

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

Fall 2017

02 Getting Started

Dr. Spencer Smith

Faculty of Engineering, McMaster University

September 8, 2017



Getting Started

- LiCS overview by Dan
- Administrative details
- Introductions
- Questions on suggested reading?
- Project choices
- Software tools
- Software Engineering for Scientific Computing literature

Administrative Details

- Benches and white boards
- Use folder structure given in repo
- Post any questions as issues in our repo
- Problem statement due Friday, Sept 15 by 11:59 pm

Benches and Glassboards



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 Plan 10%
6. Module Guide (MG) 10%
7. Module Interface Specification (MIS) 10%
8. Final Documentation (including revised versions of previous documents, plus the source code and a testing report) 35%

Administrative Details: Report Deadlines

Problem Statement	Week 02	Sept 15
System Requirements Specification (SRS)	Week 05	Oct 4
Verification and Validation Plan	Week 07	Oct 25
Module Guide (MG)	Week 09	Nov 8
Module Interface Specification (MIS)	Week 11	Nov 22
Final Documentation	Week 13	Dec 6

- 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 25
V&V Present	Week 06	Week of Oct 16
MG Present	Week 08	Week of Oct 30
MIS Present	Week 10	Week of Nov 13
Implementation Present	Week 12	Week of Nov 27

- Tentative dates
- Specific schedule depends on final class registration and need
- Informal presentations with the goal of improving everyone's written deliverables

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?

Questions on Suggested Reading?

- Smith2016 [11]
- SmithEtAl2007 [12]

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.
- 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 [14]
 - ▶ 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 [15]

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

SE For SC Literature

- CAS 741 process is document driven, adapted from the waterfall model [4, 13]
- Many say a document driven process is not used by, nor suitable for, scientific software.
 - ▶ Scientific developers naturally use an agile philosophy [1, 2, 3, 9],
 - ▶ or an amethodical process [5]
 - ▶ or a knowledge acquisition driven process [6].
- Scientists do not view rigid, process-heavy approaches, favorably [2]
- Reports for each stage of development are counterproductive [8, p. 373]
- Up-front requirements are impossible [2, 10]
- What are some arguments in favour of a rational document driven process?

Counter Arguments

- Just because document driven is not used, does not mean it will not work
- Documentation provides many benefits [7]:
 - ▶ 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

References I



Karen S. Ackroyd, Steve H. Kinder, Geoff R. Mant, Mike C. Miller, Christine A. Ramsdale, and Paul C. Stephenson.

Scientific software development at a research facility.
IEEE Software, 25(4):44–51, July/August 2008.



Jeffrey C. Carver, Richard P. Kendall, Susan E. Squires, and Douglass E. Post.

Software development environments for scientific and engineering software: A series of case studies.

In *ICSE '07: Proceedings of the 29th International Conference on Software Engineering*, pages 550–559, Washington, DC, USA, 2007. IEEE Computer Society.

References II



Steve M. Easterbrook and Timothy C. Johns.
Engineering the software for understanding climate
change.

Comuting in Science & Engineering, 11(6):65–74,
November/December 2009.



Carlo Ghezzi, Mehdi Jazayeri, and Dino Mandrioli.
Fundamentals of Software Engineering.

Prentice Hall, Upper Saddle River, NJ, USA, 2nd edition,
2003.

References III



Diane Kelly.

Industrial scientific software: A set of interviews on software development.

In Proceedings of the 2013 Conference of the Center for Advanced Studies on Collaborative Research, CASCON '13, pages 299–310, Riverton, NJ, USA, 2013. IBM Corp.



Diane Kelly.

Scientific software development viewed as knowledge acquisition: Towards understanding the development of risk-averse scientific software.

Journal of Systems and Software, 109:50–61, 2015.

References IV



David Lorge Parnas.

Precise documentation: The key to better software.

In *The Future of Software Engineering*, pages 125–148, 2010.



Patrick J. Roache.

Verification and Validation in Computational Science and Engineering.

Hermosa Publishers, Albuquerque, New Mexico, 1998.



Judith Segal.

When software engineers met research scientists: A case study.

Empirical Software Engineering, 10(4):517–536, October 2005.

References V



Judith Segal and Chris Morris.

Developing scientific software.

IEEE Software, 25(4):18–20, July/August 2008.



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.

References VI



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.



Hans van Vliet.

Software Engineering (2nd ed.): Principles and Practice.

John Wiley & Sons, Inc., New York, NY, USA, 2000.



Greg Wilson, Jennifer Bryan, Karen Cranston, Justin Kitzes, Lex Nederbragt, and Tracy K. Teal.

Good enough practices in scientific computing.

CoRR, abs/1609.00037, 2016.

References VII



Gregory V. Wilson.

Where's the real bottleneck in scientific computing?

Scientists would do well to pick some tools widely used in the software industry.

American Scientist, 94(1), 2006.