IS-ENES2 HighRes ESM performance resulting from OASIS updates

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Abstract

The efficiency of core OASIS3-MCT coupler functionalities (interpolation+communication) grows with a factor of ten compared to the former OASIS3 performances. Together with a better estimation of load balancing in our coupled systems, this work had a positive impact on coupling efficiency in our HR M4 simulations. Ideas on OASIS coupling future challenges are discussed to prepare our Earth System Models to Exascale supercomputing.

Executive Summary

The increasing parallelism of climate models, particularly for high resolution configurations as the ones used in this work-package, necessarily requires scalability for each of their components (Amdahl's law). The OASIS coupling library is one of them for three (EC-Earth3, HadGEM3 and ARPEGE5-NEMO) of the five coupled models used in this IS-ENES2 Work-package 9. The enhancements of the OASIS library during the project length are supposed to ensure a high scalability on the PRACE tier-0 class of machines and allow to perform efficiently high resolution multi-model multi-member simulations (HR M4).

The efficiency of core OASIS3-MCT coupler functionalities (interpolation+communication) grows with a factor of ten compared to the former OASIS3 performances. The various functionalities added in the version 3.0 do not downgrade the library performances. At the same time, better coupling techniques were generalized. The LUCIA tool is now distributed together with the OASIS reference version and helps to reduce load imbalance in our configurations. Load imbalance is reduced below 15% in any of our HR M4.

The parallel calculation of interpolation weights is now an urgent and necessary development that should be included in the OASIS official release. We believe that the simplicity, the non intrusiveness of the OASIS library, and the compatibility with an extended range of existing models will convince many new users to equip their models with an OASIS based interface. However, the coupling library must be enhanced to face the growing complexity of our coupled systems (Earth System Models) and to simplify its calculations to fit single precision platform requirements.

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1. Coupler/coupling performances

1.1 OASIS parallelism

The increasing parallelism of climate models, particularly for high resolution configurations as the ones used in this work-package, necessarily requires scalability for each of their components (Amdahl's law). The OASIS coupling library is one of them for three (EC-Earth3, HadGEM3 and ARPEGE5-NEMO) of the five coupled models used in this IS-ENES2 Work-package 9. Targeted platforms are PRACE and national supercomputers currently available. The enhancements of the OASIS library during the project length are supposed to keep a high scalability on this kind of machine. Performances on more advanced platforms (GPU, KNL, ARM ...) are out of the scope of this document.

1.2 Real coupling cost, load balancing

A coupling operation can be basically decomposed into two main operations: interpolation and communication. There is no particular reason to expect low parallelism for the first. All possible scalability losses come from the latter but, assuming that this operation (i) does not require all-to-all communications[1] and (ii) is performed at a relatively low frequency in comparison to other model tasks, it is important that this additional cost stays small.

However, a coupled configuration often implies that computations of individual components were performed concurrently, with an associated load imbalance. This load imbalances is known to be, most of the time, the major factor of performance losses and is usually chosen as a main indicator of "coupling cost" in climate models [1]. For that reason, this document will better focus on that aspect when a performance measure on real models will be presented.

1Only a global conservation operation (CONSERV) requires such MPI communications but is not necessarily included in a coupling configuration (local conservative interpolation can be chosen instead)

2. CMIP6 models performances

2.1 OASIS coupler theoretical performances

The legacy OASIS3 coupler, based on a separate executable centralizing coupling operations, was replaced, before the beginning of the IS-ENES2 project, by the OASIS3-MCT library, enabling the direct communication of coupling fields and the parallelisation of interpolations between processes of the models (also named *components* of the coupled system).

The WP9 High Resolution (HR) CGCMs already benefited from this major improvement, as reported in [2]. During the last four years, two new versions of OASIS3-MCT were made available and the last one (3.0) were recently tested in WP9 frameworks. Recent OASIS3-MCT developments aims to add functionalities rather than improve the overall performances of the tool. For example, the OASIS functionality making possible the coupling between components sharing the same processes (zooms, large model subroutines like atmosphere chemistry) is now available in the current version [3].

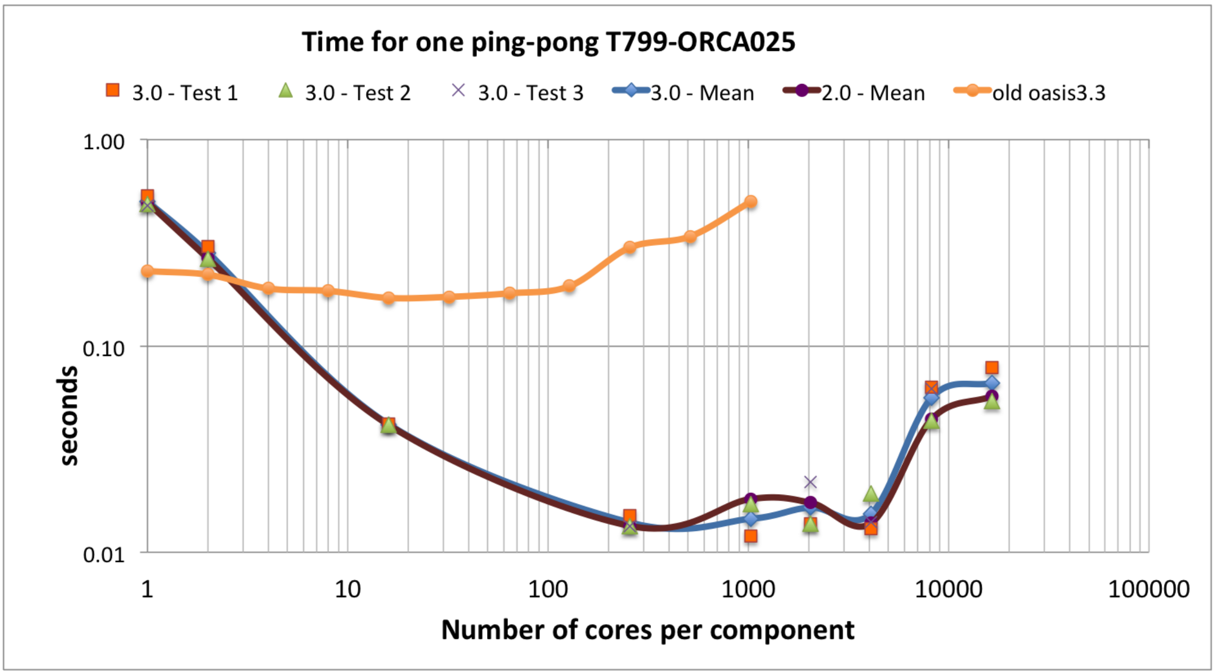


Figure 1: Performances of a "ping-pong" exchange between two toy models discretised on T799 (~25Km) Gaussian grid and ORCA025 (~25Km) lat-lon tripolar grid. Measurements made for several OASIS versions on CURIE (PRACE tier-0) thin nodes, for various decompositions from 1 to 20.000 horizontal domains. The interpolation used is the SCRIP nearest neighbours, Gaussian weighted (source: Sophie Valcke, CERFACS)

Figure 1 shows a comparison of performances between several OASIS versions, in a dedicated test called "ping-pong". In this test, a coupling field (here exchanged between grids at resolutions[2] comparable to those of the work-package coupled systems) is sent

2T799: 850,000 horizontal grids points and ORCA025 1,470,000 horizontal grid points by a varying parallel decomposition toy model, received by a second model of the same kind and immediately sent back to the first. The duration of a fixed number of exchanges (100), reproduced three times, is supposed to give a good approximation of OASIS performances, that are dependant of the toy model parallelisation.

Results shows a factor of ten between peak performance of OASIS3 (used before the beginning of the project, orange line) and the new 2.0 (violet line) and 3.0 (blue line) versions of OASIS3-MCT. The various functionalities added in the version 3.0 do not downgrade the library performances: the three tests performed with 3.0 version on the CURIE[3] supercomputer exhibit a restitution time close to the mean value of tests performed on the same machine with version 2.0.

The raw value of these performances shows a scaling until 100 cores, and stays under 0.1 s per exchange up to 10,000 cores. The work-package HR models currently requires no more than 1,000 cores, and for them, the time spent for one exchange is supposed to be rather equal to 0.02 s.

2.2 Coupler performances on real models

The necessary evaluation of computing performances during the IS-ENES2 WP9 leaded to discussions with aim to precisely assess what performances meant in this context, particularly regarding to coupling. These discussions were useful to contribute to [1]. This article proposes a standard set of metrics and describes the corresponding methods to simply obtain them. An international exercise (CPMIP) should soon take benefit of the large and common campaign of climate modelling (CMIP6) to fulfil the first database that gathers computing performances of a large diversity of models at worldwide scale. The five modelling groups involved in WP9 already updated their results. They are presented in a separate document [4].

Several results are meaningful in the present work. The “coupling cost” metric isolates from the whole simulation cost this part which is directly related to an imperfect load balancing between components of the coupled system. We detail on Table 1 the differences with the measurements performed at the beginning of the IS-ENES2 project. The unit represents the fraction of the total CPU wasted during the simulation, or said differently, the amount of time spent by every model processes to wait a coupled variable.

Models	First measurement (2014)	Final measurement (2016)
ARPEGE5-NEMO	13%	1%
EC-Earth3	24.7%	4%
HadGEM3-GC2	n/a	15%

Table 1: Load imbalance (% of the total CPU cost) of HR models

3CURIE platform: Chip: Sandy Bridge, Total core #: 80,640, Clock Speed: 2.7Ghz, Clock cycle concurrency: 8,URL: http://goo.gl/RR5kfc

The given numbers are rather synthetic. An analysis on more configurations are detailed in the next paragraph. It is already important to notice that a better knowledge of this potential loss of performances is observed in the community, even though tools to measure it and methods to reduce it are difficult to share.

A more direct measurement of OASIS performances (the cost of interpolations only) was done at the beginning of the project. After discussions, this metric was not directly included in the CPMIP metrics, due to its small impact on the total simulation cost. The interpolation cost, but also the communication time spent to exchange coupling fields, can become significant at higher resolution (range of NWP resolution models -10Km-) and larger decompositions (>5,000) as shown in Figure 1, but this is not the case for the models we are studying here. The WP9 HR models, despite the large size of exchanged variables, not necessarily exhibit the highest coupling costs amongst the models used in our community. Sequential coupling with exchange of 3D fields at each model time step can significantly increase the number of MPI messages required and have a measurable impact of the overall performances. But, as shown in global-regional coupling [5] or in the coupling between global 3D components with different resolutions [6], this cost remains negligible. In the first example (global-regional coupling), measurements show the crucial effect of the "bundle" option[4] provided by OASIS (with a reduction by a factor of three). In the second (global-global coupling), the huge reduction in time, that the OASIS based hybrid approach allows, is nothing compared to the small communication/interpolation extra cost.

2.3 Load balancing

The numbers shown in Table 1 seem to suggest that a better load balancing can be achieved in our coupled systems. This impression must be mitigated, taking into account that the growing complexity of our models significantly makes more complicated the coupling algorithm and leaves room for unavoidable sequentiality. In CMIP6 versions of EC-Earth or CNRM-CM, a small executable of runoff routing or interpolation is necessarily called at the end of the atmosphere calculations, and must be taken into account for an appropriate load balancing with the ocean component. In more advanced systems, like the Earth System Model currently developed at MetOffice (UKESM), more components have to be organized to avoid CPU losses but also deadlock in algorithms.

4Multiple fields can be interpolated in a single matrix multiplication and exchanged via a single communicator

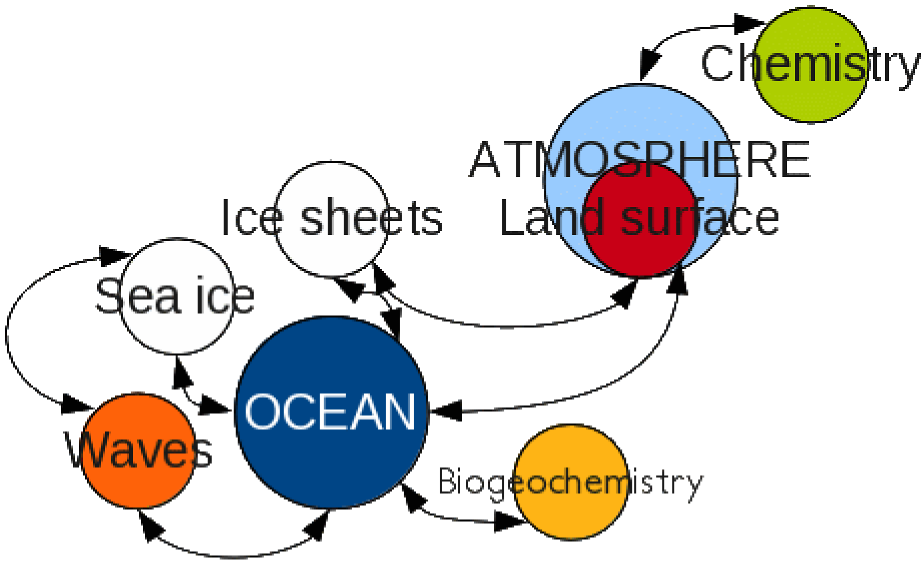
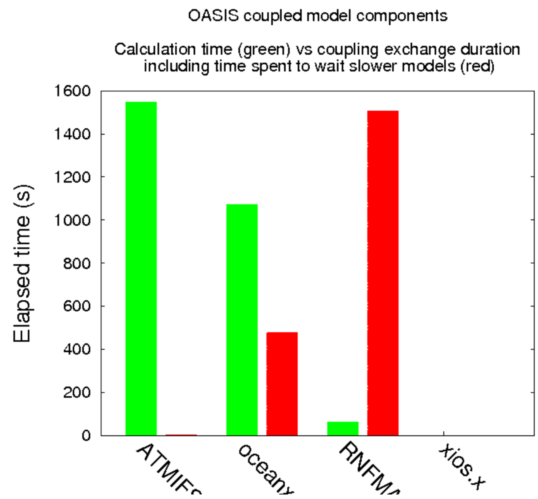


Figure 2: Complexity of near present ESMs (source: Richard Hill, Met Office)

The load balancing issue is now a well known issue in the community of Research Software Engineers, including in the Climate Modellers community. In the OASIS community, this problem is not solved by the coupling library itself. The OASIS library toolkit approach differs from framework solutions, such as CESM, which includes algorithms able to minimize load balancing [7]. Each OASIS user has to find the optimum number of resources allocated to each component such that, amongst other constraints, the load imbalance is minimized. A specific tool [8] was developed for this purpose (LUCIA). It is now distributed together with the OASIS reference version and helps to tune an increasing number of OASIS based configurations.

A recent improvement was made necessary to investigate a recurrent problem in one of the WP9 HR coupled system (EC-Earth). The two plots presented in Figure 3-a and 3-b are produced by the post-processing analysis tool LUCIA after a one month long simulation. It gives the comparative times spent by each component of the EC-Earth coupled system (IFS, NEMO and a small runoff model). Figure 3a (3b) is the result of a simulation using 128 computing cores of Mare Nostrum III for NEMO and 256 (512) cores for IFS.



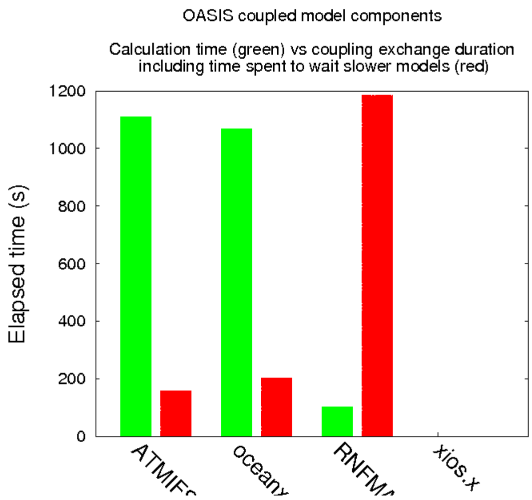


Figure 3-a & 3-b: Load balancing analysis of EC-Earth coupled system with different parallel decomposition of IFS (256 & 512) and the same decomposition of NEMO (128)

The 3-a figure presents a largely unbalanced setting. The time spent by IFS doing calculations (first green column) is about 450 s larger than the time spent by NEMO doing theirs. The fastest model (NEMO) logically spends 450 s waiting (second red column). In comparison, the time spent by IFS to wait its coupling fields is negligible (first red column).

On the second experiment presented in the 3-b, the number of IFS allocated resources is multiplied by two. Consequently, the IFS calculation time is reduced to 1100 s. This number is now practically equal to the time spent by NEMO doing its calculations and the coupled system should be balanced. However, the two models are both waiting during about 200 s.

This large difference can be explained by the unusual coupling frequency of atmosphere-ocean exchanges (each model time step = 900 s) and the IFS time stepping profile: the expensive calculation of the radiative scheme is called every four time steps. A finer analysis conducted by BSC with PARAVER [9] reveals that, using the 512-128 decomposition, NEMO and IFS calculations on one time step alternatively exhibit the larger or the smaller duration.

The LUCIA tool was modified to produce the same plot than Figure 3, but for the 40 first coupling time steps. On Figure 4-a (up) and 4-b (down), we present the results respectively for the same 256-128 and 512-128 decomposition than plotted in Figure 3. Three horizontal stripes represent computing (green) and waiting time (red) along 20 coupling time steps of the simulation (x axis), for IFS (upper), NEMO (middle) and runoff (lower). In 4-a, red segments (waiting time) are only visible for NEMO. It means that, at each coupling time step, NEMO is faster than IFS. In 4-b, the waiting time appears alternatively on IFS or NEMO stripes. It means that, NEMO and IFS are alternatively waiting each other.

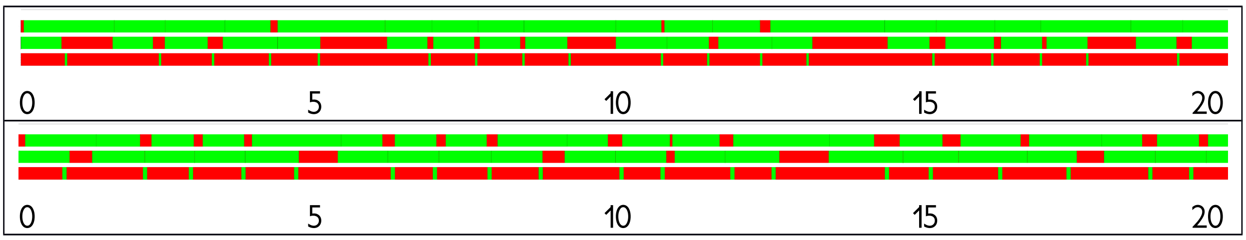


Figure 4-a & 4-b: same than Figure 3, but along the time axis (x)
for the 20 first coupling time steps

There is at the moment no solution to this issue, assuming that radiation scheme cannot be immediately separated from the original IFS code and computed in parallel of the other calculations. However, our tool analysis is now able to evaluate the minimal load imbalance that can be found for this configuration.

3. Bound to "Exascale" ?

The IS-ENES2 WP9 contributed to a test bed for the latest OASIS improvements. The involved laboratories reported their problems, worked together to better understand what computing performance means from a coupling perspective and proposed solutions to their actual issues. At the same time, the WP activities contributed to give a better view on the future of coupling technologies, thanks to common activities, dedicated support and participations to workshops [10,11,12].

3.1 Model resolution

The leading question of the last few years concerning coupling was in link with the increase in parallelism of the coupled system components. It has a strong impact on OASIS evolution (from OASIS3 separate and sequential executable to the parallel OASIS3-MCT library), but also on the design of new coupling libraries (e. g. YAC [13]) and/or IO toolkits (e. g. XIOS [14]). Requirement for more parallelism was guided from the evolution of HPC market, which progressively switched from vector machines, dedicated to supercomputer market, to scalar ones, based on general market processors. The constantly evolving landscape in HPC market will have a new impact on climate model design, and consequently, on coupling technologies. The end of Moore's law [15] and the path for the convergence of CPU based machines and Deep Learning prone structures (e. g. Intel Knights Mill/ARM) will limit the growth of easily available computing power. In addition, recent developments in numerics (e.g. [16]) pave the way for different gain in effective resolution. Combined with technical limits in scalability (unavoidable communications, increases in halo size), numerics (time step decreases when horizontal resolution increases) and physics/dynamics (e.g. (i) limit at about 10km for hydrostatic approximation, that comes with extra calculations, (ii) increase in vertical resolution, harder to decompose in independent MPI or OpenMP processes and (iii) computational load imbalance due to heterogeneity of local processes occurring independently at high resolution), the evolution of climate modelling not necessarily leads to much more parallelism and larger significant increases in model resolution, at least not at global scales. On the other hand, the present trend, which consists in adding more components in an existing coupled system, can be considered to be continued in the next years, towards a possible convergence between NWP and climate models. This could mean that couplers like OASIS would be used by broader communities, in more complex systems. Technically speaking, intra-node communications between components (based on a share memory library, e. g. OpenMP) could be preferred to inter-communications. In that case, a community coupler should include this communication technique in addition to the one available in the MPI-based MCT library.

3.2 Coupling requirements

Unless this will probably have a major influence only for a few configurations, scalability will remain mandatory for coupling in the ten years to come. Will the currently available scalability in OASIS be sufficient ? Even in a context of reasonable growth in resolution, the parallel calculation of interpolation weights is now an urgent and necessary

development that should be included in the OASIS official release. We do not believe that a dynamic definition of these weights during the simulation will be mandatory soon, and we know that a calculation in a pre-processing phase, with existing tools such as ESMF, is a satisfactory solution for most of our users. But a renewal of the legacy SCRIP interpolation library would be appreciated and an integrated solution would probably find users rapidly. We are convinced that, anticipating a new growth in Many Integrated Core (MIC) processors (KNL), a simple OpenMP solution would fit the requirements of most of the OASIS-based configurations. The interpolation package is quite isolated from the main code and we believe that there is room for a separated update. If the SCRIP library could be replaced, the new interpolations could addressed a widely debated but still pending question: what a "conservative" interpolation (local or global) means in a context of mask mismatch between grids ? Could this operation be performed efficiently (i.e. avoiding all-to-one/one-to-all MPI communications) ? On the same topic of interpolation enhancements, OASIS would provide a simple test bed for the most recent updates in the field of coupling physics, e.g. as described in [17].

Due to the domination of Intel platforms and its associated compiler, the last decade offered a pause in the porting activities. It is quite obvious that emerging architectures will come with diverse compilers, with a risk of incompatibility with our most widely used programming languages such as FORTRAN. The full compatibility of Intel MIC systems (Intel Xeon Phi) is ensured, with interesting potential of improvements for scalability (OpenMP) and vectorisation, but processors like ARM, better suited for Deep Learning software and shoo-in for Exascale computing, would be much more difficult to handle. However, it is not fully excluded that experimental and computation demanding configurations would be developed on such platforms. As a first step, the coupling of existing breakthrough developments [18] on GPU platforms (generally associated to traditional CPU in the same supercomputer) would be an interesting approach to become more familiar with this unavoidable kind of architecture.

The OASIS coupling library must give support to a growing number of laboratories in the path towards increased complexity in coupled systems. Such Earth System Models, both global and regional (possibly requiring 3D coupling for biogeochemistry, atmospheric chemistry, etc) are currently in development or even already in use in our community [6,19], and beyond [20]. In addition, the need to increase task parallelism leads to split existing codes between separated executables for better parallel performances [21]. We believe that the simplicity, the non intrusiveness of the OASIS library, and the compatibility with an extended range of existing models such as ocean wave [22], NWP atmosphere [23], coastal ocean [24], atmospheric chemistry [25], ESMs [26], finite element ocean [27] or land surface models [28] will convince number of new users to equip their models with an OASIS based interface. However, the coupling library must be enhanced to face this growing complexity. It is already obvious that the OASIS parameter file ("namcouple") loses its readability when coupling field number exceeds the range number of 10/20. To cope with this difficulty, scripts were already developed to automatically create this parameter file, anticipating what could be a meta-parameter file, that would be useful to distribute with the OASIS official release. Another issue rises with the inclusion of a coupled system in larger frameworks, such as assimilation codes [29]. In these configurations, the use of coupled components can be transitory along the execution, requiring from the coupled communication system to be switched off when not used. The use of a local communicator by OASIS[5] can also be required.

Another large scale evolution of modelling already observed in our community is the trend towards computing simplification. Following hardware requirements (notably on ARM-based light consumption architectures), double precision calculations are systematically avoided when not needed, and even when this simplification involve (slight) biases on results [30]. Is the same idea interesting for performance in coupling ? Even though their contribution to the total model cost is small, our interpolations would benefit of such simplification. Could reduced communications, the first contribution to the OASIS cost for highly parallel configurations, be assessed in future version of our library ? Coupling is located at such a key position in our systems that OASIS library can be chosen as solution to the emerging issue of asynchronism.

To conclude, at the confluence of simplification of computations and increase of coupled system concurrency, emerging configurations propose an increase of resolution, but only in limited areas. This solution strongly reduces the computing cost needed in high resolution configurations, and offers studies of the same spatial scales on the area of interest [31]. In GCMs, traditional approaches promote grid stretching, e.g. [32], or refinement e.g. [33]. Unfortunately, both solution have important limitations. A third idea, the coupling between a GCM and a regional model [34], proposes solutions to time step gap and parametrisation heterogeneity between grids. This solution also presents implementation difficulties, particularly if vertical resolution between regional and global model differs. This strongly suggests that OASIS improvements in surface pressure and orography coupling field interpolation, jointly with vertical interpolation implementation, should be carried to facilitate the set up of this range of configurations e.g. [35].

5Instead of MPI_COMM_WORLD, that can be required by the assimilation workflow

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