CS601: Software Development for Scientific Computing

Autumn 2021

Week1: Overview

Who this course is for?

- Anybody who wishes to develop “computational thinking“
  - A skill necessary for everyone, not just computer programmers
  - More on this later…

Course Takeaways

- Non-CS majors:
  - Write code and
  - Develop software (not just write standalone code)
    - Numerical software
- CS-Majors:
  - Face mathematical equations and implement them with confidence

What is this course about?

Software Development

+

Scientific Computing

Software Development

- *Software development is the process of conceiving, specifying, designing, programming, documenting, testing, and bug fixing involved in creating and maintaining applications, frameworks, or other software components.*

Software development is a process of writing and maintaining the source code, but in a broader sense, it includes all that is involved between the conception of the desired software through to the final manifestation of the software, …

- Wikipedia on “Software Development”

Scientific Computing

- Also called computational science
  - *Development of models to understand systems (biological, physical, chemical, engineering, humanities)*

Collection of tools, techniques, and theories required to solve on a computer mathematical models of problems in science and engineering

This course NOT about..

- Software Engineering
  - Systematic study of Techniques, Methodology, and Tools to build correct software within time and price budget (topics covered in CS305)
    - People, Software life cycle and management etc.
- Scientific Computing
  - Rigorous exploration of numerical methods, mathematical models, and theories
  - Programming models (topics covered in CS410)

Who this course is for?

- You are interested in scientific computing
- You are interested in high-performance computing
- You want to build / add to a large software system

Why C++ ?

- C/C++/Fortran codes form the majority in scientific computing codes
- Catch a lot of errors early (e.g. at *compile-time* rather than at *run-time)*
- Has features for *object-oriented* software development
- Known to result in codes with better *performance*

Who this course is for?

- Anybody who wishes to develop "computational thinking"
  - A skill necessary for everyone, not just computer programmers
  - An approach to problem solving, designing systems, and understanding human behavior that draws on concepts fundamental to computer science.

Computational Thinking - Examples

- How difficult is the problem to solve? And what is the best way to solve?
- Modularizing something in anticipation of multiple users
- Prefetching and caching in anticipation of future use
- Thinking recursively
- Reformulating a seemingly difficult problem into one which we know how to solve by reduction, embedding, transformation, simulation
  - Are approximate solutions accepted?
  - False positives and False negatives allowed? etc.
- Using abstraction and decomposition in tackling large problem
- ...

Computational Thinking – 2 As

- Abstractions
  - Our "mental" tools
  - Includes: <u>choosing right abstractions</u>, operating at multiple <u>layers</u> of abstractions, and defining <u>relationships</u> among layers
- Automation
  - Our "metal" tools that <u>amplify</u> the power of "mental" tools
  - Is mechanizing our abstractions, layers, and relationships
    - Need precise and exact notations / models for the "computer" below ("computer" can be human or machine)

Computing - 2 As Combined

- Computing is the automation of our abstractions
- Provides us the ability to scale
  - Make infeasible problems feasible
    - E.g. SHA-1 not safe anymore
  - Improve the answer's precision
    - E.g. capture the image of a black-hole

Summary: choose the right abstraction and computer

Example - Factorial

- `n! = n x (n-1) x (n-2) x . . . x 3 x 2 x 1`

  `(n–1)! = (n-1) x (n-2) x . . . x 3 x 2 x 1`

  therefore,

  Definition1: `n! = n x (n-1)!`

  is this definition complete?

  - plug 0 to n and the equation breaks.

  Definition2:

$$n! = \begin{cases} n \times (n-1)! & \text{when } n>=1 \\ 1 & \text{when } n=0 \end{cases}$$

Exercise 1

- Does this code implement the definition of factorial correctly?

```
int fact(int n){
    if(n==0)
       return 1;

    return n*fact(n-1);

}
```

Example - Factorial

Definition2:

$$n! = \begin{cases} n \times (n-1)! & \text{when } n>=1 \\ 1 & \text{when } n=0 \end{cases}$$

is this definition complete?

- `n!` is not defined for negative `n`

Solution - Factorial

```
int fact(int n){
    if(n<0)
        return ERROR;
    if(n==0)
        return 1;

    return n*fact(n-1);

}
```

Exercise 2

- In how many `flops` does the code execute?

  `1 flop = 1` step executing ***any*** arithmetic operation

```
int fact(int n){
    if(n<0)
        return ERROR;
    if(n==0)
        return 1;

    return n*fact(n-1);

}
```

Exercise 3

- Does the code yield correct results for any n?

```
int fact(int n){
    if(n<0)
        return ERROR;
    if(n==0)
        return 1;

    return n*fact(n-1);

}
```