EUROPEAN COMMISSION

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INFRASTRUCTURE FOR THE EUROPEAN NETWORK FOR EARTH SYSTEM MODELLING

IS-ENES2 DELIVERABLE (D -N°: 10.2)

Interim report on status of benchmark suite

File name: {IS-ENES2_D10.2.pdf}

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Reporting period: **01/10/2014 – 31/03/2016**

Release date for review: **27/01/2016**

Final date of issue: **14/03/2016**

Revision table			
Version	**Date**	**Name**	**Comments**
1	27/01/16	Irina Fast	First release for internal review
2	02/02/16	Eric Maisonnave	Internal review
3	14/03/16	Irina Fast	Final version with reviewer's comments integrated

Abstract

This deliverable describes the current development status of the ENES Benchmark Suite, a collection of real application benchmarks used to model Earth System. The suite is assembled from applications of varying complexity ranging from simple computational and communication kernels to fully coupled Earth System Models (ESMs). Here, we focus on the description of already available benchmarks: CMCC-CESM-NEMO, EC-EARTH, IPSLCM, and MPI ESM1. The Redmine project management tool is employed to ensure the availability of up-to-date benchmarks and performance data.

Project co-funded by the European Commission's Seventh Framework Programme (FP7; 2007-2013) under the grant agreement n°312979		
Dissemination Level		
PU	Public	X
PP	Restricted to other programme participants including the Commission Services	
RE	Restricted to a group specified by the partners of the **IS-ENES2** project	
CO	Confidential, only for partners of the **IS-ENES2** project	

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Glossary

CDO	Climate Data Operators
CESM	Community Earth System Model
CHSY	Core Hours per Simulated Year
CM	Climate Model
CMCC	Centro Euro-Mediterraneo sui Cambiamenti Climatici (Euro-Mediterranean Center on Climate Change)
CMIP5/6	Coupled Model Intercomparison Project Phase 5/6
COSMO	Consortium for Small-scale Modelling
COSMO-CLM	COSMO Climate Limited-area Model
CPMIP	Computational Performance Model Intercomparison Project
DKRZ	Deutsches Klimarechenzentrum (German Climate Computing Center)
ENES	European Network for Earth System modelling
ESM	Earth System Model
FCA	Fabric Collective Accelerator
Flop	Floating point operation
FTP	File Transfer Protocol
GB	Gigabyte (10^9 bytes)
GFlop	10^9 Flop
HPC	High Performance Computer / Computing
ICON	Icosahedral Non-hydrostatic general circulation model
I/O	Input / Output
IPCC AR5	Intergovernmental Panel on Climate Change Fifth Assessment Report
IPSL	Institut Pierre Simon Laplace
IS-ENES2	Infrastructure for the European Network of Earth System Modelling Phase 2
JRA	Joint Research Activity
LiU	Linköping University
MD5	Message-Digest Algorithm 5
MPI	Max-Planck Institut
MXM	Mellanox Messaging Accelerator
NEMO	Nucleus for European Modelling of the Ocean
NSC	National Supercomputer Centre at LiU
OASIS3-MCT	OASIS3 - Model Coupling Toolkit coupler
OpenPALM	Open source parallel coupler
RAM	Random Access Memory
SYPD	Simulated Years Per Day
UM	Uncoupled Model (in this document)
YAC	Yet Another Coupler

Executive Summary

This report describes the current development status of the ENES Benchmark Suite, a collection of real application benchmarks used to model Earth System. The suite is assembled from applications of varying complexity ranging from simple computational and communication kernels to fully coupled Earth System Models (ESMs) in order to address different performance-relevant aspects of climate models. Here, we focus on the description of already available benchmarks: ***CMCC-CESM-NEMO, EC-EARTH, IPSLCM,*** *and* ***MPI-ESM1****. The Redmine project management tool is employed to ensure the availability of up-to-date benchmarks and performance data (https://redmine.dkrz.de/projects/enes-benchmark-suite). A detailed description of the final version of ENES Benchmark Suite will be subject of the deliverable D10.4.*

1. Introduction

The main objectives of the JRA2 (Joint Research Activity 2) within IS-ENES2 project is to assemble a benchmark suite based on real models used in climate research as well as collect key performance data on different HPC systems and make them available to the climate modelling community. The core of the suite is formed by four coupled Earth System Models (ESMs), but stand-alone models, couplers, and performance sensitive computational and communication kernels are included too. Thus, the ENES benchmarks represent the compute and data workloads that are characteristic for climate research applications and stress almost all features of the computing systems: floating-point and integer performance, memory bandwidth, I/O sub-systems, network interconnects etc. The benchmarks will serve the following purposes:

1. Improvement of the benchmarking of the HPC systems for procurements
2. Reduction of the time needed for porting of climate research applications to new systems
3. Monitoring of system performance throughout the operational lifecycle especially after machine, firmware, and software upgrades/updates
4. Provision of test cases based on real applications for computer scientists
5. Comparison of the performance of different ESMs on different computing systems in order to develop an understanding of factors affecting performance of some/all ESMs
6. Preparation of ESMs for extreme scale computing capabilities
7. Support of European climate researchers in assessing of computing time requirements and selection of most appropriate HPC system by providing performance reference for different ESMs on different HPC systems

In the next section we describe the status of different application benchmarks prepared so far and provide performance measurements. Section 3 outlines future work.

2. ENES Benchmark Suite

To ensure the availability and usability of the benchmarks and to allow for regular updates of benchmark codes and scripts, instructions for benchmark execution, and performance data we use the Redmine project management tool. The top project “ENES Benchmark Suite” (https://redmine.dkrz.de/projects/enes-benchmark-suite) has a number of subprojects devoted to a single benchmark application or application category. The integration of such features as wiki, forums, issue trackers, and development roadmap made Redmine particularly appropriate for managing of the suite. Furthermore, Redmine automatically tracks number of downloads and computes MD5 checksums for provided files thus supporting the dissemination of benchmarks.

The core of the ENES benchmark suite consists of four state-of-the-art European Earth System Models. All four ESMs have contributed to the CMIP5 project, which provided data bases for the IPCC AR5, and will also contribute to the CMIP6 project starting 2016-2017.

To exclude coupling costs and ESM load imbalance from the performance analysis four uncoupled models (UM) are also included in the suite. *Table 1* gives an overview about full model benchmarks (coupled and uncoupled) belonging to the ENES Benchmark Suite.

Table 1: *List of climate model benchmarks and the current availability status. The number of grid boxes is an indicator for the problem size to be solved. The following abbreviations have been used: ESM - Earth System Model, UM - Uncoupled Model, A – Atmosphere, O – Ocean, NX, NY, NZ number of grid cells along the x-, y-, and z-axes in the model.*

Benchmark	Model type	Grid	Number of grid cells NX x NY x NZ	Status
CMCC-CESM-NEMO	ESM	0.23x0.31 ORCA025L50	A: 1152 x 768 x 30 O: 1442 x 1021 x 50	Available (on request)
EC-EARTH	ESM	T255 L91 ORCA1L46 T511L91 ORCA025L75	A: 512 x 256 x 91 O: 362 x 332 x 46 A: 1024x 512 x 91 O: 1021 x 1442 x 75	Available[1]
IPSLCM	ESM	VLR LR	A: 96 x 95 x 39 O: 182 x 49 x 31 A: 144 x 142 x 79 O: 362 x 332 x 75	Available (on request)
MPI-ESM1	ESM	MR	A: 192 x 96 x 95 O: 802 x 404 x 40	Available
COSMO-CLM	UM	EU11 (regional)	A: 450 x 438 x 40	In preparation
ECHAM	UM	LR	A: 192 x 96 x 47	In preparation
ICON	UM	R2B07 LAM_r0416m	A: 1.310.720 x 96 A: 3.514.368 x 50	Available
NEMO	UM	ORCA025L50	O: 1021 x 442 x 50	In preparation

Another group of benchmarks included in the suite will address the coupling technologies in ESMs by defining a set of applications based on toy models coupled via OASIS3-MCT, OpenPALM, and YAC couplers. A description of the coupler benchmarks will be given in the upcoming deliverable D10.3 “Report on benchmark suite for evaluation of coupling strategies”.

Furthermore, kernels representing compute-intensive algorithms and communication patterns that are characteristic for climate models will be part of the suite. The kernels will be derived from the new generation atmospheric model ICON and the widely used ocean model NEMO. The NEMO Tracer Advection kernel can be downloaded at https://redmine.dkrz.de/projects/nemo-kernels.

Finally, test cases for Fortran 2003 and Fortran 2008 features required by climate models will be provided within the category “Fortran ISO benchmarks”.

[1] Due to license issues the EC-EARTH benchmark is not freely available yet.

Below, more detailed descriptions of the already available benchmarks and scalability data are provided.

2.1 CMCC-CESM-NEMO Benchmark

Status

The CMCC–CESM–NEMO model [1] is the physical basis of the new CMCC (Centro Euro-Mediterraneo sui Cambiamenti Climatici) Earth System Model. The model is derived from the NCAR coupled model CESM, where the ocean component is NEMO rather than the NCAR ocean model. In CMCC-CESM-NEMO all the climate components (atmosphere, ocean, land and sea-ice) are fully coupled via CPL7 CESM internal coupler.

The source code of CMCC-CESM-NEMO model has been updated to the latest stable release CESM 1.2.2. The NEMO ocean model has been updated to the NEMO 3.4 release. An optimization concerning the communication of the MPI processes involved in the NEMO North fold boundary condition has been integrated (see section on the performance reference).

IS-ENES2 partners can access the CMCC-CESM-NEMO model source code and input data through FTP. Credentials can be requested by email (piergiuseppe.fogli@cmcc.it).

A detailed step by step guide for download, configuration, and execution of CMCC-CESM-NEMO can be found on Redmine.

Redmine project: https://redmine.dkrz.de/projects/cmcc-cesm-nemo-benchmark

Performance reference

The performance of an ESM is strictly related to two factors:

1. The performance of the each component (atmosphere, ocean, land, etc.)
2. The load balance of the computational resources among all the components

In order to optimize the usage of available computational resources, it is needed to both improve the parallel efficiency of each component and to allocate them in the best way trying to synchronize the execution and to minimize the processes idle time.

To this aim, the analysis of scalability of each CMCC-CESM-NEMO component has been carried out, executing it in coupled mode. The main outcome of this analysis is the execution time of each component on a different number of cores. This information allows (i) to define the best distribution of the computational resources, given the total number of cores allocated for the job and (ii) to identify the bottlenecks to the parallel efficiency.

The analysis of scalability has been performed on the ATHENA system, an iDataPlex cluster equipped with Intel SandyBridge cores, located at the CMCC Supercomputing Center. Details on the system are reported in *Table 2*.

Table 2: *ATHENA Architectural parameters*

Design Parameters	IBM iDataPlex SandyBridge (CMCC)
Processor	Intel Xeon Sandy Bridge
Cores/Node	16
Hardware Threads	2
Flop/clock/core	8
Flop / Node (GFlop)	332.8
Clock Speed (GHz)	2.6
RAM / core (GB)	4
Number of Nodes	482
Network	InfiniBand 4x FDR

The charts in *Figure 1*, *Figure 2*, and *Figure 3* show respectively the Execution Time (for 1 day simulation), the Simulated Years Per Day (SYPD) and the Speedup of the two main components: ocean and atmosphere. The minimum number of cores allocated for each component (32 for ocean and 64 for atmosphere) is given by the memory required by the component itself and the memory available on the Athena node.

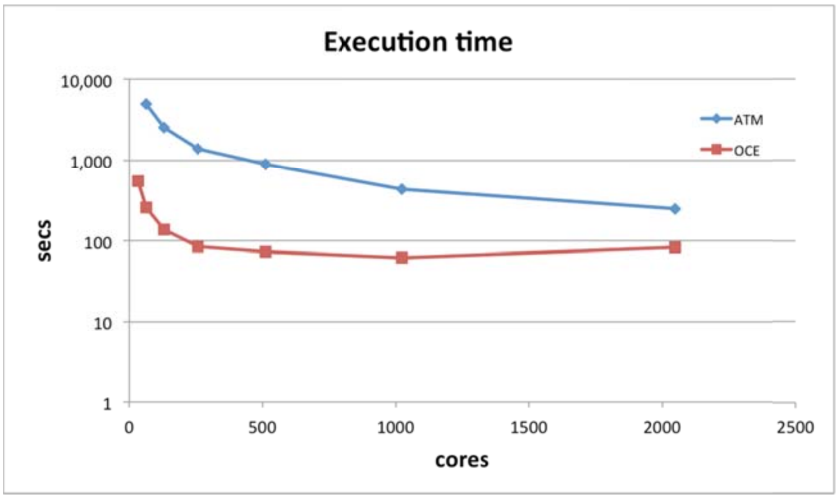

Figure 1: *Execution time of the main CMCC-CESM-NEMO components*

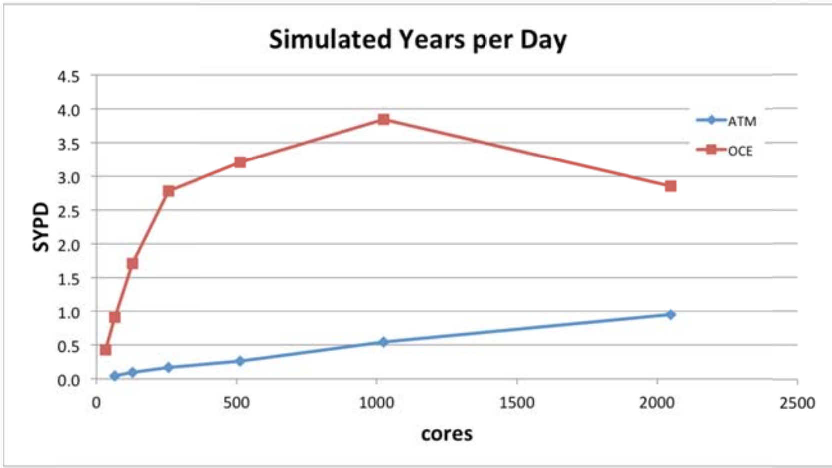

Figure 2: *SYPD of the main CMCC-CESM-NEMO components*

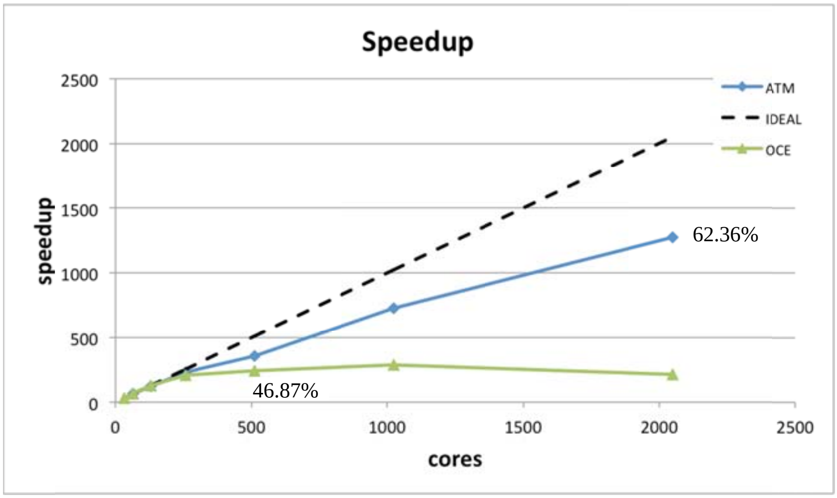

Figure 3: *Speedup of the main CMCC-CESM-NEMO components*

The bottleneck in terms of execution time is the atmospheric component. However, the parallel efficiency of the ocean component is already very low (~47%) on 512 cores. In order to improve it, the optimization of the north-fold algorithm implementation [2] has been integrated and the analysis of scalability has been repeated only on the ocean component.
The new version of the ocean model scales up 512 cores (*Figure 4*) with a good efficiency (~65%). The SYPD of the optimized version w.r.t. the old one is more than double on 2048 cores (*Figure 5*).

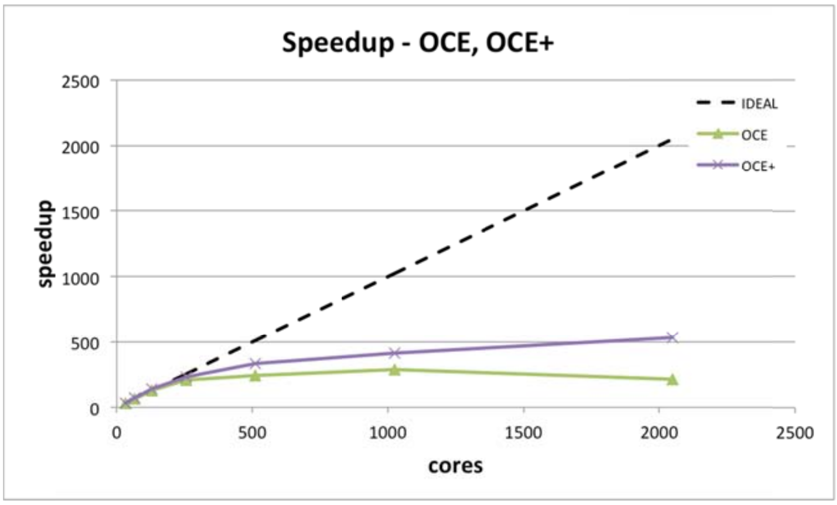

Figure 4: *Speedup of the ocean component (comparison between the original and the optimized version)*

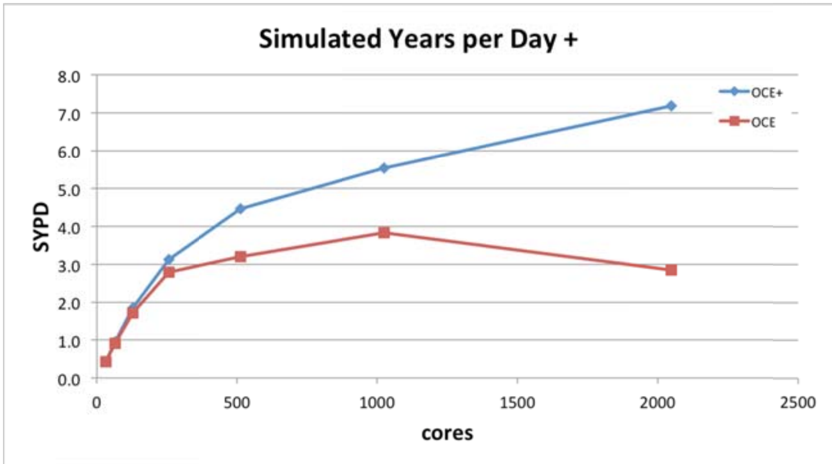

Figure 5: *SYPD of the ocean component (comparison between the original and the optimized version)*

Performance analysis of the single components allows to define the best configuration (reported in *Figure 6*) on the Athena system, following the requirements of the CESM framework (fully concurrent except the atmosphere run sequentially with the ice, rof, and land components; coupler run on a subset of the atmosphere processors, concurrently run with the land and ice).

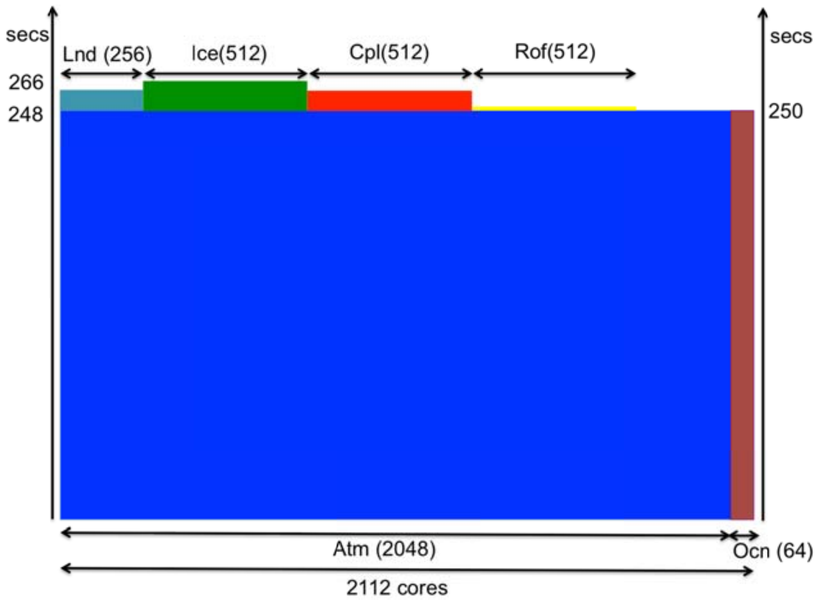

Figure 6: *CMCC-CESM –NEMO best configuration on the Athena system*

Table 3 reports the main metrics for ESMs performance evaluation, their explanation and related values for the configuration represented in *Figure 6*.

Table 3: *CMCC-CESM-NEMO performance evaluation metrics*

Performance metric	Explanation	Value
Resolution	Grid point distance	Atm, Lnd: 0.23 x 0.31, ~26km (lat) x ~35km (lon) (0.25L30) Ocn, Ice: ~28Km (0.25L50) Rof: ~56Km (0.5°)
Complexity	Number of prognostic variables of the main components (Atm and Ocn) Number and dimension of variables (2D or 3D) in restart files of the main components (Atm and Ocn)	Atm: 34 Ocn: 6 Atm (2D): 34 Atm (3D): 51 Ocn (2D): 15 Ocn (3D): 20
SYPD	Simulated years per day	~ 0.86
CHSY	Core hours per simulated year	59,100
ASYPD	Actual simulated years per day (taking into account pending time)	0.042
Memory bloat	Actual/ideal memory consumption	Actual (Ocn+Atm): 288 GB Ideal (Ocn+Atm): 18 GB
Coupler cost	Time spent in coupling/overall time	4.7%
Load imbalance	Time spent waiting for coupler (or other components) / overall time	3.4%
#Grid points		Atm: ~ 26,542,080 Ocn: ~ 73,614,100
Parallelization	Resources allocation allowing the best load balance among components	2048 (Atm) + 512 (Ice) + 64 (Ocn) + 256 (Lnd) + 512 (Rof) + 512 (Cpl) Lnd, Ice, Cpl, Rof sequential to Atm

2.2 EC-EARTH Benchmark

Status

NSC and LiU are working on the benchmarking of the EC-EARTH 3.2beta version which is a pre-release CMIP6 version of EC-Earth. Due to the license issues of EC-EARTH, it is difficult to make the benchmark suite *freely* available via the ENES Portal as envisioned in the work package description. Hence we are focusing on writing a best practice guide for building and benchmarking EC-EARTH. Currently, we are doing performance analysis of the atmosphere only runs of EC-EARTH.

Redmine project: https://redmine.dkrz.de/projects/ec-earth-benchmark/

Performance reference

The benchmarking is done on the Triolith system at NSC (https://www.nsc.liu.se/systems/triolith/) using Intel compiler version 15.0.3.187, Intel MKL version 11.2.3, Intel MPI version 5.0.3.048. The EC-EARTH compilation depends on a number of external libraries such as hdf5, netcdf, gribapi, gribex etc. Normally HPC systems have these libraries already installed, but for benchmarking we have decided to compile these libraries with the same versions of compiler and MPI as is used for compiling EC-EARTH.

The script ‘install_libs.sh’ for building all the necessary libraries is provided in Redmine (https://redmine.dkrz.de/projects/ec-earth-benchmark/wiki/Instructions). The script can download and install all the necessary packages. However for the gribex package, the script needs the path for the local copy of the tar file as gribex is no longer available for download.

For compilation of EC-EARTH we follow the standard EC-EARTH build procedure. For benchmarking purpose, a new *benchmark-triolith* platform section is defined in *config-build.xml* file which is also provided on the Redmine site mentioned above. The *benchmark-triolith* platform is the adaptation of the existing triolith platform in build configuration file with some changes relevant to our benchmarking environment.

The atmosphere only runs of EC-EARTH were done for the standard resolution (T255L91) and the high resolution (T511L91) grids. The runs were profiled with Allinea perf-report tool (http://www.allinea.com/products/allinea-performance-reports) which gives insight on percentage of time spent on Compute, MPI, I/O and others part of the code. In the *Table 4* the percentage times are shown.

Table 4: *Proportion of time spent in compute, MPI and I/O parts of EC-EARTH code (atmosphere only).*

Grid	Ranks	Compute %				MPI %			I/O %
		Total (t_c)	Scalar ops[1]	Vector ops[1]	Memory access[1]	Total (t_m)	Collective[2]	Pt-to-pt[2]	
T255L91	64	65.4	34.6	11.9	48.2	33.8	43.2	56.9	0.7
T511L91	64	76.6	29.8	11.4	58.5	22.9	38.1	61.9	0.8

[1] with respect to the total compute fraction (t_c)
[2] with respect to the total MPI fraction (t_m)

It can be seen that for 64 ranks both standard and high resolution runs are compute-bound. However, a high percentage of compute time is used for memory access. Also, most numeric operations are scalar operation. Hence the code is not properly vectorized. For the runs MPI collectives are taking more time than the point-to-point communication. The results presented here are preliminary. In future we will run it on a larger number of cores and compare the results on different platforms.

2.3 IPSLCM Benchmark

Status

IPSL Coupled Earth System model is a full earth system model. In addition to the physical atmosphere-land-ocean-sea ice model, it also includes a representation of the carbon cycle, the stratospheric chemistry and the tropospheric chemistry with aerosols. The benchmark includes sources, utilities and additional files required to run and check a short simulation. IPSL Coupled Earth System model benchmark is available for two different generations of IPSLCM [3]: IPSLCM5 and IPSLCM6.

IPSLCM5: 2010-2016

IPSLCM5 benchmark exists since 2010 when IPSLCM5 has been frozen for CMIP5. Regular updates have been done to include additional platforms. Practically, IPSLCM5 benchmark (a tar file including: sources, compiling tools, input files, output files as examples, README) is available on request by email to Arnaud.Caubel@lsce.ipsl.fr

Since 2010, IPSLCM5 benchmark is automatically launched for a short simulation period (3 simulated months) each couple of days, on two different platforms, to check the environment and to verify reproducibility. This is called *trusting*. Summarized information is available through a webservice [4]. Since 2010, five different systems have been monitored: two successive platforms at IDRIS (French national supercomputer centre/CNRS): vargas (IBM, 2008-2013) and ada (IBM 2013-now) and three successive platforms at TGCC (French national supercomputer centre/CEA): mercure (NEC SX-9, 2009-2012), titane (Bull, 2009-2013) and curie (Bull, 2011-now).

An important milestone was the publication [5] of a comparison of the preindustrial climate of the IPSL-CM5A-LR model on different computers used at IPSL. These simulations have been studied and compared on five different supercomputers. This study shows how comparable is the simulated climate.

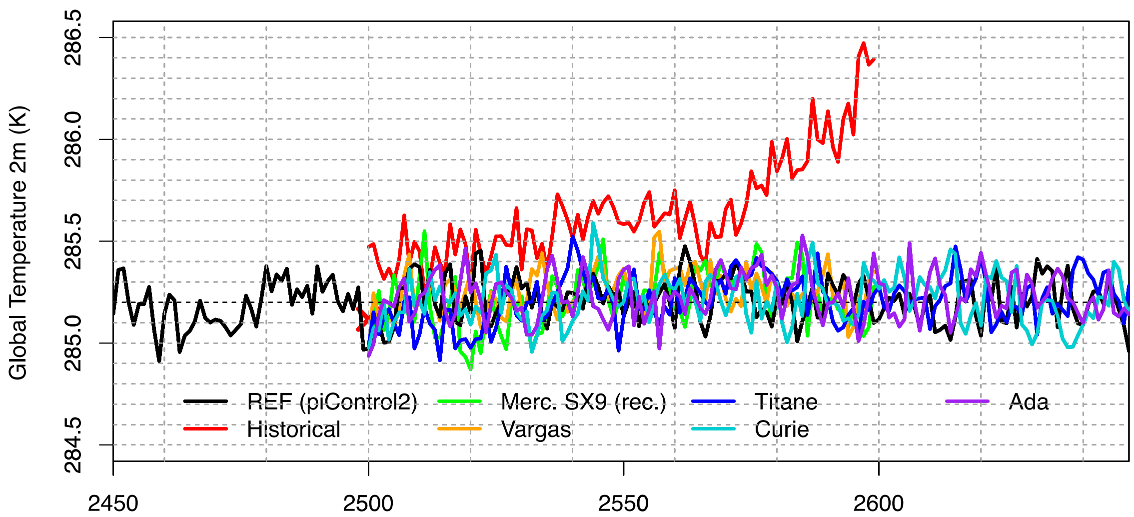

Figure 7: *Global mean temperature at 2m in piControl2 (solid black line, reference simulation on Mercure SX-9), piControl2M0 (in green, perturbed simulation on SX-9), piControl2V0 (in orange, on Vargas), piControl2T0 (in blue, on Titane), piControl2C0 (in light blue, on Curie) and piControl2A0 (in purple, on Ada). The historical simulation (Historical) is in red. The red cross highlights the common starting date for all simulations (but Historical).*

IPSLCM6: 2015-2019

IPSLCM6 is still under development and will be used for CMIP6 starting in 2016. A preliminary benchmark version exists, but, because this model still under development, is not frozen. IPSL is planning to produce a frozen version of IPSLCM6 benchmark in the second trimester of 2016. Nevertheless, since May 2015, a release candidate 0 version of IPSLCM6 has been used for *trusting* on two different supercomputers curie (Bull) at TGCC and ada (IBM) at IDRIS. Summarized information is also available through the same webservice [4].

Redmine project: https://redmine.dkrz.de/projects/ipsl-cm

Performance reference

As usual IPSLCM is based on three different executables running simultaneously and load balancing requires specific optimization. This version of IPSLCM6 release candidate 0 benchmark has been used to determine the number of cores required by each executable to keep a balanced workload for two different resolutions. For IPSLCM6-VLR with 96x95x39 atmosphere resolution mesh (LMDZ) and 182x149x31 oceanic resolution mesh (NEMO ORCA2), 27 simulated years per day could be achieved with a total of 128 cores. For IPSLCM6-LR with 144x142x79 atmosphere resolution mesh (LMDZ) and 362x332x75 oceanic resolution mesh (NEMO eORCA1), 6 simulated years per day could be achieved with a total of 480 cores. The *Figure 8* shows that the maximum speed of whole coupled system will be approximately the same than the “slowest” component one. Consequently, the optimization work consists in finding the optimal scalability for the slowest component and attributing resources for each model accordingly to this number. This work was done using LUCIA, a load balancing tool for Oasis coupled systems [6].

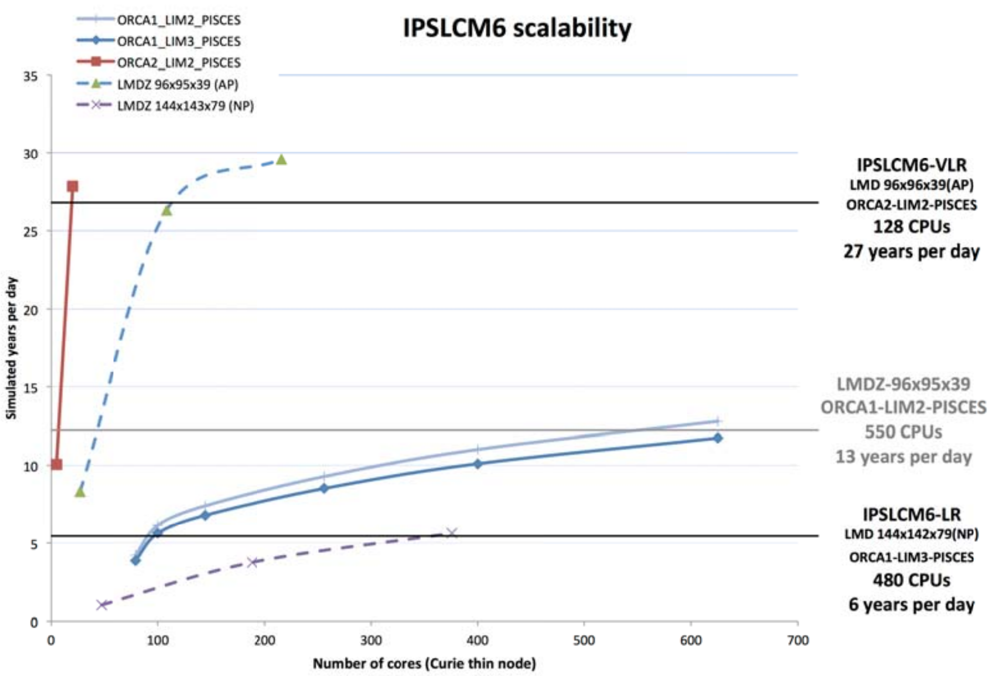

Figure 8: *IPSLCM6 scalability. The figure shows the number of simulated years per day for atmospheric and oceanic component of IPSLCM at different resolution and on different numbers of cores on one computer (Bull, curie, TGCC). For IPSLCM6-VLR with 96x95x39 atmosphere resolution mesh (LMDZ) and 182x149x31 oceanic resolution mesh (NEMO ORCA2 LIM2 PISCES), 27 simulated years per day could be achieved with a total of 128 cores. For IPSLCM6-LR with 144x142x79 atmosphere resolution mesh (LMDZ) and 362x332x75 oceanic resolution mesh (NEMO eORCA1 LIM3 PISCES), 6 simulated years per day could be achieved with a total of 480 cores. For the third possible configuration with 96x95x39 atmosphere resolution mesh (LMDZ) and 362x332x75 oceanic resolution mesh (NEMO eORCA1 LIM2 PISCES), the number of cores used by the ocean could be increased and 13 simulated years per day could be achieved with a total of 550 cores.*

2.4 MPI-ESM1 Benchmark

Status

MPI-ESM1 (Max-Planck Institute Earth System Model) is a state-of-the-art global Earth System Model consisting of components ECHAM/JSBACH that simulate atmosphere, land surface, soil, and vegetation processes and MPIOM/HAMOCC that describe ocean, sea ice and ocean biogeochemistry. ECHAM/JSBACH and MPIOM/HAMMOC run as separate executables coupled via the OASIS3-MCT coupler.

All public releases of the MPI-ESM1 benchmark package are put on the Files area of the Redmine project 'MPI-ESM1 Benchmark' for download. The corresponding input data sets can be downloaded from the Cloud Storage maintained by DKRZ.

Redmine project: https://redmine.dkrz.de/projects/mpi-esm-benchmark

Performance reference

The prepared benchmark experiment simulates the historical climate in years 1850-1851 at MR spatial model resolution.
The benchmark was executed on the DKRZ Mistral cluster [7] using

- Intel Compiler version 16.0.1
- Bullx MPI version 1.2.8.3 with Mellanox libraries MXM (version 3.3.3002) and FCA (version 2.5.2393)
- CDO version 1.7.0 (for evaluation)

Figure 9 shows the speedup curve for MPI-ESM1. The measurements cover the range from 24 (1 Mistral node) to 864 (36 Mistral nodes) cores and imply an ideal (linear) speedup of factor 36. The actual speedup amounts to 16. The scalability of the coupled model is limited by the behaviour of the atmospheric component ECHAM (nor shown here). According to the detailed profiling analysis the scalability of ECHAM is affected by non-scaling global data transpositions needed to re-arrange data between spectral and grid point spaces. The other performance bottleneck is high-frequency (every 6 hours) serial data output. The amount of output time on the total simulation time increases from 5% for 24 cores to 57% for 864 cores (not shown). This issue will be fixed in the next release of ECHAM6 by implementing asynchronous output via dedicated I/O servers.

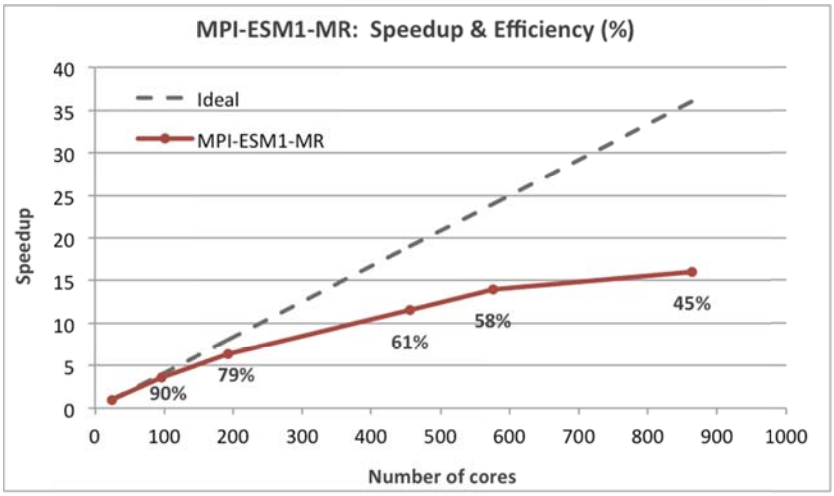

Figure 9: *Linear and measured speedup curves for MPI-ESM1 model. Numbers at data points indicate the parallel efficiency defined here as ratio between actual speedup and ideal speedup. Please, note that speedup and efficiency data refer to the execution time on 24 cores.*

The measured benchmark execution times correspond to the number of simulated years per day shown in *Figure 10*. Throughput rates above 20 SYPD (which is a prerequisite for spin up, tuning and performing of ensemble experiments within reasonable time frames) can be achieved for total number of cores higher than 576 (24 Mistral nodes).

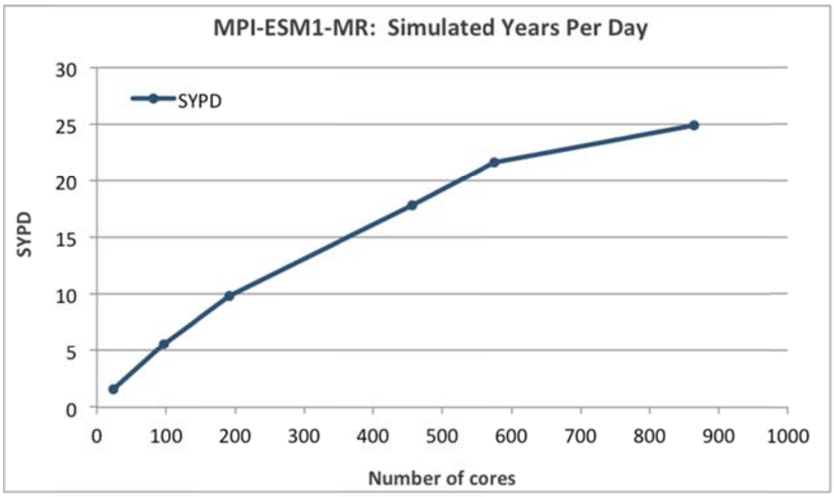

Figure 10: *Simulated Years per Day that can be achieved with MPI-ESM1-MR for different numbers of cores.*

3. Outlook

We have reported on the current development status of the ENES Benchmark Suite consisting of real applications from European climate modelling research.

Our next steps are:

1. Update of model source codes to the model versions to be used for the CMIP6 experiments. It is expected that finalized source code of the most ESMs will be released in the second half of 2016.
2. Make further benchmark packages available
3. Extended performance analysis of all benchmarks using common set of performance metrics for example as defined in the IS-ENES WP9 [8] and, possibly, CPMIP protocol.
4. Comparison of performance on different HPC systems

The final version of the ENES benchmark Suite will be described in the deliverable D10.4 “Report on the suite of base benchmarks and comparison of the performance on available platforms” that is due in January 2017.

References

[1] Fogli; P.G., D. Iovino. CMCC–CESM–NEMO: toward the new CMCC Earth System Model, Research Papers Issue RP0248 December 2014

[2] Epicoco I., S. Mocavero, G. Aloisio: “Performance Optimization of NEMO Oceanic Model at High Resolution”, EGU2014, April 27-May 2, 2014, Vienna, Austria

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