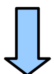
第４回　並列計算法

大規模並列計算

”大規模”問題とは？

自由度が多い問題 (計算時間が長く，記憶容量が必要な問題)



分散メモリ並列計算機の利用

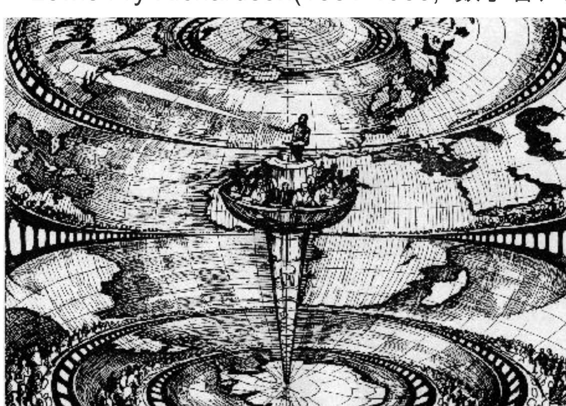
より自由度が多い問題 (大規模問題) ：広域・高解像度

より多くの計算機の利用 (大規模計算機システム)

大規模なデータを大規模なシステムで処理すること

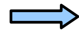
リチャードソンの夢

Lewis Fry Richardson(1881-1953，数学者、気象学者)



気象予報の原型を提案
第１次世界大戦のデータを使用し、
6 時間後を予測
--> 手計算で２ヶ月かかる。

“64000 人の計算者を巨大ホールに集め、指揮者に従い整然と計算を行えば、
実際の天候の変化と同じぐらいの速さで予報が行える。”
Richardson, L.F. : Weather Prediction by Numerical Process, University Press, 1922.

 並列計算の基本概念

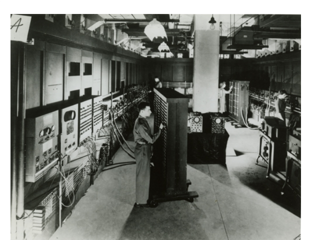
コンピュータの開発

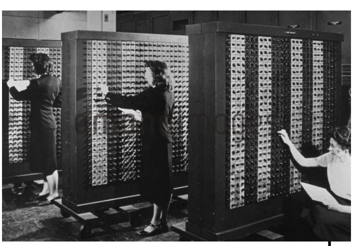
John von Neumann (1903-1957，数学者)

von Neumann architecture ;
CPU(中央演算装置) とアドレス付けされた記憶装置、それらをつなぐ Bus で構成される。
=> 記憶装置に保存されたプログラムを実行する　(Stored-program computer)
– First Draft of a Report on the EDVAC, 1945 --

* 「博士の異常な愛情」の Dr. Strangelove のモデルの一人と言われている。

ENIAC(Electronic Numerical Integrator and Computer), 1946
- 世界初の電子汎用コンピュータ
- 弾道計算を目的にしているが、マンハッタン計画の Neumann がこの計算機に深く関わる
- John W. Mauchly, John P. Eckert により開発
- EDVAC へ引き継がれる
- 真空管を使用





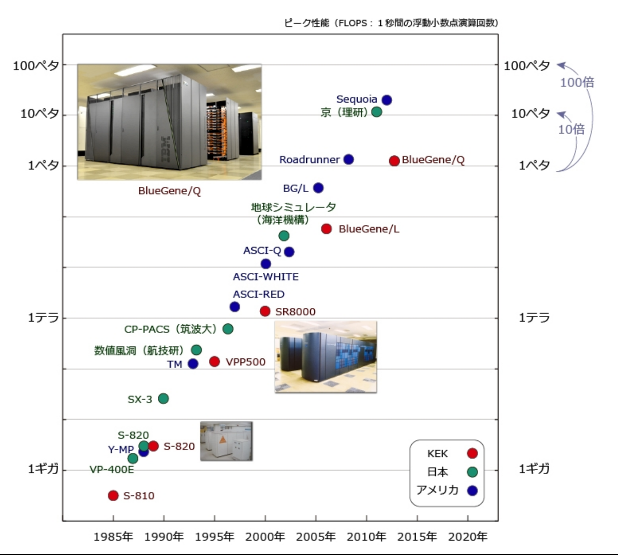
コンピュータの開発

UNIVAC I (UNIVersal Automatic Computer), 1950
- John W. Mauchly, John P. Eckert により開発
- 世界最初の商用コンピュータ
- 真空管の本数は ENIAC の 3 分の 1 程度
- 磁気テープ搭載
- プログラム内蔵方式

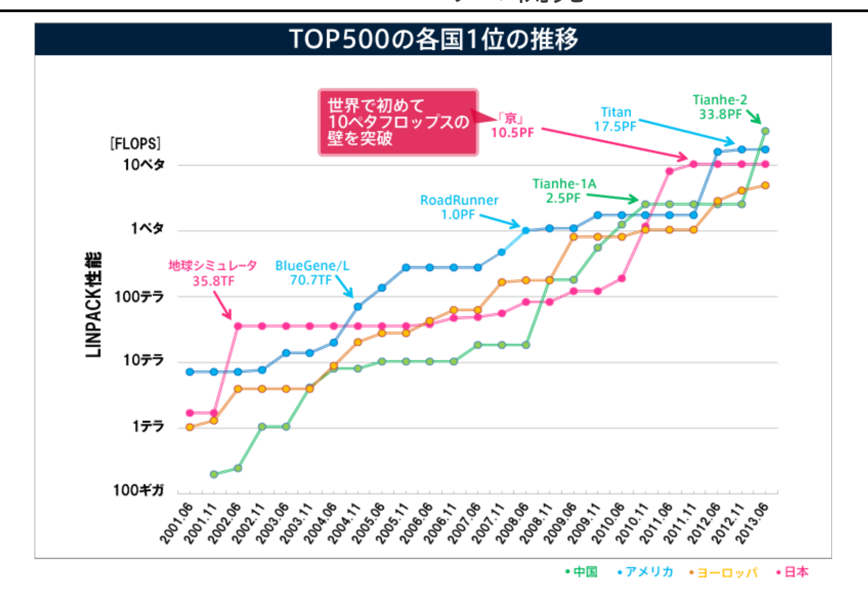
IBM 1401, 1959
- トランジスタ集積回路
- 搭載ソフトウェア
    - FORTRAN II, COBOL ...

以降、マイクロプロセッサの時代へ

コンピュータの開発



コンピュータの開発



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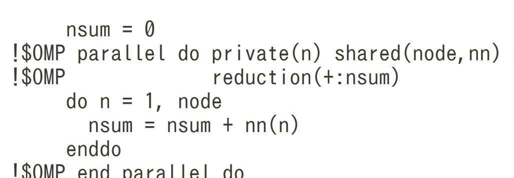
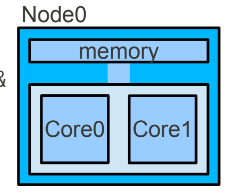
並列計算方法

共有メモリ型並列計算

- 各演算装置 (CPU/Core) は同一のメモリにアクセス
- ループを分割することにより高速化
- プログラミングが容易 (一部のみ並列化可能)
- データ構造の変更が無い
- メモリ容量の削減はされない



```
      nsum = 0
!$OMP parallel do private(n) shared(node,nn) &
!$OMP                 reduction(+:nsum)
      do n = 1, node
        nsum = nsum + nn(n)
      enddo
!$OMP end parallel do
```



do n=1,5　　do n=5,10

並列計算方法

分散メモリ型並列計算

- 各演算装置 (CPU/Core) は各々のメモリにアクセス
- データを分割することにより高速化
- プログラミングが比較的難しい（全体を並列化）
- データ構造の変更が必要（領域分割）
- メモリ容量が削減される

```
nsum = 0
do n = 1, node
  nsum = nsum + nn(n)
enddo
mpi_allreduce(nsum,nsumr,1,mpi_integer,&
              mpi_sum,mpi_comm_world,ierr)
nsum = nsumr
```

Network
CN0 CN1
memory memory
Core0 Core0

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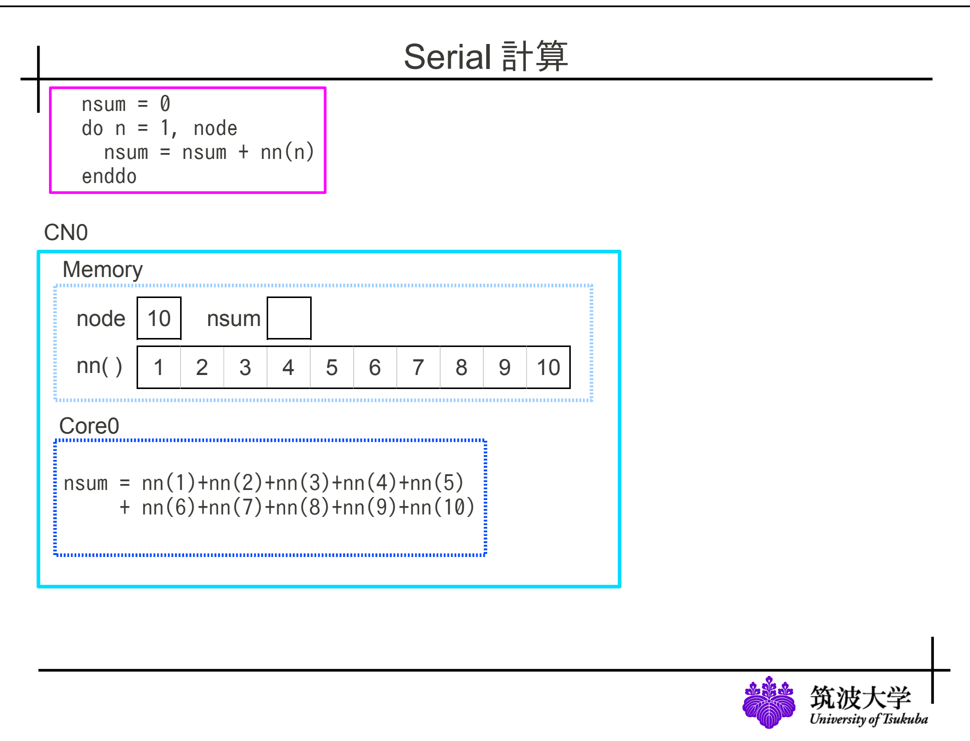

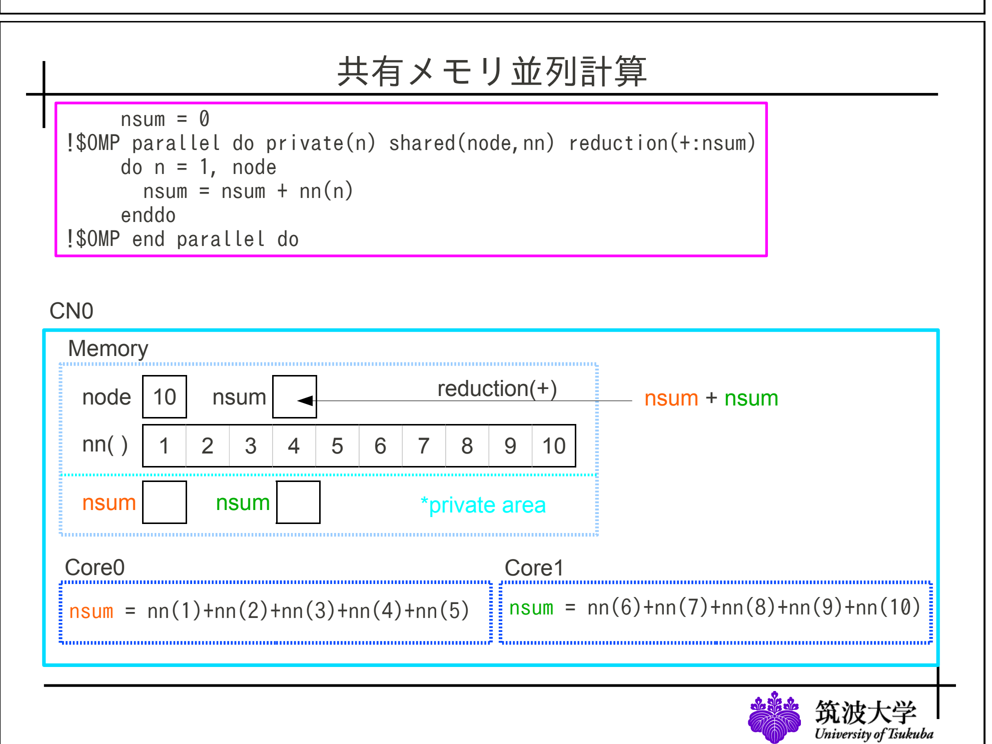

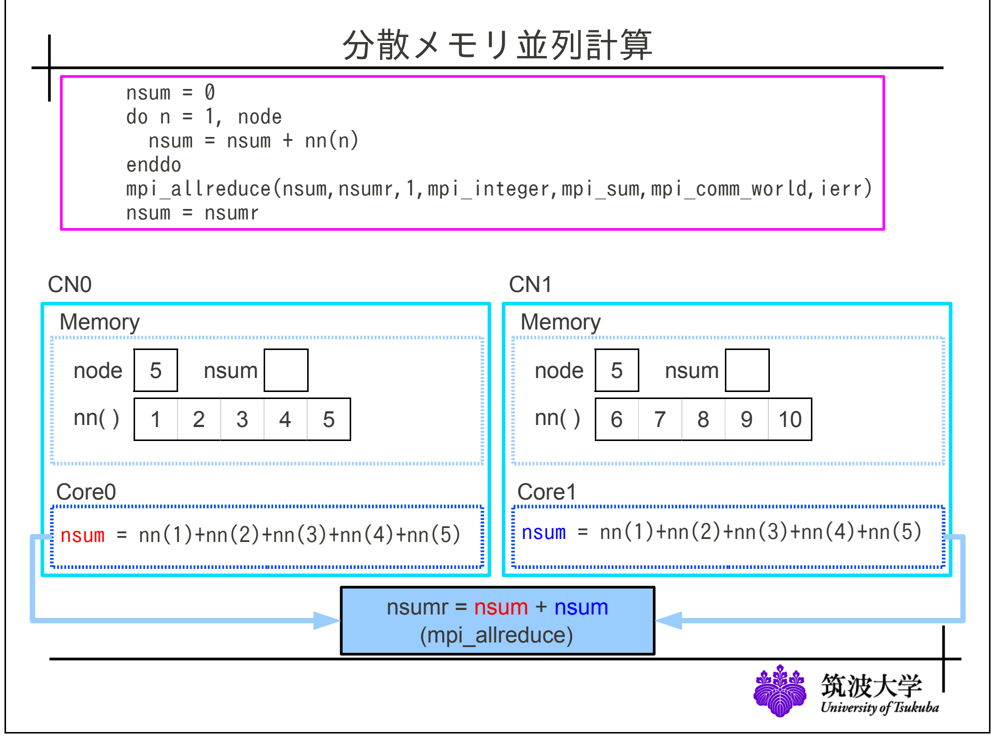

What is OpenMP ?

OpenMP is a set of compile directives and callable runtime library routines that extend that Fortran (and other languages) to express shared memory parallelization.

1) http://www.openmp.org/

Hello world (single)

```
program  hello_world
 integer :: mythread
 mythread = 0
 write(6,*) mythread,  'Hello World'
end program hello_world
```

Hello world (OMP)

```
program  hello_world_omp
 integer :: mythread
 mythread = 0
 !$OMP parallel private( mythread )
 !$ mythread = omp_get_thread_num()
  wirte(6,*) mythread,  'Hello World'
 !$OMP end parallel
end program hello_world_omp
```

Why should we use OpenMP ?

Merit

- Easy to parallelize (for simple loop!)
  MPI programming require the change over the entire your code.
  MPI programming require the data partitioning. (for the specified parallelization)

Hello world (single)

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 !$OMP end parallel
end program hello_world_omp
```

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Why should we use OpenMP ?

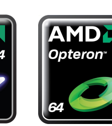
Merit

- Easy to parallelize (for simple loop!)
  MPI programming require the change over the entire your code.
  MPI programming require the data partitioning. (for the specified parallelization)
- Easy to construct the OpenMP environment.
  Can you do the clustering for some computers and setting up the MPI library?

Shared memory parallel computing needs:

- Multi Core/CPU Computer

⇨ If you buy the computer now, it have the dual or quad core CPU(s).



2006.11. Intel started to sell the "first" Quad core CPU (codename:Clovertown)
2007. 9. AMD started to sell the "native" Quad core CPU (codename:Barcelona)

- OpenMP library

⇨ The major compiler (intel, PGI and NAG?) has had the OpenMP option.

Parallerization using OpenMP

The rules of OpenMP

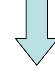
!$OMP ○○○ ×××	:	OpenMP directive
!$ ○ = × ＊ △	:	It is done only OpenMP
! ○×△	:	Comments

```
program  hello_world_omp
 integer :: mythread
 mythread = 0
 !$OMP parallel private( mythread )
 !$ mythread = omp_get_thread_num()
  wirte(6,*) mythread,  'Hello World'
 !$OMP end parallel
end program hello_world_omp
```

- `!$OMP parallel private( mythread )` → Parallel Construct (start)
- `!$ mythread = omp_get_thread_num()` → OMP Function (to get the my thread number)
- `end program hello_world_omp` → Parallel Construct (end)

OpenMP sample program

```
program  welcome_to_parallel_world_omp
 integer :: mythread
 mythread = 0
 write(6,*) mythread,  'Hello Parallel World'
 !$OMP parallel private( mythread )
 !$ mythread = omp_get_thread_num()
  write(6,*) mythread,  'Parallel Computing'
 !$OMP end parallel
  write(6,*) mythread,  'Good-by'
end program welcome_to_parallel_world_omp
```



Run with 4 threads

```
0  Hello Parallel World
0  Parallel Computing
1  Parallel Computing
2  Parallel Computing
3  Parallel Computing
0  Good-by
```

Outline of Running on OpenMP

```
program  welcome_to_parallel_world_omp
 integer :: mythread
 mythread = 0
 write(6,*) mythread, 'Hello Parallel World'

 !$OMP parallel private( mythread )
 !$ mythread = omp_get_thread_num()
  write(6,*) mythread,'Parallel Computing'
 !$OMP end parallel

  write(6,*) mythread,'Good-by'
end program welcome_to_parallel_world_omp
```

Master thread

write(6,*) 'Hello Parallel World'

write(6,*)'Parallel Computing'

Thread0 Thread1 Thread2 Thread3

Slave threads

write(6,*) 'Good-by'

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Parallel and Worksharing Construct

2. Worksharing construct

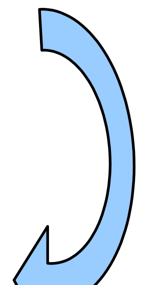
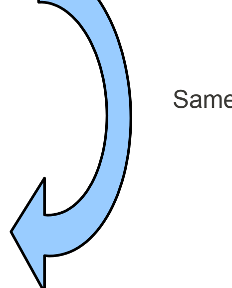
```
!$OMP parallel
 !$OMP do
   do i = 1, n
    ........
   enddo
 !$OMP enddo
!$OMP end parallel
```

Direction to do worksharing in Parallel Construct

- do directions
- single directions
- workshare directions

3.Unitted Worksharing construct

```
!$OMP parallel do
   do i = 1, n
    ........
   enddo
!$OMP end parallel do
```

Same !

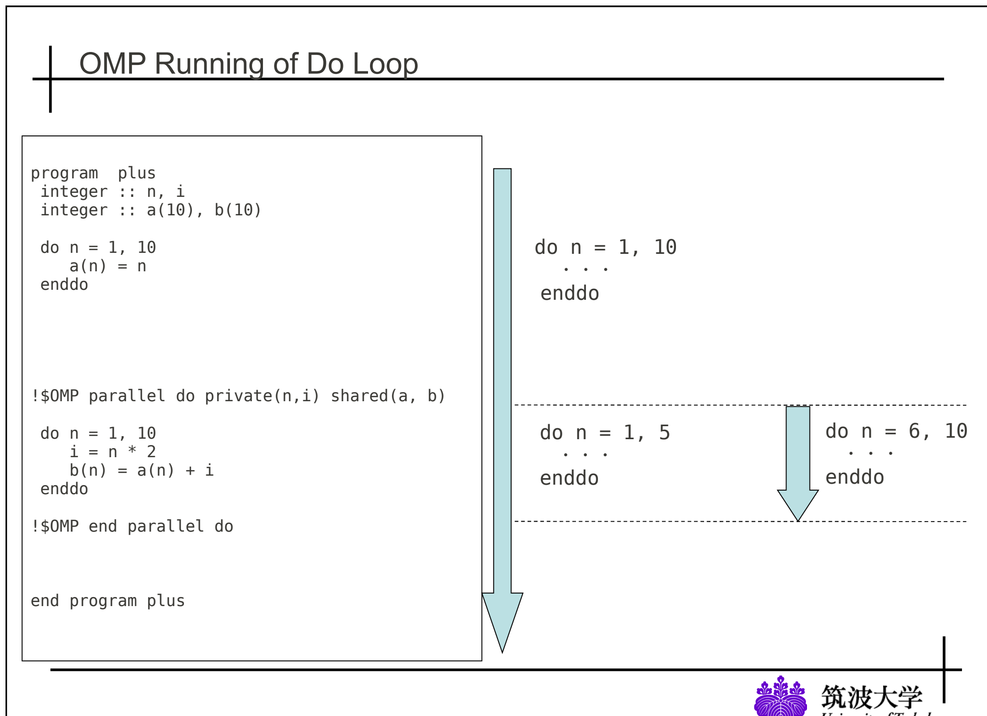
Parallel and Worksharing Construct

2. Worksharing construct

```
!$OMP parallel
 !$OMP do
   do i = 1, n
    ........
   enddo
 !$OMP enddo
   m = n * 2
 !$OMP do
   do j = 1, m
    ........
   enddo
 !$OMP enddo
!$OMP end parallel
```

3.Unitted Worksharing construct

```
!$OMP parallel do
   do i = 1, n
    ........
   enddo
!$OMP end parallel do
   m = n * 2
!$OMP parallel do
   do j = 1, m
    ........
   enddo
!$OMP end parallel do
```


OMP Running of Do Loop
program plus
integer :: n, i
integer :: a(10), b(10)
do n = 1, 10
a(n) = n
enddo
!$OMP parallel do private(n,i) shared(a, b)
do n = 1, 10
i = n * 2
b(n) = a(n) + i
enddo
!$OMP end parallel do
end program plus
do n = 1, 10
. . .
enddo
do n = 1, 5
. . .
enddo
do n = 6, 10
. . .
enddo
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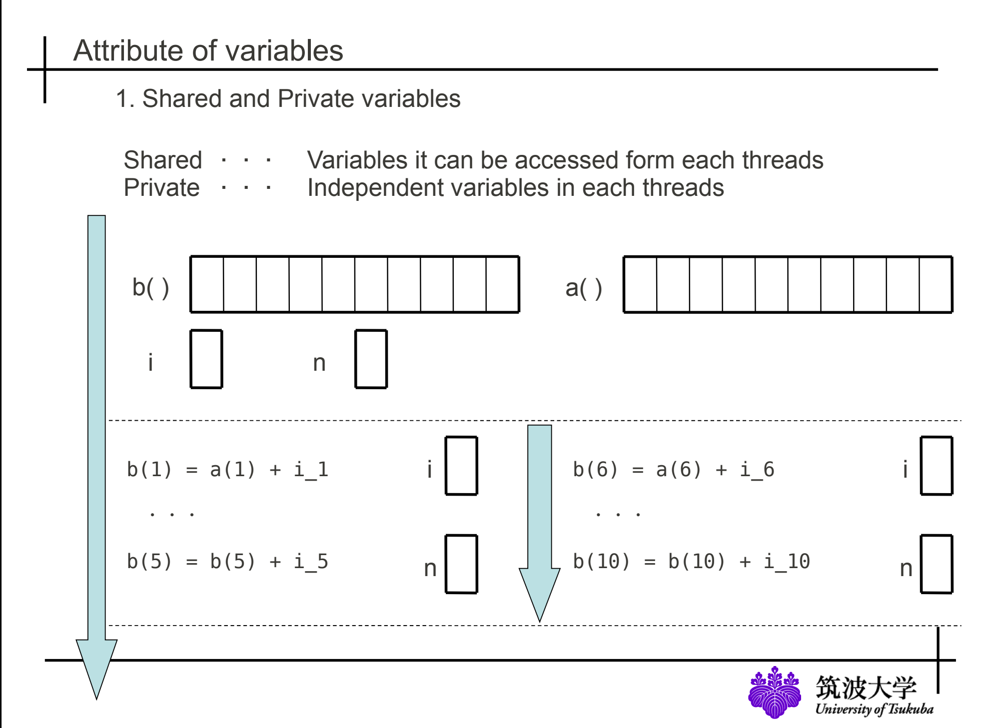
Attribute of variables
1. Shared and Private variables
Shared ・・・ Variables it can be accessed form each threads
Private ・・・ Independent variables in each threads
b( )
a( )
i
n
b(1) = a(1) + i_1
. . .
b(5) = b(5) + i_5
i
n
b(6) = a(6) + i_6
. . .
b(10) = b(10) + i_10
i
n
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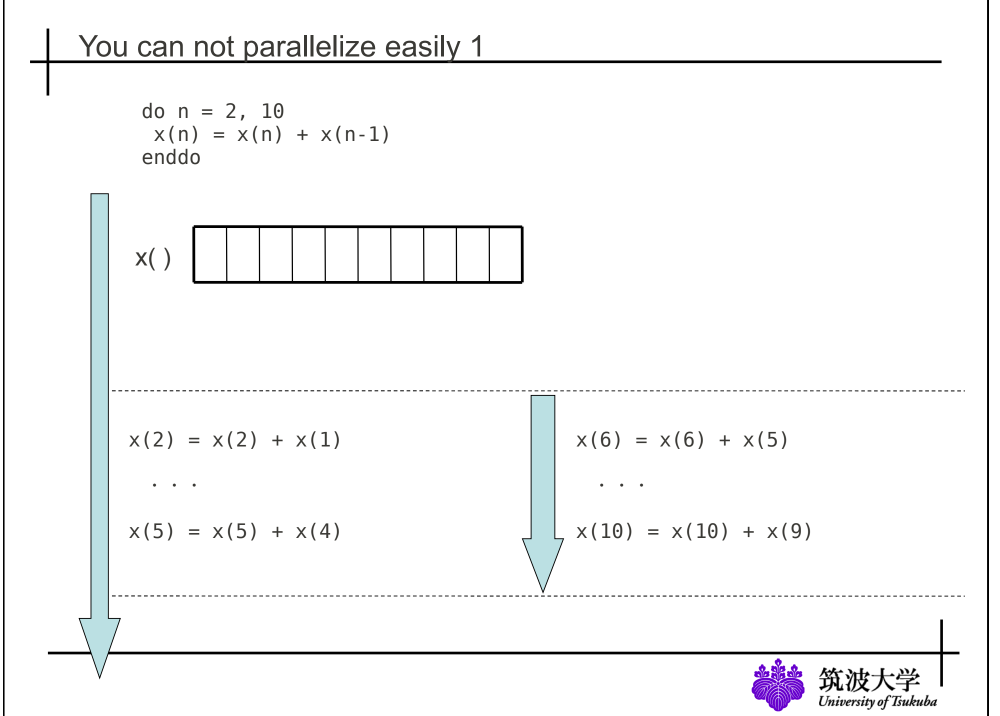
You can not parallelize easily 1
do n = 2, 10
x(n) = x(n) + x(n-1)
enddo
x( )
x(2) = x(2) + x(1)
. . .
x(5) = x(5) + x(4)
x(6) = x(6) + x(5)
. . .
x(10) = x(10) + x(9)
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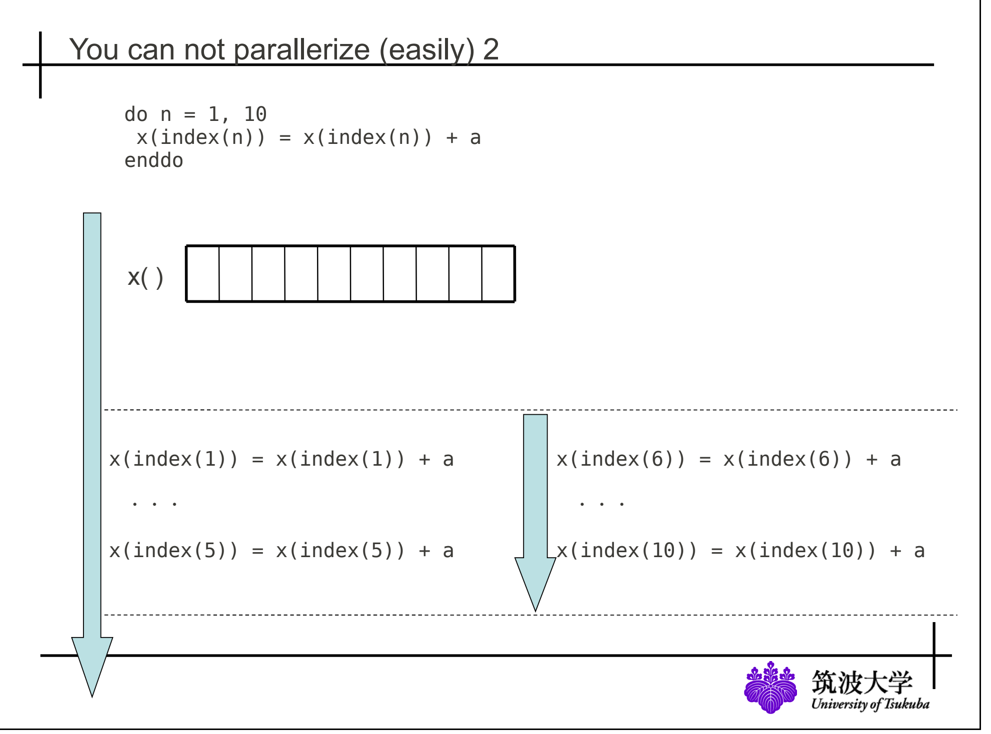
You can not parallerize (easily) 2
do n = 1, 10
x(index(n)) = x(index(n)) + a
enddo
x( )
x(index(1)) = x(index(1)) + a
. . .
x(index(5)) = x(index(5)) + a
x(index(6)) = x(index(6)) + a
. . .
x(index(10)) = x(index(10)) + a
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You can not parallerize (easily) 3

Example: Calculation of the sum

```
do i = 1, num
 a(i) = i
enddo

s = 0
do i=1, num
  s = s + a(i)
enddo
```

Variables “s” is ,
- Private ?
- Shared ?

You can not parallerize (easily) 3

Example: Calculation of the sum

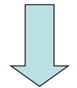
```
do i = 1, num
 a(i) = i
enddo

s = 0
do i=1, num
  s = s + a(i)
enddo
```

Case 1. If “s” is private

```
do i = 1, num
 a(i) = i
enddo

s = 0
!$OMP parallel do private(s,i) shared(a,num)
do i=1, num
  s = s + a(i)
enddo
!$OMP end parallel do
```



Results

s = 0

You can not parallerize (easily) 3

```
 s = 0
!$OMP parallel do private(s,i) shared(a,num)
 do i=1, num
   s = s + a(i)
 enddo
```

```
s = 0                                   s

    s =  s + a(i)                       s          s =  s + a(i)               s
1:  1 =  0 +  1                                6:  6 =  0 +  6
2:  3 =  1 +  2                                7: 13 =  6 +  7
3:  6 =  3 +  3                                8: 21 = 13 +  8
4: 10 =  6 +  4                                9: 30 = 21 +  9
5: 15 = 10 +  5                               10: 40 = 30 + 10

    s = 15                                         s = 40

s = 0
```


You can not parallerize (easily) 3

Example: Calculation of the sum

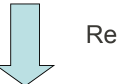
```
do i = 1, num
 a(i) = i
enddo

s = 0
do i=1, num
  s = s + a(i)
enddo
```

Case2. If “s” is shared.

```
do i = 1, num
 a(i) = i
enddo

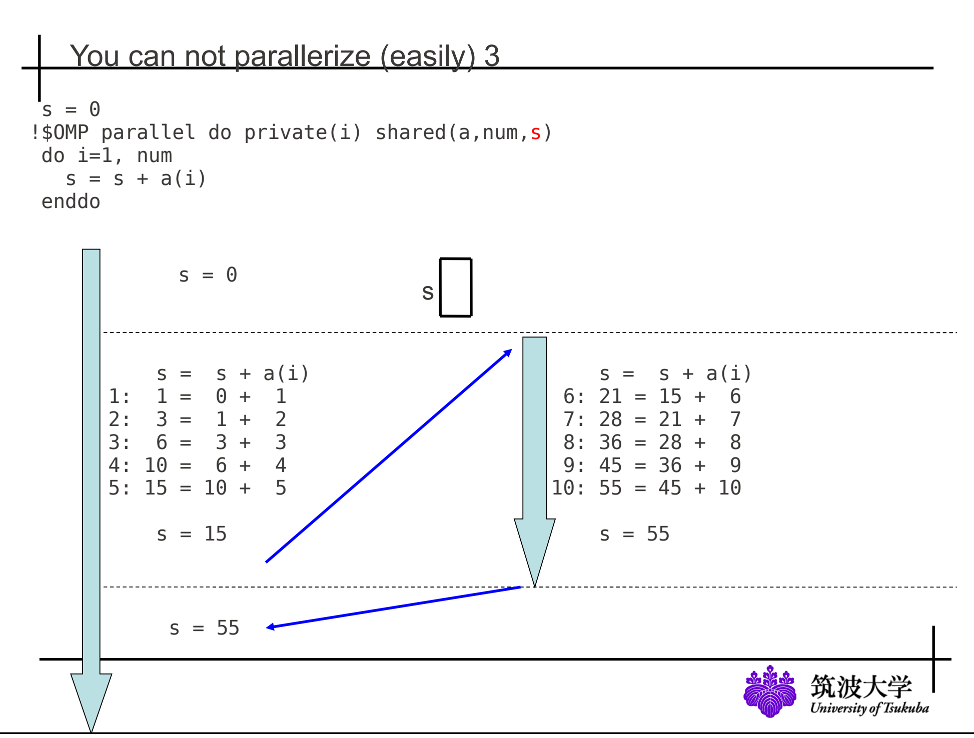
s = 0
!$OMP parallel do private(i) shared(a,num,s)
do i=1, num
  s = s + a(i)
enddo
!$OMP end parallel do
```



Results

s = 55 (num=10)

You can not parallerize (easily) 3



You can not parallerize (easily) 3

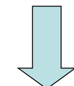
Example: Calculation of the sum

```
do i = 1, num
 a(i) = i
enddo

s = 0
do i=1, num
  s = s + a(i)
enddo
```

```
do i = 1, num
 a(i) = i
enddo

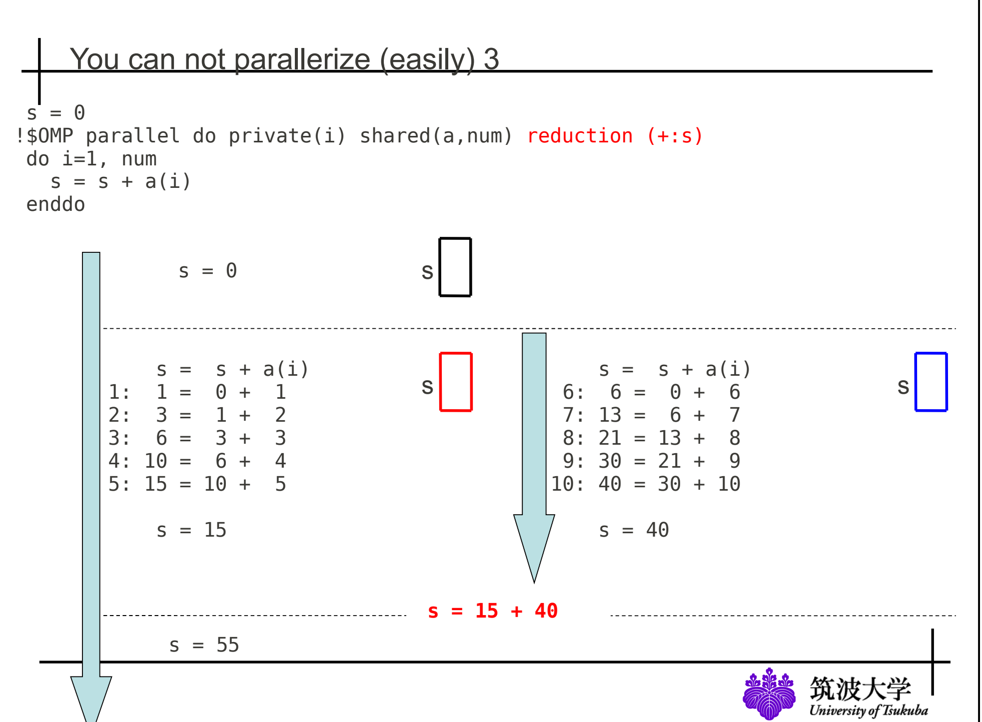
s = 0
!$OMP parallel do private(i) shared(a,num) &
!$               reduction(+:s)
 do i=1, num
   s = s + a(i)
 enddo
!$OMP end parallel do
```



Result

s = 55

You can not parallerize (easily) 3



Basic Styles

```
 s = 0
!$OMP parallel do private(i) shared(a,num) reductio (+:s)
 do i=1, num
   s = s + a(i)
 enddo
!$OMP end parallel do
```

!$OMP parallel do ・・・ United worksharing direction

!$ private(variable1， variable2，) ・・・ Private variables direction

!$ shared(variable1， variable2，) ・・・ Shared variables direction

!$ reduction (Operation ： variable1， variable2，) ・・・ Variable direction

Compile & Run the OpenMP program

If you use Intel Fortran Compiler, you can complile with “-openmp” option.

$ ifort –openmp *****.f90

* You can see the OMP option in compiler manual

You should define the number of threads, as follows;

* bash

```
$ export OMP_NUM_THREADS=4
```

* csh

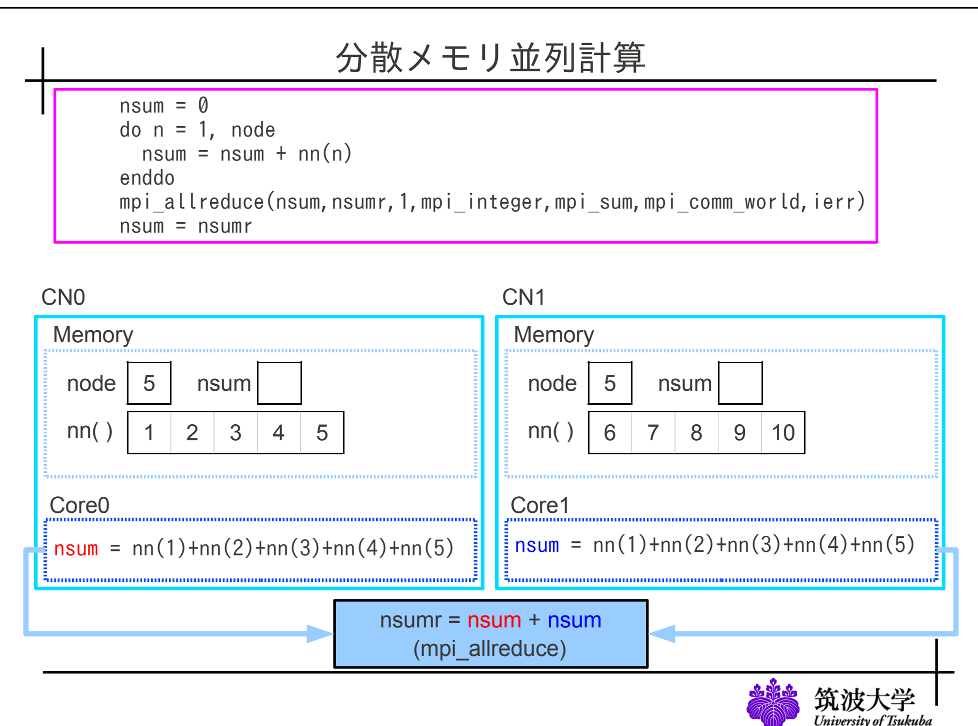
```
$ setenv OMP_NUM_THREADS 4
```

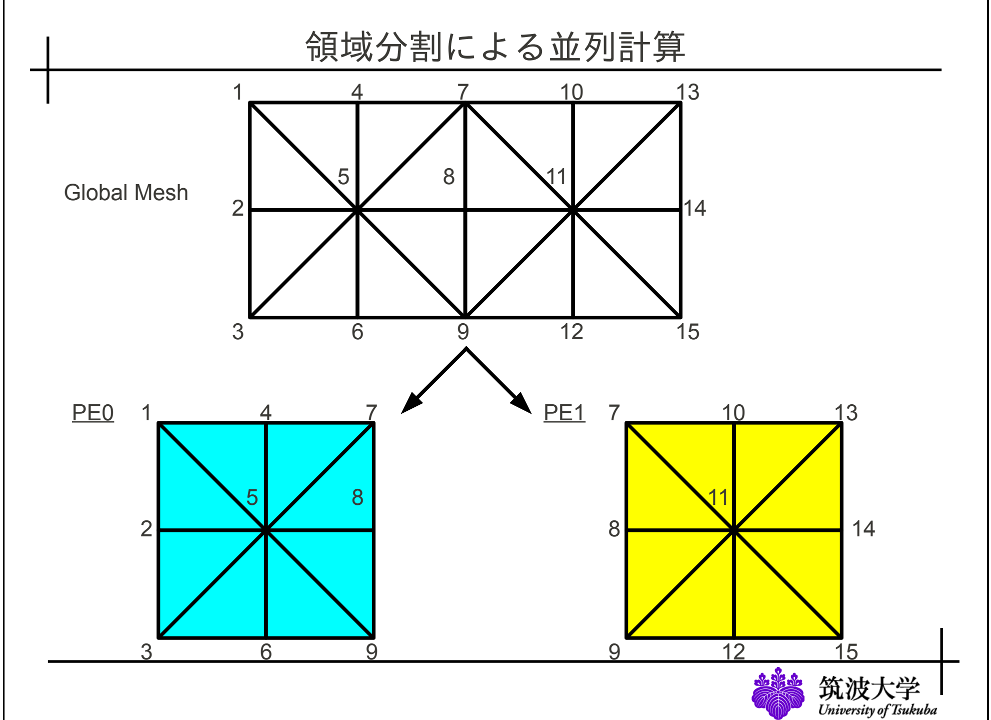
* Windows

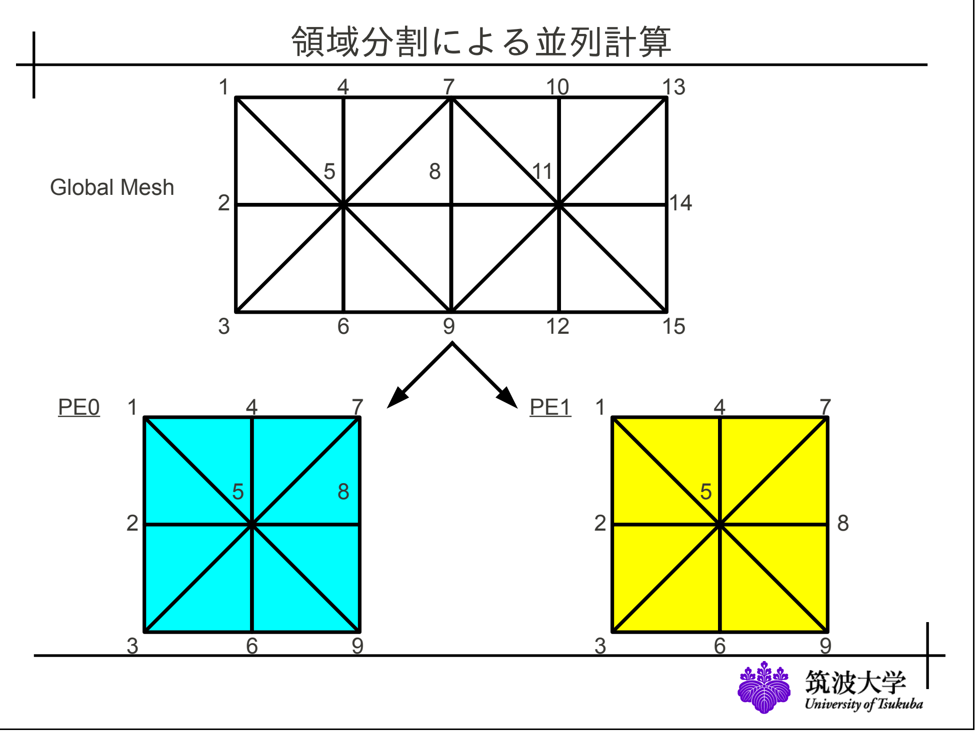
```
$ set OMP_NUM_THREADS=4
```

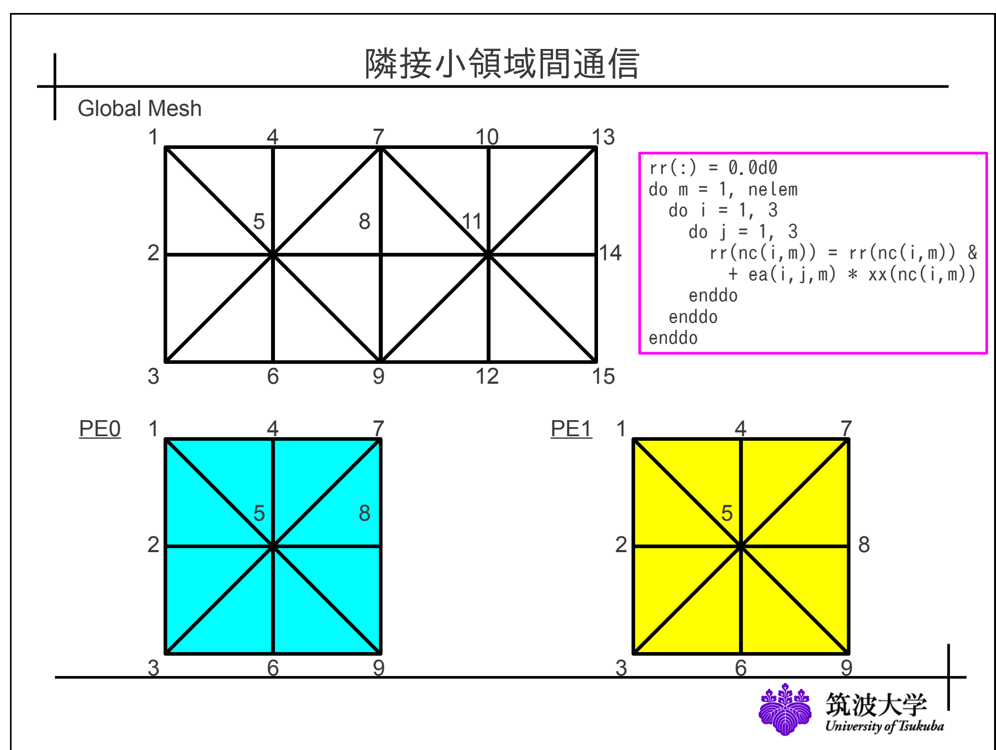
Finally, you can run the exe file

```
$  ./a.out
```









隣接小領域間通信
Global Mesh
rr(:) = 0.0d0
do m = 1, nelem
do i = 1, 3
do j = 1, 3
rr(nc(i,m)) = rr(nc(i,m)) &
+ ea(i,j,m) * xx(nc(i,m))
enddo
enddo
enddo
PE0
PE1
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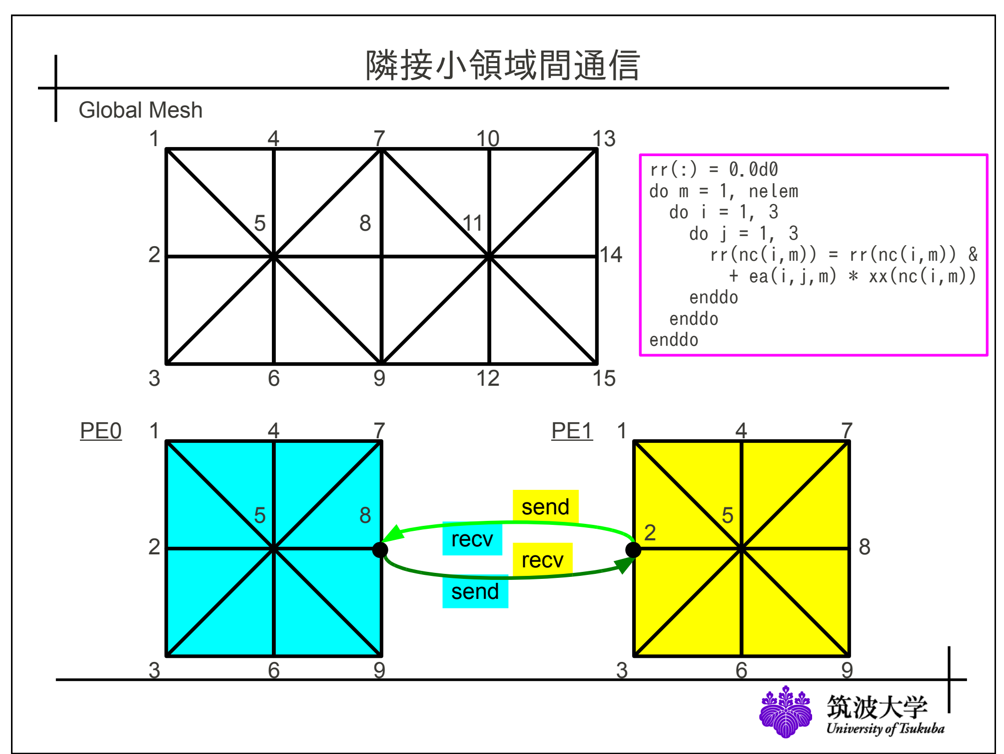

隣接小領域間通信
Global Mesh
rr(:) = 0.0d0
do m = 1, nelem
do i = 1, 3
do j = 1, 3
rr(nc(i,m)) = rr(nc(i,m)) &
+ ea(i,j,m) * xx(nc(i,m))
enddo
enddo
enddo
PE0
PE1
send
recv
recv
send
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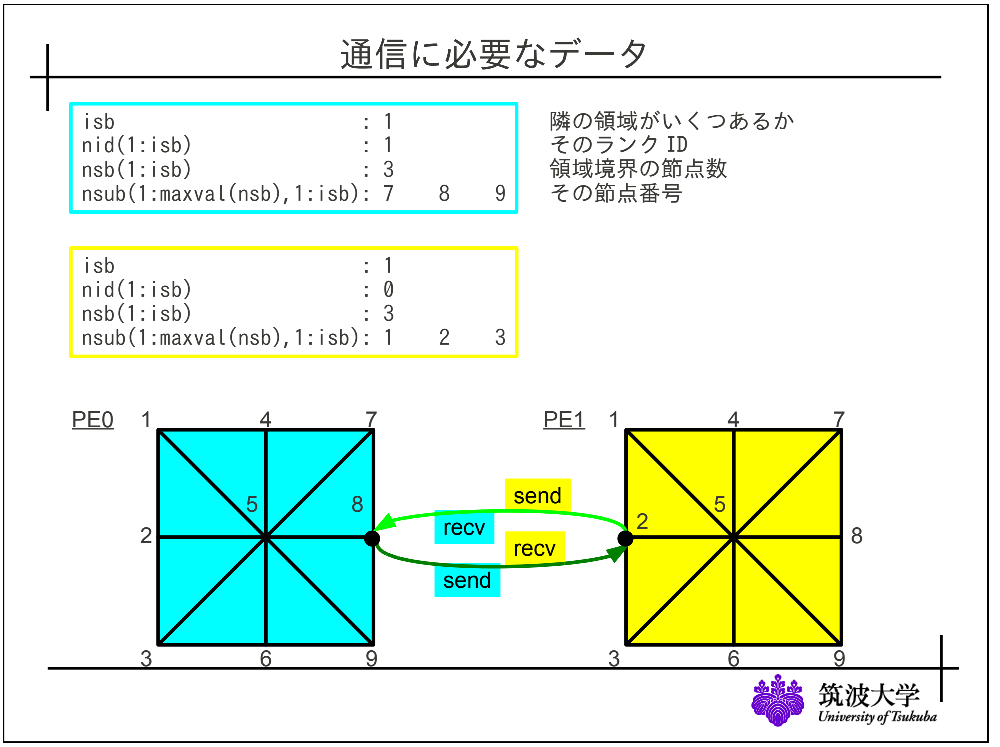

通信に必要なデータ
isb : 1
nid(1:isb) : 1
nsb(1:isb) : 3
nsub(1:maxval(nsb),1:isb): 7 8 9
隣の領域がいくつあるか
そのランク ID
領域境界の節点数
その節点番号
isb : 1
nid(1:isb) : 0
nsb(1:isb) : 3
nsub(1:maxval(nsb),1:isb): 1 2 3
PE0
PE1
send
recv
recv
send
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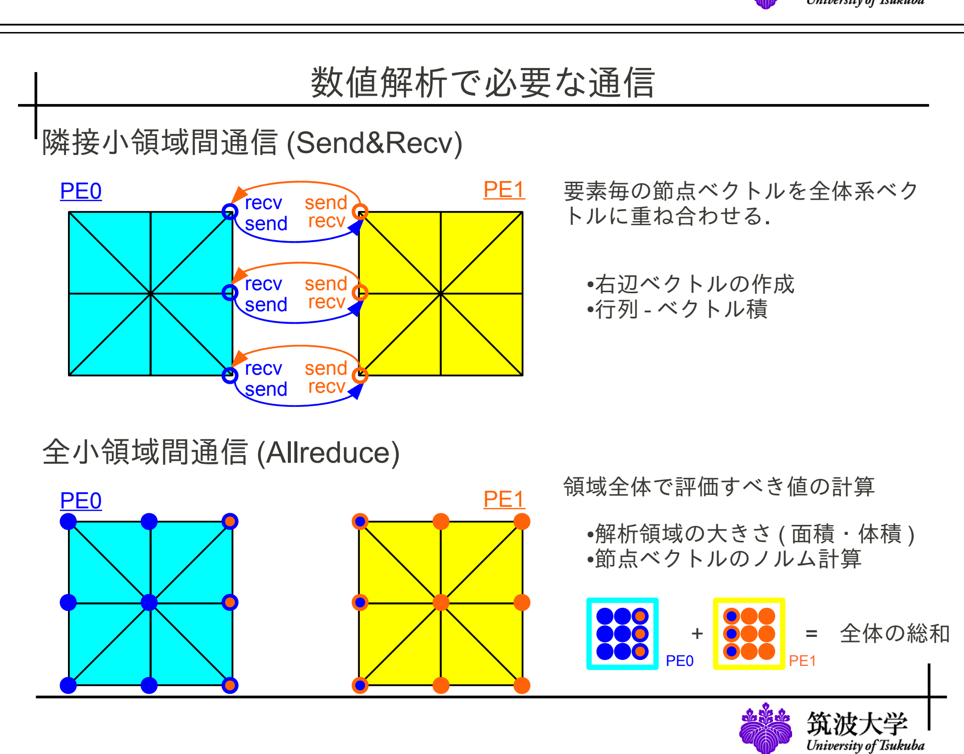

数値解析で必要な通信
隣接小領域間通信 (Send&Recv)
PE0
PE1
recv
send
要素毎の節点ベクトルを全体系ベクトルに重ね合わせる.
•右辺ベクトルの作成
•行列 - ベクトル積
全小領域間通信 (Allreduce)
領域全体で評価すべき値の計算
•解析領域の大きさ (面積・体積)
•節点ベクトルのノルム計算
PE0
PE1
= 全体の総和
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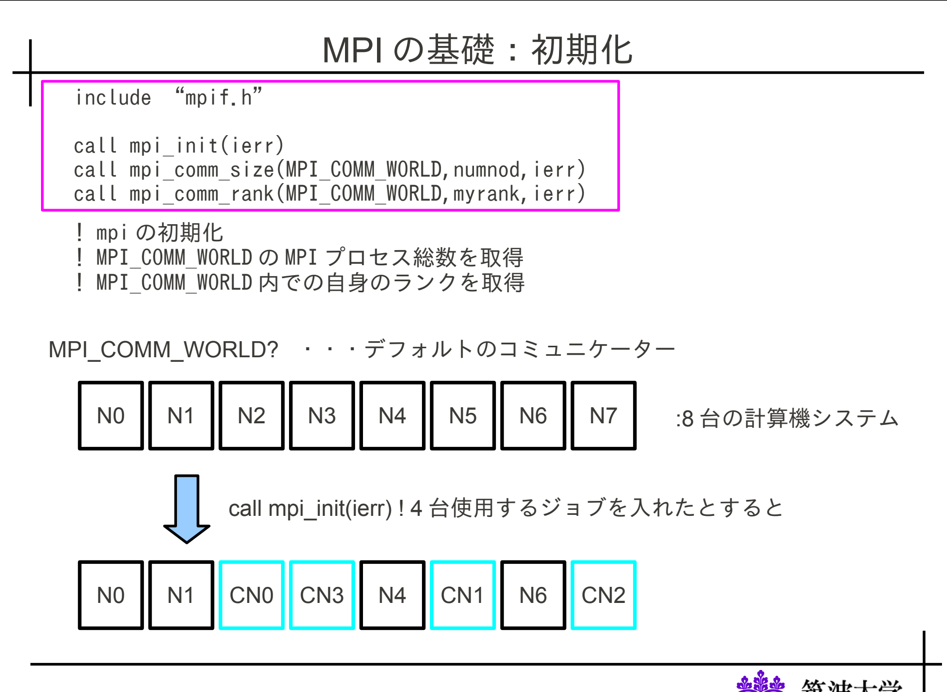

MPI の基礎： Send & Recv

Non Blocking Communication : MPI_ISEND, MPI_IRECV and MPI_WAIT

```
!Buffer Setting
   do i = 1, isb
     do j = 1, nsb(i)
       buf_s(j,i) = dat(nsub(j,i))
     enddo
   enddo

!Send <=> Recv
   do i = 1, isb
     icount = nsb(i)
     ncomID = naid(i)
     call MPI_ISEND( buf_s(1,i), icount, MPI_DOUBLE_PRECISION, &
                     ncomID, 0, MPI_COMM_WORLD, irqs(i), ierr)
     call MPI_IRECV( buf_r(1,i), icount, MPI_DOUBLE_PRECISION, &
                     ncomID, 0, MPI_COMM_WORLD, irqr(i), ierr)
   enddo

!Synchronization
   call MPI_WAITALL( isb, irqs(1), istatus, ierr)
   call MPI_WAITALL( isb, irqr(1), istatus, ierr)
```

```
isb                       : 1
nid(1:isb)                : 1
nsb(1:isb)                : 3
nsub(1:maxval(nsb),1:isb): 7    8    9
```

```
isb                       : 1
nid(1:isb)                : 0
nsb(1:isb)                : 3
nsub(1:maxval(nsb),1:isb): 1    2    3
```

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MPI の基礎： Send & Recv

Non Blocking Communication : MPI_ISEND, MPI_IRECV and MPI_WAIT

```
!Buffer Setting
   do i = 1, isb
     do j = 1, nsb(i)
       buf_s(j,i) = dat(nsub(j,i))
     enddo
   enddo

!Send <=> Recv
   do i = 1, isb
     icount = nsb(i)
     ncomID = naid(i)
     call MPI_ISEND( buf_s(1,i), icount, MPI_DOUBLE_PRECISION, &
                     ncomID, 0, MPI_COMM_WORLD, irqs(i), ierr)

!Synchronization
   call MPI_WAITALL( isb, irqs(1), istatus, ierr)
   call MPI_WAITALL( isb, irqr(1), istatus, ierr)
```

送信データの先頭アドレス

送信データの個数

送信データの型

エラーコード

送信リクエスト

コミュニケーター名

tag(とりあえず Send と Recv で同じ値を)

宛先のコミュニケーター内のランク

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MPI の基礎： Send & Recv

Non Blocking (MPI_ISEND/IRECV) と Blocking(MPI_SEND/RECV) の違い

```
!Send <=> Recv
   do i = 1, isb
     icount = nsb(i)
     ncomID = naid(i)
     call MPI_ISEND( buf_s(1,i), icount, MPI_DOUBLE_PRECISION, &
                     ncomID, 0, MPI_COMM_WORLD, irqs(i), ierr)
     call MPI_IRECV( buf_r(1,i), icount, MPI_DOUBLE_PRECISION, &
                     ncomID, 0, MPI_COMM_WORLD, irqr(i), ierr)
   enddo
!Synchronization
   call MPI_WAITALL( isb, irqs(1), istatus, ierr)
   call MPI_WAITALL( isb, irqr(1), istatus, ierr)
!
!   do i = 1, isb
!     icount = nsb(i)
!     ncomID = naid(i)
!     call MPI_SEND( buf_s(1,i), icount, MPI_DOUBLE_PRECISION, &
!                    ncomID, 0, MPI_COMM_WORLD, ista_s, ierr)
!     call MPI_RECV( buf_r(1,i), icount, MPI_DOUBLE_PRECISION, &
!                    ncomID, 0, MPI_COMM_WORLD, ista_r, ierr)
!   enddo
```

MPI の基礎： Send & Recv

Non Blocking (MPI_ISEND/IRECV) と Blocking(MPI_SEND/RECV) の違い

Blocking

MPI_SEND がコールされ，そのデータが相手に MPI_RECV されて送受信が完了．これが正常に終了するまで，次の作業には進めない．

Non-Blocking

MPI_ISEND がコールされる．ただし，送受信が完了していなくても，別の別の処理を開始することが可能．送受信を完了するには MPI_WAIT をコールする必要がある．

```
!
!   do i = 1, isb
!     icount = nsb(i)
!     ncomID = naid(i)
!     call MPI_SEND( buf_s(1,i), icount, MPI_DOUBLE_PRECISION, &
!                    ncomID, 0, MPI_COMM_WORLD, ista_s, ierr)
!     call MPI_RECV( buf_r(1,i), icount, MPI_DOUBLE_PRECISION, &
!                    ncomID, 0, MPI_COMM_WORLD, ista_r, ierr)
!   enddo
```

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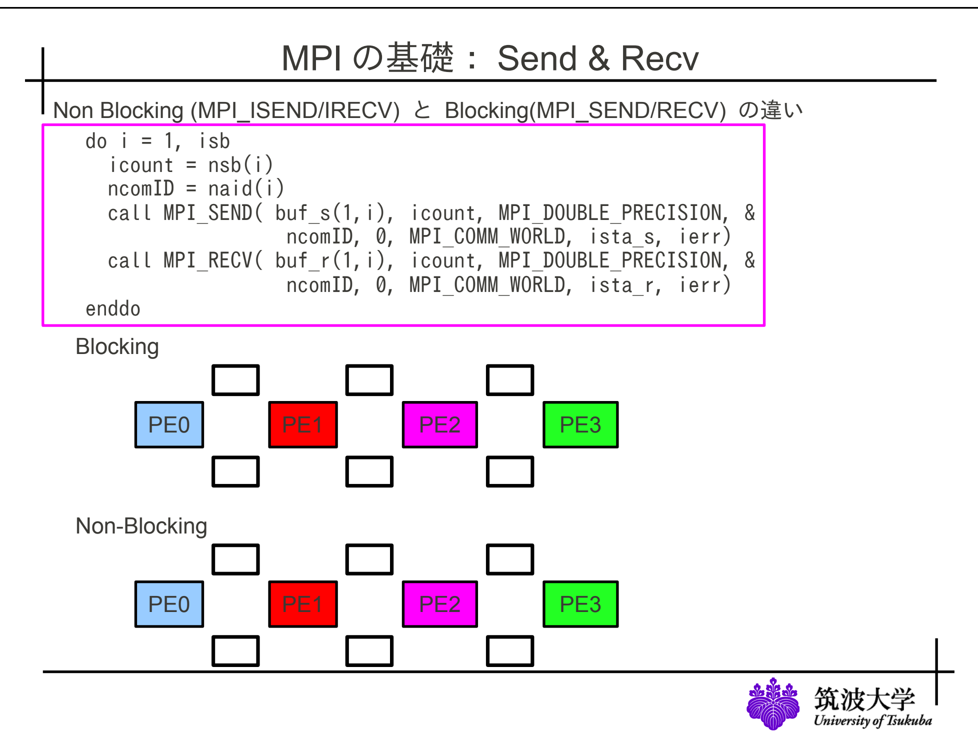

MPI の基礎： Allreduce

```
dots = 0.0d0
do n = 1, node
  dots = dots + r(n)*r(n)/ndb(n)
enddo

call MPI_ALLREDUCE( dots, dotr, 1, MPI_DOUBLE_PRECISION, &
                    MPI_SUM, MPI_COMM_WORLD, ierr )
```

節点重複数

全小領域間通信 (Allreduce)

PE0　PE1

PE0 + PE1 = 全体の総和

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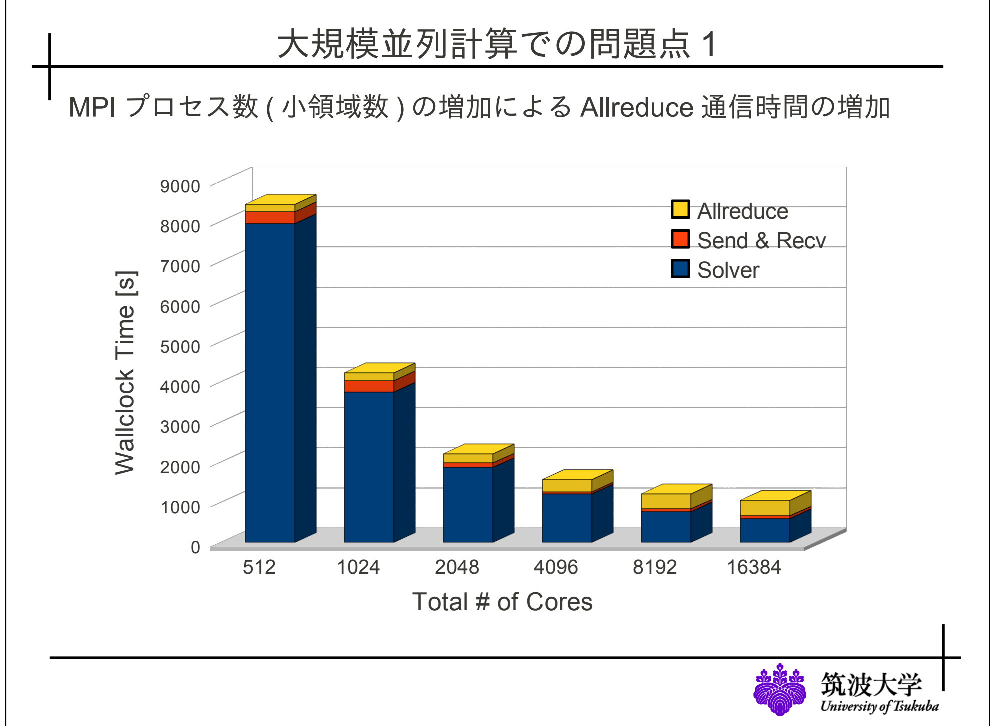

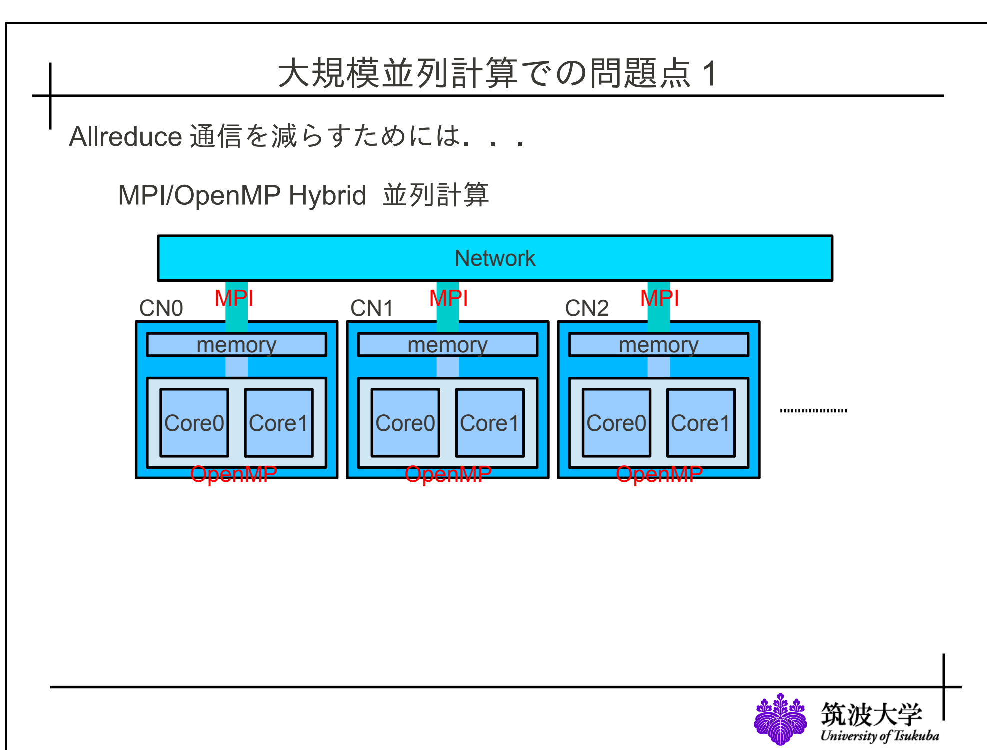

大規模並列計算での問題点 1
Allreduce 通信を減らすためには．．．
MPI/OpenMP Hybrid 並列計算
Network
MPI
CN0
CN1
CN2
memory
Core0
Core1
OpenMP
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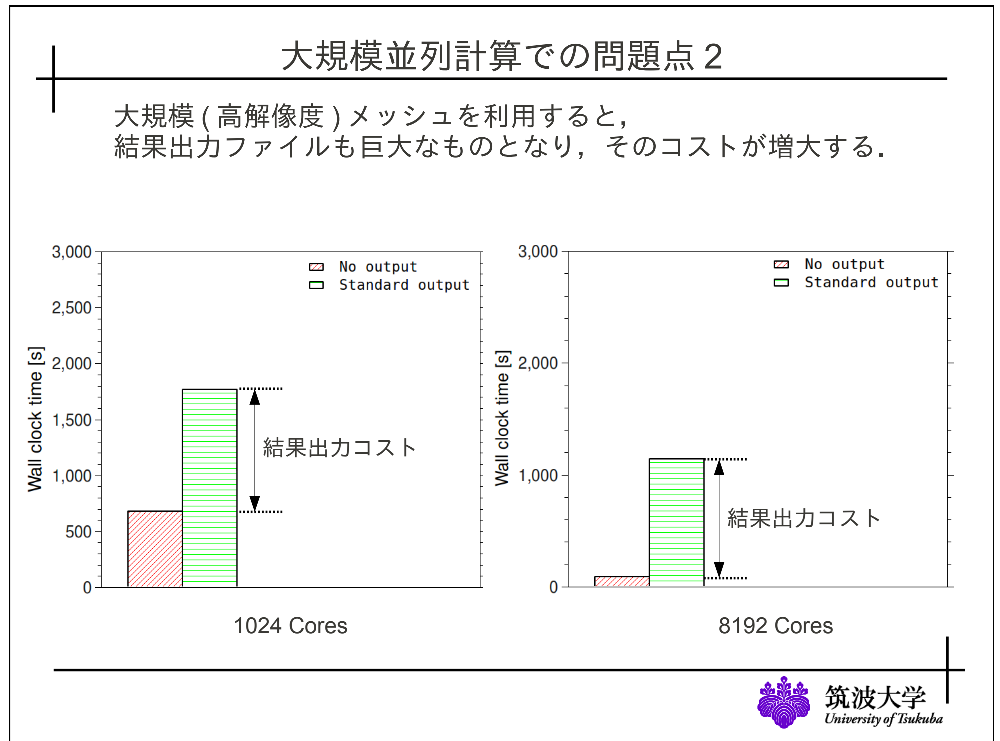
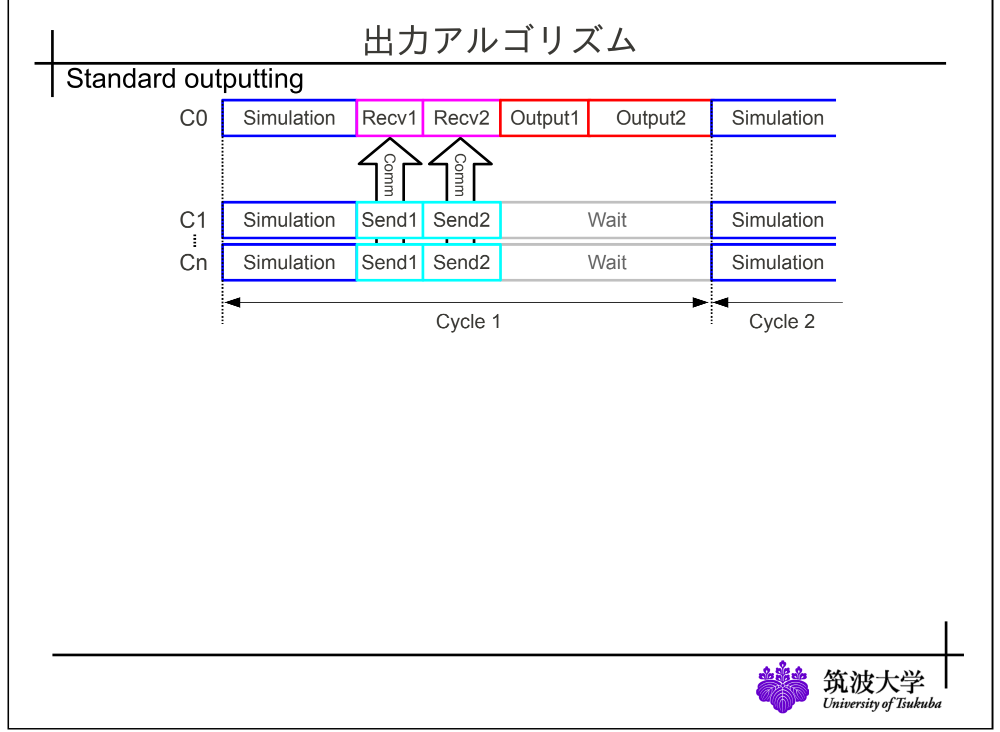
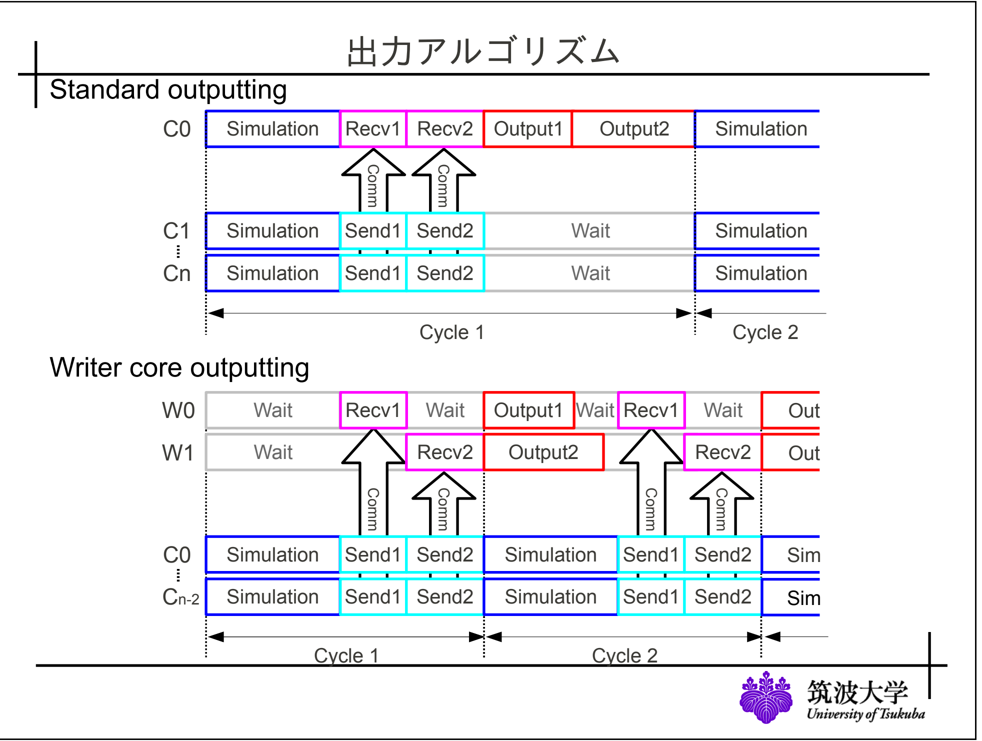


大規模並列計算での問題点 2
大規模 (高解像度) メッシュを利用すると，
結果出力ファイルも巨大なものとなり，そのコストが増大する．
No output
Standard output
Wall clock time [s]
結果出力コスト
1024 Cores
8192 Cores
筑波大学
University of Tsukuba



出力アルゴリズム
Standard outputting
C0
C1
Cn
Simulation
Recv1
Recv2
Output1
Output2
Send1
Send2
Wait
Comm
Cycle 1
Cycle 2
筑波大学
University of Tsukuba



出力アルゴリズム
Standard outputting
Writer core outputting
W0
W1
C0
Cn-2
Simulation
Recv1
Recv2
Output1
Output2
Send1
Send2
Wait
Out
Sim
Comm
Cycle 1
Cycle 2
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Writer Cores の性能

0.125 day simulation of Katrina Hurricane on SL15x04 grid
Output every 15 minutes,
4 files (Elevation, Velocity, Atmospheric pressure, Wind Stress)
Explicit method.

Wall clock time [s]
3,000
2,000
1,000
0

No output
Standard output
1 writer core
2 writer cores
4 writer cores
8 writer cores

1024 Cores

8192 Cores

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MPI の基礎：コミュニケータの分割

```
call mpi_init(ierr)
call mpi_comm_dup(MPI_COMM_WORLD, MPI_COMM_GBL)
call mpi_comm_size(MPI_COMM_GBL,numnod_gbl,ierr)
call mpi_comm_rank(MPI_COMM_GBL,myrank_gbl,ierr)
call mpi_comm_group(MPI_COM_GBL,GROUP_GBL,ierr)
n1 = numnod_gbl/2
n2 = numnod_gbl-n1
do i = 1, n1
  ilist(i) = i-1
enddo
call mpi_group_incl(GROUP_GBL,n1,ilist(1),GROUP1,ierr)
call mpi_comm_create(MPI_COMM_GBL,GROUP1,MPI_COMM_GR1,ierr)
do i = 1, n2
  ilist(i) = n1+i-1
enddo
call mpi_group_incl(GROUP_GBL,n2,ilist(1),GROUP2,ierr)
call mpi_comm_create(MPI_COMM_GBL,GROUP2,MPI_COMM_GR2,ierr)
```

コミュニケータを複製

全体のグループを作成

GROUP_GBL から
GROUP1 を作成

GROUP1 からなる
コミュニケータを作成

0 1 2 3

0 1 0 1

: MPI_COMM_WORLD
: MPI_COMM_GR1
: MPI_COMM_GR2

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結果出力方法

POSIX I/O

Ascii output

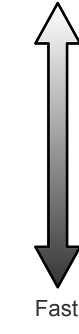
```
do i = 1, nnode
  write(60,*)  uu(i)
enddo
```

Binary output (formatted)

```
inquire(iolength=length) a
open(60,access='direct', recl=length)
irec=0
do i = 1, nnode
  irec=irec+1
  write(60,rec=irec)  uu(i)
enddo
```

Binary output (unformatted)

```
open(60,format='unformatted')
write(60)  (uu(i), i=1,nnode)
```



ただし， endian 問題があり，異なる環境 (CPU， OS 等) により
互換性が失われる場合がある．

結果出力方法

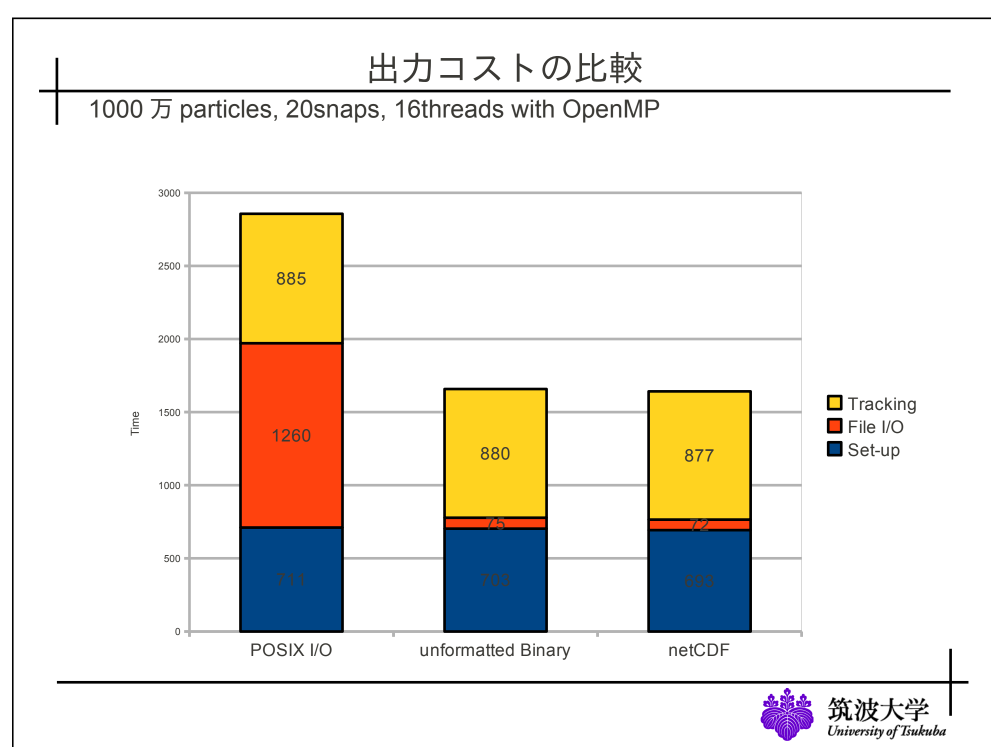
NetCDF (Network Common Data Form)

- University Corporation Atmospheric Research (UCAR) が開発．
- Library と幾つかの tool のパッケージ
- C/C++/Fortran， その他の言語 (Perl, Python, Ruby, Matlab 等) でも利用可能

```
use netCDF
ist=nf90_create('fort.60',nf90_64bit_offset,ncid)
ist=nf90_def_dim(ncid,'Total_Num_of_Nodes',nnode,id_nnode)
ist=nf90_def_var(ncid,'Velocity_u',nf90_double,id_nnode,id_varU)
ist=nf90_enddef(ncid)

ist=nf90_put_var(ncid,id_varU,uu,start=(/1/),count=(/nnode/))
ist=nf90_close(ncid)
```

```
$ gfortran -c -I$NETCDF_INC wirte_nc.f90
$ gfortran -o write_nc.exe write_nc.o -L$NETCDF_LIB -lnetcdf
```



大規模並列計算での軽微な問題点

Problems on 32,768 (=2^{15}) MPI process

Range of 32bit Integer number (-2^{31}~2^{31})

- Metis 4.0 requires 4*(# of MPI)^2 for memory allocation.

Limit of maximum total number of sub-directories. *1

- ext3 file system has the limit. (max: 31,998)

GlobalDir/PE00000/mesh.data, bc.data, comm.data

:

/PE31997/mesh.data, bc.data, comm.data

Memory allocation related to # of MPI

```
isb                     : 1
nid(1:isb)              : 1
nsb(1:isb)              : 3
nsub(1:maxval(nsb),1:isb): 7    8    9
```

Sometimes nsub is allocated as,
allocate(nsub(1:nnode/nproc,1:nproc))

*1 The newest ext4 file system don't have such a limitation.