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

Fall 2017

02 Getting Started

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September 7, 2018

Getting Started

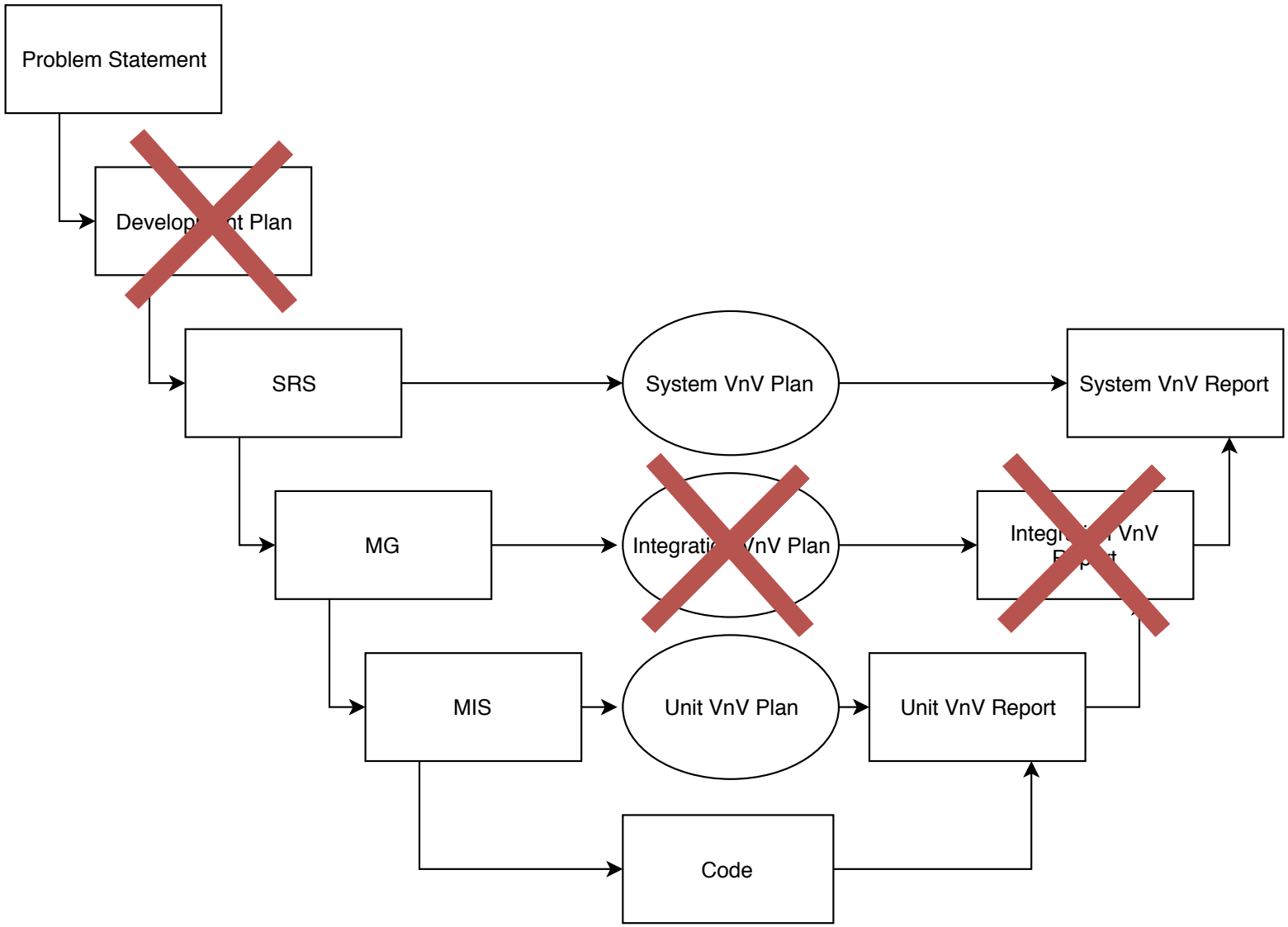
- Administrative details
- Any more introductions?
- Project choices
- Software tools
- Questions on suggested reading?
- Software Engineering for Scientific Computing literature

Administrative Details

- Classes are 1.5 hours long :-)
- Use folder structure given in repo (will be updating)
- Post any questions as issues in our repo
- Problem statement due Friday, Sept 15 by 11:59 pm

Benches and Glassboards

Administrative Details: Our Deliverables



Administrative Details: Grade Assessment

1. Presentations and class discussion 10%
2. Quality of GitHub issues provided to classmates 5%
3. Problem Statement 0%
4. System Requirements Specification (SRS) 20%
5. Verification and Validation (VnV) Plan 15%
   - 5.1 System VnV Plan 10%
   - 5.2 Unit VnV Plan 5%
6. Module Guide (MG) 5%
7. Module Interface Specification (MIS) 15%
8. Final Documentation 30%
   - 8.1 Problem Statement, SRS, System VnV Plan, MG, MIS, Unit VnV Plan (Revised)
   - 8.2 Code
   - 8.3 System VnV Report
   - 8.4 Unit VnV Report

Administrative Details: Report Deadlines

Problem Statement	Week 02	Sept 14
System Requirements Specification (SRS)	Week 05	Oct 4
System VnV Plan	Week 07	Oct 22
Module Guide (MG)	Week 09	Nov 5
Module Interface Specification (MIS)	Week 11	Nov 19
Unit VnV Plan	Week 13	Dec 3
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

Administrative Details: Presentations

SRS Present	Week 04	Week of Sept 24
Syst. VnV Present	Week 06	Week of Oct 15
MG Present	Week 08	Week of Oct 29
MIS Present	Week 10	Week of Nov 12
Unit VnV or Implement Present	Week 12	Week of Nov 26

- Tentative dates
- Specific schedule depends on final class registration and need
- Informal presentations with the goal of improving everyone's written deliverables
- You will be assigned to ask questions of your colleagues

Introductions

- Your name
- Degree program
- Academic background
- Experience with:
  - 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
- Ideally, 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
- 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 [15]
  - 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 [16]

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
- Create an issue

LaTeX

- A typesetting language
- Some initial information in course repo
- Start from an example
  - The lectures notes
  - The Blank Project Template
  - The problem statement

Suggested Reading Questions?

- Smith2016 [11]
- SmithEtAl2007 [13]
- ParnasAndClements1986 [9]
- Solar Water Heating System Example

Literature on SE applied to SCS

- Highlights problems with SE
  - Miller2006 [7]
  - Hatton2007 [4]
  - Sleipner A oil rig collapse [8, p. 38]
  - Patriot missile disaster [8, p. 36]
- Highlights gap/chasm between SE and SC
  - Kelly2007 [6]
  - Storer2017 [14]
- Studies of SE applied to SC
  - CarverEtAl2007 [3]
  - Segal2005 [10]

Literature on SE applied to SCS

- Reproducibility
  - BaileyEtAl2016 [1]
  - BenureauAndRougier2017 [2]
- Future of SE for SC
  - JohansonAndHasselbring2018 [5]
  - Smith2018 [12]

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