High Performance Parallel Programming (CS61064)

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Lecture notes, materials, assignments and tests

- Login to Moodle from CSE homepage.
- Enroll as Student in Course
  - High Performance Parallel Programming (HP3_2018s)
- Your password is HP3_2018s
- Do not forget to mention your roll number at ID Number field.

References

1. “Using OpenMP” by Barbara Chapman, Gabriele Jost and Ruud van der Pas

2. “MPI: The Complete Reference” by Marc Snir, Jack Dongarra, Janusz S. Kowalik, Steven Huss-Lederman, Steve W. Otto, David W. Walker

3. “Parallel Programming with MPI” by Peter Pacheco

Why HPC?

- Weather forecast
- Share market forecast
- Many body interaction
- Massive Database search
- High throughput screening
- Intelligent game design
- Real time analysis
- Flexibility over the search space
- Simulation: Atoms to Planets

The first era (1940s-1960s)

Control Data Corporation (CDC) 6600

The Cray Era (1975-1990)

Cray 1, 1976

1980s

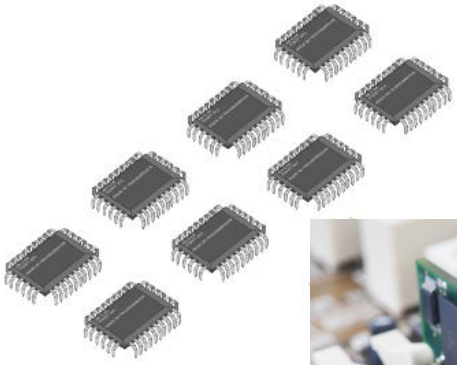
Vectors processors
Shared memory

The cluster Era (1990-2010)

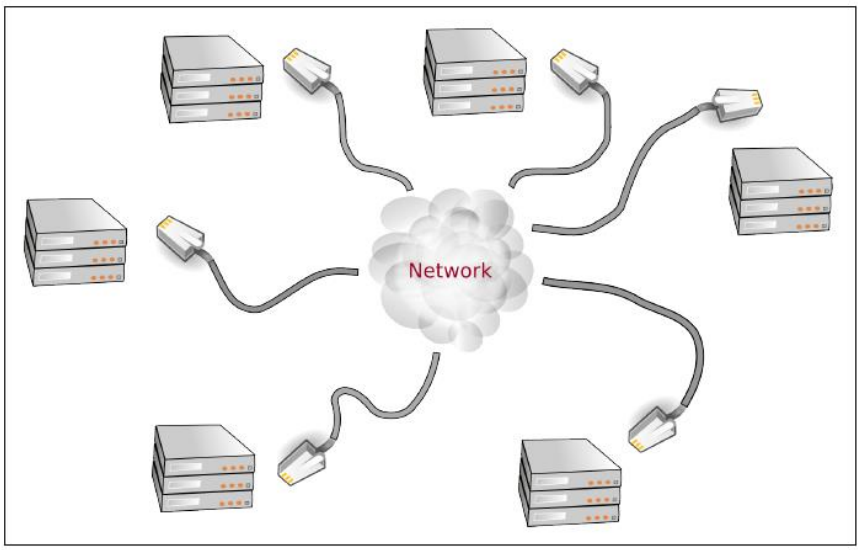
Current Scenario

- The GPGPU and Hybrid Era (2000-
- https://www.top500.org/

Shared or Private



Shared or Private



Grandness

- WRF (Weather Research Forecast) ConUS (CONtinental Usa) 2.5km 6hr benchmark
  - Single P6: ~40 hr (though theoretically ~4hr)
  - 4 nodes (128 cores): 0.6 hr
  - 64 nodes (1024 cores): 9 min

Matrix Multiplication

```
for (i = 0; i < N; i++) {
    for (j = 0; j < N; j++) {
        sum = 0;
        for (k = 0; k < N; k++) {
            sum = sum + M1[i][k] * M2[k][j];
        }
        M12[i][j] = sum;
        }
}
```

Concurrency

- int X;
  - X = 12 * 2 + 6 / 2 – 3^3 + (2 + 1)
- int X, Y;
  - Y = 12 * 2;
  - X = Y + 6 / 2 – 3^3 + (2 + 1)
- int X, Y;
  - Y = 6 * 2 ;
  - X = Y * 2 + 6 / 2 – 3^3 + (2 + 1)

Amdahl's law

- If a proportion (in time) **P** of a code can get **S** speed up then total speedup will be (less than)

$$\frac{1}{(1-P)+\frac{P}{S}}$$

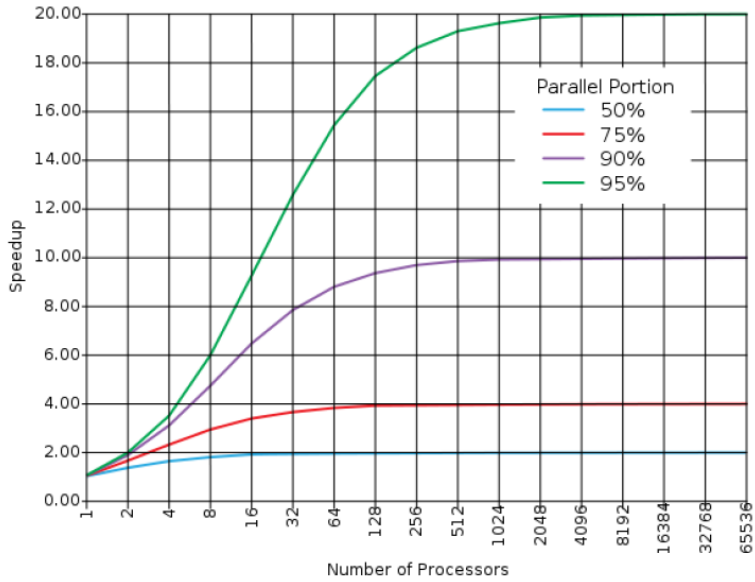
- Improving **P** is more important than improving **S** that is often more difficult too.

Amdahl's law

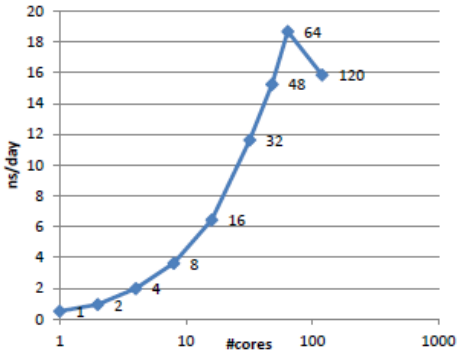
- **An example -**
  - if 95% of a program can be parallelized
  - ...but remaining 5% cannot
  - theoretical maximum speed-up is...
  - ...with infinite processors
  - ...and no overhead

20

Amdahl's law



The scaling limit



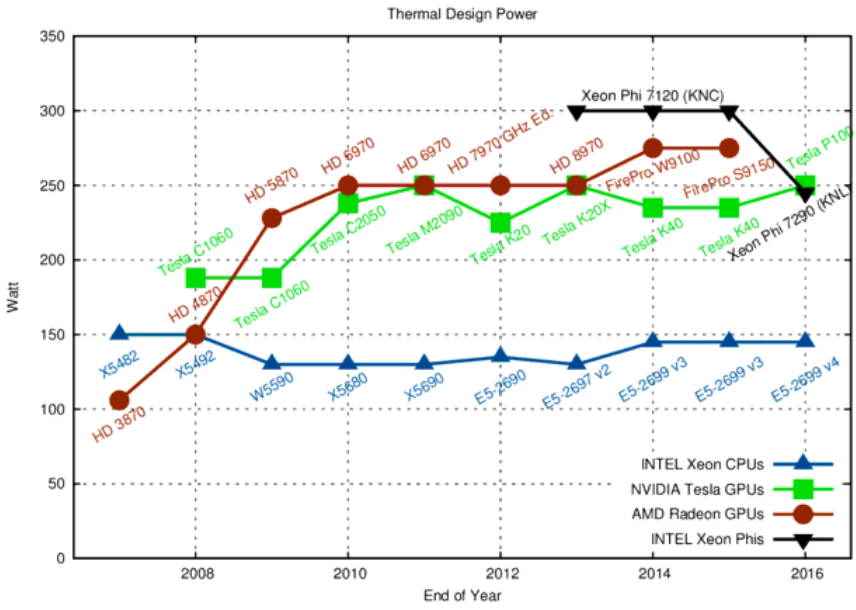
Molecular Dynamics Simulation (using Gromacs)

Take home message

- Do you need infinite number of computing and storage power?

~~**Possibly**~~ **NO!!**

Power requirement and Cooling

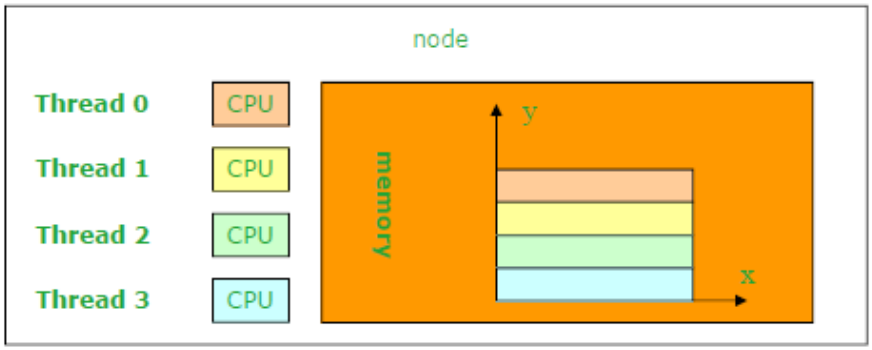


Parallel Software Models and Languages

- **Programming Models**
  - Shared Memory (OpenMP)
  - Message Passing (MPI)
  - Hardware Accelerators (CUDA, OpenCL)
  - Hybrid

- **Programming Language:**
  - C
  - C++
  - Fortran

Shared Memory



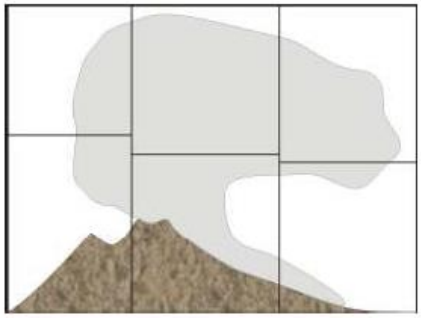
Shared Memory

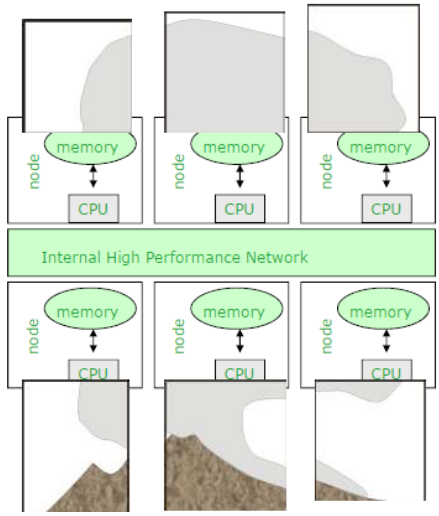
OpenMP

- **Main Characteristics**
  - Compiler directives
  - Medium grain
  - Intra node parallelization
  - Loop or iteration partition
  - Shared memory
  - Many HPC App
- **Open Issues**
  - Thread creation overhead
  - Memory/core affinity
  - Interface with MPI

Private Memory

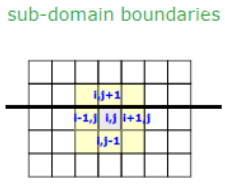
Message Passing

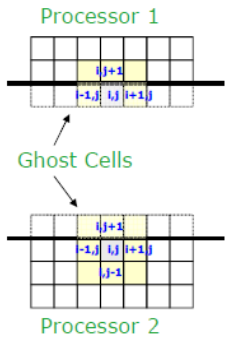


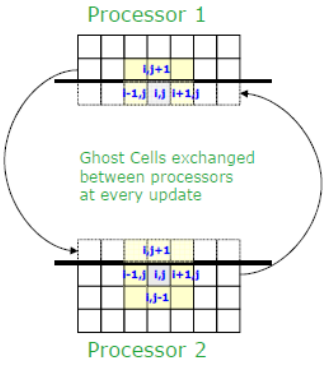


Private Memory

Message Passing







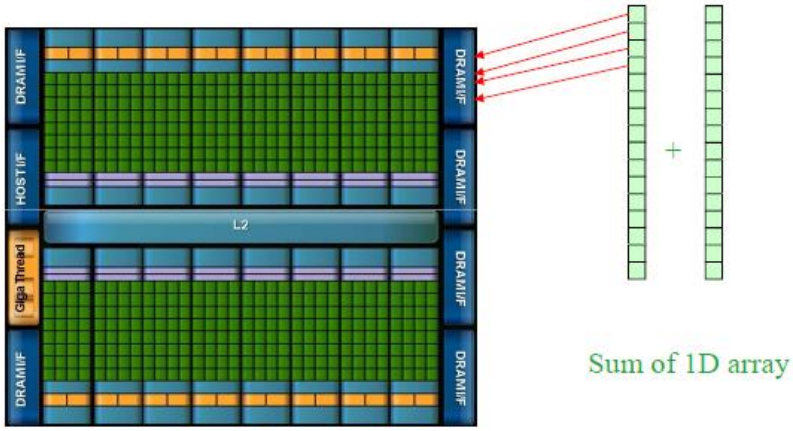
Private Memory

MPI

- **Main Characteristics**
  - Library
  - Coarse grain
  - Inter node parallelization
  - Domain partition
  - Distributed memory
  - Almost all HPC parallel App

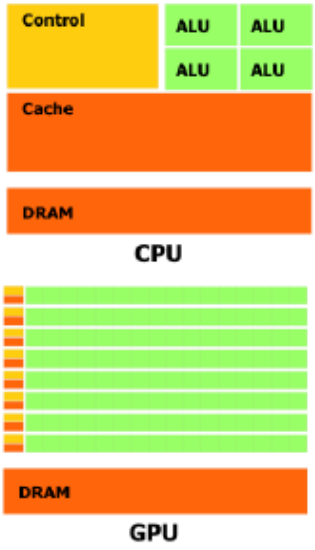
- **Open Issues**
  - Latency
  - OS Jitter
  - Scalability

Accelerator / GPGPU

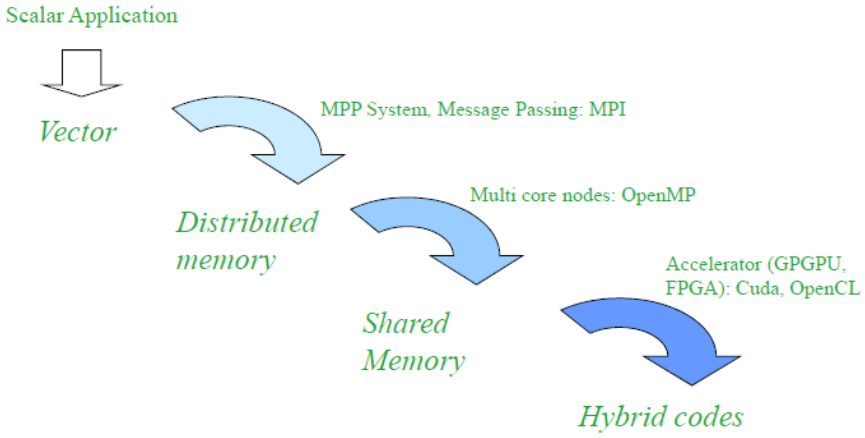


CUDA - OpenCL

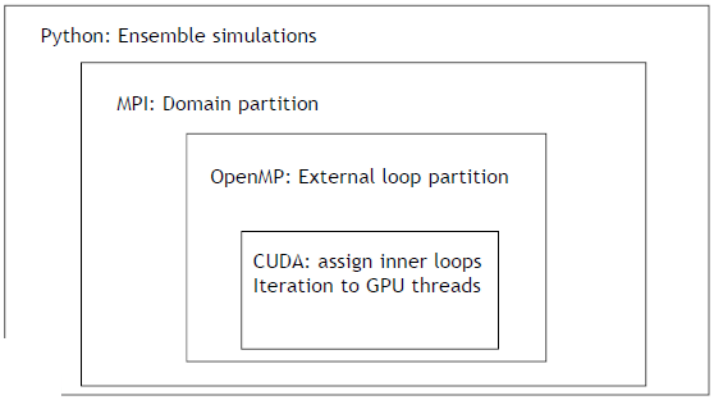
- **Main Characteristic**
  - Ad-hoc compiler
  - Fine grain
  - Offload parallelization (GPU)
  - Single iteration parallelization
  - Few HPC App
- **Open Issue**
  - Memory copy
  - Standard
  - Tools
  - Integration with other languages



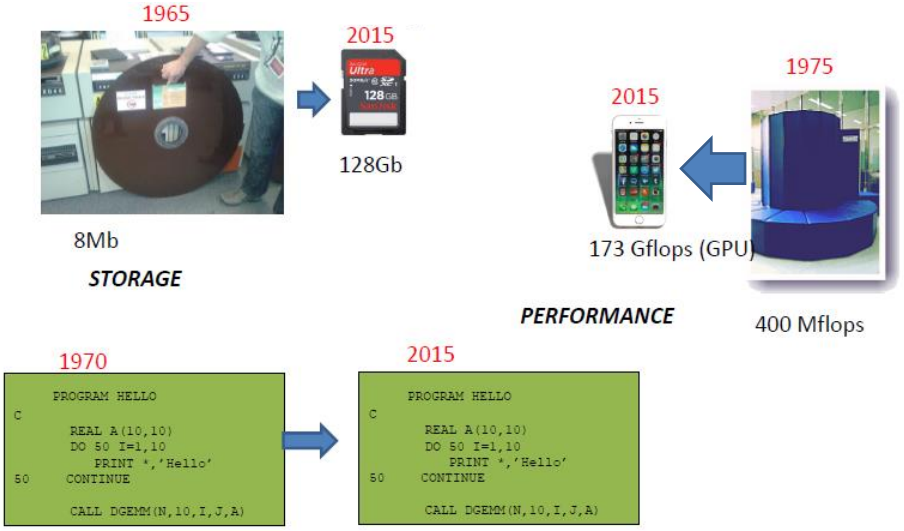
Hybrid Parallel Programming



Hybrid Parallel Programming



Advances: Hardware vs Software



Real HPC Crisis: Software

A supercomputer application and software are usually much more long-lived than a hardware

- Hardware life typically four-five years at most.
- Fortran and C are still the main programming models

Programming is stuck

- Arguably hasn't changed so much since the 70's

Software is a major cost component of modern technologies.

- The tradition in HPC system procurement is to assume that the software is free.

It's time for a change

- Complexity is rising dramatically
- Challenges for the applications on Petaflop systems
- Improvement of existing codes will become complex and partly impossible.
- The use of O(100K) cores implies dramatic optimization effort.
- New paradigm as the support of a hundred threads in one node implies new parallelization strategies
- Implementation of new parallel programming methods in existing large applications can be painful

Software Difficulties

- Legacy applications (includes most scientific applications) not designed with good software engineering principles. Difficult to parallelise programs with many global variables, for example.
- Memory/core decreasing.
- I/O heavy impact on performance, esp. for BlueGene where I/O is handled by dedicated nodes.
- Checkpointing and resilience.
- Fault tolerance over potentially many thousands of threads.
  - In MPI, if one task fails all tasks are brought down.

Summary

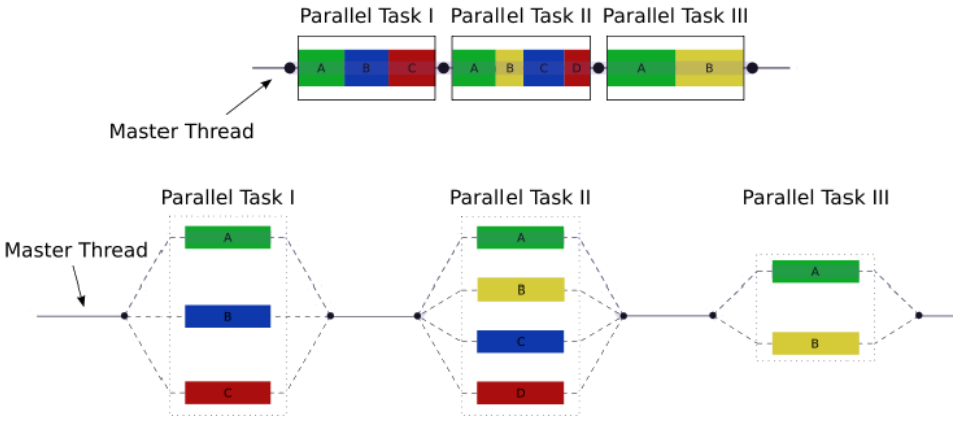
- HPC is only possible via parallelism and this must increase to maintain performance gains.
- Parallelism can be achieved at many levels but because of limited code scalability with traditional cores increasing role for accelerators (e.g. GPUs, MICs). The Top500 is becoming now becoming dominated by hybrid systems.
- Hardware trends forcing code re-writes with OpenMP, OpenCL, CUDA, OpenACC, etc in order to exploit large numbers of threads.
- Unfortunately, for many applications the parallelism is determined by problem size and not application code.
- Energy efficiency (Flops/Watt) is a crucial issue. Some batch schedulers already report energy consumed and in the near future your job priority may depend on predicted energy consumption.

OpenMP

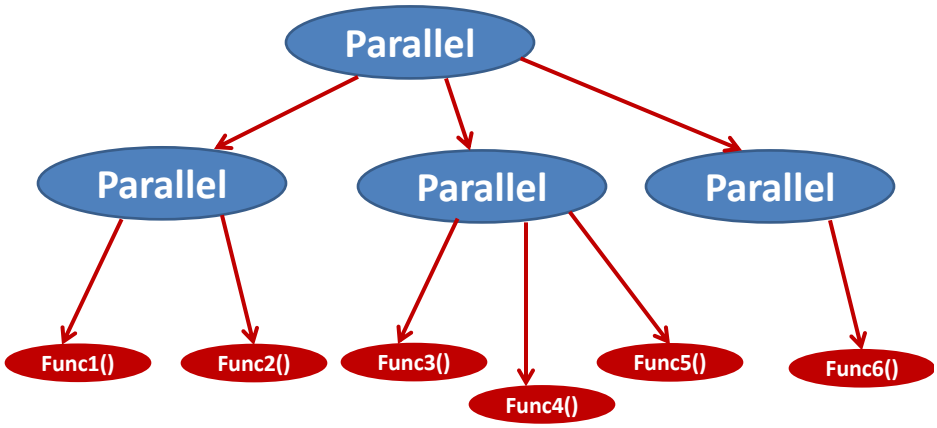
Facts

- Very easy to use!
- Based on preprocessor directives
- Same code for both serial and parallel applications (with caveats)
- Automatically distributes workload
- Synchronization between a subset of threads is not allowed.
- Runs **ONLY** in shared-memory
- Doesn't help if our problem does not fit in memory

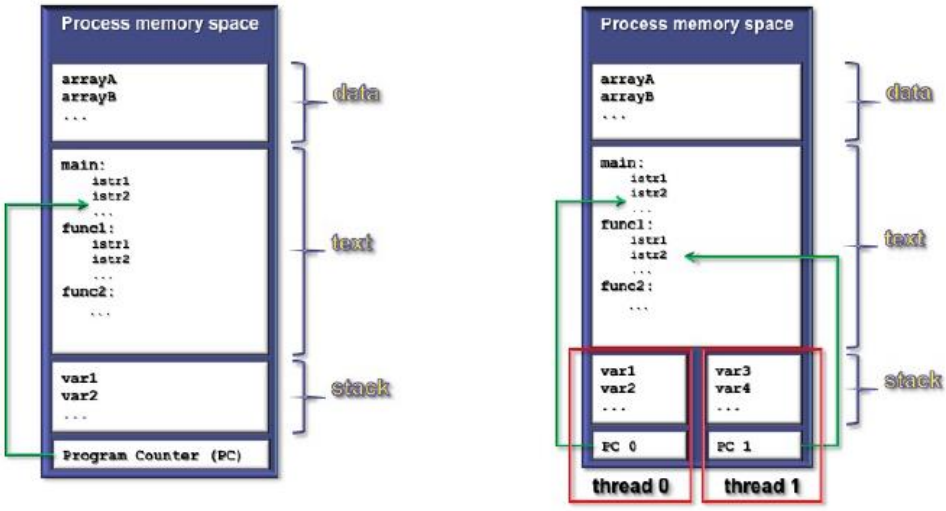
Overview



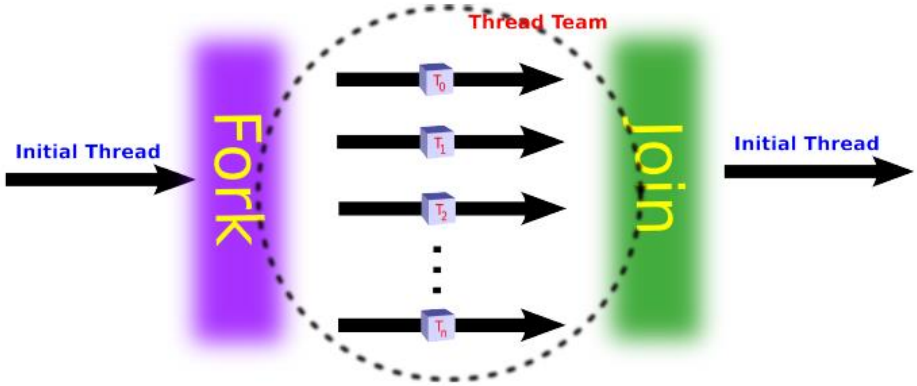
Overview



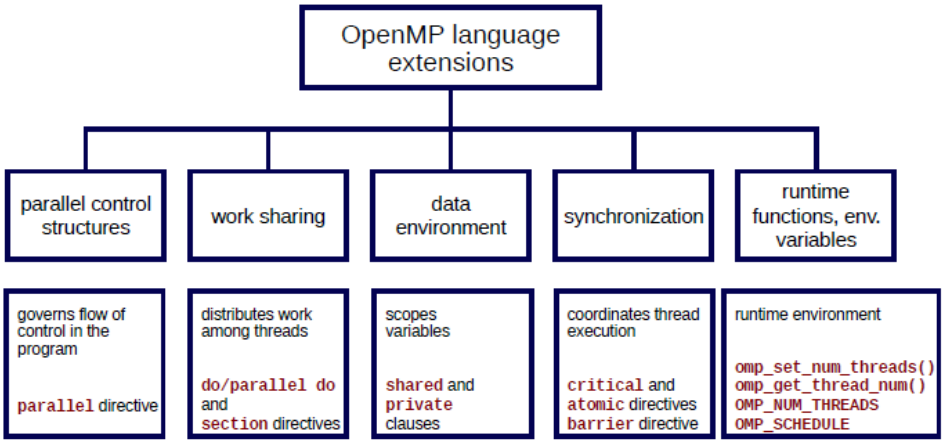
Multi-threaded process



Execution Model



OpenMP core elements



Your first openMP program

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

int main()
{
        #pragma omp parallel
        {
                printf("Hello world!\n");
        }
        return 0;
}
```

Your first openMP program

Check your system support: locate omp.h

/usr/lib/gcc/x86_64-redhat-linux/4.8.2/include/omp.h

Compilation: g++ -fopenmp first_openMP.c

Conditional Compilation:

```
#ifdef _OPENMP
        printf("Compiled with OpenMP support:%d",_OPENMP);
#else
        printf("Compiled for serial execution.");
#endif
```

Execution: ./a.out

Flags:

GNU: **-fopenmp** for Linux, Solaris, AIX, MacOSX, Windows.
IBM: **-qsmp=omp** for Windows, AIX and Linux.
Sun: **-xopenmp** for Solaris and Linux.
Intel: **-openmp** on Linux or Mac, or **-Qopenmp** on Windows
PGI: **-mp**

Your first openMP program

```
$ ./a.out
Hello world!
Hello world!
Hello world!
Hello world!
Hello world!
Hello world!
Hello world!
Hello world!
```

Setting Environmental Variable

- **Know your shell**

  $ echo $SHELL

  $ /bin/bash

$ export OMP_NUM_THREADS=16

Lecture 03-04

Your first openMP program

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

int main()
{
        #pragma omp parallel
        {
                printf("Hello world!\n");
        }
        return 0;
}
```

Setting Environmental Variable and Executing

```
//Know your shell
$ echo $SHELL
$ /bin/bash
//Setting environmental variables
$ export OMP_NUM_THREADS=8
//Compilation
$ g++  -fopenmp  first_openMP.c
//Execution
$ ./a.out
Hello world!
Hello world!
Hello world!
Hello world!
Hello world!
Hello world!
Hello world!
Hello world!
```

Directives

- **Syntactically directives are just comments**
  - **#pragma omp** *directive-name [clause[[,] clause]...] new-line*
- **Examples**
  - #pragma omp parallel
- **Clause is one of the followings**
  - if(scalar-expression)
  - private(variable-list)
  - firstprivate(variable-list)
  - default(shared | none)
  - shared(variable-list)
  - copyin(variable-list)
  - reduction(operator: variable-list)
  - num_threads(integer-expression)
- **Multiple directive names are not allowed**
  - #pragma omp parallel barrier

parallel construct

#pragma omp parallel

- Forms a team of *N* threads before starting executing parallel region
- *N* is set by *OMP_NUM_THREADS* environment or using function *omp_set_num_threads()*
- Semantics is (almost) same as serial program

Comments on *parallel* construct

- At most one **if** clause can appear on the directive (serial/parallel)
- It is unspecified whether any side effects inside the **if** expression or **num_threads** expression occur.
- Only a single **num_threads** clause can appear on the directive. The **num_threads** expression is evaluated outside the context of the parallel region, and must evaluate to a positive integer value.
- The order of evaluation of the **if** and **num_threads** clauses is unspecified.
- A nested parallel region is executed by a team composed of one thread. The default behavior may be changed by using either the runtime library function **omp_set_nested.**
- If the **num_threads** clause is present then it supersedes the number of threads requested by the **omp_set_num_threads** library function or the **OMP_NUM_THREADS** environment variable only for the parallel region it is applied to. Subsequent parallel regions are not affected by it.

Run time library functions

#include <omp.h>

- omp_get_num_threads() returns number of threads
- omp_get_thread_num() returns the thread ID of the current thread
- omp_set_num_threads() sets number of threads
- omp_get_wtime() returns the wall clock time in sec
- omp_get_max_threads()
- omp_get_num_procs()
- omp_in_parallel()
- omp_set_dynamic()
- omp_get_dynamic()
- omp_set_nested()
- omp_get_nested()

Example -2

```
# include <stdio.h>
# include <omp.h>
int main ( int argc, char *argv[] ) {
 int id;
 double wtime;
 printf ( "Number of processors available = %d\n", omp_get_num_procs ( ) );
 printf ( "Number of threads =           %d\n",  omp_get_max_threads ( ) );
 wtime = omp_get_wtime ( );
 printf ( "OUTSIDE the parallel region.\n" );

 id = omp_get_thread_num ( );
 printf ( "HELLO from process %d\n Going INSIDE the parallel region:\n ", id ) ;

# pragma omp parallel \
 private ( id )  {
  id = omp_get_thread_num ( );
  printf ("  Hello from process %d\n", id );
 }
 wtime = omp_get_wtime ( ) - wtime;

 printf ( "Back OUTSIDE the parallel region.\nNormal end of execution.\nElapsed wall clock time = %f\n", wtime );
 return 0;
}
```

Example -2

Initialization:

export OMP_NUM_THREADS=16

Compilation:

g++ -fopenmp example.c

Execution:

./a.out

Example -2

```
Number of processors available = 8
Number of threads =          16
OUTSIDE the parallel region.
HELLO from process 0
Going INSIDE the parallel region:
 Hello from process 4
 Hello from process 0
 Hello from process 2
 Hello from process 14
 Hello from process 12
 Hello from process 13
 Hello from process 3
 Hello from process 7
 Hello from process 1
 Hello from process 8
 Hello from process 9
 Hello from process 10
 Hello from process 11
 Hello from process 5
 Hello from process 6
 Hello from process 15
Back OUTSIDE the parallel region.
Normal end of execution.
Elapsed wall clock time = 0.001034
```

Example -3

What will be the output?

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

int main()
{
        int ii;
        #pragma omp parallel
        {
                for(ii = 0; ii < 10; ++ii)
                        printf("iteration %d\n", ii);
        }
        return 0;
}
```

There is a loop. I wish to make it parallel.

WRONG

Example -4

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

int main()
{
    int i,j,n,m,temp,a[100][100];
    n=m=7;
    for(i=0;i<=n*m-1;i++) {
        temp=i/m+1;
        j=i%m+1;
        sleep(1);
        a[temp][j]=temp+100*(j-1);
    }
    for(i=0;i<=n*m-1;i++) {
        temp=i/m+1;
        j=i%m+1;
        if(i%m==0) printf("\n");
        printf("%d\t",a[temp][j]);
    }
    printf("\n");
    return 0;
}
```

```
$ ./a.out

1   101   201   301   401   501   601
2   102   202   302   402   502   602
3   103   203   303   403   503   603
4   104   204   304   404   504   604
5   105   205   305   405   505   605
6   106   206   306   406   506   606
7   107   207   307   407   507   607
```

Example -4

```
#include <stdio.h>
#include <unistd.h>
#include <omp.h>
int main()
{
    int i,j,n,m,temp,a[100][100];
    n=m=7;
    #pragma omp parallel
    {
        for(i=0;i<=n*m-1;i++) {
            temp=i/m+1;
            j=i%m+1;
            sleep(1);
            a[temp][j]=temp+100*(j-1);
        }
    }
    for(i=0;i<=n*m-1;i++) {
        temp=i/m+1;
        j=i%m+1;
        if(i%m==0) printf("\n");
        printf("%d\t",a[temp][j]);
    }
    printf("\n");
    return 0;
}
```

```
$ ./a.out

1   0   201   0   401   0   601
0   102   0   302   0   502   0
3   0   203   0   403   0   603
0   104   0   304   0   504   0
5   0   205   0   405   0   605
0   106   0   0   0   506   606
7   0   207   0   407   0   607
```

Example -4

```
#include <stdio.h>
#include <unistd.h>
#include <omp.h>
int main()
{
    int i,j,n,m,temp,a[100][100];
    n=m=7;
    #pragma omp parallel private (temp, j)
    {
        for(i=0;i<=n*m-1;i++) {
            temp=i/m+1;
            j=i%m+1;
            sleep(1);
            a[temp][j]=temp+100*(j-1);
        }
    }
    for(i=0;i<=n*m-1;i++) {
        temp=i/m+1;
        j=i%m+1;
        if(i%m==0) printf("\n");
        printf("%d\t",a[temp][j]);
    }
    printf("\n");
    return 0;
}
```

```
$ ./a.out

1   101   201   301   401   501   601
2   102   202   302   402   502   602
3   103   203   303   403   503   603
4   104   204   304   404   504   604
5   105   205   305   405   505   605
6   106   206   306   406   506   606
7   107   207   307   407   507   607
```

Work-sharing Constructs

- **for Construct**
  - **#pragma omp for** *[clause[[,] clause] ...] new-line*
    for-loop
  - ***Clause***
    - **private(***variable-list***)**
    - **firstprivate(***variable-list***)**
    - **lastprivate(***variable-list***)**
    - **reduction(***operator***:** *variable-list***)**
    - **ordered**
    - **schedule(***kind[***,** *chunk_size]***)**
    - **nowait**

Work-sharing Constructs

- **for (***init-expr***;** *var logical-op b***;** *incr-expr***)**
  - **init-expr/incr-expr: same as C**
  - **var:** A signed integer variable. If this variable would otherwise be shared, it is implicitly made private for the duration of the for. This variable must not be modified within the body of the for statement. Unless the variable is specified lastprivate, its value after the loop is indeterminate.
  - **logical-op:** >, <, >=, <=
  - ***lb*, *b*, and *incr:*** Loop invariant integer expressions. There is no synchronization during the evaluation of these expressions. Thus, any evaluated side effects produce indeterminate results.

Loop Construct

```
void nowait_example(int n, int m, floa t *a, floa t *b, floa t *y, floa t *z)
{
        #pragma omp parallel
        {
                #pragma omp for nowait
                        for (int i=1; i<n; i++)
                                b[i] = (a[i] + a[i-1]) / 2.0;
                #pragma omp for nowait
                        for (int i=0; i<m; i++)
                                y[i] = sqrt(z[i]);
        }
}
```

Example -5

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

int main()
{
    int i,x=0, a[10],b[10];

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

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

    printf("%d\n",x);
    return 0;
}
```

```
$ ./a.out
165
$
```

Example -5

```
#include <stdio.h>
#include <omp.h>
int main()
{
      int i,x=0, a[10],b[10];
      for(i=0;i<10;i++) {
            a[i]=i;
            b[i]=10-i;
      }
      #pragma omp parallel
      {
            for(i=0;i<10;i++) {
                  x = x + a[i]*b[i];
            }
      }
      printf("%d\n",x);
      return 0;
}
```

```
$ gcc -Wall -fopenmp example3_openMP.c
$ ./a.out
620
$ ./a.out
834
$ ./a.out
350
$ ./a.out
213
$ ./a.out
138
$ ./a.out
186
$ ./a.out
221
$ ./a.out
106
$ ./a.out
403
$
```

Example -5

```
#include <stdio.h>
#include <omp.h>
int main()
{
      int i,x=0, a[10],b[10];
      for(i=0;i<10;i++) {
            a[i]=i;   b[i]=10-i;
      }
      #pragma omp parallel
      {
            #pragma omp for reduction (+:x)
                  for(i=0;i<10;i++) {
                        x = x + a[i]*b[i];
                  }
      }
      printf("%d\n",x);
      return 0;
}
```

```
$ ./a.out
165
$
```

Reduction Clause

- sum is the reduction variable
- cannot be declared shared
  - threads would overwrite the value of sum
- cannot be declared private
  - private variables don't persist outside of parallel region
- specified reduction operation performed on individual values from each thread

Reduction Operand

Operator	Initial value
+	0
*	1
-	0
&	~0
|	0
^	0
&&	1
\|\| | 0