# Elements of OpenMP and MPI

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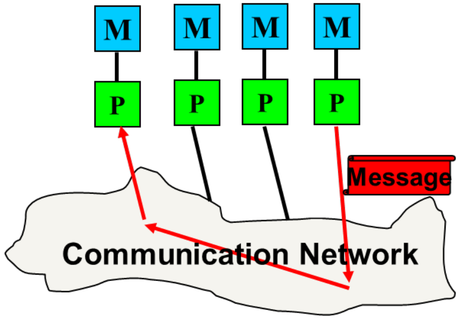
High Performance Computing

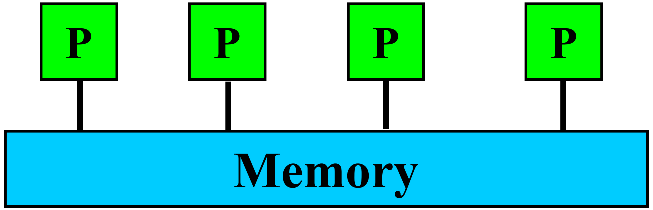
# Two Paradigms for Parallel Programming

- Distributed Memory
  - message passing
  - explicit programming required




- Special design:
  - cache coherency protocol over interconnect
  - behaves like non-uniform shared memory

- Shared Memory
  - common address space for a number of CPUs
  - access efficiency may vary → SMP, (cc)NUMA
    (memory access time depends on the memory location relative to the processor)
  - many programming models
  - potentially easier to handle
  - hardware and OS support required



# Two Paradigms for Parallel Programming

## Distributed Memory

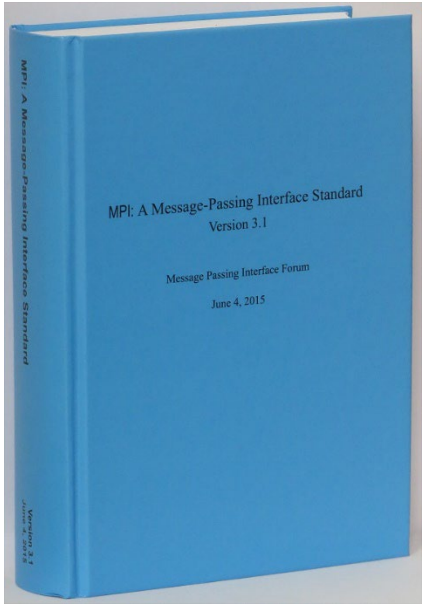
- **Same program on each processor/machine (SPMD) or**
  Multiple programs with consistent communication structure (MPMD)
- **Program written in a sequential language**
  - all variables process-local
  - no implicit knowledge of data on other processors
- **Data exchange between processes**
  - send/receive messages via appropriate library
  - most tedious, but also the most flexible way of parallelization
- Parallel library discussed here:
  - Message Passing Interface, **MPI**

## Shared Memory

- **Single Program on single machine**
  - UNIX Process splits off **threads**, mapped to CPUs for work distribution
- **Data**
  - may be process-global or thread-local
  - exchange of data not needed, or via suitable synchronization mechanisms
- **Programming models**
  - explicit threading (hard)
  - directive-based threading via **OpenMP** (easier)
  - automatic parallelization (very easy, but mostly not efficient)

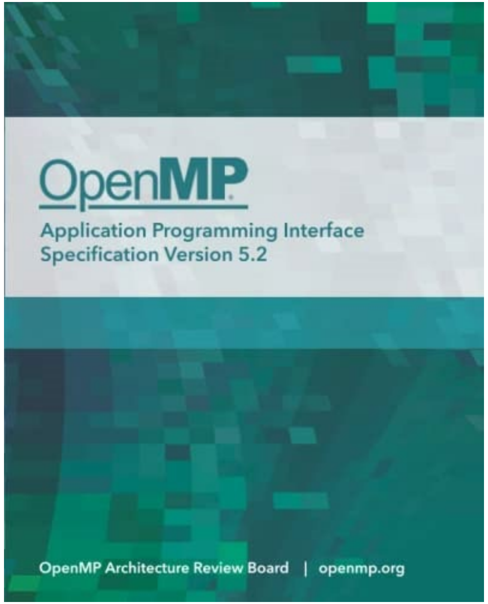
# Standards-Based Parallelism

**MPI Standard**




https://www.mpi-forum.org/docs/

**OpenMP Standard**



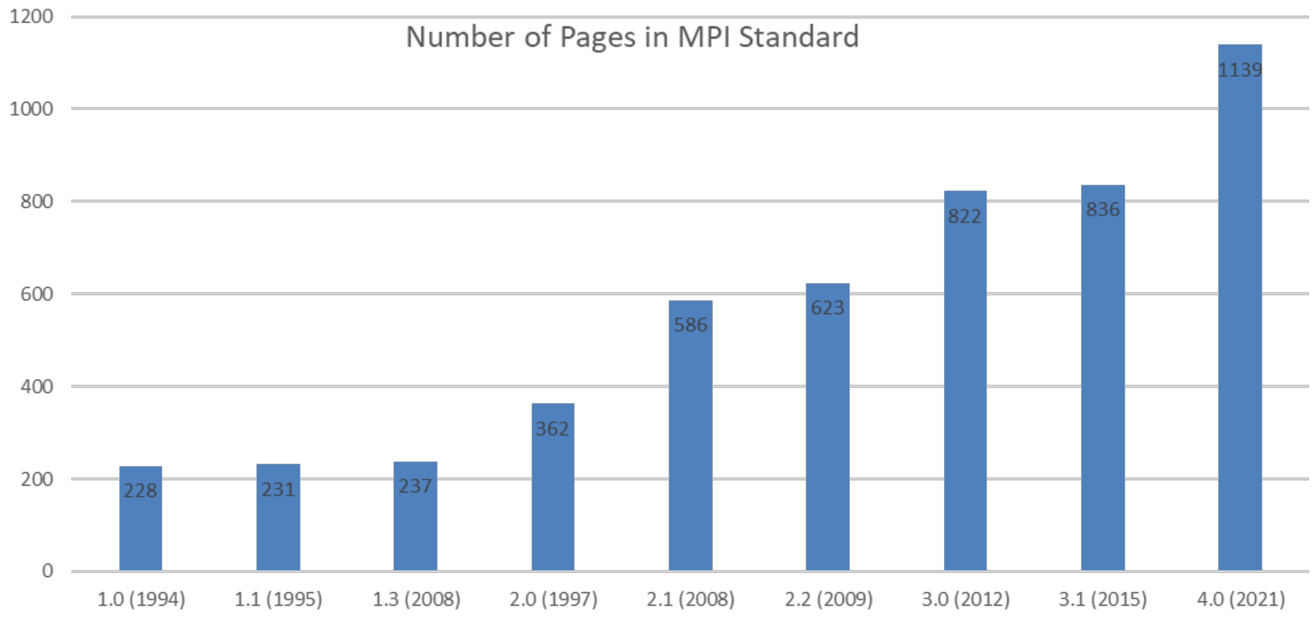

https://www.openmp.org/specifications/

# Two Paradigms for Parallel Programming

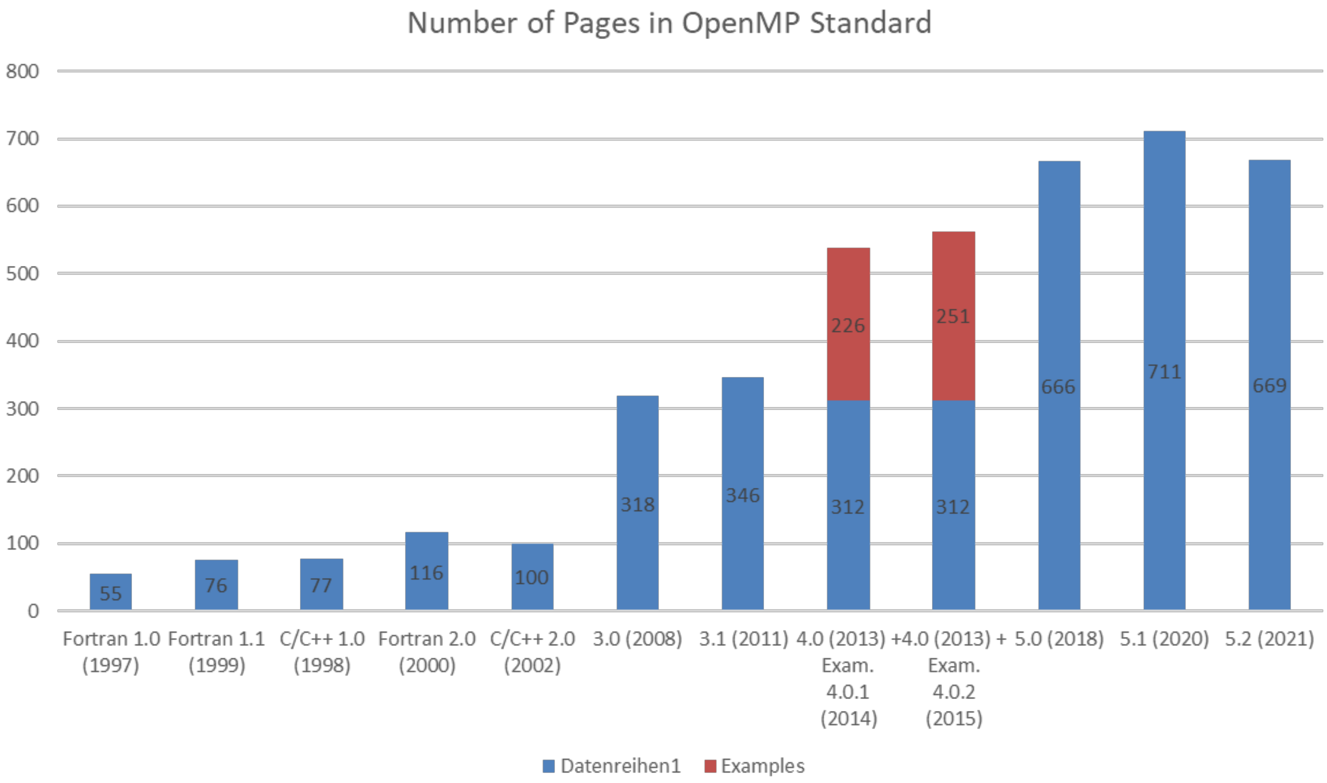
- **MPI Standard**
  - MPI version 1.0 in May 1994
  - MPI version 2.0 in July 1997
  - MPI version 3.0 in September 2012
  - MPI version 4.0 in June 2021
  - MPI version 4.1 in November 2023.
- **Base Languages**
  - Fortran
  - C
- **Resources**
  - http://www.mpi-forum.org

- **OpenMP Standard**
  - OpenMP 1.0 in 1997 (Fortran) / 1998 (C, C++)
  - OpenMP 3.0 (May 2008)
    - tasking etc.
  - OpenMP 4.0 (July 2013)
    - SIMD, affinity policies, accelerator support
  - OpenMP 5.0 (Nov 2018)
    - two new tool interfaces , multilevel memory systems
  - OpenMP 5.2 (Nov 2021)
    - improvements and refinements
- **Base Languages**
  - Fortran
  - C, C++
- **Resources**
  - http://www.openmp.org

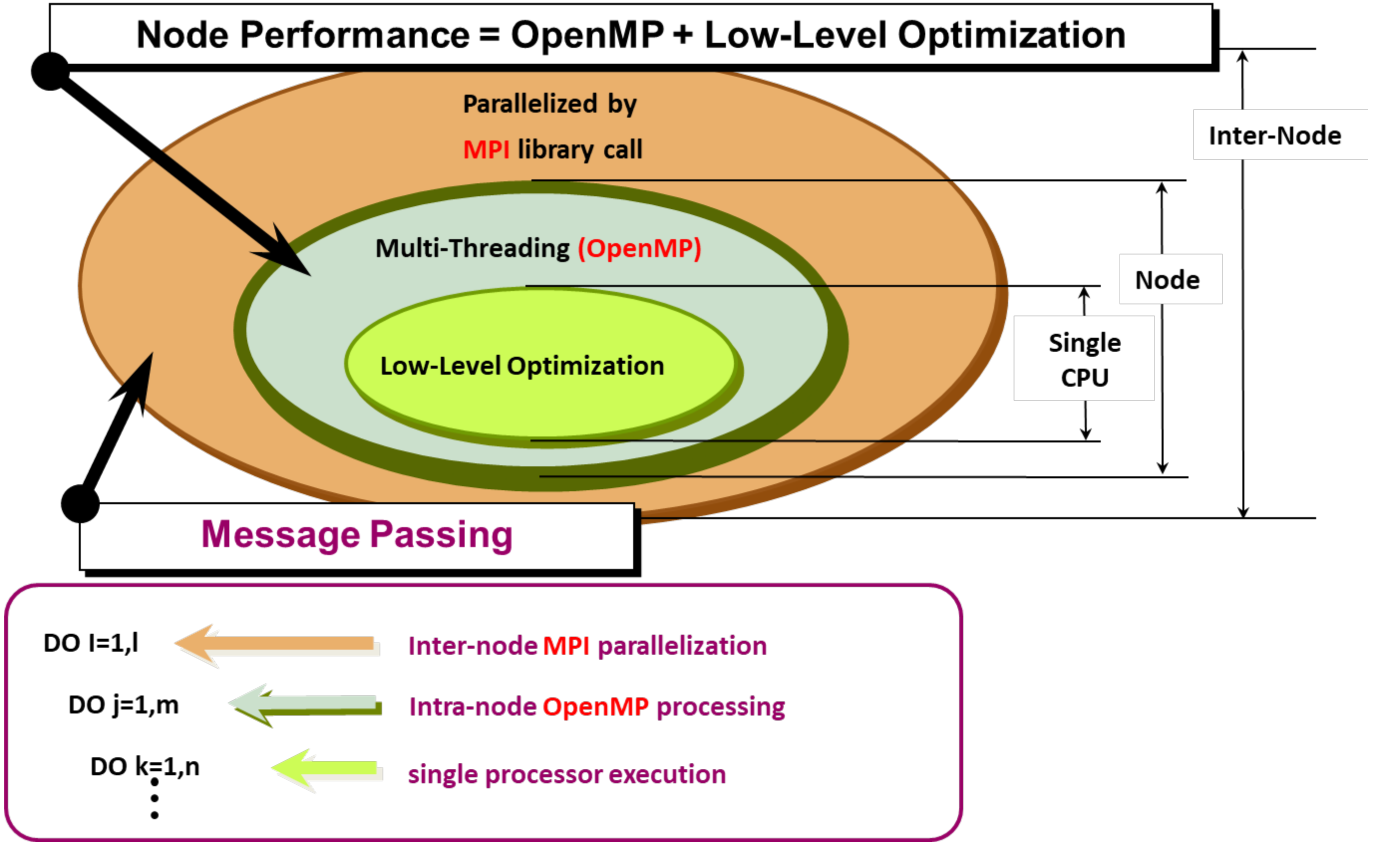
# MPI Standard



# OpenMP Standard



# Typical Parallelization Hierarchy



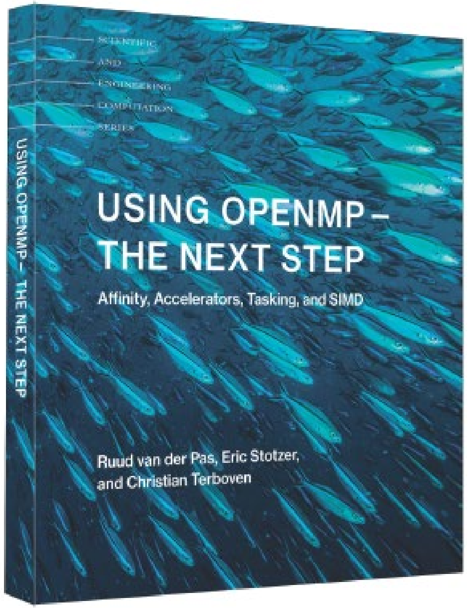
# OpenMP

Principles of Directive Driven Shared Memory Parallelism

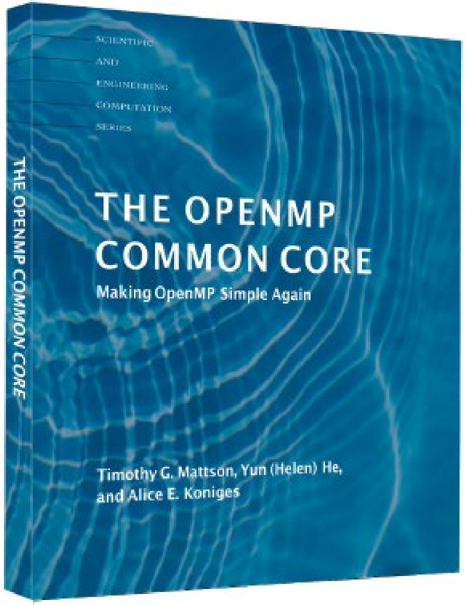
# OpenMP Architecture Review Board (ARB)

The mission of the OpenMP ARB (Architecture Review Board) is to standardize directive-based multi-language high-level parallelism that is performant, productive and portable.

# Recent Books about OpenMP

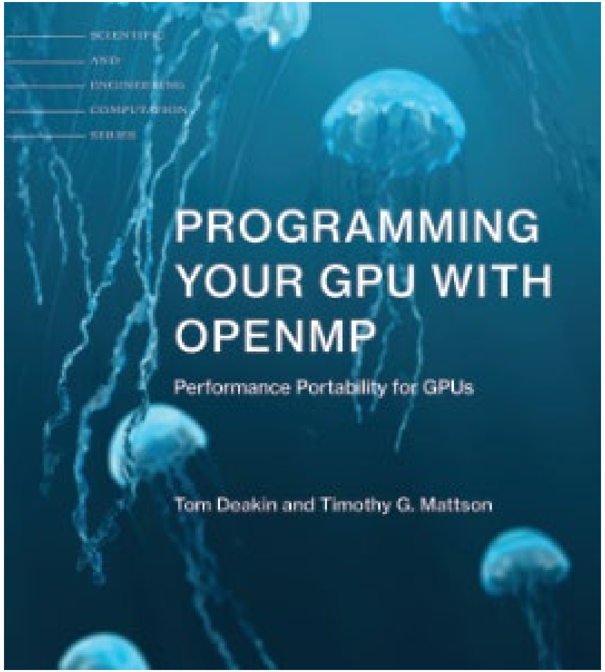



Covers all of the
OpenMP 4.5 features, 2017



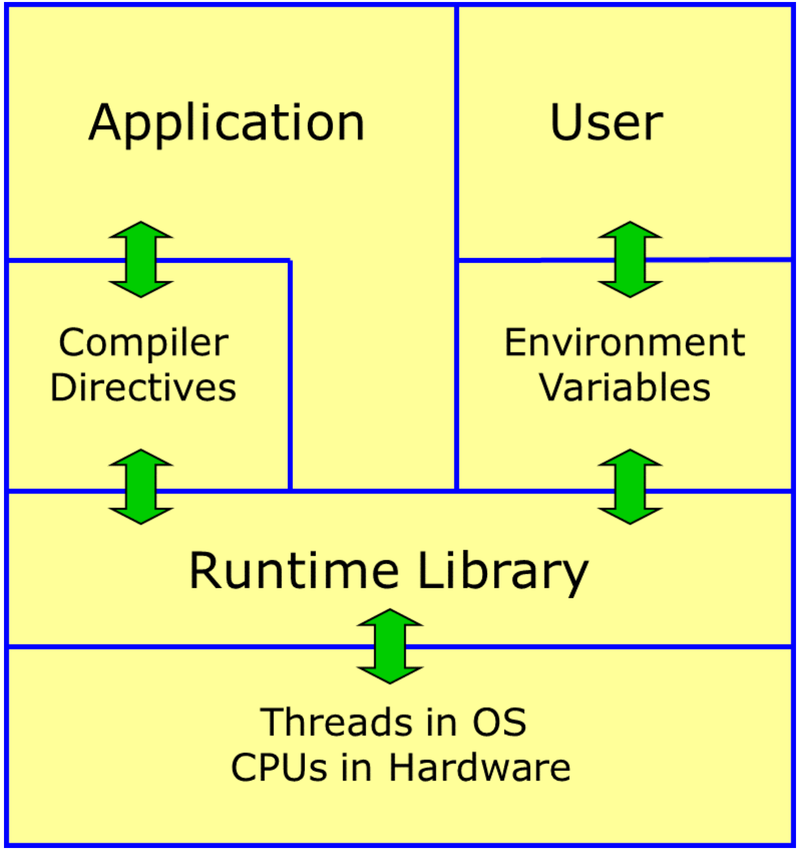

Introduces the
OpenMP Common Core, 2019

# Recent Books about OpenMP



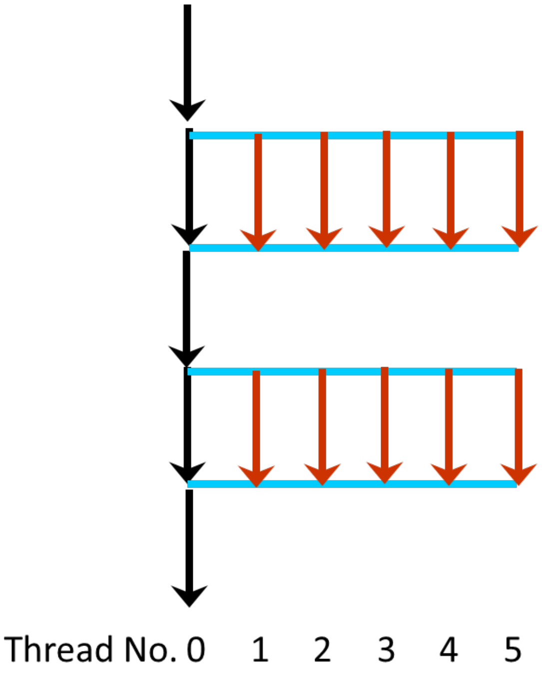

Covers all about Accelerator Programming, 2023

# Two Paradigms for Parallel Programming




- **Operating system view:**
  - parallel work done by **threads**
- **Programmer's view:**
  - **directives**: comment lines in code, e.g.
    - `!$omp parallel`
    - `#pragma omp parallel`
  - library routines, e.g.
    - `omp_get_num_threads()`
    - `omp_get_thread_num()`
    - `omp_get_max_threads()`
- **User's view:**
  - **environment variables** determine:
    resource allocation, scheduling strategies and other (implementation-dependent) behaviour, e.g.
    - `OMP_NUM_THREADS`
    - `OMP_SCHEDULE`
    - `OMP_NESTED`

# Two Paradigms for Parallel Programming




- Program start: only initial thread (formerly known as master thread) runs
- Parallel region: team of worker threads is generated (“fork”)
- Threads synchronize when leaving parallel region (“join”)
- Only initial thread executes sequential part (worker threads persist, but are inactive)
- Task and data distribution possible via directives
- Nesting of parallel regions:
  - allowed, but level of support implementation dependent
- Usually optimal:
  - one thread per processor core
  - other resource mappings are allowed/possible

# Parallel region: Simplest Program Example: Fortran

```
program hello
  use omp_lib
  implicit none
  integer :: nthr, myth

!$omp parallel private(myth)

!$omp single
  nthr = omp_get_num_threads()
!$omp end single

  myth = omp_get_thread_num()

  write(*,*) "Hello from ", myth, "of ", nthr
!$omp end parallel

end program hello
```

- **Parallel region directive:**
  - enclosed code executed by **all** threads
  - may include subprogram calls („dynamic region“)
- **Special function calls:**
  - module `omp_lib` provides interface
  - here: get number of threads and index of executing thread
- **Data scoping:**
  - uses a **clause** on the directive
  - `myth` thread-local: **private**
  - `nthr` process-global: **shared**

(will be discussed in more detail later)

# Parallel region: Simplest Program Example: C/C++

```
#include <stdio.h>
#include <omp.h>
int nthr, myth;
int main(int arc, char *argv[])
{
#pragma omp parallel private(myth)
  {
    #pragma omp single
    nthr = omp_get_num_threads();

    myth = omp_get_thread_num();
    printf("Hello from %i of %i\n", myth, nthr);
  }
}
```

- **Parallel region directive:**
  - enclosed code executed by **all** threads
  - may include subprogram calls („dynamic region“)
- **Special function calls:**
  - Include file <omp.h>
  - here: get number of threads and index of executing thread
- **Data scoping:**
  - uses a **clause** on the directive
  - `myth` thread-local: **private**
  - `nthr` process-global: **shared**

(will be discussed in more detail later)

# Compiling and Running an OpenMP Program

**Compile Fortran (e.g. with Intel compiler):**

```
ifort -qopenmp -o hello.exe hello.f90
```

**Compile C (e.g. with Intel compiler):**

```
icc -qopenmp -o hello.exe hello.f90
```

**Run:**

```
export OMP_NUM_THREADS=4
./hello.exe
 Hello from 0 of  4
 Hello from 2 of  4
 Hello from 3 of  4
 Hello from 1 of  4
```

ordering not reproducible

**Compile for serial run (e.g. with Intel compiler):**

```
ifort -qopenmp-stubs -o hello.exe hello.f90
```

- special switch for „stub library“

- **Special compiler switch**
  - activates OpenMP directives
  - generates threaded code
  - further suboptions may be available
  - each compiler has something **different** here
- **OpenMP environment**
  - defines runtime behaviour
  - here: number of threads used
- **Serial functionality of program**
  - (dis)order of output

# OpenMP Fortran Syntax

- Specifications:
  - Fortran 77 style

```
include "omp_lib.h"
```

  - Fortran 90 module (**preferred**)

```
use omp_lib
```

- Directives:
  - fixed form source:

```
C$OMP <directive> [<clause [(<args>)]>, …]
```

sentinel starting in column 1, also : ***$OMP, !$OMP**

free form source (preferred):

```
!$OMP <directive> [<clause [(<args>)]>, …]
```

- Conditional compilation:

```
 myid = 0
!$ myid = omp_get_thread_num()
```

  - In fixed form also sentinels *$, c$

- Continuation line:

```
!$OMP <directive> &
!$OMP <clause>
```

# OpenMP C/C++ Syntax

- Include file:

```
#include <omp.h>
```

- Preprocessor  directive:  uses pragma feature

```
#pragma omp <directive> [clause …]
```

- Conditional compilation: OpenMP switch sets preprocessor macro

```
#ifdef _OPENMP

  … /* do something */
#endif
```

- Continuation line:

```
#pragma omp directive \
   clause
```

# OpenMP Syntax: Remarks on Clauses

- Many (but not all) OpenMP directives support clauses
  - more than one may appear on a given directive
- Clauses specify additional information associated with the directive
  - modification of directive's semantics
- "Simplest example" from above:
  - `private(…)` appears as clause to the `parallel` directive
- The specific clause(s) that can be used depend on the directive

# OpenMP Syntax: Structured Block

- **Defined by braces in C/C++**
- **If explicitly specified in Fortran:**
  - code between begin/end of an OpenMP construct must be a complete, valid Fortran block
- **Single point of entry:**
  - no `GOTO` into block (Fortran), no `setjmp()` to entry point (C)
- **Single point of exit:**
  - `RETURN`, `GOTO`, `EXIT` outside block are prohibited (Fortran)
  - `longjmp()` and `throw()` must not violate entry/exit rules (C, C++)
  - **exception:** termination via `STOP` or `exit()`

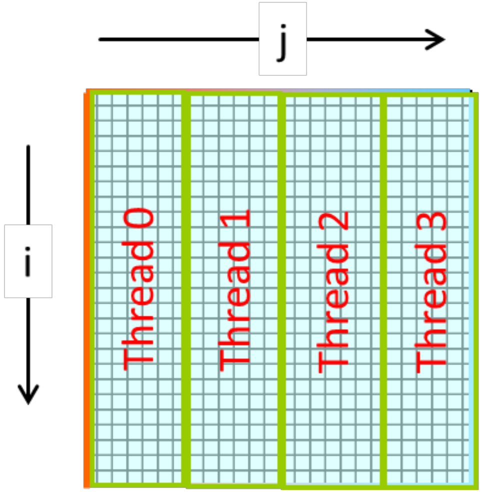
- **Block structure example:**
  - C version of simplest program

```
#include <omp.h>

int main() {
  int numth = 1;
#pragma omp parallel
  {
     int myth = 0; /* private */
#ifdef _OPENMP
#pragma omp single
      numth = omp_get_num_threads();
      /* block above: one statement */
      myth = omp_get_thread_num();
#endif
      printf("Hello from %i of %i\n",\
             myth,numth);
   }  /* end parallel */
}
```

# Work Sharing in OpenMP (1): Fortran

- **Making parallel regions useful …**
  - divide up work between threads
- **Example:**
  - working on an array processed by a nested loop structure




```
real :: a(ndim, ndim)
…
!$omp parallel
!$omp do
do j=1, ndim
  do i=1, ndim
    …
    a(i, j) = …
  end do
end do
!$omp end do
  …
!$omp end parallel
```

j-loop is sliced

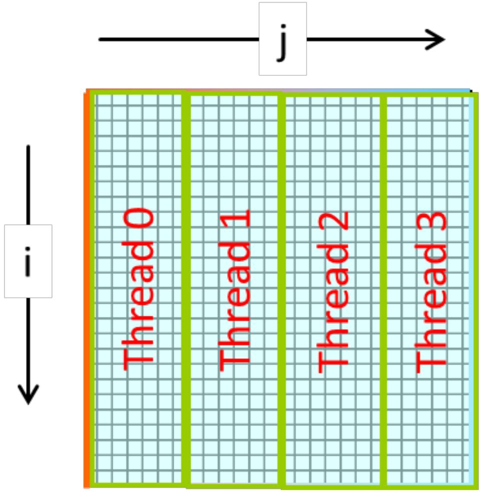
synchronization between threads

further parallel execution

- iteration space of **directly nested loop** is sliced

# Work Sharing in OpenMP (1): C/C++

- **Making parallel regions useful …**
  - divide up work between threads
- **Example:**
  - working on an array processed by a nested loop structure




```
float a[ndim][ndim];

int main(int arc, char *argv[])
{
#pragma omp parallel
  {
#pragma omp for
    for(int j=0;j<ndim;j++) {
      for(int i=0;i<ndim;i++) {
        a[i][j]= …;
      }
    }
   …
  }
}
```

j-loop is sliced

synchronization between threads

further parallel execution

  - iteration space of **directly nested loop** is sliced

# Work Sharing in OpenMP (2)

- **Synchronization behaviour:**
  - all threads (by default) **wait for completion** at the end of the work sharing region („barrier“)
  - following references and definitions to an array element by **other** threads are therefore OK.
- **Slicing of iteration space:**
  - „loop scheduling“
  - default behaviour is implementation dependent
  - usually as equal as possible chunks of largest possible size
- **Additional clauses on `!$OMP DO / #pragma omp for`**
  - will be discussed in advanced OpenMP talk

- **Fortran syntax:**

```
!$omp do [clause]
do ...
   ...   // loop body
end do
```

- **C/C++ syntax:**

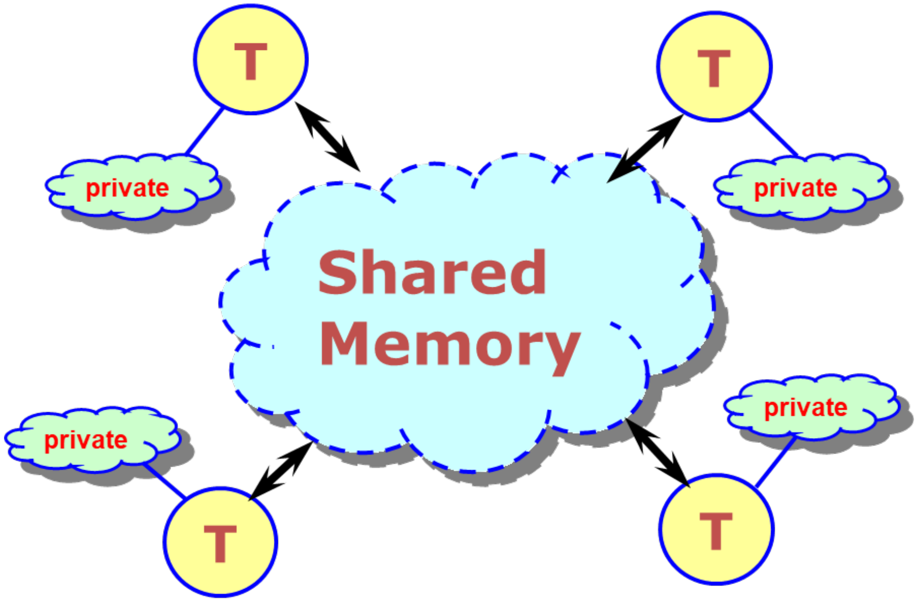
```
#pragma omp for [clause]
for ( ... )  {
       ...   // loop body
}
```

- **Restrictions on loop structure:**
  - trip count must be **computable** at entry to loop

    **disallowed:** C style loops modifying the loop variable, or otherwise violating the require-ment, Fortran `do while` loop without loop control;
  - loop body with single entry and single exit point

# Memory Model

- **Two kinds of memory exist in OpenMP**




- **Threads access globally shared memory**
- **Data can be shared or private**
  - shared data – one instance of an entity available to all threads
  - private data – each per-thread copy only available to thread that owns it
- **Data transfer** transparent to programmer
- **Synchronization** takes place (is mostly implicit)
- **threadprivate variables**
  - see advanced OpenMP talk

# Data-Sharing Attributes

- By default most variables are shared
  - local variables outside the scope of construct
  - static/global (C/C++) or save/common (Fortran) variables

```
int s = 1;

#pragma omp parallel
{
  int p = omp_get_thread_num();
  printf("s=%d p=%d\n", s, p);
}
```

- Except
  - variables* defined inside the construct are private
    - i.e. declared inside `{}`-block or `BLOCK/END BLOCK`
  - variables* local to functions/routines called from within the region are private
  - loop iteration variables of worksharing loops are private

* non-static (C/C++) or without save attribute (Fortran)

# Data-Sharing Attribute Clauses

- Clauses for explicitly specifying how a variable should be treated
  - supported by several directives, e.g., `parallel`, `do`/`for`, `single`, `sections`, `task`, …
- Clauses:
  - `shared(var1, var2, …)`
  - `private(var1, var2, …)`
  - private + special operation
    - `firstprivate(var1, var2, …)`
    - `lastprivate`, for `do`/`for` construct
- Change default:
  - Fortran `default(shared|private|firstprivate|none)`
  - C/C++: `default(shared|none)`
  - best practice: `default(none)`
    - every variable referenced must appear in a `shared`/`private`/… clause
    - avoids incorrect assumptions about shared/private

# Scoping: Second-Simplest Example: Fortran

- Summation inside a loop

```
real :: s, stot
stot = 0.0
!$omp parallel private(s)
s = 0.0
!$omp do
do i=1, ndim
     … ! workload
     s = s + …
end do
!$omp end do

!$omp critical
  stot = stot + s
!$omp end critical

!$omp end parallel
```

- **Note:** large workload inside loop improves threaded performance

- require thread-individual variable for partial sum calculated on each thread
- **but:** private copies of variables are **undefined** at entry to, and become **undefined** at exit of the parallel region
- **therefore:** collect partial sums to a **shared** variable defined after the worksharing region
- **updates** to shared variable must be specially protected:

→ use a **critical region**

→ only one thread at a time may execute (mutual exclusion)

(performance impact due to explicit synchronization)

# Scoping: Second-Simplest Example: C/C++

- Summation inside a loop

```
 float s, stot;
 stot = 0.;
#pragma omp parallel private(s)
  {
    s = 0.;
#pragma omp for
    for(int i=0;i<ndim;i++) {
      … // workload
      s = s + … ;
    }
#pragma omp critical
    {
      stot = stot + s;
    }
  }
```

- **Note:** large workload inside loop improves threaded performance

- require thread-individual variable for partial sum calculated on each thread
- **but:** private copies of variables are **undefined** at entry to, and become **undefined** at exit of the parallel region
- **therefore:** collect partial sums to a **shared** variable defined after the worksharing region
- **updates** to shared variable must be specially protected:

→ use a **critical region**

→ only one thread at a time may execute (mutual exclusion)

(performance impact due to explicit synchronization)

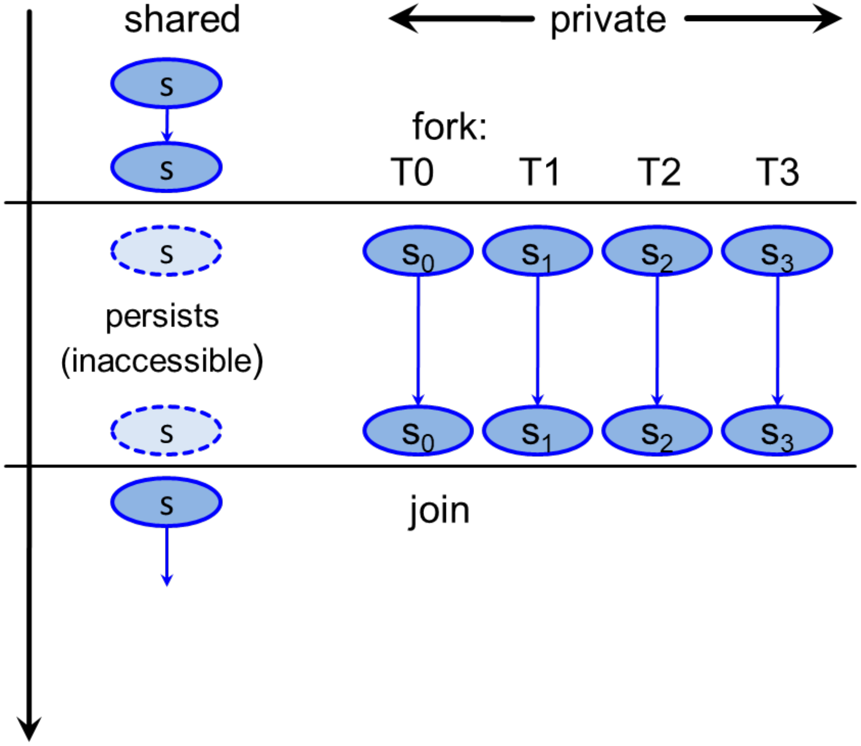
# Private Variables – Masking: Fortran

```
real :: s

  s = …

!$omp parallel private(s)
  s = …
  … = … + s
!$omp end parallel

  … = … + s
```




- **Masking relevant for**
  - privatized variables defined in scope outside the parallel region

# Private Variables – Masking: C/C++

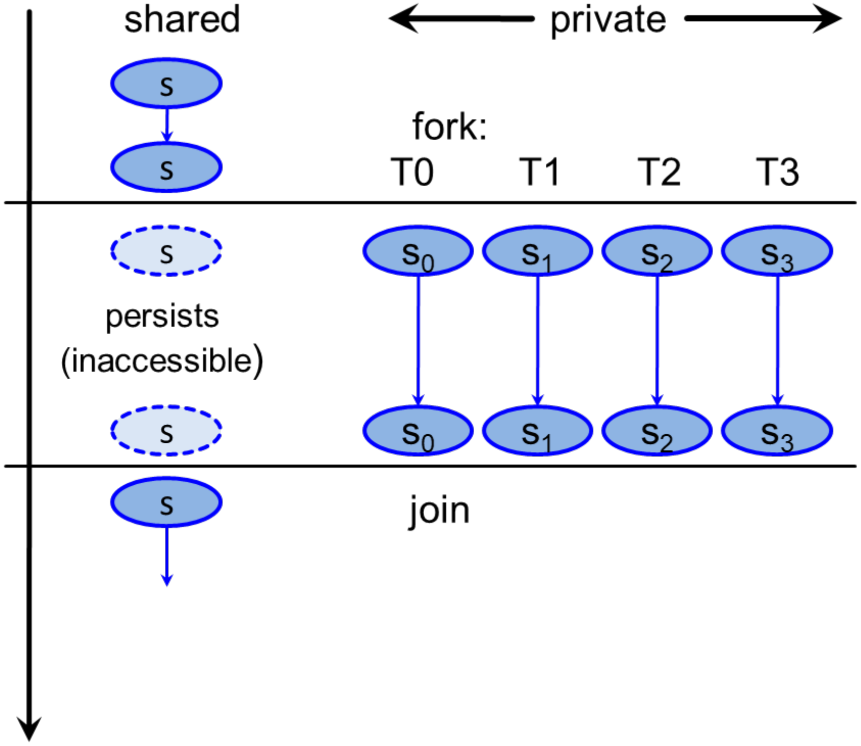
```
float s;

  s = … ;

#pragma omp parallel private(s)
{
  s = … ;
  … = … + s;
}

  … = … + s;
```

- **Masking relevant for**
  - privatized variables defined in scope outside the parallel region



# The firstprivate Clause: Fortran

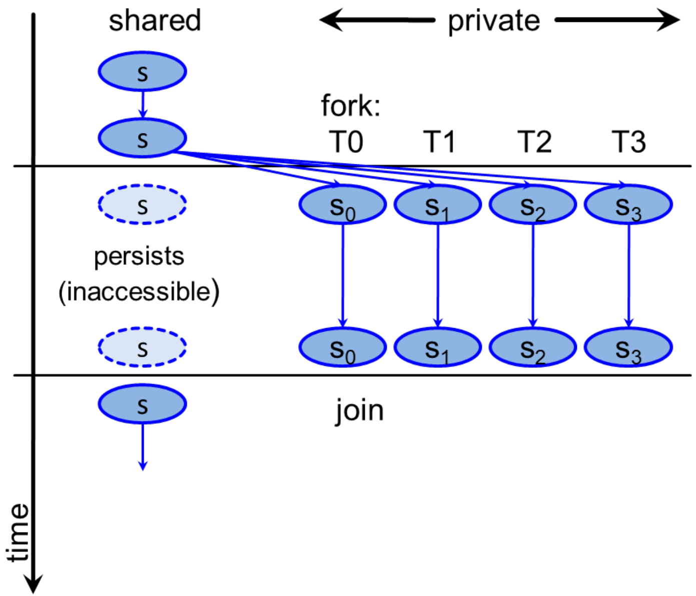
```
real :: s

  s = …

!$omp parallel firstprivate(s)

  … = … + s
!$omp end parallel

  … = … + s
```




- **Extension of private:**
  - value of master copy is transferred to private variables
  - **restrictions:** not a pointer, not assumed shape, not a subobject, master copy not itself private etc.

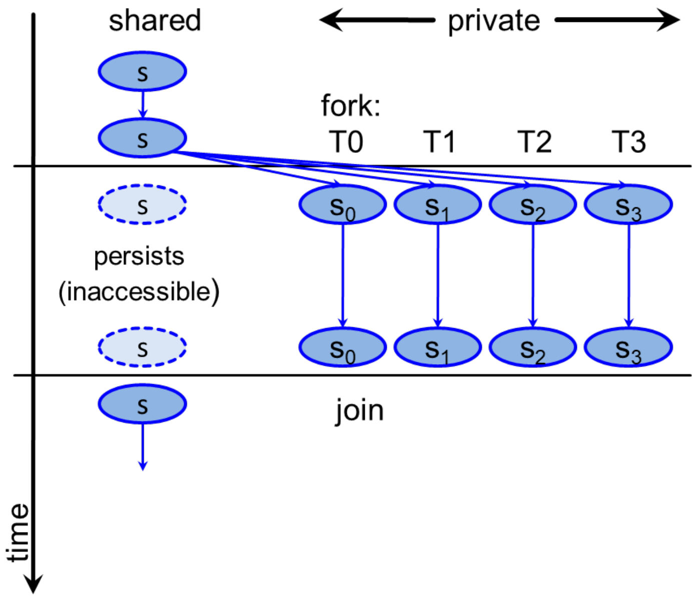
# The firstprivate Clause: C/C++

```
float s;

  s = … ;

#pragma omp parallel firstprivate(s)
{
  … = … + s;
}


  … = … + s;
```




- **Extension of private:**
  - value of master copy is transferred to private variables
  - **restrictions:** not a pointer, not assumed shape, not a subobject, master copy not itself private etc.

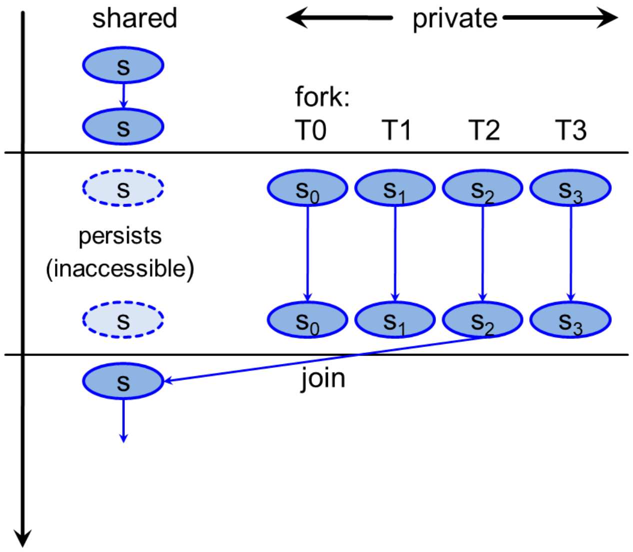
# The lastprivate Clause: Fortran

```
real :: s

  s = …
!$omp parallel
!$omp do lastprivate(s)
  do i = …
     s = …
  end do
!$omp end do
!$omp end parallel
  … = … + s
```

on work sharing directive

- **When to use?**
  - as little as possible
  - legacy code



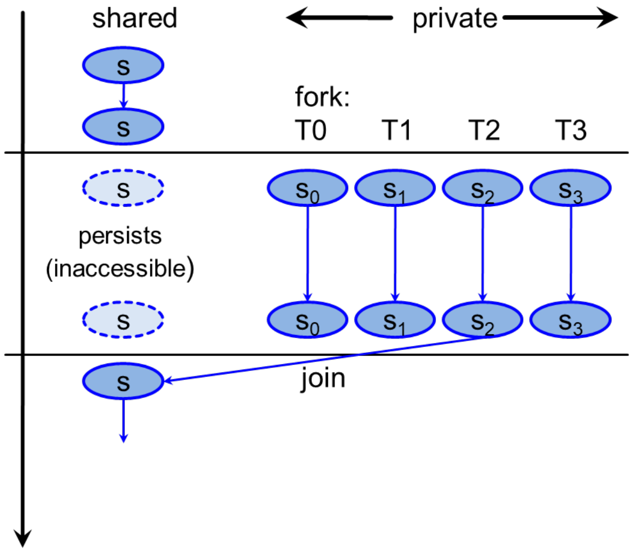

- **Extension of private:**
  - additional semantics for work sharing
  - value from thread which executes last iteration of loop is transferred back to master copy (which must be allocated if it is a dynamic entity)
  - restrictions similar to `firstprivate`

# The lastprivate Clause: C/C++

```
float s;

  s = …;
#pragma omp parallel
  {
#pragma omp for lastprivate(s)
    for(int i=0; i<ndim; i++) {
      s = …;
    }
  }
 … = … + s;
```

on work sharing directive

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- **Extension of private:**
  - additional semantics for work sharing
  - value from thread which executes last iteration of loop is transferred back to master copy (which must be allocated if it is a dynamic entity)
  - restrictions similar to **`firstprivate`**

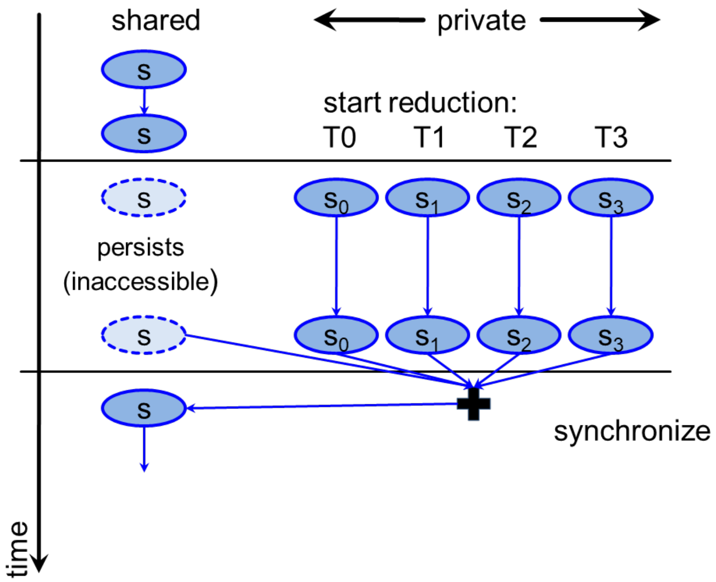
# Reduction Operations (1): Fortran

```
real :: s

!$omp parallel
!$omp do reduction(+:s)
  do i = …
    …
      s = s + …
  end do
!$omp end do
  … = … * s
!$omp end parallel
```

s is still shared here

**Note:** this improves on the summation example
(no explicit critical region needed)



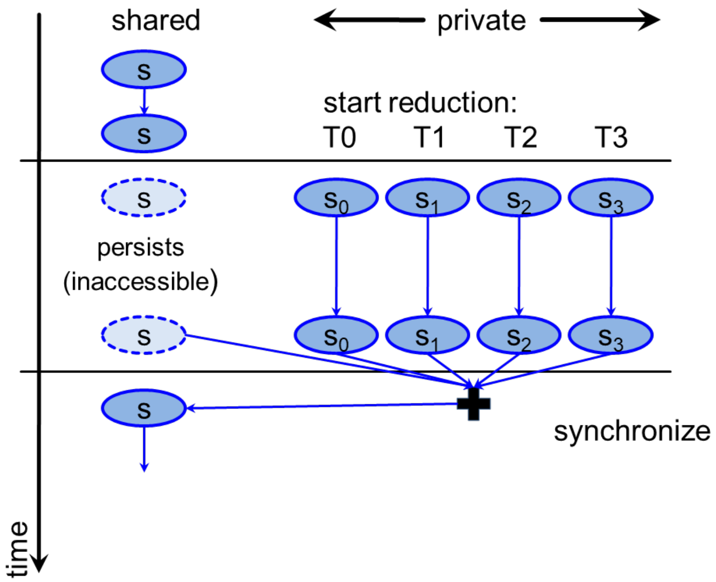

- **At synchronization point:**
  - reduction operation is performed
  - result is transferred to master copy
  - restrictions similar to `firstprivate`

# Reduction Operations (1): C/C++

```
float s;

#pragma omp parallel
  {
#pragma omp for reduction(+:s)
     for(int i=0;i<ndim;i++) {
        ...;
        s = s + …;
     }
    … = … * s;
  }
```

s is still shared here




Note: **Note:** this improves on the summation example (no explicit critical region needed)

- **At synchronization point:**
  - reduction operation is performed
  - result is transferred to master copy
  - restrictions similar to `firstprivate`

# Reduction Operations (2): Fortran

- **Initial value of reduction variable**
  - depends on operation

| Operation | Initial Value |
|---|---|
| + | 0 |
| - | 0 |
| * | 1 |
| .and. | .true. |
| .or. | .false. |
| .eqv. | .true. |
| .neqv. | .false. |
| MAX | min(type) |
| MIN | max(type) |
| IAND | all bits set |
| IEOR | 0 |
| IOR | 0 |

- **Consistency required**
  - operation specified in clause vs. update statement
- **Multiple reductions:**
  - multiple scalars, or an array:

```
real :: x, y, z
!$OMP do reduction(+:x, y, z)
```

```
real :: a(n)
!$OMP do reduction(*:a)
```

```
!$OMP do reduction(+:x, y) &
!$OMP    reduction(*:z)
```

# Reduction Operations (2): C/C++

- **Initial value of reduction variable**
  - depends on operation

| Operation | Initial Value |
|---|---|
| + | 0 |
| - | 0 |
| * | 1 |
| & | ~ 0 |
| \| | 0 |
| ^ | 0 |
| && | 1 |
| \|\| | 0 |
| max | min(type) |
| min | max(type) |

- **Consistency required**
  - operation specified in clause vs. update statement

- **Multiple reductions:**
  - multiple scalars, or an array:

```
float x, y, z;
#pragma omp for reduction(+:x, y, z)
```

lower bound, length

```
float a[n];
#pragma omp for reduction(*:a[0:n])
```

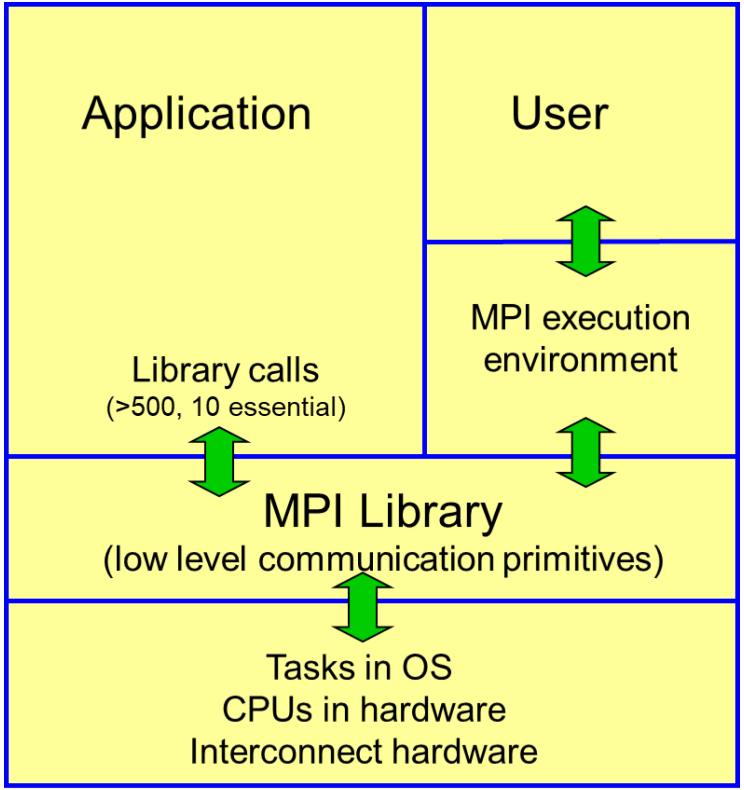
```
#pragma omp for reduction (+:a[0:n]) \
    reduction (*:b[0:n],c[0:n])
```

# MPI

Principles of Message Passing on Distributed Memory Architectures

High Performance Computing

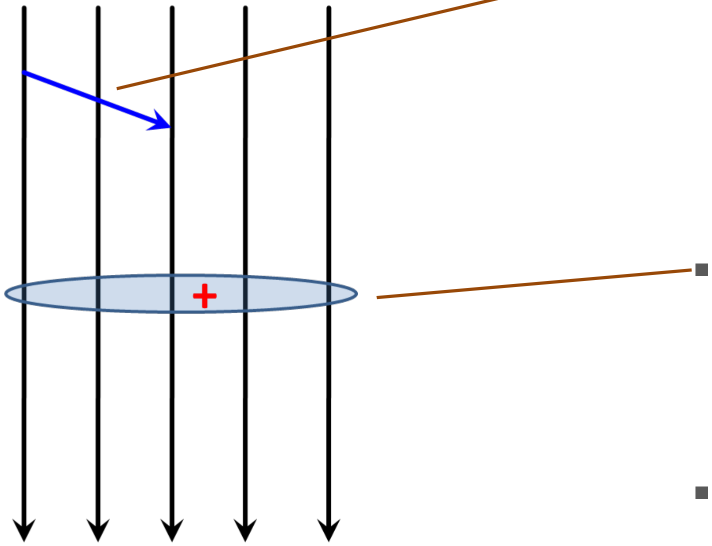
# MPI Architecture




- **Operating system view:**
  - parallel work done by **tasks**
- **Programmer's view:**
  - library routines for
    - coordination
    - communication
    - synchronization
- **User's view:**
  - MPI execution environment provides
    - resource allocation
    - startup method
    - and other (implementation-dependent) behaviour

# MPI Parallel Execution

- **Tasks run throughout program execution**
  - all variables are local



- **Startup phase:**
  - establishes communication context („communicator“) among all tasks
- **Point-to-point data transfer:**
  - usually between pairs of tasks
  - usually coordinated
  - may be blocking or non-blocking
  - explicit synchronization is needed for non-blocking
- **Collective communication:**
  - between all tasks or a subgroup of tasks
  - MPI 2 blocking-only (→ MPI 3)
  - reductions, scatter/gather operations
- **Clean shutdown**

# MPI C and Fortran Interfaces

- **Required header files:**
  - C: `#include <mpi.h>`
  - Fortran: `include 'mpif.h'`
  - Fortran90: `USE MPI`

- **Bindings:**
  - C: `error = MPI_Xxxx(parameter,.....);`
  - Fortran: `call MPI_XXXX(argument,...,ierror)`
  - MPI constants (global/common): All upper case in C

- **Arrays:**
  - C: indexed from 0
  - Fortran: indexed from 1

# MPI Error Handling

- **Fortran MPI routines**
  - `ierror` argument — cannot be omitted!
- **C MPI routines**
  - return an `int` — may be ignored
- **Return value `MPI_SUCCESS`**
  - indicates that all went ok
- **Default:**
  - abort parallel computation in case of other return values
  - but can also define error handlers

# Initialization and Finalization (1)

- **Each processor must start/terminate an MPI process**
  - Usually handled automatically
  - More than one process per processor is mostly possible
- **First call in MPI program: initialization of parallel machine**
  - Fortran: `call MPI_INIT(ierror)`
  - C: `MPI_Init(&argc, &argv);`
- **Last call: clean shutdown of parallel machine**
  - Fortran: `call MPI_FINALIZE(ierror)`
  - C: `MPI_Finalize();`
- Only process with rank 0 (see later) is guaranteed to return from `MPI_Finalize`
- Stdout/stderr of each MPI process
  - usually redirected to console where program was started
  - many options possible, depending on implementation

# Initialization and Finalization (2)

- **Frequent source of errors**: **`MPI_Init()`** in C

  **C binding:**

  ```
  int MPI_Init(int *argc, char ***argv);
  ```

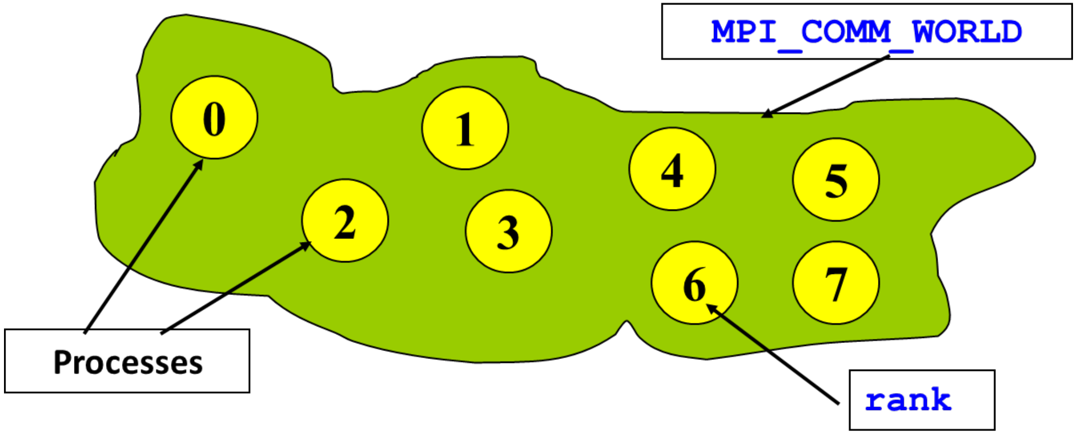
- **If `MPI_Init()` is called in a function** (bad idea anyway), this function must have pointers to the original data:

  ```
  void init_all(int *argc, char***argv) {
     MPI_Init(argc, argv);
     …
  }
  …
  init_all(&argc, &argv);
  ```

- Depending on implementation, mistakes at this point might even go unnoticed until code is ported

# Communicator and Rank (1)

- **MPI_Init** defines "communicator" **MPI_COMM_WORLD**:




- **MPI_COMM_WORLD** defines the processes that belong to the parallel machine
- other communicators (subsets) are possible
- **rank** labels processes inside a communicator

# Communicator and Rank (2)

- The rank identifies each process within a communicator (e.g. **MPI_COMM_WORLD**):
  - obtain rank in Fortran:

    ```
    integer rank, ierror
    call MPI_COMM_RANK(MPI_COMM_WORLD, rank, ierror)
    ```

  - obtain rank in C:

    ```
    int rank;
    MPI_Comm_rank(MPI_COMM_WORLD, &rank);
    ```

  - **rank = **0, 1, 2, … , (number of MPI tasks – 1)
- Obtain number of MPI tasks in communicator:
  - in Fortran:

    ```
    integer size, ierror
    call MPI_COMM_SIZE(MPI_COMM_WORLD, size, ierror)
    ```

  - in C:

    ```
    int size;
    MPI_Comm_size(MPI_COMM_WORLD, &size);
    ```

# Communicator and Rank (3)

- `MPI_COMM_WORLD` is
  - effectively an **MPI-global** variable and required as argument for nearly all MPI calls
- `rank`
  - is target label for MPI messages
  - can drive user-defined directives what each process should do:

Fortran

```
if (rank == 0)  then
  ... ! do work for rank 0
else
  ... ! do work for other ranks
end if
```

C

```
if (rank == 0){
  ... // do work for rank 0
}
else {
  ... // do work for other ranks ***
}
```

# A Very Simple MPI Program: Fortran

```fortran
program hello
 use mpi
 implicit none

 integer :: rank, size, ierror

 call MPI_INIT(ierror)
 call MPI_COMM_SIZE(MPI_COMM_WORLD, size, ierror)
 call MPI_COMM_RANK(MPI_COMM_WORLD, rank, ierror)

 write(*,*) 'Hello World! I am ',rank,' of ',size

 call MPI_FINALIZE(ierror)
end program
```

# A Very Simple MPI Program: C/C++

```
#include <stdio.h>
#include <mpi.h>

int main(int argc, char *argv[]) {

  int rank, size;

  MPI_Init(&argc, &argv);
  MPI_Comm_size(MPI_COMM_WORLD,&size);
  MPI_Comm_rank(MPI_COMM_WORLD, &rank);

  printf("Hello World! I am %i of %i\n", rank, size);

  MPI_Finalize();
}
```

# Compiling and Running MPI Code

- **Compile time:**
  - include files or module information file needed
- **Link time:**
  - MPI library required
- **Most implementations**
  - provide `mpif77`, `mpif90`, `mpicc` and `mpiCC` wrappers
  - not standardized, so variations must be expected e.g., with Intel-MPI (`mpiifort`, `mpiicc` etc.)
- **Startup facilities**
  - `mpirun` (legacy)
  - `mpiexec`
  - site and implementation dependent

- **Compile**:
  - Fortran: `mpif90 -o hello hello.f90`
  - C: `mpicc -o hello hello.c`
- **Run on 4 processors**:

`mpirun -np 4 ./hello` or

`mpiexec -n 4 ./hello`

- **Output**:

```
Hello World! I am 3 of 4
Hello World! I am 1 of 4
Hello World! I am 0 of 4
Hello World! I am 2 of 4
```

order undefined

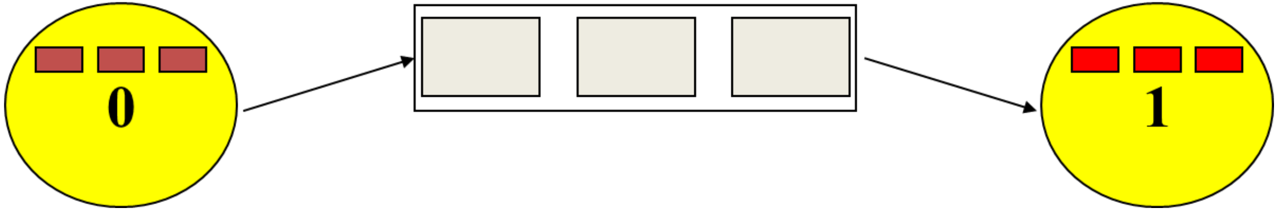
# MPI Process Communication

- **Communication between two processes:**

  Sending / Receiving of MPI-Messages

- **MPI-Message:**

  Array of elements of a particular MPI datatype




- **MPI data types:**
  - basic data types
  - derived data types

# Basic Fortran and C Data Types

Most important basic data types:

Fortran

| MPI datatype | FORTRAN datatype |
| --- | --- |
| MPI_CHARACTER | CHARACTER(1) |
| MPI_INTEGER | INTEGER |
| MPI_REAL | REAL |
| MPI_DOUBLE_PRECISION | DOUBLE PRECISION |
| MPI_COMPLEX | COMPLEX |
| MPI_LOGICAL | LOGICAL |
| MPI_BYTE | |
| MPI_PACKED | |

C

| MPI datatype | C datatype |
| --- | --- |
| MPI_CHAR / MPI_SHORT | signed char / short |
| MPI_INT / MPI_LONG | signed int / long |
| MPI_UNSIGNED_CHAR / … | unsigned char / … |
| MPI_FLOAT / MPI_DOUBLE | float / double |
| MPI_LONG_DOUBLE | long double |
| MPI_BYTE | |
| MPI_PACKED | |

# Basic Fortran and C Data Types in MPI 4.1

Table 3.1: Predefined MPI datatypes corresponding to Fortran datatypes

| MPI datatype | Fortran datatype |
|---|---|
| MPI_INTEGER | INTEGER |
| MPI_REAL | REAL |
| MPI_DOUBLE_PRECISION | DOUBLE PRECISION |
| MPI_COMPLEX | COMPLEX |
| MPI_LOGICAL | LOGICAL |
| MPI_CHARACTER | CHARACTER(1) |
| MPI_BYTE | |
| MPI_PACKED | |

Table 3.3: Predefined MPI datatypes corresponding to both C and Fortran datatypes

| MPI datatype | C datatype | Fortran datatype |
|---|---|---|
| MPI_AINT | MPI_Aint | INTEGER(KIND=MPI_ADDRESS_KIND) |
| MPI_OFFSET | MPI_Offset | INTEGER(KIND=MPI_OFFSET_KIND) |
| MPI_COUNT | MPI_Count | INTEGER(KIND=MPI_COUNT_KIND) |

Table 3.4: Predefined MPI datatypes corresponding to C++ datatypes

| MPI datatype | C++ datatype |
|---|---|
| MPI_CXX_BOOL | bool |
| MPI_CXX_FLOAT_COMPLEX | std::complex<float> |
| MPI_CXX_DOUBLE_COMPLEX | std::complex<double> |
| MPI_CXX_LONG_DOUBLE_COMPLEX | std::complex<long double> |

Table 3.2: Predefined MPI datatypes corresponding to C datatypes

| MPI datatype | C datatype |
|---|---|
| MPI_CHAR | char (treated as printable character) |
| MPI_SHORT | signed short int |
| MPI_INT | signed int |
| MPI_LONG | signed long int |
| MPI_LONG_LONG_INT | signed long long int |
| MPI_LONG_LONG (as a synonym) | signed long long int |
| MPI_SIGNED_CHAR | signed char (treated as integral value) |
| MPI_UNSIGNED_CHAR | unsigned char (treated as integral value) |
| MPI_UNSIGNED_SHORT | unsigned short int |
| MPI_UNSIGNED | unsigned int |
| MPI_UNSIGNED_LONG | unsigned long int |
| MPI_UNSIGNED_LONG_LONG | unsigned long long int |
| MPI_FLOAT | float |
| MPI_DOUBLE | double |
| MPI_LONG_DOUBLE | long double |
| MPI_WCHAR | wchar_t (defined in <stddef.h>) (treated as printable character) |
| MPI_C_BOOL | _Bool |
| MPI_INT8_T | int8_t |
| MPI_INT16_T | int16_t |
| MPI_INT32_T | int32_t |
| MPI_INT64_T | int64_t |
| MPI_UINT8_T | uint8_t |
| MPI_UINT16_T | uint16_t |
| MPI_UINT32_T | uint32_t |
| MPI_UINT64_T | uint64_t |
| MPI_C_COMPLEX | float _Complex |
| MPI_C_FLOAT_COMPLEX (as a synonym) | float _Complex |
| MPI_C_DOUBLE_COMPLEX | double _Complex |
| MPI_C_LONG_DOUBLE_COMPLEX | long double _Complex |
| MPI_BYTE | |
| MPI_PACKED | |

# MPI Data Types Cont'd

- **`MPI_BYTE`: Eight binary digits**
  - hack value, do not use

- `MPI_PACKED`: can implement new data types → however, it is more flexible to use …

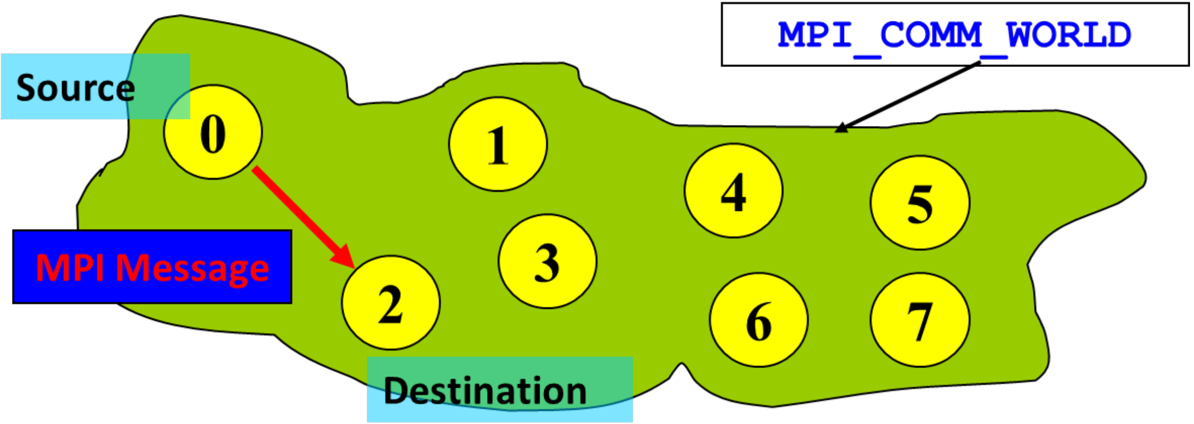
- **Derived data types**: Built at run time from basic data types

- **Data type matching**: Same MPI data type in SEND and RECEIVE call
  - type must match on both ends in order for the communication to take place

- **Support for heterogeneous systems/clusters**
  - implementation-dependent
  - automatic data type conversion between systems of differing architecture may be needed

# Point-to-Point Communication

- Communication between exactly two processes within the communicator




- Identification of source and destination via the rank within the communicator!
- Blocking: MPI call returns after completion of the corresponding send/receive operation

# Blocking Standard Send: MPI_Send

- Fortran: `call MPI_SEND (buf, count, datatype, dest, tag, comm, ierror)`
- `C: MPI_Send (&buf, count, datatype, dest, tag, comm)`

  - `buf / &buf`: starting address of data buffer to be sent
  - `count`: number of elements to be sent
  - `datatype`: MPI data type of elements to be sent
  - `dest`: rank of destination process
  - `tag`: message marker
  - `comm`: communicator shared by source & destination
  - `ierror`: error code (Fortran-only)

- Completion of `MPI_Send`:
  - status of `dest` is not defined – message may or may not have been received after return!
- Send buffer may be reused after `MPI_Send` returns

# MPI_Send Example

- Example:
  send array of 10 integers to task no. 5

```fortran
integer count, dest, tag
integer, allocatable :: field(:)
…
count=10; dest=5; tag=0
allocate(field(count));
call MPI_SEND(field, count, MPI_INTEGER, &
        dest, tag, MPI_COMM_WORLD, ierror)
```

```c
int count, dest, tag;
int *field;
…
 count=10; dest=5; tag=0;
 field = (int*)malloc(count*sizeof(int));
 MPI_Send(field, count, MPI_INTEGER,
          dest, tag, MPI_COMM_WORLD);
```

- **Source and destination may coincide**
  - beware potential deadlocks!

# Blocking Standard Receive: MPI_Recv

- `MPI_Recv`: 1. receive data
  2. complete
- Fortran: `call MPI_RECV (buf, count, datatype, source, tag, comm, status, ierror)`
- C: `MPI_Recv(&buf, count, datatype, source, tag, comm, &status)`

  - `buf` — size of buffer **must** be ≥ size of message
  - `count` — **maximum** number of elements to receive
  - `source, tag` — **wildcards** may be used (`MPI_ANY_SOURCE`, `MPI_ANY_TAG`)
  - `status` — information from the message that was received (**is a complex object** - see next slide)

# Handling Status Information

- **MPI status provides additional information about the message**
  - size, source, tag, error code – may not be otherwise known if wildcards are used
  - can also use MPI_STATUS_IGNORE in some contexts

- **MPI_status in Fortran**

```
integer :: status(MPI_STATUS_SIZE)
```

  - Array of integers of size MPI_STATUS_SIZE
  - index values for query: MPI_SOURCE, MPI_TAG, MPI_ERROR

- **MPI_status in C/C++**

```
MPI_Status status;
```

  - Structure of type MPI_Status
  - hand a reference to MPI_Recv
  - component names for query: status.MPI_SOURCE, status.MPI_TAG, status.MPI_ERROR

- Inquiring message length needs an additional MPI call:
  - Fortran: `call MPI_GET_COUNT(status, datatype, count, ierror)`
  - C: `MPI_Get_count(&status, datatype, &count);`
    - count is output argument
    - datatype must be the same datatype used in the MPI call that produced the status variable

# MPI_Recv Example: Fortran

- **Example: receive array of REALs from any source**

```
integer count, countrecv, status(MPI_STATUS_SIZE)
  real field(count)
  ...
  call MPI_RECV(field, count, MPI_REAL,
      &        MPI_ANY_SOURCE, MPI_ANY_TAG,
      &        MPI_COMM_WORLD, status, ierror)
  write(*,*) 'Received from ', status(MPI_SOURCE),
      &          ' with tag ', status(MPI_TAG)
```

- **Obtain number of actually received items:**

```
call MPI_GET_COUNT(status, MPI_REAL, countrecv, ierror)
```

# MPI_Recv Example: C/C++

- **Example: receive array of floats from any source**

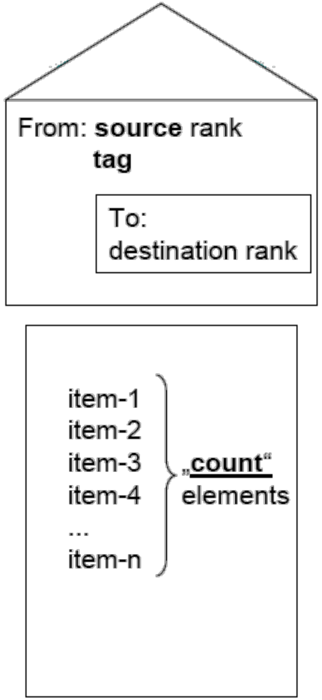
```
int count, countrecv;
MPI_Status status;
field = (float *)malloc(count*sizeof(float));
…
MPI_Recv(field, count, MPI_FLOAT, MPI_ANY_SOURCE,
   MPI_ANY_TAG, MPI_COMM_WORLD, &status);
printf("Received from %i with tag %i count: %i \n",
  status.MPI_SOURCE, status.MPI_TAG)
```

- ```
  MPI_Get_count(&status, MPI_FLOAT, &countrecv);
  ```
  ```

# Requirements for Point-to-Point Communication

**For a communication to succeed:**

- sender must specify a valid destination.
- receiver must specify a valid source rank (or **`MPI_ANY_SOURCE`**).
- communicator must be the same (e.g., **`MPI_COMM_WORLD`**).
- tags must match.
- message datatypes must match.
- receiver's buffer must be large enough (otherwise result is undefined!)



# Summary of Basic MPI API Calls

- **Beginner's MPI procedure toolbox:**
  - `MPI_Init` let's get going
  - `MPI_Comm_size` how many are we?
  - `MPI_Comm_rank` who am I?
  - `MPI_Send` send data to someone else
  - `MPI_Recv` receive data from some-/anyone
  - `MPI_Get_count` how many items have I received?
  - `MPI_Finalize` finish off

- **Standard send/receive calls** provide most simple way of point-to-point communication
- **Send/receive buffer** may safely be reused after the call has completed
- `MPI_Send` must have a specific target/tag, `MPI_Recv` does not

# First Complete MPI Example in Fortran

Write a parallel program in which a master process collects some data (e.g., numbers to sum up) from the others

```
program collect
  use mpi
  implicit none
  integer :: i,size,rank,ierror, &
             status(MPI_STATUS_SIZE)
  integer :: number,sum
  call MPI_INIT(ierror)
  call MPI_COMM_RANK (MPI_COMM_WORLD,&
             rank,ierror)
```

```
 if(rank.eq.0) then
    sum=0
    call MPI_COMM_SIZE(MPI_COMM_WORLD,&
                size,ierror)
   do i=1,size-1
     call MPI_RECV(number,1, &
      MPI_INTEGER, MPI_ANY_SOURCE, &
      MPI_ANY_TAG, MPI_COMM_WORLD, &
       status, ierror)
      sum=sum+number
   enddo
  write(*,*) 'The sum is ',sum
 else
  call MPI_SEND(rank,1,MPI_INTEGER, &
        0, 0, MPI_COMM_WORLD, ierror)
 endif
 call MPI_FINALIZE(ierror)
end program
```

# First Complete MPI Example in C

Write a parallel program in which a master process collects some data (e.g., numbers to sum up) from the others

```
#include <mpi.h>

int main(int argc, char *argv[]) {
  int i, size, rank;
  int sum, number;
  MPI_Status status;

  MPI_Init(&argc, &argv);
  MPI_Comm_rank(MPI_COMM_WORLD, &rank);
```

```
 if(rank==0){
   sum=0;
   MPI_Comm_size(MPI_COMM_WORLD,&size);
   for(i=0;i<size-1;i++) {

    MPI_Recv(&number,1,MPI_INT,MPI_ANY_SOU
    RCE ,MPI_ANY_TAG, MPI_COMM_WORLD,
    &status);
       printf("Got number: %i\n", number);
       sum+=number;
    }
    printf("The sum is %i\n", sum);
  }
  else {
    MPI_Send(&rank,1,MPI_INT, 0,
   0,MPI_COMM_WORLD);
  }
  MPI_Finalize();
}
```

# First Complete MPI Example

**Remarks:**

- **gathering results** from processes is a very common task in MPI – there are more efficient ways to do this (see advanced talk).
- this is a **reduction operation** (summation). There are more efficient ways to do this (see advanced talk).
- the 'master' process waits for one receive operation to be completed before the next one is initiated. There are more efficient ways... You guessed it!
- ‘master-worker' schemes are quite common in MPI programming
- error checking is rarely done in MPI programs – debuggers are often more efficient if something goes wrong
- every process has its own `sum` variable, but only the master process actually uses it