CAS 741, CES 741 (Development of Scientific Computing Software)

Fall 2019

01 Introduction

Dr. Spencer Smith

Faculty of Engineering, McMaster University

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Introduction to CAS 741 (CES 741)

- Administrative details
- Brief overview of course
- Introductions
- Course outline
- Requirements

Administrative Details

- New Grad Stdnt Orientation: Mon, Sept 9, 10 am – 1 pm
- Lectures: Mon and Thurs, 10:30 am – 12:00 noon
- Avenue for grade tracking
  - http://avenue.mcmaster.ca/
  - Consider putting a picture up on Avenue
- We'll also use git on GitLab for the course material
  - https://gitlab.cas.mcmaster.ca/
  - Create your account by logging in, option to set CAS password to MacID password
  - Course material and issue tracking at https://gitlab.cas.mcmaster.ca/smiths/cas741
- Your projects will be hosted on GitHub
  - https://github.com/
  - Create an account, if you do not already have one
  - Give the instructor (me) master access to your repo

Overview of the Course

- Application of software engineering methodologies to improve the quality of scientific computing software
- What is the definition of scientific computing?
- What are some examples of scientific computing and scientific computing software?
- What is the definition of software engineeing?
- What are some techniques, tools and principles for software engineering?

Scientific Computing (SC)

- Scientific computation consists of using computer tools to simulate mathematical models of real world systems so that we can better understand and predict the system's behaviour.
- Examples
  - Temperature of fuel-pin in nuclear reactor
  - Flow of pollutant in groundwater
  - Displacement of a structure
  - Thickness of cast film
  - Temperature of water in a solar water heating tank over time
  - Ordinary Differential Equation solver
  - Root finding solver etc.
- Includes analysis, design and "exploration"

Software Engineering (SE)

- SE is an area of engineering that deals with the development of software systems that
  - Are large or complex
  - Exist in multiple versions
  - Exist for large period of time
  - Are continuously being modified
  - Are built by teams
- SE is "application of a systematic, disciplined, quantifiable approach to the development, operation and maintenance of software" (IEEE 1990)
- D. Parnas (1978) defines SE as "multi-person construction of multi-version software"
- Like other areas of engineering, SE relies heavily on mathematical techniques (logic and discrete math)
- SE might be applied to SC for software certification

SE Tools, Techniques and Principles

- Tools
  - Programming languages
  - Version control software (git, svn, etc)
  - Debugger
  - Profiler
  - ...
- Techniques
  - Documentation
  - Testing
  - Program families
  - Code generation
  - ...
- Principles
  - Information hiding
  - Least privelege
  - ...

Instructor

- Instructor
  - Dr. Spencer Smith (`smiths@mcmaster.ca`)
  - ITB/167
  - Drop in or make an appointment

Introduction: Dr. Spencer Smith

- Associate Professor, Department of Computing and Software.
- B.Eng.C.S, Civil Engineering Department, McMaster University.
  M.Eng., Ph.D., Civil Engineering Department, McMaster University.
- P.Eng. (Licensed Professional Engineer in Ontario).
- Teaching: Software design, scientific computing, introduction to computing, communication skills, software project management.
- Research: Application of software engineering methodologies to improve the quality of scientific computing software.

Introductions

- Your name
- Degree program
- Academic background
- Experience with:
  - Physics
  - Scientific computing
  - Continuous math
  - Discrete math
  - Software engineering
  - Software development technology
    - Git
    - GitHub or GitLab
    - LaTeX
    - Make etc.
- What do you hope to get out of this course?

Course Introduction

- Calendar description
  - Principles of software development for reliable and sustainable scientific and engineering software
  - Systematic process for development and documentation of
    - Requirements
    - System architecture
    - Detailed design
    - Implementation
    - Verification and Validation Plan
    - Verification and Validation Report

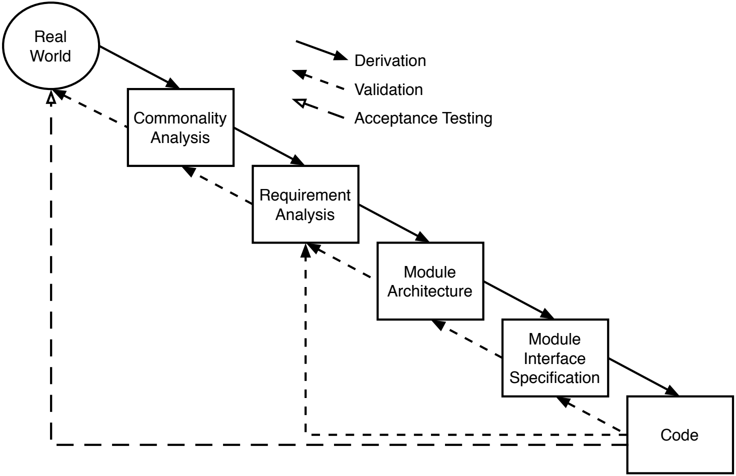
Course Project

- Select a candidate SC problem
  - Requires approval from instructor
  - Will accommodate your interests as much as feasible
  - Select a project related to your research
  - Scope needs to be feasible within one term
- Milestones
  1. Software Requirements Specification (SRS)
  2. Module Guide (MG)
  3. Module Interface Specification (MIS)
  4. Implementation (and appropriate programming language)
  5. VnV Plan
  6. VnV Report
- Deliverables can potentially be modified to provide project flexibility

Project Selection: Desired Qualities

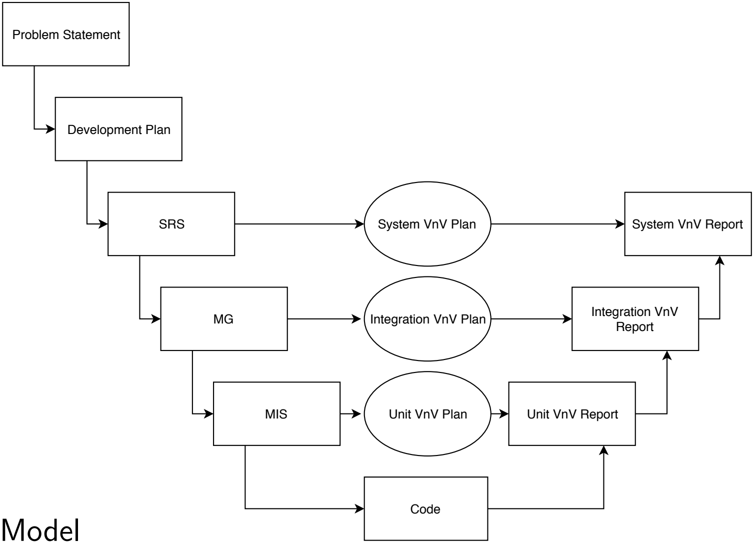
- Related to scientific computing
- Simple, but not trivial
- If feasible, select a project related to your research
- Possibly re-implement existing software
- Each student project needs to be unique
- Possibly a specific physical problem
- Possibly a (family of) general purpose tool(s)
- Some examples follow, the links are just places to get started

"Faked" Rational Design Process



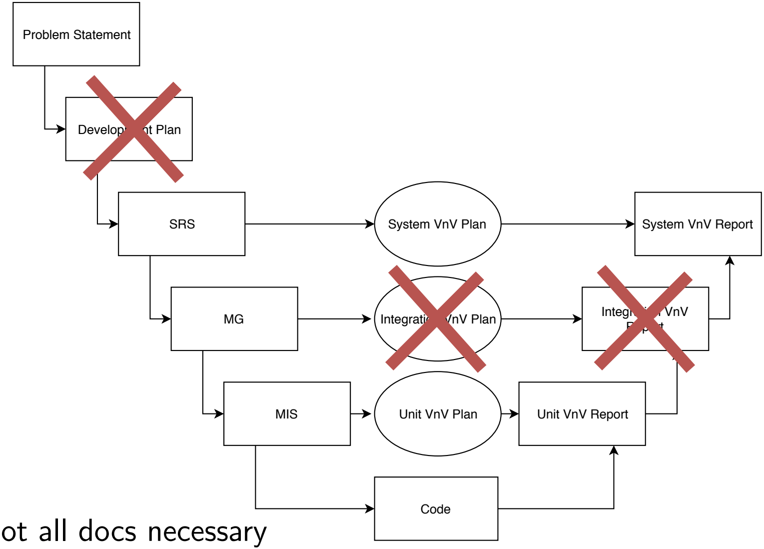
See Parnas and Clements 1986 about "Faking It"

Our “Faked” Process



V Model

Our Deliverables



Not all docs necessary

Course Structure

- Student and instructor presentations
- Classroom discussions
- Will present a subset of your documentation for in-class feedback
- Structure from our documentation
- Use GitHub issue tracker for feedback from other students

Grade Assessment

1. Presentations and class discussion 5%
2. "Domain Expert" and secondary reviewer roles 10%
3. Problem Statement 0%
4. System Requirements Specification (SRS) 15%
5. System Verification and Validation (VnV-Syst) Plan 15%
6. Module Guide and Module Interface Specification (MG and MIS) 15%
7. Final Documentation (including revised versions of previous documents, plus the source code, unit testing plan, reflection report and testing reports (System and Unit)) 40%
8. Drasil simple physics example, pull request accepted 5% (Bonus)

Policy Statements

- Ideas to improve the course are welcomed
- Missed/late work please communicate in advance, or a penalty of 20 % per working day
- If there is a problem with discrimination please contact the Department Chair, or other appropriate body

Academic Dishonesty

- Academic dishonesty consists of misrepresentation by deception or by other fraudulent means
- Can result in serious consequences, e.g. the grade of zero on an assignment, loss of credit with a notation on the transcript, and/or suspension or expulsion from the university.
- It is your responsibility to understand what constitutes academic dishonesty
- Three examples of academic dishonesty
  - Plagiarism
  - Improper collaboration
  - Copying or using unauthorized aids in tests and examinations
- Academic dishonesty will not be tolerated!

Assigned Reading

As often as possible, hyperlinks are included for references in the lecture slides

- W. Spencer Smith. A rational document driven design process for scientific computing software.
  In Jeffrey C. Carver, Neil Chue Hong, and George Thiruvathukal, editors, *Software Engineering for Science*, chapter Section I – Examples of the Application of Traditional Software Engineering Practices to Science, pages 33–63. Taylor & Francis, 2016
- W. Spencer Smith, Lei Lai, and Ridha Khedri.

  Requirements analysis for engineering computation: A systematic approach for improving software reliability.
  Reliable Computing, Special Issue on Reliable Engineering Computation, 13(1):83–107, February 2007

Assigned Reading

- David L. Parnas and P.C. Clements. A rational design process: How and why to fake it. *IEEE Transactions on Software Engineering*, 12(2): 251–257, February 1986
- Solar Water Heating System Example
- Solar Water Heating System Example SRS (Generated by Drasil)
- Projectile Example SRS (Generated by Drasil)
- Recommended reading order for SRS documents
  - Goal Statement
  - Instance Models
  - Requirements
  - Introduction
  - Specific System Description