CRAY T3E
Parallelization of grid–based applications

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Agenda

- ❑ Numerical solution of the Laplace equation (serial)
- ❑ Numerical solution of the Laplace equation (parallel)
- ❑ Intermezzo on Cray T3E hardware
- ❑ Parallel implementation

The Laplace equation

The Laplace equation in two dimensions:

$-\Delta u = f$ on $\Omega = (0,1) \text{ x } (0,1)$

$u = g$ on $d\Omega$ (Dirichlet)

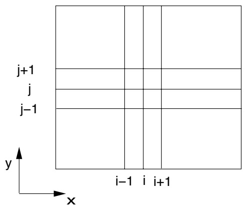
Approximate solution required:

* Define a mesh or grid consisting of points (xi, yj)

* Compute the (approximate) solution in these grid points

Discretization

Discretization on the computational domain by means of finite differences:

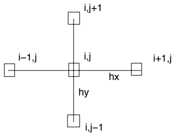


Several approaches to compute u(i,j) based on its neighbouring points. This is called a *stencil*.

Note that the distances in x– and y–direction do not need to be equal (non–equidistant).

Stencil

The stencil we will use is the following (5–point):



The solution method we will use is iterative.
Its general form is:

u(i,j) = F(u(i,j),u(i–1,j),u(i+1,j),u(i,j–1),u(i,j+1),f,hx,hy)

In words: the new value of u(i,j) is computed from the old and new values from itself and its neighbours

For simplicity, assume: hx = hy = h

Discretization

$$\Delta = \delta^2 u/\delta x^2 + \delta^2 u/\delta y^2$$

$$\delta u/\delta x = \frac{u(i+1/2) - u(i-1/2)}{h}$$

$$\delta^2 u/\delta x^2 \text{ ––––> } \frac{u(i+1,j) - 2u(i,j) + u(i-1,j)}{h^2}$$

$$\delta^2 u/\delta y^2 \text{ ––––> } \frac{u(i,j+1) - 2u(i,j) + u(i,j-1)}{h^2}$$

Then:

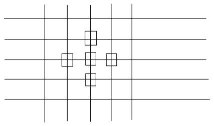
$$-u(i+1,j) + 2u(i,j) - u(i-1,j) - u(i,j+1) + 2u(i,j) - u(i,j-1) = h*h*f(i,j)$$

$$u(i,j) = 0.25*h*h*f(i,j) + 0.25*(u(i-1,j)+u(i+1,j)+u(i,j-1)+u(i,j+1))$$

Example iterative methods

Point Jacobi:
unew(i,j) = 0.25*(h*h*f(i,j) + uold(i–1,j) + uold(i+1,j) + uold(i,j–1) + uold(i,j+1))

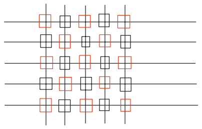
Point Gauss–Seidel:
unew(i,j) = 0.25*(h*h*f(i,j) + unew(i–1,j) + uold(i+1,j) + unew(i,j–1) + uold(i,j+1))



Example iterative methods

Red–Black Gauss–Seidel:
unew(i,j) = 0.25*(h*h*f(i,j) + unew(i–1,j) + uold(i+1,j) + unew(i,j–1) + uold(i,j+1))

Two sweeps:
red sweep: all red points
black sweep: all black points



Treatment of boundaries

Dirichlet boundary conditions:
$u = g$ on $d\Omega$

Suppose, the number of internal grid points is N*N
Then, including the boundaries, the total number of points is (N+2)*(N+2)

Then, the distance between two neighbouring points is h = 1/(N+1)

Internal points range: i = 1, ..., N
j = 1, ..., N

Before start of iteration process, initialize the boundary point solution to g, and use it in the stencil calculations

Basic serial algorithm

The basic serial algorithm looks as follows:

```
Input

Initialize grid
Initialize boundary values

while ((no convergence) .and. (no_max_iter))

    Sweep over red points
    Sweep over black points
    Determine convergence
    uold = unew

end while

Output
```

Detailed serial algorithm

"Initialize grid"

Remember:

$$-\Delta u = f \quad \text{on} \quad \Omega = (0,1) \times (0,1)$$
$$u = g \quad \text{on} \quad d\Omega$$

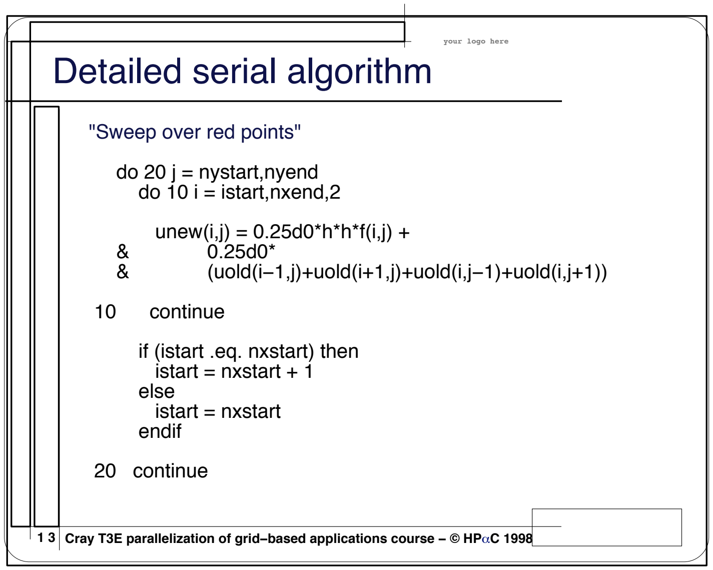
```
      do 40 j = nystart–1,nyend+1
        do 40 i = nxstart–1,nxend+1
          x(i,j)      = dble(i)/dble(nx+1)
          y(i,j)      = dble(j)/dble(ny+1)
          f(i,j)      = funcf(x(i,j),y(i,j),itype)
          uexact(i,j) = uexactf(x(i,j),y(i,j),itype)
          uold(i,j)   = 0.0d0
 40   continue
```

itype denotes the kind of testproblem

Detailed serial algorithm

"Initialize boundary values"

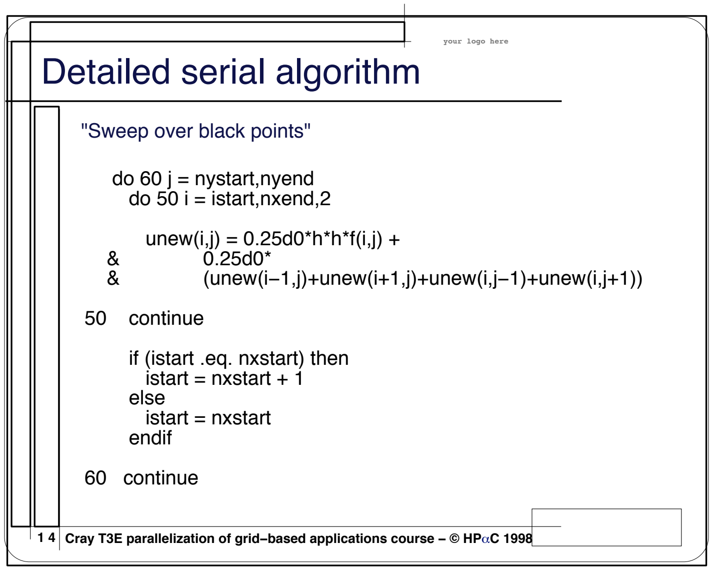
```
c
c  south boundary
c
      if (south .eq. –1) then

        j = 0
        do 51 i = 0,nx+1
          xx     = x(i,j)
          yy     = y(i,j)
          u(i,j) = exp(–(xx–yy)*(xx–yy))
 51       continue
      endif
c
c  north boundary
c
      if (north .eq. –1) then

        j = ny+1
        do 61 i = 0,nx+1
          xx     = x(i,j)
          yy     = y(i,j)
          u(i,j) = exp(–(xx–yy)*(xx–yy))
 61       continue
      endif
c
c  west boundary   ..............................
```



Detailed serial algorithm

"Sweep over red points"

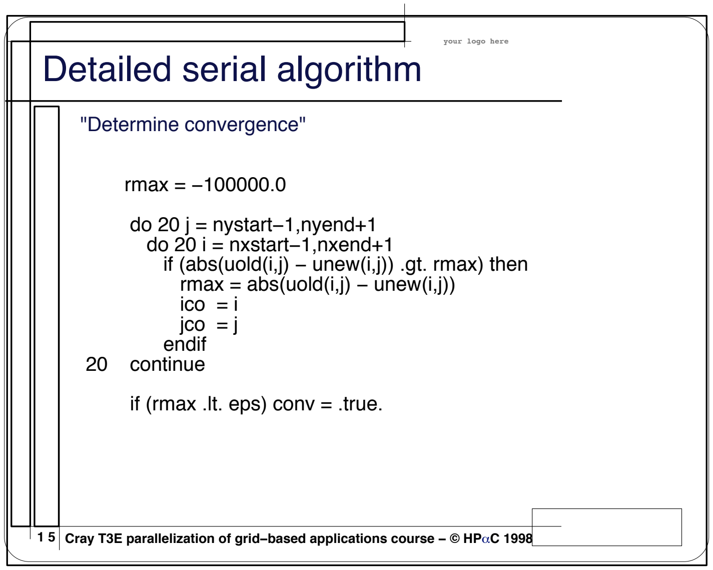
```
    do 20 j = nystart,nyend
       do 10 i = istart,nxend,2

          unew(i,j) = 0.25d0*h*h*f(i,j) +
    &            0.25d0*
    &            (uold(i–1,j)+uold(i+1,j)+uold(i,j–1)+uold(i,j+1))

 10     continue

       if (istart .eq. nxstart) then
          istart = nxstart + 1
       else
          istart = nxstart
       endif

 20   continue
```



Detailed serial algorithm

"Sweep over black points"

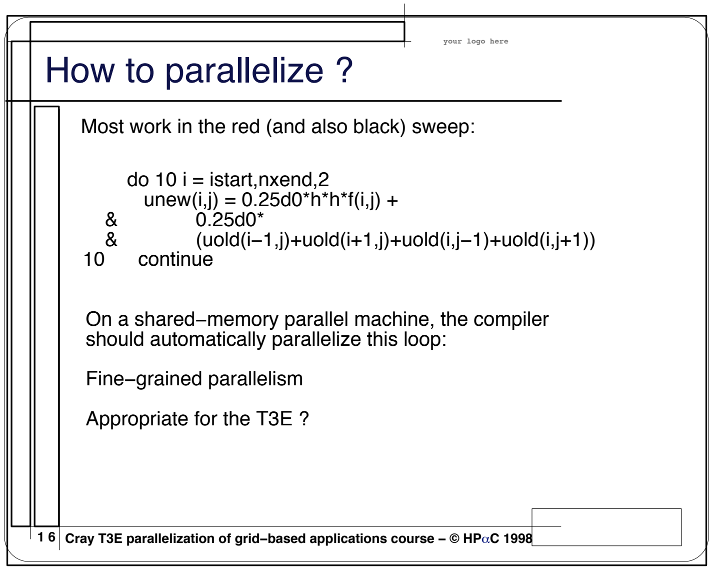
```
    do 60 j = nystart,nyend
       do 50 i = istart,nxend,2

          unew(i,j) = 0.25d0*h*h*f(i,j) +
   &             0.25d0*
   &             (unew(i–1,j)+unew(i+1,j)+unew(i,j–1)+unew(i,j+1))

 50    continue

       if (istart .eq. nxstart) then
          istart = nxstart + 1
       else
          istart = nxstart
       endif

 60   continue
```



Detailed serial algorithm

"Determine convergence"

```
      rmax = –100000.0

       do 20 j = nystart–1,nyend+1
          do 20 i = nxstart–1,nxend+1
             if (abs(uold(i,j) – unew(i,j)) .gt. rmax) then
                rmax = abs(uold(i,j) – unew(i,j))
                ico  = i
                jco  = j
             endif
 20    continue

       if (rmax .lt. eps) conv = .true.
```



How to parallelize ?

Most work in the red (and also black) sweep:

```
       do 10 i = istart,nxend,2
          unew(i,j) = 0.25d0*h*h*f(i,j) +
   &             0.25d0*
   &             (uold(i–1,j)+uold(i+1,j)+uold(i,j–1)+uold(i,j+1))
10     continue
```

On a shared–memory parallel machine, the compiler should automatically parallelize this loop:

Fine–grained parallelism

Appropriate for the T3E ?

Coarse–grained parallelism

So, let’s go for coarser–grained parallelism:

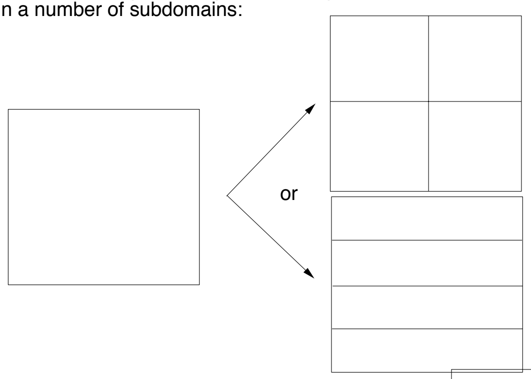
- less synchronization points
- less communication (when implemented on a distributed memory machine)

Typically, domain decomposition is used to accomplish coarse–grained parallelism

Note that domain decomposition parallelism can be applied on both shared memory and distributed memory machines

Domain decomposition

Domain decomposition splits the computational domain in a number of subdomains:



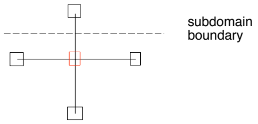
Domain decomposition

Each subdomain is devoted to a processor

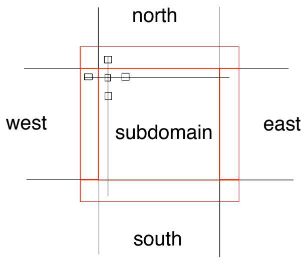
The processor executes the numerical algorithm for the points in its subdomain:

```
       do 10 i = istart,nxend,2
          unew(i,j) = 0.25d0*h*h*f(i,j) +
     &           0.25d0*
     &           (uold(i–1,j)+uold(i+1,j)+uold(i,j–1)+uold(i,j+1))
 10    continue
```

Immediately, it becomes clear where the problems are:



Domain decomposition

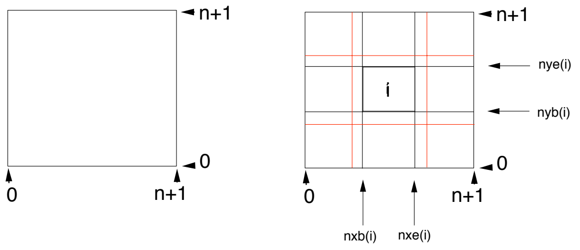


So, each subdomain computes the solution in its internal area. For the points at the internal boundary, it needs input from neighbouring subdomains

Grid points numbering

Global domain:

Global numbering is kept in subdomains:



So, arrays in subdomains run from nxb(i)−1 to nxe(i)+1, and from nyb(i)−1 to nyb(i)+1

Implementation aspects

For the remainder, we make a few assumptions on the parallel implementation:

- Distributed memory model
- Each processor only knows the subdomain it is responsible for
- T3E in mind: SPMD (= Single Program Multiple Data)
- MPI
- One of the MPI instances takes care of the administrational issues (and also of its own subdomain)
- General subdomain configurations (nx blocks in x–direction, ny blocks in y–direction)
- In MPI, the processor id's range from 0 to nprocs–1
- We assume the processor with id = 0 to do the global administration issues

Basic parallel algorithm

```
MPI initialization
Input, and communication of input
Initialize (sub)grid, determine neighbours
Initialize boundary values

while ((no convergence) .and. (no_max_iter))

    Sweep over red points
    Communicate red values at internal boundaries
    Sweep over black points
    Communicate black values at internal boundaries

    Determine convergence (in subdomain)
    Communicate to single PE (my_id = 0)
    Determine global convergence (one PE)
    Communicate convergence result

end while

Output
```

Note that each processor runs the same program !

Detailed parallel algorithm

"MPI initialization"

```
call MPI_INIT(ierr)
call MPI_COMM_RANK(MPI_COMM_WORLD, myid, ierr)
call MPI_COMM_SIZE(MPI_COMM_WORLD, numprocs, ierr)
```

numprocs comes from:

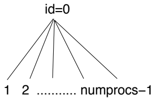
mpirun −np *numprocs executable*

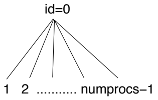
myid is the id of the process/processor

Detailed parallel algorithm

"Input, and communication of input"

```
  if (myid .eq. 0) then


     ibuffer(1) = isubs
     ibuffer(2) = kbx            blocks in x−direction
     ibuffer(3) = kby            blocks in y−direction
     ibuffer(4) = nmax           max. iterations

     itag = 1

     do id = 1,numprocs−1
        call MPI_SEND(ibuffer,4,MPI_INTEGER,id,itag,
 &                   MPI_COMM_WORLD,ierr)
     enddo

     rbuffer(1) = omega          relaxation parameter, assume 1.0
     rbuffer(2) = eps            relative accuracy

     itag = 2

     do id = 1,numprocs−1
        call MPI_SEND(rbuffer,2,MPI_DOUBLE_PRECISION,id,itag,
 &                   MPI_COMM_WORLD,ierr)
     enddo

  else
       ...........  next page ..........
```





Detailed parallel algorithm

"Input, and communication of input"

```
     ....  previous page .....

  else

c
c  Slaves receive data and compute related parameters
c

        call MPI_RECV(ibuffer,4,MPI_INTEGER,0,1,
    &                 MPI_COMM_WORLD,istat,ierr)

        isubs   = ibuffer(1)
        kbx     = ibuffer(2)
        kby     = ibuffer(3)
        nmax    = ibuffer(4)

        kblock = kbx*kby

        call MPI_RECV(rbuffer,2,MPI_DOUBLE_PRECISION,0,2,
    &                 MPI_COMM_WORLD,istat,ierr)

        omega = rbuffer(1)
        eps   = rbuffer(2)

     endif
```

Detailed parallel algorithm

"Initialize (sub)grid, determine neighbours"

```
      do 201 ky = 1,kby
        do 201 kx = 0,kbx−1

          ibls((ky−1)*kbx+kx) = nint(dble(       kx*nx)/dble(kbx))+1
          ible((ky−1)*kbx+kx) = nint(dble((kx+1)*nx)/dble(kbx))
          jbls((ky−1)*kbx+kx) = nint(dble((ky−1)*ny)/dble(kby))+1
          jble((ky−1)*kbx+kx) = nint(dble(      ky*ny)/dble(kby))

 201    continue
c
c  Now, slave myid is responsible for the global points:
c
c                 ibls(myid) to ible(myid) in X−direction
c                 jbls(myid) to jble(myid) in Y−direction
```

Note:

- kbx and kby were input values, and have been communicated to each id
- Each processor (id) runs this code !
- Each processor knows on which grid points every other processor works on

Detailed parallel algorithm

"Initialize (sub)grid, determine neighbours"

```
c
c  Next, determine neighbours of myid
c

      myid_div = myid/kbx
      myid_mod = mod(myid,kbx)

      south = myid − kbx
      if (myid_div .eq. 0) south = −1

      north = myid + kbx
      if (myid_div .eq. kby−1) north = −1

      west = myid − 1
      if (myid_mod .eq. 0) west = −1

      east = myid + 1
      if (myid_mod .eq. kbx−1) east = −1

      neighbours(1) = north
      neighbours(2) = south
      neighbours(3) = west
      neighbours(4) = east
```

9	10	11
6	7	8
3	4	5
0	1	2

So, each processor (id) knows the id's of its (max. 4) neighbours

Detailed parallel algorithm

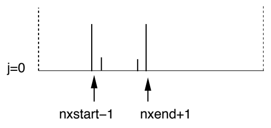
Basically, the administration is ready now:

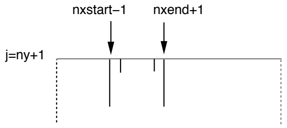
- Each processor knows on which part of the global domain it works
- Each processor knows the lower and upper bounds of its arrays, and can allocate them
- Each processor knows its own id, and knows the id’s of its neighbours
- Furthermore, each processor knows which of its neighbours is north, south, east or west
- If there is no neighbour on either of the 4 sides (subdomain has a global boundary), the neighbour is set to −1

Detailed parallel algorithm

"Initialize boundary values"

```
c
c  south boundary
c
       if (south .eq. −1) then

         j = 0
         do 51 i = nxstart−1,nxend+1
           xx     = x(i,j)
           yy     = y(i,j)
           u(i,j) = exp(−(xx−yy)*(xx−yy))
 51        continue
       endif
c
c  north boundary
c
       if (north .eq. −1) then

         j = ny+1
         do 61 i = nxstart−1,nxend+1
           xx     = x(i,j)
           yy     = y(i,j)
           u(i,j) = exp(−(xx−yy)*(xx−yy))
 61        continue
       endif
c
c  west boundary    ....................
```





So, basically no changes compared to serial algorithm

Detailed parallel algorithm

"Sweep over red points"

```
   do 20 j = nystart,nyend
      do 10 i = istart,nxend,2

        unew(i,j) = 0.25d0*h*h*f(i,j) +
   &            0.25d0*
   &            (uold(i−1,j)+uold(i+1,j)+uold(i,j−1)+uold(i,j+1))

 10     continue

      if (istart .eq. nxstart) then
        istart = nxstart + 1
      else
        istart = nxstart
      endif

 20   continue
```

So, no changes compared to serial algorithm, provided that:

- input for internal boundary points is up−to−date (must have come from neighbouring subdomains)

Detailed parallel algorithm

"Sweep over black points"

```
   do 60 j = nystart,nyend
     do 50 i = istart,nxend,2

       unew(i,j) = 0.25d0*h*h*f(i,j) +
  &            0.25d0*
  &            (unew(i−1,j)+unew(i+1,j)+unew(i,j−1)+unew(i,j+1))

 50   continue

     if (istart .eq. nxstart) then
       istart = nxstart + 1
     else
       istart = nxstart
     endif

 60   continue
```

The same holds here:

No changes compared to serial algorithm, provided that input for internal boundary points is available

Detailed parallel algorithm

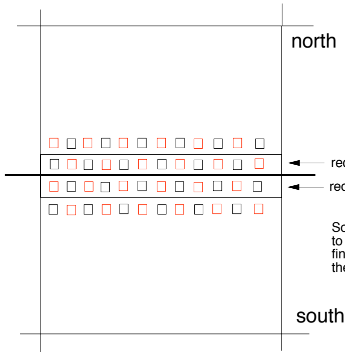
"Communicate red values at internal boundaries"

Several issues to take care of:

- What to communicate ?
  which values
- How to communicate ?
  which order or strategy

Detailed parallel algorithm

"Communicate red values at internal boundaries"
Which values to communicate ?



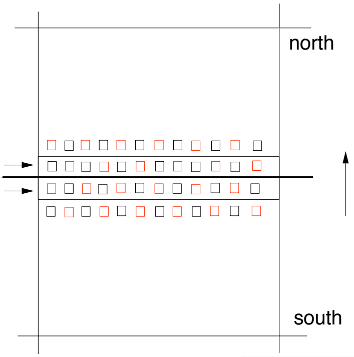
red values needed as input for south

red values needed as input for north

So, at each internal boundary, you need to find out which the red values are: find the first (in this case leftmost), and then increment by 2

Detailed parallel algorithm

"Communicate red values at internal boundaries"



nystart in "north" = nyend+1 in "south"

nyend in "south" = nystart–1 in "north"

In order to understand the concept, assume the south subdomain sends to the north subdomain

Detailed parallel algorithm

"Communicate red values at internal boundaries"

```
      if (nnorth .ge. 0) then                determine *if* there is a north neighhbour

        if (color .eq. 1) then               color=1 (communicate red), color=0 (communicate black)
c
c  Red
c
          if (mod(nyend,2) .eq. 1) then                 red    points: (even,even) and (odd,odd)
            if (mod(nxstart,2) .eq. 1) then              black points: (even,odd) and (odd,even)
              istart = nxstart
            else
              istart = nxstart + 1
            endif
          else
            if (mod(nxstart,2) .eq. 1) then
              istart = nxstart + 1
            else
              istart = nxstart
            endif
          endif

        else
c
c  Black    ..........
c
            ......
        endif
      endif
```

Note: this code is executed in
the south subdomain

Detailed parallel algorithm

"Communicate red values at internal boundaries"

```
      nnorth = neighbours(1)                id of MPI–instance that takes care of north
                                            neighbour
      do i = istart,nxend,2
         rbufnorth(i) = unew(i,nyend)       fill a buffer array to use in MPI_SEND
      enddo

      length = nxend+1–(nxstart–1)+1        determine number of values to send
      itag   = 4*(niter–1)+103

      call MPI_SEND(rbufnorth,length,MPI_DOUBLE_PRECISION,nnorth,itag,
     &            MPI_COMM_WORLD,ierr)
```

itag characterizes this specific message. It is important to have each different message to have a different tag value;

nnorth is the destination of the message

Note: this code is executed in the south subdomain

Detailed parallel algorithm

"Communicate red values at internal boundaries"

```
    if (nsouth .ge. 0) then              determine *if* there is a south neighbour

      if (color .eq. 1) then             color=1 (communicate red), color=0 (communicate black)
c
c  Red
c
        if (mod(nystart–1,2) .eq. 1) then       red    points: (even,even) and (odd,odd)
          if (mod(nxstart,2) .eq. 1) then       black points: (even,odd) and (odd,even)
            istart = nxstart
          else
            istart = nxstart + 1
          endif
        else
          if (mod(nxstart,2) .eq. 1) then
            istart = nxstart + 1
          else
            istart = nxstart
          endif
        endif

      else
c
c  Black
c
        ........
      endif
    endif
```

Note: this code is executed in the north subdomain

Detailed parallel algorithm

"Communicate red values at internal boundaries"

```
      nsouth = neighbours(2)                id of MPI–instance that takes care of south
                                            neighbour

      length = nxend+1–(nxstart–1)+1        determine number of values to receive
      itag   = 4*(niter–1)+103

      call MPI_RECV(rbufsouth,length,MPI_DOUBLE_PRECISION,nsouth,itag,
     &            MPI_COMM_WORLD,istat,ierr)

      do i = istart,nxend,2                 store the received values in the appropriate
         unew(i,nystart–1) = rbufsouth(i)   array
      enddo
```

Note that the value of itag should correspond with the value in the corresponding MPI_send message

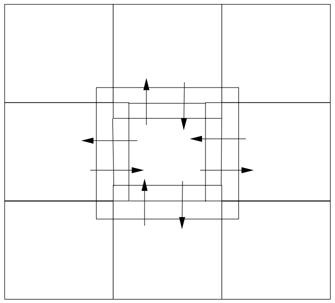
nsouth is the source of the message

Note: this code is executed in the north subdomain

Detailed parallel algorithm

"Communicate red values at internal boundaries"

Which communication strategy ?

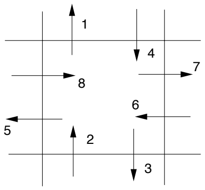


So, exchange of 8 messages between a subdomain and its neighbours

Detailed parallel algorithm

A safe strategy is the following:

- Each subdomain sends its north boundary to its north neighbour (if any)
  Then, each subdomain receives from its south neighbour (if any)
- Next, each subdomain sends its south boundary to its south neighbour (if any)
  Then, each subdomain receives from its north neighbour (if any)
- Next, each subdomain sends its west boundary to its west neighbour (if any)
  Then, each subdomain receives from its east neighbour (if any)
- Next, each subdomain sends its east boundary to its east neighbour (if any)
  Then, each subdomain receives from its west neighbour (if any)



Detailed parallel algorithm

"Sweep over black points"

Basically equivalent to the "sweep over red points"

"Communicate black values at internal boundaries"

Basically equivalent to the "communication of red values at internal boundaries"

Detailed parallel algorithm

"Determine convergence (in subdomain)"

```
      rmax = –100000.0

      do 20 j = nystart–1,nyend+1
         do 20 i = nxstart–1,nxend+1
            if (abs(uold(i,j) – unew(i,j)) .gt. rmax) then
               rmax = abs(uold(i,j) – unew(i,j))
               ico  = i
               jco  = j
            endif
 20   continue
```

So, no changes compared to serial version, except that no global decision on convergence can be taken yet

Detailed parallel algorithm

"Communicate to single PE (my_id = 0)"

```
c
c  Send convergence results to master
c
      if (myid .ne. 0) then
         rbuffer(1) = rmax
         itag = 100000 + 2*(n–1) + 1
         call MPI_SEND(rbuffer,1,MPI_DOUBLE_PRECISION,0,itag,
     &                MPI_COMM_WORLD,ierr)
c
c  Wait for message of master to continue or not
c
      ........
```

So, each processor (except 0) sends its maximum difference to processor 0, and then starts waiting for a message from processor 0 on what to do further

Detailed parallel algorithm

"Determine global convergence"

```
        if (myid .ne. 0) then
           "subdomains send to processor 0"         see previous slide
        else
c
c  Master receives local convergence results and decides whether
c  to continue or not

           rmax_ar(0) = rmax

           itag = 100000 + 2*(n–1) + 1
           do id = 1,numprocs–1
              call MPI_RECV(rbuffer,1,MPI_DOUBLE_PRECISION,id,itag,      source could be –1
    &                    MPI_COMM_WORLD,istat,ierr)
              rmax_ar(id) = rbuffer(1)
              if (rmax_ar(id) .gt. rmax) rmax = rmax_ar(id)
           enddo

           signal = 0
           if (rmax .lt. eps) then
              conv = .true.
              signal = 1
           endif

        endif
```

Detailed parallel algorithm

"Communicate convergence result"

```
        if (myid .eq. 0) then
c
c  Master send slaves message to continue or not
c
           itag = 100000 + 2*(n–1) + 2
           do id = 1,numprocs–1
              call MPI_SEND(signal,1,MPI_INTEGER,id,itag,
    &                    MPI_COMM_WORLD,ierr)
           enddo

        endif
```

So, each subdomain receives one integer ("signal"):

- * signal = 1:   global convergence, stop
- * signal = 0:   no global convergence yet, continue

Detailed parallel algorithm

"Communicate convergence result"

```
c
c  Wait for message of master to continue or not
c
           signal = –1
           itag   = 100000 + 2*(n–1) + 2

           call MPI_RECV(signal,1,MPI_INTEGER,0,itag,
    &                    MPI_COMM_WORLD,istat,ierr)
```

Message received from processor 0
Depending on signal (0 or 1), continue or not

Exercise 1

Write an MPI program for *nprocs* processors which splits a square computational domain into a number of subdomains. The number of subdomains in the x–direction is *kbx*, in the y–direction *kby*. Assume that *nprocs* = *kbx***kby*.

kbx and *kby* are input to process 0. Assume the subdomain numbers range from 0 to *nprocs*–1.

Desired output: for each subdomain, print its north, south, east and west neighbour. If a subdomain does not have a neighbour in a certain direction, print –1.

Exercise 2

Copy the directory with the example red–black solver to your own directory. In subroutine "rbcomm", the communication between the subdomains takes place, as described earlier.

As you can see, this is the safe strategy.

Change the strategy to, e.g., a less safe strategy by having each subdomain sending to all its neighbours, and then receiving from all its neighbours.

Determine whether this influences the elapsed execution time.