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

Fall 2020

02 Getting Started

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Getting Started

- Administrative details
- Additional introductions
- Traditional project choices
- Drasil project choices
- Software tools
  - Git, GitLab and GitHub (Issue Creating Exercise)
  - LaTeX
  - Make
- Questions on suggested reading?
- Software Engineering for Scientific Computing literature

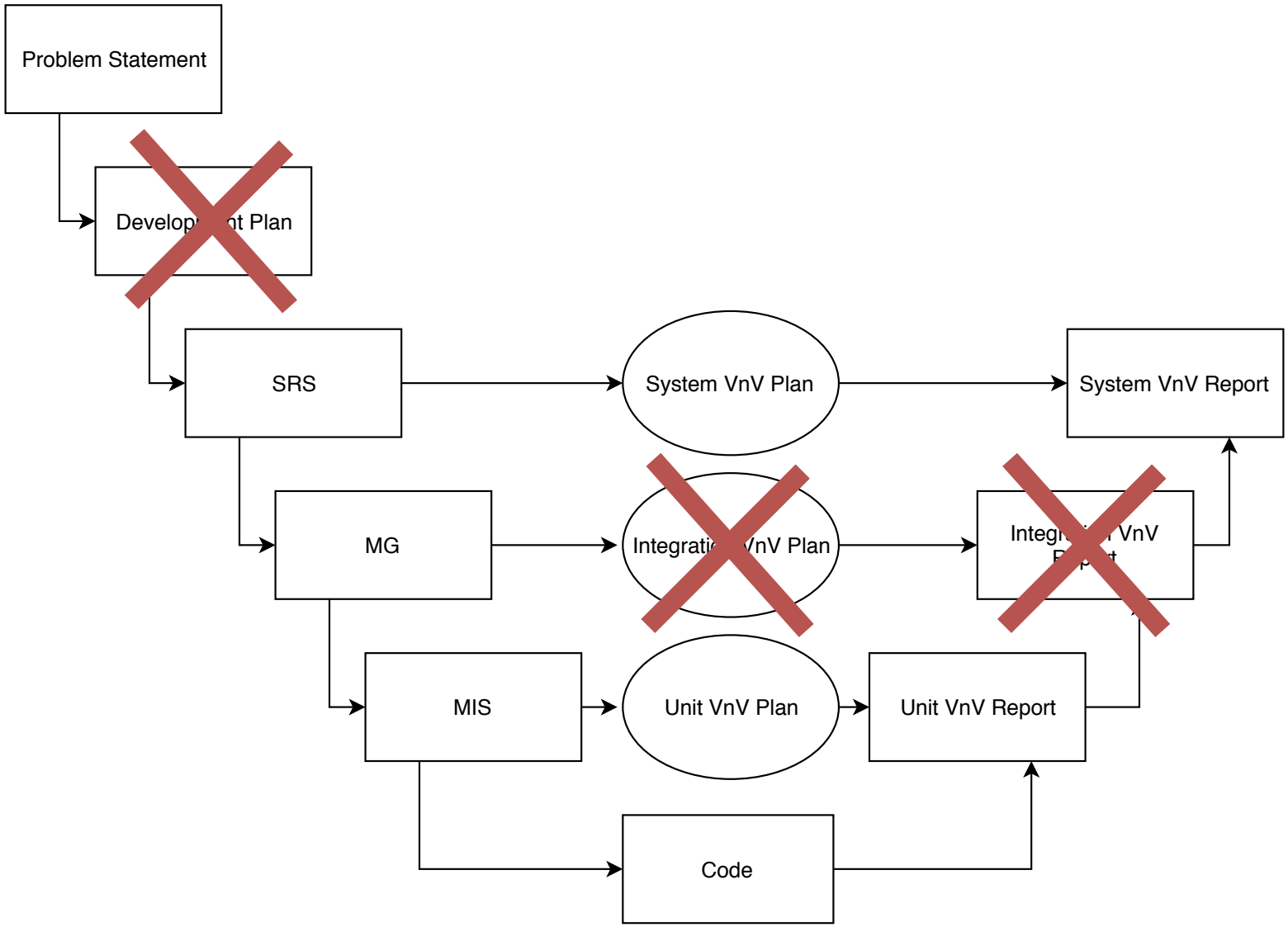
Administrative Details

- Can everyone access GitLab?
  https://gitlab.cas.mcmaster.ca/smiths/cas741
- Use folder structure given in repo (will be updating)
- Create a GitHub account if you don't already have one
- Add `smiths` to your GitHub repos
- Problem statement
  - Problem statement due Mon, Sept 21 by 11:59 pm
  - Assign the instructor an issue to review your problem statement
- Issue creating exercises due Fri, Sept 18 by 1:00 pm
- 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

Administrative Details: Our Deliverables



Administrative Details: Presentations (Draft Deadlines)

SRS Present	Week 05?	Week of Sept 30?
POC Demo	Week 06?	Week of Oct 6?
Syst. VnV Present	Week 07?	Week of Oct 21?
MG + MIS Syntax Present	Week 9?	Week of Nov 4?
MIS Semantics Present	Week 11?	Week of Nov 18?
Unit VnV or Implement Present	Week 12/13?	Week of Nov 28?

- 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: Draft Report Deadlines

Issue Creation Exercise	Week 02	Sept 18
Problem Statement	Week 03	Sept 21
System Requirements Specification (SRS)	Week 06?	Oct 7?
System VnV Plan	Week 08?	Oct 28
Module Guide (MG) + Mod Int Spec (MIS)?	Week 10?	Nov 25
Final Documentation	Week 14?	Dec 9?

- 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: Optional Study Participation

- You will be contacted by Oluwaseun (Olu) Owojaiye for potential participation in a study
- "Traditional" versus "Generative" for software development
- If you participate you will be interviewed and asked to record some details of how you spend your development time
- Participation is entirely voluntary
- The course instructor will not know who has participated
- Participation or non-Participation will not effect your grade
- Olu will visit our class on Thursday to discuss further

Introductions

- 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

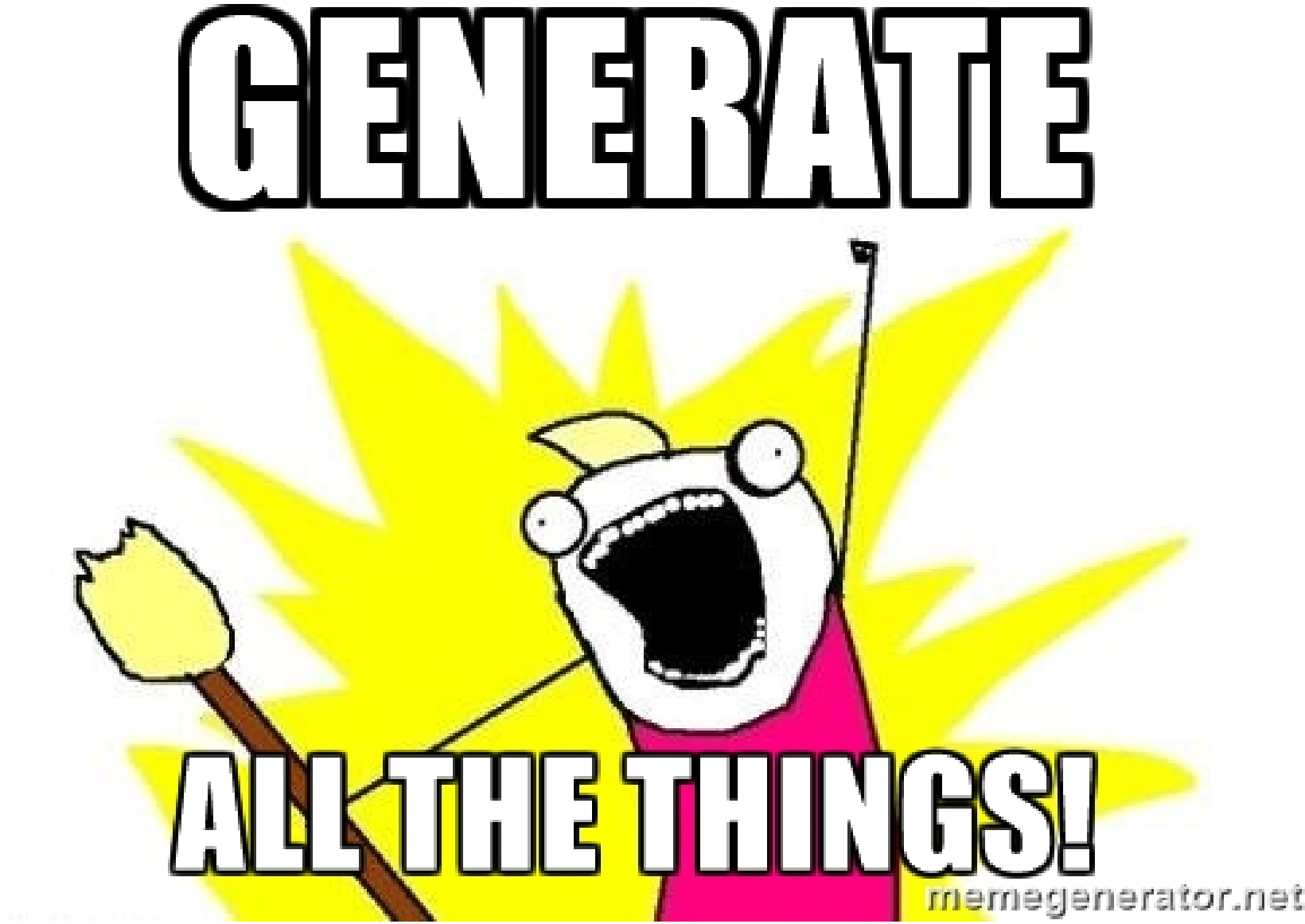
- Related to scientific computing
- Simple, but not trivial
- If feasible, select a project related to your research
- Possibly re-implement existing software
- Each student project needs to be unique
- A specific physical problem
- Some examples follow, the links are just places to get started

Project Selection: Specific Physical Problem

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

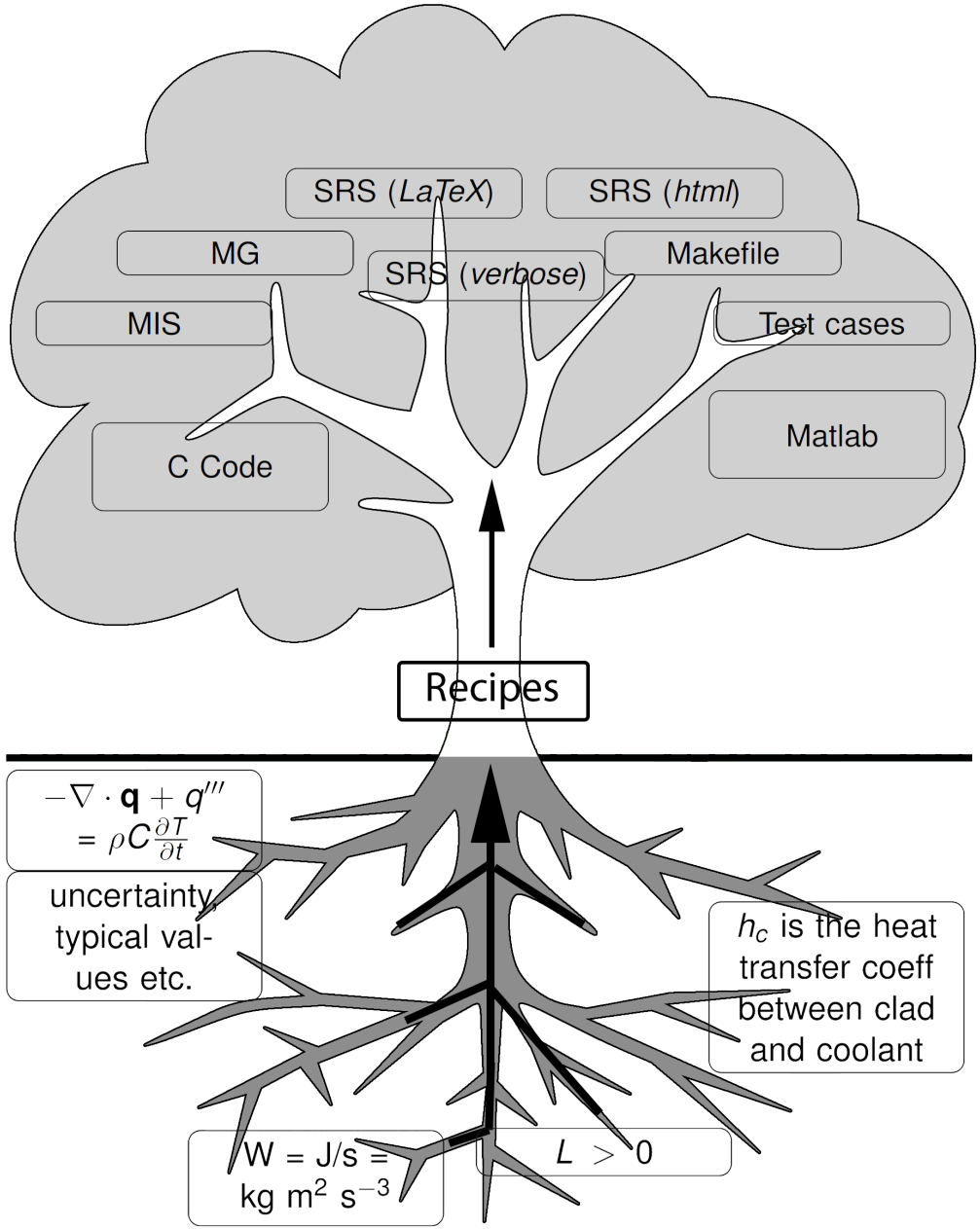
Project Selection: Family of General Purpose Tools

- 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.


GENERATE
ALL THE THINGS!
memegenerator.net

Knowledge Capture

Drasil


SRS (*LaTeX*)
SRS (*html*)
MG
SRS (*verbose*)
Makefile
MIS
Test cases
C Code
Matlab
Recipes
$-\nabla \cdot \mathbf{q} + q''' = \rho C \frac{\partial T}{\partial t}$
uncertainty, typical values etc.
h_c is the heat transfer coeff between clad and coolant
W = J/s = kg m^2 s^{-3}
$L > 0$

Introduction to Drasil

- Drasil uses a generative approach
- Knowledge is captured in a Domain Specific Language (DSL)
- Documentation (in tex and html) and code (in Java, C++, C#, Python and Swift) are generated
- Changes are propagated throughout documentation and code
- Consistency and completeness checks
- Reuse throughout document, between documents and between projects

Project Selection (Drasil): Specific Physical Problems

- Set of explicit equations with the variables of interest isolated on one side of the equation (like GlassBR, or Projectile)
- First order Initial value problem (like NoPCM)
- Examples
  - Cooling of a uniform temperature body over time
  - Charging or discharging of a capacitor
  - Flow into a reservoir
  - Population growth
  - Blood alcohol level over time
  - Some potential problems
  - Worked example in a physics or chemistry textbook, using equations, like solving for the forces in a statically indeterminate structure

Project Selection Ideas/Questions

1. Naveen
2. Liuyin
3. Tiago
4. John
5. Gaby
6. Seyed Shayan Mousavi Masouleh
7. Xingzhi
8. Siddharth (Sid)
9. Andrea
10. Nafiseh (audit)
11. Mohamed
12. Elizabeth
13. Xuanming
14. Jamil
15. Ting-Yu
16. Leila
17. Parsa
18. Salah Gamal aly Hessien

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
- Instructions for setting up a Virtual Machines

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 Friday, Sept 18, 1:00 pm
- Create 2 issues for case studies in Drasil repo
- https://jacquescarette.github.io/Drasil/
- Select any case study that interests you and review the SRS
- Create issues at https://github.com/JacquesCarette/Drasil/issues
- At `smiths` (Since you cannot assign issues as guests)
- Consider using SRS checklist (except for major revision history)
- Additional guidance in SRS Template
- Please do not create issues related to pdf file formatting inconsistencies
- Issues that are questions are fine (use question label)

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, favourably [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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