New version of EULAG with 3d domain decomposition

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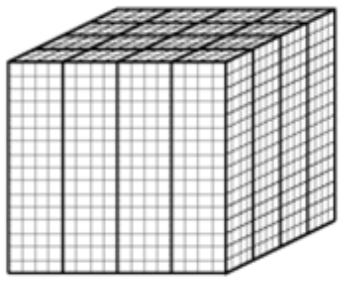
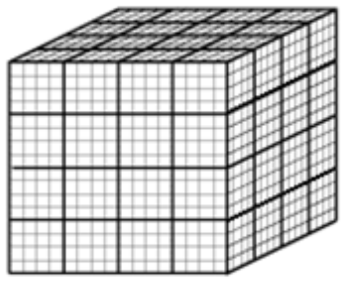
Codename Eulag 3p


2D


3D

Description of new features and optimizations

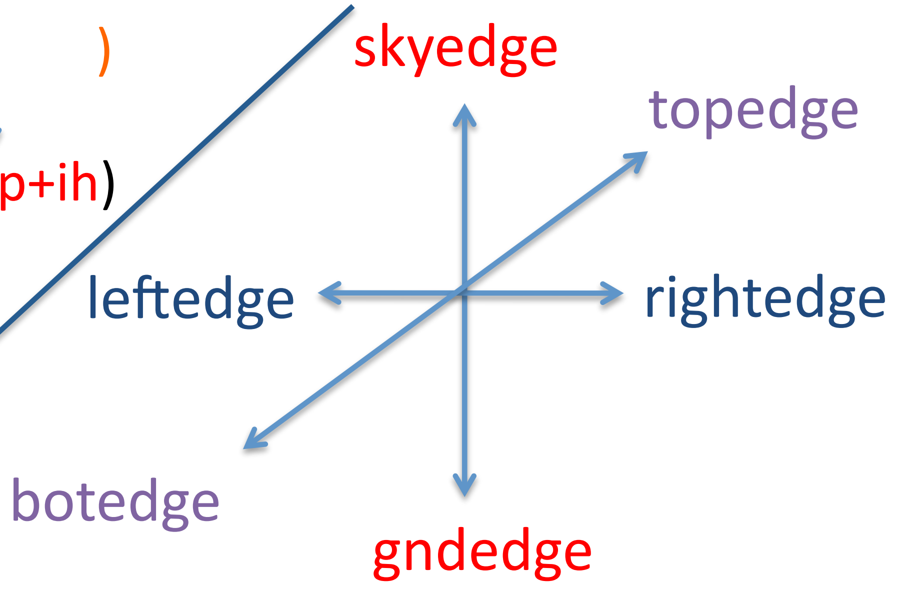
Loops and boundaries

Modified array declarations: 1-ih:mp+ih, l)

dimension u(1-ih:np+ih, 1-ih:mp+ih, 1-ih:lp+ih)

Loops throughout the code are now:

```
 do k=1,lp  (instead of do k=1,l )
      do j=1,mp
          do i=1,np
              ……
           enddo
      enddo
  enddo
```



New boundaries: gndedge and skyedge

```
If(ibcz.eq.1) then
       if (gndedge.eq.1) then
        do  j=jllim,julim
         do  i=illim,np
        v1(i,j,1)=vdyf(x(i-1,j,1),x(i,j,1),f1(i,j,1),
    *              .5*(h(i-1,j,1)+h(i,j,1)))
          enddo
        enddo
     endif  ! gndedge = 1
```

Processor grid and configuration

Processor grid is now defined by nprocz as well, e.g.:

```
        parameter (nprocx=4, nprocy=2, nprocz=4)
```

Processor position on the grid is now defined by lpos as well.
E.g., retrieval of the actual position (ia,ja,ka) from (i,j,k)
on a given processor is defined by:

```
 do 4 k=1,lp
     ka = (lpos-1)*lp + k
        do 4 j=1,mp
           ja = (mpos-1)*mp + j
              do 4 i=1,np
                 ia = (npos-1)*np + i
```

Updates and global operations

Update calls have now additional arguments, e.g.:

```
 call update(  ue,np,mp,lp,np,mp,lp,iup)
```

also there is a new type of update in the vertical direction only:

```
call updategs(pe,np+rightedge,mp+topedge,lp+skyedge,
     .                  np+1,mp+1,lp+1,iupz)
```

akin to iupx,iupy

Global operations (max,min,sum) also need additional arguments, e.g.:

```
 dftav=globsum(temp,1-ih,np+ih,1-ih,mp+ih,1-ih,lp+ih,
     .              1,np,1,mp,1,lp)
```

Optimizations

Petascale simulations with very large number of cores demand more focus on optimizing communication layer.

Processor geometry setup - new default Cartesian MPI topology option parameter(icart=1)

- Using icart=1 informs MPI system about the geometry of the task
- Results in several % smaller wall time, allows for more effective profiling in SCALASCA which is now able to understand mesh structure
- Invisible to the rest of the Eulag code …
- …. but, processors are usually numbered differently than for traditional icart=0 option, if you need to know how neighboring cores are distributed,

use peGNW,peGSW,peGSE,peGNE,
. peGW,peGE,peGN,peGS,
. peZNW,peZSW,peZSE,peZNE,
. peZW,peZE,peZN,peZS,
. peZ,peG,peW,peE,peN,peS,
. peNW,peSW,peSE,peNE

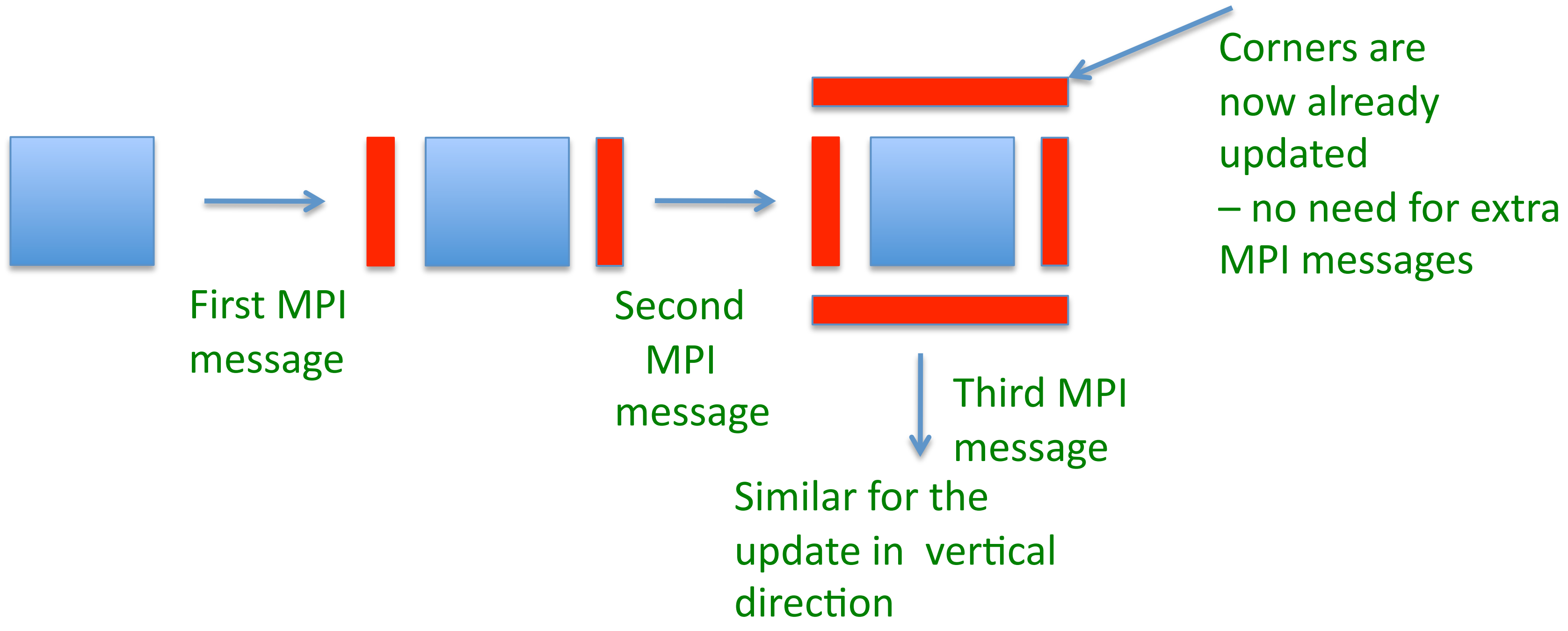
Z stands for “Zenith”

G stands for “Ground”

(replaces traditional peleft,peright,peabove,pebelow, etc.)

Brand new update subroutine

• Traditional set of update subroutine (update, updatelr, updatebt, updatew, update2) replaced with one subroutine update3dsplitn
• Invisible to the users, traditional calls to update, updatelr, updatebt, etc. are now WRAPPERS only (translating simple old way of calling to the fully universal update3dsplitn)
• New update3dsplitn limits number of MPI messages to three, but two of them communicating the domain WITH HALO


Corners are now already updated – no need for extra MPI messages
First MPI message
Second MPI message
Third MPI message
Similar for the update in vertical direction

Further halo update optimizations

- New update3dsplitn allows for overlapping computations and communications
- New set of OPTIONAL subroutines are defined and can be used as in the following example:

```
    call updatelrbeg(f1,np+rightedge,mp,lp,np+1,mp,lp,1,1)
     do 403 j=1,lp+skyedge
     do 403 i=1,np
 403 f2(i,1,j)=donor(c2,c2,v2(i,1,j))
     call updatelrend(f1,np+rightedge,mp,lp,np+1,mp,lp,1,1)
```

Last parameter for update..beg and update…end is a number of buffer (because one may wish to update more than one variable)

- Full update can be done in a sequence:

```
call updatelrbegf(f1,np+rightedge,mp,lp,np+1,mp,lp,1,1)
…..
call updatelrendf(f1,np+rightedge,mp,lp,np+1,mp,lp,1,1)
call updatebtbegf(f1,np+rightedge,mp,lp,np+1,mp,lp,1,1)
…..
call updatebtendf(f1,np+rightedge,mp,lp,np+1,mp,lp,1,1)
call updategsbegf(f1,np+rightedge,mp,lp,np+1,mp,lp,1,1)
……
call updategsendf(f1,np+rightedge,mp,lp,np+1,mp,lp,1,1)
```

Further halo update optimizations #2

- For nonperiodic boundary conditions, you don’t need to update outer boundaries of the computational domain, which are usually far from each other inside the machine.
The only exception is *vbcad* subroutine.

- Therefore, there is an important change in DEFAULT behavior –
For nonperiodic b.c. there is no update on outer domain borders

- On the other hand, for periodic boundary conditions it is often unnecessary to update variables inside the domain. For these two purposes, new set of BORDER ONLY updates are defined:

```
if(ibcz.eq.1) then
     call updategsbor(p,np,mp,lp,np,mp,lp,1) ! updategsborbeg and updategsborend possible
      if(skyedge.eq.1) then
        do 10 j=1,mp
          do 10 i=1,np
 10           p(i,j,lp)=p(i,j,lp+1)
       endif
```

Global communication optimizations

• Global summation, max and min operations are necessary for elliptic solver but EXTREMELY expensive (and relative cost growing)

•Therefore, there is a need to minimize number of AlltoAll operations

•It is done by global operations (sum, max, min or combined) on vectors

Example:

globsumvbor - sums u,v,w outflow, inflow and weights in vbcad within 1 global communication instead of 9 (especially useful when you call vbcad every timestep)

globsumv, globmaxv, globsumaxv – sums, finds max, or both at the same global communication for vector of data

Example (from gcrk):

```
eetabs(1)=qrlsum
eetabs(2)=qrlmax
call globsumaxv(eetabs,eetabd,2)
  eer=eetabd(1)
eem=amax1(eem,sqrt(eetabd(2)))
```

```
call MPI_OP_CREATE
.(sumax,commute,MPI_SUMAX,err)
 function sumax(wrkin,wrkinout,ihalf,itype)
      do i=1,ihalf
      wrkinout(i)=wrkin(i)+wrkinout(i)
      wrkinout(ihalf+i)=amax1(wrkinout(ihalf+i)
.                             ,wrkin(ihalf+i))
```

Other optimizations

• In principle, it is not necessary to compute all the norms for exit conditions from GCRK iterations at each timestep since they need expensive global communication. Threshold for these computations:

```
parameter(itertrem=0.5)  ! Could be any number between (0,1)
```

defines at which fraction of the last number of GCRK iterations, the norms for GCRK exit conditions will be computed.

• Computations of precon_bcz coefficients now takes place once per gcrk call in precon_bcz_ini

• Parallel tridiagonal solver, necessary if nprocz > 1 is implemented in tdmapar subroutine. Variables isequp, iseqdn initialized in blockdata blanelas choose details of algorithms (default: 7, failsafe: 1)

• Parallel NETCDF long and short tape write is now called by iowrite/ioread and iowrsh/iorsh subroutines as the standard Fortran tape

Compiler setup

• Cray supercomputers and Linux clusters, very popular these days, offer various compilers (PGI, Intel, Cray, Pathscale, GNU), which makes maintenance of library, compiling and submission scripts difficult

• Set of new environmental variables has been introduced to facilitate switching between the compilers, optimization levels and submission methods:

```
##################################################################################
##
#### Choose compiler if more then one available
##
##   0 - Default compiler
##   1 - PGI compiler
##   2 - Intel compiler
##   3 - Pathscale compiler
##   4 - Cray  compiler
##   5 - GNU compiler
##
###################################################################################
setenv COMPILER 4
```

```
###################################################################
###########
####  Define level of compiler optimization
##    0  - no optimization at all (for very fast compilation)
##    1  - full set of diagnostic and debugging options
##    2  - default optimization   (different for different machines)
##    3  - strong  optimization   (recommended by compiler vendors)
##    4  - maximum optimization   (usually -O4 or -O5 with IPA)
###################################################################
###########
setenv COMPOPTI 0
###################################################################
###########
##
#### Define special option for code instrumentation for profiling
#### Default: setenv CODEINST 0
##   0 - No instrumentation (default)
##   1 - Scalasca instrumentation with skin
##   2 - Tau compiler instrumentation
##   3 - Tau PDT instrumentation
##
###################################################################
###########
setenv CODEINST 0
```

Architectures

Recently, Eulag has been successfully run on the following modern architectures (setups available):

- Intel Linux cluster (JANUS @ CU, Boulder)
- IBM Power 7 (ICM, Poland)
- Bluegene/P (ICM, Poland)
- Cray XE 6 (CSCS, Switzerland)
- Cray XT5m (NCAR, Boulder)

Optimizations discussed are not fully tested, IFASTSUBS 0 and IOVER 0 available to switch to generic "failsafe" mode without optimizations

Known problems:

- Each new machine is likely to cause some problems
- Standard optimizations of some newer versions of PGI

may not work, always try COMPOPTI 0 to see if it helps.

Parallelization status

- Tested and work: 2D/3D Eulerian/SL solver, GCRK, bulk moist models, ILES/SGS 1/SGS 2, ANALIZ 1 mode, velocity predictor

- Untested: WORD 4 time integration, grid adaptivity, , SGS 2 for ibcz=1 seems incomplete, although parallelized

- Not parallelized/implemented yet: single core mode, zonal absorbers, parallel diagnostic packages, efficient precon_bcz for ibcz=1, MHD, unstructured

- Serial NETCDF and slices subroutines are not fully parallelized and/or not up to date