CAS 741 (Development of Scientific Computing Software)

Winter 2024

02 Getting Started

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Getting Started

- Administrative details
- Problem statements
- More information on Drasil
- Project choice discussion
- Software tools
  - Git, GitLab and GitHub
  - Continuous integration
  - LaTeX
  - Make
- Questions on suggested reading?
- Software Engineering for Scientific Computing literature
- Start Projectile example

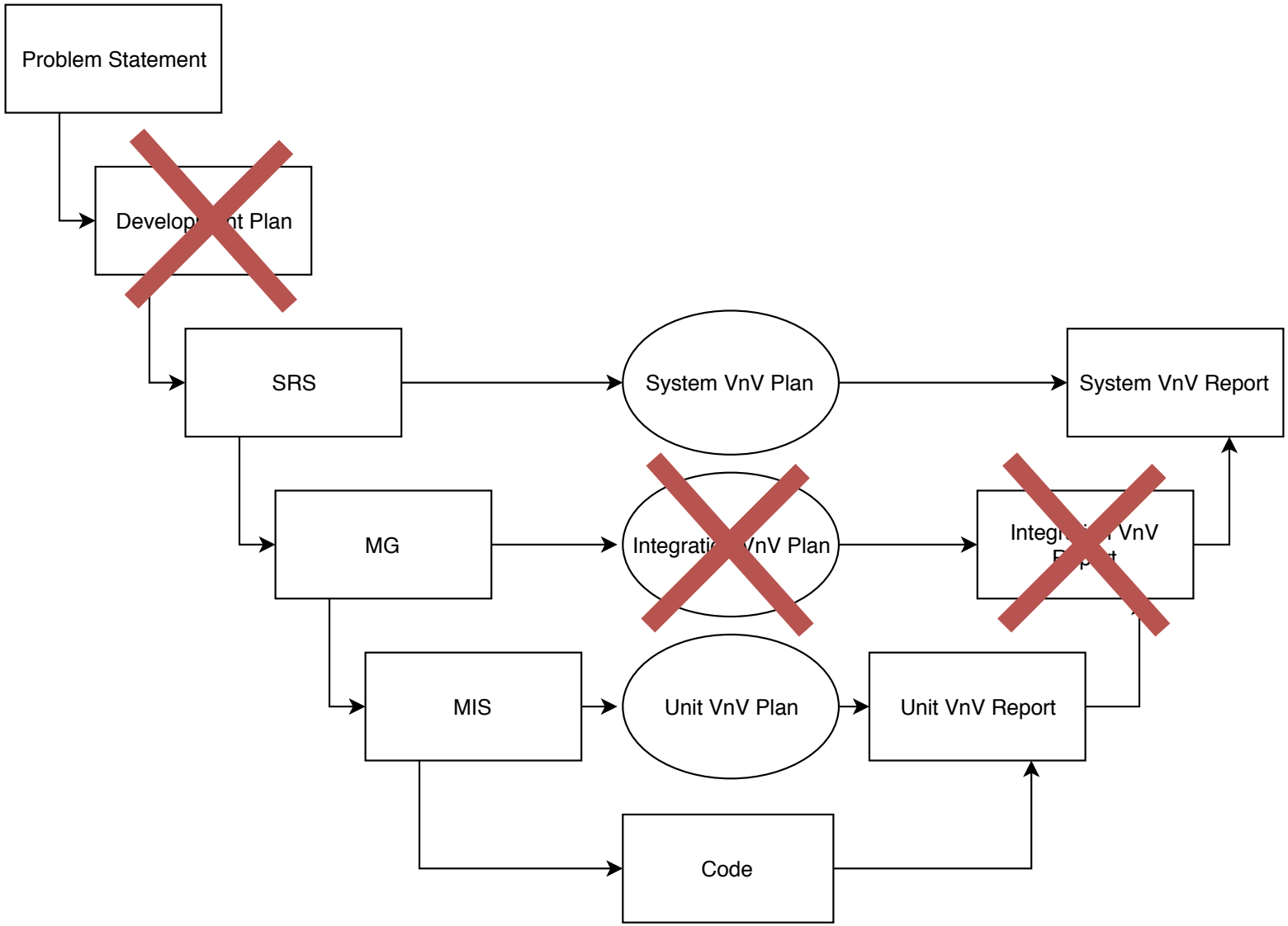
Administrative Details

- Teams channel created
- Can everyone access our course repo on GitLab?
- Create a GitHub account if you don't already have one
- Use the GitHub template to create a new repo
- Add `smiths` to your GitHub repo
- Create a fork (on GitLab) and a merge request to modify Repos.csv with your project details
- Problem statement
  - Problem statement due Fri, Jan 19 by 11:59 pm
  - Assign an issue to instructor to review
- Feel free to add me to you Linked-In network
- Participation grades will be posted before the end of the term, providing an opportunity to improve

Administrative Details: Domain Expert

- Create issues for their partner's written deliverables
- Asks questions during their partner's presentations

Administrative Details: Our Deliverables



Administrative Details: Report Deadlines

Problem Statement	Week 02	Jan 19
System Req. Spec. (SRS)	Week 04	Feb 2
System VnV Plan	Week 06	Feb 16
MG + MIS	Week 09	Mar 15
Drasil Code	Week 09	Mar 15
Final Documentation	Week 13	Apr 12

- 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 for a **written** doc, please ask
- When ready, assign issues to your primary and secondary reviewers
- GitHub issues due two days after assignment deadlines
- From Drasil Code onward, Drasil projects no longer need to maintain traditional SRS

Administrative Details: Presentations

SRS	Week 03/04	Week of Jan 23, 30
Syst. VnV	Week 06	Week of Feb 13
POC Demo	Week 06, 07	Week of Feb 13, 27
MG + MIS Syntax	Week 09	Week of Mar 13
MIS Semantics	Week 09	Week of Mar 13
Drasil	Week 11	Week of Mar 27
Unit VnV/Implement	Week 12	Week of Apr 3

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

Presentation Schedule

TBD

Presentation Schedule

- 4 presentations each (please check)
- If you will miss a presentation, please trade with someone else
- Implementation presentation could be used to run a code review, or code walkthrough

Problem Statement

- Modify the Problem statement from the template repo
- Written in LaTeX (or other text-based file format)
- Due electronically (on GitHub) by deadline
- Generated files should NOT be under source control (except pdf)
- Comments used to give advice, you can use for your own reviews
- Remove comments via `\newif\ifcomments\commentsfalse`

Problem Statement Cont'd

- Abstractly state the problem to be solved
  - **What** problem
  - **Not how** to solve
- Characterize the problem in terms of inputs and the outputs
- State why the problem is important
- Give context
  - Stakeholders?
  - Environment for the software?
  - A page description should be sufficient

Sample Project Statements

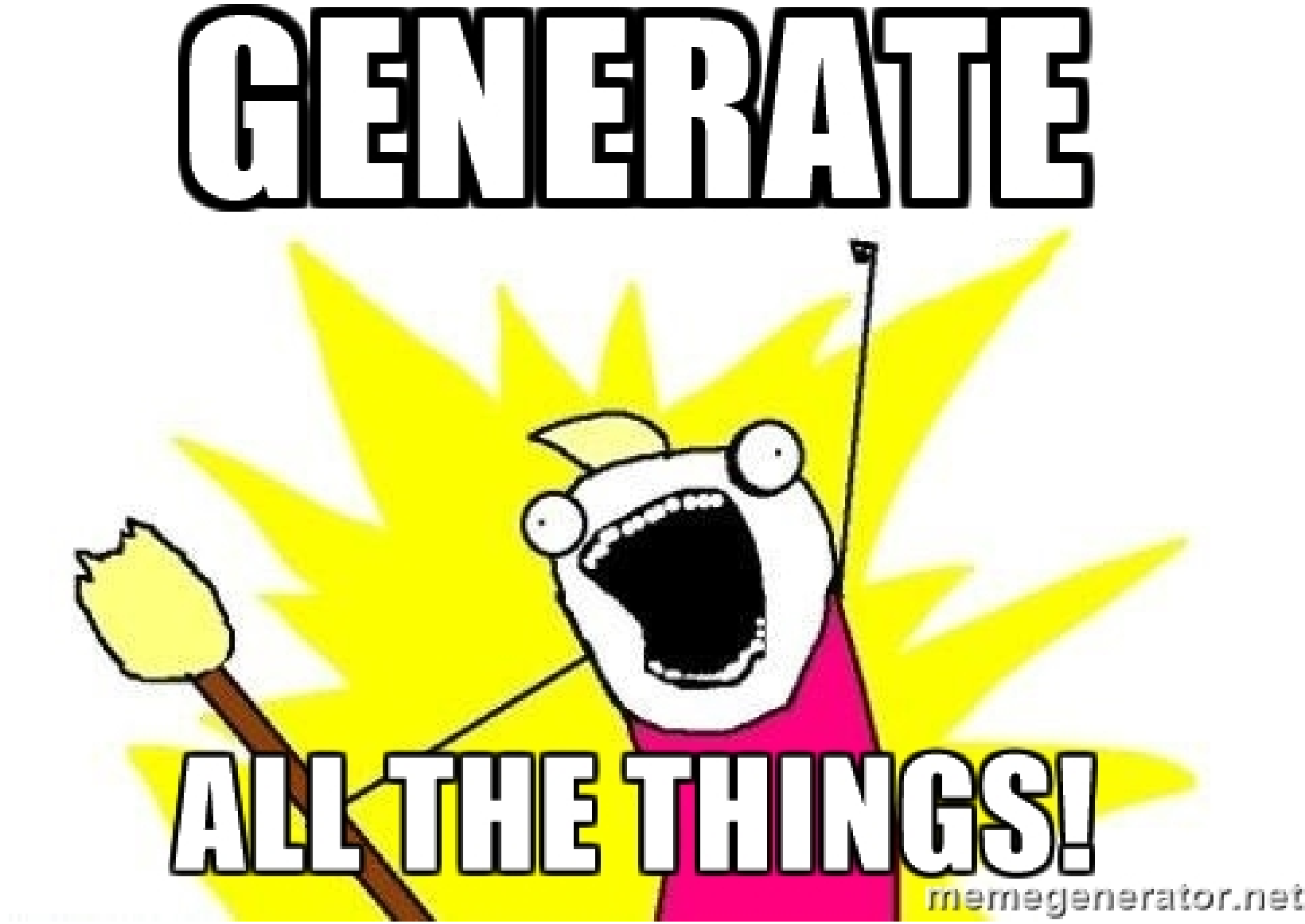
- Solar Cooker
- SpectrumImageAnalysisPy
- Aqueous Speciation Diagram Generator
- FloppyFish
- PyERT - For GPS trip data analysis
- EMA (watch to monitor older adults with lumbar spinal disorders)
- MTO Bridge

Goals

- Refine problem statement into high level goals
- Selling points for your project (could include you learning new skills)
- Goals should be measurable
- Usually around 5 goals
- Explain goals that are not obvious
- Include goals and stretch goals

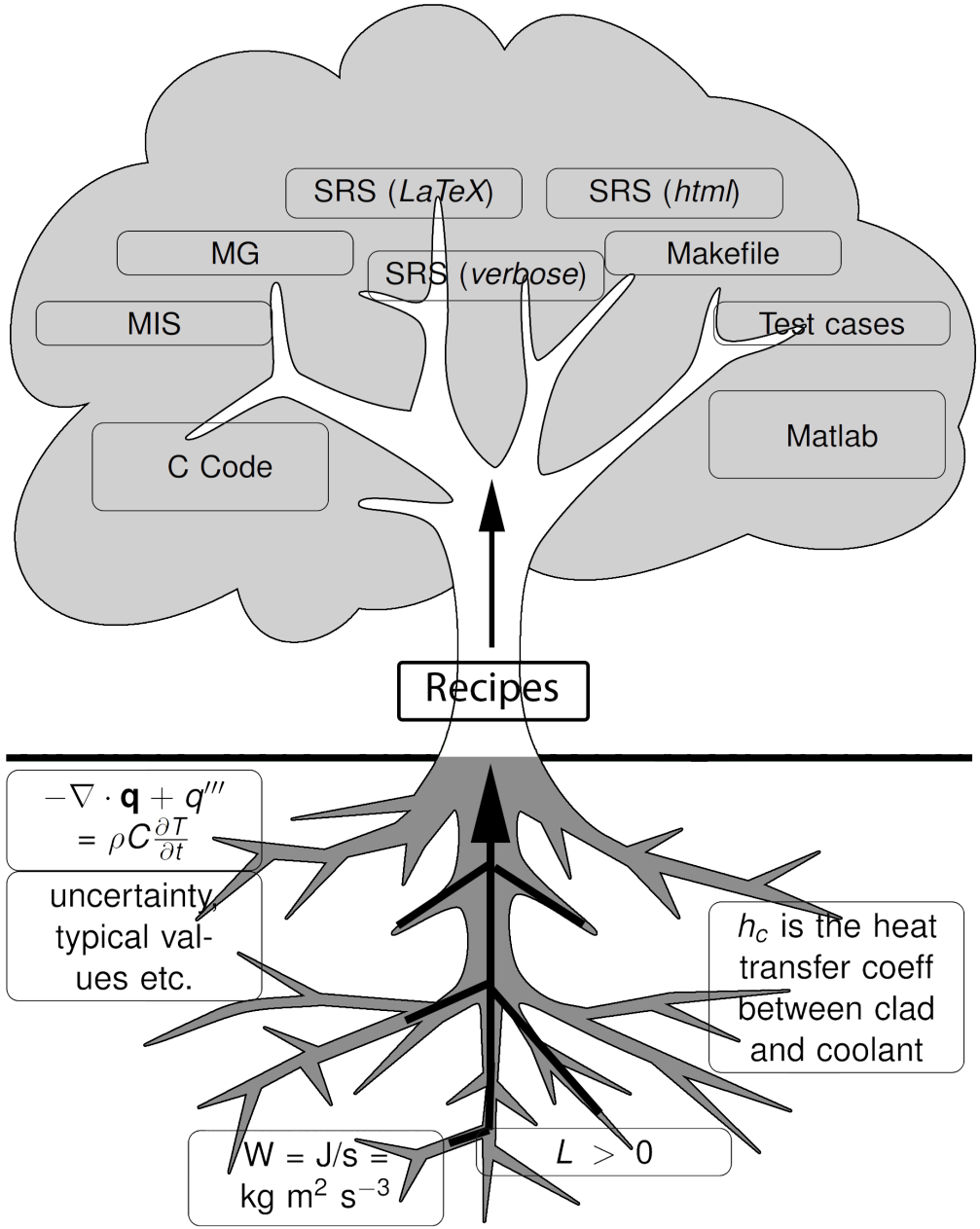
Sample Goals

- Skeleton Key
- Hot Mesh Solutions
- Smart Farm Solutions


GENERATE
ALL THE THINGS!
memegenerator.net

Knowledge Capture

Drasil


SRS (*LaTeX*)
SRS (*html*)
MG
SRS (*verbose*)
Makefile
MIS
Test cases
Matlab
C Code
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 Ideas/Questions

Let's discuss some of your project ideas

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
- Shared Team's Video on git and GitHub with extra material
- Shared Team's Video on Continuous Integration with extra material

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

Continuous Integration

- Building and testing software on every push to the code repository (see Fowler)
- Requires:
  - A version control system
  - A fully automated build system
  - An automated test system
  - An automated system for other tasks, like code checking (linting), doc building, web-site updating
  - An integration build system
- A good idea for your projects
- A useful skill to have

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 Project Template
  - The problem statement

Make

- Software Carpentry: Automation and Make
- The 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]

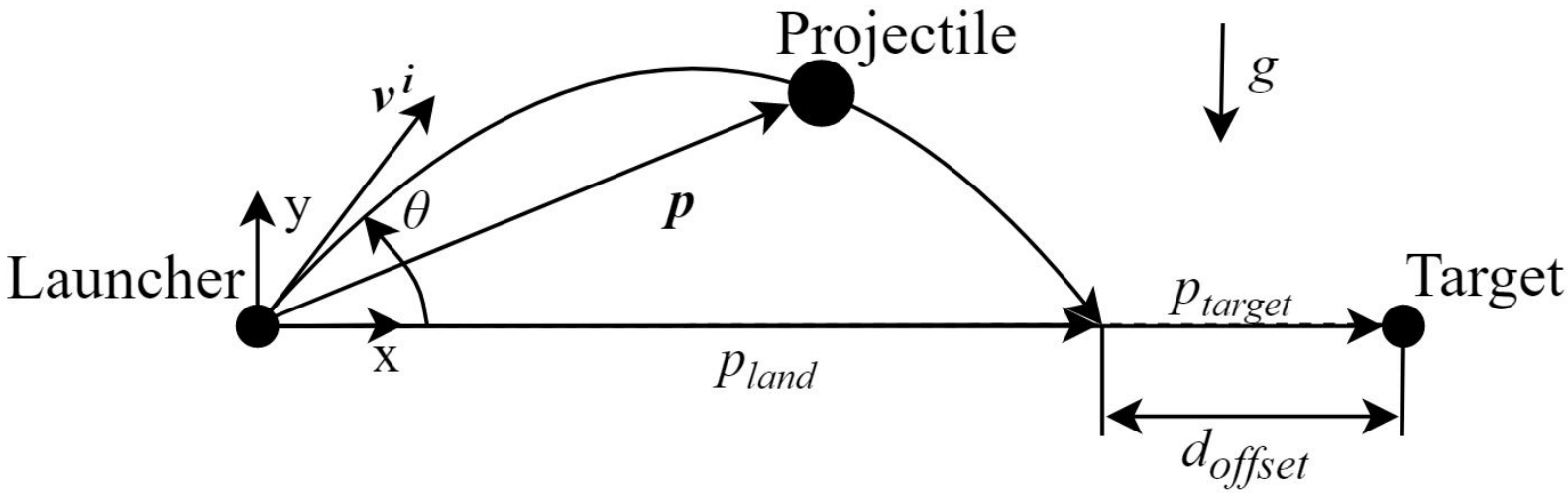
Literature on SE applied to SCS

- 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]

Requirements for Projectile



- Goal(s)?
- Inputs?
- Outputs?
- Simplifying assumptions?
- Kinematic theories for translational motion?
- Refined Theories Projectile SRS

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