Parallelism in LMDZ

A short survival guide for those who feel diagonally stuck in a parallel world

LMDZ course, December 17th 2014

LMDZ5 DOCUMENTATION:
http://lmdz.lmd.jussieu.fr/utilisateurs/manuel-de-reference-1/lmdz5-documentation/view

Why go parallel ?

• To have simulations run faster by using multiple cores to share the workload, each working “as independently as possible” (i.e.: with the minimum communication/interaction with the other cores).

• To benefit from modern architectures (from laptops to supercomputers).

Which parallelism is implemented in LMDZ ?

• LMDZ is designed so that it can be compiled and run in serial (sequential) or parallel mode (in various forms, MPI, OpenMP, or mixed MPI/OpenMP, as will be discussed later).

• The implementation of the parallel modes has been thought of, and done (Yann Meurdesoif, LSCE, IPSL), so that it can easily benefit from all hardware platforms. The various aspects of parallelism in the code have moreover been coded as to be the least intrusive for users and developers.

MPI and OpenMP parallelism paradigms

MPI : Distributed Memory parallelism

• The code to be executed is replicated on all CPUs in as many processes.

• Each process runs independently and by default does not have access to the other precesses' memory.

• Data is shared via a **message passing interface library** (OpenMPI, MPICH, etc.) which uses the interconnection network of the machine. Efficiency then essentially relies on the quality of the interconnection network.

• The number of processes to use is given at runtime: mpirun -n 8 gcm.e

OpenMP : Shared memory parallelism

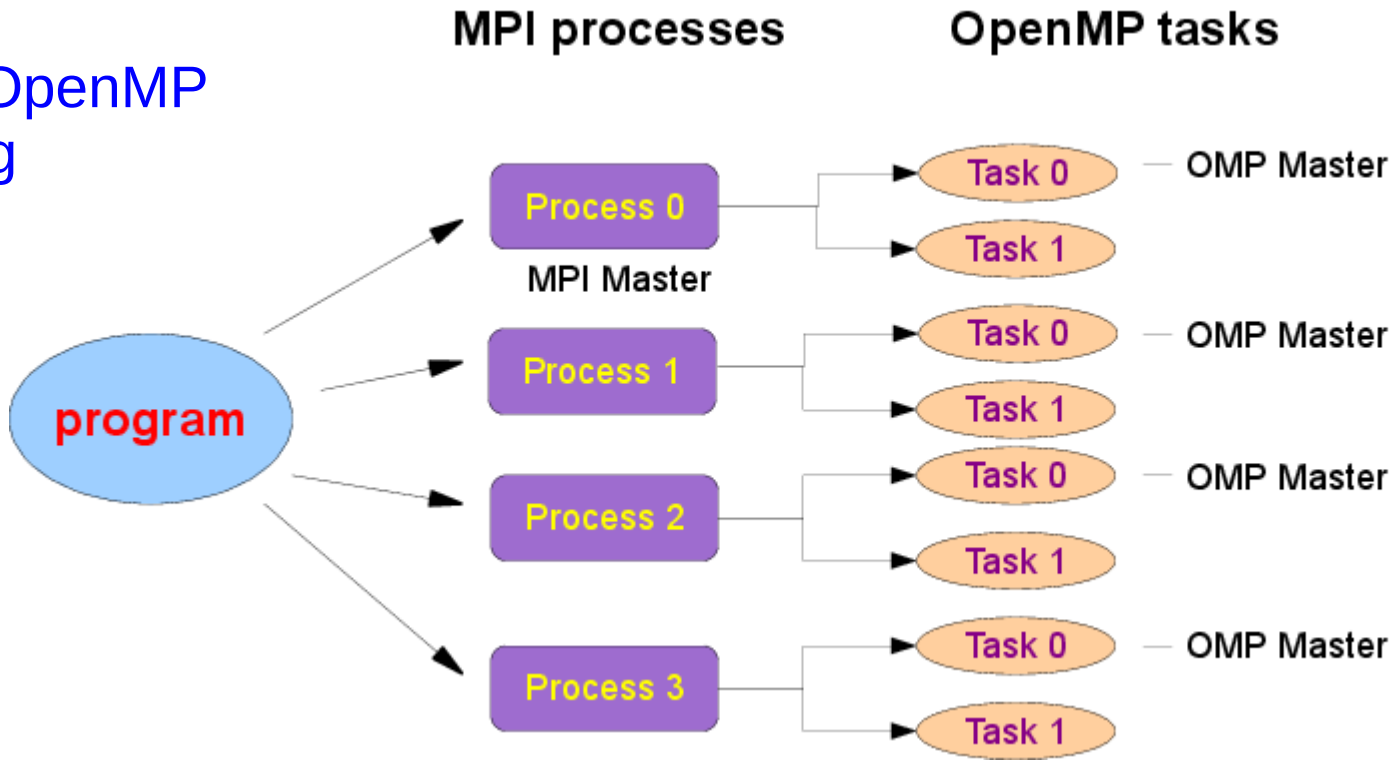
• This parallelism is based on the principle of multithreading. Multiple tasks (threads) run concurrently within a process.

• Each task essentially has (shared) **access to the global memory** of the process.

• Loops are parallelized using directives (!$OMP ... , which are included in the source code where they appear as comments) interpreted by the compiler.

• The number of OpenMP threads to used is set via an environment variable OMP_NUM_THREADS (e.g.: OMP_NUM_THREADS=4)

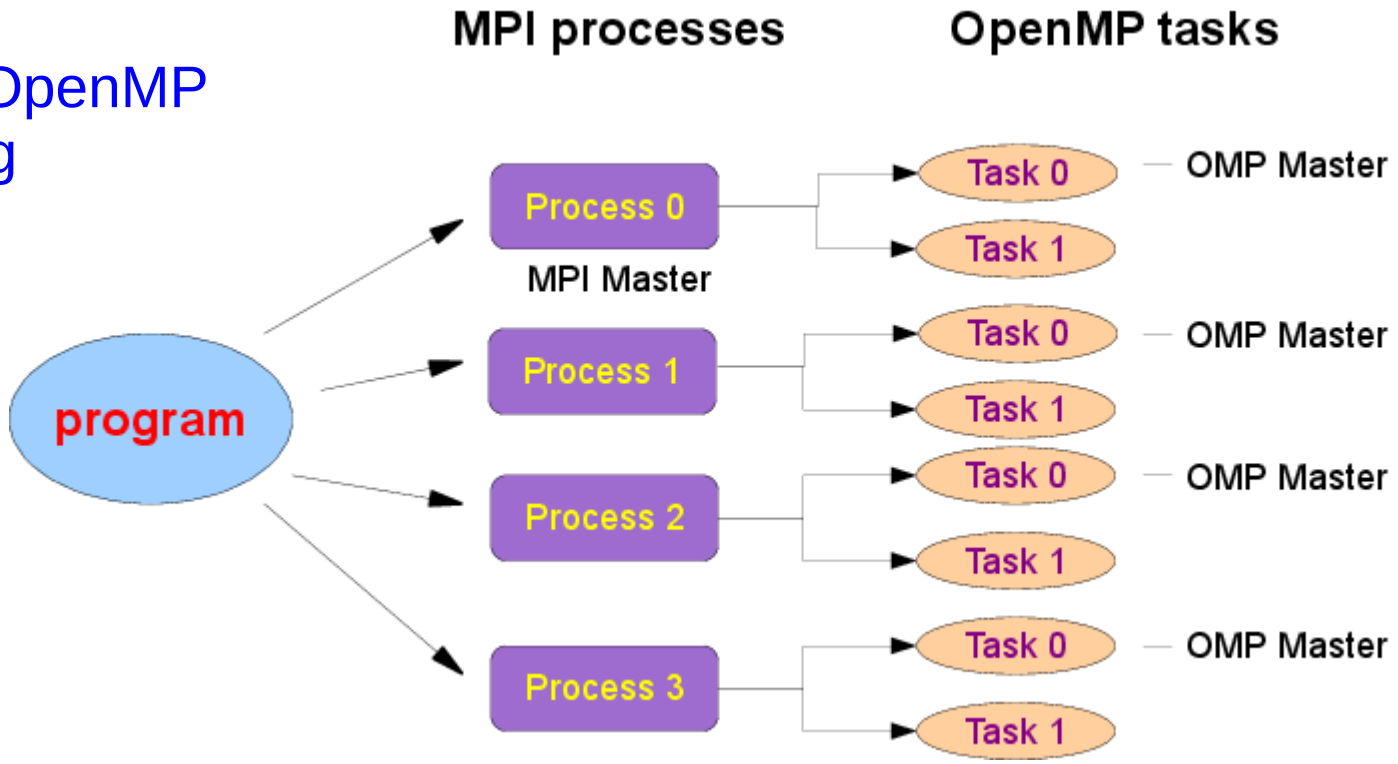
Hybrid MPI/OpenMP programming



- Each MPI process launches OpenMP threads which have access to its global memory. (threads also have private memory for specific variables)

- In LMDZ, MPI and OpenMP are differently implemented to best fit requirements. The number of OpenMP threads per MPI process is fixed and remains the same throughout a simulation.

Hybrid MPI/OpenMP programming



Different parallization approaches in the dynamics and physics

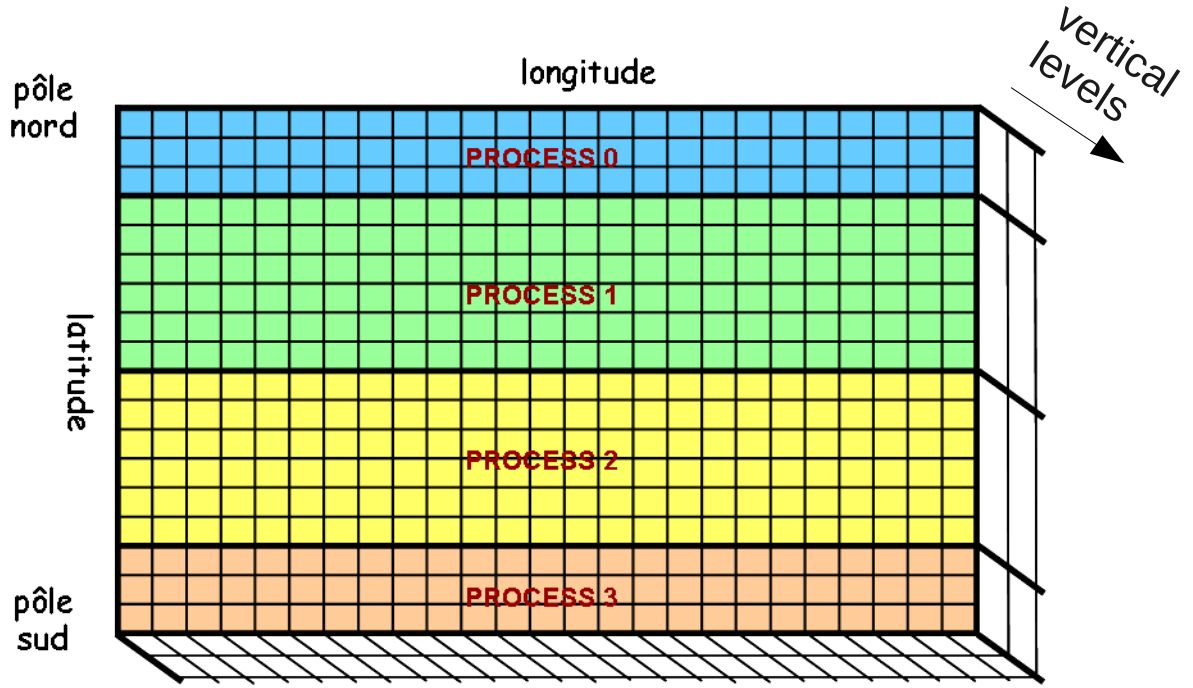
- In the dynamics

  Short time steps; many interactions between neighbouring meshes, and therefore numerous cases of data exchange and synchronizations. The subtler part of the parallelism in the code..

- In the physics

  longer time steps; **no interaction** between neighbouring columns of the atmosphere.

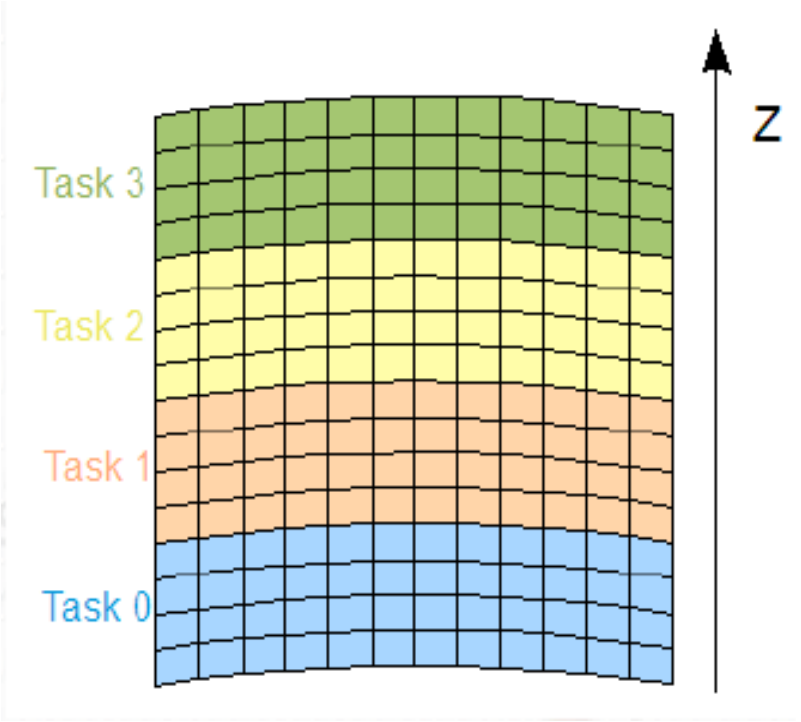
Parallelism in the dynamics



=> MPI tiling

- Tiling is by bands of latitude.
- A minimum of 3 latitude bands per MPI process is mandatory.
- But the work load is not the same for all latitudes (essentially because of the polar filter).
- Use option *adjust=y* (in *gcm.def*) to dynamically optimize (during the run) the band distribution of processes.
  - Run the GCM (in MPI mode only!) over at least a few thousand time steps to obtain a Bands_**x**x**_*prc.dat file.
  - Re-run the simulation using option *adjust=n* (with the Bands_* file in the run directory)
    NB: if there is no Bands_* file, the GCM creates one with a uniform balance between processes

Parallelism in the dynamics

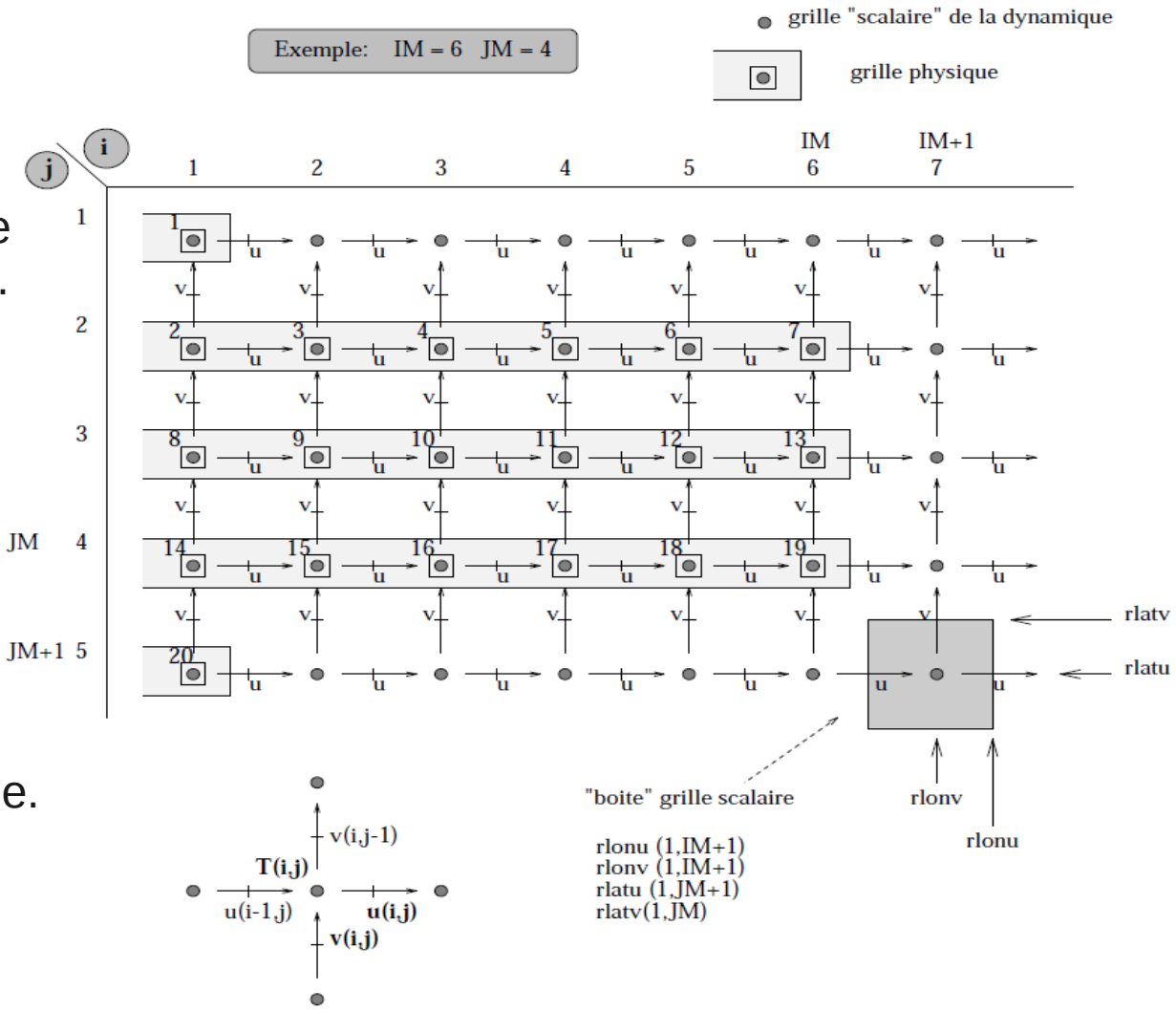


=> OpenMP split

- The split is done along the vertical levels only (the outermost loop in most computations).
- An indicate size of blocs to assign to each thread can be specified using option *omp_chunck*=... in gcm.def.
- In practice, target chunks of 4 or 5 vertical levels for each OpenMP task (an optimal compromise, but which may depend on the machine on which the code is run).

Parallelism in the physics

- The physics handles physical phenomena which interact within a single atmospheric column: radiation, convection boundary layer, etc.
- Individual columns of atmosphere **do not interact** with one another.
- The paralellization strategy is to distribute the colums of atmosphere over all cores.
- The physics grid : klon_glo geographic points over klev vertical levels.
  First node (1) => North pole,
  last node (klon_glo) => South pole.

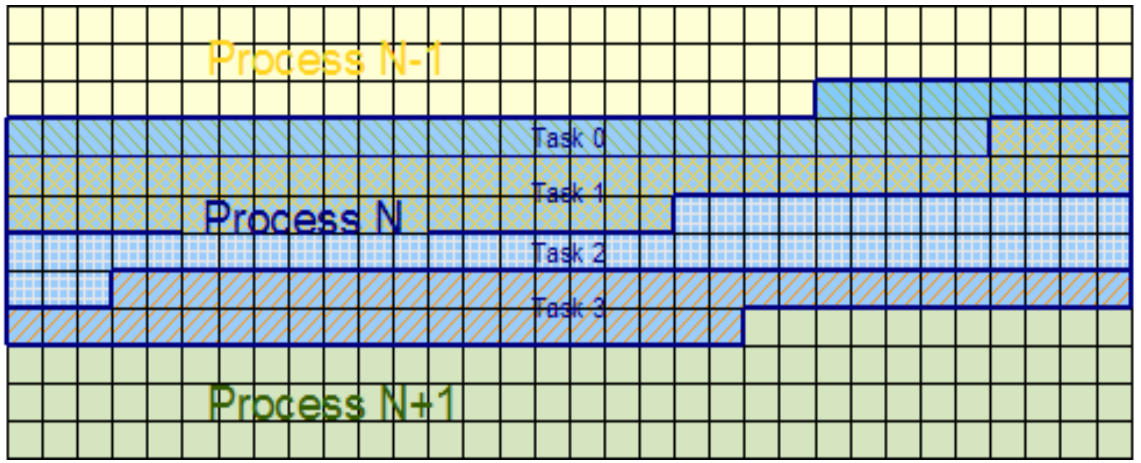


Parallelism in the physics

- The columns from the global domain are first distributed among the MPI processes.
  - The global domain : klon_glo columns of atmosphere

- The columns of each MPI domain are assigned to the OpenMP tasks assigned to the that process :
  - In each MPI domain : klon_mpi columns : Σ klon_mpi = klon_glo
  - In each OpenMP domain : klon_omp columns : Σ klon_omp = klon_mpi

- In practice, the size of the local domain klon is **an alias** of klon_omp (so as to behave exactly as when running the serial code).
  - ➔ Never forget that klon varies from one core to another.



Some code parameters linked to parallelism

Global grid : module mod_grid_phy_lmdz

- klon_glo : number of horizontal nodes of the global domain (1D grid)
- nbp_lon : number of longitude nodes (2D grid) = iim
- nbp_lat : number of latitude nodes (2D grid) = jjm+1
- nbp_lev : number of vertical levels = klev or llm

MPI grid : module mod_phys_lmdz_mpi_data

- klon_mpi : number of nodes in the MPI local domain.
- klon_mpi_begin :start index of the domain on the 1D global grid.
- klon_mpi_end : end index of the end of the domain on the 1D global grid.
- ii_begin : longitude index of the beginning of the domain (2D global grid).
- ii_end : longitude index of the end of the domain (2D global grid).
- jj_begin : latitude index of the beginning of the domain (2D global grid).
- jj_end : latitude index of the end of the domain (2D global grid).
- jj_nb : number of latitude bands = jj_end-jj_begin+1
- is_north_pole : .true. If the process includes the North pole.
- is_south_pole : .true. If the process includes the south pole.
- is_mpi_root : .true. If the process is the MPI master.
- mpi_rank : rank of the MPI process.
- mpi_size : total number of MPI processes.

Some code parameters linked to parallelism

OpenMP grid : module mod_phys_lmdz_mpi_data

- klon_omp : number of nodes in the local OpenMP domain.
- klon_omp_begin: beginning index of the OpenMP domain within the MPI domain.
- klon_omp_end : end index of the OpenMP domain.
- is_omp_root : .true. If the task is the OpenMP master thread.
- omp_size : number of OpenMP threads in thhe MPI process.
- omp_rank : rank of the OpenMP thread.

Coding constraints in the physics

• Nothing specific to worry about (compared to serial case) if :
  - There is no interaction between atmospheric columns
  - No global or zonal averages need be computed
  - There are no input or output files to read or write

• One mandatory thing to enforce for OpenMP : all variables declared as SAVE or in « common » blocks must be protected by an !$OMP THREADPRIVATE clause, for instance :

```
REAL, SAVE :: save_var
!$OMP THREADPRIVATE(save_var)
```

• Arrays must be allocated with the local size klon, since klon may vary from a core to another; for instance :

```
ALLOCATE (myvar(klon))
```

Warning! Note that in the general case, myvar(1) or myvar(klon) are neither North nor South poles.

• Use the logical variables, is_north_pole et is_south_pole if a specific treatment for the poles is required

Data transfer in the physics

- Care is required if :
  - there is some interaction between atmospheric columns
  - some zonal or global averages need be computed
  - files must be read or written

=> Then, some transfers between MPI processes and OpenMP tasks will be required:

- All **transfer routines are encapsulated** and transparently handle communications between MPI processes and OpenMP tasks.

- All are include in module : mod_phys_lmdz_transfert_para

The transfer interfaces handle data of all the basic types :
REAL
INTEGER
LOGICAL
CHARACTER : only for broadcast

The transfer interfaces moreover can handle fields of 1 to 4 dimensions.

Data transfer in the physics (continued)

Broadcast : the master process duplicates its data to all processes and tasks.

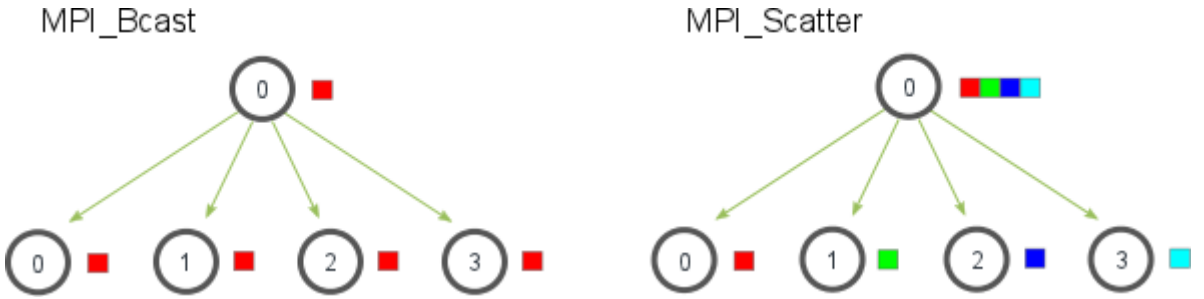
Independently of the variable's dimensions

CALL bcast(var)

Scatter : the master task has a field on the global grid (klon_glo) which is to be scattered to the local grids (klon).

The first dimension of the global field must be klon_glo, and the one of the local field must be klon

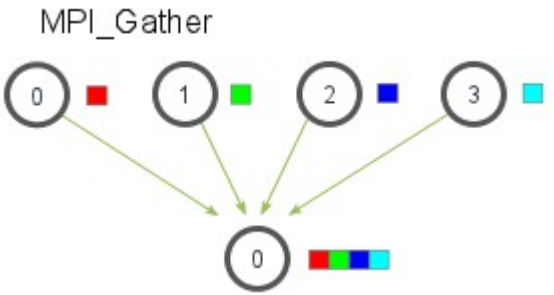
CALL scatter(field_glo,field_loc)



Gather : a field defined on the local grids (klon) is gathered on the global grid of the master process (klon_glo).

The first dimension of the global field must be klon_glo, and the one of the local field must be klon

CALL gather(field_loc,field_glo)



Figures from: http://mpitutorial.com/mpi-scatter-gather-and-allgather/

Scatter2D : same as Scatter exept that the global field is defined on a 2D grid of : nbp_lon x nbp_lat.

The first and second dimensions of the global field must be (nbp_lon,nbp_lat), and the first dimension of the local field must be klon

```
CALL scatter2D(field2D_glo,field1D_loc)
```

Gather2D : gather data on the 2D grid of the master process.

```
CALL gather2D(Field1D_loc,Field2D_glo)
```

Some examples

Reading physics parameters from files physiq.def and config.def

- Done in conf_phys.F90
- The master task read the value (call getin('VEGET',ok_veget_omp) within an !$OMP MASTER clause) and then duplicates it to the other tasks (after the !$OMP END MASTER , there is an ok_veget = ok_veget_omp)

Reading the initial state for the physics : startphy.nc

- Done in phyetat0.F
- The master task of the master process (if(is_mpi_root.and.is_omp_root) or equivalently if(is_master)) reads the field on the global grid and then scatters it to the local grids using the scatter routine.
- Encapsulated in the get_field routine of the iostart module.

Writing the final state for the physics : restartphy.nc

- Done in phyredem.F
- Encapsulated in routine put_field of the iostart module, put_field first does a gather to collect all the local fields into a global field. Then the master task of the master process writes the field in the restart file restarphy.nc.

Illustrative example of load data from a file, (simplified) extracted from phylmd/read_map2D.F90

```
USE dimphy
USE netcdf
USE mod_grid_phy_lmdz
USE mod_phys_lmdz_para
...

REAL, DIMENSION(nbp_lon,nbp_lat) :: var_glo2D
REAL, DIMENSION(klon_glo)        :: var_glo1D
REAL, DIMENSION(klon)            :: varout

! Read variable from file. Done by master process MPI and master thread OpenMP
  IF (is_mpi_root .AND. is_omp_root) THEN
     NF90_OPEN(filename, NF90_NOWRITE, nid)
     NF90_INQ_VARID(nid, varname, nvarid)

     start=(/1,1,timestep/)
     count=(/nbp_lon,nbp_lat,1/)
     NF90_GET_VAR(nid, nvarid, var_glo2D,start,count)
     NF90_CLOSE(nid)

     ! Transform the global field from 2D to 1D
     CALL grid2Dto1D_glo(var_glo2D,var_glo1D)
  ENDIF

! Scatter global 1D variable to all processes
  CALL scatter(var_glo1D, varout)
```

Writing output IOIPSL files and rebuilding the results

- Each MPI process writes data for its domain in a distinct file. One thus obtains as many files histmth_00XX.nc files as processes were used for the simulation.

- The domain concerned by a given IOIPSL file is defined with a call to histbeg, which is encapsulated in histbeg_phy (module iophy.F).

- Data is gathered on the master (rank 0) OpenMP task for each process. Each MPI process then calls the IOIPSL routine histwrite, which is encapsulated in histwrite_phy (module iophy.F).

- **Warning**: what is mentioned above is only true for **outputs in the physics**; it is also possible to make some outputs in the dynamics (triggered via ok_dyn_ins and ok_dyn_ave in *run.def*), but for these, data is moreover gathered on the master process so that there is only one file on output (which is a major bottleneck, performance-wise) => should only be used for debugging.

Writing output IOIPSL files and rebuilding the results

Once the simulation finished, one must gather the data in a single file.
This requires using the rebuild utility:

```
rebuild -o histmth.nc histmth_00*.nc
```

- rebuild is a utility distributed with IOIPSL
  See « How to install IOIPSL and the rebuild utility» in the LMDZ website FAQ
  (http://lmdz.lmd.jussieu.fr/utilisateurs/faq-en)

- In the IDRIS and CCRT supercomputing centres, rebuild is available to all, along with other common tools :

IDRIS
Ada/Adapp : /smphome/rech/psl/rpsl035/bin/rebuild

CCRT
Curie : /home/cont003/p86ipsl/X64/bin/rebuild

The XIOS library

- Next generation of the output library (IOIPSL not upgraded any more, will become depreciated).

https://forge.ipsl.jussieu.fr/ioserver

- Having installed the XIOS library (reference versions on global IPSL account on Ada and Curie), compile LMDZ using the “-io xios” option:

makelmdz_fcm -mem -parallel [mpi|omp|mpi_omp] -io xios .....

- Set flag “ok_all_xml=y” in run.def in order to control the ouputs in the X**.nc files from the related *.xml files. Or leave “ok_all_xml=n” to control outputs as with IOIPSL, from the output.def file

- With XIOS, output files can be generated as single files (no need to rebuild output files), by setting type=”one_file” par_access=”collective” parameters in the attributes of the “file” definition in the xml:

<file_definition type=”one_file” par_access=”collective” ..... >

Mixed bag of thoughts, advice and comments

- To run on a « local » machine (typically a multicore laptop):
  - An MPI library must be installed, and the « arch » files must be correspondingly modified to compile the model: 'makelmdz_fcm -arch local [-mem] ...'
  - It is always best to be able to use as much memory as possible: ulimit -s unlimited
  - It is also important to reserve enough private memory for OpenMP tasks: export OMP_STACKSIZE=200M
  - Use 'mpiexec -np n ...' to run with n processes, and 'export OMP_NUM_THREADS=m' to use m OpenMP tasks
  - Some examples and advice are given here (in English and French): http://lmdz.lmd.jussieu.fr/utilisateurs/guides/lmdz-parallele-sur-pc-linux-en

- To run on clusters (Climserv, Ciclad, Gnome, ...) and machines of supercomputing centres (IDRIS, CCRT,..):
  - Check the centre's documentation to see how to specify the number of MPI processes, OpenMP tasks, local limitations (memory, run time) for batch submission of jobs, etc.
  - Some information on appropriate job headers for some of the machines widely used at IPSL is gathered here (in French): https://forge.ipsl.jussieu.fr/igcmg/wiki/IntegrationOpenMP

Illustrative Example of a purely MPI job (loadleveler) on Ada (IDRIS)

> cat Job_MPI

```
# ########################
# ##     ADA IDRIS    ##
# ########################
# @ job_name = test
# @ job_type = parallel
# @ output = $(job_name).$(jobid)
# @ error =  $(job_name).$(jobid)
# Number of MPI processes to use
# @ total_tasks = 32
# Maximum (wall clock) run time hh:mm:ss
# @ wall_clock_limit = 0:30:00
# Default maximum memory per process is 3.5Gb, but one
# can ask for up to 7.0Gb with less than 64 processes
# @ as_limit = 3.5gb
# End of job header
# @ queue


poe ./gcm.e  > gcm.out  2>&1
```

> llsubmit Job_MPI

Illustrative Example of a mixed MPI/OpenMP job (loadleveler) on Ada

> cat Job_MPI_OMP

```
# ########################
# ##     ADA IDRIS    ##
# ########################
# @ job_name = test
# @ job_type = parallel
# @ output = $(job_name).$(jobid)
# @ error =  $(job_name).$(jobid)
# Number of MPI processes to use
# @ total_tasks = 16
# Number of OpenMP threads per MPI process
# @ parallel_threads = 4
# Maximum (wall clock) run time hh:mm:ss
# @ wall_clock_limit = 0:30:00
# Maximum memory per process is 3.5Gb x parallel_threads if more
# than 64 processes; 7.0Gb x parallel_threads otherwise
# @ as_limit = 14.0gb
# End of job header
# @ queue

# Set the private stack memory for each thread
export OMP_STACKSIZE=200M

poe ./gcm.e  > gcm.out  2>&1
```

> llsubmit Job_MPI_OMP

libIGCM

• The modipsl/libIGCM environment manages IPSL models (LMDZOR, LMDZORINCA, IPSLCM5, LMDZREPR, ORCHIDEE_OL) as a platform which simplifies extraction, installation and setting up simulations on the supercomputers “traditionally” used at IPSL; documentation available on

http://forge.ipsl.jussieu.fr/igcmg_doc/wiki/Doc

• The distributed job headers and a few parameters may still need be modified (e.g. memory requirements and maximum allowed run time).

• Recombination of the output files (rebuild) is automatically done.

• There are regularly modipsl/libIGCM courses (organized by Josefine Ghattas & Anne Cozic) ; sometimes in French and sometimes in English.

http://forge.ipsl.jussieu.fr/igcmg_doc/wiki/Train

To summarize

► In the physics, as long as there is no communication between columns, you can develop and modify code “as if in serial”. Only mandatory requirement (for OpenMP): variables which have a SAVE attribute have to be declared as !$OMP THREADPRIVATE.

➔ Do take the time to check the correct integration of modifications! Results should be identical (bitwise) when the number of processes or OpenMP threads is changed (at least when compiling in 'debug' mode).

► In the dynamics, parallelism is much more intrinsic; one should really take the time to understand the whole system before modifying any line of code.

► One can compile in any of the following parallel modes: mpi, omp or mpi_omp
makelmdz_fcm -mem -parallel [mpi|omp|mpi_omp] .....

► A run should use as many cores as possible, without forgetting that the maximum number of MPI processes = number of nodes along the latitude / 3 and that it is usually best to use 1 OpenMP task for every 4 or 5 points along the vertical.

► To optimize the workload among different MPI processes, run a first month with *adjust=y* in run.def. And then use the obtained bands_resol_Xprc.dat files for the following simulations.