

Parallel computing

MPI, OpenMP, using GPU

Claudia Blaas-Schenner
VSC Research Center, TU Wien



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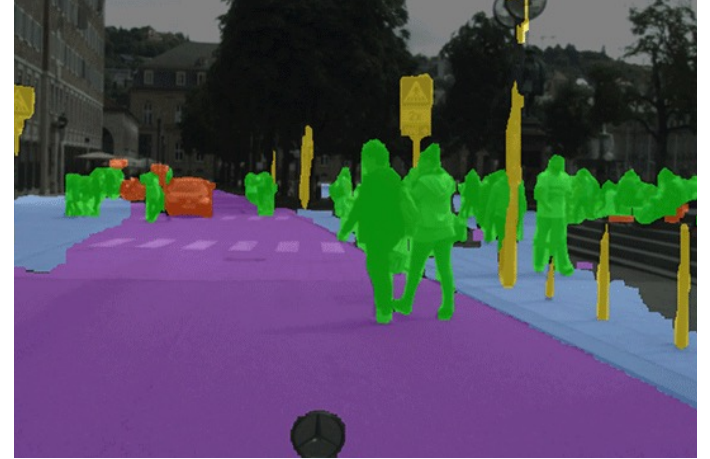
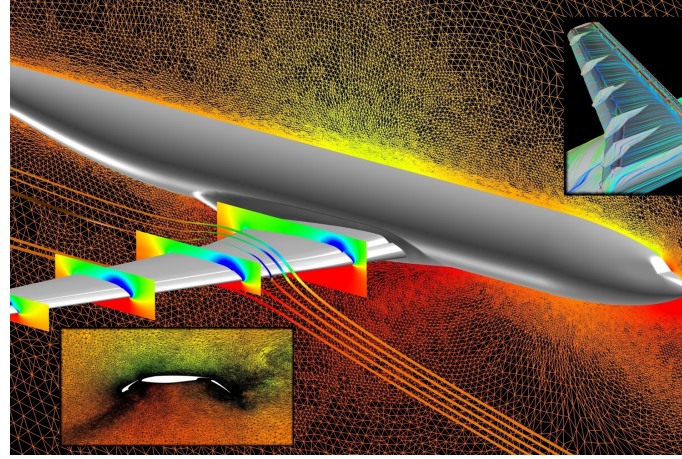
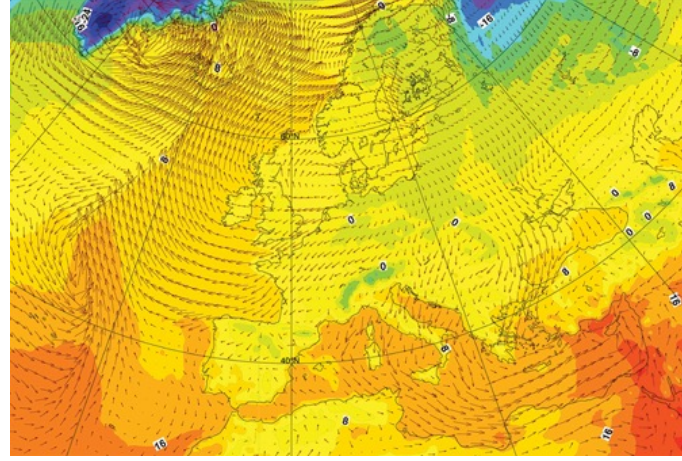
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HPC solves societal challenges



*The days when scientists did not have to care about the hardware are over,
and so are the days when compute centers did not have to worry about the scientific application!*

source:
www.prace-ri.eu

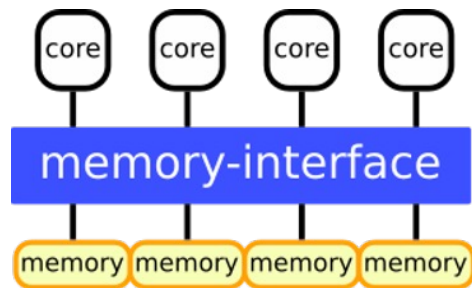
remarkable repeated success stories:

- recurring core part of Nobel Prizes in Physics & Chemistry
- saving billions with better weather forecasting
- improving human health with genomics, personalized medicine
- 3-4% better fuel efficiency of aircraft & wind turbines every year
- disrupting communication, transportation and manufacturing
- design of future materials from scratch based on desired properties
- batteries & supercapacitors
- artificial intelligence, machine learning, sensors, open data

OpenMP: shared memory (socket, node)

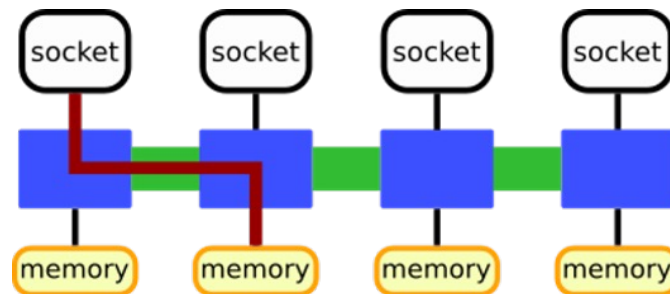
MPI: distributed memory (socket, node, **cluster**)

CUDA: accelerated nodes



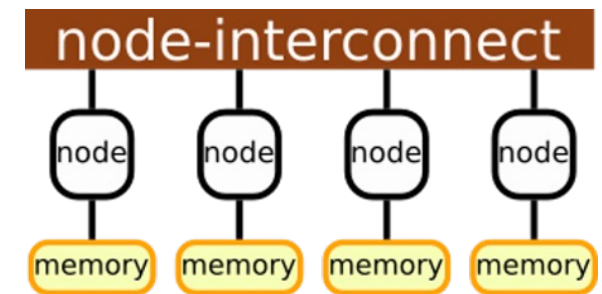
socket

UMA (uniform memory access)
SMP (symmetric multi-processing)



node

ccNUMA (cache-coherent non-uniform ...)
first touch, pinning!



cluster

NUMA (non-uniform memory access)
fast access to own memory only

Amdahl's law

$$T_{\text{parallel}, p} = f \cdot T_{\text{serial}} + (1-f) \cdot T_{\text{serial}} / p$$

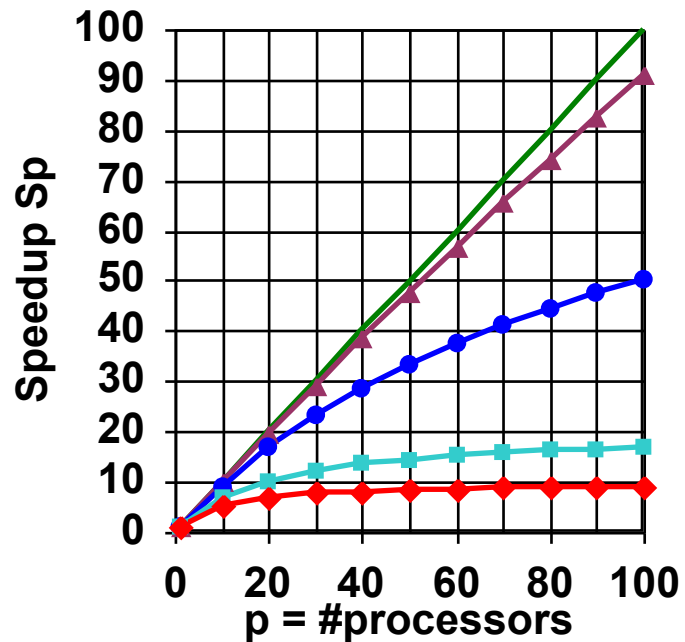
f ... sequential part of code

neglecting time for communication

$$S_p = T_{\text{serial}} / T_{\text{parallel}, p} = 1 / (f + (1-f) / p)$$

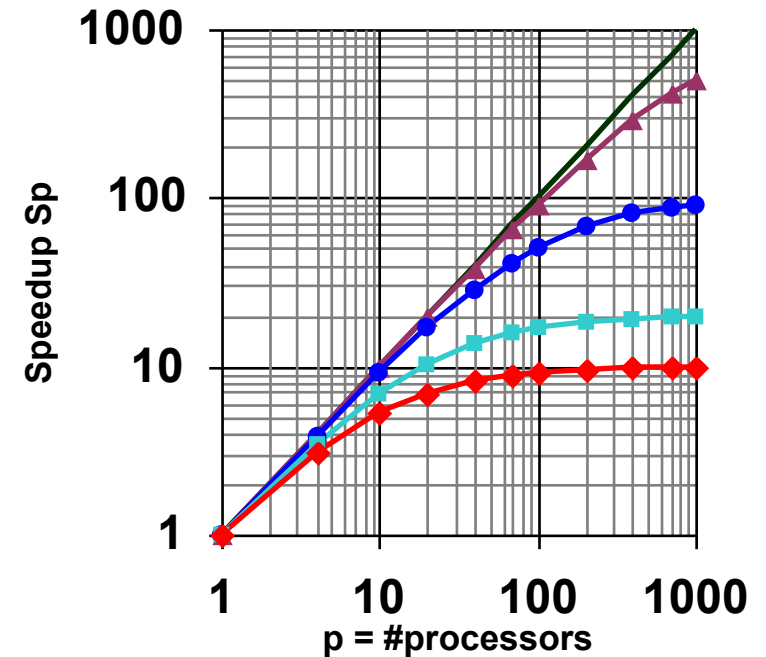
Speedup is limited: $S_p < 1 / f$

neglecting load imbalance



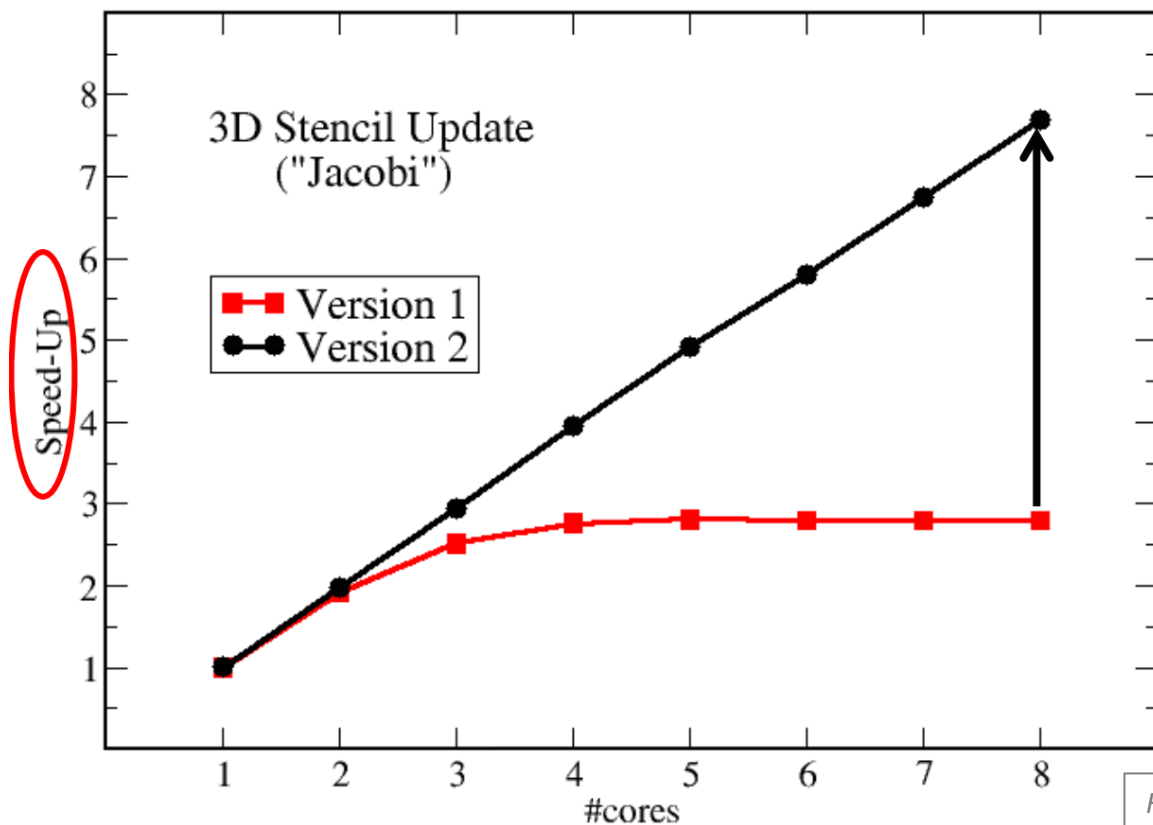
- $S_p = p$ (ideal speedup)
- $f=0.1\% \Rightarrow S_p < 1000$
- $f= 1\% \Rightarrow S_p < 100$
- $f= 5\% \Rightarrow S_p < 20$
- $f= 10\% \Rightarrow S_p < 10$

Figures courtesy of
Rolf Rabenseifner.

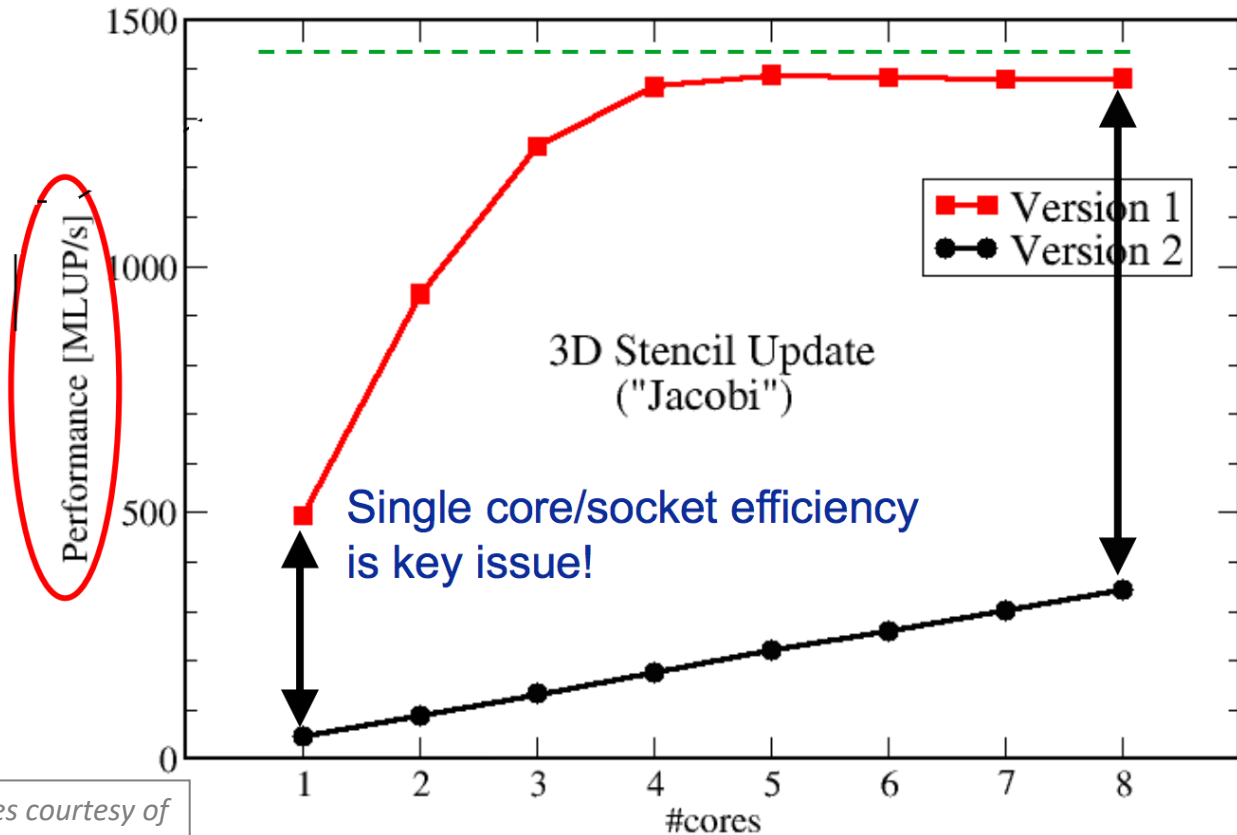


Speedup = ratio – no absolute performance !

scalability vs. performance

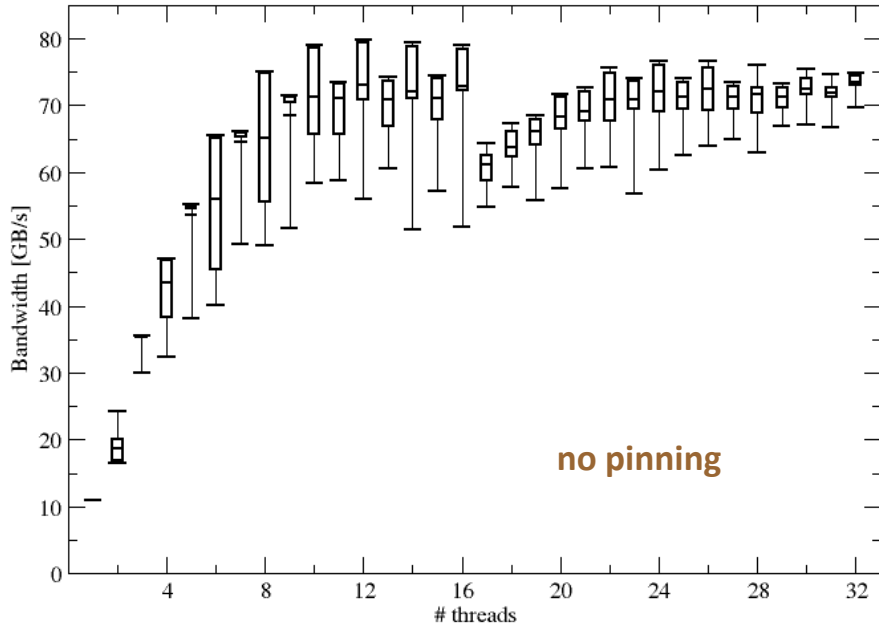


Figures courtesy of Georg Hager.

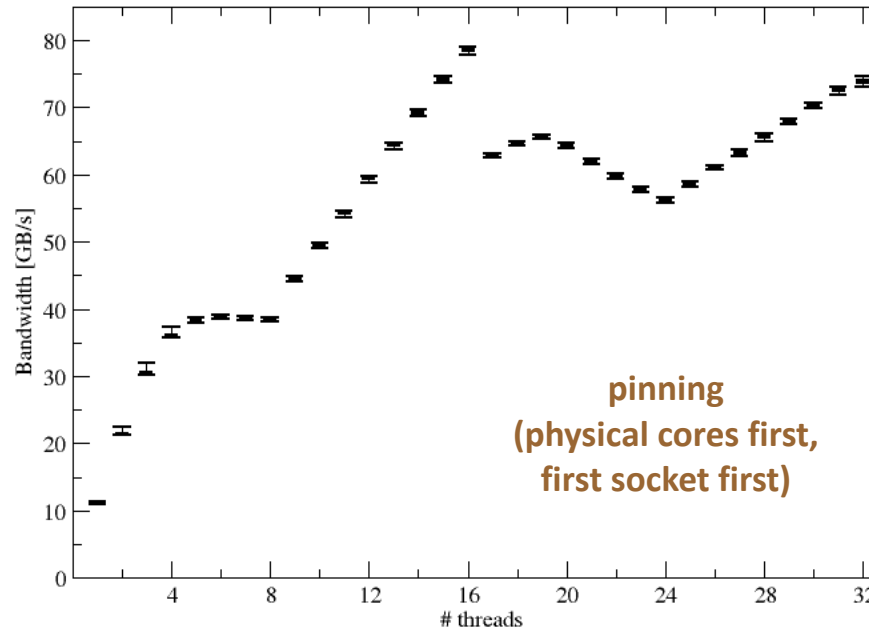
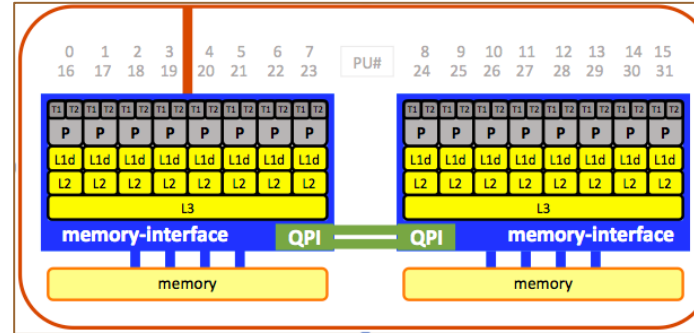


$$3D \text{ Stencil Update ("Jacobi")}: y(i, j, k) = b * (x(i-1, j, k) + x(i+1, j, k) + x(i, j-1, k) + x(i, j+1, k) + x(i, j, k-1) + x(i, j, k+1))$$

pinning ?



no pinning



pinning
(physical cores first,
first socket first)

OpenMP
STREAM benchmark

Benchmark & plots
courtesy of
Georg Hager.

MPI will give the very same picture !

why should we care
about **pinning** ?

- eliminating performance variations
- making use of architectural features
- avoiding resource contention



HPC = computation – communication – I/O

LATENCY	← typical values →	BANDWIDTH	HPC	
1–2 ns	L1 cache	100 GB/s	computation node / core	<i>exclusive</i>
3–10 ns	L2/L3 cache	50 GB/s		
100 ns	memory	10 GB/s	communication message passing	<i>exclusive (BF)</i>
1–10 μs	HPC networks	1–8 GB/s		
50 μs	Gigabit Ethernet	100 MB/s	I/O parallel FS	<i>shared with all users</i>
500 μs	Solid state disk	100 MB/s		
10 ms	Local hard disk	50 MB/s		
50 ms	Internet	10 MB/s		

Understand HW features!

Know your code!

Know the sys. environment!

→ Take control!

→ Avoiding slow data paths is the key to most performance optimizations!



OpenMP

standard - defined for C/C++ and Fortran

[OpenMP 5.2 Specifications \(PDF\) and Reference Guides \(PDF\)](#)

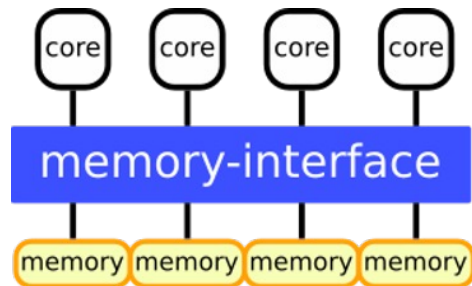
OpenMP: shared memory (socket, node)

Several sockets with multi-processors (node)

- memory is shared among all CPUs
- single / global address space
- uniform / non-uniform memory access

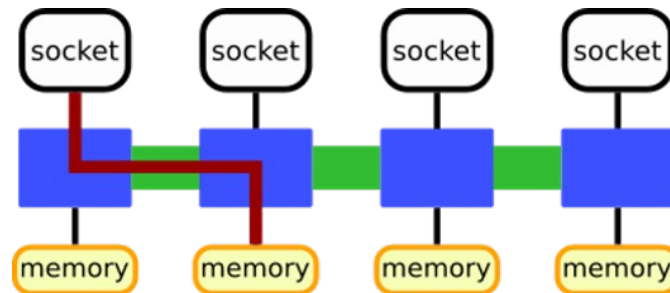
OpenMP works only on shared memory!

- **socket** - UMA
- **node** - ccNUMA



socket

UMA (uniform memory access)
SMP (symmetric multi-processing)



node

ccNUMA (cache-coherent non-uniform ...)
first touch, pinning!

- the **easiest way to parallelize** your code
- requires a shared memory system (allows to exploit node level parallelism)
- portable across shared memory architectures (standard since 1997)
- extension to C/C++ and Fortran
(using directives, environment variables, and some library routines)
- focuses mostly on **parallelizing loops with independent iterations**
(less and less true with each version)

philosophy of OpenMP

- parallelization with as little modification to the sequential program as possible
- incremental approach to parallelization



- **thread** is a set of sequential instructions that are executed in order
- **thread** is a software construct - **core** is a hardware construct
 - often each thread in a program is mapped to a single core
- **shared memory model** assumes that all threads read and write from the same memory
- **distributed memory model** means that no shared memory is available (in this case communication has to be done by sending messages)

To start with OpenMP is easy

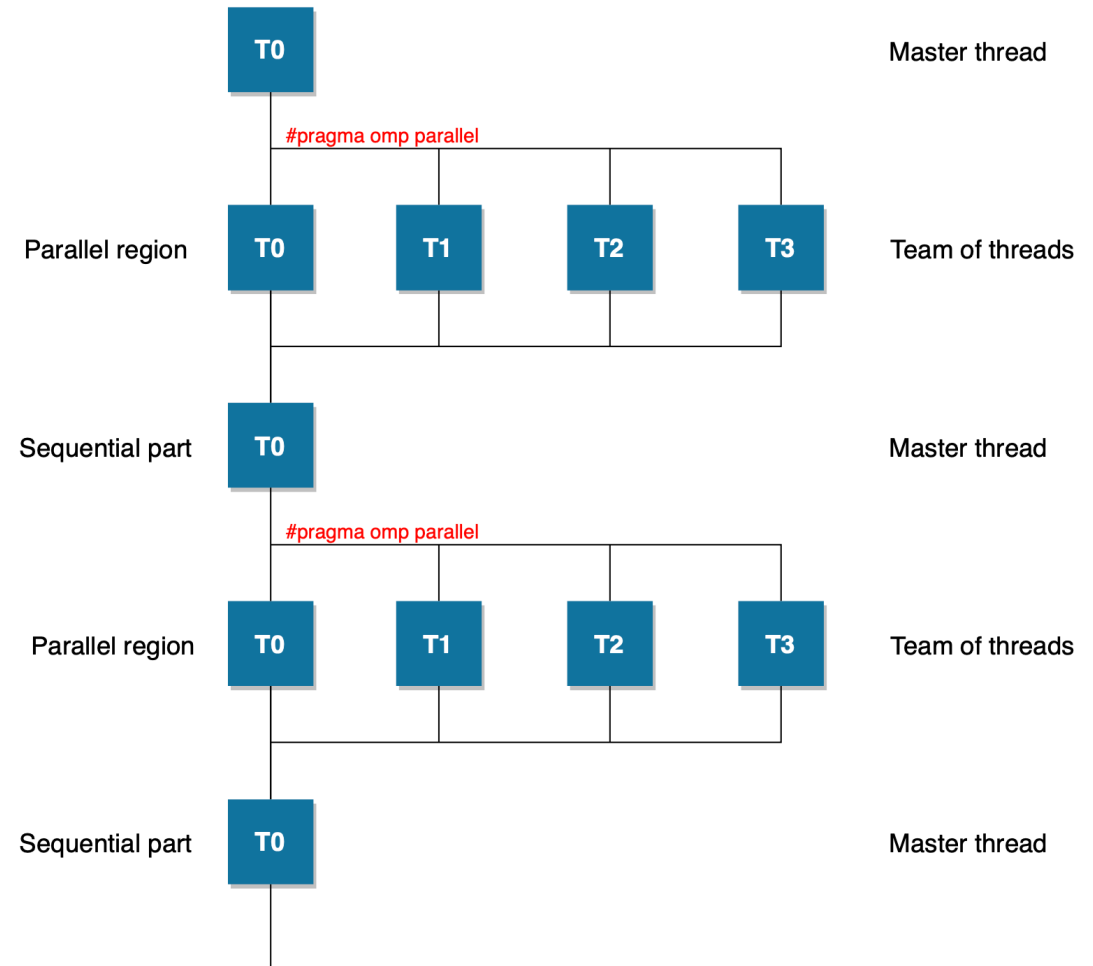
```
#pragma omp parallel for
for (i = 0; i < n; i++)
{
    out[i] = in [i];
}
```

Divides the loop iterations into pieces that are then executed in parallel by different threads.

→ it must be possible to determine the number of iterations at the time the loop starts execution

fork-join model

- program begins as a single process (**master thread**)
- at the **beginning** of a parallel region a **team of threads** is created
- at the **end** of a parallel region **threads synchronize** (implied barrier)
- at the end of a parallel region execution **continues sequentially**



- OpenMP **directive format**

```
#pragma omp directive_name [clause, [[,] clause] ... ]
```

- a **parallel region** creates a team of threads that (potentially) execute the workload

```
#pragma omp parallel  
{  
    printf("Hello World!\n");  
}
```

→ code is executed redundantly

- the **header file `omp.h`** provides library functions
- **`omp_get_num_threads()`** → returns the number of threads in the current team
- **`omp_get_thread_num()`** → returns the thread id (0 to `omp_get_num_threads()-1`)

```
#pragma omp parallel
{
    if (omp_get_thread_num() == 0)
        printf(" Number of threads: %1d \n", omp_get_num_threads());

    printf(" Hello world from thread %1d \n", omp_get_thread_num());
}
```

- **compile**
cc -fopenmp program.c
- **run**
./a.out

- **prints**
Number of threads: 3
Hello world from thread 2
Hello world from thread 0
Hello world from thread 1

- there is **no guarantee in which order** the threads are executed
- if a specific order is desired this has to be enforced (might be **very expensive**)
- the thread id can be used to divide the work among threads (a lot of boilerplate)

OpenMP provides facilities to automatically divide the work among the threads in a team

- the corresponding directives are called **worksharing directives** (e.g., **for**)
- **reduction**, combining multiple values into a single one, is a common pattern

- the **number of threads** used by OpenMP can be set by using environment variables

set number of threads for the entire session

```
export OMP_NUM_THREADS=4; ./program
```

or only for one execution of the program

```
OMP_NUM_THREADS=4 ./program
```

- the **default**, often the number of hyperthreads in the system, is usually **not** an optimal choice

→ **rule of thumb:** number of threads = number of cores

- **shared memory model:** all threads can write and read from main memory
- there are two types of variables
 - **shared** variables are common to all threads (usually arrays, global variables, ...)
 - **private** variables are duplicated on each thread (local variables, loop counters, ...)
- **by default all variables are shared**
- exceptions
 - local variables defined inside an OpenMP directive
 - loop control variables for a parallel for loop
 - variables that are declared in a called function
- **a variable can be explicitly declared as private or shared**

- OpenMP is easy to write, but it is also easy to get wrong.
- OpenMP **delegates a lot of responsibility to the programmer.**
- ensure that the code can be parallelized
 - make sure that the **loop iterations are independent**
- **NO race conditions!** - a program with a race condition is always wrong...
a race condition occurs when multiple threads are allowed to access the same memory location and at least one access is a write

example - pi serial

```
#include <time.h>
#include <stdio.h>
#include <math.h>

int main(int argc, char *argv[])
{
    int num_threads, i, n = 10000000;
    double pi, sum, h, x;
    double time, time_s, time_e;
    double PI25DT = 3.141592653589793238462643;

    num_threads = 1;

    h = 1.0 / (double)n;
    sum = 0.0;

    time_s = clock();

    for (i = 0; i < n; i++)
    {
        x = h * ((double)i + 0.5);
        sum += 4.0 / (1.0 + x*x);
    }

    pi = h * sum;

    time_e = clock();

    printf("serial, time, pi, error: %1d, %.3f, %.16f, %.16f\n",
        num_threads, ((time_e-time_s)/1e3), pi, fabs(pi-PI25DT));
}
```

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

int main(int argc, char *argv[])
{
    int num_threads, i, n = 10000000;
    double pi, sum, h, x;
    double time, time_s, time_e;
    double PI25DT = 3.141592653589793238462643;

    #pragma omp parallel
    {
        #pragma omp single
        num_threads = omp_get_num_threads();
    }

    h = 1.0 / (double)n;
    sum = 0.0;

    time_s = omp_get_wtime();

    #pragma omp parallel for private(x) shared(h) reduction(+:sum)
    for (i = 0; i < n; i++)
    {
        x = h * ((double)i + 0.5);
        sum += 4.0 / (1.0 + x*x);
    }

    pi = h * sum;

    time_e = omp_get_wtime();

    printf ("num_threads, time, pi, error: %02d, %.3f, %.16f, %.16f\n",
           num_threads, ((time_e-time_s)*1e3), pi, fabs(pi-PI25DT));
}
```

results - pi OpenMP



- `cd PI`
- `ml OpenMPI/4.1.1-GCC-10.2.0-Java-1.8.0_221`
- `vi pi_openmp.c`
- `cc -fopenmp -o pi_openmp pi_openmp.c`
- `OMP_NUM_THREADS=1 ./pi_openmp` → 1, 2, 4, 8, 16, 32

```
num_threads, time, pi, error: 01, 34.713, 3.1415926535897309, 0.00000000000000622
num_threads, time, pi, error: 02, 18.123, 3.1415926535899228, 0.0000000000001297
num_threads, time, pi, error: 04, 8.933, 3.1415926535896697, 0.0000000000001235
num_threads, time, pi, error: 08, 4.363, 3.1415926535898038, 0.000000000000107
num_threads, time, pi, error: 16, 2.618, 3.1415926535898024, 0.0000000000000093
num_threads, time, pi, error: 32, 1.352, 3.1415926535898024, 0.0000000000000093
```

MPI

standard - defined for C/C++ and Fortran

[MPI: A Message-Passing Interface Standard Version 4.0 \(PDF\)](#)

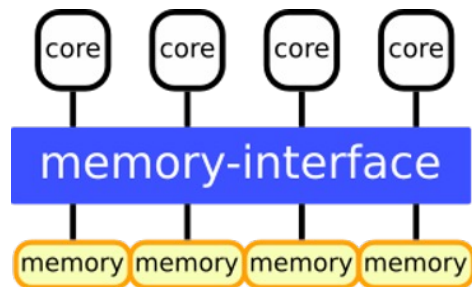
python (not part of the MPI standard): <https://mpi4py.readthedocs.io/>

■

MPI: distributed memory (socket, node, cluster)

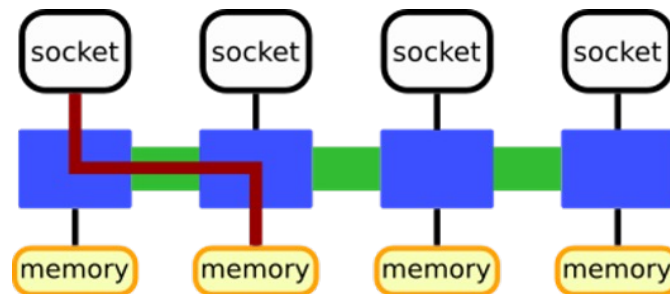
Several sockets with multi-processors (node)

- memory is shared among all CPUs
- single / global address space
- uniform / non-uniform memory access



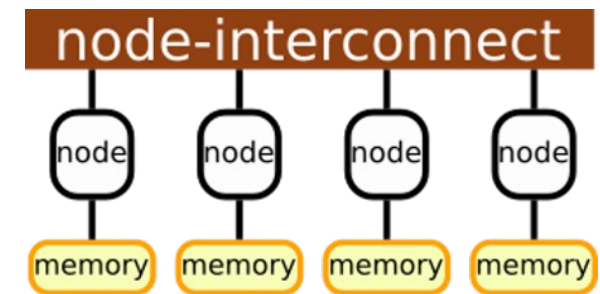
socket

UMA (uniform memory access)
SMP (symmetric multi-processing)



node

ccNUMA (cache-coherent non-uniform ...)
first touch, pinning!



cluster

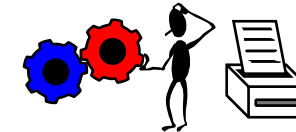
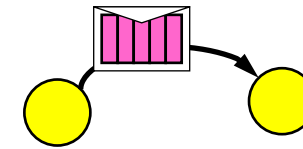
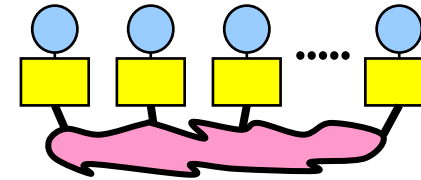
NUMA (non-uniform memory access)
fast access to own memory only

MPI works everywhere!

Multi-computers with various architectures (cluster)

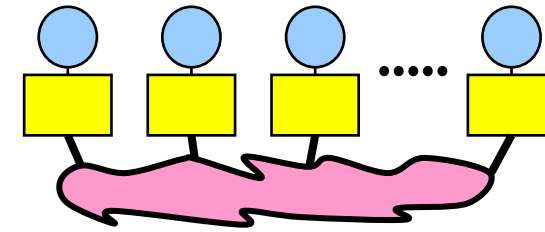
- set of nodes interconnected by a network
- each node has separated memory
- slower access to memories of other processors

- **overview, process model and language bindings**
 - one program on several processors
 - work and data distribution
 - starting several MPI processes
- **messages and point-to-point communication**
 - the MPI processes can communicate
- **nonblocking communication**
 - to avoid idle times, serializations, and deadlocks
- **collective communication**
 - e.g. broadcast, reduction, ...



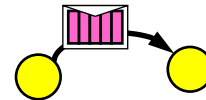
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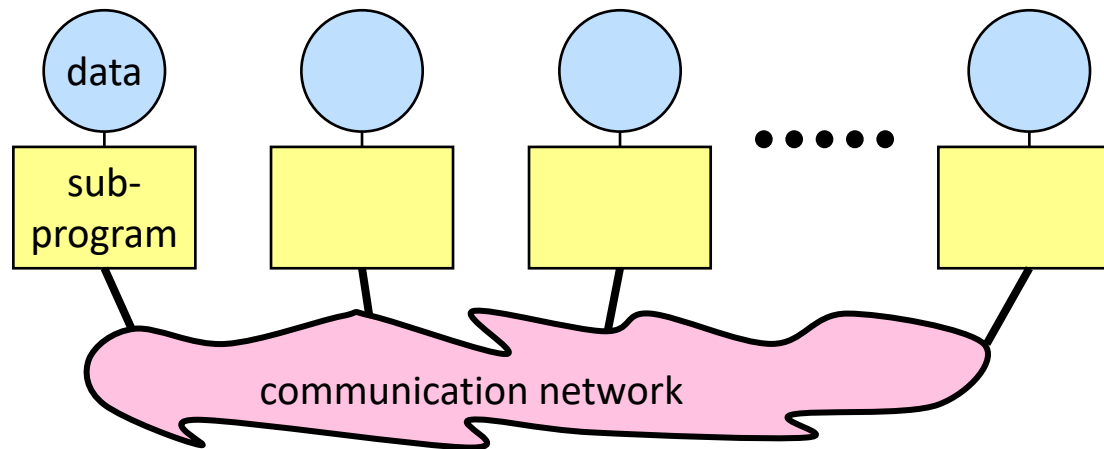
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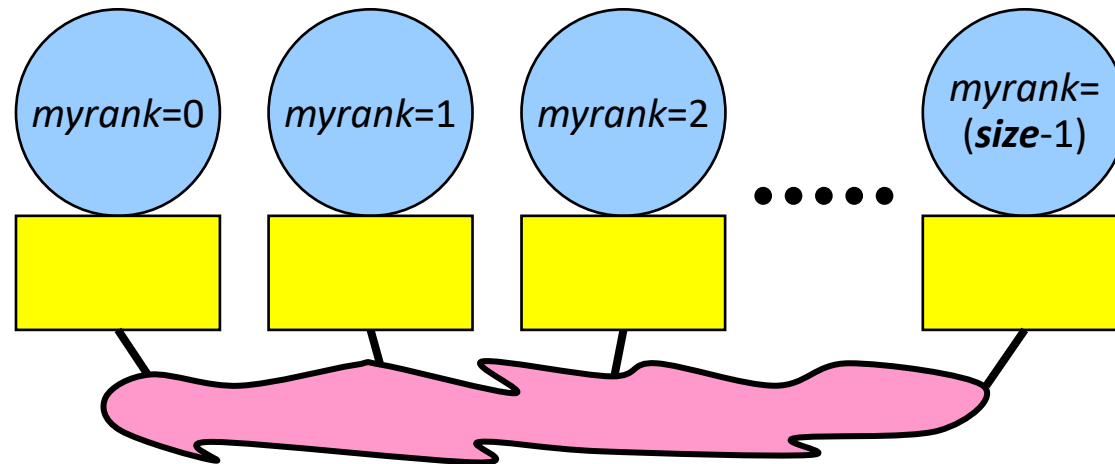


each processor in a message passing program runs a *sub-program*

- written in a conventional sequential language, e.g., C, Fortran, or python
- typically the same on each processor (SPMD), all variables are private
- communicate via special send & receive routines (*message passing*)



- the system of *size* processes is started by special MPI initialization program
- the value of *myrank* is returned by special library routine
- all distribution decisions are based on *myrank*

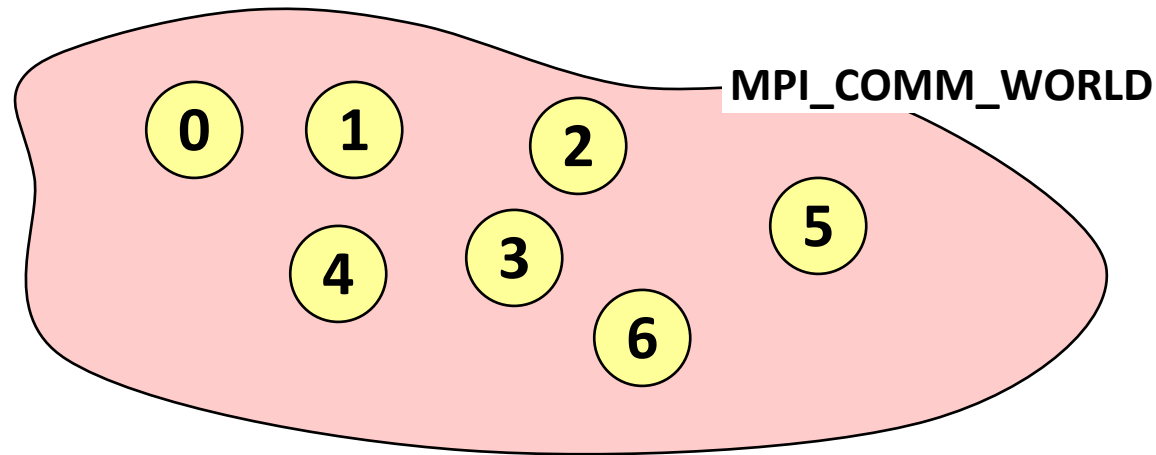


- must be linked with an MPI library → `mpicc`
- must be started with the MPI startup tool → `mpirun -n # ./a.out`

```
#include <mpi.h>
#include <stdio.h>
int main(int argc, char *argv[])
{
    MPI_Init(&argc, &argv);
    ...
    MPI_Finalize();
}
```

- MPI function format → `MPI_XXXXXX (parameter, ...);`

- all processes (= sub-programs) of one MPI program are combined in the **communicator MPI_COMM_WORLD** (predefined handle)
- **size** is the number of processes in a communicator
- each process has its own **rank** in a communicator starting with 0 – ending with (size-1)



example: Hello world!

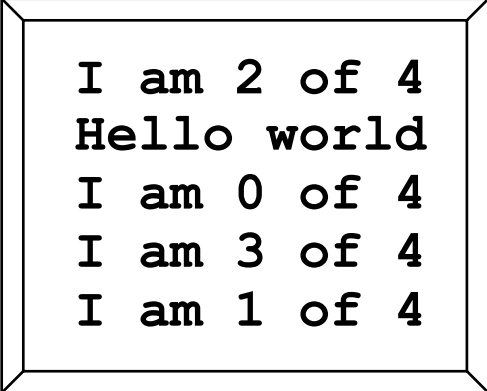
```
#include <mpi.h>
#include <stdio.h>
int main(int argc, char *argv[])
{
    int rank, size;

    MPI_Init(&argc, &argv);

    MPI_Comm_rank(MPI_COMM_WORLD, &rank);
    MPI_Comm_size(MPI_COMM_WORLD, &size);

    if (my_rank == 0)
    {
        printf ("Hello world!\n");
    }
    printf("I am process %i out of %i\n", rank, size);

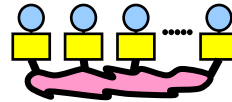
    MPI_Finalize();
}
```



```
I am 2 of 4
Hello world
I am 0 of 4
I am 3 of 4
I am 1 of 4
```

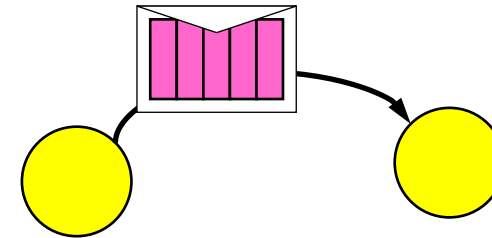

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- the MPI processes can communicate



- **nonblocking communication**


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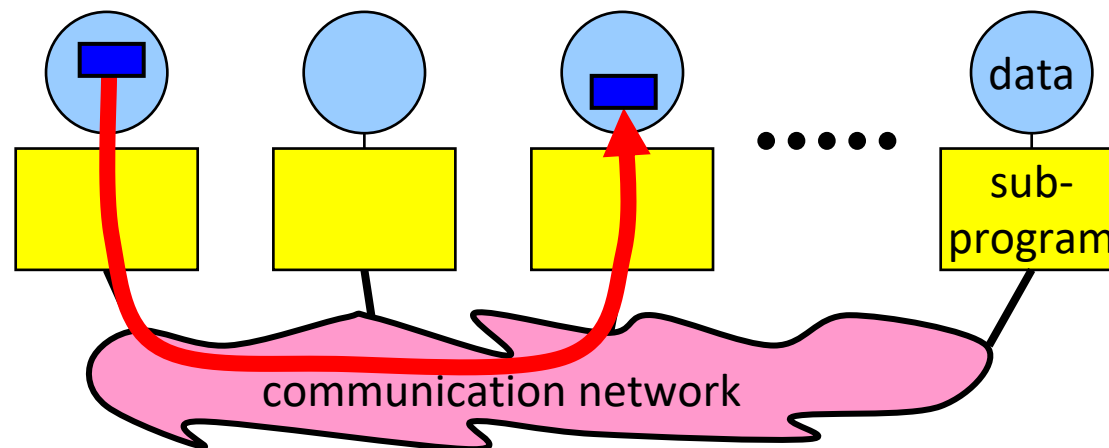


- **collective communication**

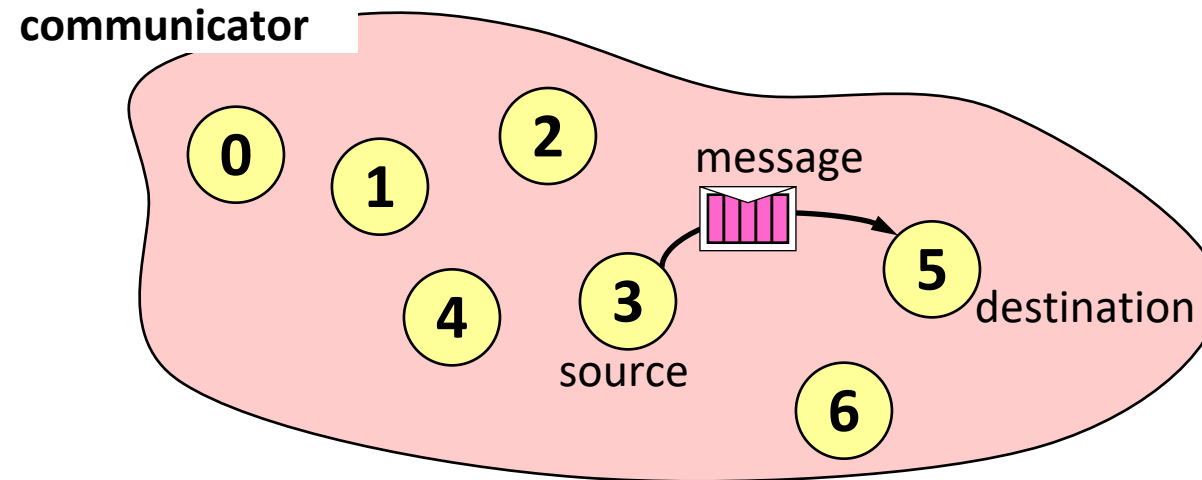
- e.g. broadcast, reduction, ...



- **messages** are packets of data moving between MPI processes
 - necessary information for the message passing system:
 - sending process
 - receiving process
 - source location
 - destination location
 - source data type
 - destination data type
 - source data size
 - destination buffer size
- } i.e., the ranks
- } 



- communication between **two** processes
- **source** process sends message to **destination** process
- communication takes place within a **communicator**, e.g., MPI_COMM_WORLD
- processes are identified by their **ranks** in the communicator



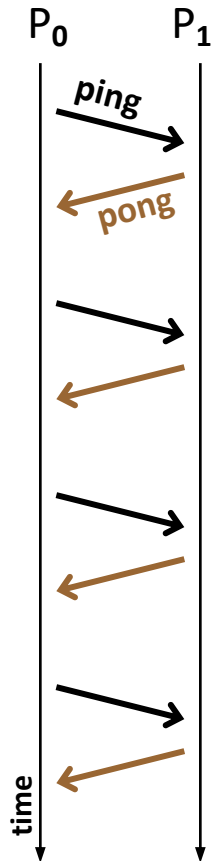
example: ping pong

```
start = MPI_Wtime();

for (i = 1; i <= 50; i++)
{
    if (my_rank == 0)
    {
        MPI_Send(buffer, 1, MPI_FLOAT, 1, 17, MPI_COMM_WORLD);
        MPI_Recv(buffer, 1, MPI_FLOAT, 1, 23, MPI_COMM_WORLD, &status);
    }
    else if (my_rank == 1)
    {
        MPI_Recv(buffer, 1, MPI_FLOAT, 0, 17, MPI_COMM_WORLD, &status);
        MPI_Send(buffer, 1, MPI_FLOAT, 0, 23, MPI_COMM_WORLD);
    }
}

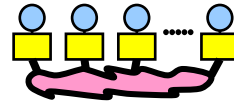
finish = MPI_Wtime();

if (my_rank == 0)
    printf("Time for one messsage: %f micro seconds.\n",
          finish - start) / (2 * 50) * 1e6 );
```



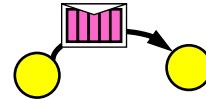
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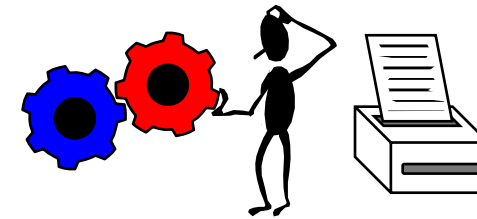
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- the MPI processes can communicate



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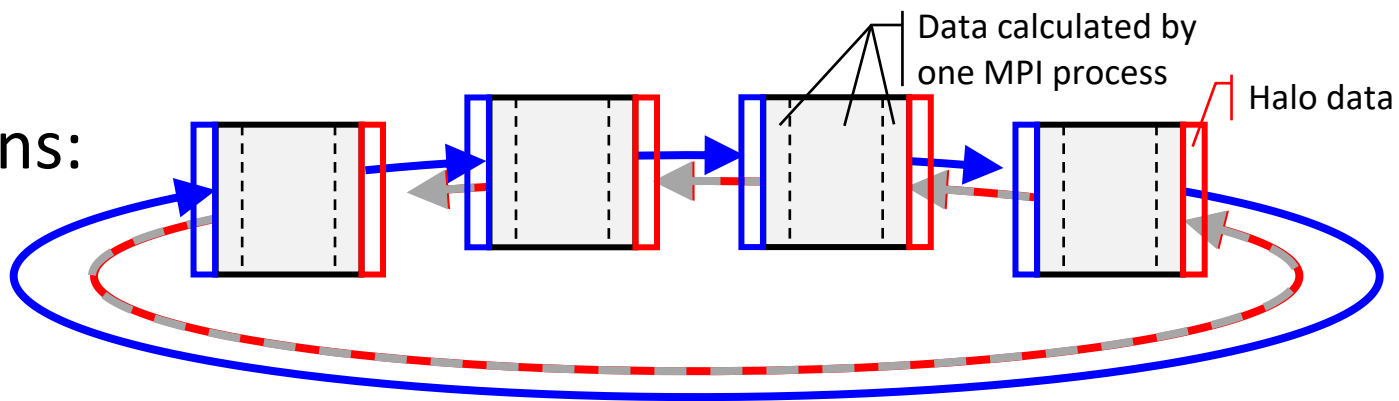
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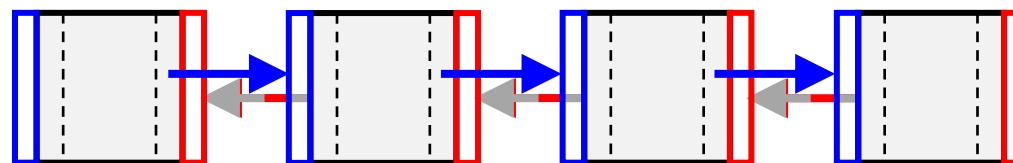


- to avoid idle times, serializations and deadlocks
- halo communication

cyclic boundary conditions:



non-cyclic boundary:

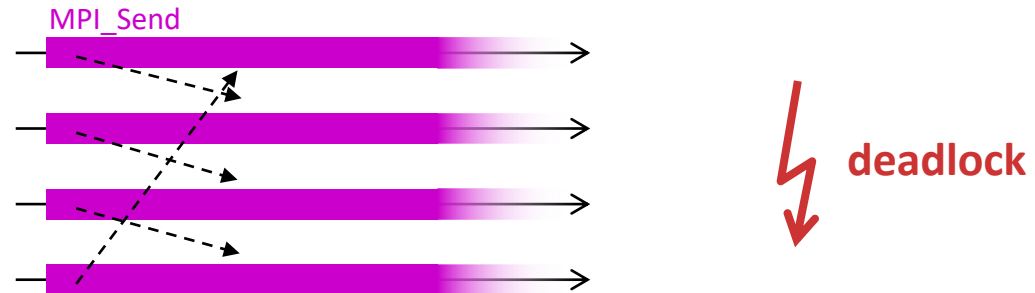


blocking → risk deadlocks & serializations

cyclic boundary:

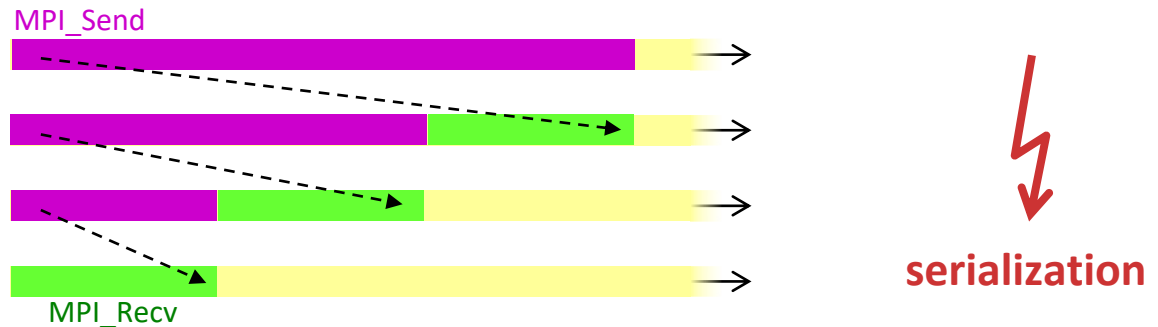
```
MPI_Send(..., right, ...)  
MPI_Recv( ..., left, ...)
```

if the MPI library chooses the synchronous protocol
timelines of all processes



non-cyclic boundary:

```
if (myrank < size-1)  
  MPI_Send(..., right, ...);  
if (myrank > 0)  
  MPI_Recv( ..., left, ...);
```

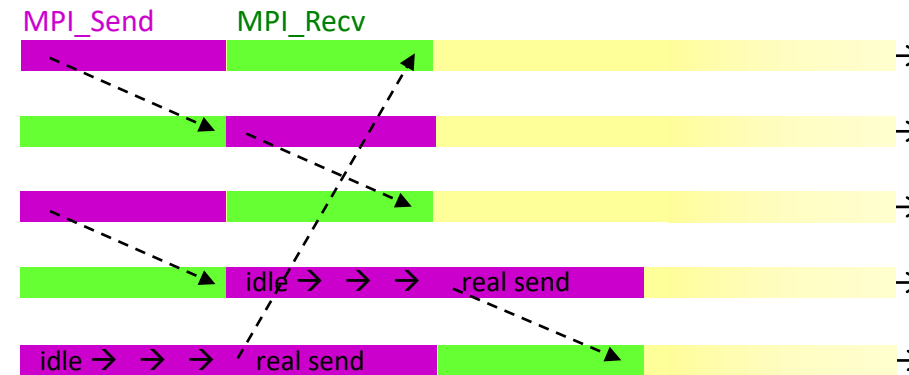
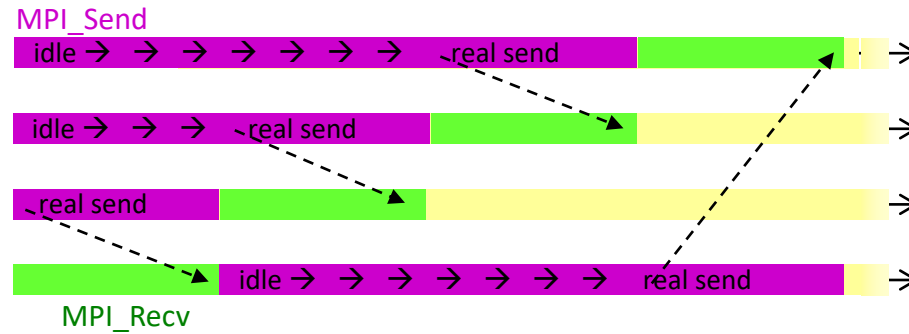


cyclic communication → other bad ideas

```
if (myrank < size-1) {  
  MPI_Send(..., right, ...);  
  MPI_Recv( ..., left, ...);  
} else {  
  MPI_Recv( ..., left, ...);  
  MPI_Send(..., right, ...);  
}
```

```
if (myrank%2 == 0) {  
  MPI_Send(..., right, ...);  
  MPI_Recv( ..., left, ...);  
} else {  
  MPI_Recv( ..., left, ...);  
  MPI_Send(..., right, ...);  
}
```

if the MPI library chooses the synchronous protocol
timelines of all processes

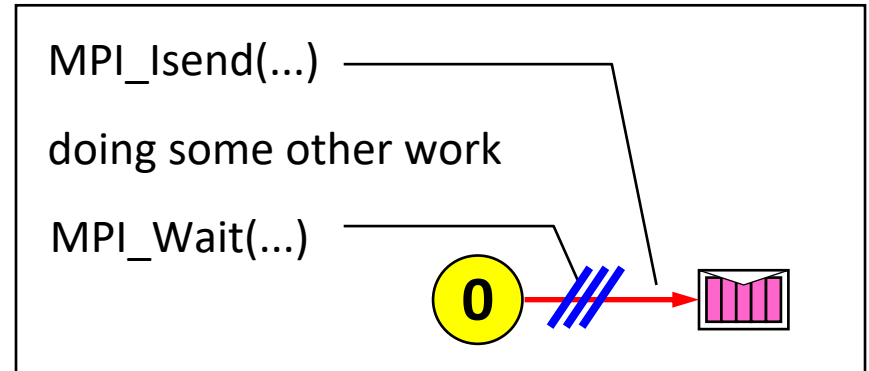



serialization



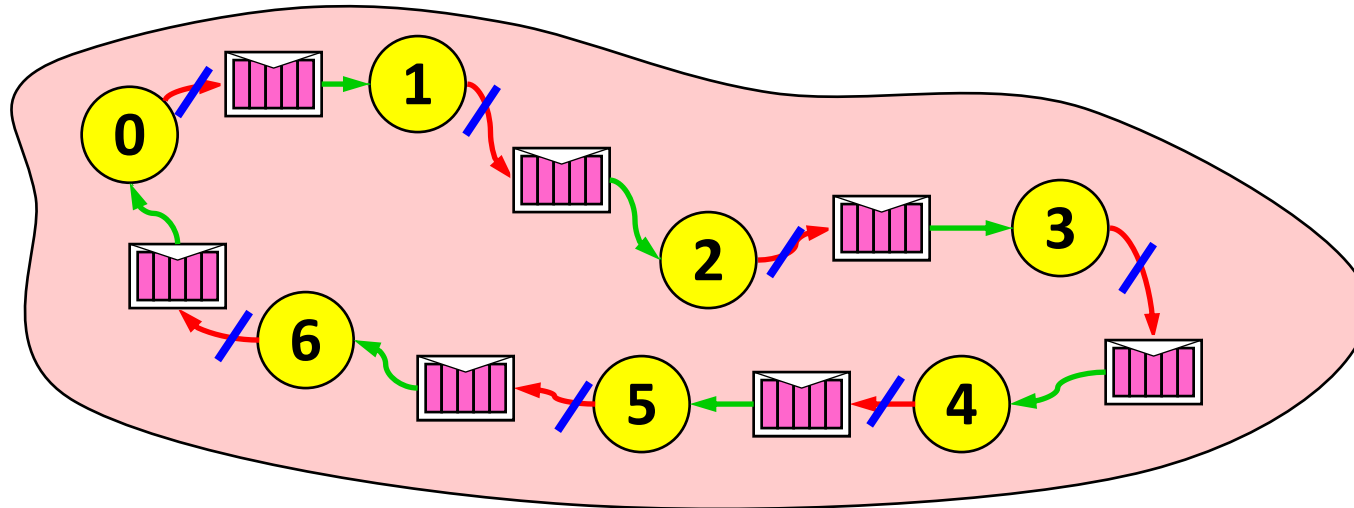
separate communication into **three phases**:

- initiate nonblocking communication
 - routine name starting with MPI_I...
 - incomplete
 - local, returns immediately, returns independently of any other process' activity
- do some work (perhaps involving other communications?)
- wait for nonblocking communication to **complete**
 - the send buffer is read out, or
 - the receive buffer is filled in

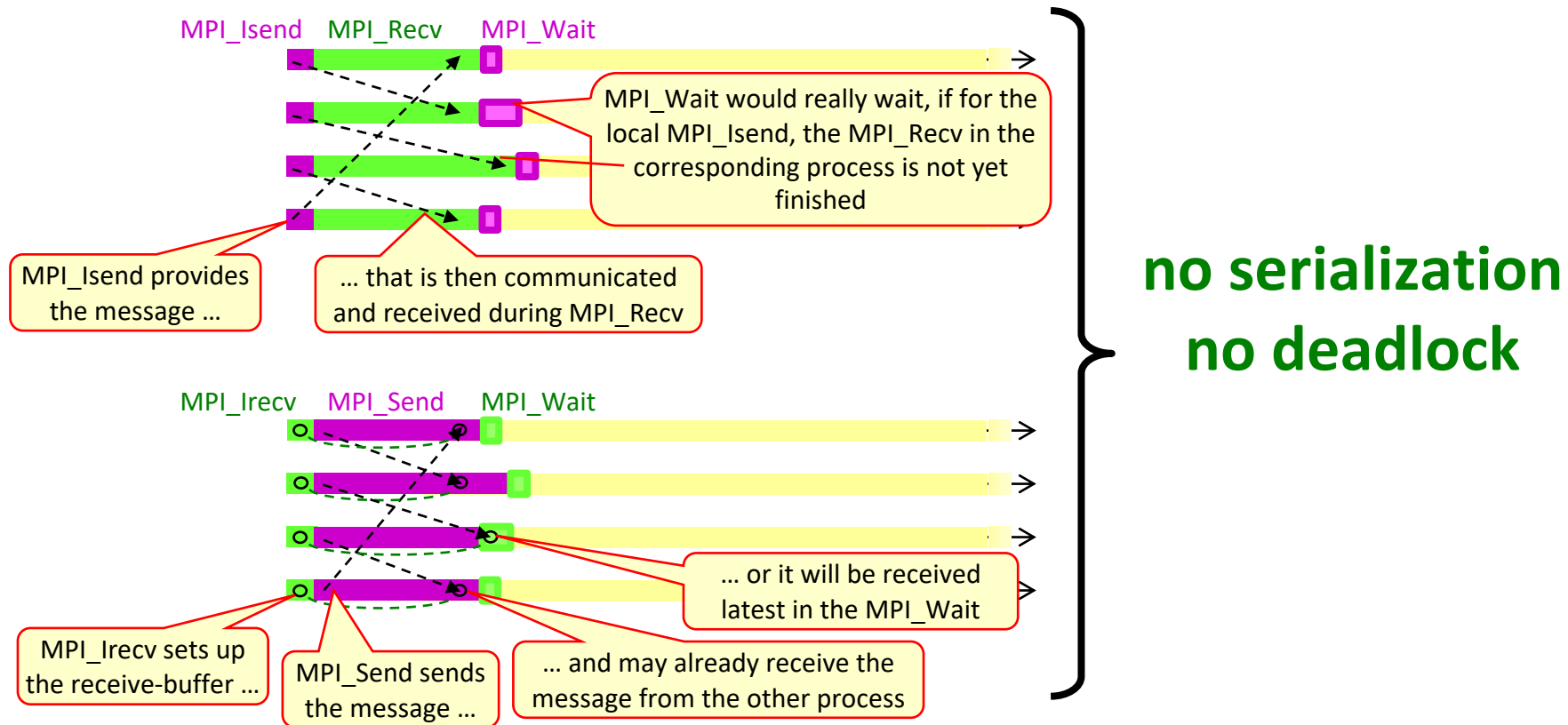


the definition of nonblocking
is clarified in
MPI-4.0
reading: [MPI-4.0/2.4](#) & [MPI-4.0/3.7](#)

- Initiate nonblocking send
 - in the ring example: Initiate nonblocking send to the right neighbor
- Do some work:
 - in the ring example: Receiving the message from left neighbor
- Now, the message transfer can be completed
- Wait for nonblocking send to complete /



nonblocking timelines



→ to avoid idle times, serializations and deadlocks

(as if overlapping of communication with other communication)

→ real overlapping of

- several communications
- communication and computation

→ other MPI features: **Send-Receive in one routine**

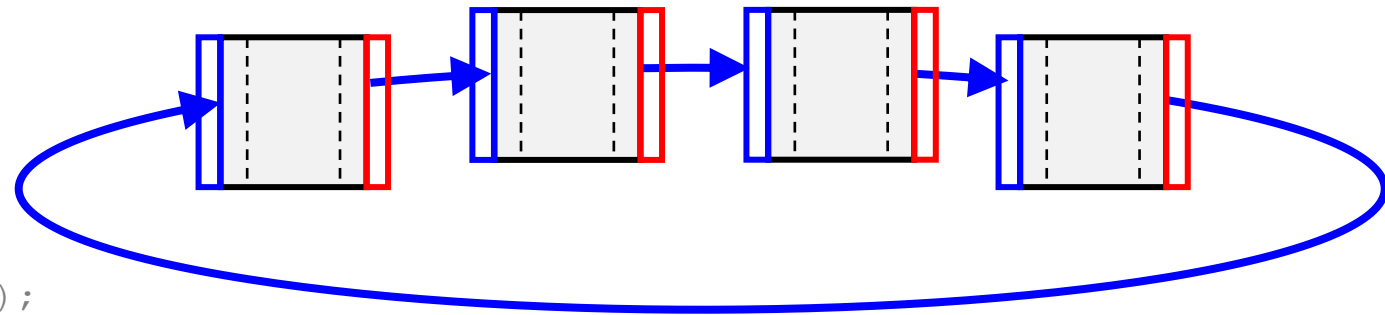
- MPI_Sendrecv & MPI_Sendrecv_replace (blocking → prevent serializations & deadlocks)
- combines the triple “MPI_Irecv + Send + Wait” into one routine
- MPI_Isendrecv & MPI_Isendrecv_replace (nonblocking → minimize idle times) ← **new MPI 4.0**

example: ring

```
int snd_buf, rcv_buf;
int right, left;
int sum, rank, size, i;
MPI_Status status;
MPI_Request request;

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

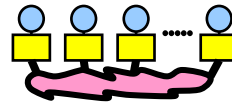
right = (rank+1) % size;
left = (rank-1+size) % size;
sum = 0;
snd_buf = rank;
for( i = 0; i < size; i++)
{
    MPI_Issend(&snd_buf, 1, MPI_INT, right, 17, MPI_COMM_WORLD, &request);
    MPI_Recv ( &rcv_buf, 1, MPI_INT, left, 17, MPI_COMM_WORLD, &status);
    MPI_Wait(&request, &status);
    snd_buf = rcv_buf;
    sum += rcv_buf;
}
printf ("PE%i:\tSum = %i\n", my_rank, sum);
MPI_Finalize();
```



Synchronous send (Issend) instead of standard send (Isend) is used only to demonstrate the use of the nonblocking routine resolves the deadlock (or serialization) problem. A real application would use standard **Isend()**.

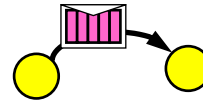
- **overview, process model and language bindings**

- one program on several processors
- work and data distribution
- starting several MPI processes



- **messages and point-to-point communication**

- the MPI processes can communicate



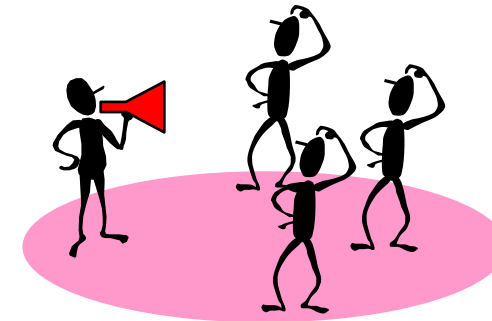
- **non-blocking communication**

- to avoid idle times, serializations, and deadlocks



- **collective communication**

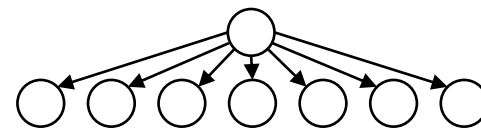
- e.g. broadcast, reduction, ...



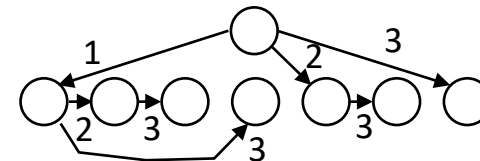
- **all processes in a communicator** processes are involved
- can be built out of point-to-point communications, but ...
- allow **optimized** internal implementations (by MPI libraries)
- examples:
 - **broadcast**, scatter, gather
 - **reduction operations** (global sum, maximum, etc.)
 - barrier synchronization (do NOT use in production code!)
 - neighbor communication in a virtual process grid

You need not to care about it !
It is the job of the MPI library !!!

Should be faster than
any programming
with point-to-point
messages!



Sequential algorithm
 $O(\# \text{ processes})$



Tree based algorithm
 $O(\log_2(\# \text{ processes}))$

example - pi serial

```
#include <time.h>
#include <stdio.h>
#include <math.h>

int main(int argc, char *argv[])
{
    int num_threads, i, n = 10000000;
    double pi, sum, h, x;
    double time, time_s, time_e;
    double PI25DT = 3.141592653589793238462643;

    num_threads = 1;

    h = 1.0 / (double)n;
    sum = 0.0;

    time_s = clock();

    for (i = 0; i < n; i++)
    {
        x = h * ((double)i + 0.5);
        sum += 4.0 / (1.0 + x*x);
    }

    pi = h * sum;

    time_e = clock();

    printf("serial, time, pi, error: %1d, %.3f, %.16f, %.16f\n",
        num_threads, ((time_e-time_s)/1e3), pi, fabs(pi-PI25DT));
}
```



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

int main(int argc, char *argv[])
{
    int rank, size, i, n = 10000000;
    double mypi, pi, sum, h, x;
    double time, time_s, time_e;
    double PI25DT = 3.141592653589793238462643;

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

    h = 1.0 / (double)n;
    sum = 0.0;
```

```
    time_s = MPI_Wtime ();

    for (i = rank; i < n; i += size )
    {
        x = h * ((double)i + 0.5);
        sum += 4.0 / (1.0 + x*x);
    }

    mypi = h * sum;
    MPI_Reduce(&mypi, &pi, 1, MPI_DOUBLE, MPI_SUM, 0, MPI_COMM_WORLD);

    time_e = MPI_Wtime ();

    if (rank == 0)
        printf ("size, time, pi, error: %02d, %.3f, %.16f, %.16f\n",
                size, ((time_e-time_s)*1e3), pi, fabs(pi-PI25DT));

    MPI_Finalize();
}
```

results - pi MPI



- `cd PI`
- `ml OpenMPI/4.1.1-GCC-10.2.0-Java-1.8.0_221`
- `vi pi_mpi.c`
- `mpicc -o pi_mpi pi_mpi.c`
- `mpirun -n 1 ./pi_mpi` → 1,2,4,8,16,32

```
size, time, pi, error: 01, 35.339, 3.1415926535897309, 0.00000000000000622
size, time, pi, error: 02, 17.625, 3.1415926535899850, 0.0000000000001918
size, time, pi, error: 04, 9.157, 3.1415926535896861, 0.0000000000001070
size, time, pi, error: 08, 4.955, 3.1415926535898069, 0.000000000000138
size, time, pi, error: 16, 2.451, 3.1415926535897931, 0.0000000000000000
size, time, pi, error: 32, 2.789, 3.1415926535897847, 0.0000000000000084
```

no standard

different options

GPU

ISO standard parallelism

OpenACC

OpenMP

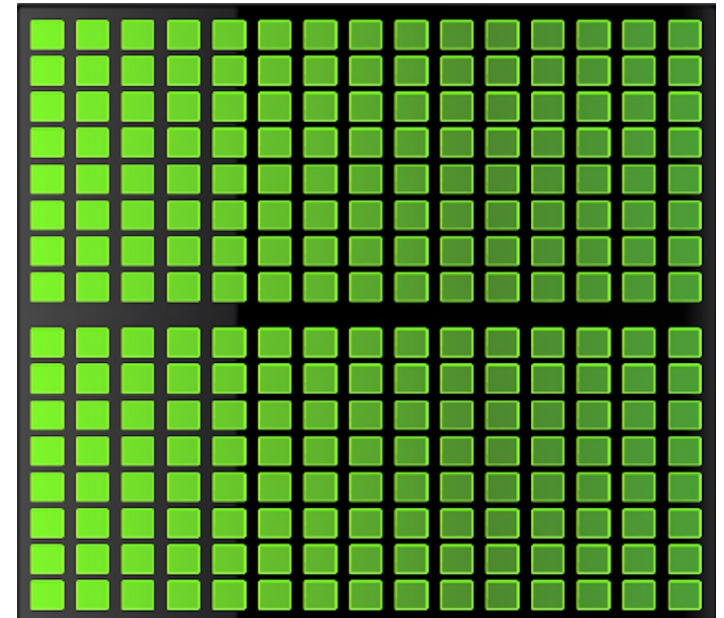
CUDA



- GPU & GPU are fundamentally different
- **CPU is a latency reducing architecture** - optimized for serial tasks
 - + very large main memory
 - + very fast clock speed
 - + latency optimized via large caches
 - + small number of threads can run very quickly
 - relatively low memory bandwidths
 - cache missed very costly
 - low performance / watt



- GPU & GPU are fundamentally different
- **GPU is all about hiding latency** - optimized for parallel tasks
 - + high-bandwidths main memory
 - + significantly more compute resources
 - + latency tolerant via parallelism
 - + high throughput
 - + high performance / watt
 - relatively low memory capacity
 - low per-thread performance



Thank you for your attention!

<http://sctrain.eu/>

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