Parallelization
programming

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Contents

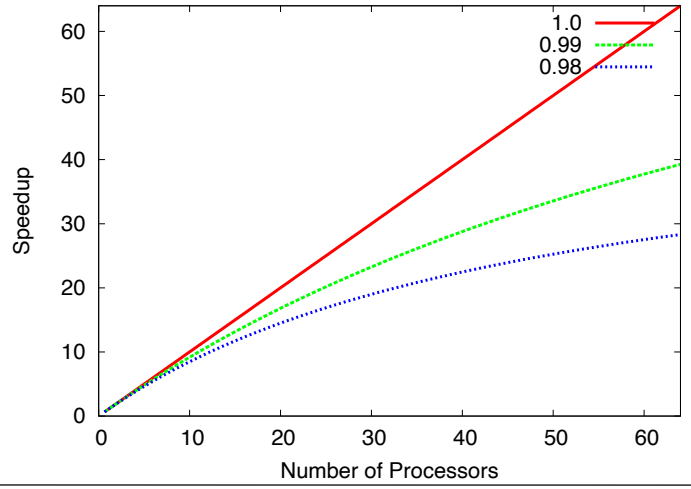
Amdahl's Law

- Describes the relation between the parallel portion of your code and the expected speedup

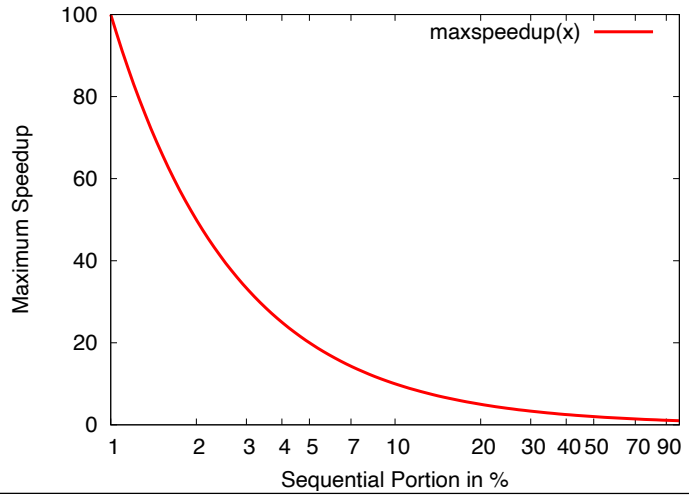
$$speedup = \frac{1}{(1-P) + \frac{P}{N}}$$

- P = parallel portion
- N = number of processors used in parallel part
- P/N is the ideal parallel speed-up, it will always be less

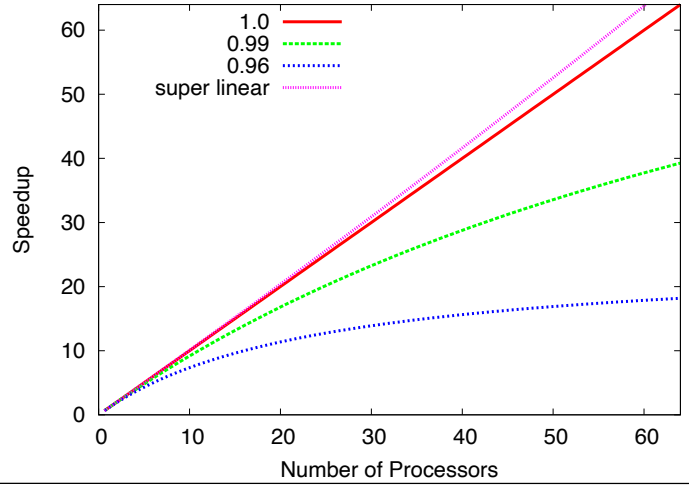
Amdahl's Law



Amdahl's Law



Super Linear speed up



Concurrency and Parallelism

- Concurrency and parallelism are often used synonymously.

  Concurrency: The independence of parts of an algorithm (= independent of each other).

  Parallelism (also parallel execution): Two or more parts of a program are executed at the same moment in time.

Concurrency is a necessary prerequisite for parallel execution
for parallel execution
but
Parallel execution is only one possible consequence of concurrency.

Concurrency vs. Parallelism

- Concurrency: two or more threads are in progress at the same time:

- Parallelism: two or more threads are executing at the same time

Multiple cores needed

Learning

Classical CPU's are sequential

There is an enormous **sequential** programming knowledge build into compilers and know by most programmers.

Parallel Programming is requiring new skills and new tools.

Start to parallelise simple problems and keep on learning along the way to complex real-world problems.

Recognizing Sequential Processes

- Time is inherently sequential
  - Dynamics and real-time, event driven applications are often difficult to parallelize effectively
    - time stepping modeling code
    - Many games fall into this category
- Iterative processes
  - The results of an iteration depend on the preceding iteration
    - conjugate gradient methods
    - Audio encoders

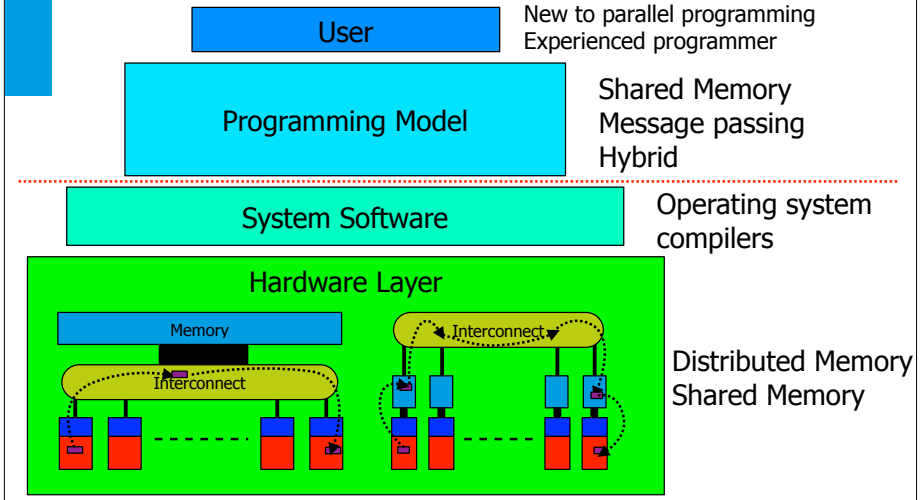
Parallel Programming Models

- Parallel programming models exist as an abstraction above hardware and memory architectures.
- Which model to use is often a combination of what is available and personal choice. There is no "best" model, although there certainly are better implementations of some models over others.

Parallel Programming Models

- Shared Memory
  - tasks share a common address space, which they read and write asynchronously.
- Threads (functional)
  - a single process can have multiple, concurrent execution paths. Example implementations: POSIX threads & OpenMP
- Message Passing
  - tasks exchange data through communications by sending and receiving messages. Example: MPI-2 specification.
- Data Parallel languages
  - tasks perform the same operation on their partition of work. Example: Co-array Fortran (CAF), Unified Parallel C (UPC), Chapel
- Hybrid

Programming Models



Parallel Programming Concepts

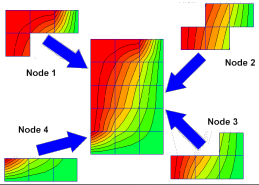
- Work distribution
  - Which parallel task is doing what?
  - Which data is used by which task?
- Synchronization
  - Do the different parallel tasks meet?
- Communication
  - Is communication between parallel parts needed?
- Load Balance
  - Does every task has the same amount of work?
  - Are all processors of the same speed?

Distributing Work and/or Data

- Work decomposition
  - based on loop counter
- Data decomposition
  - all work for a local portion of the data is done by the local processor
- Domain decomposition
  - decomposition of work and data

```
do i=1,100
  1: i=1,25
  2: i=26,50
  3: i=51,75
  4: i=76,100

A(1:10,1:25)
A(1:10,26:50)
A(11:20,1:25)
A(11:20,25:50)
```



Synchronization

```
Do i=1,100                    i=1..25 | 26..50 | 51..75 | 76..100
   a(i) = b(i)+c(i)              execute on the 4 processors
Enddo
                              BARRIER synchronization
Do i=1,100
   d(i) = 2*a(101-i)          i=1..25 | 26..50 | 51..75 | 76..100
Enddo                            execute on the 4 processors
```

- Synchronization
  - causes overhead
  - idle time, when not all tasks are finished at the same time

Communication

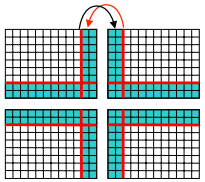
- communication is necessary on the boundaries

A(1:25)
A(26:50)
A(51:75)
A(76:100)

```
do i=2,99
   b(i) = b(i) + h*(a(i-1)-2*a(i)+a(i+1))
end do

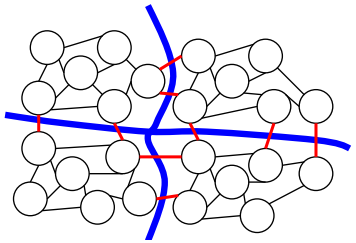
e.g. b(26) = b(26) + h*(a(25)-2*a(26)+a(27))
```

- domain decomposition



Load Imbalance

- Load imbalance is the time that some processors in the system are idle due to:
  - less parallelism than processors
  - unequal sized tasks together with too little parallelism
  - unequal processors

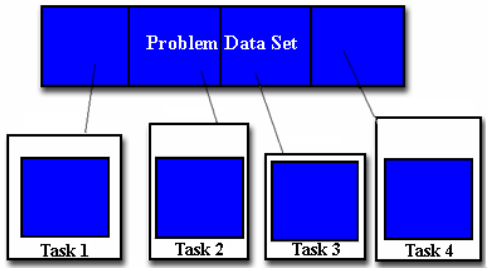


Examples of work distribution

- Domain Decomposition
- Master Worker
- Task Decomposition

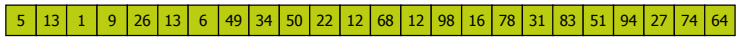
Domain Decomposition

- First, decide how data elements should be divided among processors
- Second, decide which tasks each processor should be doing



Domain Decomposition

Find the largest element of an array



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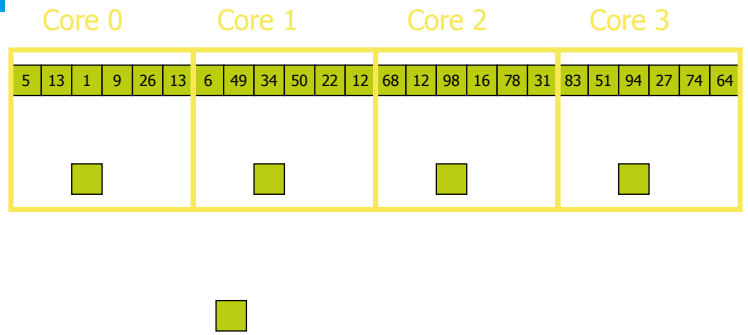

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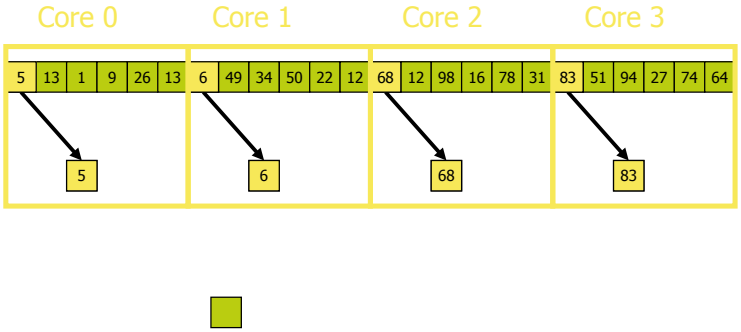

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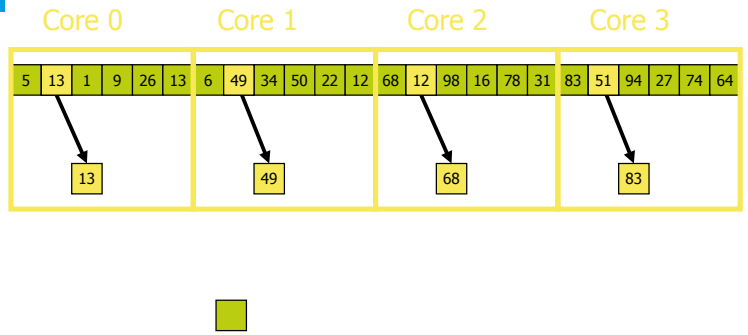

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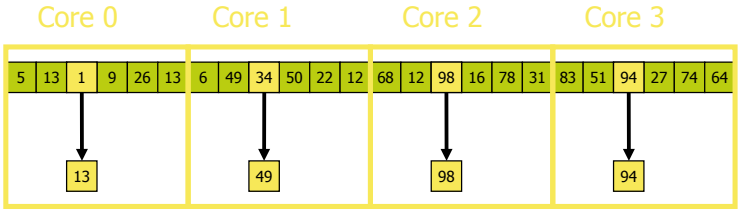

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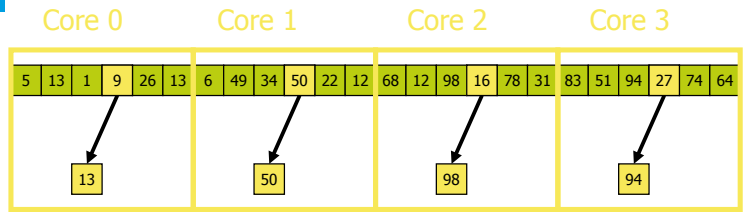

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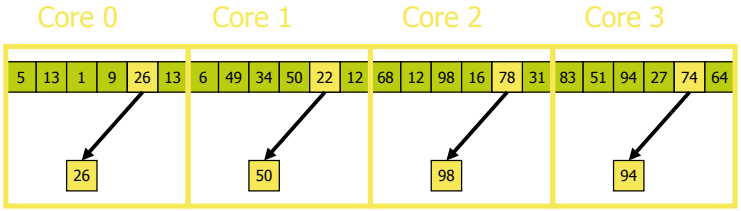

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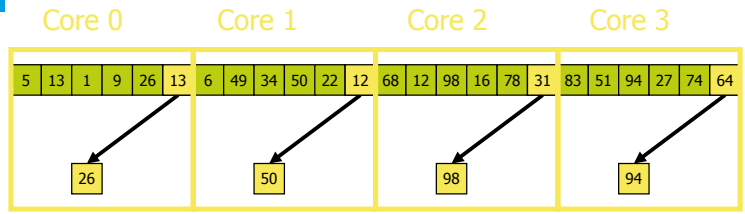

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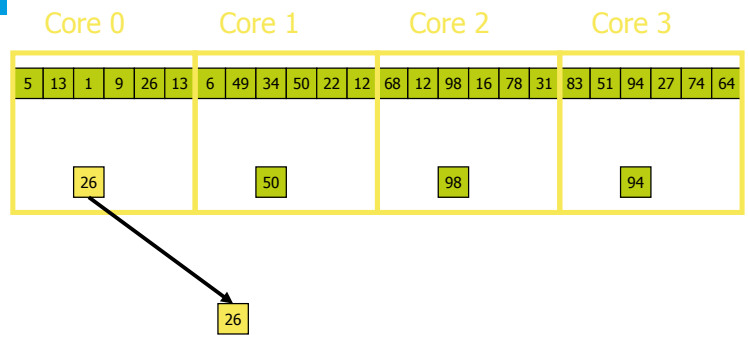
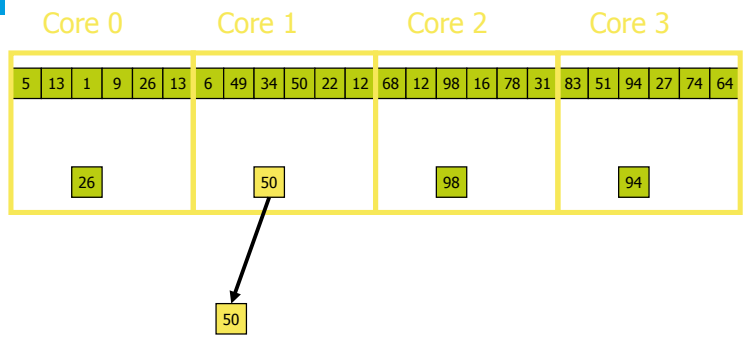


TUDelft

Domain Decomposition

Find the largest element of an array



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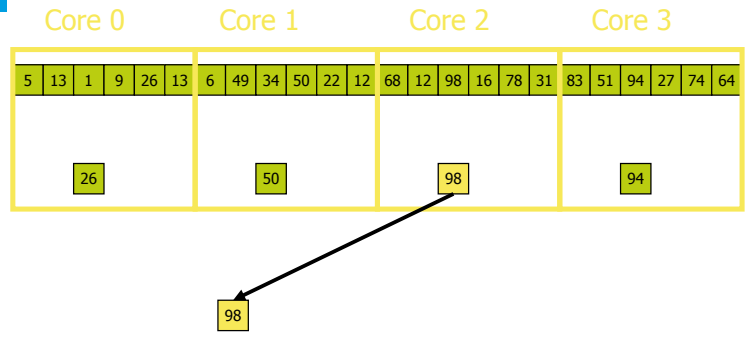
Domain Decomposition

Find the largest element of an array



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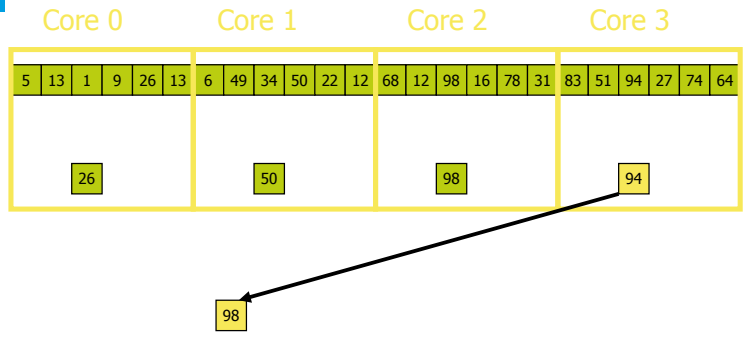

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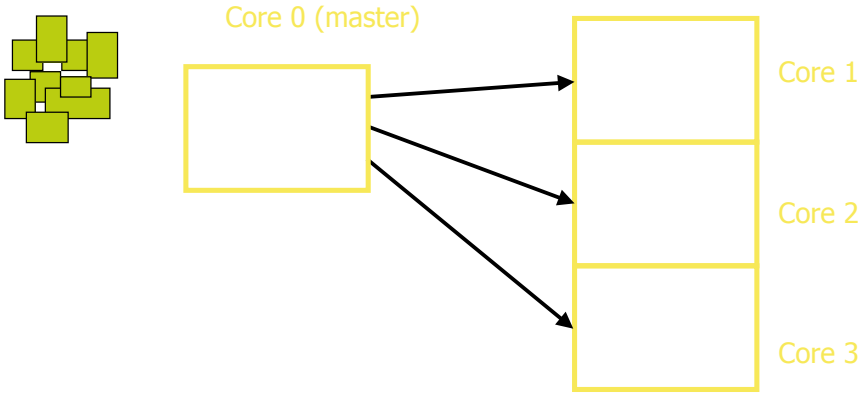
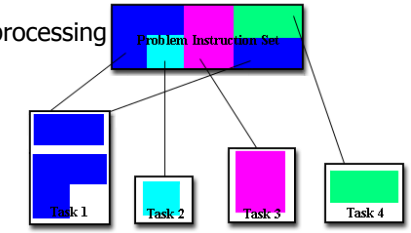
Master Worker

Get a heap of work done

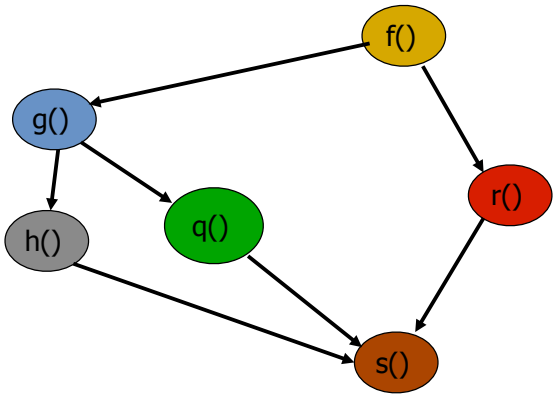


Functional Decomposition

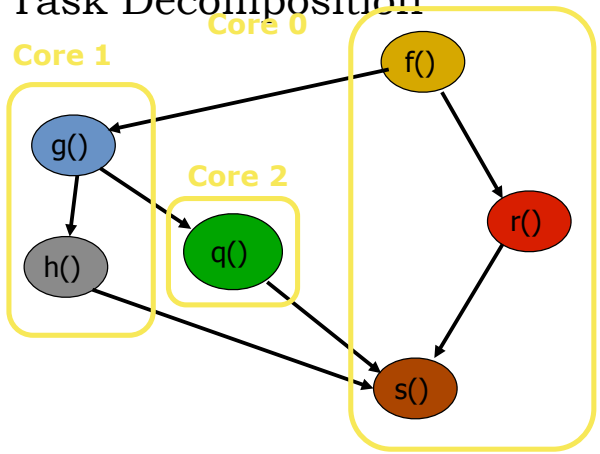
- The problem is decomposed according to the work that must be done. Each task then performs a portion of the overall work.
- Divide computation based on natural set of independent tasks
  - Assign data for each task as needed
- Example: pipeline seismic data pre-processing
  - static-correction
  - deconvolution
  - nmo correction
  - stacking
  - ....



Task/Functional Decomposition



Task Decomposition



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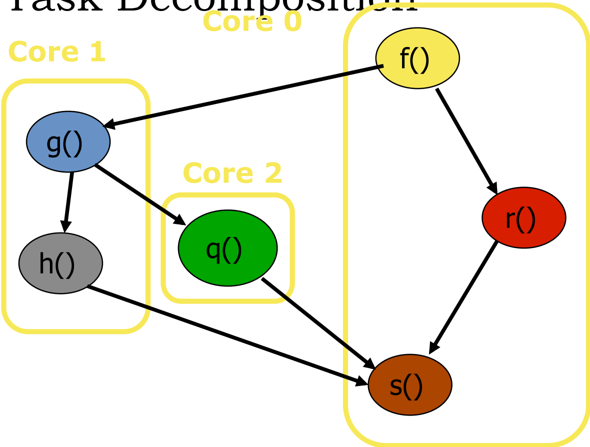

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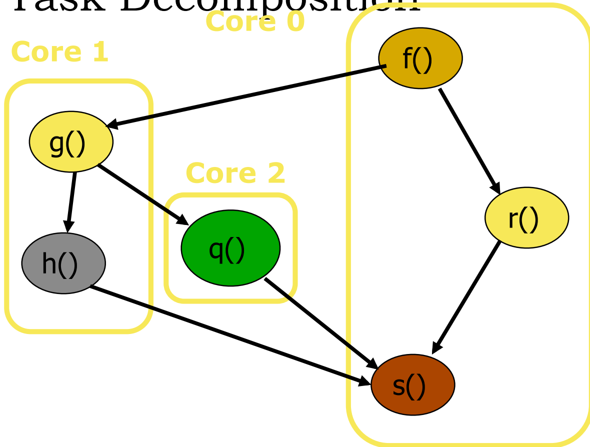
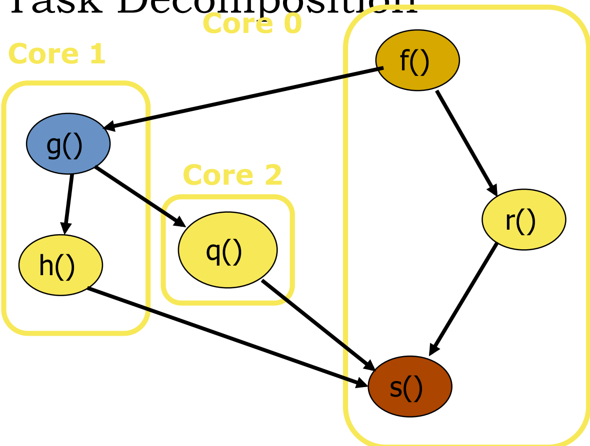


Task Decomposition



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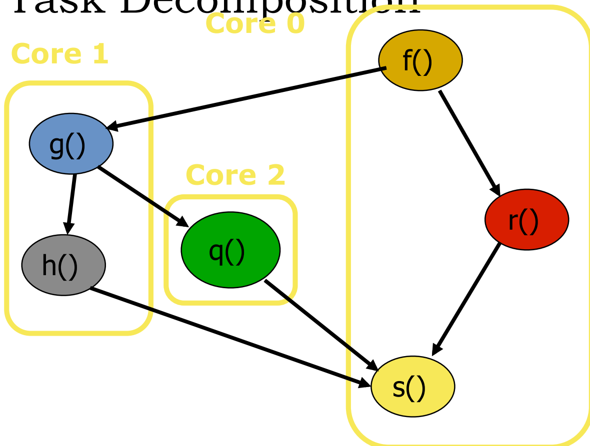
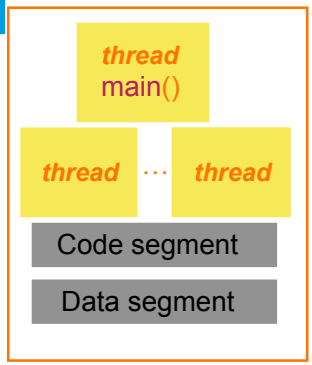


Shared Memory Parallelism

- Introduction to Threads
  - Exercise: Racecondition
- OpenMP Programming Model
  - Scope of Variables: Exercise 1
  - Synchronisation: Exercise 2
- Scheduling
  - Exercise: OpenMP scheduling
- Reduction
  - Exercise: Pi
- Shared variables
  - Exercise: CacheTrash
- Tasks
- Future of OpenMP

Processes and Threads



Modern operating systems load programs as processes
- Resource holder
- Execution

A process starts executing at its entry point as a thread

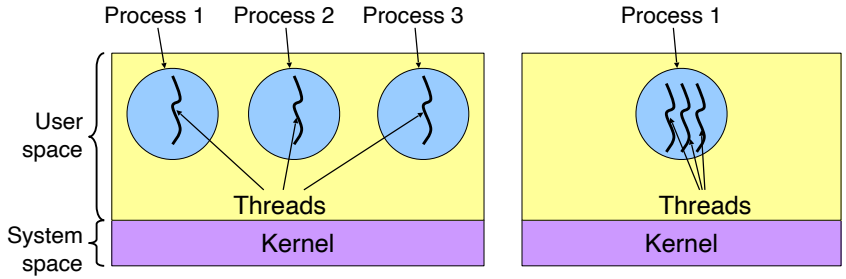
Threads can create other threads within the process

All threads within a process share code & data segments

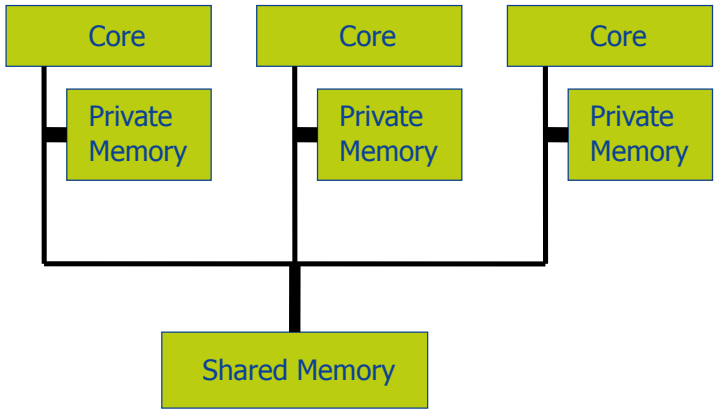
Threads have lower overhead than processes

Threads: "processes" sharing memory

- Process == address space
- Thread == program counter / stream of instructions
- Two examples
  - Three processes, each with one thread
  - One process with three threads



The Shared-Memory Model



What Are Threads Good For?

Making programs easier to understand

Overlapping computation and I/O

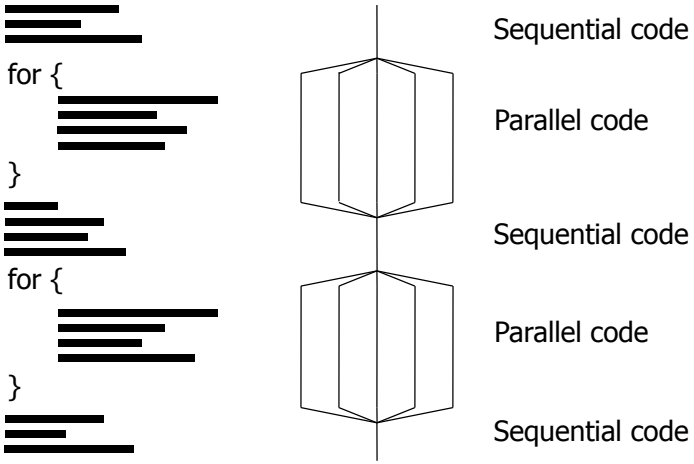
Improving responsiveness of GUIs

Improving performance through parallel execution
- with the help of OpenMP

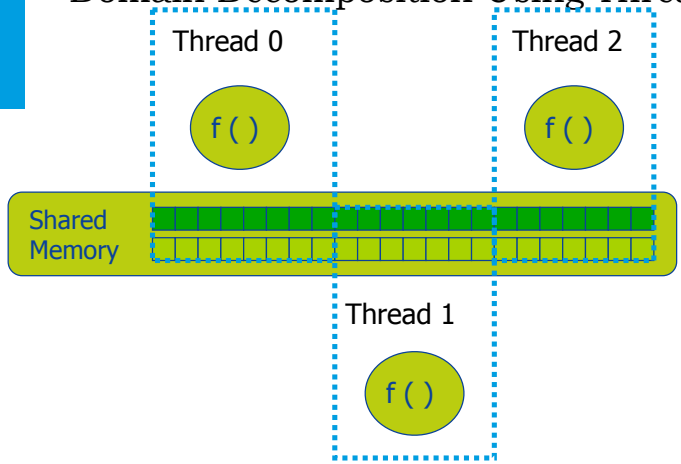
Fork/Join Programming Model

- When program begins execution, only master thread active
- Master thread executes sequential portions of program
- For parallel portions of program, master thread ***forks*** (creates or awakens) additional threads
- At ***join*** (end of parallel section of code), extra threads are suspended or die

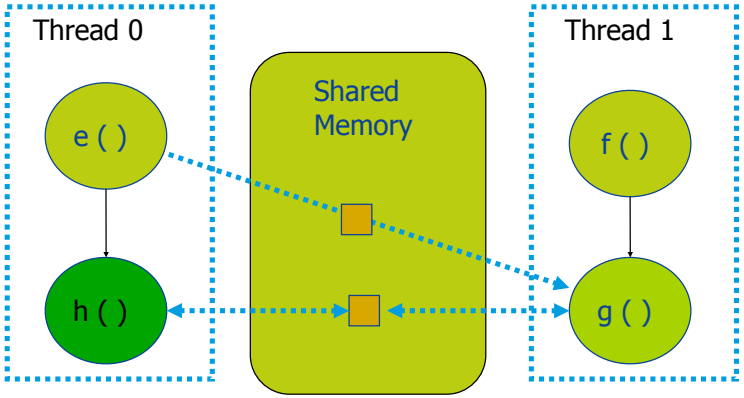
Relating Fork/Join to Code (OpenMP)



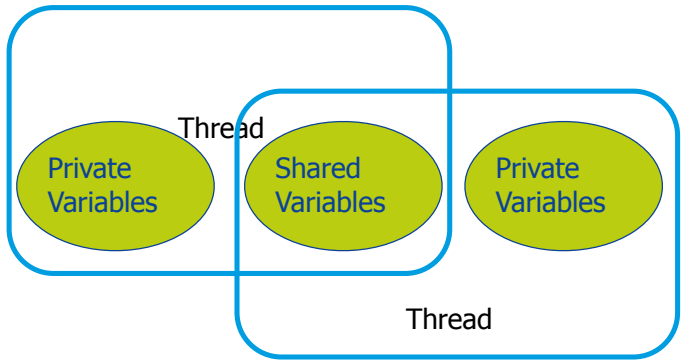
Domain Decomposition Using Threads



Task Decomposition Using Threads



Shared versus Private Variables

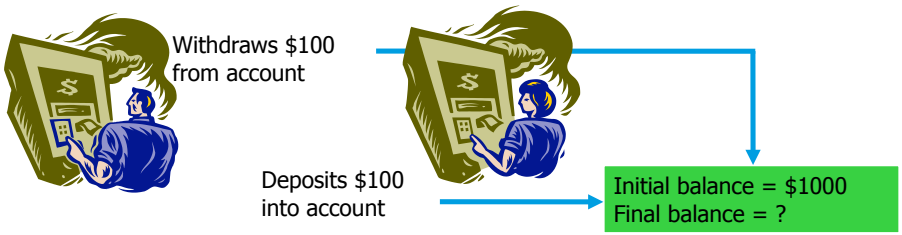


Race Conditions

Parallel threads can "race" against each other to update resources

Race conditions occur when execution order is assumed but not guaranteed

Example: un-synchronised access to bank account



Race Conditions

Time	Withdrawal	Deposit
T_0	Load (balance = $1000)	
T_1	Subtract $100	Load (balance = $1000)
T_2	Store (balance = $900)	Add $100
T_3		Store (balance = $1100)

Code Example in OpenMP exercise: HPCource/RaceCondition

```
for (i=0; i<NMAX; i++) {
    a[i] = 1;
    b[i] = 2;
}
#pragma omp parallel for shared(a,b)
for (i=0; i<12; i++) {
    a[i+1] = a[i]+b[i];
}
```

```
1: a= 1.0,  3.0,  5.0,  7.0,  9.0, 11.0, 13.0, 15.0, 17.0, 19.0, 21.0, 23.0
4: a= 1.0,  3.0,  5.0,  7.0,  9.0, 11.0, 13.0,  3.0,  5.0,  7.0,  9.0, 11.0
4: a= 1.0,  3.0,  5.0,  7.0,  9.0, 11.0, 13.0, 15.0, 17.0, 19.0, 21.0, 23.0
4: a= 1.0,  3.0,  5.0,  7.0,  9.0, 11.0, 13.0, 15.0, 17.0, 19.0, 21.0, 23.0
```


Code Example in OpenMP

```
thread    computation
0         a[1] = a[0] + b[0]
0         a[2] = a[1] + b[1]
0         a[3] = a[2] + b[2]  <--| Problem
1         a[4] = a[3] + b[3]  <--| Problem
1         a[5] = a[4] + b[4]
1         a[6] = a[5] + b[5]  <--| Problem
2         a[7] = a[6] + b[6]  <--| Problem
2         a[8] = a[7] + b[7]
2         a[9] = a[8] + b[8]  <--| Problem
3         a[10] = a[9] + b[9] <--| Problem
3         a[11] = a[10] + b[10]
```


How to Avoid Data Races

- Scope variables to be local to threads
  - Variables declared within threaded functions
  - Allocate on thread's stack
  - TLS (Thread Local Storage)
- Control shared access with critical regions
  - Mutual exclusion and synchronization
  - Lock, semaphore, event, critical section, mutex…

Examples variables

Domain Decomposition

Sequential Code:

```
int a[1000], i;
for (i = 0; i < 1000; i++) a[i] = foo(i);
```


Domain Decomposition

Sequential Code:

```
int a[1000], i;
for (i = 0; i < 1000; i++) a[i] = foo(i);
```

Thread 0:

```
for (i = 0; i < 500; i++) a[i] = foo(i);
```

Thread 1:

```
for (i = 500; i < 1000; i++) a[i] = foo(i);
```


Domain Decomposition

Sequential Code:

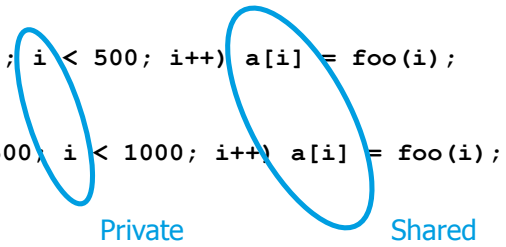
```
int a[1000], i;
for (i = 0; i < 1000; i++) a[i] = foo(i);
```

Thread 0:

```
for (i = 0; i < 500; i++) a[i] = foo(i);
```

Thread 1:

```
for (i = 500; i < 1000; i++) a[i] = foo(i);
```



Task Decomposition

```
int e;

main () {
   int x[10], j, k, m;   j = f(k);   m = g(k); ...
}

int f(int *x, int k)
{
   int a;   a = e * x[k] * x[k];   return a;
}

int g(int *x, int k)
{
   int a;   k = k-1;  a = e / x[k];   return a;
}
```

Task Decomposition

```
int e;

main () {
   int x[10], j, k, m;   j = f(k);   m = g(k);
}
```

Thread 0

```
int f(int *x, int k)
{
   int a;   a = e * x[k] * x[k];   return a;
}
```

Thread 1

```
int g(int *x, int k)
{
   int a;   k = k-1;   a = e / x[k];   return a;
}
```


Task Decomposition

`int e;` Static variable: Shared

```
main () {
   int x[10], j, k, m;   j = f(k);   m = g(k);
}
```

Thread 0

```
int f(int *x, int k)
{
   int a;   a = e * x[k] * x[k];   return a;
}
```

Thread 1

```
int g(int *x, int k)
{
   int a;   k = k-1;   a = e / x[k];   return a;
}
```


Task Decomposition

```
int e;
```

Heap variable: Shared

```
main () {
   int x[10], j, k, m;   j = f(x, k);   m = g(x, k);
}
```

Thread 0

```
int f(int *x, int k)
{
   int a;   a = e * x[k] * x[k];   return a;
}
```

Thread 1

```
int g(int *x, int k)
{
   int a;   k = k-1;   a = e / x[k];   return a;
}
```


Task Decomposition

```
int e;

main () {
   int x[10], j, k, m;   j = f(k);   m = g(k);
}
```

Function's local variables: Private

Thread 0

```
int f(int *x, int k)
{
   int a;   a = e * x[k] * x[k];   return a;
}
```

Thread 1

```
int g(int *x, int k)
{
   int a;   k = k-1;   a = e / x[k];   return a;
}
```

Shared and Private Variables

- Shared variables
  - Static variables
  - Heap variables
  - Contents of run-time stack at time of call
- Private variables
  - Loop index variables
  - Run-time stack of functions invoked by thread

What Is OpenMP?

- Compiler directives for multithreaded programming
- Easy to create threaded Fortran and C/C++ codes
- Supports data parallelism model
- Portable and Standard
- Incremental parallelism
  - ➡ Combines serial and parallel code in single source

OpenMP is not …

Not Automatic parallelization
– User explicitly specifies parallel execution
– Compiler does **not** ignore user directives even if wrong

Not just loop level parallelism
– Functionality to enable general parallel parallelism

Not a new language
– Structured as extensions to the base
– Minimal functionality with opportunities for extension

Directive based

- Directives are special comments in the language
  - Fortran fixed form: `!$OMP, C$OMP, *$OMP`
  - Fortran free form: `!$OMP`

Special comments are interpreted by OpenMP compilers

```
      w = 1.0/n
      sum = 0.0
!$OMP PARALLEL DO PRIVATE(x) REDUCTION(+:sum)
      do I=1,n
        x = w*(I-0.5)
        sum = sum + f(x)
      end do
      pi = w*sum
      print *,pi
      end
```

Comment in Fortran but interpreted by OpenMP compilers

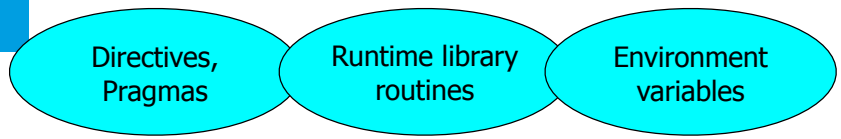
C example

`#pragma omp` directives in C

- Ignored by non-OpenMP compilers

```
  w = 1.0/n;
  sum = 0.0;
#pragma omp parallel for private(x) reduction(+:sum)
  for(i=0, i<n, i++) {
    x = w*((double)i+0.5);
    sum += f(x);
  }
  pi = w*sum;
  printf("pi=%g\n", pi);
}
```


Architecture of OpenMP



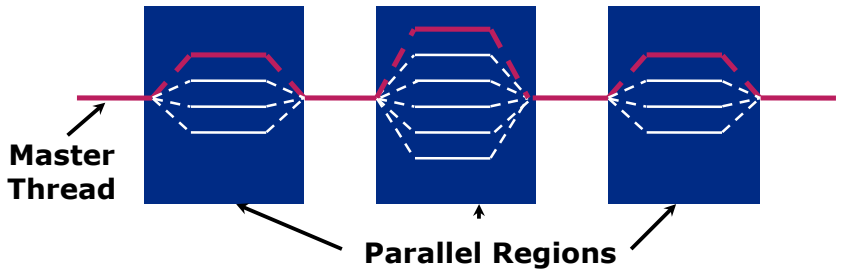
- Control structures
- Work sharing
- Synchronization
- Data scope attributes
  - private
  - shared
  - reduction
- Orphaning

- Control & query routines
  - number of threads
  - throughput mode
  - nested parallism
- Lock API

- Control runtime
  - schedule type
  - max threads
  - nested parallelism
  - throughput mode

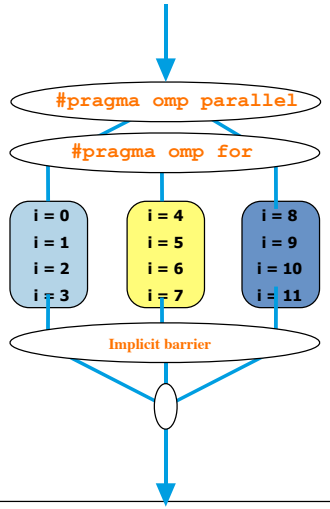
Programming Model

- Fork-join parallelism:
  - Master thread spawns a team of threads as needed
  - Parallelism is added incrementally: the sequential program evolves into a parallel program



Work-sharing Construct

```
#pragma omp parallel
#pragma omp for
   for(i = 0; i < 12; i++)
      c[i] = a[i] + b[i]
```



Threads are assigned an independent set of iterations

Threads must wait at the end of work-sharing construct

Combining pragmas

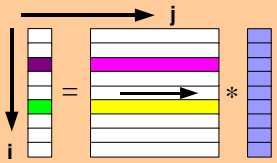
These two code segments are equivalent

```
#pragma omp parallel
{
    #pragma omp for
    for (i=0; i< MAX; i++) {
       res[i] = huge();
    }
}
```

```
#pragma omp parallel for
    for (i=0; i< MAX; i++) {
         res[i] = huge();
    }
```


Matrix-vector example

```
#pragma omp parallel for default(none) \
        private(i,j,sum) shared(m,n,a,b,c)
for (i=0; i<m; i++)
{
   sum = 0.0;
   for (j=0; j<n; j++)
     sum += b[i][j]*c[j];
   a[i] = sum;
}
```



TID = 0

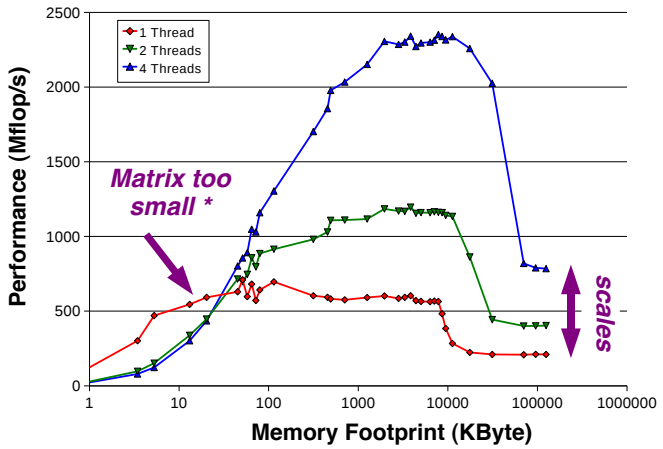
```
for (i=0,1,2,3,4)
 i = 0
 sum = Σ  b[i=0][j]*c[j]
   a[0] = sum
 i = 1
 sum = Σ  b[i=1][j]*c[j]
   a[1] = sum
```

TID = 1

```
for (i=5,6,7,8,9)
 i = 5
 sum = Σ  b[i=5][j]*c[j]
   a[5] = sum
 i = 6
 sum = Σ  b[i=6][j]*c[j]
   a[6] = sum
```

etc

Performance is matrix size dependent



OpenMP parallelization

- OpenMP Team := Master + Workers
- A Parallel Region is a block of code executed by all threads simultaneously
  - The master thread always has thread ID 0
  - Thread adjustment (if enabled) is only done before entering a parallel region
  - Parallel regions can be nested, but support for this is implementation dependent
  - An "if" clause can be used to guard the parallel region; in case the condition evaluates to "false", the code is executed serially
- A work-sharing construct divides the execution of the enclosed code region among the members of the team; in other words: they split the work

Data Environment

- OpenMP uses a shared-memory programming model
  - Most variables are shared by default.
  - Global variables are shared among threads
    C/C++: File scope variables, static
- Not everything is shared, there is often a need for "local" data as well

Data Environment

... not everything is shared...

- Stack variables in functions called from parallel regions are PRIVATE
- Automatic variables within a statement block are PRIVATE
- Loop index variables are private (with exceptions)
  C/C+: The first loop index variable in nested loops following a `#pragma omp for`

About Variables in SMP

- Shared variables
  Can be accessed by every thread thread. Independent read/write operations can take place.
- Private variables
  Every thread has it's own copy of the variables that are created/ destroyed upon entering/leaving the procedure. They are not visible to other threads.

serial code	**parallel code**
global	shared
auto local	local
static	use with care
dynamic	use with care

Data Scope clauses

attribute clauses

```
default(shared)

shared(varname,…)

private(varname,…)
```


The Private Clause

Reproduces the variable for each thread

- Variables are un-initialised; C++ object is default constructed
- Any value external to the parallel region is undefined

```
void* work(float* c, float *a, float
*x, int N)
{
  float x, y; int i;
 #pragma omp parallel for private(x,y)
     for(i=0; i<N; i++) {
       x = a[i]; y = b[i];
       c[i] = x + y;
     }
}
```


Synchronization

- Barriers `#pragma omp barrier`
- Critical sections `#pragma omp critical()`
- Lock library routines

```
omp_set_lock(omp_lock_t *lock)

omp_unset_lock(omp_lock_t *lock)

....
```


OpenMP Critical Construct

```
#pragma omp critical [(lock_name)]
```

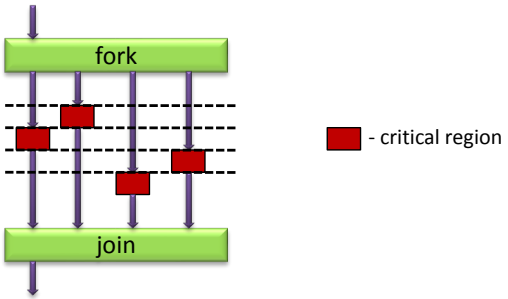
Defines a critical region on a structured block

All threads execute the code, but only one at a time. Only one calls `consum()` thereby protecting R1 and R2 from race conditions.

Naming the critical constructs is optional, but may increase performance.

```
float R1, R2;
#pragma omp parallel
{ float A, B;
#pragma omp for
  for(int i=0; i<niters; i++){
    B = big_job(i);
#pragma omp critical(R1_lock)
    consum (B, &R1);
    A = bigger_job(i);
#pragma omp critical(R2_lock)
    consum (A, &R2);
  }
}
```

OpenMP Critical

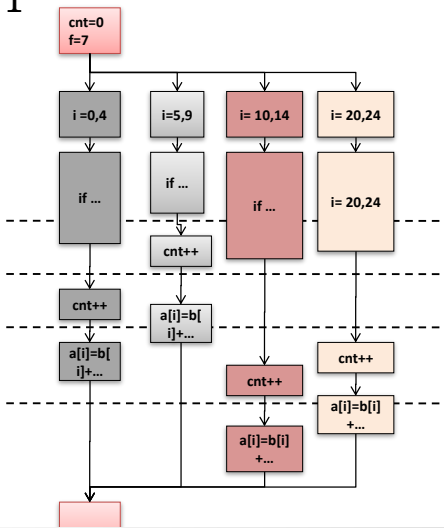


All threads execute the code, but only one at a time. Other threads in the group must wait until the current thread exits the critical region. Thus only one thread can manipulate values in the critical region.

Critical Example 1

```
cnt = 0;
f = 7;
#pragma omp parallel
{
   #pragma omp for
      for (i=0;i<20;i++){
         if(b[i] == 0){

            #pragma omp critical
               cnt ++;
          } /* end if */
          a[i]=b[i]+f*(i+1);
       } /* end for */
} /* omp end parallel */
```



Critical Example 2

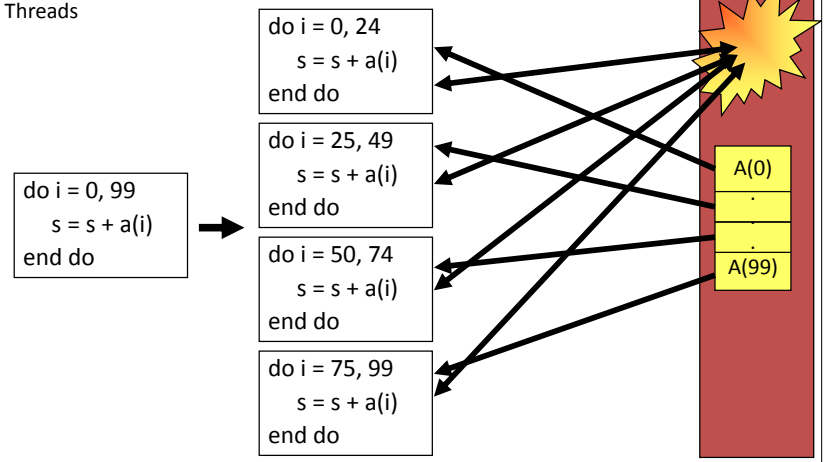
```
int i;

#pragma omp parallel for
for (i = 0; i < 100; i++) {

s = s + a[i]; }
```


Critical Example 2

Pseudo-Code
Here: 4 Threads



OpenMP Single Construct

- Only one thread in the team executes the enclosed code
- The Format is:

```
#pragma omp single [nowait][clause, ..]{
        "block"
}
```

- The supported clauses on the single directive are:

```
private (list)
firstprivate (list)
```

NOWAIT: the other threads will not wait at the end single directive

OpenMP Master directive

```
#pragma omp master {
        "code"
}
```

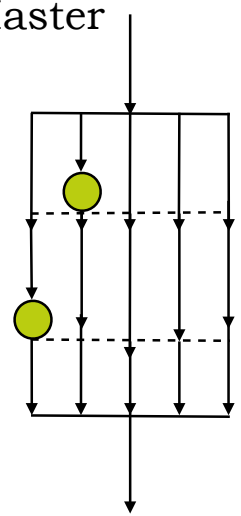
- All threads but the master, skip the enclosed section of code and continue
- There is no implicit barrier on entry or exit !

```
#pragma omp barrier
```

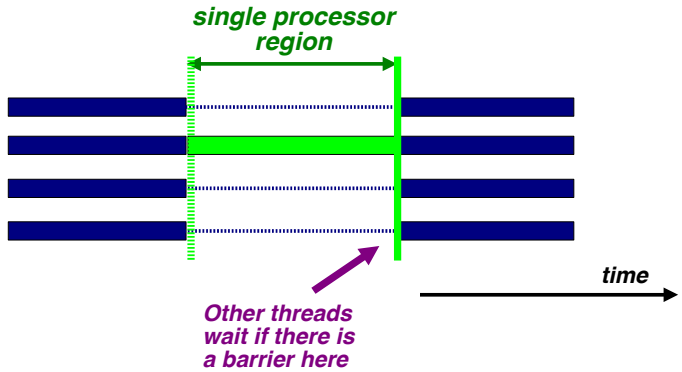
- Each thread waits until all others in the team have reached this point.

Work Sharing: Single Master

```
#pragma omp parallel
{
     ....
#pragma omp single [nowait]
{
     ....
}
#pragma omp master
{
     ....
}
     ....
#pragma omp barrier
}
```



Single processor



Work Sharing: Orphaning

- Worksharing constructs may be outside lexical scope of the parallel region

```
#pragma omp parallel
{
      ....
      dowork( )
      ....
}
 ....
```

```
void dowork( )
{
   #pragma omp for
   for (i=0; i<n; i++) {
        ....
   }
}
```


Scheduling the work

- schedule (static | dynamic | guided | auto [, chunk]) schedule (runtime)

static [, chunk]

- Distribute iterations in blocks of size "chunk" over the threads in a round-robin fashion
- In absence of "chunk", each thread executes approx. N/P chunks for a loop of length N and P threads

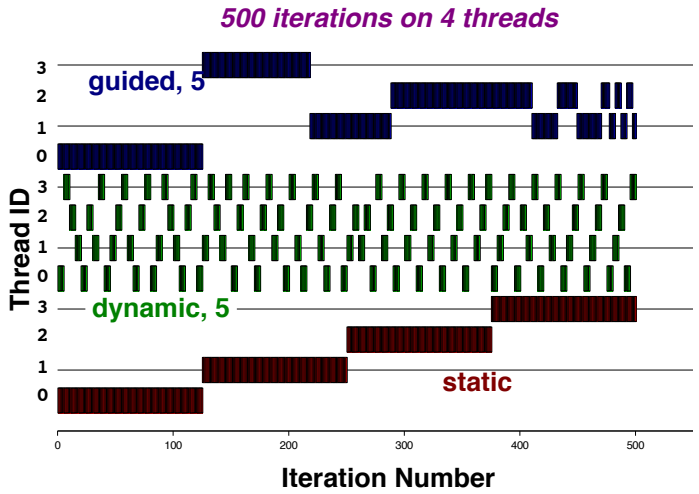
Thread	0	1	2	3
*no chunk**	1-4	5-8	9-12	13-16
chunk = 2	1-2 9-10	3-4 11-12	5-6 13-14	7-8 15-16

- **dynamic [, chunk]**
  - Fixed portions of work; size is controlled by the value of chunk
  - When a thread finishes, it starts on the next portion of work
- **guided [, chunk]**
  - Same dynamic behavior as "dynamic", but size of the portion of work decreases exponentially

runtime

- Iteration scheduling scheme is set at runtime through environment variable OMP_SCHEDULE

Example scheduling



Environment Variables

- The names of the OpenMP environment variables must be UPPERCASE
- The values assigned to them are case insensitive

```
OMP_NUM_THREADS

OMP_SCHEDULE "schedule [chunk]"

OMP_NESTED { TRUE | FALSE }
```


Exercise: OpenMP scheduling

- How OpenMP can help parallelize a loop, but as a user you can help in making it better ;-)
- On the git clone: cd HPCourse/OMP_schedule
- The README has instructions:
  This works best with an Intel compiler that uses an auto-parallelizer to generate threaded code
- This exercise requires already some knowledge about OpenMP.
  The OpenMP website at
  https://www.openmp.org/
  can be helpful to get started.

OpenMP Reduction Clause

```
reduction (op : list)
```

The variables in "*list*" must be shared in the enclosing parallel region

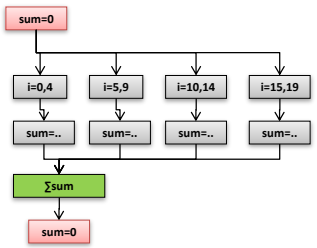
Inside parallel or work-sharing construct:

- A PRIVATE copy of each list variable is created and initialized depending on the "op"
- These copies are updated locally by threads
- At end of construct, local copies are combined through "op" into a single value and combined with the value in the original SHARED variable

Reduction Example

```
#pragma omp parallel for
reduction(+:sum)
   for(i=0; i<N; i++) {
     sum += a[i] * b[i];
   }
```

Local copy of *sum* for each thread
All local copies of *sum* added together and stored in "global" variable



C/C++ Reduction Operations

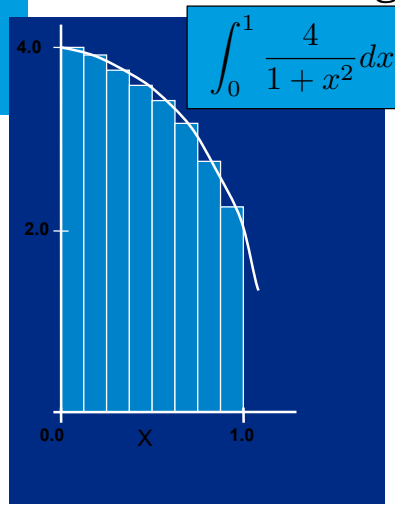
A range of associative and commutative operators can be used with reduction
Initial values are the ones that make sense

Operator	Initial Value
+	0
*	1
-	0
^	0

Operator	Initial Value
&	~0
|	0
&&	1
||	0

FORTRAN:
intrinsic is one of MAX, MIN, IAND, IOR, IEOR
operator is one of +, *, -, .AND., .OR., .EQV., .NEQV.

Numerical Integration Example



$$\int_0^1 \frac{4}{1+x^2} dx = \pi$$

```
static long num_steps=100000;
double step, pi;

void main()
{  int i;
   double x, sum = 0.0;

   step = 1.0/(double) num_steps;
   for (i=0; i<num_steps; i++){
      x = (i+0.5)*step;
      sum = sum + 4.0/(1.0 + x*x);
   }
   pi = step * sum;
   printf("Pi = %f\n",pi);
}
```


Numerical Integration to Compute Pi

```
static long num_steps=100000;
double step, pi;

void main()
{  int i;
   double x, sum = 0.0;

   step = 1.0/(double) num_steps;
   for (i=0; i<num_steps; i++){
      x = (i+0.5)*step;
      sum = sum + 4.0/(1.0 + x*x);
   }
   pi = step * sum;
   printf("Pi = %f\n",pi);
}
```

Parallelize the numerical integration code using OpenMP

What variables can be shared?

`step, num_steps`

What variables need to be private?

`x, i`

What variables should be set up for reductions?

`sum`

Solution to Computing Pi

```
static long num_steps=100000;
double step, pi;

void main()
{  int i;
   double x, sum = 0.0;
   step = 1.0/(double) num_steps;
#pragma omp parallel for private(x) reduction(+:sum)
   for (i=0; i<num_steps; i++){
      x = (i+0.5)*step;
      sum = sum + 4.0/(1.0 + x*x);
   }
   pi = step * sum;
   printf("Pi = %f\n",pi);
}
```

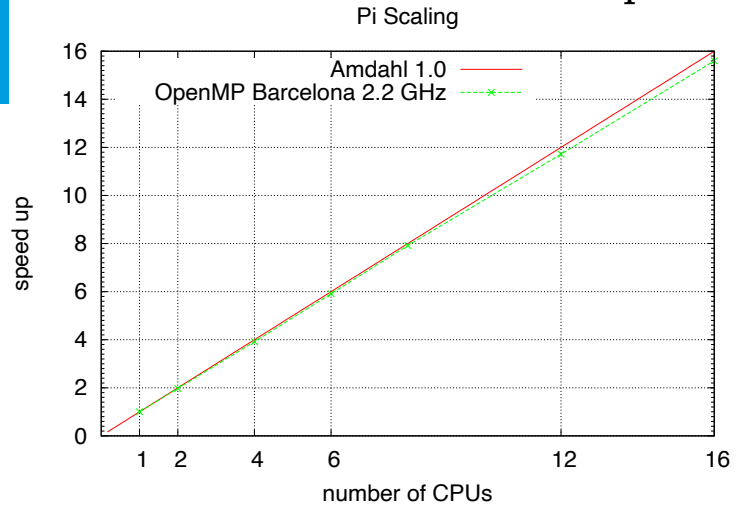
Let's try it out

- Go to example MPI_pi and will work with openmp_pi2.c

Exercise: PI with MPI and OpenMP

cores	OpenMP
1	9.617728
2	4.874539
4	2.455036
6	1.627149
8	1.214713
12	0.820746
16	0.616482

Exercise: PI with MPI and OpenMP



Cuda Computing PI

```
float step = 1.0f / (float)NSET;
float sum = 0.0f;

PiSimple2<<<GRIDDIM, BLOCKDIM>>>
    (d_partials, step, NSET);
CUT_CHECK_ERROR("***PiSimple2
    execution failed!!!***");



CUDA_SAFE_CALL(cudaMemcpy(h_partia
    ls, d_partials,
    fSmallArraySize,
    cudaMemcpyDeviceToHost) );

for (j = 0; j < GRIDDIM; j++)
{
    sum += h_partials[j];
}
Pi = step * sum;
```

```
__global__ void
PiSimple2( float* g_partialOut, float step,
    int NSamples)
{
  const int tid = blockDim.x * blockIdx.x +
    threadIdx.x;
  const int blocksize = blockDim.x;
  const int THREAD_N = blockDim.x * gridDim.x;
  float x, partialsum = 0.0f;

for(int i = tid; i < NSamples; i += THREAD_N){
      x = (i * 0.5f)*step;
      partialsum = partialsum + 4.0f / (1.0f
                  + x*x);
  }

 __shared__  float threadsum[BLOCKDIM];
threadsum[threadIdx.x] = partialsum;

  __syncthreads();
  float blocksum = 0;
  if (threadIdx.x == 0)   {
    const int blockindex = blockIdx.x;
    for (int i = 0; i < blocksize; i++)
        blocksum += threadsum[i];
    g_partialOut[blockindex] = blocksum;
  }
}
```

Exercise: Shared Cache Trashing

- Let's do the exercise: CacheTrash

About local and shared data

- Consider the following example:

```
for (i=0; i<10; i++){
    a[i] = b[i] + c[i];
}
```

- Let's assume we run this on 2 processors:
  - processor 1 for i=0,2,4,6,8
  - processor 2 for i=1,3,5,7,9

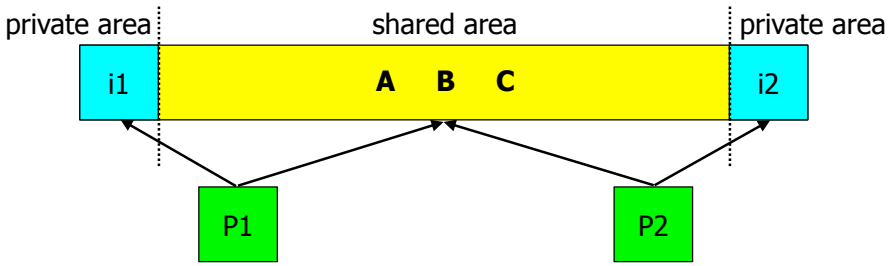
About local and shared data

Processor 1

```
for (i1=0,2,4,6,8){
    a[i1] = b[i1] + c[i1];
}
```

Processor 2

```
for (i2=1,3,5,7,9){
    a[i2] = b[i2] + c[i2];
}
```



About local and shared data

processor 1 for i=0,2,4,6,8
processor 2 for i=1,3,5,7,9

- This is not an efficient way to do this!

Why?

Doing it the bad way

- Because of cache line usage

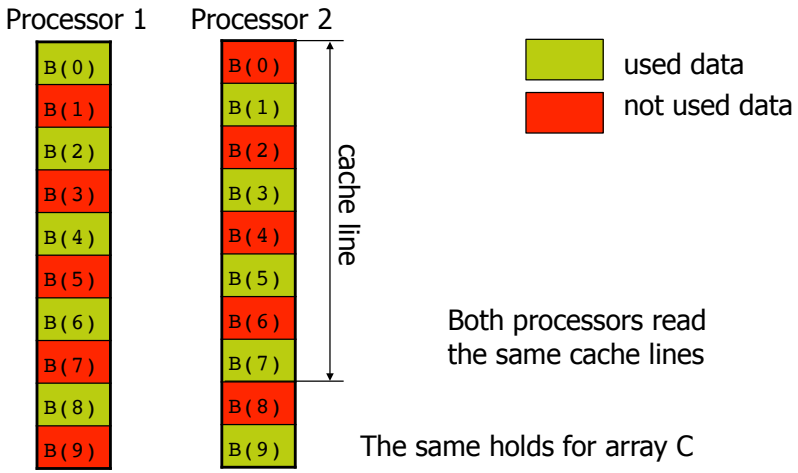
```
for (i=0; i<10; i++){
    a[i] = b[i] + c[i];
}
```

- b[] and c[]: we use half of the data
- a[]: false sharing

False sharing and scalability

- The Cause:
  Updates on independent data elements that happen to be part of the same cache line.
- The Impact:
  Non-scalable parallel applications
- The Remedy:
  False sharing is often quite simple to solve

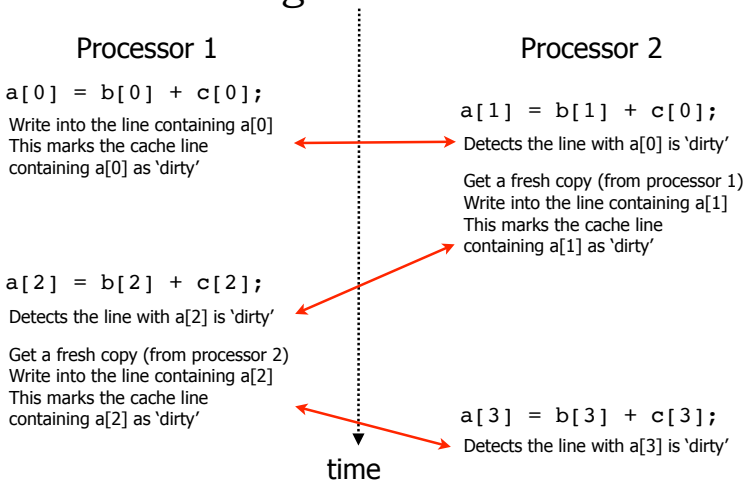
Poor cache line utilization



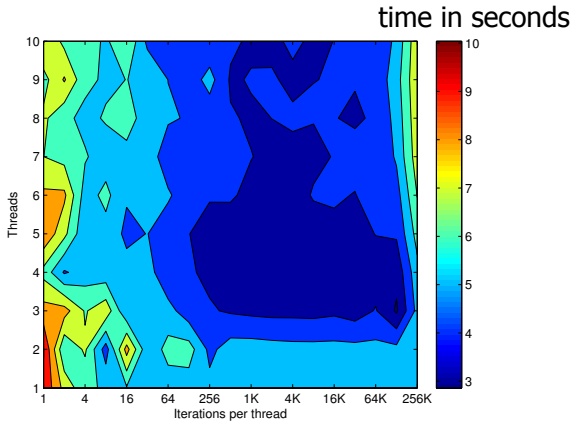
Both processors read the same cache lines

The same holds for array C

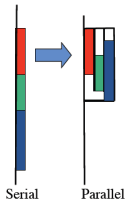
False Sharing



False Sharing results



OpenMP tasks



- What are tasks
  - Tasks are independent units of work
  - Threads are assigned to perform the work of each task.
    - Tasks may be deferred
    - Tasks may be executed immediately
    - The runtime system decides which of the above
- Why tasks?
  - The basic idea is to set up a task queue: when a thread encounters a task directive, it arranges for some thread to execute the associated block at some time. The first thread can continue.

The Tasking Example

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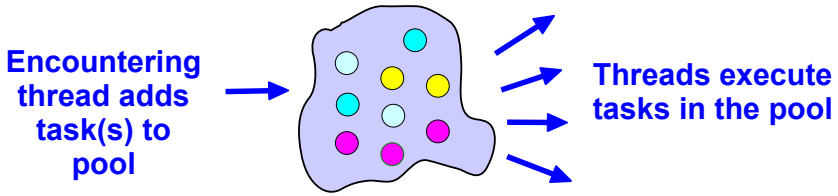


Developer specifies tasks in application
Run-time system executes tasks

OpenMP tasks

Tasks allow to parallelize irregular problems
- Unbounded loops
- Recursive algorithms
- Manger/work schemes

A task has
- Code to execute
- Data environment (It owns its data)
- Internal control variables
- An assigned thread that executes the code and the data

OpenMP has always had tasks, but they were not called "task".

– A thread encountering a parallel construct, e.g., "for", packages up a set of implicit tasks, one per thread.
– A team of threads is created.
– Each thread is assigned to one of the tasks.
– Barrier holds master thread till all implicit tasks are finished.

OpenMP tasks

```
#pragma omp parallel -> A parallel region creates a team of threads;
#pragma omp single
{
  ...                -> One thread enters the execution
#pragma omp task
  { ... }            -> pick up threads „from the work queue"
  …
#pragma omp taskwait
}                    -> the other threads wait at the end of the single
```


Summary

- First tune single-processor performance
- Tuning parallel programs
  - Has the program been properly parallelized?
    - Is enough of the program parallelized (Amdahl's law)?
    - Is the load well-balanced?
  - location of memory
    - Cache friendly programs: no special placement needed
    - Non-cache friendly programs
      - False sharing?
  - Use of OpenMP
    - try to avoid synchronization (`barrier, critical, single, ordered`)

Plenty of Other OpenMP Stuff

Scheduling clauses

Atomic

Barrier

Master & Single

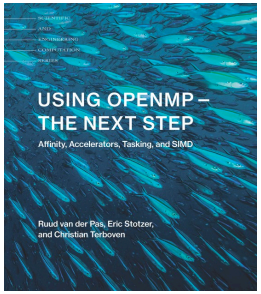
Sections

Tasks (OpenMP 3.0)

API routines

OpenMP references

https://mitpress.mit.edu/books/using-openmp-next-step



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Compiling and running OpenMP

- Compile with -openmp flag (intel compiler) or -fopenmp (GNU)
- Run program with variable:

```
export OMP_NUM_THREADS=4
```

OpenACC

- Set of directives to support accelerators
  - Developed by PGI and HPE-Cray:
  - Used to support all vendors: PGI now part of Nvidia
  - Intel's MIC's not supported anymore
  - AMD Fusions processors: only support by HPE-Cray
- OpenMP 5.0 also aims at GPU's and real open standards
  - might replace OpenACC in the future.
  - not yet same compiler support of all vendors: Intel? AMD?

OpenACC example

```
void convolution_SM_N(typeToUse A[M][N], typeToUse B[M][N]){
        int i, j, k;
        int m=M, n=N;
        // OpenACC kernel region
        // Define a region of the program to be compiled into a sequence of kernels
        // for execution on the accelerator device
        #pragma acc kernels pcopyin(A[0:m]) pcopy(B[0:m])
        {
          typeToUse c11, c12, c13, c21, c22, c23, c31, c32, c33;

          c11 = +2.0f;  c21 = +5.0f;  c31 = -8.0f;
          c12 = -3.0f;  c22 = +6.0f;  c32 = -9.0f;
          c13 = +4.0f;  c23 = +7.0f;  c33 = +10.0f;

          // The OpenACC loop gang clause tells the compiler that the iterations of the loops
          // are to be executed in parallel across the gangs.
          // The argument specifies how many gangs to use to execute the iterations of this loop.
          #pragma acc loop gang(64)
          for (int i = 1; i < M - 1; ++i) {

          // The OpenACC loop worker clause specifies that the iteration of the associated loop are
      to be
          // executed in parallel across the workers within the gangs created.
          // The argument specifies how many workers to use to execute the iterations of this loop.
              #pragma acc loop worker(128)
              for (int j = 1; j < N - 1; ++j){
                  B[i][j] = c11 * A[i - 1][j - 1]  +  c12 * A[i + 0][j - 1]  +  c13 * A[i + 1][j - 1]
                    +       c21 * A[i - 1][j + 0]  +  c22 * A[i + 0][j + 0]  +  c23 * A[i + 1][j + 0]
                    +       c31 * A[i - 1][j + 1]  +  c32 * A[i + 0][j + 1]  +  c33 * A[i + 1][j +
      1];
              }
          }
        }//kernels region
      }
```

MPI

Message Passing

- Point-to-Point
- Requires explicit commands in program
  - Send, Receive
- Must be synchronized among different processors
  - Sends and Receives must match
  - Avoid Deadlock -- all processors waiting, none able to communicate
- Multi-processor communications
  - e.g. broadcast, reduce

MPI advantages

- Mature and well understood
  - Backed by widely-supported formal standard (1992)
  - Porting is "easy"
- Efficiently matches the hardware
  - Vendor and public implementations available
- User interface:
  - Efficient and simple
  - Buffer handling
  - Allow high-level abstractions
- Performance

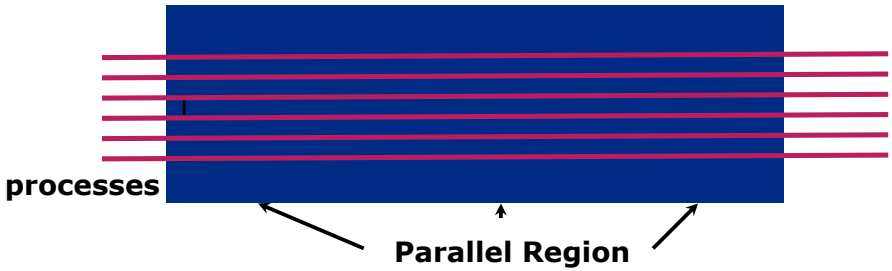
MPI disadvantages

- MPI 2.0 includes many features beyond message passing

- Execution control environment depends on implementation

Programming Model

- Explicit parallelism:
  - All processes starts at the same time at the same point in the code
  - Full parallelism: there is no sequential part in the program



Work Distribution

- All processors run the same executable.
- Parallel work distribution must be explicitly done by the programmer:
  - domain decomposition
  - master worker

A Minimal MPI Program (C)

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

int main( int argc, char *argv[] )
{
    MPI_Init( &argc, &argv );
    printf( "Hello, world!\n" );
    MPI_Finalize();
    return 0;
}
```


A Minimal MPI Program (Fortran 90)

```
program main
use MPI
integer ierr

call MPI_INIT( ierr )
print *, 'Hello, world!'
call MPI_FINALIZE( ierr )
end
```

Starting the MPI Environment

- **`MPI_INIT ( )`**

  Initializes MPI environment. This function must be called and must be the first MPI function called in a program (exception: **`MPI_INITIALIZED`**)

  Syntax

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

MPI_INIT ( IERROR )
INTEGER IERROR
```

  NOTE: Both C and Fortran return error codes for all calls.

Exiting the MPI Environment

- **`MPI_FINALIZE ( )`**

  Cleans up all MPI state. Once this routine has been called, no MPI routine (even **`MPI_INIT`**) may be called

  Syntax

```
int MPI_Finalize ( );

MPI_FINALIZE ( IERROR )
INTEGER IERROR
```

  MUST call MPI_FINALIZE when you exit from an MPI program

C and Fortran Language Considerations

- Bindings
  - C
    - All MPI names have an **`MPI_`** prefix
    - Defined constants are in all capital letters
    - Defined types and functions have one capital letter after the prefix; the remaining letters are lowercase
  - Fortran
    - All MPI names have an **`MPI_`** prefix
    - No capitalization rules apply
    - last argument is an returned error value

Finding Out About the Environment

- Two important questions that arise early in a parallel program are:
  - How many processes are participating in this computation?
  - Which one am I?
- MPI provides functions to answer these questions:
  - **`MPI_Comm_size`** reports the number of processes.
  - **`MPI_Comm_rank`** reports the *rank*, a number between 0 and size-1, identifying the calling process

Better Hello (C)

```
#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 );
    printf( "I am %d of %d\n", rank, size );
    MPI_Finalize();
    return 0;
}
```

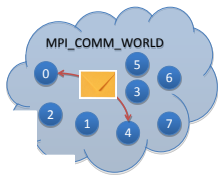

Better Hello (Fortran)

```
program main
use MPI
integer ierr, rank, size

call MPI_INIT( ierr )
call MPI_COMM_RANK( MPI_COMM_WORLD, rank, ierr )
call MPI_COMM_SIZE( MPI_COMM_WORLD, size, ierr )
print *, 'I am ', rank, ' of ', size
call MPI_FINALIZE( ierr )
end
```

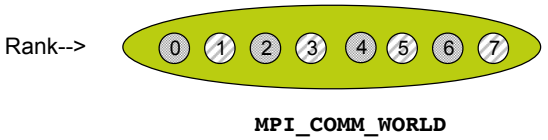

Some Basic Concepts

- Processes can be collected into *groups*.
- Each message is sent in a *context*, and must be received in the same context.
- A group and context together form a *communicator*.
- A process is identified by its *rank* in the group associated with a communicator.
- There is a default communicator whose group contains all initial processes, called **`MPI_COMM_WORLD`**.



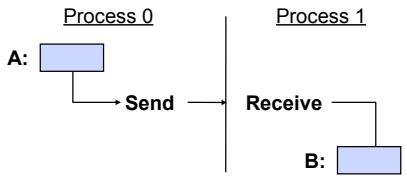
Communicator

- Communication in **`MPI`** takes place with respect to communicators
- **`MPI_COMM_WORLD`** is one such predefined communicator (something of type **`"MPI_COMM"`**) and contains group and context information
- **`MPI_COMM_RANK`** and **`MPI_COMM_SIZE`** return information based on the communicator passed in as the first argument
- Processes may belong to many different communicators



MPI Basic Send/Receive

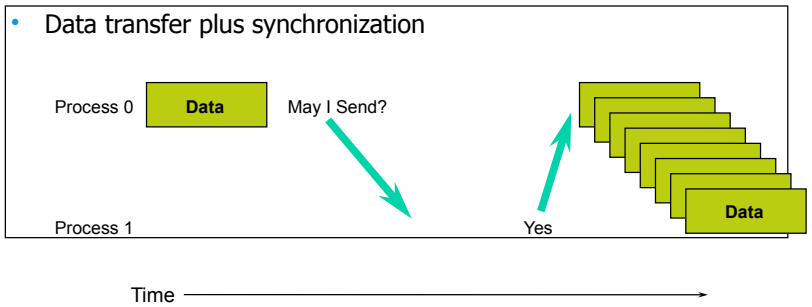
- Basic message passing process. Send data from one process to another



- Questions
  - To whom is data sent?
  - Where is the data?
  - What type of data is sent?
  - How much of data is sent?
  - How does the receiver identify it?

MPI Basic Send/Receive

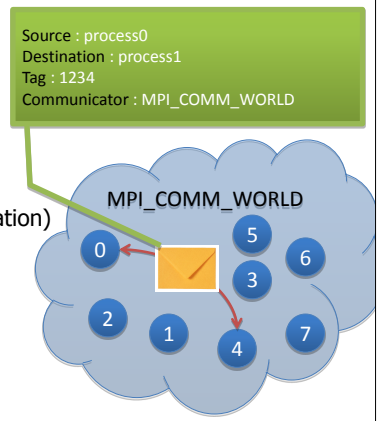
- Data transfer plus synchronization



- Requires co-operation of sender and receiver
- Co-operation not always apparent in code
- Communication and synchronization are combined

Message Organization in MPI

- Message is divided into data and envelope
- data
  - buffer
  - count
  - datatype
- envelope
  - process identifier (source/destination)
  - message tag
  - communicator



MPI Basic Send/Receive

- Thus the basic (blocking) send has become:
  `MPI_Send ( start, count, datatype, dest, tag, comm )`
  - Blocking means the function does not return until it is safe to reuse the data in buffer. The message may not have been received by the target process.
- And the receive has become:
  `MPI_Recv( start, count, datatype, source, tag, comm, status )`
  - The source, tag, and the count of the message actually received can be retrieved from `status`

MPI C Datatypes

MPI datatype	C datatype
MPI_CHAR	signed char
MPI_SHORT	signed short int
MPI_INT	signed int
MPI_LONG	signed long int
MPI_UNSIGNED_CHAR	unsigned char
MPI_UNSIGNED_SHORT	unsigned short int
MPI_UNSIGNED_LONG	unsigned long_int
MPI_UNSIGNED	unsigned int
MPI_FLOAT	float
MPI_DOUBLE	double
MPI_LONG_DOUBLE	long double
MPI_BYTE	
MPI_PACKED	

MPI Fortran Datatypes

MPI FORTRAN	FORTRAN datatypes
MPI_INTEGER	INTEGER
MPI_REAL	REAL
MPI_REAL8	REAL*8
MPI_DOUBLE_PRECISION	DOUBLE PRECISION
MPI_COMPLEX	COMPLEX
MPI_LOGICAL	LOGICAL
MPI_CHARACTER	CHARACTER
MPI_BYTE	
MPI_PACKED	

Is MPI Large or Small?

- Is MPI large (128 functions) or small (6 functions)?
  - MPI's extensive functionality requires many functions
  - Number of functions not necessarily a measure of complexity
  - Many programs can be written with just 6 basic functions

  MPI_INIT **MPI_COMM_SIZE** **MPI_SEND**
  MPI_FINALIZE **MPI_COMM_RANK** **MPI_RECV**

- MPI is just right
  - A small number of concepts
  - Large number of functions provides flexibility, robustness, efficiency, modularity, and convenience
  - One need not master all parts of MPI to use it

Example: PI in Fortran 90 and C

```
#include "mpi.h"
#include <math.h>
int main(int argc, char *argv[])
{
    int done = 0, n, myid, numprocs, i, rc;
    double PI25DT = 3.141592653589793238462643;
    double mypi, pi, h, sum, x, a;
    MPI_Init(&argc,&argv);
    MPI_Comm_size(MPI_COMM_WORLD,&numprocs);
    MPI_Comm_rank(MPI_COMM_WORLD,&myid);
    while (!done)  {
            if (myid == 0) {
                    printf("Enter the number of intervals: (0 quits) ");
                    scanf("%d",&n);
            }
            MPI_Bcast(&n, 1, MPI_INT, 0, MPI_COMM_WORLD);
            if (n == 0) break;
            h   = 1.0 / (double) n;
            sum = 0.0;
            for (i = myid + 1; i <= n; i += numprocs) {
                    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);
            if (myid == 0)
                    printf("pi is approximately %.16f, Error is %.16f\n",pi, fabs(pi - PI25DT));
    }
    MPI_Finalize();
    return 0;
}
```

work distribution

```
      program main
      use MPI
      double precision  PI25DT
      parameter (PI25DT = 3.14159265358979323846264338327950288419716939937510d0)
      double precision  mypi, pi, h, sum, x, f, a
      integer n, myid, numprocs, i, ierr
c                               function to integrate
      f(a) = 4.d0 / (1.d0 + a*a)
      call MPI_INIT( ierr )
      call MPI_COMM_RANK( MPI_COMM_WORLD, myid, ierr )
      call MPI_COMM_SIZE( MPI_COMM_WORLD, numprocs, ierr )
 10   if ( myid .eq. 0 ) then
         write(6,98)
 98      format('Enter the number of intervals: (0 quits)')
         read(5,'(i10)') n
      endif
      call MPI_BCAST( n, 1, MPI_INTEGER, 0,MPI_COMM_WORLD, ierr)
      if ( n .le. 0 ) goto 30
      h = 1.0d0/n
      sum  = 0.0d0
      do 20 i = myid+1, n, numprocs
         x    = h * (dble(i) - 0.5d0)
         sum = sum + f(x)
 20   continue
      mypi = h * sum
      call MPI_REDUCE( mypi, pi, 1, MPI_DOUBLE_PRECISION,
     +                 MPI_SUM, 0, MPI_COMM_WORLD,ierr)
      if (myid .eq. 0) then
         write(6, 97) pi, abs(pi - PI25DT)
 97      format('  pi is approximately: ', F18.16,
     +          '  Error is: ', F18.16)
      endif
      goto 10
 30   call MPI_FINALIZE(ierr)
      end
```

work distribution

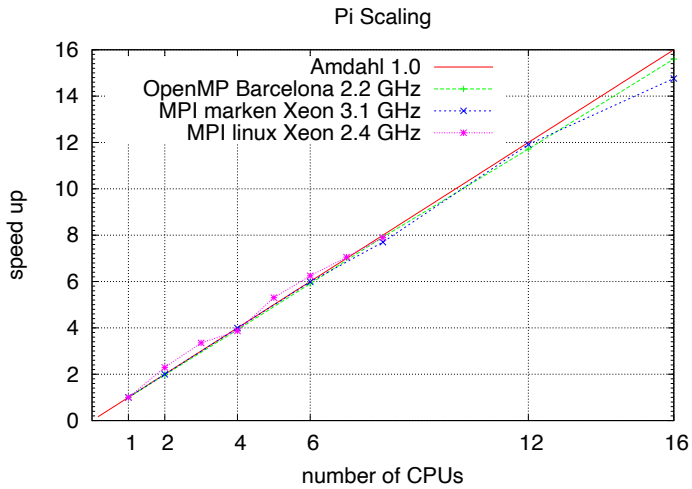
Exercise: PI with MPI and OpenMP

- Compile and run for computing PI parallel
- From git HPCourse/MPi_pi
- There is a README with instructions.
- It is assumed that you use mpich1 and has PBS installed as a job scheduler. If you have mpich2 let me know.
- Use qsub to submit the mpi job (an example script is provided) to a queue.

Exercise: PI with MPI and OpenMP

cores	OpenMP	marken	linux
1	9.617728	14.10798	22.15252
2	4.874539	7.071287	9.661745
4	2.455036	3.532871	5.730912
6	1.627149	2.356928	3.547961
8	1.214713	1.832055	2.804715
12	0.820746	1.184123	
16	0.616482	0.955704	

Exercise: PI with MPI and OpenMP



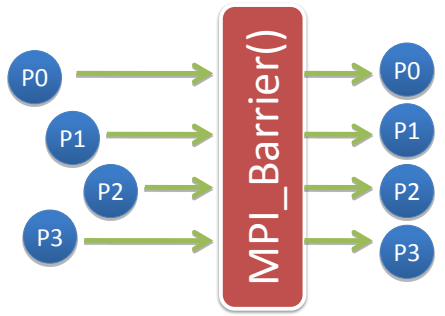
Collective Communications in MPI

- Communication is co-ordinated among a group of processes, as specified by communicator, not on all processes
- All collective operations are blocking and no message tags are used (in MPI-1)
- All processes in the communicator group must call the collective operation
- Collective and point-to-point messaging are separated by different "contexts"
- Three classes of collective operations
  - Data movement
  - Collective computation
  - Synchronization

Collective calls

- MPI has several collective communication calls, the most frequently used are:
  - Synchronization
    - Barrier
  - Communication
    - Broadcast
    - Gather Scatter
    - All Gather
  - Reduction
    - Reduce
    - All Reduce

MPI_Barrier()



Creates barrier synchronization in a communicator group comm. Each process, when reaching the MPI_Barrier call, blocks until all the processes in the group reach the same MPI_Barrier call.

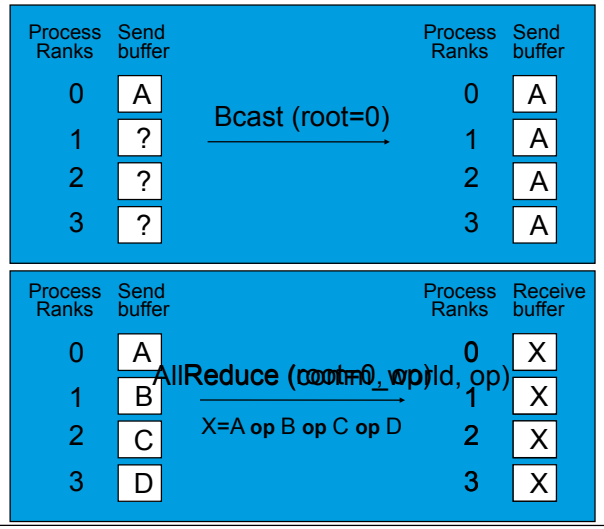
MPI Basic Collective Operations

- Two simple collective operations

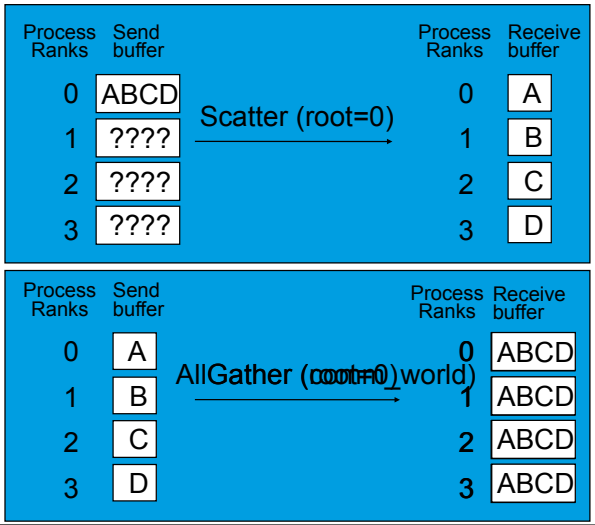
```
MPI_BCAST( start, count, datatype, root, comm )
MPI_REDUCE( start, result, count, datatype, operation,
  root, comm )
```

- The routine **MPI_BCAST** sends data from one process to all others
- The routine **MPI_REDUCE** combines data from all processes, using a specified operation, and returns the result to a single process
- In many numerical algorithms, **SEND/RECEIVE** can be replaced by **BCAST/REDUCE**, improving both simplicity and efficiency.

Broadcast and Reduce



Scatter and Gather



MPI Collective Routines

- Several routines:

MPI_ALLGATHER	**MPI_ALLGATHERV**	**MPI_BCAST**
MPI_ALLTOALL	**MPI_ALLTOALLV**	
MPI_GATHER	**MPI_GATHERV**	
MPI_REDUCE_SCATTER	**MPI_REDUCE**	**MPI_ALLREDUCE**
MPI_SCATTERV	**MPI_SCATTER**	

- **All** versions deliver results to all participating processes
- **"V"** versions allow the chunks to have different sizes

- **MPI_ALLREDUCE, MPI_REDUCE, MPI_REDUCE_SCATTER,** and take both built-in and user-defined combination functions

Built-In Collective Computation Operations

MPI Name	Operation
MPI_MAX	Maximum
MPI_MIN	Minimum
MPI_PROD	Product
MPI_SUM	Sum
MPI_LAND	Logical and
MPI_LOR	Logical or
MPI_LXOR	Logical exclusive or (xor)
MPI_BAND	Bitwise and
MPI_BOR	Bitwise or
MPI_BXOR	Bitwise xor
MPI_MAXLOC	Maximum value and location
MPI_MINLOC	Minimum value and location

Extending the Message-Passing Interface

- Dynamic Process Management
  - Dynamic process startup
  - Dynamic establishment of connections
- One-sided communication
  - Put/get
  - Other operations
- Parallel I/O
- Other MPI-2 features
  - Generalized requests
  - Bindings for C++/ Fortran-90; inter-language issues

When to use MPI

- Portability and Performance
- Irregular Data Structures
- Building Tools for Others
  - Libraries
- Need to Manage memory on a per processor basis

When *not* to use MPI

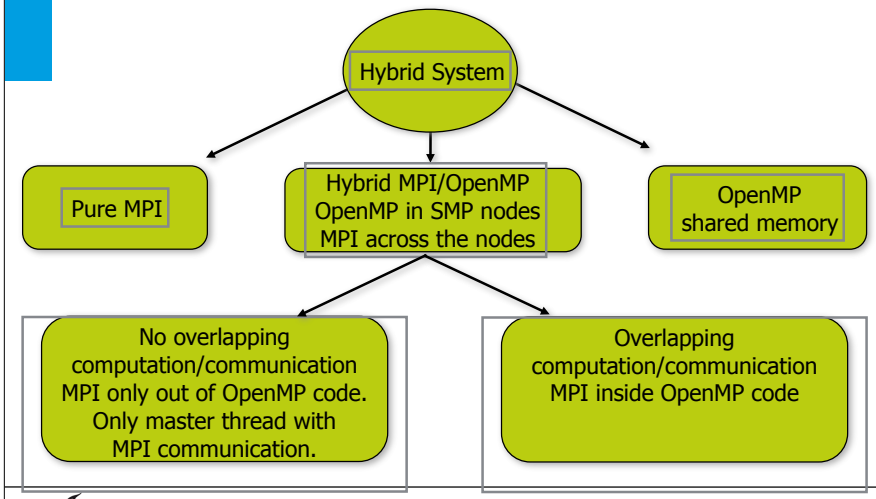
- Number of cores is limited and OpenMP is doing well on that number of cores
  - typically 16-32 cores in SMP
- Course: Introduction to MPI course
  - June 2022: …

Summary

MPI Summary

- MPI Standard widely accepted by vendors and programmers
  - MPI implementations available on most modern platforms
  - Several MPI applications deployed
  - Several tools exist to trace and tune MPI applications
- Simple applications use point-to-point and collective communication operations
- Advanced applications use point-to-point, collective, communicators, datatypes, one-sided, and topology operations

Hybrid systems programming hierarchy



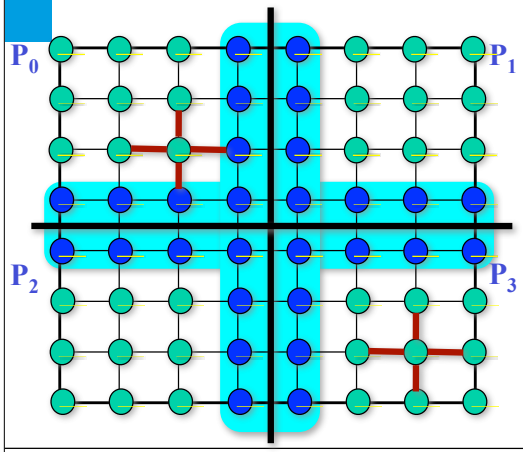
Hybrid OpenMP/MPI

- Natural paradigm for clusters of SMP's
- May offer considerable advantages when application mapping and load balancing is tough
- Benefits with slower interconnection networks (overlapping computation/communication)

- Requires work and code analysis to change pure MPI codes
- Start with auto parallelization?
- Link shared memory libraries…check various thread/MPI processes combinations
- Study carefully the underlying architecture

- What is the future of this model? Could it be consolidated in new languages?
- Connection with many-core?

Overlapping computation/communication: Example



Suppose we wish to solve the PDE

$$-\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}\right)=f(x,y)$$

Using the Jacobi method: the value of u at each discretization point is given by a certain average among its neighbors, until convergence.

Distributing the mesh to SMP clusters by Domain Decomposition, it is clear that the GREEN nodes can proceed without any comm., while the Blue nodes have to communicate first and calculate later.

MPI/OpenMPI: Overlapping computation/ communication

Not only the master but other threads communicate. Call MPI primitives in OpenMP code regions.

```
if (my_thread_id < # ){
    MPI_… (communicate needed data)
} else
    /* Perform computations that to not need
    communication */
    .
    .
}
/* All threads execute code that requires
    communication */
    .
    .
```



```
for (k=0; k < MAXITER; k++){
    /* Start parallel region here */
    #pragma omp parallel private(){
            my_id = omp_get_thread_num();

            if (my_id is given "halo points")
                    MPI_SendRecv("From neighboring MPI process");
            else{
                    for (i=0; i < # allocated points; i++)
                            newval[i] = avg(oldval[i]);
            }

            if (there are still points I need to do) /* Thi
                    for (i=0; i< # remaining points; i++)
                            newval[i] = avg(oldval[i]);

            }
            for (i=0; i<(all_my_points); i++)
                            oldval[i] = newval[i];
    }
    MPI_Barrier(); /* Synchronize all MPI processes here */
}
```


Hiding IO with IO-Server

Use more nodes to act as IO-Servers (pseudo code)

Text

Compute Node

```
do i=1,time_steps
  compute(j)
  checkpoint(data)
end do

subroutine checkpoint(data)
  MPI_Wait(send_req)
  buffer = data
  MPI_Isend(IO_SERVER, buffer)
end subroutine
```

I/O Server

```
do i=1,time_steps
  do j=1,compute_nodes
    MPI_Recv(j, buffer)
    write(buffer)
  end do
end do
```

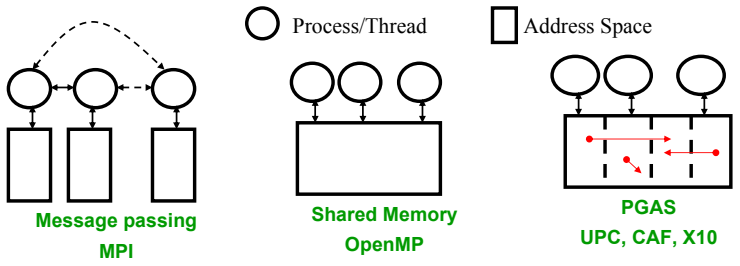
PGAS

- What is PGAS?
- How to make use of PGAS as a programmer?

Partitioned Global Address Space

- **Explicitly parallel, shared-memory like programming model**
- **Global addressable space**
  - Allows programmers to declare and "directly" access data distributed across the machine
- **Partitioned address space**
  - Memory is logically partitioned between *local* and *remote* (a two-level hierarchy)
  - Forces the programmer to pay attention to data locality, by exposing the inherent NUMA-ness of current architectures
- **Single Processor Multiple Data (SPMD) execution model**
  - All threads of control execute the **same** program
  - Number of threads fixed at startup
  - Newer languages such as X10 escape this model, allowing fine-grain threading
- **Different language implementations:**
  - **UPC** (C-based), CoArray Fortran (Fortran-based), Titanium and X10 (Java-based)

Partitioned Global Address Space

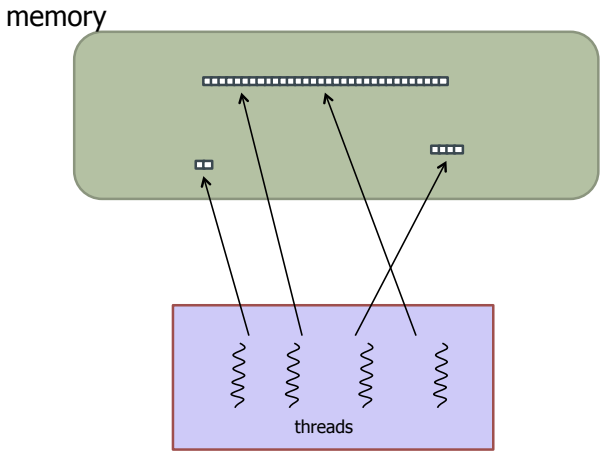


- **Computation is performed in multiple places.**
- **A place contains data that can be operated on remotely.**
- **Data lives in the place it was created, for its lifetime.**
- **A datum in one place may point to a datum in another place.**
- **Data-structures (e.g. arrays) may be distributed across many places.**

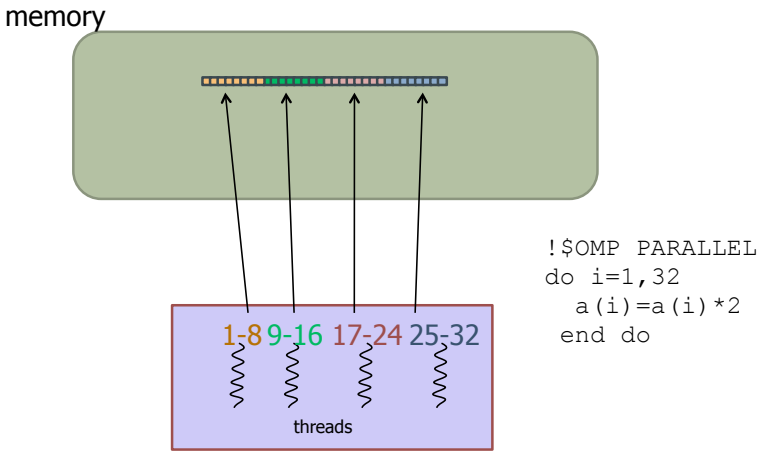
Shared Memory (OpenMP)

- Multiple threads share global memory
  - Most common variant: OpenMP
- Program loop iterations distributed to threads, more recent task features
  - Each thread has a means to refer to private objects within a parallel context
- Terminology
  - Thread, thread team
- Implementation
  - Threads map to user threads running on one SMP node
  - Extensions to multiple servers not so successful

OpenMP

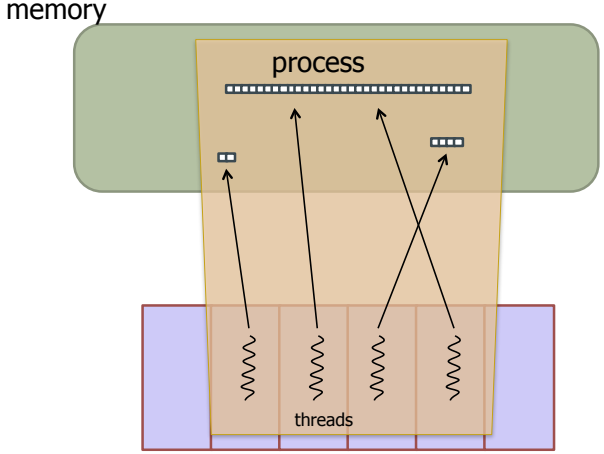


OpenMP: work distribution




```
!$OMP PARALLEL
do i=1,32
  a(i)=a(i)*2
 end do
```


OpenMP: implementation

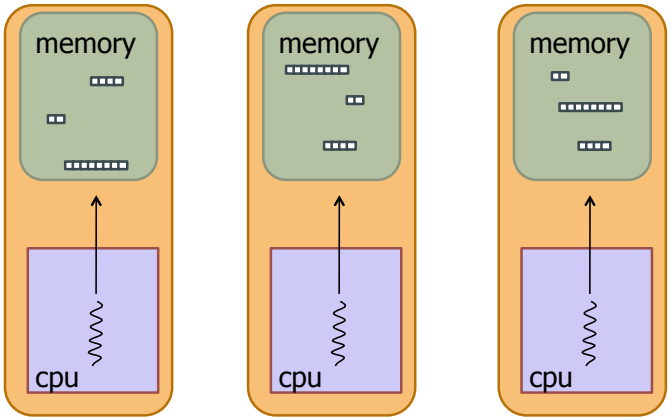


Message Passing (MPI)

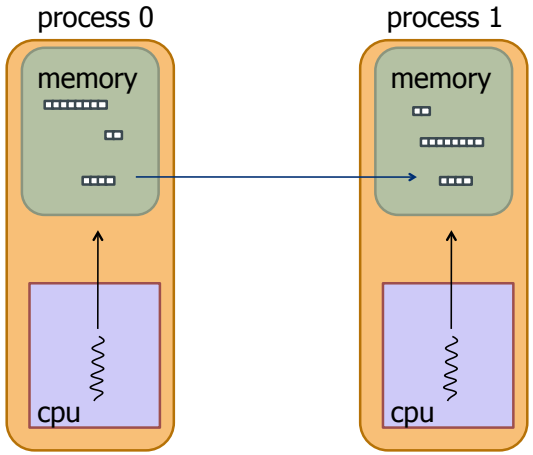
- Participating processes communicate using a message-passing API
- Remote data can only be communicated (sent or received) via the API.
- MPI (the Message Passing Interface) is the standard
- Implementation:
  - MPI processes map to processes within one SMP node or across multiple networked nodes
  - API provides process numbering, point-to-point and collective messaging operations

MPI

processes



MPI

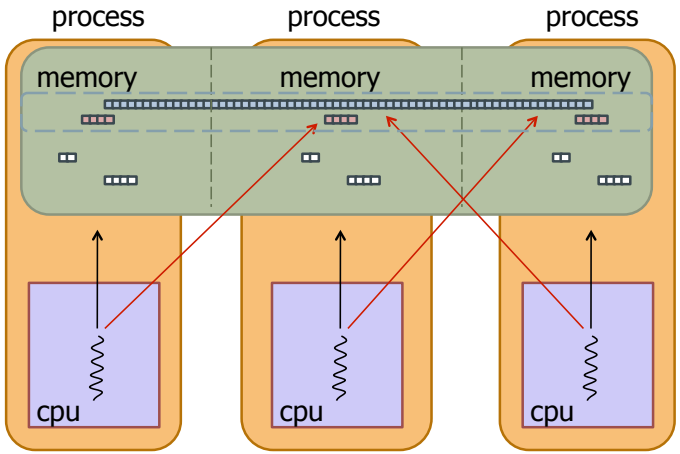



```
MPI_Send(a,...,1,…)  MPI_Recv(a,...,0,…)
```


Partitioned Global Address Space

- Shortened to PGAS
- Participating processes/threads have access to local memory via standard program mechanisms
- Access to remote memory is directly supported by the PGAS language

PGAS



PGAS languages

Partitioned Global Address Space (PGAS):

- Global address space – any process can address memory on any processor
- Partitioned GAS – retain information about locality
- Core idea– hardest part of writing parallel code is managing data distribution and communication; make that simple and explicit
- PGAS Languages try to simplify parallel programming (increase programmer productivity).

Data Parallel Languages

- **Unified Parallel C** (UPC) is an extension of the C programming language designed for high performance computing on large-scale parallel machines.
  http://upc.lbl.gov/
- **Co-array Fortran** (CAF) is part of Fortran 2008 standard. It is a simple, explicit notation for data decomposition, such as that often used in message-passing models, expressed in a natural Fortran-like syntax.
  http://www.co-array.org
- both need a global address space (which is not equal to SMP)

UPC

- Unified Parallel C:
  - An extension of C99
  - An evolution of AC, PCP, and Split-C
- Features
  - SPMD parallelism via replication of *threads*
  - Shared and private address spaces
  - Multiple memory consistency models
- Benefits
  - Global view of data
  - One-sided communication

Co-Array Fortran

- Co-Array Fortran:
  - An extension of Fortran 95 and part of "Fortran 2008"
  - The language formerly known as F--
- Features
  - SPMD parallelism via replication of *images*
  - *Co-arrays* for distributed shared data
- Benefits
  - Syntactically transparent communication
  - One-sided communication
  - Multi-dimensional arrays
  - Array operations

Basic execution model co-array F--

- Program executes as if replicated to multiple copies with each copy executing asynchronously (SPMD)
- Each copy (called an image) executes as a normal Fortran application
- New object indexing with [] can be used to access objects on other images.
- New features to inquire about image index, number of images and to synchronize

CAF (F--)

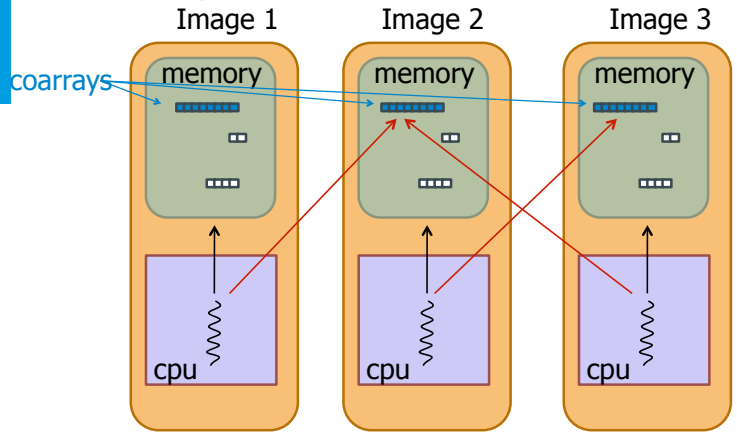
parallel

```
REAL, DIMENSION(N)[*] :: X,Y
   X(:) = Y(:)[Q]
```

Array indices in parentheses follow the normal Fortran rules within one memory image.

Array indices in square brackets provide an equally convenient notation for accessing objects across images and follow similar rules.

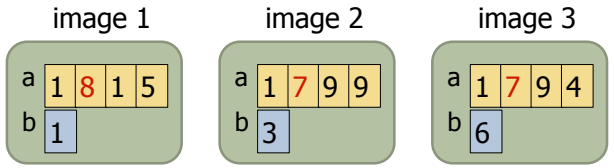
Coarray execution model



Remote access with square bracket indexing: a(:)[2]

Basic coarray declaration and usage

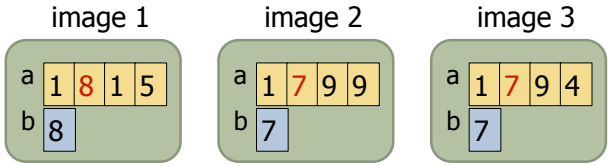
```
integer :: b
integer :: a(4)[*] !coarray
```




```
b=a(2)
```

Basic coarray declaration and usage

```
integer :: b
integer :: a(4)[*] !coarray
```




```
b=a(2)
```


Basic coarray declaration and usage

```
integer :: b
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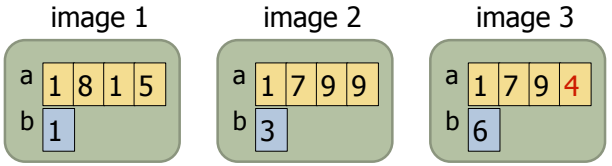
Text

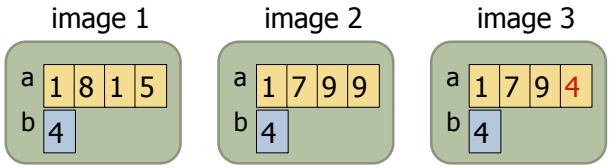



```
b=a(4)[3]
```


Basic coarray declaration and usage

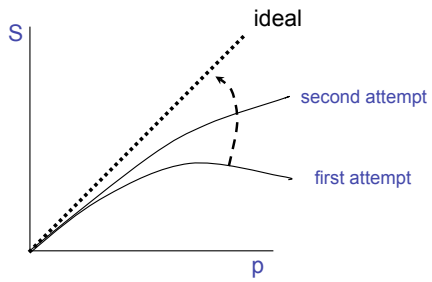
```
integer :: b
integer :: a(4)[*] !coarray
```

Text




```
b=a(4)[3]
```

Performance Tuning



Performance tuning of parallel applications is an iterative process

Compiling MPI Programs

Compiling and Starting MPI Jobs

- Compiling:
  - Need to link with appropriate MPI and communication subsystem libraries and set path to MPI Include files
  - Most vendors provide scripts or wrappers for this (mpxlf, mpif77, mpicc, etc)
- Starting jobs:
  - Most implementations use a special loader named mpirun
    - **`mpirun -np <no_of_processors> <prog_name>`**
  - In MPI-2 it is recommended to use
    - **`mpiexec -n <no_of_processors> <prog_name>`**

MPICH: a Portable MPI Environment

- MPICH is a high-performance portable implementation of MPI (both 1 and 2).
- It runs on MPP's, clusters, and heterogeneous networks of workstations.
- The CH comes from Chameleon, the portability layer used in the original MPICH to provide portability to the existing message-passing systems.
- In a wide variety of environments, one can do:

```
mpicc -mpitrace myprog.c
mpirun -np 10 myprog
upshot myprog.log
```

to build, compile, run, and analyze performance.

MPICH2

MPICH2 is an all-new implementation of the MPI Standard, designed to implement all of the MPI-2 additions to MPI.

- separation between process management and communications
- use daemons (mpd) on nodes
- dynamic process management,
- one-sided operations,
- parallel I/O, and others

- http://www.mcs.anl.gov/research/projects/mpich2/

Compiling MPI programs

- From a command line:
  `mpicc -o prog prog.c`
- Use profiling options (specific to mpich)
  - **-mpilog** Generate log files of MPI calls
  - **-mpitrace** Trace execution of MPI calls
  - **-mpianim** Real-time animation of MPI (not available on all systems)
  - **--help** Find list of available options
- The environment variables `MPICH_CC`, `MPICH_CXX`, `MPICH_F77`, and `MPICH_F90` may be used to specify alternate C, C++, Fortran 77, and Fortran 90 compilers, respectively.

example hello.c

```
#include "mpi.h"
#include <stdio.h>
int main(int argc ,char *argv[])
{
  int myrank;
  MPI_Init(&argc, &argv);
  MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
  fprintf(stdout, "Hello World, I am process
  %d\n", myrank);
  MPI_Finalize();
  return 0;
}
```


Example: using MPICH1

```
-bash-3.1$ mpicc -o hello hello.c
-bash-3.1$ mpirun -np 4 hello
Hello World, I am process  0
Hello World, I am process  2
Hello World, I am process  3
Hello World, I am process  1
```

Example: details

- If using frontend and compute nodes in machines file use
  `mpirun -np 2 -machinefile machines hello`
- If using only compute nodes in machine file use
  `mpirun -nolocal -np 2 -machinefile machines hello`
  - -nolocal - don't start job on frontend
  - -np 2 - start job on 2 nodes
  - -machinefile machines - nodes are specified in machines file
  - hello - start program hello

Notes on clusters

- Make sure you have access to the compute node (ssh keys are generated ssh-keygen) and ask your system administrator.
- Which mpicc are you using
  - $ which mpicc
- command line arguments are not always passed to mpirun/mpiexec (depending on your version). In that case make a script which calls your program with all its arguments

MPICH2 daemons

- `mpdtrace`: output a list of nodes on which you can run MPI programs (runs mpd daemons).
  - The -l option lists full hostnames and the port where the mpd is listening.
- `mpd` starts an mpd daemon.
- `mpdboot` starts a set of mpd's on a list of machines.
- `mpdlistjobs` lists the jobs that the mpd's are running.
- `mpdkilljob` kills a job specified by the name returned by `mpdlistjobs`

  `mpdsigjob` delivers a signal to the named job.

MPI - Message Passing Interface

- MPI or MPI-1 is a library specification for message-passing.
- MPI-2: Adds in Parallel I/O, Dynamic Process management, Remote Memory Operation, C++ & F90 extension …
- MPI Standard:
  http://www-unix.mcs.anl.gov/mpi/standard.html
- MPI Standard 1.1 Index:
  http://www.mpi-forum.org/docs/mpi-11-html/node182.html
- MPI-2 Standard Index:
  http://www-unix.mcs.anl.gov/mpi/mpi-standard/mpi-report-2.0/node306.htm
- MPI Forum Home Page:
  http://www.mpi-forum.org/index.html

MPI tutorials

- http://www.nccs.nasa.gov/tutorials/mpi_tutorial2/mpi_II_tutorial.html
- https://fs.hlrs.de/projects/par/par_prog_ws/
- Course: Introduction to MPI
  - 50/50 lecture and exercises

MPI Sources

- The Standard (3.0) itself:
  - at http://www.mpi-forum.org
  - All MPI official releases, in both PDF and HTML
- Books:
  - *Using MPI: Portable Parallel Programming with the Message-Passing Interface*, by Gropp, Lusk, and Skjellum, MIT Press, 1994.
  - *Parallel Programming with MPI*, by Peter Pacheco, Morgan-Kaufmann, 1997.
- Other information on Web:
  - at http://www.mcs.anl.gov/mpi
  - pointers to lots of stuff, including other talks and tutorials, a FAQ, other MPI pages
  - http://mpi.deino.net/mpi_functions/index.htm

Job Management and queuing

Job Management and queuing

- On a large system many users are running simultaneously.
- What to do when:
  - The system is full and you want to run your 512 CPU job?
  - You want to run 16 jobs, should others wait on that?
  - Have bigger jobs priority over smaller jobs?
  - Have longer jobs lower/higher priority?
- The job manager and queue system takes care of it.

MPICH1 in PBS

```
#!/bin/bash
#PBS -N Flank
#PBS -V
#PBS -l nodes=11:ppn=2
#PBS -j eo

cd $PBS_O_WORKDIR
export nb=`wc -w < $PBS_NODEFILE`
echo $nb

mpirun -np $nb -machinefile $PBS_NODEFILE ~/bin/
migr_mpi \
        file_vel=$PBS_O_WORKDIR/grad_salt_rot.su \
        file_shot=$PBS_O_WORKDIR/cfp2_sx.su
```


Job Management and queuing

- PBS (maui):
  - http://www.clusterresources.com/pages/products/maui-cluster-scheduler.php
  - Torque resource manager http://www.clusterresources.com/pages/products/torque-resource-manager.php
- Sun Grid Engine
  - http://gridengine.sunsource.net/
- SLURM
  - http://slurm.schedmd.com
- Luckily their interface is very similar (qsub, qstat, ...)

queuing commands

- qsub
- qstat
- qdel
- xpbsmon

qsub

```
#PBS -l nodes=10:ppn=1
#PBS -l mem=20mb
#PBS -l walltime=1:00:00
#PBS -j eo
```

submit:

```
qsub -q normal job.scr
```

output:

```
jobname.ejobid
jobname.ojobid
```

qstat

- available queue and resources

```
qstat -q
```

- queued and running jobs

```
qstat (-a)
```


qdel

- deletes job from queue and stops all running executables

```
qdel jobid
```


Submitting many jobs in one script

```
#!/bin/bash -f
#
export xsrc1=93
export xsrc2=1599
export dxsrc=3
xsrc=$xsrc1

while (( xsrc <= xsrc2 ))
do
echo ' modeling shot at x=' $xsrc

cat << EOF > jobs/pbs_${xsrc}.job
#!/bin/bash
#
#PBS -N fahud_${xsrc}
#PBS -q verylong
#PBS -l nodes=1:ppn=1
#PBS -V

program with arguments

EOF

qsub jobs/pbs_${xsrc}.job
(( xsrc = $xsrc + $dxsrc))
done
```

Be careful !

submitting job-arrays with slurm

```
#!/bin/bash
#SBATCH --job-name=mega_array   # Job name
#SBATCH --nodes=1                    # Use one node
#SBATCH --ntasks=1                   # Run a single task
#SBATCH --time=00:10:00              # Time limit hrs:min:sec
#SBATCH --output=array_%A-%a.out     # Standard output and error log
#SBATCH --array=1-5                  # Array range
pwd; hostname; date

#Set the number of runs that each SLURM task should do
PER_TASK=1000

# Calculate the starting and ending values for this task based
# on the SLURM task and the number of runs per task.
START_NUM=$(( ($SLURM_ARRAY_TASK_ID - 1) * $PER_TASK + 1 ))
END_NUM=$(( $SLURM_ARRAY_TASK_ID * $PER_TASK ))

echo This is task $SLURM_ARRAY_TASK_ID, which will do runs $START_NUM to
$END_NUM

# Run the loop of runs for this task.
for (( run=$START_NUM; run<=END_NUM; run++ )); do
  echo This is SLURM task $SLURM_ARRAY_TASK_ID, run number $run
  #Do your stuff here
done
```

Exercise: PI with MPI and OpenMP

- Compile and run for computing PI parallel
- MPI_pi directory
- Check the README for instructions.
- It is assumed that you use mpich1 and has PBS installed as a job scheduler. If you have mpich2 let me know.
- Use qsub to submit the mpi job (an example script is provided) to a queue.

Exercise: PI with MPI and OpenMP

cores	OpenMP	marken (MPI)	linux (MPI)
1	9.617728	14.10798	22.15252
2	4.874539	7.071287	9.661745
4	2.455036	3.532871	5.730912
6	1.627149	2.356928	3.547961
8	1.214713	1.832055	2.804715
12	0.820746	1.184123	
16	0.616482	0.955704	

Exercise: OpenMP Max

- Find the maximum number in a random generated array.
- on github HPCource/OMP_MAX
- There is a README for instructions.
- The exercise focus on using the available number of cores in an efficient way.
- Also inspect the code and see how the reductions are done, is there another way of doing the reductions?

Exercise: OpenMP details

- More details is using OpenMp and shared memory parallelisation
- collection of code is in HPCource/PowerGroup
- Unpack tar file and check the README for instructions.
- These are 'old' exercises from SGI and give insight in problems you can encounter using OpenMP.
- It requires already some knowledge about OpenMP. The OpenMP F-Summary.pdf from the website can be helpful.

END