CPA – Parallel Computing

Informatics Engineering Degree

S1. Introduction to Parallel Computing Frameworks

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Content

Section 1

Programming in "C"

- A brief remind on "C"

"C" Language

"C" is a general purpose programming language

- Features: compiled, portable and efficient
- Java and C++ inherit the sintax of "C"
- A simple language kernel, additional functionality by means of software libraries.
- One of the most used languages in supercomputing

```
void daxpy(int n, double a, double *x, double *y)
{
    int i;
    for (i=0; i<n; i++) {
        y[i] = a*x[i] + y[i];
    }
}
```

Variables and Basic Types

All variables used must be previously declared

- Integer: `char`, `int`, `long`; modifier `unsigned`
- Enumerated: `enum` (equivalent to an integer)
- Floating Point: `float`, `double`
- Void type: `void` (special usage)
- Derived type: `struct`, arrays, pointers

```
char c;
int i1,i2;
enum {NORTE,SUR,ESTE,OESTE} dir;
unsigned int k;
const float pi=3.141592;
double r=2.5,g;
```

```
c = 'M';
i1 = 2;
i2 = -5*i1;
dir = SUR;
k = (unsigned int) dir;
g = 2*pi*r;
```

New types can be defined using `typedef`

```
typedef enum {ROJO,VERDE,AZUL,AMARILLO,BLANCO,NEGRO} color;
color c1,c2;
```


Sentences and Expressions

There are different types of sentences:

- Declaration of types and variables (inside/outside of the function)
- Expression, typically an assignment `var=expr`
- Composed sentence (`{...}` block)
- Conditions (`if`, `switch`), loops (`for`, `while`, `do`)
- Others: void sentences (`;`), jump (`goto`)

Expressions:

- Assignations: `=`, `+=`, `-=`, `*=`, `/=`; increments: `++`, `--`
- Arithmetic: `+`, `-`, `*`, `/`, `%`; bit-wise: `~`, `&`, `|`, `^`, `<<`, `>>`
- Logic: `==`, `!=`, `<`, `>`, `<=`, `>=`, `||`, `&&`, `!`
  Zero is equivalent to "false" and any other value stands for "true"
- Ternary operator: `a? b: c`

Examples of flow control sentences

```
if (j>0) valor = 1.0;
else valor = -1.0;
```

```
if (i>1 && (qi[i]-1.0)<1e-7) {
  zm1[i] *= 1.0+sk1[i-1];
  zm2[i] *= 1.0+sk1[i-1];
} else {
  zm1[i] *= 1.0+sk0[i-1];
  zm2[i] *= 1.0+sk0[i-1];
}
```

```
for (i=0;i<n;i++) x[i] = 0.0;
```

```
k = 0;
while (k<n) {
  if (a[k]<0.0) break;
  z[k] = 2.0*sqrt(a[k]);
  k++;
}
```

```
switch (dir) {
  case NORTH:
    y += 1; break;
  case SOUTH:
    y -= 1; break;
  case EAST:
    x += 1; break;
  case WEST:
    x -= 1; break;
}
```

```
for (i=0;i<n;i++) {
  y[i] = b[i];
  for (j=0;j<i;j++) {
    y[i] -= L[i][j]*y[j];
  }
  y[i] /= L[i][i];
}
```


Arrays and Pointers

Array: collection of variables of the same type

- Length defined in the declaration
- Elements accessed by an index (starting in 0)

```
#define N 10
int i;
double a[N],s=0.0;
for (i=0;i<N;i++)
  s = s + a[i];
```

Multidimensional arrays: `double matriz[N][M];`
Strings are arrays of type `char` ending with the character `'\0'`

Pointer: variable containing the memory address of other variable or value

- In the declaration, * is added before the name of the variable
- Operator & returns the address of a variable
- Operator * enables accessing the value pointed to

```
double a[4] =
 {1.1,2.2,3.3,4.4};
double *p,x;
p = &a[2];
x = *p;
*p = 0.0;
p = a;  /* &a[0] */
```

More about pointers

Pointer arithmetics

- Basic operations: `+`, `-`, `++`
- The increment/decrement is proportional to the pointed type size

```
char *s =
    "Parallel Computing";
char *p = s;
while (*p!='C') p++;
```

NULL pointer

- It values zero (`NULL`)
- It is an invalid pointer normally used to indicate a failure

```
double w,*p;
if (!p)
  error("Invalid Pointer");
else w = *p;
```

Generic Pointer

- Type: `void*`
- It can be casted to point to a variable of any type

```
void *p;
double x=10.0,z;
p = &x;
z = *(double*)p;
```

Multiple level pointer: `double **p` (pointer to pointer)

Structs

Structs: a collection of heterogeneous data

- Members can be accessed with `.` (or `->` in the case of struct pointers)

```
struct complex {
  double re,im;
};
struct complex c1, *c2;
c1.re = 1.0;
c1.im = 2.0;
c2 = &c1;
c2->re = -1.0;
```

```
typedef struct {
  int i,j,k;
  const char *label;
  double data[100];
} mystruct;

mystruct s;
s.label = "NEW";
```

Functions

A "C" program has at least one function (`main`)

Functions return a value (unless the funtion type were `void`)

```
double rad2deg(double x) {
  return x*57.29578;
}
```

```
void message(int k) {
 printf("Fin etapa %d\n",k);
}
```

The arguments of a function receive the values indicated in the call (references can be achieved through pointers)

```
float fun1(float a,float b){
  float c;
  c = (a+b)/2.0;
  return c;
}
...
w = fun1(6.0,6.5);
```

```
void fun2(float *a,float *b){
  float c;
  c = ((*a)+(*b))/2.0;
  if (fun3(c)*fun3(*a)<=0.0)
    *b = c;
  else *a = c;
}
...
fun2(&x,&y);
```

Functions can be declared before their definition (prototypes)

Software library functions

String processing `<string.h>`

- String copy (`strcpy`), string compare (`strcmp`)
- Memory copy (`memcpy`), memory set (`memset`)

Input-Output `<stdio.h>`

- Standard: `printf`, `scanf`
- Files: `fopen`, `fclose`, `fprintf`, `fscanf`

Standard tools `<stdlib.h>`

- Dynamic memory management: `malloc`, `free`
- Conversions: `atof`, `atoi`

Mathematic functions `<math.h>`

- Functions and Operations: `sin`, `cos`, `exp`, `log`, `pow`, `sqrt`
- Rounding: `floor`, `ceil`, `fabs`

Example with files

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

void readdata( char *filename )
{
  FILE *fd;
  int i,n,*ia,*ja;
  double *va;
  fd = fopen(filename,"r");
  if (!fd) {
    perror("Error - fopen");
    exit(1);
  }
  fscanf(fd,"%i",&n);        /* number of data to be read */
  ia = (int*) malloc(n*sizeof(int));
  ja = (int*) malloc(n*sizeof(int));
  va = (double*) malloc(n*sizeof(double));
  for (i=0;i<n;i++) {
    fscanf(fd,"%i%i%lf",ia+i,ja+i,va+i);
  }
  fclose(fd);
  process(n,ia,ja,va);
  free(ia); free(ja); free(va);
}
```


Variable Types

Global variables

- They are declared outside any function block
- They can be accessed from any point of the program
- They are allocated in the data segment

Local variables

- They are declared inside a function block
- They are only accessible by the sentences of the function block
- They are created in the (*stack*), and destroyed when leaving the function

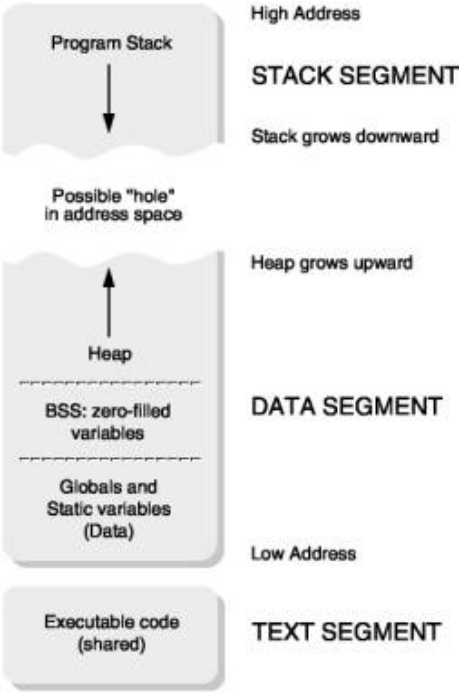
Static variables

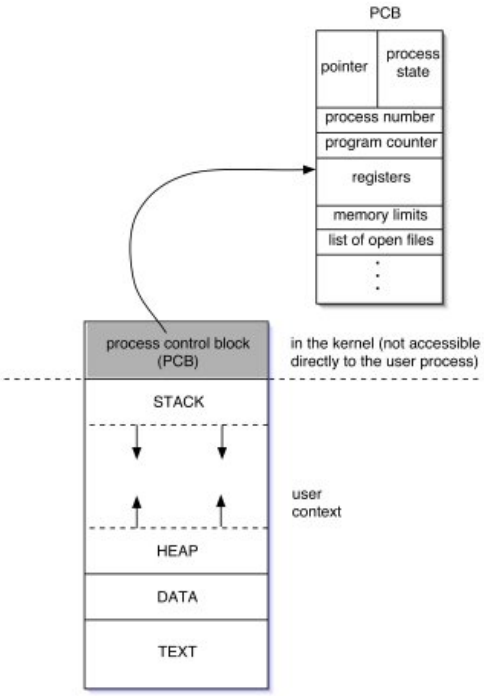
- Modifier `static`
- Local scope but persistent between successive calls

Dynamic memory allocated variables

- Variables pointing to memory allocated with `malloc`, persist until `free` function is called
- They are created in the *heap*

Memory model of Unix processes



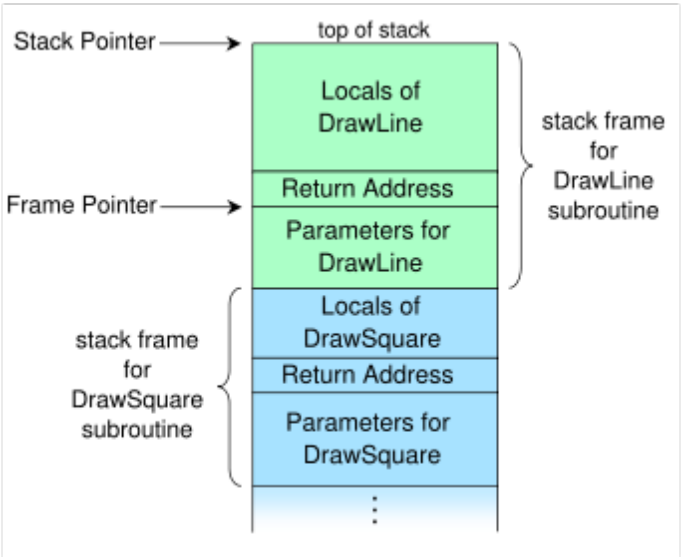


Stack

The arguments of a function are treated as local variables

When entering in a function:

1. all the arguments are inserted in the stack
2. the return address is stacked also
3. local variables are created in the stack



When executing `return` or leaving the function, the whole context created is destroyed

Section 2

Usage of Parallel Computers

- Development cycle
- Cluster for the laboratory
- Running parallel programs

Development cycle

The process of compiling consist of:

- Preprocessing: The "C" source code is modified according to a set of instructions (preprocessing directives)
- Compiling: The object code (binary) is created from the already preprocessed code
- Linking: It merges the object codes from the different modules and external libraries to generate the final executable

The development cycle is completed with the following actions:

- Automatisation of complex program compiling (`make`)
- Error debugging (`gdb`, `valgrind`)
- Performance analysis (`gprof`)

Preprocessing

Before the compiling, preprocessing takes place (the cpp command is automatically invoked)

- `include`: It inserts the content from other file
- `define`: It defines constants and macro-expressions (including arguments)
- `if`, `ifdef`: enables skiping part of the code during the compilation
- `pragma`: compiler directive

```
#include "myheader.h"

#define PI 3.141592
#define DEBUG_
#define AVG(a,b) ((a)+(b))/2

#ifdef DEBUG_
  printf("variable i=%d\n",i);
#endif
```


Compiling and Linking

Compiling: `cc`

- For each `*.c` file, a `*.o` object file is generated
- It comprises the machine code of the functions and variables, as well as a list of unsolved symbols

Linking (*link*): `ld`

- It solves all the unsolved dependencies using the `*.o` files and external software libraries (`*.a`, `*.so`)

ej.c

```
#include <stdio.h>
extern double f1(double);
int main() {
  double x = f1(4.5);
  printf("x = %g\n",x);
  return 0;
}
```

f1.c

```
#include <math.h>
double f1(double x) {
  return 2.0/(1.0+log(x));
}
```

```
$ gcc -o ej ej.c f1.c -lm
```

Parallel program compilation

OpenMP is based on directives `#pragma omp`

- A compiler without OpenMP support ignores these directives
- Modern compilers have these support, provided that a special option is included in the compilation and linkage

```
$ gcc -fopenmp -o prgomp prgomp.c
```

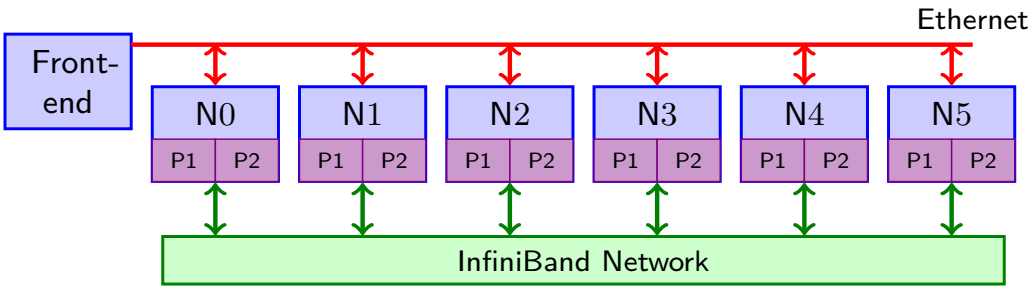
MPI provides the `mpicc` command

- Invokes `cc` adding all the necessary options for MPI codes (MPI software libraries, `mpi.h` path)
- Eases the compilation in different computers and environments
- `mpicc -show` shows the options available
- Also availbe for other languages: `mpicxx`, `mpif77`, `mpif90`

```
$ mpicc -o prgmpi prgmpi.c
```


Cluster for the laboratory

Hardware configuration: 6 biprocessors linked with InfiniBand



Each node:

- 2 AMD Opteron 16 Core 6272 processor, 2.1Ghz, 16MB
- 32GB DDR3 1600 memory
- 500GB, SATA 6 GB/s HD
- InfiniBand QDR 40Gbps adapter

In total: 12 proc, 192 cores, 192 GB

Parallel computing: Front-End

The *front-end* enables users to interact with the cluster

Accessing the front-end:

```
$ ssh -X user@kahan.dsic.upv.es
```

For routine tasks. (Do not run costly executions)

- Editing and compiling programs
- Short test runs

Useful commands:

- Files/directories: `cd`, `pwd`, `ls`, `cp`, `mkdir`, `rm`, `mv`, `scp`, `less`, `cat`, `chmod`, `find`
- Processes: `w`, `kill`, `ps`, `top`
- Editors and others: `vim`, `emacs`, `pico`, `man`

Lab cluster: Network

Gigabit Ethernet

- Auxiliar network, only for the O.S. traffic (`ssh`, NFS)

InfiniBand

- High bandwidth network with low latency, perfect for clusters
- Evolution from other networks such as Myrinet
- Bidirectional bus, with serveral transfer rates (simple, doble, ...); links can be grouped by 4 or 12

	SDR	DDR	QDR
1X	2.5 Gbps	5 Gbps	10 Gbps
4X	10 Gbps	20 Gbps	**40 Gbps**
12X	30 Gbps	60 Gbps	120 Gbps

- Coding ratio 8B/10B: Effective communication bandwidth of 32 Gbps
- Latency: theoric 100ns, in practice around 1-2μs
- Switched topology (using a *switch*)

Running parallel programs

OpenMP: Executables can be run directly

Usually the number of threads should be indicated

```
$ OMP_NUM_THREADS=4 ./prgomp
```

Other option is to export the variables

```
$ OMP_NUM_THREADS=4; OMP_SCHEDULE=dynamic
$ export OMP_NUM_THREADS OMP_SCHEDULE
$ ./prgomp
```

MPI: use `mpiexec` (or `mpirun`) commands

Options: choose hosts, architecture

```
$ mpiexec -n 4 prgmpi <args>
$ mpiexec -n 6 -host node1,node2,node5 prgmpi
```

MPMD mode

```
$ mpiexec -n 2 program1 : -n 2 program2
```


Wueue system

The Queue system (or job scheduler or resource manager) is a software that enables sharing a cluster among different users

- The user can run "jobs" usually in *batch* mode (non interactive) using one or several nodes
- A job is a particular execution with a set of attributes (nodes, maximum execution time, etc.)
- Job scheduling policies are defined
- The system accounts the resources used (hours)
- Objective: maximize usage and minimize waiting time

Working procedure:

1. A job is defined and then submitted to a queue, which returns an identifier.
2. Depending on the workload, after a waiting time the job is run.
3. The output is obtained when the job finishes.

Lab cluster: Queues (1)

TORQUE is a queue system based on PBS (*Portable Batch System*)

Example of a job `prac1.sh`

```
#PBS -q cpa
#PBS -l nodes=1:ppn=8,walltime=2:00:00
cd $HOME/prac/p1
./imagenes
```

- `-q`: name of the queue to submit the job
- `-l`: list of resources (nodes, memory, architecture,...)
- `-N`: name of the job
- `-m`,`-M`: sends an e-mail
- `-j`: merges the standard output and error in a single file

For MPI, use `mpiexec` (`-n` is)

Lab cluster: Queues (2)

For the submission of a job:

```
$ qsub prac1.sh
3482.kahan
```

At the end, two files are created in the current directory: `prac1.o3482` (output) y `prac1.e3482` (error)

For browsing the status of the job:

```
$ qstat
Job id            Name      User    Time   S Queue
----------------- --------- ------- ------ - -----
3482.kahan        prac1.sh  alum1   0      Q cpa
```

Possible status: queued (`Q`), running (`R`), ended (`E`)

Job cancelling: `qdel`