Implementation of XIOS in the Atmospheric Component of the Unifed Model

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Abstract

Weather and climate science make heavy use of ensembles of model simulations to provide estimation of uncertainty arising from a range of causes (e.g. [1]). Current practice is to write each ensemble member (simulation) out to disk as it is running, and carry out an ensemble analysis at the end of the simulation. Such analysis will include simple statistics, as well as detailed analysis of some ensemble members. However, as model resolutions increase (with more data per simulation), and ensemble sizes increase (more instances), the storage and analysis of this data is becoming prohibitively expensive — many major weather and climate sites are looking at managing in excess of an exabyte of data within the next few years. This become problematic for an environment where we anticipate running such ensembles on exascale machines which may not themselves include local storage of sufficient size where data can be resident for long periods of analysis.

There are only two possible strategies to cope with this data deluge - data compression (including "thinning", that is the removal of data from the output) and in-flight analysis. We discuss here some first steps with the latter approach. We exploit the XML IO server (XIOS, [2]) to manage the output from simulations and to carry out some initial analysis en-route to storage.

We have achieved three specific ambitions: (1) We have adapted a current branch of the Met Office Unified Model to replace much of the diagnostic system with the XIOS. (2) We have exploited a single executable MPI environment to run multiple UM instances with output sent to XIOS, and (3) We have demonstrated that simple ensemble statistics can be calculated in-flight, including both summary statistics of individual ensemble members, and cross-member statistics such as means and extremes.

With this ability, we can in principle avoid having all data needing to reside on fast disk when the ensemble simulation is complete. This would allow, for example, deployment on an exascale machine with burst-buffer migrating data directly to tape (or to the wide area network).

Keywords: ensemble

1. Introduction

As increasing computer power has become available, the weather and climate community have put effort into increasing the spatial resolution within the simulation domain, increasing the domain of simulation (spatial and/or temporal), expanded use of, or complexity of, data assimilation to improve initial conditions, and increasing the number of simulations within "ensembles". Such ensembles are collections of simulations which address the same problem, but where some key aspect of each simulation differs from the others.

Ensembles typically vary along one or more of four axes: initialisation, boundary conditions, physical parameters, and modelling system (aka "Model"). Initialisation ensembles are the mainstay of numerical weather prediction - choosing the right set of initialisations is a science in and of itself [3]. Ensembles along the other dimensions are more normally used in climate science (e.g. the coupled model intercomparison projects such as CMIP6, [4]), but are also increasingly used at shorter timescales for weather related problems. In all cases, the ensembles are used to sample uncertainty - see [1] for an example from climate science, and [5] for a more philosophical discus-sion of how ensembles are used to sample uncertainty.

Whatever the use, the workflows associated with ensembles are becoming problematic: when ensemble simulations are run in parallel on the same platform they can swamp the available bandwidth to, and volume available at, local storage systems. When they are run sequentially, the volume issues remain, and workflow and queuing delays become new hurdles to surmount. Whether simulations are run sequentially or in parallel the current mode of usage is to write out all the data from each simulation and post-process to produce "ensemble statistics", and at many sites this can be difficult, especially for large, long, and high-resolution ensembles. Managing the workflows has become an exercise in logistics [6]. These ensembles are also a major contributor to the vast archives of data held at major weather and climate sites, and together with the cost of adequate disk, the cost of even tape archive is becoming problematic. All these problems are expected to increase in the next few years, not only is there increasing scientific focus on large ensembles (e.g. [7]), problems with getting models ready for exascale [8] will probably mean the first usage of exascale machines in weather and climate will be for large ensembles.

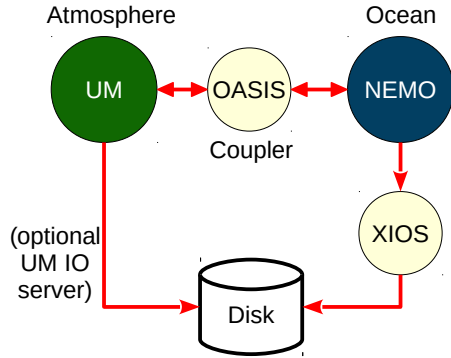There are only two possible strategies to cope with this data

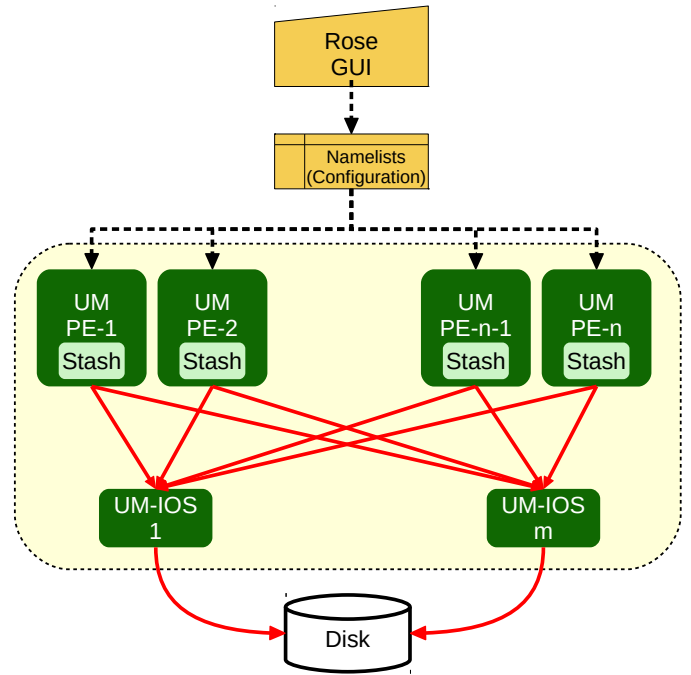Figure 1: Schematic of the existing UK climate mode.

Figure 2: The Unified Model Configuration and output data flow (for an atmosphere only instance): configuration files define the domain decomposition (the number of processing elements, PEs) and the outputs required. Output is written to "STASH" and then, in the IO server configurtion, written to multiple IO server instances, which each write to disk. One MPI context (shown in yellow) covers the entire activity. Control flow shown in black, data flow in red.

deluge - data compression (including "thinning", that is the removal of data from the output) and in-flight analysis. In this paper we introduce some first steps with the latter approach. In particular, we demonstrate the use of a single executable climate ensemble system developed so that each member simulation shares access to an extra component - an IO server - which carries out data reductions before writing data to disk.

Section 2 discusses the climate model environment and introduces the particular IO server that is being used. Section 3 introduces the software that was developed to support the ensemble system and section 5 reports on our experiences with the system. Section **??** discusses related work, and in section 6 we summarise our achievements and signpost some of our plans for further work.

2. Context

Climate modelling in the UK is predominantly done using variants of the Unified Model, running standalone in "atmosphere only mode" [**?**], or in coupled mode [**?**]. The coupled variant is depicted in Figure 1: the UM atmosphere is coupled via the OASIS coupler [9] to a NEMO [10] ocean. NEMO uses the XIOS [2] to write to disk, and the UM atmosphere either writes directly to disk, or uses an internal UM IO server.

The XIOS already has support for user configurable data reductions, and has already been used to manage ensembles [11], so was a natural target for investigating ensemble support.

2.1. The Unified Model

Devloped jointly by the Met Office, its partner organizations, and the academic climate and weather research community, the UM is the model chiefly used to run numerical simulations in the UK academic and research-centre environments. Much of this work is undertaken on ARCHER, accounting for 2000 MAU annually. The model is run in a wide range of configurations varying from low-resolution, high-fidelity Earth System models (UKESM [12]), to very high-resolution climate (PRIMAVERA), to ultra high-resolution process studies (PARACON). The UM is an MPI-OMP code written in FORTRAN, with a small amount of C. The UM has very few software dependencies, principally the communications library (GCOM),

which is simply a wrapper for MPL, and, depending on precisely how the model is configured, possible dependencies on NetCDF and HDF5. The UM is managed through a workflow system, which combines a model configuration system Rose [13] and workflow scheduling engine Cylc [14].

2.1.1. Climate Configuration

While the UM can be configured with time varying sea-surface acillary fields to mimic fully interactive atmosphere-ocean coupling, it is more commonly the case that a fully coupled configuration is employed. Figure 1 outlines the components of the coupled model - the UM (atmosphere) and NEMO (ocean) run asynchronously with a defined coupling frequency. Fields are exchanged between the two componenets by meaans of the OASIS coupler, which performs the required conservative regridding between UM (lat-long) and NEMO (tri-polar) grids. The UM currently manages its output through its proprietary IO server scheme and NEMO uses XIOS to output diagnostics (prognostics are handled differently.)

2.1.2. Current UM IO scheme

The UM diagnostics system, commonly referred to as STASH, has been developed over 25 years into a highly configurable and versatile scheme for extracting and filtering UM fields. Recent advances have seen the successful development of CF-NetCDF capability circumventing the writing data in UM format. Diagnostics are made available for selection through the Rose GUI, where in addition, they can be configured for
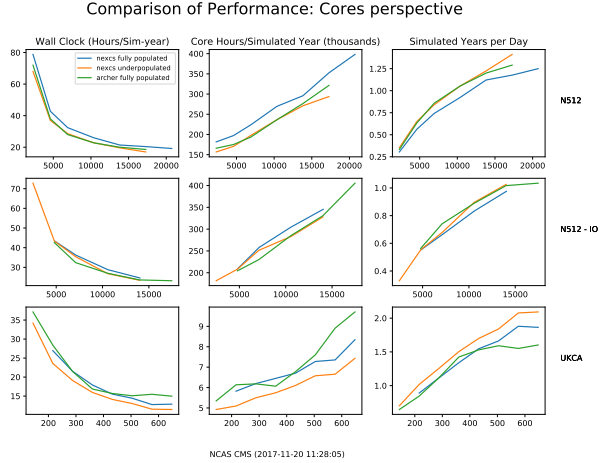
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Figure 3: UM atmosphere strong scaling for a high resolution (N512) model with and without IO, and for a low resolution (N96) model with atmospheric chemistry included. All plots display wall clock time against number of cores.

temporal and spatial processing. Rose generates FORTAN namelists from user choices - the workflow is sketched in Figure 2 - which are read at runtime to control model execution. The UM IO scheme is a client-server model; diagnostics are processed and buffered on the compute PEs then moved to the servers (UM-IOS in Figure 2) to be written to disc. The number and placement of server processes is configurable.

2.1.3. Resolution and Performance

Climate models typically run at low or high resolution. Low resolution is designated as N96 with 96x2 zonal grid points for resolution of 135km at the equator; high resolution is designated N512, which translates to 25km on the equator. We are currently running N1280 (5km) and developing N2560 (2.5km).

Figure 3 shows the results of some scaling runs for a high-resolution (N512) atmosphere-only climate model, which is essentially the model used throughout this work, on ARCHER and NEXCS (part of the MO Cray XC40), with and without IO. IO was managed through the UM IO servers (see Figure 2), which implement achynchronous IO to write data in the proprietary UM data format. The figure also shows scaling behaviour for a low-resoulsion model which includes an expensive atmospheric chemistry scheme. All runs were performed with two OMP threads (required for the UM IO server). The N512 model scales reasonably well out to 15000 cores both and without IO - changes to the IO profile can have significant impact on performance through increased stalling resulting from inappropriate buffering and/or simply overmatcing the machine IO bandwidth (recall that ARCHER is a very heavily loaded machine).)

2.2. XIOS

XIOS (XML IO Server) is a software system devloped at IPSL (Institute Pierre Simon Laplace) through IS-ENES (Infrastructure for the European Network of Earth System Modelling) [15], CONVERGENCE, ICOMEX, and ESiWACE [16]. XIOS is organized around a heirarchical description of its data through an external XML file providing a simple interface for the user. XIOS provides dedicated servers for asynchronous output to overlap with computation, parallel I/O for single file output and posssible performance improvement and simplified down stream data workflow, in addition to multiple file (one per IO server) output. XIOS also offers the prospect of *in situ* data analysis (our use of the phrase *in flight* is based on this potential).

XIOS is 90,000 lines of C++; it is open source software (under CeCiLL licence) and avaailable at http://forge.ipsl.jussieu.fr/ioserver. The XIOS build system is based on FCM [17] with support for Intel and Cray compilers. We have built and run XIOS with Intel and Cray compliers. Our use of XIOS is based primarily on revision 1404.

XIOS is based on a client-server arctitecture, whereby each compute processor interacts with an XIOS client to expose agreed data fields through a mininmalist interface. The set of fields to be exposed is defined by entries in the XML file. A simple FORTRAN call is all that the model needs to do to offload data to XIOS, thus:

```
call xios_send_field("field_id", field)
```

where "field_id" is a reference to the XML descripion of the field which includes grid and domain information, and `field` is the address of the field data.

XIOS supports multiple data filters and transformations including, importantly for this work, reductions over an axis.

2.2.1. XML

The contents of the XML file are distinguished by `context`, which may represent a model or a component of a model. In the following XML snippet, we have defined the `atmosphere` context with associated XML elements referencing axis (typically the vertical or pressure axis in a climate model), domain (the horizontal structure), grid (combinations of domains and axes), field (specifying a set of `field_ids` and their associated grids (a given `field_id` can be output on multiple grids)), and file (specifying output frequency, filename, other purely file-related criteria.) The XML file will typically comprise of several contexts, each associated with a logically appropriate model or component.

```
<simulation>
  <context id="atmospere" >
    <axis_definition    src="./axis_def.xml"   />
    <domain_definition  src="./domain_def.xml"/>
    <grid_definition    src="./grid_def.xml"   />
    <field_definition   src="./field_def.xml" />
    <file_definition    src="./file_def.xml"   />
  </context>
  <context id="other" >
  ....
  </context>
</simulation>
```
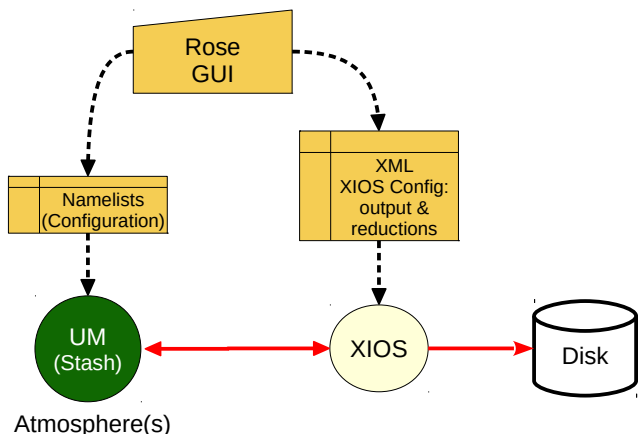
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Figure 4: Maintaining the look and feel of UM diagnostics: the Rose GUI is used to configure both the UM atmosphere via namelists, and the XIOS output. The UM reads the XML files and integrates them with the STASH system and sends the fields to the XIOS server.

Judging from our experience with NEMO, the XML file is a very slowly changing object, ie model output is defined once and hardly changes over time. Use of XIOS in the UM research environment will require a much more quickly evolving XML configuration, and the abilty to easily modify it through methods incorporated into the well established UM model configuration infrastructure - this is a must to enure its acceptance by the UM community.

3. Software Structure

There were four distinct software activities required to develop our ensemble system based on XIOS:

1. The XIOS system had to be inserted alongside the existing diagnostic system (we did not in these experiments completely replace the existing diagnostic system)
2. We had to work out how to get XIOS to deliver ensemble statstics,
3. We had work out how to get XIOS to control the ensemble,
4. We had to develop methods of configuring the model ensemble system to request the required diagnostics.

3.1. XIOS in the UM

Given the maturity of the Rose system and its familarity in the UM user community, it was essential that we did not develop a new diagnostic interface. Our goal was to maintian the look and feel of the current system to enable easy user uptake of the new XIOS functionality. Figure 4 shows the steps to achieve our objective. The diagnostic choices must be translated into an XML format to be read by XIOS and the UM itself must be modified to hand off data to XIOS.

3.1.1. STASH to XML utility

UM diagnostics are selected and configured through a Rose interface. The user selects a diagnostic and associates it with three "profiles", namely, time, domain, and usage. The time
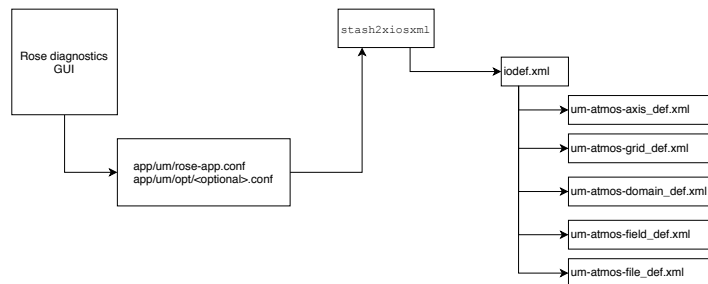

Figure 5: Work flow for creating XML files from STASH requests. The familiar Rose GUI isolates the user from details about XIOS XML. `stash2xiosxml` reads configuration files generated by Rose to create an XML description of the diagnostic output.

and domain profiles represent specifications for temporal and spatial processing for the selected diagnostic (time meaning or accumulation, spatial meaning or subspacing, for example); the usage profile, which, in combination with an output stream, determines the file structure for the diagnostic. We wished to maintain the familiar diagnostics interface for use with XIOS; this was achieved through the addition of XIOS output streams to complement regular UM output streams, and the developmemt of a utility to identify diagnostics destined for XIOS and translate their traditional STASH description into XML.

We have developed `stash2xiosxml` to make the translation. `stash2xiosxml` is a Python utility which loads Rose suite configuration files into a heirarchical data structure, extracts and collates information relevant for XIOS diagnostics, cross references with data held in the STASHMaster file to retrieve grid information, and writes the XML. Figure 5 is a schematic of the steps involved in XML creation; Rose creates possibly many configuration files which are inputs to `stash2xiosxml`; the XIOS standard XML file iodef.xml is output along with its subcomponents.

Of the 4017 possible diagnostcs availble to a standard atmosphere UM model, we can handle the 3672 which are avaialable on the main model time step. Diagnostics available on other time steps (the radiation time step for example, which is typically a large multiple of the model time step) need special handling and are not not covered in this work.

3.1.2. New code in the UM

Files added to the UM named with the prefix `um_xios` represent new code. The additional files are located in `/um/src/control/xios` and comprise approximately 3000 lines of code. Figure 6 indicates where the new code impacts the UM. The majority of work is done in the model initialisation stages with only minimal changes required to intercept and redirect diagnostics to XIOS. The global communicator is split by a native XIOS call in `um_xios_init_mpi` which returns the communicator for use by the model. The additional XIOS functionality is entirely independent from all other UM IO. Checkpoint files, logging files, and any diagnostics selected not to use XIOS, are handled through traditional UM means.
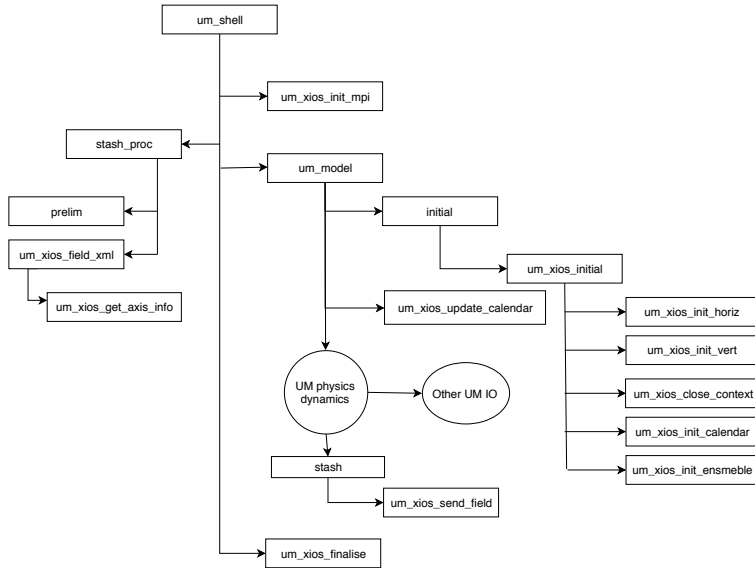
Figure 6: Areas in the UM where use of XIOS impacts the code. Diagnostics are intercepted in the routine stash. All other UM IO (logging, checkpointing, and diagnostics not directed to XIOS) is handled in the traditional manner.
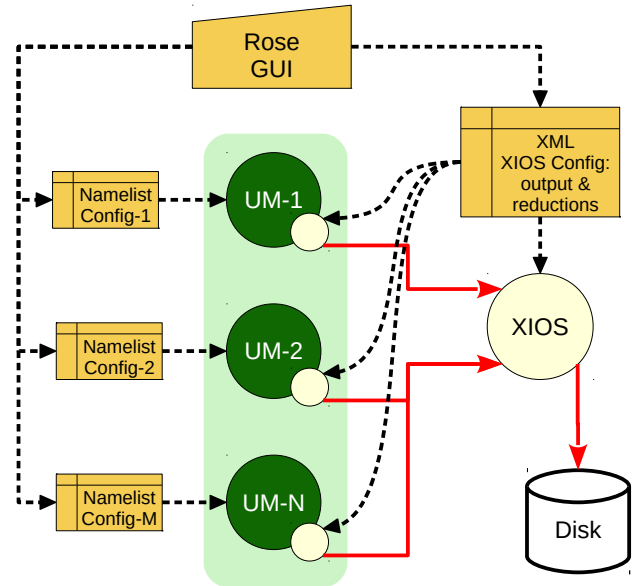

Figure 7: Key control and data flow concepts for XIOS control of a UM ensemble. The XIOS controls the output of each UM instance by exploiting XIOS clients within each process of each UM instance. Output from the clients goes through XIOS server instances to disk.
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3.1.3. Build system and job submission

Minor changes were made to the Rose GUI and UM build configuration files to accommodate the use of the XIOS library. Minor changes were made to the Rose GUI and the scripts which generate the job submission file to enable the launch of the UM and XIOS in MPMD mode.

4. XIOS UM ensemble

In order to take full advantage of the existing XIOS reduction capabilities, we introduced the idea of the *ensemble axis*. This simply attaches an extra dimension to the data generated by the ensemble to indicate to which ensemble member a particular field belongs. This greatly simplifies `context` management in XIOS, since now the entire ensemble is associated with a single `context` - XIOS simply sees an (n+1)-dimensional data set for the ensemble, where for a single model it saw an n-dimensional data set. Applying reductions over the ensemble axis provides the mechanism for generating ensemble statistics.

Figure 7 describes the key features of our XIOS UM ensemble configuration. From the XIOS viewpoint, the UM ensemble is simply a model - XIOS clients reside on each PE and send fields to XIOS servers. An individual ensemble member runs in its familiar environment - exactly as before.

Several XML files are augmented for the ensemble case; the additonal ensemble axis feeds through to ensemble XML grid, and file definitions. An ensemble grid would appear thus:

```
<grid_definition>
  <grid id="um-atmos_grid">
    <domain domain_ref="um-atmos_domain" />
    <axis axis_ref="um-atmos_vertical" />
    <axis axis_ref="ensemble" />
  </grid>
```

```
</grid_definition>
```

Attaching this grid to a field will result in its output of data for all ensemble members.

4.1. UM code for an ensemble

For the ensemble case, the model communicator provided by `um_xios_init_mpi` (see section 3.1.2) is split again for each ensemble member. Individual ensemble member models run on their own model communicators, and as previously for the single model case, non-XIOS IO (read and write input, logging files, check points...) are handled in their own separate ensemble-member spaces.

Other than additions to `whatroutine` to ensure that each memeber executable runs in a specific directory (a requirement imposed by the Rose infrastructure) and minor additions to accommodate setting up the ensemble axis, the code described in Figure 6 suffices for the ensemble case.

4.2. Rose ensemble configuration

As set up through Rose, a UM simulation is defined as a collection of configuration files (in INI format). On job submission, (i) Rose creates namelists from the configuration files; (ii) creates a work space on the HPC; (iii) copies the namelists (and other data) into the work space; (iv) sets up and submits a PBS script to run the parallel job. We have developed a Rose ensemble member set up task to perform items (i)-(iii), which, in conjunction with the use of Rose optional override configuration files to specify parameters for each ensemble member, creates the appropriate environment for each member to run in on the HPC. An oviride file typically contains one line to specify an initial condition or a parameter value.

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A separate task to run the ensemble then creates the appropriate MPMD aprun command for submission of multipe UM instances and XIOS.

4.3. Configuring ensemble output

XIOS currently supports max, min, and mean reductions. Our interest is primarily in the ensemble mean. It is a general feature of XIOS that data transformations are performed on the the basis of the target grid for the output field. In the example in section 4, the target grid spanned all ensemble members; a reduction over the ensemble axis is achieved by appopriately defining the grid on which to output the field. In the following, the ensemble-reduction grid `um-atmos_grid-reduce` includes instruction to reduce over the ensemble axis with operation `average`.

```
<grid id="um-atmos_grid-reduce">
   <domain domain_ref="um-atmos_domain" />
   <axis axis_ref="um-atmos_vertical" />
   <scalar id="3d-ensmean">
     <reduce_axis operation="average" />
   </scalar>
</grid>
```

Our Python utility `stash2xiosxml` (section 3.1.1) includes support for creating XML for ensemble reductions.

5. Results

Our underlying UM configuration is GA7.0 UM 10.7 AMIP [18] which we run at both low resolution (N96) and high resolution (N512). The model was configured to run for 9 model hours for ensemble runs, or 24 model hours for single mode runs, with data output hourly. We selected diagnostics from several UM physics and dynamics sections, to include 2-d and 3-d fields, output as instantaneous or time accumulations for total 50 fields, with the aim to mimic typical near-future climate integeration data volumes. Table 1 shows the number of PEs running the models. For N512, this represents a typical production-run resource usage; fewer PEs than is normal were used for N96.

5.1. Single UM

A key requirement for an IO (or more appropriately a diagnotics) server is that it is capable of managing its activity (data processing and writing to disc) asynchronously and without stalling or throttling the main computation (keeping 50,000 processors idle while data is written to disc is an expensive prospect). Our main single UM test focussed on confirming that XIOS is capable of handling large amounts of data without impacting model computation times. Our confguration creates 214GB of data, which translates to 77TB/model year, which exceeds our current N512 production output rate by a factor of 35. XIOS provides many opportunities for performamce optimisations which we have not explored, nevertheless, the results in Table 3 with 6 XIOS servers in multipe-file mode, clearly

Resolution	PEs
N96	96
N512	5184

Table 1: Single model core counts

indicate that XIOS is effectively hiding IO from computation. The 7% XIOS overhead is an acceptable penalty for the rate of data production seen here. Single file output can incur a larger IO overhead and requires more tuning for opimal preformance, which is out of scope here, and perhaps of less interest in the longer term with the increased interest in data sharding [**?**].

5.2. UM ensembles

We applied our developments to ensembles of N96 and N512 models. Results from our initial experiments are presented in Figure 8. Data points in blue are for XIOS multiple-file output, and in red for single-file output (note, as for the single model case, we have made no attempt to optimise the XIOS configuration). The ensembles are congfigured to write diagnostics for all members and the ensemble avarages for all fields. This configuration is **not** how we anticipate production runs to work but servers as a test case.

5.2.1. N96

The multiple-file ensemble performance is encouraging with relatively flat peformance over the range of ensemble sizes - perfect performance is represented by horizontal lines. The 100-member ensemble is generating 45TB/mode year.

5.2.2. N512

We initially ran the N512 model at two processor decompositions - in Figure 8, N512 runs labelled with a (1) used on 960 PEs/ensemble member, those labelled (2) ran with 5184 PEs/ensemble member. It is worth noting that these (and all) emsembles ran *out of the box* - to our knowledge XIOS had not been tested under these conditions - our 10-member ensemble requiring half of ARCHER to run on. The 10-member ensemble is generating 467TB/model year. Scaling for the N512 ensemble is less encouraging at first glance. It is clear that single-file output, based on MPI-IO has a significant impact on performance, and while multiple-file output performs better, its scaling is not ideal.

These initial tests conflate two issues; (i) internal XIOS scaling and; (ii) speed to write to disc. Figure 9 shows some preliminary results aimed at better understandng how internal XIOS operations scale with ensemble size. These runs write out only the ensemble averages, are configured for multiple-file output, and data is writtem to /tmp to eliminate the actual time to write to disc. The figure shows data for multiple runs (with significant jitter) and lines are best fits to the scattered data points. There is no clear candidate responsible for the gradual relative slowing - but nor is the lack of scaling as critical as might be assumed from results in Figure 8.

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Resolution	Ensemble Size	
	100	10
N96	9600	
N512		54000

Table 2: Maximum core counts for the largest ensembles

	no IO	XIOS	UM IO (single PE)
run time	3??	400	830
IO overhead		30	428

Table 3: Single model N512 IO performance. The integration ran for 24 model hours to create 214GB of diagnostic output (equivalent to 77TB/year.) All times in seconds and model initialisation time removed.
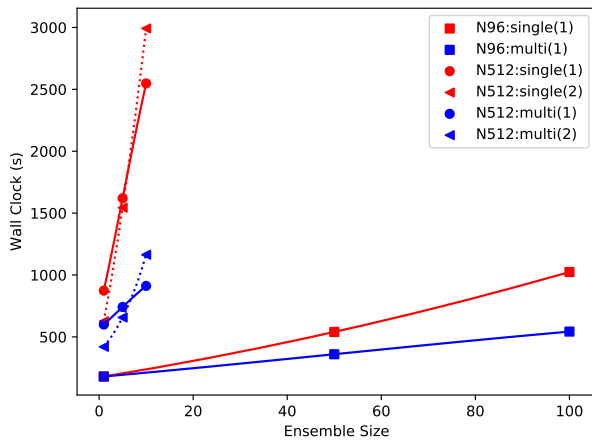

Figure 8: Scaling curves for ensemble writing using N96 and N512 ensembles for single file output and multiple file output. Each N96 emsemble member ran on 96 PEs. N512 runs labelled (1) used 960 PEs/ensemble member; those labelled (2) used 5184 PEs/ensemble member.
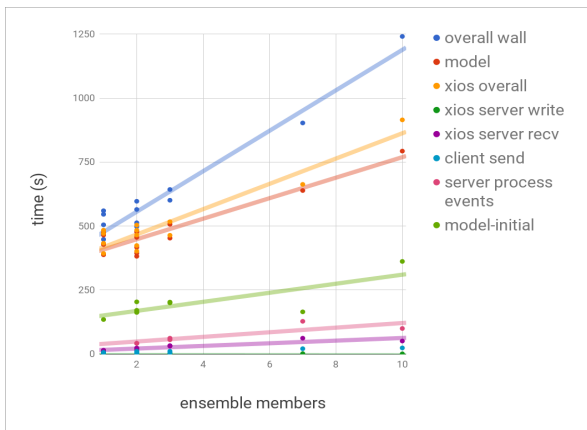

Figure 9: N512 ensemble with a multiple-file XIOS configuration with output to /tmp. Timings for several internal XIOS operations are reported, along with timings for a represetative ensemble member at each ensembe size (showing flat performace as expected). Multiple runs are reported for selected ensemble sizes showing moderate jitter.

6. Summary and Further Work

We have achieved three specific ambitions: (1) We have adapted a current branch of the Met Office Unified Model to replace much of the diagnostic system with the XIOS. (2) We have exploited a single executable MPI environment to run multiple UM instances with output sent to XIOS, and (3) We have demonstrated that simple ensemble statistics can be calculated in-flight, including both summary statistics of individual ensemble members, and cross-member statistics such as means and extremes.

In our current setup, failure of a single ensemble member will crash the entire ensemble; we have inherited UM checkpointing of course, so restarting the ensemble is possible, but ideally we should be able to manage such a failure more gracefully. We can imagine a scenario whereby we would trap ensmeble member errors and subsequently send *missing data* or otherwise signal the faiure to XIOS; a modified XIOS would handle the situation in a manner to be determined.

There is scope to greatly improve the range of ensemble processing capability within XIOS and indeed in the entire ensemble management activity.

We note that the Met Office have expressed an interest in assisting us to put our UM branch into a UM release in light of our successes and in view of their anticipated use of XIOS in LFric [19].

Acknowledgements

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