Computational aspects and performance evaluation of the IFS-XIOS integration

Xavier Yepes-Arbós, BSC
Mario C. Acosta, BSC
Gijs van den Oord, NLeSC
Glenn Carver, ECMWF

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1. Introduction
Introduction

• Earth system models have benefited of the exponential growth of supercomputing power
• This allows to use more complex computational models to find more accurate solutions
• As a consequence, the generated amount of data has grown considerably
• However, since the I/O was not significant enough in the past, not much attention was paid to improve it
Introduction

• Due to this reason, some Earth system models output data using inefficient sequential I/O schemes

• This type of 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

• This is the case of one of the I/O schemes of IFS
Introduction

• IFS is a global forecasting system developed by ECMWF
• It has two different output schemes:
  • The Météo-France (MF) I/O server which is fast and efficient from a computational point of view. It is only used at ECMWF, such its operational forecasts
  • A sequential I/O scheme which is slow and inefficient from a computational point of view. It is used by non-ECMWF users, this is, in OpenIFS and in the IFS version of EC-Earth
• IFS is also used as a component of the EC-Earth model
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 files to netCDF files
  • Transform data to be CMIP-compliant (CMORization)
  • 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 experiments using the T511L91-ORCA025L75 configuration under the H2020 PRIMAVERA project
- Experiments require to output a lot of fields, causing a considerable slowdown in the EC-Earth execution time
- 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
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

- Netherlands eScience Center (NLeSC)/Koninklijk Nederlands Meteorologisch Instituut (KNMI)
- European Centre for Medium-Range Weather Forecasts (ECMWF)
2. Components description
The Integrated Forecast System (IFS) is a global data assimilation and forecasting system developed by ECMWF.

It writes using the GRIB format (standard in weather forecast).

It can use two different output schemes:
- The MF I/O server
- A sequential I/O scheme
XIOS

- The XML Input/Output Server (XIOS) is an asynchronous MPI parallel I/O server developed by IPSL
- It writes using the netCDF format
- Written data is CMIP-compliant (CMORized)
- It is able to post-process data online to generate diagnostics
3. IFS-XIOS integration
Scheme of the IFS-XIOS integration

IFS process 0
IFS process 1
IFS process N-1

Library calls

XIOS client 0
XIOS client 1
XIOS client N-1

Asynchronous MPI

XIOS server 0
XIOS server M-1

‘M’ XIOS processes (XIOS scope)

System calls

output.nc

System file (scripts & output files)

iodef.xml

Post-processing on client side. E.g. horizontal interpolations
Post-processing on server side. E.g. netCDF compression

model

run_parallel

... cp $foo_path/iodef.xml .
mkdir xios_output
Ifs setstripe -c 4 xios_output ...

... aprun -n 'N' ifsMASTER :
   -n 'M' xios_server.exe
   ....

<file_definition>
  <file name="xios_output/3D" output_freq="3h">
    <field field_ref="t" operation="instant" />
  </file>
</file_definition>
Development steps

• XIOS setup
  • Initialization
  • Finalization
  • Context: calendar and geometry (axis, domain and grid)
  • \textit{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

• FullPos integration to support vertical post-processing: grid-point fields only
Development steps

• XIOS setup
  • Initialization
  • Finalization
  • Context: calendar and geometry (axis, domain and grid)
  • *lddef.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

• **FullPos integration** to support vertical post-processing: grid-point fields only
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)
NPROMA blocks gather

• The IFS data arrays do not match with the XIOS ones:
  • IFS_data_array(NPROMA, NFLEVG, NFIELDSD, 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
FullPos integration

• FullPos is a post-processing package currently used by IFS
• The use of FullPos is necessary to perform vertical interpolations not supported by XIOS
• It is called as usual, and afterwards, data is sent to XIOS
• For now, it is only possible to output grid-point fields
4. Performance analysis and optimization
Execution overview

• Two different experiments according to if we use FullPos or not:
  • *Pre-FullPos*: it outputs both grid-point and spectral fields. NetCDF files size: 3.2 TB
  • *Post-FullPos*: it outputs only grid-point fields. NetCDF files size: 2.5 TB

• For both experiments:
  • Octahedral reduced Gaussian grid. Horizontal resolution: T1279 (16 km)
  • 702 MPI processes, each with 6 OpenMP threads
  • 10 days of forecast with a time step of 600 seconds

• Three optimizations applied:
  • Parallelization using OpenMP threads (both exp.) [XIOS v2]
  • Optimized compilation of XIOS with -O3 (both exp.) [XIOS v3]
  • Computation and communication overlap (only *Pre-FullPos*)
Execution overview

• Execution times of this presentation correspond to *Post-FullPos*, except the third optimization

• Execution times:
  • Sequential output: 9391 seconds
  • MF I/O server: 7453 seconds
  • IFS-XIOS integration: 7682 seconds [XIOS v1]
  • IFS with FullPos but no I/O: 7443 seconds
Threading with OpenMP

• We used OpenMP to parallelize the NPROMA blocks gather
• Although it does not have a big impact, it avoids the rest of threads to be idle while the master is working
• The execution time is reduced 80 seconds, from 7682 seconds to 7602 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:

```plaintext
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%
```
Optimized compilation of XIOS

- Someone previously reported a bug 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

<table>
<thead>
<tr>
<th>report</th>
<th>Performance report</th>
<th>Whole time from XIOS init and finalize</th>
<th>7562.36 s</th>
</tr>
</thead>
<tbody>
<tr>
<td>report</td>
<td>Performance report</td>
<td>total time spent for XIOS</td>
<td>40.3018 s</td>
</tr>
<tr>
<td>report</td>
<td>Performance report</td>
<td>time spent for waiting free buffer</td>
<td>0.463693 s</td>
</tr>
<tr>
<td>report</td>
<td>Performance report</td>
<td>Ratio</td>
<td>0.00613159 %</td>
</tr>
</tbody>
</table>

Server

<table>
<thead>
<tr>
<th>report</th>
<th>Performance report</th>
<th>Time spent for XIOS</th>
<th>7562.37</th>
</tr>
</thead>
<tbody>
<tr>
<td>report</td>
<td>Performance report</td>
<td>Time spent in processing events</td>
<td>1382.16</td>
</tr>
<tr>
<td>report</td>
<td>Performance report</td>
<td>Ratio</td>
<td>18.2768 %</td>
</tr>
</tbody>
</table>

- The execution time is reduced 103 seconds, from 7602 seconds to 7499 seconds
Overlapping computation and communication

- The trace shows that after an output time step, there is a delay in the communications of the next two time steps (**MPI_Waitany** and **MPI_Alltoallv**)

- There is a conflict between intra IFS communications and IFS to XIOS communications
Overlapping computation and communication

Approach of the current output scheme:

• 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

IFS time steps

<table>
<thead>
<tr>
<th>0</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>n</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_0G_0S_0$</td>
<td>$C_1G_1S_1$</td>
<td>$C_2G_2S_2$</td>
<td>$C_3G_3S_3$</td>
<td>$C_nG_nS_n$</td>
</tr>
</tbody>
</table>

$C_x$ - Update calendar
$G_x$ - Gather
$S_x$ - Send
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:

IFS time steps

<table>
<thead>
<tr>
<th>0</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>n</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_0$</td>
<td>$G_0$</td>
<td>$S_0C_1$</td>
<td>$G_1$</td>
<td>$S_1C_2$</td>
</tr>
</tbody>
</table>

- $C_x$ - Update calendar
- $G_x$ - Gather
- $S_x$ - Send
Overlapping computation and communication

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

- The execution time is reduced 122 seconds \textit{(Pre-FullPos)}.
5. Evaluation
Optimal number of XIOS servers
Comparison test

Average execution time

Execution time (seconds)

Output scheme

Seq. output
MF I/O server
XIOS v3
IFS-FullPos no I/O
Comparison test adding GRIB to netCDF post-processing

Average execution time

Execution time (seconds)

Output scheme

Seq. output
MF I/O server
XIOS v3
6. Conclusions
Conclusions

• We have presented an easy-to-use development
• The integration with no optimization already improved the execution time:
  • Sequential output 9391 seconds (20.7% of overhead) → IFS-XIOS integration 7682 seconds (3.1% of overhead)
• Using OpenMP to parallelize the NPROMA blocks gather, the execution time is reduced by 80 seconds
  • It is really important to make an scalable gather, because it could become a bottleneck for future higher grid resolutions
Conclusions

• Using an optimized compilation of XIOS, the execution time is reduced by 103 seconds
  • This optimization proves that it is important to compile external libraries using the best optimization flags

• Using a better overlapping between IFS computation and XIOS communication, the execution time is reduced by 122 seconds (*Pre-FullPos* experiment)
  • It is sometimes necessary to analyse in which places computation and communication can be effectively overlapped
Conclusions

• Performance highlights of the most optimized version:
  • It only has a 0.7% of overhead
  • Within 56 seconds IFS outputs 2.5 TB of data

• When post-processing to convert GRIB to netCDF files is taken into account:
  • The post-processing takes 9.2 hours (sequentially performed, as in EC-Earth)
  • Thus, the most optimized version is a 5.7x faster than the sequential output and a 5.4x 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
Conclusions

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  • Increase the performance and efficiency of the whole model
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  • Save thousands of computing hours
  • Save storage space, because it will only store processed data ready to be used

Save money!
Ongoing and future work

• Use FullPos to transform fields from spectral space to grid-point space, post-process and send them to XIOS
• 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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