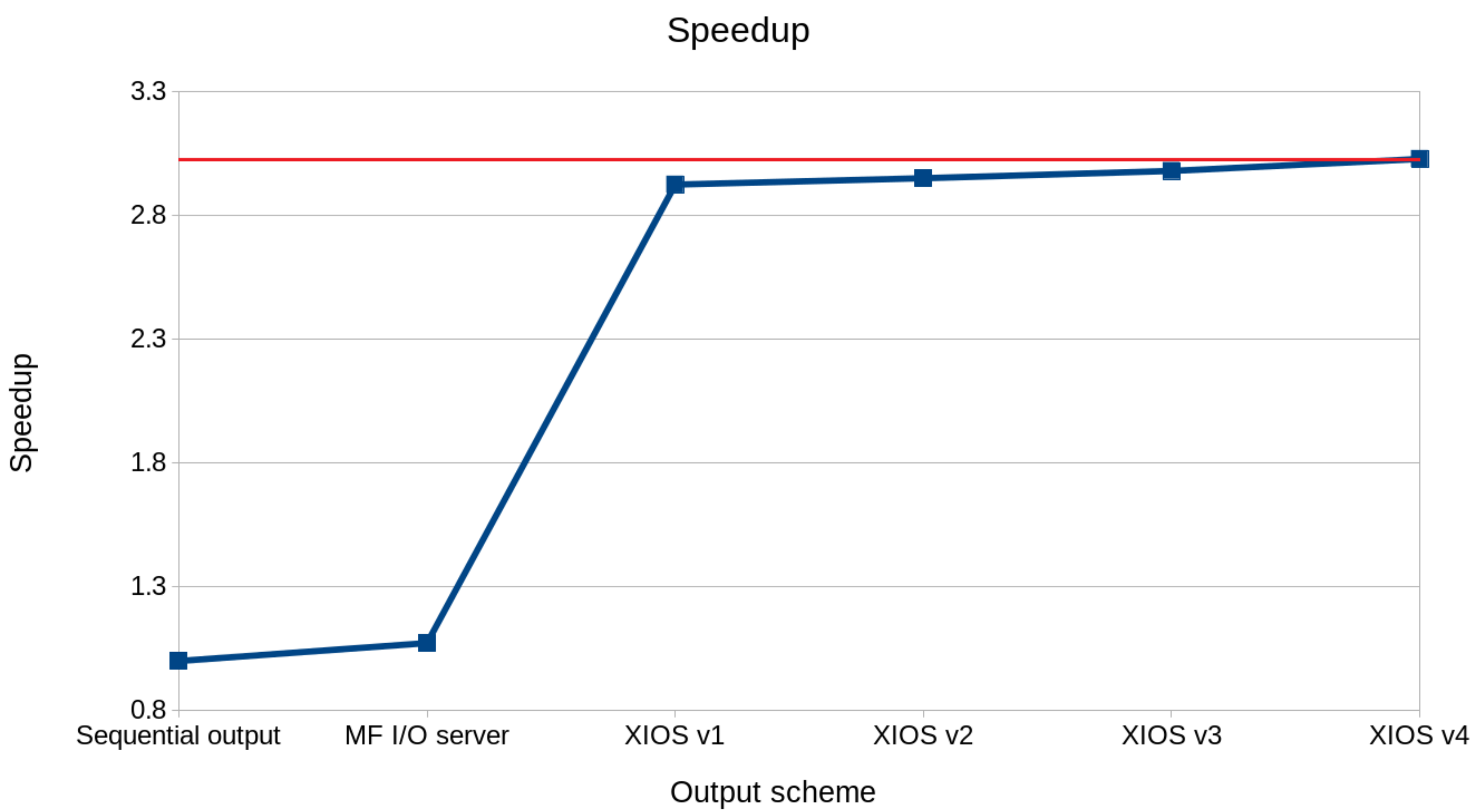

*MF I/O server includes FullPos calls

Comparison test with additional computational resources and GRIB to netCDF post-processing

- In this test, we add to the IFS processes of the sequential I/O scheme the equivalent of the computational resources needed to run XIOS
- XIOS uses 10 cores spread along 10 nodes
- Then, the execution times with the additional resources are:
  - XIOS v4 (702 IFS + 10 XIOS) → 7507 seconds
  - Seq. I/O (702 IFS) → 22734 seconds
  - Seq. I/O (702 + 10 cores = 712 IFS) → 22583 seconds
  - Seq. I/O (702 + 120 cores* = 822 IFS) → 21962 seconds

*According to the IFS affinity used, 10 nodes = 120 cores

7. Conclusions

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Conclusions

- The integration with no optimization already improved the execution time:
  - Sequential output 9054 seconds (23% of overhead) → IFS-XIOS integration 7773 seconds (5.6% of overhead)
- Performance highlights of the most optimized version:
  - It is slightly faster than the MF I/O server (but without FullPos calls): 7519 s vs. 7507 s
  - It is only 151 seconds slower than no output (2% of overhead)
  - Within 151 seconds IFS outputs 3.2 TB of data
- When post-processing to convert GRIB to netCDF files is taken into account:
  - The post-processing takes 13680 seconds (3.8 hours)
  - Thus, the most optimized version is a 202% faster than the sequential output and a 182% faster than the MF I/O server

Conclusions

- These numbers denote that we have implemented an scalable and efficient development that will address the I/O issue
- In EC-Earth, this new I/O development will:
  - Increase the performance and efficiency of the whole model
  - Perform online post-processing operations
  - Save thousands of computing hours
  - Save storage space, because it will only store processed data ready to be used

Ongoing work

- Add FullPos features into the IFS-XIOS integration to:
  - Convert spectral fields to grid-point fields before sending them to XIOS
  - Use vertical interpolations such as pressure or PV level

  Ensure a user-friendly output configuration file
- Increase the usability and the robustness of the IFS-XIOS integration by managing XIOS elements in runtime: fields, files, domain, axis, etc.

Future work

- Performance analysis and optimization of the final integration reusing the explained optimization techniques and maybe new ones
- The development done for IFS will be ported to OpenIFS
- Adapt the EC-Earth model to generate online diagnostics from OpenIFS and NEMO components through XIOS

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Thank you!

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Appendix

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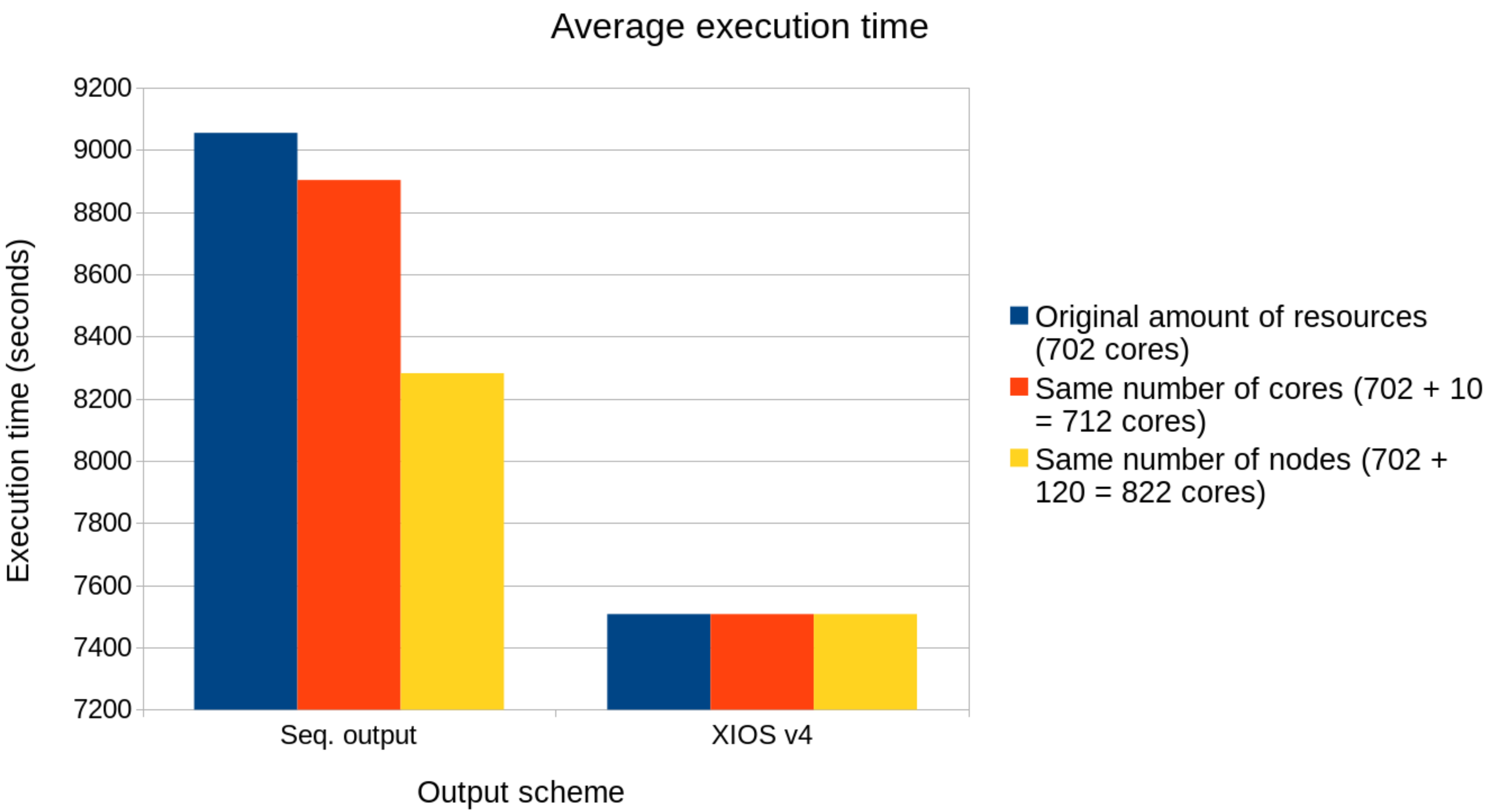
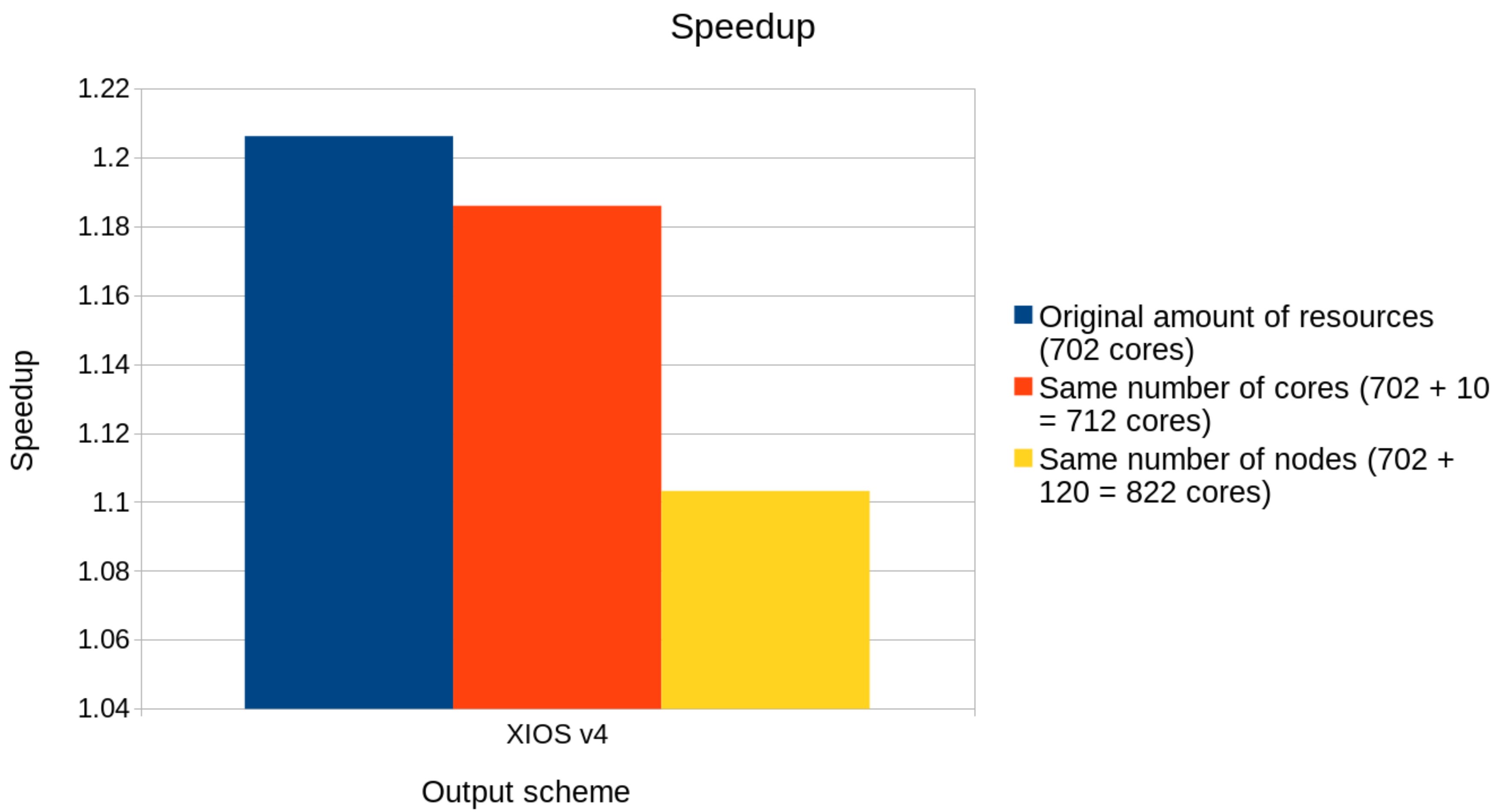
Comparison test with additional computational resources



Comparison test with additional computational resources



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Comparison test with additional computational resources and GRIB to netCDF post-processing

Comparison test with additional computational resources and GRIB to netCDF post-processing