Centro Euro-Mediterraneo per i Cambiamenti Climatici

Issue RP0100
July 2010

Scientific Computing and Operation (SCO)

DEFINITION OF AN ESM BENCHMARK FOR EVALUATING PARALLEL ARCHITECTURES

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SUMMARY Different approaches exist for evaluating the computational performance of a parallel system. These approaches are based on the appliance of some benchmarking tools for evaluating either the whole system or some of its subcomponents (i.e. I/O system, memory bandwidth, node interconnection, etc). Different kind of benchmarks can be considered: real program benchmarks are based on real applications; kernel benchmarks include some key codes normally abstracted from actual programs (i.e. linear algebra operations); component benchmarks are focused on the evaluation of computer's basic components; synthetic benchmarks are built taking statistics of all types of operation from many application programs and writing a program based on a proportional invocation of such operations.

This report describes the development of an ESM (Earth System Model) benchmark, based on real applications, for evaluating the performance of a parallel system and its suitability for running climate models. The development of the ESM benchmark started from the composition of an evaluation suite that includes some of the most significant ESM models adopted in the climate community. The selection of the ESM models has been made within the ENES community involving all the main climate centers in Europe. Finally, we have defined a metric as index for measuring the system's performance. The benchmark will be used for both comparing different parallel architectures and highlighting the hotspots of the target one. The benchmark's results can provide useful hints for tuning and better configuring the analyzed system.

Keywords: benchmark, parallel system, ESM evaluation suite

JEL: C63

The work here presented carried out with support of the funding of the european project IS-ENES.

INTRODUCTION

Earth system models are the only analytical tools available for prediction of the future climate evolution either under natural conditions or under the influence of humankind. The development and use of realistic climate models requires a sophisticated software infrastructure and access to the most powerful supercomputers and data handling systems. Several scientific institutions, universities, governmental organizations and industrial partners in Europe have developed a world class expertise in different aspects of Earth System Modeling and have contributed to international assessments of climate change. The complex processes of a high-resolution climate system model, that better simulates the interactions and feedbacks among the physical and biological processes, include: atmosphere, ocean, land, soils, permafrost, vegetation cover, sea ice, land ice, carbon and other biogeochemical cycle, clouds and related microphysics, hydrology, atmospheric chemistry, aerosols, ice sheets, human systems. Current models already provide improved simulation and prediction of changes in temperature and precipitation, and extreme weather events.

EVALUATION SUITE

The main goal of this report is to define and describe the initial contents of the Benchmark Evaluation Suite, which gathers key existing and developing ESMs belonging to the IS-ENES partners. Even though the selection of the applications belonging to the Evaluation Suite has been initially based on the ESMs developed by IS-ENES project partners, it must not be considered a closed list. The list can be extended, as the scientific research evolves, with other ESMs available in the community. The main purpose of this report regards the definition of a suite of climate models to be used for:

- evaluating the performances of the models themselves on existing parallel architectures
- benchmarking the parallel architectures and defining the critical aspects that climate models stress
- profiling and optimizing current ESMs and related infrastructure on the available architectures
- highlighting the bottlenecks, the strengths and weaknesses of each of the models to guide the design and development of future optimized ESMs for the upcoming peta and exascale architectures.

A multitude of climate models is actually available worldwide. They differ each other both for computational requirements and scientific reliability of the prediction and modelization of the climate behavior and its impacts. In order to define the evaluation suite we have discussed some relevant selection criteria, described below:

1. Interest for the model. The main criteria adopted is based on the estimation about how much the model is of interest for IS-ENES partners. From a pragmatic point of view, all of the models, belonging to the Evaluation Suite, should be maintained, ported and optimized on the major parallel architectures. More a model is of interest more it will be maintained, optimized and analyzed. The interest for a model has to be measured evaluating the plans that a partner has for porting, optimizing, providing support on it.
2. Model spread. This criteria measures how much the model can be relevant for

a wider climate community. It consists in the number of climate centers that regularly use the model for production.

3. Supported platforms. This criteria is strictly related to the availability of the model on different parallel architectures. More are the platform where the model is already ported and analyzed, less will be the effort to support new architectures.

4. Performance requirements. A qualitative evaluation of memory, cpu, I/O, network use. The metric could be low/medium/high.

5. Model extension. The criteria refers to the number of model components integrated within the couple model.

6. Potentiality for peta-exascaling. This is a qualitative criteria that defines how much a model could scale up to exaflop architectures and how difficult is to modify the model for the exascale platforms.

7. Level of model documentation. The availability of a good documentation related to the model is relevant for maintaining the model and for running the evaluation suite.

ESM MODELS

The Evaluation Suite gathers existing models used by partners to provide other tasks with an application-focused lead for understanding ESMs performance and improving them for current state-of-the-art computing systems and for future, such as for peta and exascale architectures. An initial set of applications has been defined, taking into account both partners experience and knowledge and selection criteria described in the previous section. The Evaluation Suite will include two different categories of applications: (i) coupled models, often used by climatologists to evaluate the complexity of the system as the range of model components involved (i.e., physical, chemical, and biological) and their interactions, and (ii) stand-alone models, generally used for performing high-resolution simulations in the short period. The suite overview synthesizes models features. In particular:

- The configuration referring to a test case run. This configuration is used for testing/benchmarking the model.
- A description of the model (for coupled models each component has to be analyzed).
- A description of platforms on which the model has been tested and the execution details, such as libraries, compilation flags, etc.
- Details about scalability such as the execution time, the I/O time and the communication time with different number of cores.
- Recommendations about potential for Peta/Exascaling and optimization and related expected effort.

In the next section the following models will be described:

- CMCC-MED from CMCC.
- ARPEGE-NEMO from CERFACS.
- IPSLCM5 from CNRS-IPSL.
- HadGEM3 from METOFFICE.
- MPI-M from MPI.
- NEMO from IPSL.
- ECHAM5 from MPI-M.

ESM MODELS

CMCC-MED

Model's name :
CMCC-MED

Reference person :
Silvio Gualdi, gualdi@bo.ingv.it, CMCC

Version :
2.0

Brief description :
Three components fully coupled climate model with mediterranean sea region

ESM Infrastructure :
OASIS3 ver. 2.5 (CMCC parallel version)

Download :
For information about the code download, please contact the reference person

Input configuration :
The coupled model is made of:
Echam5 T159L31
OPA 8.2 global
Nemo 1/16° for Mediterranean sea

Length of model run: 1 month

Oasis configuration:
total number of exchanged fields 35
exchanged fields 17 (Echam -> Oasis -> OPA)
exchanged fields 9 (Echam -> Oasis -> Nemo)
exchanged fields 6 (OPA -> Oasis -> Echam)
exchanged fields 3 (Nemo -> Oasis -> Echam)
coupling period: 2h 40'

Echam5:
Region: Global
Resolution: T159L31 (480 x 240)
time step: 240 sec

OPA:
Region: Global
Resolution: 2¡ (182 x 149)
time step: 600 sec

Nemo:
Region: Mediterranean Sea
Resolution: 1/16¡ (871 x 253)
time step:

Input files dimension :
Echam5: 912MB
OPA: 96MB
NEMO: 1.6GB
OASIS: 1.1GB
restart files (1 month):
Echam5: 1.23GB
OPA: 102MB
Nemo: 1.5GB
OASIS3: 30,5MB

Output files dimension :
Echam5: 9.2GB
Nemo: 18GB
OPA: 1.5GB

Platforms

Execution platform Ulysses / NEC-SX9

Details of the execution platform :
CPU Type: SX9
CPU Speed: 3.2 GHz
number of nodes: 7
SMP size: 16 vector CPUs
Memory: 512 GB per node
Interconnection: IXS
Teoretical Peak Performance: 11.2 TFLOPS
Installed Libraries: Blas, Lapack, MPI, OpenMP
C compiler: sxcc
Fortran compiler: sxf90
profiler: SXFtrace

Libraries :
Oasis: -lnetcdf
Echam: -llapack -lblas -lnetcdf
OPA: -lnetcdf
Nemo: -lnetcdf

Compilation flags for each component :

OASIS: -Pstack -pi auto nest=3 line=10000 exp=iminim, rmaxim, rminim, grid_search_bilin -Ep -sx9 -Wf,"-P nh" -Wf,"-pvctl noassume loopcnt=5000000 vworksz=100M" -Wf,"-A idbl4" -Wf,"-msg o" -Wf,"-pvctl fullmsg" -Wf,"-L fmtlist transform map summary noinclist" -Chopt -Wf,"-ptr byte"

Echam: -Popenmp -Chopt -sx9 -Wf,-init heap=zero stack=zero -Wf,-K a -Wf"-L source fmtlist noinclist mrgmsg summary transform map objlist" -Ep -pi line=1000 -Wf,-pvctl chgpwr fullmsg,-msg o,-ptr byte

OPA: -Ep -Pstack -sx9 -Chopt -Wf,-P nh -Wf,-pvctl noassume loopcnt=200000 vworksz=4M -Wf,-A idbl4 -Wf,-msg o -Wf,-pvctl fullmsg -Wf,-L fmtlist transform map summary noinclist

Nemo: -size_t64 -dw -Wf÷A dbl4÷sx9 -pi auto -P stack -C vopt -Wf"-init stack=nan" -Wl"-f nan" -Wf"-P nh" -Wf,-pvctl noassume loopcnt=10000 -L transform -Wf,"-msg o" -Wf,"-L fmtlist transform map summary noinclist"

Scalability details :
The performance, reported below, refers to 1 month run. In the experiment, the number of processes for OPA, Nemo and Echam are constant:
OPA: 1 proc - Nemo: 6 procs - Echam: 8 procs

# Cores for OASIS	# Total cores	Wall clock (s)
1	16	4320.95
2	17	4032.18
3	18	3963.80
7	22	3898.64
9	24	3856.03
11	26	3864.05
13	28	3790.30
15	30	3786.89
17	32	3774.50
26	41	3793.12
33	48	3822.48

Recommendation

Expected potential for Peta/Exascaling :
low

Expected effort to reach potential Peta/Exascaling :
Improve kernels to be able to scale to high number of processes.
Increase resolution of the models.

Expected potential for optimization :
medium

Expected effort to reach the optimization potential :
Optimize I/O operations in order to improve simulation time.
Reduce bank conflicts on vector machines.

ARPEGE-NEMO

Name of the model :
ARPEGE-NEMO

Reference person :
Eric Maisonnave, eric.maisonnave@cerfacs.fr, CERFACS

Version :
ARPEGE-Climat v5.2 - NEMO v3.2

Brief description :
CGCM high definition

ESM Infrastructure :
OASIS v3 (pseudo parallel) - OASIS v4 (work in progress)

Download :
Due to component licence restriction, CERFACS does not provide any version of the coupled model

Reference for detailed information :
For general information on ARPEGE-NEMO workflow, see LEGO: Grid Compliant Climate Model Analysis.
For information on porting and tuning the high-resolution configuration, document to come.

Input configuration :
The coupled model consists on:
ARPEGE-5 T359L31 (possibly higher resolution)
NEMO-3 1/4° (possibly 1/12° - 1D configuration also available)

Length of model run: 1 month

Oasis configuration
OASIS-3 Pseudo-parallel mode (possibly OASIS-4)
Coupling period: 3h
Coupling fields (reduced configuration)
O2A: surface temperatures, albedo
A2O: heat fluxes, water fluxes (without calving and runoff), non solar heat flux derivative

ARPEGE-5
Region: Global
Resolution: T359L31 (360 x 180)
time step: 900 sec

NEMO-3
Region: Global
Resolution: 1/4 (1442 x 1021)
time step: 1080 sec

Input files dimension :
ARPEGE: 87 MB
NEMO: 384 GB
OASIS: 8 GB

restart files (1 month):
ARPEGE: 48 MB
NEMO: 8.4 GB
OASIS3: 50 MB

Output files dimension :
Monthly means:
ARPEGE: 4.5GB
NEMO: 745 MB

Platforms

Execution platform : Meteo-France NEC-SX9
(but also SGI Altix, IBM JS21/BG-L/BG-P at lower resolution)

Details of the execution platform :
CPU Type: SX9
CPU Speed: 3.2 GHz
Number of nodes: 6
SMP size: 16 vector CPUs
Memory: 1 TB per node
Teoretical Peak Performance: 102 GFLOPS/proc

Installed Libraries:
Blas, Lapack, MPI, OpenMP, Netcdf

Development tools:
C compiler: sxcc
Fortran compiler: sxf90
profiler: SXFtrace

Libraries :
Oasis: -lnetcdf
Echam: -llapack -lblas -lnetcdf
OPA: -lnetcdf
Nemo: -lnetcdf

Compilation flags for each component :
Oasis/NEMO/ARPEGE: -Ep -Pstack -dwW -Wf-A idbl4 -pvctl vwork=stack fullmsg-sx9 -Wf,-P nh

General comments :
Slow-down at GPFS file copy stage
Multi-core communications slower than intra-core
About 1.7 faster than SX8R configuration

Scalability details :
1 month long simulation, NEMO on 4 cores, one OASIS without additional resource. The number of cores below refer to ARPEGE (but NEMO always faster)

# Cores	Wall clock (s)
4	7416
5	6912
7	6516

Recommendation

Expected potential for Peta/Exascaling :
medium

Expected effort to reach potential Peta/Exascaling :
Weak-scaling: increase of the resolution for Terascale
Strong-scaling: code rewriting for Peta/Exascale

Expected potential for optimization :
medium

Expected effort to reach the optimization potential :
Porting on MPP platforms: fully parallel coupling (OASIS4) and IO improvements

IPSLCM5

Name of the model :
IPSLCM5

Reference person :
Arnaud Caubel arnaud.caubel@lsce.ipsl.fr
Marie-Alice Foujols foujols@ipsl.jussieu.fr, IPSL

Version :
v.3

Brief description :
Ocean-sea ice-atmosphere-land climate model, ready for Earth System Model (chemistry, marine biogeochemistry and carbon cycle added)

ESM Infrastructure :
OASIS v3 (pseudo parallel)

Download :
For information about the code download, please contact the reference person

Input configuration :
The IPSLCM5 model consists on:
LMDZ4+ORCHIDEE (CMIP5)
NEMO v3.2

Length of model run: 5 days

Region: Global

Oasis configuration:
Total number of exchanged fields 21
Exchanged fields 17 (LMDZ4 -> Oasis -> NEMO)
Exchanged fields 4 (NEMO -> Oasis -> LMDZ4)
Coupling period: 24h

LMDZ4
Resolution: 280x280x19 (280x280x39 also possible if more memory available)
Time step: 72 s (dynamics) and 30 min (physics)

NEMO
Region: Global
Resolution: ORCA05 1/2° (511x722x31)
time step: 40 min

Input files dimension :
LMDZ4/ORCHIDEE: 140 MB
NEMO: 1.1GB
OASIS: 900 MB (9GB with calculated weights for runoff)

restart files (5 days):
LMDZ4/ORCHIDEE: 600 MB
NEMO : 1.5 GB
OASIS: 23 MB

Output files dimension :
LMDZ4/ORCHIDEE: 315 MB (histday.nc and histhf.nc)
NEMO: 650 MB

Platforms

Execution platform BSC MareNostrum, IBM PPC
Bull, NEC SX-8/9, IBM Power6, SGI for lower resolutions

Details of the execution platform :
CPU Type: IBM PPC
CPU Speed: 2.3 GHz
number of cores: 72 (LMDZ) + 20 (NEMO) +2 (Oasis)
SMP size: 4 cores per nodes
Memory: 8 GB per node, ie a maximum of 3 LMDZ MPI process per node at this resolution (280x280x19)
Teoretical Peak Performance: 94,2 TFLOPS

Installed Libraries:
NetCDF, Blas, Lapack, MPI 1, OpenMP

Development tools:
C compiler: mpicc
Fortran compiler: xlf90_r
Profiler: Paraver

Libraries :
Oasis: -lnetcdf
LMDZ4: -llapack -lblas -lnetcdf
Nemo: -lnetcdf

Compilation flags for each component :
Oasis: -O2 -qextname=flush -q64 -qarch=ppc970 -qtune=ppc970 -qrealsize=8
LMDZ4: -O3 -qstrict -qarch=ppc970 -qtune=ppc970 -qcache=auto -q64 -qautodbl=dbl4
Nemo: -O2 -qsave -qstrict -qrealsize=8 -qsuffix=cpp=F90 -qextname=flush -qsource -qlargepage -qmaxmem=-1

Scalability details :
5 days run for LMDZ (MPI only), 1 day run for NEMO (on MareNostrum). Performances depend on the repartition of MPI process on nodes (1/4, 2/4 or 3/4).

# Cores (LMDZ)	Wall clock (s)	# Cores (NEMO)	Wall clock (s)
1	50000	5	760
2	18805	10	382
4	12524	20	201
8	8610	27	141
16	4389	32	125
24	3213		
32	2830		
40	2329		
45	1881		
48	1700		
56	1561		
60	1484		
72	1350		
80	1316		

for 5 days run

Cores (LMDZ)	Cores (Nemo)	Cores (Oasis)	Cores (total)	Wall clock (s)
72	20	2	94	1270

Recommendation

Expected potential for Peta/Exascaling :
High

Expected effort to reach potential Peta/Exascaling :
Weak-scaling: increase of the resolution
Strong-scaling: dynamical core code rewriting for Peta/Exascale from scratch or from a shared kernel

Expected potential for optimization :
High
Use OpenMP to increase the scalability and the number of cores used by LMDZ4 (OpenMP is available in LMDZ4 sources but running with it needs investigation on BSC).
IO server allows asynchronous outputs and increases scalability

Expected effort to reach the optimization potential :
Hybrid parallelisation based on MPI/OPenMP need more investigation on all platforms
Use of IO server in standard configuration

HADGEM3A

Name of the model :
Unified Model: HadGEM3A configuration

Reference person :
Steve.Mullerworth@metoffice.gov.uk

Version :
v7.4

Brief description :
Atmosphere model

ESM Infrastructure :
Input set up through user interface. No coupler (can be used coupled to NEMO through OASIS)

Download :
Provided on CD. License is required

Input configuration :
Configuration is defined by a User Interface, and different configurations can be supplied. A typical configuration is a resolution of 192 points E-W by 145 points N-S on 63 atmospheric levels, running with a 20 minute time-step for 1 month

Input files dimension :
Typically 4GB

Output files dimension :
Configurable - minimum 2GB

Platforms

Execution platform <u>**IBM Power 6**</u>

Details of the execution platform :
CPU Type: IBM Power 6
SMP size: 32 cores per node, 100 nodes

Libraries :
GCOM, mass

Compilation flags for each component :
: -qextname -qsuffix=f=f90 -qarch=pwr6 -qtune=pwr6 -qrealsize=8 -qintsize=8 -NS32768

Scalability details :
One month run

# Cores	Wall clock (s)
32	5800
64	3080
96	2240
128	1800

Recommendation

Expected potential for Peta/Exascaling :
Low

Expected potential for optimization :
Medium

MPI-M

Name of the model :
MPI-M

Reference person :
Marco Giorgetta, marco.giorgetta@zmaw.de, MPI-M

Version :
COSMOS-1.2.1.1

Brief description :
Earth system model consisting of coupled atmosphere, ocean, and land, includes carbon cycle

ESM Infrastructure :
IMDI SCE/SRE, OASIS3

Download :
Available for download upon request from the following URL: http://www.mpimet.mpg.de/en/wissenschaft/modelle/model-distribution.html

Input configuration :
"ASOB" configuration, i.e. coupled climate carbon cycle model ECHAM5J/MPIOM. Setup like Control run for preindustrial conditions, as done for ENSEMBLES stream 2. Length of integration in this case = 20 years

The IPSLCM5 model consists on:
ECHAM5
MPIOM

<u>Length of model run</u>: 20 years

Region: Global

<u>Oasis configuration</u>:
Total number of exchanged fields 25
Exchanged fields 17 (ECHAM5J -> Oasis -> MPIOM)
Exchanged fields 8 (MPIOM -> Oasis -> ECHAM5J)
Coupling period: 24h

<u>ECHAM5J</u>
Resolution: T31L19 (96x48)
Time step: 2400 sec

<u>MPIOM</u>
Region: Global
Resolution: 3°
time step: 8640 sec

Input files dimension :
58MB

<u>restart files (5 days)</u>:
36MB

Platforms

Execution platform <u>**Blizzard, IBM P6 parallel SMP**</u>

Libraries :
IBM MPI, lapack, essl, blas, mass, netcdf-3.6.3, hdf5-1.8.2, szip-2.1 zlib-1.2.3

Compilation flags for each component :
MPIOM: -q64 -qsuffix=cpp=f90 -O3 -qsuppress=1518-061:1518-128 -qstrict -qarch=pwr6 -qtune=balanced -qzerosize -qessl -qhot -qxflag=nvecvter -qxflag=nsmine -qfloat=fltint -qextname -qdpc=e -qrealsize=8
ECHAM5: -q64 -qsuffix=cpp=f90 -qsuppress=1500-036 -O3 -qlist -qreport -qxflag=nvectver -qxflag=nsmine -qarch=auto -qtune=auto -qcache=auto -qfloat=fltint -qzerosize -qessl -bdatapsize:64k -bstackpsize:64k -qextname
OASIS3:-q64 -qfixed=72 -qsuffix=cpp=F -qtbtable=full -O3 -qstrict -qMAXMEM=-1 -Q -qarch=auto -qtune=auto -qcache=auto -qfloat=fltint -qzerosize -qessl -qextname -qdpc=e -qrealsize=8

General comment :
The selected model configuration is typical for millennia time scale simulations. The primary goal is to achieve a high turnover rate (many years per 24 hr wall clock time). Hence the model runs at low resolution. This is a special challenge on computers like Blizzard (IBM Power 6), which have a large number of relatively slow processors. Gaining speed by parallelization is difficult for low resolution models. But high resolution models would still have a lower turnover rate.

Scalability details :
No scalability data is available for this platform

Execution platform tornado, AMD cluster

Libraries :
OpenMPI, acml, acml_mv, netcdf-4.0.1-without-hdf5, rdmacm, libverbs, numa, dl, nsl, util, pthread

Compilation flags for each component :
-Mpreprocess -O2 -Kieee -fastsse -Mnorecursive -Mextend -tp amd64e -byteswapio -r8

Scalability details :

# Cores (ECHAM)	# Cores (MPIOM)	# Cores (total)	Wall clock (s)
8	3	12	339
16	15	32	175
36	27	64	135

Recommendation

Expected potential for Peta/Exascaling :
Low

Expected effort to reach potential Peta/Exascaling :Switch to a new dynamical core, and software infrastructure

Expected potential for optimization :
High
Use OpenMP to increase the scalability and the number of cores used by LMDZ4 (OpenMP is available in LMDZ4 sources but running with it needs investigation on BSC).
IO server allows asynchronous outputs and increases scalability

COMPONENT MODELS

Component model's name ARPEGE-Climat Version: v5
License policy: "ARPEGE-Climat Software Licence Agreement", which must be signed by each user (contact CNRM, Meteo-France)
Programming Language(s): Fortran
Libraries: BLAS, LAPACK
Parallelization method supported: MPI1 (MPICH, OpenMPI, LAM tested), possibly OpenMP

Component model's name LMDZ4 - ORCHIDEE
Version: CMIP5
License policy: CeCILL licenses
Programming Language(s): Fortran
Libraries: NetCDF, MPI, OpenMP, Lapack, Blas
Parallelization method supported: MPI1, OpenMP

Component model's name OASIS3
Version: v.3
License policy: Lesser GNU General Public License (LGPL) see https://oasistrac.cerfacs.fr/
Programming Language(s): C, Fortran
Libraries: NetCDF, MPI, OpenMP
Parallelization method supported: MPI1, MPI2, OpenMP (Pseudo parallelism IPSL/CERFACS and field parallelism CMCC method)

Component model's name Echam
Version: v.5
License policy: "MPI-M Software Licence Agreement", which must be signed by each user
Programming Language(s): Fortran
Libraries: NetCDF, MPI, OpenMP, Lapack, Blas
Parallelization method supported: MPI1, MPI2, OpenMP

Component model's name OPA
Version: v. 8.2
License policy: CeCILL license (public license)
Programming Language(s): F95
Libraries: NetCDF, MPI
Parallelization method supported: MPI1, MPI2

Component model's name Nemo3
Version: v.3.2
License policy: CeCILL license (public license) see http://www.nemo-ocean.eu/user/register
Programming Language(s): Fortran90/95
Libraries: NetCDF, MPI, xml
Parallelization method supported: MPI1 (MPICH, OpenMPI, LAM tested)

Component model's name HadGEM3A
Version: v7.4
License policy: License available for academic/research users
Programming Language(s): FORTRAN + some C
Libraries: GCOM
Parallelization method supported: MPI. Some OpenMP currently being developed

Component model's name MPIOM
License policy: "MPI-M Software Licence Agreement", to be signed by each user, see http://www.mpimet.mpg.de/en/wissenschaft/modelle/model-distribution.html
Programming Language(s): Fortran, C
Libraries: NetCDF, CDI, MPI
Parallelization method supported: MPI1, MPI2, OpenMP

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