Development constraints *including presentation of constraints due to shared code with Arp/Ifs*

Filip Váňa

filip.vana@chmi.cz

ONPP / ČHMÚ - LACE

Outline

- Basic rules
- Parallelization principles
- Concept of NPROMA
- Data structures

Basic code rules

Coding rules and conventions (Karim's talk)

- Coding rules and conventions (Karim's talk)
- Bit reproducibility (with respect to different NPROMA values and different no. of PEs)

- Coding rules and conventions (Karim's talk)
- Bit reproducibility (with respect to different NPROMA values and different no. of PEs)
- Platform independence optimized for Scalar and Vector platforms

- Coding rules and conventions (Karim's talk)
- Bit reproducibility (with respect to different NPROMA values and different no. of PEs)
- Platform independence optimized for Scalar and Vector platforms
- Parallel code allows parallel computation, supports MPI and OpenMP standards

- Coding rules and conventions (Karim's talk)
- Bit reproducibility (with respect to different NPROMA values and different no. of PEs)
- Platform independence optimized for Scalar and Vector platforms
- Parallel code allows parallel computation, supports MPI and OpenMP standards
- MPI/OpenMP called only through MPL/OML modules (wrappers), CDSTRING should be set to the name of the caller routine

 Source code written in FORTRAN (F90, F77) and C (soon also C++)

- Source code written in FORTRAN (F90, F77) and C (soon also C++)
- DGEMM is only standard library routine

- Source code written in FORTRAN (F90, F77) and C (soon also C++)
- DGEMM is only standard library routine
- Error trapping usable for operational applications

- Source code written in FORTRAN (F90, F77) and C (soon also C++)
- DGEMM is only standard library routine
- Error trapping usable for operational applications
- 64 bit arithmetic and 64 bit addressing

- Source code written in FORTRAN (F90, F77) and C (soon also C++)
- DGEMM is only standard library routine
- Error trapping usable for operational applications
- 64 bit arithmetic and 64 bit addressing
- Spectral model = specific timestep organization $(S \to M \to L \to G \to L \to M \to S)$

- Source code written in FORTRAN (F90, F77) and C (soon also C++)
- DGEMM is only standard library routine
- Error trapping usable for operational applications
- 64 bit arithmetic and 64 bit addressing
- Spectral model = specific timestep organization $(S \to M \to L \to G \to L \to M \to S)$
- No a prior ordering of model fields

- Source code written in FORTRAN (F90, F77) and C (soon also C++)
- DGEMM is only standard library routine
- Error trapping usable for operational applications
- 64 bit arithmetic and 64 bit addressing
- Spectral model = specific timestep organization $(S \to M \to L \to G \to L \to M \to S)$
- No a prior ordering of model fields
- Indexing of model arrays is not arbitrary

- Source code written in FORTRAN (F90, F77) and C (soon also C++)
- DGEMM is only standard library routine
- Error trapping usable for operational applications
- 64 bit arithmetic and 64 bit addressing
- Spectral model = specific timestep organization $(S \to M \to L \to G \to L \to M \to S)$
- No a prior ordering of model fields
- Indexing of model arrays is not arbitrary
- all configurations share a single top-level call tree (the control levels has to be preserved: MASTER -> CNT0 -> CNT1 -> CNT2 -> CNT3 -> CNT4 -> STEPO
 MASTER -> CNT0 -> CVA1 -> CVA2 -> CONGRAD -> SIM4D -> CNT3 -> ...)

Parallelization

Computer architecture fundamentals:



node = collection of CPU with share a common memory

- MPI = Distributed memory parallelization available since AL08
- OpenMP = Shared memory parallelization available since AL29 (for AD code on Vector since AL32T2)
- Mixed/hybrid MPI and OpenMP parallelization available since AL35T2

Parallelization strategy - MPI

- Transposition strategy = complete data required is redistributed at various stages of a timestep so that the arithmetic computations between two consecutive transpositions can be performed without any inter-processor communication.
- Inter-processor communication is localized in a few routines and rest of the model need have no knowledge of this activity.
- Communication is realized through relatively long messages (1Mbytes) (Remember: short messages are bounded by latency of interconnect; long messages are bounded by bandwidth of interconnect)

Parallelization strategy - MPI II.

Different types of blocking strategy:

MP_TYPE = 1 blocked mode

- MP_TYPE = 2 buffered mode MPI_BSEND can return before
 the receive is called on the receiving processor. (This
 allows to reuse/destroy the sending array.)
- MP_TYPE = 3 immediate mode send and receive are returned immediately as the comms are performed in the background. Additional calls are then required to check or wait for the completion of a comm. (Sending array can be reused/destroyed only after MPI is confirmed to do so.)

GP computation

- **NPROC** Total number of processors to be used
- **NPRGPNS** Number of PEs in the North-South direction
- **NPRGPEW** Number of PEs in the East-West direction
- **LSPLIT** Allows the splitting of latitude rows

GP computation

- **NPROC** Total number of processors to be used
- **NPRGPNS** Number of PEs in the North-South direction
- **NPRGPEW** Number of PEs in the East-West direction
- **LSPLIT** Allows the splitting of latitude rows

SL comms as a specific feature

- squarer shape of domain = reduced comm volume for SL
- SL on demand targets (= reduces) the area of comms computed from VMAX2



Parallelization strategy - MPI IV.

Fourier transformation

- NPRTRW
 Number of processors in zonal/meridional decomposition

 (usually NPRTRW=NPRGPNS)
- NPRTRVNumber of processors in vertical decomposition
(usually NPRTRV=NPRGPEW)
- Decomposition along latitudes/longitudes * levels (there's no further independence across the fields).
- This means that for example Alaro/CE with 540*432 points and 87 levels reaches scalability limit for transformation at around 432*87=37584 MPI processes. (GP decomposition of the same domain and NPROMA=20 reaches its limit at around 421*540/20=11367 MPI processes.)

Parallelization strategy - MPI V.

Spectral SI calculation

- decomposition along NPRTRN = NPRTRV trivial as there's only vertical dependency for SI, (but might be more complicated for LIMPF=.T.)
- transpositions inside spectral space computation

Parallelization strategy - MPI VI.





Parallelization strategy - OpenMP

- Parallelize Loops between MPI calls
- High level (all GP computation is done within only 3 OpenMP parallel regions) and Loop level (leftovers like I/O)
- Strong sequential equivalence required to obtain bit-wise identical results - if multiple threads combine results into a single value, sequential order must be enforced (weak SE allowed but optionally only)
- Easy to implement but requires more maintenance to remain thread-save (bugs can lurk unknown)

Parallelization - MPI+OpenMP

Pros

- Lower MPI overheads
- Memory saving (if done properly!!!)
- Frees up processors for OS functions
- Helps balancing

Cons

- Whole code needs to be done (but not comms)
- Need some special care for vector platform (high values of NPROMA requires further optimization w.r.t. number of threads)

 Original code (designed for vector computers) coded with inner loops over horizontal in groups of NPROMA to give long vectors

- Original code (designed for vector computers) coded with inner loops over horizontal in groups of NPROMA to give long vectors
- No dependency in horizontal (important for avoiding memory conflicts)

- Original code (designed for vector computers) coded with inner loops over horizontal in groups of NPROMA to give long vectors
- No dependency in horizontal (important for avoiding memory conflicts)
- Physics and Dynamics computed in blocks of NPROMA

- Original code (designed for vector computers) coded with inner loops over horizontal in groups of NPROMA to give long vectors
- No dependency in horizontal (important for avoiding memory conflicts)
- Physics and Dynamics computed in blocks of NPROMA
- Bit reproducible with different NPROMA & no. of PEs

- Original code (designed for vector computers) coded with inner loops over horizontal in groups of NPROMA to give long vectors
- No dependency in horizontal (important for avoiding memory conflicts)
- Physics and Dynamics computed in blocks of NPROMA
- Bit reproducible with different NPROMA & no. of PEs
- The same design now good for cache

- Original code (designed for vector computers) coded with inner loops over horizontal in groups of NPROMA to give long vectors
- No dependency in horizontal (important for avoiding memory conflicts)
- Physics and Dynamics computed in blocks of NPROMA
- Bit reproducible with different NPROMA & no. of PEs
- The same design now good for cache
- NPROMA : Long for vector; short for scalar/cache

- Original code (designed for vector computers) coded with inner loops over horizontal in groups of NPROMA to give long vectors
- No dependency in horizontal (important for avoiding memory conflicts)
- Physics and Dynamics computed in blocks of NPROMA
- Bit reproducible with different NPROMA & no. of PEs
- The same design now good for cache
- NPROMA : Long for vector; short for scalar/cache
- Memory saving and easy OpenMP implementation

- Original code (designed for vector computers) coded with inner loops over horizontal in groups of NPROMA to give long vectors
- No dependency in horizontal (important for avoiding memory conflicts)
- Physics and Dynamics computed in blocks of NPROMA
- Bit reproducible with different NPROMA & no. of PEs
- The same design now good for cache
- NPROMA : Long for vector; short for scalar/cache
- Memory saving and easy OpenMP implementation
- Variability of NPROMA allows to keep control over memory conflicts (by over-dimensioning)

NPROMA II.

Illustration of NPROMA influence to model performance



Memory conflict

SX Shared Memory with 32 x 128 = 4096 memory banks and vector a(:)



If a(:) becomes A(NPROMA,NFLEVG) and by chance NPROMA=4096. In such case any loop over second dimension will cause bank conflict.

Memory conflict

SX Shared Memory with 32 x 128 = 4096 memory banks and vector a(:)



- If a(:) becomes A(NPROMA,NFLEVG) and by chance NPROMA=4096. In such case any loop over second dimension will cause bank conflict.
- \Rightarrow Situation becomes much better when array is overdimensioned to NPROMA=4097.

Model arrays decomposition

• usually no decomposition over levels and fields Example for GP arrays:

Model_Data(1:Decomp_2D_Field, 1:NFLEVG, 1:NFIELDS)
⇒

Model_Data(1:NPROMA, 1:NFLEVG, 1:NFIELDS, 1:NGPBLKS)

 various places (GLMS) use different decomposition ⇒ transpositions are moving data between processors to form a new decomposition

Data structures - GP space

GMV

- prognostic variables involved in the SI
- only attribute is field pointer (MU, MV,...)
- three modules:
 - YOMGV : contain the main GP arrays (GMV, GMVT1, GMV5, GMV_DEPART, GMVS, GMVT1S, GMV5S, GMVS_DEPART)
 - TYPE_GMVS: type descriptor to address the GMV arrays: (YT0, YT9, YT1, YPH9, YT5, YAUX)
 - GMV_SUBS: Contains subroutines used for setting up GMV
- usage (inside parallel regions):

```
DO JLEV=1,NFLEVG
DO JROF=KST,KPROF
```

```
PGMVT1(JROF, JLEV, YT1%MU) =PGMVT1(JROF, JLEV, YT1%MU) -POMVRL(JROF)
PGMVT1(JROF, JLEV, YT1%MV) =PGMVT1(JROF, JLEV, YT1%MV) -POMVRM(JROF)
ENDDO
```

ENDDO

Data structures - GP space II

GFL

- all other variables
- can be GP or SP
- plenty of attributes very flexible field definition through namelist

_ ...

Data structures - GP space II

GFL

. . .

- all other variables
- can be GP or SP
- plenty of attributes very flexible field definition through namelist

SL buffers

PB1(NASLB1,NFLDSLB1) PB2(NPROMA,NFLDSLB2,NGPBLKS)

buffer for interpolations

buffer to communicate non lagged to lagged dynamics

NASLB1 NFLDSLB1 NFLDSLB2 (over) number of columns in the core+halo region number of fields times vert. dimension in PB1 number of fields times vert. dimension in PB2

Data structures - Spectral space

- Module YOMSP contains:
 SPA1(NFLSUR,2) mean wind (in LAM only)
 SPA2(NSPEC2, NS2D) 2D spectral arrays
 SPA3(NFLSUR, NSPEC2,NS3D) 3D spectral arrays
- They are not NPROMA arryas!!!
 NFLSUR (over) number of vertical level (bank conflict!)
 NSPEC2 number of spectral coefficients
 NS3D, NS2D number of 3D/2D spectral fields