

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

Fall 2019

## 02 Getting Started

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# Getting Started

- Administrative details
- Any more introductions?
- Project choices
- Software tools
  - ▶ Git, GitLab and GitHub (Issue Creating Exercise)
  - ▶ LaTeX
  - ▶ Make
- Questions on suggested reading?
- Software Engineering for Scientific Computing literature

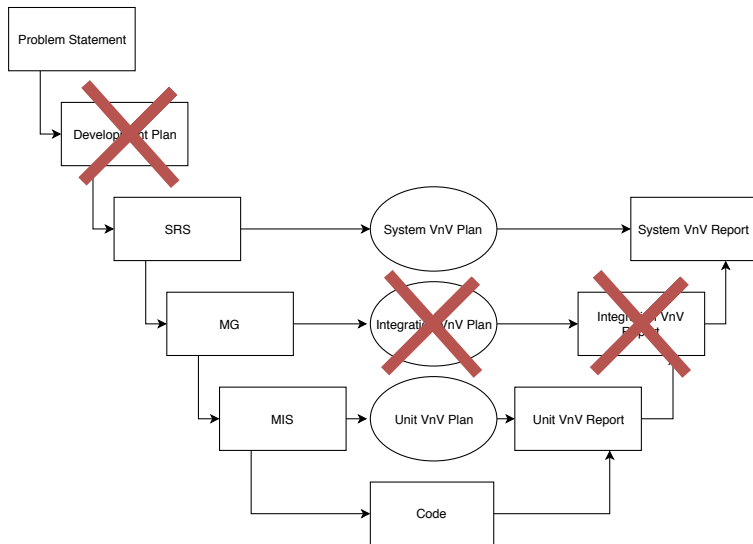
# Administrative Details

- Can everyone access GitLab?  
<https://gitlab.cas.mcmaster.ca/smiths/cas741>
- Use folder structure given in repo (will be updating)
- Post any questions as issues in our repo
- Create a GitHub account if you don't already have one
- Add `smiths` to your GitHub repos
- Problem statement
  - ▶ Problem statement due Thurs, Sept 19 by 11:59 pm
  - ▶ Assign the instructor an issue to review your problem statement
- Issue creating exercises due Thurs, Sept 19 by 10:30 am
- Feel free to add me to you Linked-In network

# Administrative Details: Domain Expert

- Creates issues for their partner's written deliverables
- Asks questions during their partner's presentations
- Implements one module following their partner's spec

# Administrative Details: Our Deliverables



# Administrative Details: Presentations

SRS Present	Week 04	Week of Sept 30
Syst. VnV Present	Week 07	Week of Oct 24
MG Present	Week 9	Week of Oct 29
MIS Present	Week 11	Week of Nov 12
Unit VnV or Implement Present	Week 13	Week of Nov 26

- Very tentative dates
- Specific schedule depends on final class registration and need
- Informal presentations with the goal of improving everyone's written deliverables
- Domain experts and secondary reviewers (and others) will ask questions

# Administrative Details: Report Deadlines

Issue Creation Exercise	Week 03	Sept 19
Problem Statement	Week 03	Sept 19
System Requirements Specification (SRS)	Week 06	Oct 10
System VnV Plan	Week 08	Oct 22
Module Guide (MG)	Week 10	Nov 5
Module Interface Specification (MIS)	Week 12	Nov 19
Final Documentation	Week 14	Dec 10

- The written deliverables will be graded based on the repo contents as of 11:59 pm of the due date
- If you need an extension, please ask
- Two days after each major deliverable, your GitHub issues will be due
- Domain expert code due 1 week after MIS deadline

# Introductions (if necessary)

- Your name
- Degree program
- Academic background
- Experience with:
  - ▶ Science (such as 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?

# 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

# Project Selection: Specific Physical Problem

- Heated rod
- Heated plate
- Double pendulum
- Rigid body dynamics
- Column buckling
- Damped harmonic oscillator
- Stoichiometric calculations (chemical balance)
- Predator prey dynamics
- Imaging: filters, edge detection etc.
- Medical Imaging
- etc.

# Project Selection: Family of General Purpose Tools

- Solution of ODEs
- Solution of  $Ax = b$
- Regression
- Interpolation
- Numerical integration
- FFT
- Mesh generation
- Finite element method
- Any chapter from a standard numerical methods textbook
- etc.

# Tool Tutorials

- Best way to learn is by doing
- Some getting started information and exercises in the [ToolTutorials](#) folder, modified from undergrad classes
- Tutorials for [se 2aa4](#) and [cs 2me3](#)
- Many other resources on-line
- Your colleagues can help too

# Git, GitLab and GitHub

- Git manages changes to documents
  - ▶ Tracks changes
  - ▶ Keeps history, you can roll back
  - ▶ Useful documentation over time
  - ▶ Allows people to work simultaneously
- Benefits for SC [25]
  - ▶ Not necessary to make a backup copy of everything, stores just enough information to recreate
  - ▶ Do not need to come up with names for backup copies - same file name, but with timestamps
  - ▶ Enforces changelog discipline
  - ▶ Facilitates identifying conflict and merging changes
- The real bottleneck in scientific computing [26]

# Git Typical Usage

First either init repo or clone (git init, git clone), then typical workflow is

1. update repo (git pull)
  2. create files
  3. stage changes to be committed (git status, git add)
  4. commit staged changes (git commit -m "message")
  5. push to remote, if using one (git push)
- Commit after every separate issue, and when need to stop working
  - Always include a meaningful and descriptive commit message for the log
  - If a push reveals conflicts, take appropriate action to merge

# GitLab and GitHub Issue Tracking

- See brief document in course repo
- See examples
- Tutorials for se 2aa4 and cs 2me3
- Create an issue

# Issue Creating Exercise

- Due by Thurs, Sept 19, 10:30 am
- Create 2 to 3 issues for case studies in Drasil repo
- <https://jacquescurette.github.io/Drasil/>
- Select any case study that interests you and review the SRS
- Create issues at <https://github.com/JacquesCurette/Drasil/issues>
- Assign issues to smiths
- Consider using SRS [checklist](#) (except for major revision history)
- Additional guidance in [SRS Template](#)

# LaTeX

- A typesetting language
- Some initial information in course repo
- Tutorials for [se 2aa4](#) and [cs 2me3](#)
- Start from an example
  - ▶ The lectures notes
  - ▶ The Blank Project Template
  - ▶ The problem statement

# Make

- Software Carpentry: Automation and Make
- The Blank Project Template

# Suggested Reading Questions?

- Smith2016 [20]
- SmithEtAl2007 [22]
- ParnasAndClements1986 [14]
- Solar Water Heating System Example

# SE For SC Literature

- CAS 741 process is document driven, adapted from the waterfall model [6, 24]
- Many say a document driven process is not used by, nor suitable for, scientific software.
  - ▶ Scientific developers naturally use an agile philosophy [1, 4, 5, 17],
  - ▶ or an amethododical process [9]
  - ▶ or a knowledge acquisition driven process [10].
- Scientists do not view rigid, process-heavy approaches, favorably [4]
- Reports for each stage of development are counterproductive [16, p. 373]
- Up-front requirements are impossible [4, 18]
- What are some arguments in favour of a rational document driven process?

# Counter Arguments

- Just because not used, doesn't mean docs shouldn't be
- Documentation provides many benefits [15]:
  - ▶ easier reuse of old designs
  - ▶ better communication about requirements
  - ▶ more useful design reviews
  - ▶ easier integration of separately written modules
  - ▶ more effective code inspection
  - ▶ more effective testing
  - ▶ more efficient corrections and improvements.
- Actually faking a rational design process
- Too complex for up-front requirements sounds like an excuse
  - ▶ Laws of physics/science slow to change
  - ▶ Often simple design patterns
  - ▶ Think program family, not individual member
- Debunking myth against up-front requirements [19]

# Literature on SE applied to SCS

- Highlights problems with SE
  - ▶ [Miller2006 \[12\]](#)
  - ▶ [Hatton2007 \[7\]](#)
  - ▶ Sleipner A oil rig collapse [[13](#), p. 38]
  - ▶ Patriot missile disaster [[13](#), p. 36]
- Highlights gap/chasm between SE and SC
  - ▶ [Kelly2007 \[11\]](#)
  - ▶ [Storer2017 \[23\]](#)
- Studies of SE applied to SC
  - ▶ [CarverEtAl2007 \[4\]](#)
  - ▶ [Segal2005 \[17\]](#)

# Literature on SE applied to SCS

- Reproducibility
  - ▶ BaileyEtAl2016 [2]
  - ▶ BenureauAndRougier2017 [3]
- Future of SE for SC
  - ▶ JohansonAndHasselbring2018 [8]
  - ▶ Smith2018 [21]

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