



# Introduction to parallel and high-performance computing (part II)

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Including adapted teaching material from books, lectures and presentations by B. Barney, B. Cumming, G. Hager, R. Rabenseifner, O. Schenk, G. Wellein

#### Roadmap – fast forward:

#### <u>Day 1, Saturday – Jan 28<sup>th</sup> (14:00-15.30)</u>

- 1. Introduction to parallel programming and high-performance computing (HPC).
- 2. Introduction 'Unix-like' HPC environments (hands on).

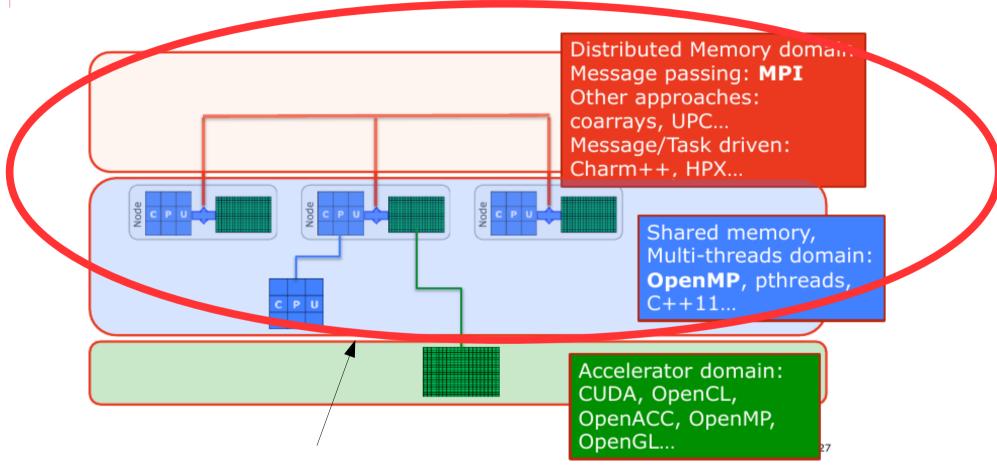
\*Homework – Introduction to Fortran or CPP, and compilation of code.

#### <u>Day 2, Monday – Jan 30<sup>th</sup> (9:30-11.00)</u>

- 1. Notes on basic code optimization (hands on).
- 2. Introduction to OpenMP (hands on).
- 3. Introduction MPI (hands on).
- 4. MPI & Python (hands on).

\*\*Exercise sheet related to the day's topics (Jan 31th, 15.45 – 17.15 ).

#### Wrap-up 1<sup>st</sup> lecture



Today we are concerned with "classical" hardware

#### Before we start...

On ALPHACRUNCHER – set the environment

>cd ~

>vi .bashrc

→ add the following lines to your .bashrc

module load gcc module rm gcc/6.1.0 module add openmpi/gcc/64/1.10.1 module load python/2.7.11

#### 1. Basic optimization of serial code

In the age of multi-1000-processor parallel computers, writing code that runs efficiently on a single CPU has grown slightly old-fashioned.

Nevertheless there can be no doubt that single-processor optimizations are of premier importance.

- → If a speed-up of two can be achieved by some simple code changes, the user will be satisfied with much fewer CPUs in the parallel case.
- → This frees resources for other users and projects, and puts hardware that was often acquired for considerable amounts of money to better use.
- → If an existing parallel code is to be optimized for speed, it must be the first goal to make the single processor run as fast as possible.

## **Profiling**

- Gathering information about a program's behaviour, specifically its use of resources, is called **profiling**.
- The most important "resource" in terms of high performance computing is **runtime**.
- → Hence, a common profiling strategy is to find out how much time is spent in the different functions, and maybe even lines, of a code in order to identify hot spots, i.e., the parts of the program that require the dominant fraction of runtime.
- These hot spots are subsequently analysed for possible optimization opportunities.
- → Software for profiling (e.g. GNU gprof,...)

### Common sense optimizations

- Very simple code changes can often lead to a significant performance boost.

- Some of those hints may **seem trivial**, but experience shows that many scientific codes can be improved by the simplest of measures.

→ e.g. do less work

```
1 logical :: FLAG
2 FLAG = .false.
3 do i=1,N
4   if(complex_func(A(i)) < THRESHOLD) then
5   FLAG = .true.
6   endif
7 enddo</pre>
```

If complex\_func() has no side effects, the only information that gets communicated to the outside of the loop is the value of **FLAG**. In this case, depending on the probability for the conditional to be true, much computational effort can be saved by leaving the loop as soon as FLAG changes state.

### Common sense optimizations II

#### **Avoid branching!**

In this multiplication of a matrix with a vector, the upper and lower triangular parts get different signs and the diagonal is ignored. The **if** statement serves to decide about which factor to use.

→ Fortunately, the loop nest can be transformed so that all if statements vanish:

```
do j=1,N
do i=1,N
if(i.ge.j) then
sign=1.d0
else if(i.lt.j) then
sign=-1.d0
else
sign=0.d0
else
sign=0.d0
endif
C(j) = C(j) + sign * A(i,j) * B(i)
enddo
enddo
enddo
```

```
1 do j=1,N
2     do i=j+1,N
3     C(j) = C(j) + A(i,j) * B(i)
4     enddo
5     enddo
6     do j=1,N
7     do i=1,j-1
8     C(j) = C(j) - A(i,j) * B(i)
9     enddo
10 enddo
```

### Data access (example)

#### Stride-N access

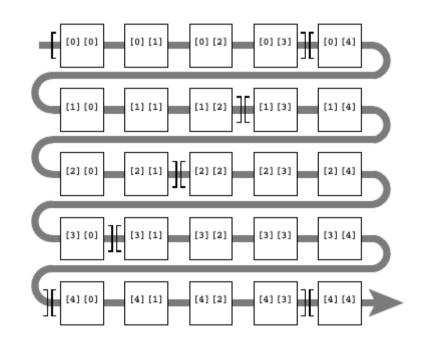
```
do i=1, N
do j=1, N
A(i,j) = i*j
enddo
enddo
```

#### (1,1)(1,3)(1,4)(1,5)(1,2)(2,4) (2,2) (2,3) (2,1) (2,5)(3,3) (3,1) (3,2) (3,4)(3,5) (4,2) (4,1)(4,3) (4,4)(4,5)(5,1)(5,2) (5,3) (5,4)(5,5)

Fortran: Column major

#### Stride-1 access

```
for(i=0; i<N; ++i) {
  for(j=0; j<N; ++j) {
    a[i][j] = i*j;
  }
}</pre>
```



C: Row major

### Small exercise on loop ordering

#### **check directory:**

- > cd zice17/scheidegger/intro to hpc/loop/
- > vi loop.f90

#### compile:

>./compile\_loop.sh

#### run:

>./test loop

#### To be done:

- a) Inspect code
- b) run code (play with array size & re-compile)

1. Basic optimization of serial code

# <u>Using SIMD instruction sets</u> <u>→ Vectorization</u>

**Vectorization** performs multiple operations in parallel on a core with a single instruction (SIMD – single instruction multiple data).

Data is loaded into vector registers that are described by their width in bits:

- -256 bit registers: 8 x float, or 4x double
- -512 bit registers: 16x float, or 8x double

**Vector units** perform arithmetic operations on vector registers simultaneously.

Vectorization is key to maximizing computational performance.

#### Vectorization illustrated

#### 

In an optimal situation all this is carried out by the compiler automatically. Compiler directives can be used to give hints as to where vectorization is safe and/or beneficial.

```
! vectorized part
rest = mod(N,4)
do i=1,N-rest,4
load R1 = [x(i),x(i+1),x(i+2),x(i+3)]
load R2 = [y(i),y(i+1),y(i+2),y(i+3)]
! "packed" addition (4 SP flops)
R3 = ADD(R1,R2)
store [r(i),r(i+1),r(i+2),r(i+3)] = R3
enddo
! remainder loop
do i=N-rest+1,N
r(i) = x(i) + y(i)
enddo
```

d[i+4]

#### Advanced Vector Extensions (AVX)

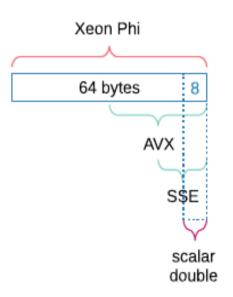


Fig. 7. Vector registers on modern CPUs: a scalar program can utilize only 1/4 of computational parallelism on AVX-enabled CPUs, e.g. the SandyBridge.

#### How to use vectorization

- use vector intrinsics (see example)
  - explicit hardware-specific instructions.
  - high performance.
  - non-portable and hard to maintain.
  - → see, e.g. https://software.intel.com/sites/landingpage/IntrinsicsGuide/
- -automatic compiler vectorization
  - compiler will vectorize where it is possible. compilers can do a poor job.
- -use libraries that are already vectorized let somebody else do the work for you.

#### Does my code vectorize?

- → Not clear a priori.
- → Compilers can generate reports that summarize which loops vectorized.
- → You can ask for different levels of detail e.g. only loops that failed to vectorize, e.g., whether to explain why a loop didn't vectorize.
- → The flags vary from compiler to compiler, e.g.:

```
- Intel: -vec-report=n , or -opt-report=n
- GCC: -ftree-vectorizer-verbose=n
- Cray: -h list=a
```

You can also use the disassemble command in **gdb\***, if you like reading assembly.

### Small example on vectorization

#### check directory:

- > cd /zice17/scheidegger/intro\_to\_hpc/vectorization/
- > vi avx-intrinsics.cpp

#### compile:

>./compile\_avx.sh

#### run:

>./avx-example

#### To be done:

a) Inspect code

## <u>Compilers</u>

- Most codes benefit, to varying degrees, from employing **compiler-based optimizations**, e.g. standard optimization options (**-O0**, **-O1**, . . .).
- Every modern compiler has command line switches that allow a (more or less) finegrained tuning of the available optimization options.
- Sometimes it is even worthwhile **trying a different compiler** just to check whether there is more performance potential. One should be aware that the compiler has the extremely complex job of mapping source code written in a high-level language to machine code, thereby utilizing the processor's internal resources as well as possible.
- However, there is no guarantee that this is actually the case and the programmer should at least be aware of the basic strategies for automatic optimization and potential stumbling blocks that prevent the latter from being applied. It must be understood that compilers can be surprisingly smart and stupid at the same time.
- A common statement in discussions about compiler capabilities is "The compiler should be able to figure that out." This is often a false assumption.

### 2. Introduction to OpenMP

(Open Multi Processing)

- OpenMP website is a good source of information:

→ openmp.org



- → You can find there:
  - tutorials and examples for all levels.
  - the standard.
  - quick references guide.

#### Some literature & other resources

#### Full standard/API specification:

- http://openmp.org

#### **Tutorials:**

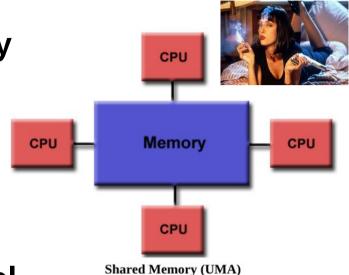
- https://computing.llnl.gov/tutorials/openMP/

#### **Books**:

- "Introduction to High Performance Computing for Scientists and Engineers" Georg Hager, Gerhard Wellein

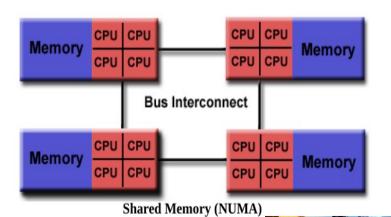
### Shared memory systems

- Process can access same GLOBAL memory
- Uniform Memory Access (UMA) model
  - Access time to memory is uniform.
  - Local cache, all other peripherals are shared.



#### Non-Uniform Memory Access (NUMA) model

- Memory is physically distributed among processors.
- Global virtual address spaces accessible from all processors.
- Access time to local and remote data is different.
- → OpenMP, but other solutions available (e.g. Intel's TBB).



### What is OpenMP?

**Application Program Interface** (API), jointly defined by a group of major computer hardware and software vendors (e.g. GNU, Intel, Cray, PGI,...).

OpenMP provides a portable, scalable model for developers of shared memory parallel applications.

Supports C/C++ and Fortran on a wide variety of architectures.

→ API may be used to explicitly direct multi-threaded, shared memory parallelism.

The API comprised of three main components:

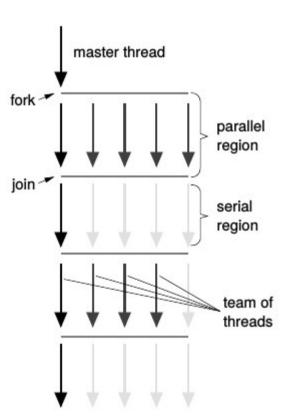
- 1) Compiler Directives
- 2) Runtime Library Routines
- 3) Environment variables

### Goals of OpenMP

- Standardization
- Ease of use:
  - → Concise and simple set of directives.
  - → Possible to get good speed-up with a handful of directives.
  - → You can incrementally add it to the code without major changes.
- Should I use OpenMP?
  - → Path least resistance to parallelize your code...
  - → For many-core architectures like Xeon Phi, lightweight threading is required since MPI does not scale there...

#### Fork and Join Model

- OpenMP uses fork and join model for threading.
- The application starts with a master thread:
  - FORK: a team of parallel worker threads is started at the beginning of each parallel block.
  - The block is executed in parallel by each thread.
  - JOIN: the worker threads are synchronized at the end of the parallel block and join with the master thread.
- Threads are numbered 0:N-1
   (N is the total number of threads).
- The master thread is always numbered 0.



#### OpenMP compiler directives

Compiler directives appear as comments in your source code and are ignored by compilers unless you tell them otherwise usually by **specifying the appropriate compiler flag**.

#### **OpenMP compiler directives are used for various purposes:**

- Spawning a parallel region.
- Dividing blocks of code among threads.
- Distributing loop iterations between threads.
- Serializing sections of code.
- Synchronization of work among threads.

#### **Compiler directives have the following syntax:**

sentinel	directive-name	[clause]
All Fortran OpenMP directives must begin with a sentinel. The accepted sentinels depend upon the type of Fortran source. Possible sentinels are:  !\$OMP C\$OMP *\$OMP	A valid OpenMP directive. Must appear after the sentinel and before any clauses.	Optional. Clauses can be in any order, and repeated as necessary unless otherwise restricted.

# **Compiling OpenMP**

- Most compilers require a flag to enable OpenMP compilation
  - → without any flag, the #pragma or !\$ directives are ignored by the compiler and a serial application is created.
- Compilers that don't understand OpenMP will simply ignore the directives (no portability problems).

```
Cray : on by default for -O1 and greater, disable with -h noomp
Intel : off by default, enable with -openmp
GNU : off by default, enable with -fopenmp
PGI : off by default, enable with -mp
```

### Runtime library

- OpenMP API includes a growing number of runtime library routines.

#### These are used for a variety of purposes:

- Setting and querying the number of threads.
- Querying a thread's unique identifier (thread ID), a thread's ancestor's identifier, the thread team size.
- Setting and querying the dynamic threads feature.
- Querying if in a parallel region, and at what level.
- Setting and querying nested parallelism.
- Setting, initializing and terminating locks and nested locks.
- Querying wall clock time and resolution.
- For C/C++, all of the runtime library routines are actual subroutines.
- For Fortran, some are actually functions, and some are subroutines.

### Runtime library (II)

- OpenMP has runtime library routines for controlling your application, including

Function:	omp_get_num_threads()			
C/ C++	int omp_get_num_threads(void);			
Fortran	integer function omp_get_num_threads()			
Description:				
Returns the total number of threads currently in the group executing the parallel block from where it is called.				
Function:	omp_get_thread_num()			
C/ C++	int omp_get_thread_num(void);			
Fortran	integer function omp_get_thread_num()			
Description:				
For the master thread, this function returns zero. For the child nodes the call returns an integer between 1 and omp_get_num_threads()-1 inclusive.				

- There are many others, however these are probably the most commonly used.

### Runtime library III

The runtime library requires that the OpenMP **header/module** is included:

```
#include <omp.h>
                                          use omp_lib
int threads = omp_get_max_threads();
                                          integer :: threads, inside, outside
int outside = omp_get_num_threads();
                                          threads = omp_get_max_threads()
int inside;
                                          outside = omp_get_num_threads()
                                          !$omp parallel
#pragma omp parallel
                                          inside = omp_get_num_threads()
  inside = omp_get_num_threads();
                                          !$omp end parallel
                                          print *, inside, ' in ', outside, ' out ',
                                                   threads, ' max'
printf("%d in, %d out, %d max \n",
       inside, outside, threads);
                   > OMP_NUM_THREADS=8 ./a.out
                   8 in, 1 out, 8 max
```

### Running OpenMP applications

 The default number of threads is set with an environment variable OMP\_NUM\_THREADS

csh/tcsh	setenv	OMP_NUM	_THREADS 8
sh/bash	export	OMP_NUM	_THREADS=8

- Compiling and running:



# "Hello world" in OpenMP (FORTRAN)

```
program hello world
     use omp lib
                    !module with API declarations
     integer :: tid !thread ID
     write(*,*) '=== serial section ==='
     write(*,*) 'hello world from thread ', omp get thread num(), ' of ', omp get num threads()
     write(*,*) '=== parallel section ==='
!Somp parallel private(tid)
!....get thead ID
     tid = omp get thread num();
!....write a personalized message from this thread
     write(*,*) 'hello world from thread ', omp get thread num(), ' of ', omp get num threads()
!....section only executed by master
     if(tid .eq. 0 ) then
       write(*,*) 'hello world from master thread with TID = ', tid
     end if
!....All threads join master thread and disband
!Somp end parallel
     end program hello world
  ______
```

### "Hello world" in OpenMP (CPP)

```
#include <omp.h>
                                         Non shared copies of
main ()
                                         data for each thread
                                                                      OpenMP directive to
   int nthreads, tid;
                                                                      indicate START
   #pragma omp parallel private(nthreads, tid).
                                                                      segment to be
                                                                      parallelized
     tid = omp_get_thread_num();
     printf("Hello World from thread = %d\n", tid);
                                                                      Code segment that
     if (tid == 0)
                                                                      will be executed in
                                                                      parallel
        nthreads = omp_get_num_threads();
         printf("Number of threads = %d\n", nthreads);
                                                                      OpenMP directive to
                                                                      indicate END
                                                                      segment to be
                                                                      parallelized
```

### Data scoping

- Any variables that existed before a parallel region still exist inside, and are **by default shared between all threads**.
- True work sharing, however, makes sense only if each thread can have its own, private variables.
- OpenMP supports this concept by defining a separate stack for every thread.
- 1. A variable that exists before entry to a parallel construct can be privatized, i.e., made available as a **private instance for every thread**, by a **PRIVATE** clause to the OMP PARALLEL directive. The private variable's scope extends until the end of the parallel construct.
- 2. The index variable of a work-sharing loop is automatically made private.
- 3. Local variables in a subroutine called from a parallel region are private to each calling thread. This pertains also to copies of actual arguments generated by the call-by-value semantics, and to variables declared inside structured blocks in C/C++. However, local variables carrying the SAVE attribute in Fortran (or the static storage class in C/C++) will be shared. Shared variables that are not modified in the parallel region do not have to be made private.

### Scope of Variables

OpenMP provides clauses that describe how variables should be shared between threads

- shared: all variables access the same copy of a variable.
  - → this is the default behavior
  - → WARNING: take care when writing to shared variables.
- private: each thread gets its own copy of the variable
  - → private copy is uninitialized.
  - → use firstprivate to initialize variable with value from master.

### Example 1:"hello world from thread"

- 1. go to /zice17/scheidegger/intro\_to\_hpc/openmp:
- > cd /zice17/scheidegger/intro\_to\_hpc/openmp
- 2. Have a look at the code
- > vi 1.hello\_world.f90 / vi 1a.hello\_world.cpp
- 3. compile by typing:
- > make
- 4. Experiment with different numbers of threads
- > export OMP\_NUM\_THREADS=1 (play around with #threads)
- > ./hello\_world.exec (FORTRAN)
- > ./1a.hello\_world.exec (CPP)

#### Example 1:"hello world from thread"

- 5. experiment with slurm (the settings)
- > cd /zice17/scheidegger/intro\_to\_hpc/openmp
- > vi submit\_openmp.sh

```
#!/bin/bash -l

#SBATCH --ntasks=1
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=8

#SBATCH --time=00:01:00

#SBATCH --job-name=test_submission
#SBATCH --output=openmp_test.out
#SBATCH --error=openmp_test.err

export OMP_NUM_THREADS=8

### openmp executable
./1.hello_world.exec
```

- 6. see 1.hello\_world.f90 line 25: !\$omp parallel private(tid)
  - → what happens if we remove private(tid) → try out!

### Shared memory model

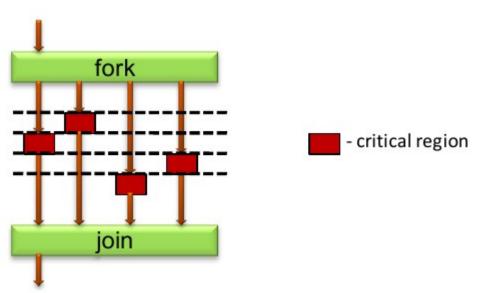
- OpenMP uses a shared memory model.
- All threads can read and write to the same memory locations simultaneously.
- By default variables are shared, so one copy is used by all threads.
- The result of computations where multiple threads attempt to read/write to a variable are undefined.
- → see /zice17/scheidegger/intro\_to\_hpc/openmp/2.example\_racing\_cond.f90
- → this is a very common parallel programming bug called race condition.

# Example 2: Race condition

```
______
     OpenMP example: Racing conditions example
     program racing cond
     use omp lib
     implicit none
     integer :: num threads, expected
     integer :: sum = 0
     num threads = omp get max threads()
     write(*,*) 'sum with ', num threads, ' threads'
!....section where we can have racing conditions
!Somp parallel
     sum = sum + omp get thread num() + 1
!Somp end parallel
!....use formula for sum of arithmetic sequence: sum(1:n) = (n+1)*n/2
     expected = (num threads + 1)*num threads/2
     if (sum .eq. expected) then
       write(*,*) "sum ", sum, ' matches the expected value'
       write(*,*) "sum ", sum, ' does not match the expected value ', expected
     endif
     end program racing cond
```

# Synchronization/critical regions

- Concurrent write access to a shared variable or, in more general terms, a shared resource, must be avoided by all means to circumvent race conditions.
- Critical regions solve this problem by making sure that at most one thread at a time executes some piece of code.
- If a thread is executing code inside a critical region, and another thread wants to enter, the latter must wait (block) until the former has left the region.



#### **Example 3: Race conditions fixed**

```
OpenMP example: Racing conditions example
      program racing cond fix
      use omp lib
      implicit none
      integer :: num_threads, expected
      integer :: sum = 0
      num threads = omp get max threads()
     write(*,*) 'sum with ', num threads, ' threads'
!....section where we can have racing conditions
!Somp parallel
!....all theads will execute block, one at at time
!Somp critical
      sum = sum + omp get thread num() + 1
!Somp end critical
!$omp end parallel
!....use formula for sum of arithmetic sequence: sum(1:n) = (n+1)*n/2
      expected = (num threads + 1)*num threads/2
      if (sum .eq. expected) then
       write(*,*) "sum ", sum, ' matches the expected value'
       write(*,*) "sum ", sum, ' does not match the expected value ', expected
      endif
      end program racing cond fix
```

### Example 2 fixed: Racing conditions

- 1. vi /zice17/scheidegger/intro\_to\_hpc/openmp/3.racing\_cond\_fix.f90
- 2. Have a look at the code
- 3. compile by typing:
- > make
- 4. Experiment with different numbers of threads

the **CRITICAL** and **END CRITICAL** directives bracket the update to **sum** so that the result is always correct.

→ WARNING: SYNCHRONIZATION (AND SERIAL CODE REGIONS) CAN QUICKLY LIMIT POTENTIAL SPEED-UP FROM PARALLELISM

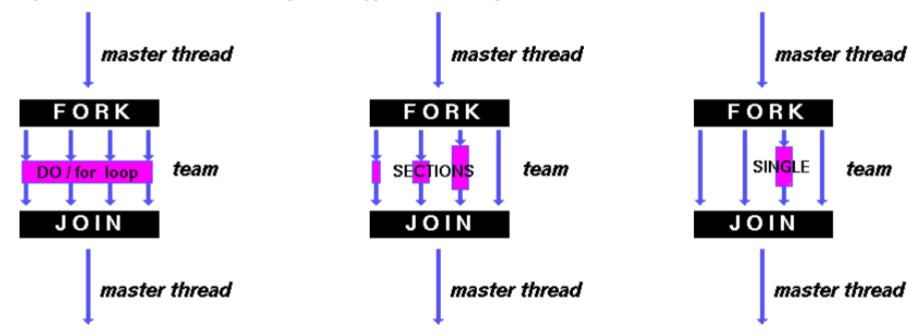
# Worksharing constructs in OpenMP

See https://computing.llnl.gov/tutorials/openMP/

**DO** / **for** - shares iterations of a loop across the team. Represents a type of "data parallelism".

**SECTIONS** - breaks work into separate, discrete sections. Each section is executed by a thread. Can be used to implement a type of "functional parallelism".

**SINGLE** - serializes a section of code



### Example: "do loops"

#### Serial code

```
double *x, *y, *z;
                                       real(kind=8) :: x(:), y(:), z(:)
int n;
                                       integer
for(int i=0; i<n; ++i) {
                                       do i=1.n
  z[i] = x[i] + y[i];
                                         z(i) = x(i) + y(i)
                             C++
                                       end do
```

#### Parallel code

- → compiler handles loop bounds for you.
- → there is a compact single-line directive.
- → !\$OMP DO (in Fortran)

```
loop index
                                            real(kind=8) :: x(:), y(:), z(:)
double *x, *y, *z;
                          variable i is
                                            integer
int n, i;
                                                         :: i, n
                           private by
#pragma omp parallel
                                            !$omp parallel
                             default
                                            !$omp_do
  #pragma omp for
                                            d i=1,n
  for(i=0; i<n; ++i) {
                                              z(i) = x(i) + y(i)
   z[i] = x[i] + y[i];
                                            end do
                                            !$omp end do
                                 C++
                                                                                 Fortran
                                            !$omp end parallel
```

→ let's attempt to parallelize the integral

$$\pi = \int_{0}^{1} \mathrm{d}x \, \frac{4}{1 + x^2}$$

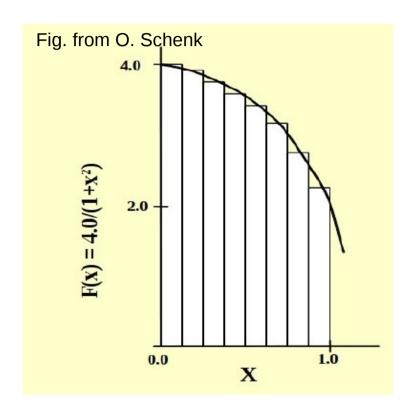
:: i, n

Fortran

by using techniques learnt so far ("summation the hard way").

→ zice17/scheidegger/intro\_to\_hpc/openmp/4.integration\_pi.f90

# Exercise 4: Computing Pi



$$\int_{0}^{1} \frac{4.0}{(1+x^{2})} dx = \pi$$

$$\sum_{i=0}^{N} F(x_i) \Delta x \approx \pi$$

```
program integration pi
     use omp lib
     implicit none
      real(8) :: pi,w,sum,x, time
      integer(8) :: i, N = 5000000000
      pi = 0.d0
      W = 1.d\theta/N
      sum = 0.d0
!....start timer
     time = -omp_get_wtime()
!SOMP PARALLEL PRIVATE(x) FIRSTPRIVATE(sum)
ISOMP DO
      do i = 1 , n
        x = w*(i-0.5d0)
        sum = sum + 4.d\theta/(1.d\theta+x*x)
      enddo
!SOMP END DO
!SOMP CRITICAL
     pi= pi + w*sum
!SOMP END CRITICAL
!SOMP END PARALLEL
!....end timer
     time = time + omp get wtime()
     write(*,*) 'The approximation of Pi =', pi
     write(*,*) 'took ', time, ' seconds'
     end program integration pi
```

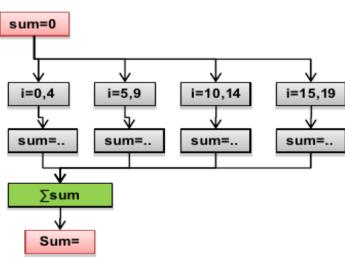
# $\frac{\text{Reductions}}{\rightarrow \text{ e.g. summation the "easy way"}}$

The **REDUCTION** clause performs a reduction on the variables that appear in the list.

→ reduction(op:list)

A private copy for each list variable is created for each thread.

At the end of the reduction, the reduction variable is applied to all private copies of the shared variable, and the final result is written to the global shared variable.



#### **Example: Reduction**

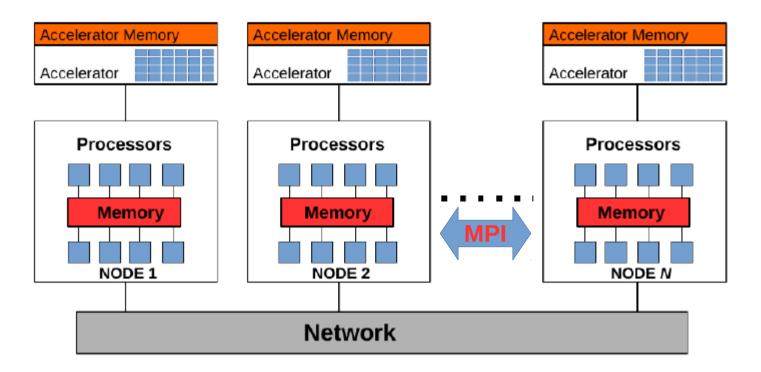
>/zice17/scheidegger/intro\_to\_hpc/openmp/4a.integration\_pi\_reduction.cpp >/zice17/scheidegger/intro\_to\_hpc/openmp/4b.integration\_pi\_reduction.f90 (play with OMP\_NUM\_THREADS & timing)

```
OpenMP example: program to approximation pi by a REDUCTION
_____
     program integration pi reduction
     use omp lib
     implicit none
     real(8) :: pi,w,x, time
     integer(8) :: i, N = 5000000000
     pi = 0.d0
     W = 1.d0/N
!....start timer
     time = -omp get wtime()
                                                                Reduction
!SOMP PARALLEL PRIVATE(x)
!SOMP DO REDUCTION(+:pi)
     do i = 1 , n
       x = w*(i-0.5d\theta)
      pi = pi + 4.d\theta/(1.d\theta + x*x)
     enddo
!SOMP END DO
I SOMP END PARALLEL
!....end timer
     time = time + omp get wtime()
     write(*,*) 'The approximation of Pi =', pi*w
     write(*,*) 'took ', time, ' seconds'
     end program integration pi reduction
```

# Break a nice mountain



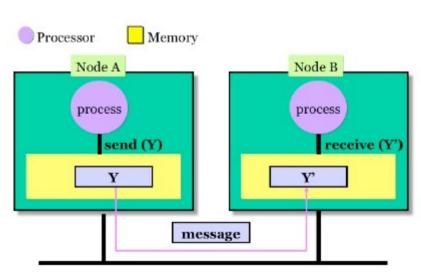
#### What is MPI?



- Ever since parallel computers hit the HPC market, there was an intense discussion about what should be an appropriate programming model for them.
- Message passing is required if a parallel computer is of the distributed memory type, i.e. if there is no way for one processor to directly access the address space of another.
- The use of explicit message passing (MP), i.e., communication between processes, is surely the most tedious and complicated but also the most flexible parallelization method.

#### Message Passing Interface (MPI)

- Resources are LOCAL (different from shared memory).
- Each process runs in an "isolated" environment. Interactions requires
   Messages to be exchanged
- Messages can be: instructions, data, synchronization.
- MPI works also on Shared Memory systems.
- Time to exchange messages is much larger than accessing local memory.
- → Massage Passing is a COOPERATIVE Approach, based on 3 operations:
- **SEND** (a message)
- **RECEIVE** (a message)
- SYNCHRONIZE



#### MPI availability

- MPI is standard defined in a set of documents compiled by a consortium of organizations : <a href="http://www.mpi-forum.org/">http://www.mpi-forum.org/</a>
- In particular the MPI documents define the APIs (application programming interfaces) for C, C++, FORTRAN77 and FORTRAN 90.
- Bindings available for Perl, Python, Java...
- In all systems MPI is implemented as a library of subroutines/functions over the network drivers and primitives.

#### <u>Messages</u>

- A message can be as simple as a **single item** (like a number) or even a **complicated structure**, perhaps scattered all over the address space.
- For a message to be transmitted in an orderly manner, some parameters have to be fixed in advance, such as:
- Which process is sending the message?
- Where is the data on the sending process?
- What kind of data is being sent?
- How much data is there?
- Which process is going to receive the message?
- Where should the data be left on the receiving process?
- What amount of data is the receiving process prepared to accept?
- → All MPI calls that actually transfer data have to specify those parameters in some way.

#### MPI: Pro's & Con's

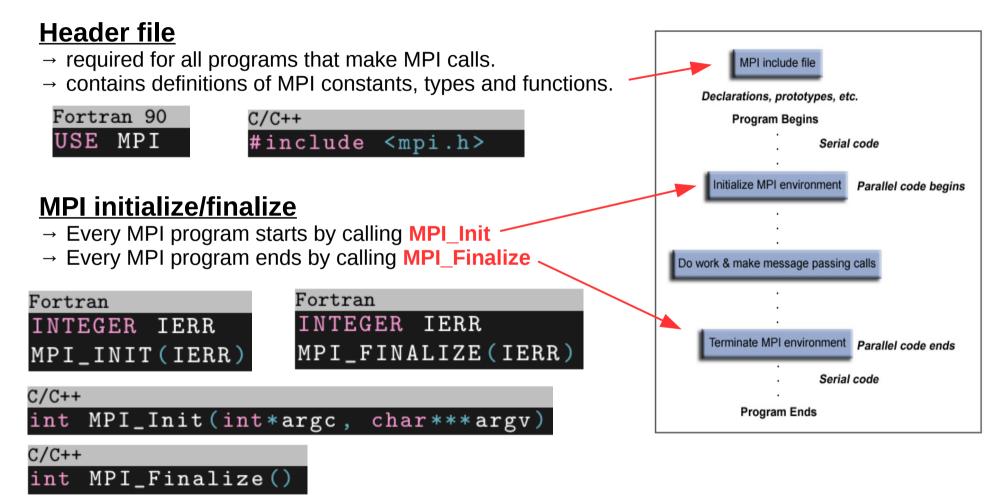
#### Pro's

- Distribute Memory → use more nodes and cores.
- Communication is the most important part of HPC.
  - → It can be (and is) highly optimized.
- MPI is portable (runs on almost any platform).
- Many current applications/libraries use MPI.
- MPI de-facto standard for distributed memory processing.

#### Con's

- Error-prone.
- Discourages frequent communications (overhead).
- Technically "hard" to implement.

# General program structure



#### **Format of MPI calls**

- → C names: case sensitive; Fortran not.
- → Programs must not declare variables or functions with the prefix MPI ...

#### MPI communicators and ranks

#### Communicator

- MPI uses objects called communicators and groups to define which collection of processes may communicate with each other.
- Most MPI routines require you to specify a communicator as an argument.
- Communicators and groups will be covered in more detail later.

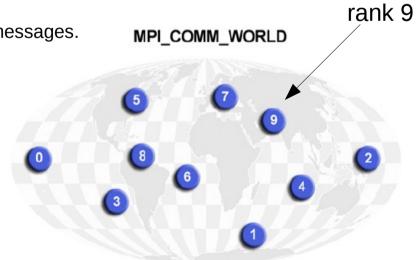
  For now, simply use MPI\_COMM\_WORLD whenever a communicator is required.
- It is the predefined communicator that includes all of your MPI processes.

#### Rank

- Within a communicator, every process has its own unique,
   integer identifier assigned by the system when the process initializes (=Rank)
- A rank is sometimes also called a "task ID". Ranks are contiguous and begin at zero.
- Used by the programmer to specify the source and destination of messages.
- Often used conditionally by the application to control program execution (if rank=0 do this / if rank=1 do that).

#### **Error Handling**

Most MPI routines include a return/error code parameter.



#### **Process Identification**

- How many processes are associated with a communicator?

```
Fortran
INTEGER COMM, SIZE, IERR
CALL MPI_COMM_SIZE(COMM, SIZE, IERR)

C/C++
MPI_Comm_size(MPI_Comm comm, int *size)
```

- How to get the rank of a process?

```
Fortran
INTEGER COMM, RANK, IERR
CALL MPI_COMM_RANK(COMM, RANK, IERR)
OUTPUT: RANK

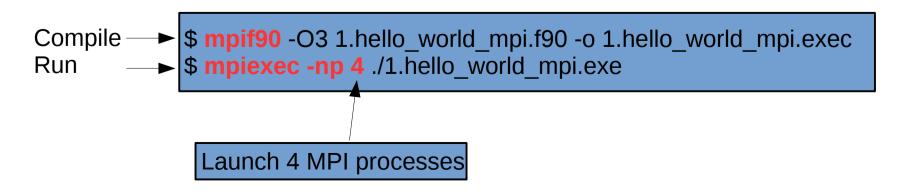
C/C++
MPI_Comm_rank(MPI_Comm comm, int *rank)
```

### Compiling and running MPI

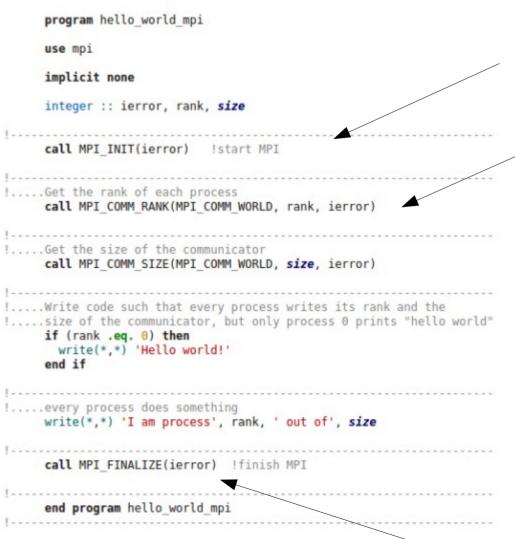
**MPI** is always available as a **library**. In order to **compile and link** an MPI program, compilers and linkers need options that specify where include files (i.e., C headers and Fortran modules) and libraries can be found.

As there is considerable variation in those locations among installations, most MPI implementations provide compiler wrapper scripts (often called mpicc, mpif90, etc.), which supply the required options automatically but otherwise behave like "normal" compilers.

Note that the way that MPI programs should be compiled and started is not fixed by the standard, so please consult the system documentation by all means.



#### "Hello World" in Fortran



This initializes the parallel environment

The MPI\_COMM\_WORLD handle describes all processes that have been started as part of the parallel program.

If required, other communicators can be defined as subsets of MPI\_COMM\_WORLD.

```
mpiexec -np 4 ./la.hello_world_mpi_cpp.exec

Hello world!
I am process 0 out of 4
I am process 2 out of 4
I am process 3 out of 4
I am process 1 out of 4
```

Note that no MPI process except rank 0 is guaranteed to execute any code beyond MPI\_Finalize().

### Hello World in MPI (Fortran/CPP)

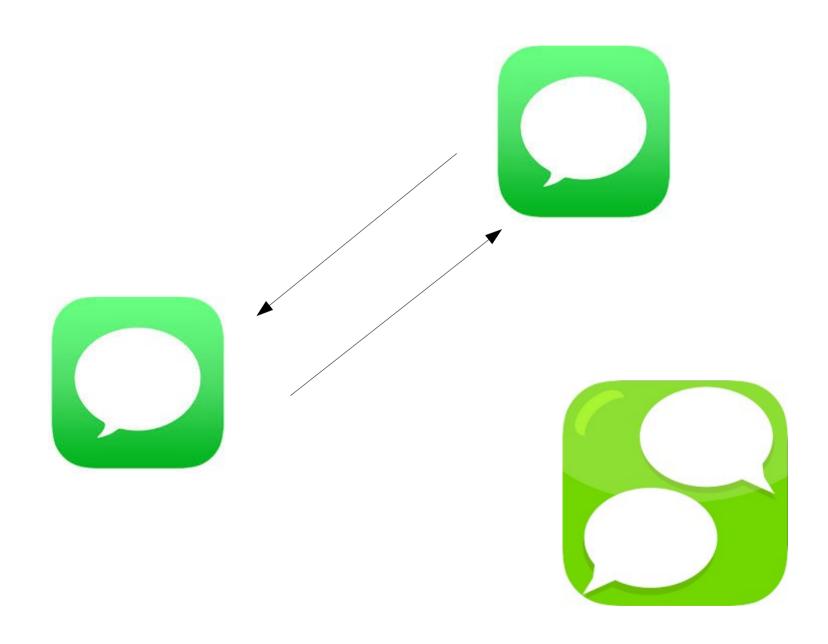
- 1. go to scheidegger/intro\_to\_hpc/MPI:
- > cd scheidegger/intro\_to\_hpc/MPI
- 2. Have a look at the code
- >vi 1.hello\_world\_mpi.f90 / 1a.hello\_world\_mpi.cpp
- 3. compile by typing:
- > make
- 4. Experiment with different numbers of MPI processes
- >mpiexec -np 4 ./1.hello\_world\_mpi.exec (-np #processes)
- >mpiexec -np 4 ./1a.hello\_world\_mpi\_cpp.exec (-np #processes)

#### Hello World in C++

The MPI bindings for the C language follow the case-sensitive name pattern MPI Xxxxx..., while Fortran is case-insensitive!

Below, I will mostly stick to the Fortran MPI bindings, and only describe the differences to C/C++ where appropriate.

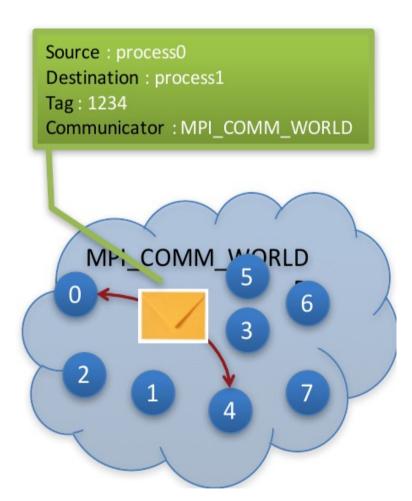
#### Messages and point-to-point communication



### Message Envelope

- Communication is performed by explicitly sending and receiving messages.
- Messages need **meta data** to describe sender and receiver as well as message contents.
- Sender and receiver are described by ranks within a group.
- Message contents given by starting address, data type, and count, where data type is:
  - → Elementary (all C and Fortran data types)
  - → Contiguous array of data types
  - → Strided blocks of data types
  - → Indexed array of blocks of data types
  - → General structure

MPI also allows messages to be tagged so that programs can deal with the arrival of messages in an orderly way.



#### Point-to-Point communication

It is the fundamental communication facility provided by a MPI library.

Communication between 2 processes.

It is conceptually simple:

- → source process A sends a message to destination process B.
- → B receives the message from A.

Communication takes place within a communicator.

Source and Destination are identified by their rank in the Communicator.

# Simple MPI communication model

Process with rank 1 sends to process with rank 2 (pseudo code)

```
Rank 1: MPI_Send(<send data buffer>, 2, MyCommunicator)
Rank 2: MPI_Recv(<recv data buffer>, 1, MyCommunicator)
```

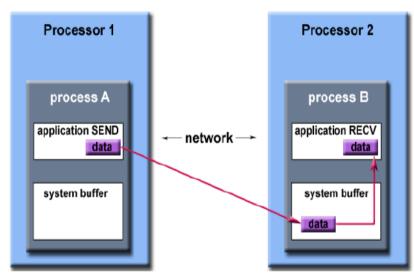
- same communicator: MyCommunicator
- send and recv buffer should be compatible:
  - → receive buffer should be large enough.
  - → data type should match.
- Rank 2 is prepare to receive data from Rank 1
  - → MPI\_Recv is called in "the right order" (deadlock).
  - → Rank 2 knows the maximum bound on the buffer size.

### Message Buffering

- In a perfect world, every send operation would be perfectly synchronized with its matching receive.
- This is rarely the case.
- The MPI implementation must be able to deal with storing the data when the two tasks are out of sync.

#### Consider the following two cases:

- → A send operation occurs 5 seconds before the receive is ready where is the message while the receive is pending?
- → Multiple sends arrive at the same receiving task which can only accept one send at a time what happens to the messages that are "backing up"?
- The MPI implementation (not the MPI standard) decides what happens to data in these types of cases. Typically, a system buffer area is reserved to hold data in transit.



#### Point-to-point communication

- "Hello World" example did not contain any real communication apart from starting and stopping processes.
- Point-to-Point communication is the fundamental communication facility provided by MPI.
- → Communication between two separate processes.
- → Source process A sends a message to destination process B.
- → B receives the message from A.
- → Communication takes place within a communicator.
- → Source and destination are identified by their rank in the communicator.

```
integer :: count, datatype, source, tag, comm,
integer :: count, datatype, dest, tag, comm, ierror
                                                         integer :: status (MPI STATUS SIZE), ierror
call MPI Send(buf,
                      ! message buffer
                                                         call MPI Recv(buf,
                                                                                ! message buffer
                     ! # of items
             count,
                                                                                ! maximum # of items
             datatype, ! MPI data type
                                                                       count,
             dest,
                     ! destination rank
                                                                       datatype, ! MPI data type
                     ! message tag (additional label)
                                                                       source, ! source rank
             tag,
             comm, ! communicator
                                                                                ! message tag (additional label)
                                                                       tag,
             ierror) ! return value
                                                                       comm,
                                                                                ! communicator
                                                                                ! status object (MPI_Status* in C)
                                                                       status,
                                                                       ierror) ! return value
```

### <u>Messages – terminology</u>

Data is exchanged in the buffer, an array of count elements of some particular MPI data type.

- → One argument that usually must be given to MPI routines is the type of the data being passed.
- → This allows MPI programs to run automatically in heterogeneous environments.

#### Messages are identified by their envelopes.

A message could be exchanged only if the sender and receiver specify the correct envelope.

body			envelope			
buffer	count	datatype	source	destination	communicator	tag

#### **Example Ping - Pong**

```
integer, parameter :: process a = 0
     integer, parameter :: process b = 1
     integer, parameter :: ping = 17 !message tag
     integer, parameter :: pong = 23 !message tag
     integer, parameter :: length = 1
     integer :: status(MPI STATUS SIZE)
     real :: buffer(length)
     integer :: i
     integer :: ierror, my rank, size
     call MPI INIT(ierror)
     call MPI COMM RANK(MPI COMM WORLD, my rank, ierror)
     call MPI Comm size(MPI COMM WORLD, size, ierror)
....the example should only be run with 2 procs, else abort
     if (size .ne. 2) then
       write(*,*) 'please run this with 2 processors'
       call MPI Finalize(ierror)
       stop
     end if
.....write a loop of number of messages iterations. Within the loop, process A sends a message
.....(ping) to process B. After receiving the message, process B sends a message (pong) to process A)
     if (my rank .eq. process a) then
      call MPI SEND(buffer, length, MPI REAL, process b, PING, MPI COMM WORLD, ierror)
       call MPI_RECV(buffer, length, MPI_REAL, process_b, PONG, MPI_COMM_WORLD, status, ierror)
     else if (my rank .eq. process b) then
       call MPI RECV(buffer, length, MPI REAL, process a, PING, MPI COMM WORLD, status, ierror)
       call MPI SEND(buffer, length, MPI REAL, process a, PONG, MPI COMM WORLD, ierror)
     end if
     write(*,*) 'Ping-pong on process complete - no deadlock on process', my rank
     call MPI FINALIZE(ierror)
     end program ping pong
```

# Example Ping - Pong

- 1. go to scheidegger/intro\_to\_hpc/MPI:
- > cd scheidegger/intro\_to\_hpc/MPI
- 2. Have a look at the code
- >vi 2.ping\_poing.f90
- 3. compile by typing:
- > make
- 4. run the code

>mpiexec -np 2 ./2.ping\_pong.exec

#### Program fragment: parallel Integration

 $\rightarrow$  we integrate f(x) = 0.5\*x in the domain [0,2]

```
integer, dimension (MPI STATUS SIZE) :: status
2 call MPI Comm size (MPI COMM WORLD, size, ierror)
  call MPI Comm rank (MPI COMM WORLD, rank, ierror)
  ! integration limits
6 a=0.d0 ; b=2.d0 ; res=0.d0
s ! limits for "me"
  mya=a+rank*(b-a)/size
                          Split work/domain wrt. all ranks available
  myb=mya+(b-a)/size
  ! integrate f(x) over my own chunk - actual work
  psum = integrate(mya, myb)
                                              Results on rank 0
  ! rank 0 collects partial results
  if (rank.eq.0) then
     res=psum
     do i=1, size-1
        call MPI Recv(tmp, &
                              ! receive buffer
19
                              ! array length
20
                               ! data type
21
                      MPI DOUBLE PRECISION, &
22
                                                                 Where is partial sum from?
                               ! rank of source
23
                              ! tag (unused here)
24
                      MPI COMM WORLD, & ! communicator
25
                      status, & ! status array (msg info)
26
                      ierror)
27
        res=res+tmp
28
     enddo
29
     write(*,*) 'Result: ',res
    ranks != 0 send their results to rank 0
  else
32
     call MPI Send (psum,
                               ! send buffer
33
                           & ! message length
34
                   MPI DOUBLE PRECISION, &
35
                               ! rank of destination 
Send partial sum from there
36
                              ! tag (unused here)
37
                   MPI COMM WORLD, ierror)
  endif
```

### **Example** – Integration

- 1. go to scheidegger/intro\_to\_hpc/MPI:
- > cd scheidegger/intro\_to\_hpc/MPI
- 2. Have a look at the code
- >vi 2a.integrate.f90 (we integrate f(x) = 0.5\*x in the domain [0,...,2])
- 3. compile by typing:
- > make
- 4. run the code
- >mpiexec -np 2 ./2a.integrate.exec
- → Play with different number of procs.
- $\rightarrow$  Change f(x) to sin(x), and also the integration bounds.

#### **Collective Communication**



# Collective communication in MPI (II)

Collective communication routines must involve all processes within the scope of a Communicator (e.g. MPI\_COMM\_WORLD).

#### **Types of Collective Operations:**

#### **Synchronization:**

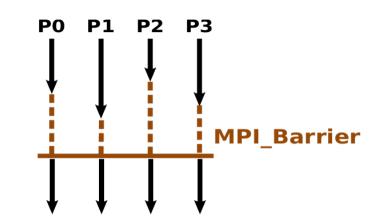
→ processes wait until all members of the group have reached the synchronization point (e.g. a barrier).

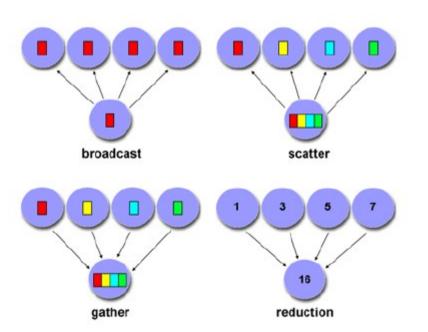
#### **Data Movement:**

→ broadcast, scatter/gather, all to all.

#### **Collective Computation (reductions):**

→ one member of the group collects data from the other members and performs an operation (min, max, add, multiply, etc.) on that data.





#### Reductions

The reduction operation allows to:

- Collect data from each process.
- Reduce the data to a single value.
- Store the result on the root processes.
- Store the result on all processes.
- Overlap communication and computation.

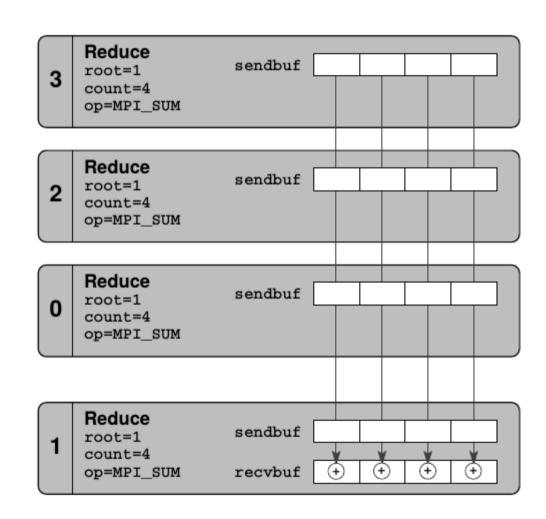
# Reduction graphically

A reduction on an array of length count (a sum in this example) is performed by MPI\_Reduce().

Every process must provide a send buffer.

The receive buffer argument is only used on the root process.

The local copy on root can be prevented by specifying MPI\_IN\_PLACE instead of a send buffer address.



### Example: Reductions → MPI\_SUM

- MPI, has mechanisms that make reductions much simpler (and in most cases) more efficient than looping over all ranks/collecting results.
- There are at the moment 12 predefined operators.

```
integer :: count, datatype, op, root, comm, ierror
call MPI Reduce (sendbuf,
                           ! send buffer
                recybuf.
                           ! receive buffer
                count.
                          ! number of elements
                datatype, ! MPI data type
                           ! MPI reduction operator
                op,
                           ! root rank
                root,
                comm.
                           ! communicator
                            ! return value
                ierror)
                                 ! send buffer (partial result)
call MPI Reduce (psum, &
                                 ! recv buffer (final result @ root)
                res, &
                1, &
                                 ! array length
                MPI_DOUBLE_PRECISION, &
                MPI SUM, &
                                 ! type of operation
```

! root (accumulate result there)

0, &

MPI COMM WORLD, ierror)

```
MPI op
                   Operation
 MPI\_MAX
                    Maximum
 MPI_MIN
                    Minimum
 MPI SUM
                      Sum
 MPI_PROD
                    Product
 MPI_LAND
                  Logical AND
 MPI_BAND
                  Bitwise AND
 MPI_LOR
                   Logical OR
                   Bitwise OR
 MPI BOR
 MPI_LXOR
               Logical exclusive OR
 MPI_BXOR
               Bitwise exclusive OR
MPI_MAXLOC
              Maximum and location
MPI MINLOC
              Minimum and location
```

```
Specific call of MPI_Reduce()
→ MPI SUM
```

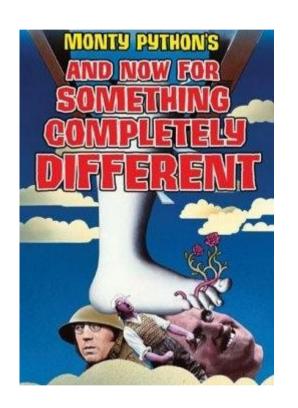
### **Example – Reduction**

```
program reduce
    use mpi
    implicit none
    integer :: rank, input, result, ierror
    call MPI Init(ierror)
    call MPI Comm rank(MPI COMM WORLD, rank, ierror)
1-----
    input = rank + 1
!....reduce the values of the different ranks in input to result of rank 0
    with the operation sum (max, logical and)
    call MPI_Reduce(input, result, 1, MPI_INT, MPI_SUM, 0, MPI_COMM_WORLD, ierror)
    if (rank .eq. 0) then
     write (*,*) 'result', result
    end if
    call MPI_Finalize(ierror)
    end program reduce
```

### Example – Reduction

- 1. go to zice17/scheidegger/intro\_to\_hpc/MPI:
- > cd zice17/scheidegger/intro\_to\_hpc/MPI:
- 2. Have a look at the code
- >vi 3.MPI\_reduce.f90
- 3. compile by typing:
- > make
- 4. run the code
- >mpiexec -np 2 ./3.MPI\_reduce.exec (experimpent with # processes)
- 5. change the "root" (line 27) from 0 to 1. What happens?

# 4. MPI & Python







### 4. MPI in Python

### See https://mpi4py.scipy.org

→ **MPI for Python** supports convenient, pickle-based communication of generic Python object as well as fast, near C-speed, direct array data communication of buffer-provider objects (e.g., NumPy arrays).

#### **Communication of generic Python objects:**

You have to use all-lowercase methods (of the Comm class), like send(), recv(), bcast(). Note that isend() is available, but irecv() is not.

Collective calls like scatter(), gather(), allgather(), alltoall() expect/return a sequence of Comm.size elements at the root or all process. They return a single value, a list of Comm.size elements, or None.

Global reduction operations reduce() and allreduce() are naively implemented, the reduction is actually done at the designated root process or all processes.

### "Hello World" in Python

Go to zice17/scheidegger/intro\_to\_hpc/alphacruncher/MPI4PY

Run with

> mpiexec -np 4 python helloworld.py

#hello.py
from mpi4py import MPI
comm = MPI.COMM\_WORLD
rank = comm.Get\_rank()
size = MPI.COMM\_WORLD.Get\_size()
print "hello world from process ", rank, " from total ", size , "processes"

### Point-to-Point Communication

>zice17/scheidegger/intro\_to\_hpc/MPI4PY/alphacruncher/pointtopoint.py

### MPI Broadcast in Python

> zice17/scheidegger/intro\_to\_hpc/MPI4PY/alphacruncher/bcast.py

### MPI Reductions in Python

- Estimate integrals using the trapezoid rule.
- A range to be integrated is divided into many vertical slivers, and each sliver is approximated with a trapezoid.

$$area \approx \sum_{i=0}^{n} \frac{[f(a) + f(b)]}{2} \cdot \Delta x = \left[ \frac{f(a) + f(b)}{2} + \sum_{i=0}^{n} f(a + i\Delta x) + f(a + (i+1)\Delta x) \right] \cdot \Delta x$$

### <u>MPI Reductions in Python</u>

```
import numpy
import sys
                                                      >zice17/scheidegger/intro to hpc/MPI4PY/alphacruncher/reduction.py
from mpi4pv import MPI
from mpi4py.MPI import ANY SOURCE
comm = MPI.COMM WORLD
                                                      Run with
rank = comm.Get rank()
size = comm.Get size()
                                                      > mpiexec -n 4 python reduction.py a b N
#takes in command-line arguments [a,b,n]
a = float(sys.argv[1])
                                                      → integration range [a,b], discretization N
b = float(sys.argv[2])
n = int(sys.argv[3])
#we arbitrarily define a function to integrate
                                                      > mpiexec -n 4 python reduction.py 0.0 1.0 1000
def f(x):
       return x*x
#this is the serial version of the trapezoidal rule
#parallelization occurs by dividing the range among procesOUTPUT = ???
def integrateRange(a, b, n):
       integral = -(f(a) + f(b))/2.0
       # n+1 endpoints, but n trapazoids
       for x in numpy.linspace(a,b,n+1):
                      integral = integral + f(x)
       integral = integral* (b-a)/n
       return integral
#h is the step size. n is the total number of trapezoids
#local n is the number of trapezoids each process will calculate
#note that size must divide n
local n = n/size
#we calculate the interval that each process handles
#local a is the starting point and local b is the endpoint
local a = a + rank*local n*h
local b = local a + local n*h
#initializing variables. mpi4py requires that we pass numpy objects.
integral = numpy.zeros(1)
total = numpy.zeros(1)
                                                                                                  Reduction
# perform local computation. Each process integrates its own interval
integral[0] = integrateRange(local a, local b, local n)
# communication
# root node receives results with a collective "reduce"
comm.Reduce(integral, total, op=MPI.SUM, root=0)
# root process prints results
if comm.rank == 0:
       print "With n =", n, "trapezoids, our estimate of the integral from"\
       , a, "to", b, "is", total
```

### **Questions?**

1. Advice – RTFM https://en.wikipedia.org/wiki/RTFM

2. Advice — http://lmgtfy.com/ http://lmgtfy.com/?q=message+passing+interface

