Com S // Cpr E // Math 5250

Numerical Analysis of High-Performance Computing

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Lecture 7: Summary up until now & Intro to C

Outline

1. Summary up until now
2. Introduction to C

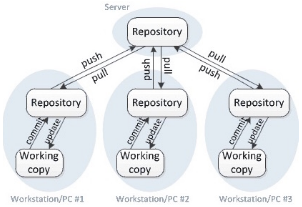
Summary up until now

Unix shell

Basic commands:

- `pwd`, `ls`, `cd`
- `cp`, `mv`, `rm`
- `rm -r`, `mkdir`

Git: distributed version control



https://homes.cs.washington.edu/~mernst/advice/version-control.html

- When you git clone a repository you get all the history (stored in .git)
- Git commands:
  - git clone – clone an existing repository
  - git status – check what files have been modified
  - git stage – add current changes into your next commit
  - git commit – commits to your clone's .git directory
  - git push – sends your recent changesets to another clone
  - git pull – pulls changesets from another clone
- The `.gitignore` file: ignore certain files in commit list

Python: multi-purpose scripting language

- Freely available, open source scripting language
- Basic Python (supports ints, floats, lists, and tuples)
- **Scripts:** can write a `.py` file that contains lists of python commands
- **Functions:** functions that can be called directly in the Python command window or by other scripts/functions
- **Modules:** a collection of related functions
- Python modules often end with a section that looks like:

```
if __name__ == "__main__":
        # some code
```

This code is not executed if the file is imported as a module, only if it is run as a script, e.g., from Unix command line:

```
$ python3 filename.py
```

Python: multi-purpose scripting language

- File output:

```
fid = open('input.data', 'w')
for k in range(0,kmax):
    value = ...
    fid.write("%12.6e" % value)
    fid.write("\n");
fid.close()
```

- File input:

```
A = np.zeros(kmax,dtype=float)
fid = open('input.data', 'r')
for k in range(0,kmax):
    linestring = fid.readline()
    linelist   = linestring.split()
    A[k]       = np.float(linelist[0])
fid.close()
```

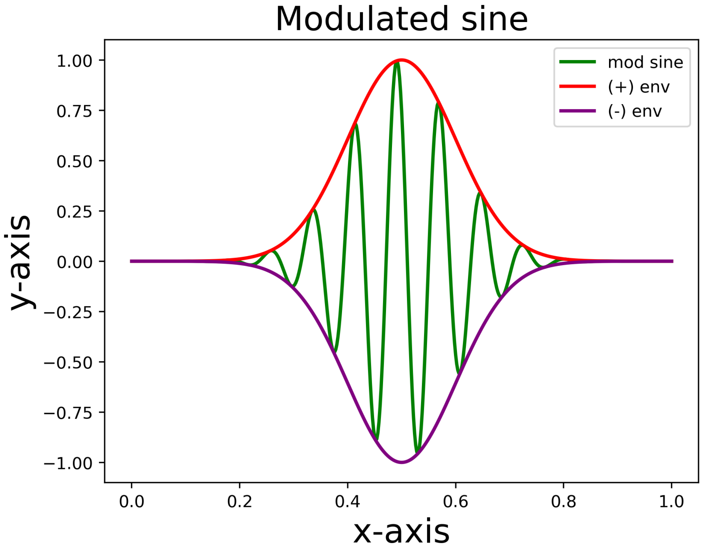
- **NumPy:** module for numerical linear algebra (e.g., `numpy.array`)
- **SciPy:** module for scientific computing (e.g., numerical integration)

Python: multi-purpose scripting language

Matplotlib: module for visualizing data in Python

```
import numpy as np
import matplotlib.pyplot as plt

x  = np.linspace(0,1,501)
y1 = np.exp(-50.0*(x-0.5)**2)*np.sin(80.0*x)
y2 = np.exp(-50.0*(x-0.5)**2)
y3 = -y2

plt.plot(x,y1,linewidth=2,color="green",label="mod sine")
plt.plot(x,y2,linewidth=2,color="red",label="(+) env")
plt.plot(x,y3,linewidth=2,color="purple",label="(-) env")
plt.legend()

plt.xlabel("x-axis",size=20); plt.ylabel("y-axis",size=20);
plt.title("Modulated sine",size=20)

plt.savefig('example2.png',dpi=400,bbox_inches='tight')
plt.show()
```

Python: multi-purpose scripting language



Introduction to C

Compiled vs. interpreted language

Not so much a feature of language syntax as of how language is converted into machine instructions.

Many languages use elements of both.

Interpeter:

- Takes commands one at a time, converts into machine code, and executes.
- Allows interactive programming at shell prompt (e.g., Python or Matlab).
- Cannot take advantage of optimizing over an entire program – does not know what instructions are coming next.
- Must translate each command while running the code, possibly many times over in a loop.
- **Bottom line:** a language that uses only an interpreter, sacrifices some **computational speed** for **coding efficiency** & **interactivity**

Compiled language

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Often large programs consist of many separate files and/or library routines – we do not want to re-compile them all when only one is changed.

Later, we will use Makefiles to handle this.

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Purpose and design of C:

- Designed to provide low-level access to memory and to provide language constructs that map efficiently to machine instructions (similar to assembly)
- Despite its low-level capabilities, the language was designed to encourage cross-platform programming and much simpler to read and write compared to assembly.

A very simple example

$ISUHPC/lectures/lecture7/codes/HelloWorld.c:

```c
#include <stdio.h>

int main()
{
   // Print a message to the screen
   printf("\n");
   printf("Hello World! My name is Cy.\n");
   printf("\n");

   // Return 0 to signify successful completion
   return 0;
}
```

- Compile by typing (in Unix):

```
$ gcc HelloWorld.c
```

- This will produce the executable: `a.out`
- Run by typing (in Unix):

```
$ ./a.out
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- Compile by typing (in Unix):

```
$ gcc HelloWorld.c -o hello
```

- This will produce the executable: `hello`
- Run by typing (in Unix):

```
$ ./hello
```

Some comments: A very simple example

Every C program must have a main function that is the entry point for the program.

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Indentation is optional (but **HIGHLY** recommended). In Python: **NOT OPTIONAL**.

Declaring variables

$ISUHPC/lectures/lecture7/codes/example1.c:

```c
#include <stdio.h>

int main()
{
    // Declare some variables
    double x = 3.0;
    double y = 0.1;
    double z;

    // Add x and y and store in z
    z = x+y;

    // Print z to screen
    printf(" z = %010.4f\n",z);

    // Return 0 to signify successful completion
    return 0;
}
```

Declaring variables

Compiling & running this code:

```
$ gcc example1.c -o ex1

$ ./ex1
 z = 3.100000
```

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Compiling & running this code:

```
$ gcc example1.c -o ex1

$ ./ex1
 z = 3.100000
```

Formating:

```
printf(" z = %f\n",z);
 z = 3.100000

printf(" z = %6.4f\n",z);
 z = 3.1000

printf(" z = %10.4e\n",z);
 z = 3.1000e+00

printf(" z = %22.16e\n",z);
 z = 3.1000000000000001e+00
```

Declaring variables

$ISUHPC/lectures/lecture7/codes/types.c:

```c
#include <stdio.h>

int main()
{
   // Standard data types
   char cyclops; // character, format: %c
   int iceman;   // 16-bit int, format: %i
   float storm;  // 32-bit float, format: %f
   double rogue; // 64-bit float, format: %f or %lf

   // Extended data types
   long int beast;       // 32-bit int, format: %li
   long long int havok; // 64-bit int, format: %lli
   long double mimic;    // 128-bit float, format: %Lf

   // Return 0 to signify completion
   return 0;
}
```

Compile-time errors

$ISUHPC/lectures/lecture7/codes/example1a.c:

```c
    // Declare some variables
    double x = 3.0;
    double y = 0.1;
    double z;

    // Add x and y and store in z
    zz = x+y;

    // Print z to screen
    printf(" z = %f\n",z);
```

Generates compile-time error:

```
$ gcc example1a.c
example1a.c:11:4: error: use of undeclared identifier 'zz'
   zz = x+y;
   ^
1 error generated.
```

A more subtle mistake

$ISUHPC/lectures/lecture7/codes/example1b.c:

```c
    // Declare some variables
    double x = 3.0;
    double y = 0.1;
    double z,zz;

    // Add x and y and store in z
    zz = x+y;

    // Print z to screen
    printf(" z = %f\n",z);
```

Generates wrong answer:

```
$ gcc example1b.c
$ ./a.out
 z = 0.000000
```

For loops in C

$ISUHPC/lectures/lecture7/codes/loop1.c:

```c
#include <stdio.h>

int main()
{
   // Declare some variables
   const int n = 8;
   int nfactorial = 1;
   int i;
   // A loop
   for (i=1; i<=n; i++)
   {
      nfactorial = nfactorial*i;
   }

   // Print to screen
   printf(" nfactorial = %i\n",nfactorial);

   return 0;
}
```

For loops in C

Answer:

```
$ gcc loop1.c
$ ./a.out
 nfactorial = 40320
```

For loops in C

Answer:

```
$ gcc loop1.c
$ ./a.out
 nfactorial = 40320
```

Format of for loops:

```
for (int i=start_index; i<=end_index; i++)
{
  // 'i' will be incremented by 1 each time
}

for (int i=start_index; i>=end_index; i--)
{
  // 'i' will be decremented by 1 each time
}

for (int i=start_index; i<=end_index; i+=2)
{
  // 'i' will be incremented by 2 each time
}
```

If-else statement in C

$ISUHPC/lectures/lecture7/codes/ifelse1.c:

```
    // Declare some variables
    double x = -1.43;
    double y = 4.5014;
    double min;

    // Check which one is smaller
    if (x<y)
    {
       min = x;
    }
    else
    {
       min = y;
    }

    // Print to screen
    printf(" min = %f\n",min);
```

If-else statement in C

Answer:

```
$ gcc ifelse1.c
$ ./a.out
 min = -1.430000
```

If-else statement in C

Answer:

```
$ gcc ifelse1.c
$ ./a.out
 min = -1.430000
```

Logical operators:

```
x == a                      // == is the logical equality test

if ( (x==a) || (x==b) )     // || is the logical 'or'

if ( (x>a) && (x<b) )       // && is the logical 'and'

if ( x != 3.8 )             // ! is the logical 'not'

if ( ( (x>a) && (x<b) ) || x==0.0 ) // use parenthesis to clarify
```

Lab assignment

Develop a script ("main program") with name **lab.c**: computing factorial of an integer *n*, exponential of a real number x, and logarithm of a real number y.

submit code and screenshot