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

Fall 2020

05 Program Families

Dr. Spencer Smith

Faculty of Engineering, McMaster University

November 20, 2020

Program Families

- Record lecture
- Olu's research project
- Administrative details
- Questions?
- Finish up on SRS
- Specification Qualities
- Motivation
- Proposed Family Methods
- Family of Linear Solvers
- Other examples (covered in "bonus" slides)
  - Family of Mesh Generators (in other set of slides)
  - Family of Material Behaviour Models (in other set of slides)

Administrative Details

- Did anyone install a VM following these instructions?
- Checklist for Problem Statement
- Repos.xlsx
- Example of the value of commit numbers and diffs
- Primary reviewers ("Domain experts") and secondary reviewers
  - Ask at least one question after presentation
  - By two days after each major deliverable, create at least 5 GitHub issues

Administrative Details: Presentations

- Presentations are about 20 minutes
- Informal
- To help you prepare your written document
- Questions from audience
- Grading out of 3
  - Generate discussion, evidence of prior thought, organized 3/3
  - Any element missing from above 2/3
  - Any two elements missing from above 1/3
  - No presentation 0/3

Administrative Details: Report Deadlines

SRS Week 06 Oct 8

- 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 on a written deliverable, please ask
- Two days after each major deliverable, your GitHub issues will be due

Administrative Details: Presentations

SRS Present Week 05 Week of Sept 28

- Informal presentations with the goal of improving everyone's written deliverables
- Primary (domain expert) and secondary reviewers (and others) will ask questions

Administrative Details: Presentation Schedule

- SRS Present
  - **Sep 28: Mohamed, Andrea, Tiago, John, Salah**
  - **Oct 1: Liz, Xingzhi, Leila, Shayan, Naveen**
  - **Oct 5: Sid, Gaby, Parsa, Ting-Yu, Xuanming**
- Primary and secondary reviewers given in Repos.xlsx file
- If you cannot make a presentation, please make an arrangement to swap with a colleague

SRS Presentations

- Project name
- Draft Goal statements
- Draft Assumptions
- Draft Input and output variables (data constraints)
- Draft General Definitions and Theoretical models
- Draft Instanced models
- Questions (from reviewers, instructor, anyone)

Presentation Guidelines (for SRS and others)

- Start all presentation with your project title and goal statements (not everyone in the audience will remember what you are doing)
- Time will go fast
  - You can gloss over domain details
  - Focus on the important/interesting things
  - Focus on questions that you have
  - You don't have to start at the "beginning" of any documents, get to the good stuff
  - Every slides should have x/total slides on it (so the moderator can judge whether you are going too fast or slow
- If virtual, try to limit frequency of slide changes and movement

Examples

- Double Pendulum
- SpectrumImageAnalysisPy
- Conformer Searching using Evolutionary Computation
- Medical Image Segmentation
- Fourier Series
- Library of Lighting Models
- Scanning Transmission Electron Microscopy
- Chemical Speciation

Questions?

- Questions about SRS?
- Any questions on the SRS Template?
- Any questions on the Writing Checklist?
- Any questions on the SRS Checklist?
- Is $a = \frac{dv}{dt}$ a TM or a DD?

Software Requirements Activities

- A software requirement is a description of how the system should behave, or of a system property or attribute
- Requirements should be abstract, unambiguous, complete, consistent, modifiable, verifiable and traceable
- Requirements should express "What" not "How"
- Formal versus informal specification
- Functional versus nonfunctional requirements
- Software requirements specification (SRS)
- Requirements template

Specification Qualities

- What are the important qualities for a specification? What makes a specification a good specification?

Specification Qualities

- Clear, unambiguous, understandable
- Consistent
- Complete
  - Internal completeness
  - External completeness
- Incremental
- Validatable
- Abstract
- Traceable

Summarized in [16, p. 406]

Clear, Unambiguous, Understandable

- Specification fragment for a word-processor
  - Selecting is the process of designating areas of the document that you want to work on. Most editing and formatting actions require two steps: first you select what you want to work on, such as text or graphics; then you initiate the appropriate action.
- What are the potential problems with this specification?

Clear, Unambiguous, Understandable

- Specification fragment for a word-processor
  - Selecting is the process of designating areas of the document that you want to work on. Most editing and formatting actions require two steps: first you select what you want to work on, such as text or graphics; then you initiate the appropriate action.
- What are the potential problems with this specification?
  - Can an area be scattered?
  - Can both text and graphics be selected?

Clear, Unambiguous, Understandable

- Specification fragment from a real safety-critical system
  - The message must be triplicated. The three copies must be forwarded through three different physical channels. The receiver accepts the message on the basis of a two-out-of-three voting policy.
- What is a potential problems with this specification?

Clear, Unambiguous, Understandable

- Specification fragment from a real safety-critical system
  - The message must be triplicated. The three copies must be forwarded through three different physical channels. The receiver accepts the message on the basis of a two-out-of-three voting policy.
- What is a potential problems with this specification?
  - Can a message be accepted as soon as we receive 2 out of 3 identical copies, or do we need to wait for receipt of the 3rd

Unambiguous, Validatable

- Specification fragment for an end-user program
  - The program shall be user friendly.
- What is a potential problems with this specification?

Unambiguous, Validatable

- Specification fragment for an end-user program
  - The program shall be user friendly.
- What is a potential problems with this specification?
  - What does it mean to be user friendly?
  - Who is a typical user?
  - How would you measure success or failure in meeting this requirement?

Unambiguous, Validatable

- Specification fragment for a linear solver
  - Given A and b, solve the linear system $Ax = b$ for x, such that the error in any entry of x is less than 5 %.
- What is a potential problems with this specification?

Unambiguous, Validatable

- Specification fragment for a linear solver
  - Given A and b, solve the linear system $Ax = b$ for x, such that the error in any entry of x is less than 5 %.
- What is a potential problems with this specification?
  - Is A constrained to be square?
  - Can A be singular?
  - Even if the problem is made completely unambiguous, the requirement cannot be validated.

Consistent

- Specification fragment for a word-processor
  - The whole text should be kept in lines of equal length. The length is specified by the user. Unless the user gives an explicit hyphenation command, a carriage return should occur only at the end of a word.
- What is a potential problems with this specification?

Consistent

- Specification fragment for a word-processor
  - The whole text should be kept in lines of equal length. The length is specified by the user. Unless the user gives an explicit hyphenation command, a carriage return should occur only at the end of a word.
- What is a potential problems with this specification?
  - What if the length of a word exceeds the length of the line?

Same Symbol/Term Different Meaning

- Can you think of some symbols/terms that have different meanings depending on the context?

Consistent

- Language and terminology must be consistent within the specification
- Potential problem with homonyms, for instance consider the symbol σ
  - Represents standard deviation
  - Represents stress
  - Represents the Stefan-Boltzmann constant (for radiative heat transfer)
- Changing the symbol may be necessary for consistency, but it could adversely effect understandability
- Potential problem with synonyms
  - Externally funded graduate students, versus eligible graduate students, versus non-VISA students
  - Material behaviour model versus constitutive equation

Complete

- Internal completeness
  - The specification must define any new concept or terminology that it uses
    - A glossary is helpful for this purpose
- External completeness
  - The specification must document all the needed requirements
    - Difficulty: when should one stop?

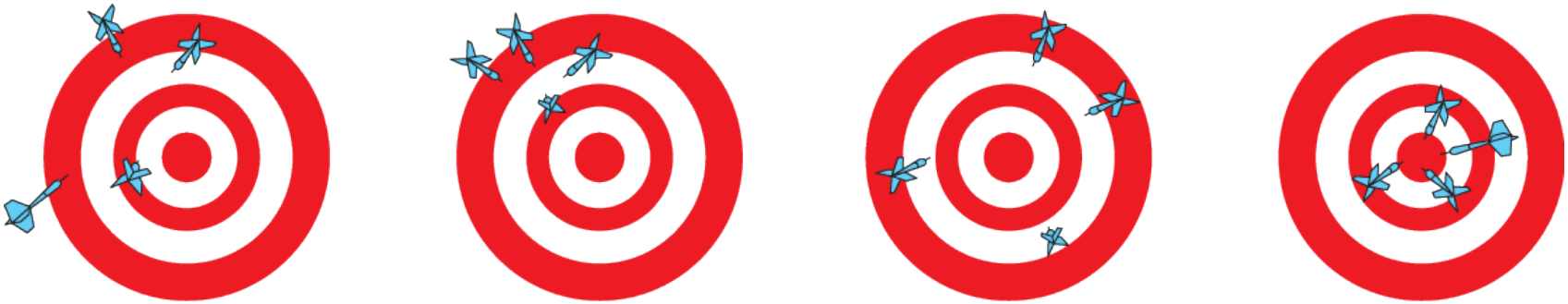
Incremental

- Referring to the specification process
  - Start from a sketchy document and progressively add details
  - A document template can help with this
- Referring to the specification document
  - Document is structured and can be understood in increments
  - Again a document template can help with this

Traceable

- Explicit links
  - Within document
  - Between documents
- Use labels, cross-references, traceability matricies
- Common sense suggests traceability improves maintainability
- Shows consequence of change
- Minimizes cost of recertification
- Additional advantages
  - Program comprehension
  - Impact analysis
  - Reuse
- Why is traceability important?

Accuracy Versus Precision



What is the distinction between accuracy and precision?

Program Family Examples

Program Families

- Can think of general purpose (or multi-purpose) SC software as a program family
- Some examples of physical models are also appropriate for consideration as a family
- A program family is a set of programs where it makes more sense to develop them together as opposed to separately
- Analogous to families in other domains
  - Automobiles
  - Computers
  - ...
- Need to identify the commonalities
- Need to identify the variabilities
- Discussed in general in [5, 12]

Background

- Program family idea since the 1970s (Dijkstra, Parnas, Weiss, Pohl, ...) - variabilities are often from a finite set of simple options [10, 11, 7]
- Families of algorithms and code generation in SC (Carette, ATLAS, Blitz++, ...) - not much emphasis on requirements [4, 25, 21, 3]
- Work on requirements for SC
  - Template for a single physical model [18, 17]
  - Template for a family of multi-purpose tool [13, 15, 14]
  - Template for a family of physical models [20, 19, 9]

Motivation

- Requirements documentation
  - Allows judgement of quality
  - Improves communication
    - Between domain experts
    - Between domain experts and programmers
    - Explicit assumptions
    - Range of applicability
- A family approach, potentially including a DSL to allow generation of specialized programs
  - Improves efficiency of product and process
  - Facilitates reuse of requirements and design, which improves reliability
  - Improves usability and learnability
  - Clarifies the state of the art

Advantages of Program Families to SC?

- Usual benefits
  - Reduced development time
  - Improved quality
  - Reduced maintenance effort
  - Increased ability to cope with complexity
- Reusability
  - Underused potential for reuse in SC
  - Reuse commonalities
  - Systematically handle variabilities
- Usability
  - Documentation often lacking in SC
  - Documentation part of program family methodology
  - Create family members that are only as general purpose as necessary
- Improved performance

Is SC Suited to a Program Family Approach?

Based on criteria from Weiss [2, 23, 24, 6, 22]

- The redevelopment hypothesis
  - A significant portion of requirements, design and code should be common between family members
  - Common model of software development in SC is to rework an existing program
  - Progress is made by removing assumptions
- The oracle hypothesis
  - Likely changes should be predictable
  - Literature on SC, example systems, mathematics
- The organizational hypothesis
  - Design so that predicted changes can be made independently
  - Tight coupling between data structures and algorithms
  - Need a suitable abstraction

Challenges

1. Validatable
   - Requirements can be complete, consistent, traceable and unambiguous, but still not validatable
   - Input and outputs are continuously valued variables
   - Correct solution is unknown a priori
   - Given $dy/dt = f(t, y)$ and $y(t_0) = y_0$, find $y(t_n)$
2. Abstract
   - If too abstract, then difficult to meet NFRs for accuracy and speed
   - Assumptions can help restrict scope, but possibly as much work as solving the original problem
     - $Ax = b$
     - $x^T Ax > 0, \forall x$
   - Algorithm selection should occur at the design stage

Challenges (Continued)

3. Nonfunctional requirements
   - Proving accuracy requirements with a priori error analysis is a difficult mathematical exercise that generally leads to weak error bounds
   - Context sensitive tradeoffs between NFRs can be difficult to specify
   - Absolute quantitative requirements are often unrealistic
4. Capture and Reuse Existing Knowledge
   - Cannot ignore the enormous wealth of information that currently exists
   - A good design will often involve integrating existing software libraries
   - Reuse software and the requirements documentation

Goal Statements for a Family of Linear Solvers?

What would be a good goal statement for a library of linear solvers?

Goal Statements for a Family of Linear Solvers

G1 Given a system of n linear equations represented by matrix A and column vector b, return x such that $Ax = b$, if possible

Theoretical Model for a Family of Linear Solvers?

- Is the theoretical model a commonality or a variability?
- What is the theoretical model for a family of linear solvers?

Theoretical Model for a Family of Linear Solvers

Given a square matrix A and column vector b, the possible solutions for x are as follows:

1. A unique solution $x = A^{-1}b$, if A is nonsingular
2. An infinite number of solutions if A is singular and $b \in span(A)$
3. No solution if A is singular and $b \notin span(A)$

[1]

Instance Model for a Family of Linear Solvers?

- Is there an instance model for a family of linear solvers?

Symbols and Terminology for a Family of Linear Solvers?

- What symbols and terminology will you need to define?

Sample Symbols and Terminology

$n : \mathbb{N}$	number of linear equations/number of unknowns
$A : \mathbb{R}^{n \times n}$	$n \times n$ real matrix
$x : \mathbb{R}^{n \times 1}$	$n \times 1$ real column vector
$b : \mathbb{R}^{n \times 1}$	$n \times 1$ real column vector
$I : \mathbb{R}^{n \times n}$	an $n \times n$ matrix where all entries are 0, except for the diagonal entries, which are 1
$\|\|v\|\|$	the norm (estimate of magnitude) of vector v
$A^{-1} : \mathbb{R}^{n \times n}$	the inverse matrix, with the property that $A^{-1}A = I$
singular	matrix A is singular if A^{-1} does not exist
residual	$\|\|b - Ax\|\|$

What Would be the Most General Binding Time?

- What would be the most general binding time for the variabilities?

What Are Some Potential Input Variabilities?

- What are some potential input variabilities? What are the associated parameters of variation?

Variability	**Parameter of Variation**
Allowed structure of A	Set of $\{$ full, sparse, banded, tridiagonal, block triangular, block structured, diagonal, upper triangular, lower triangular, Hessenberg $\}$
Allowed definiteness for A	Set of $\{$ not definite, positive definite, positive semi-definite, negative definite, negative semi-definite $\}$
Allowed class of A	Set of $\{$ diagonally dominant, Toeplitz, Vandermonde $\}$
Symmetric?	boolean
Values for n	set of $\mathbb{N}$
Entries in A	set of $\mathbb{R}$
Entries in b	set of $\mathbb{R}$

Variability	**Parameter of Variation**
Source of input	Set of { from a file, through the user interface, passed in memory }
Encoding of input	Set of {binary, text }
Format of input A	Set of {arbitrary, by row, by column, by diagonal }
Format of input b	Set of {arbitrary, ordered }

What Are Some Potential Output Variabilities?

- What are some potential output variabilities? What are the associated parameters of variation?

Output Variabilities

Variability	**Parameter of Variation**
Destination for output x	Set of $\{$ to a file, to the screen, to memory $\}$
Encoding of output x	Set of $\{$binary, text $\}$
Format of output x	Set of $\{$arbitrary, ordered $\}$
Output residual	boolean (true if the program returns the residual)
Possible entries in x	set of $\mathbb{R}$

What Are Some Potential Calculation Variabilities?

- What are some potential calculation variabilities? What are the associated parameters of variation?

Calculation Variabilities

Variability	**Parameter of Variation**
Check input?	boolean (false if the input is assumed to satisfy the input assumptions)
Exceptions generated?	boolean (false if the goal is non-stop arithmetic)
Norm used for residual	Set of {1-norm, 2-norm, ∞-norm }

References I

Howard Anton.
Elementary Linear Algebra.
Wiley, fifth edition, 1987.

Mark Ardis and David M. Weiss.
Defining families: The commonality analysis.
In *Proceedings of the Nineteenth International Conference on Software Engineering*, pages 649–650. ACM, Inc., 1997.

Blitz.
Blitz++, object-oriented scientific computing, Last Accessed in December 2001.

References II


Jacques Carette.
Gaussian elimination: A case study in efficient genericity with MetaOCaml.
Science of Computer Programming, 62(1):3–24, 2006.


Paul Clements and Linda M. Northrop.
Software product lines: practices and patterns.
Addison-Wesley Longman Publishing Co., Inc., Boston, MA, USA, 2002.


David A. Cuka and David M. Weiss.
Specifying executable commands: An example of FAST domain engineering.
Submitted to IEEE Transactions on Software Engineering, pages 1 – 12, Submitted 1997.

References III

Edsger W. Dijkstra.
Notes on structured programming.
In O. J. Dahl, E. W. Dijkstra, and C. A. R. Hoare, editors, *Structure Programming*, pages 1–82. Academic Press Ltd., London, UK, UK, 1972.

K. Kreyman and D. L. Parnas.
On documenting the requirements for computer programs based on models of physical phenomena.
SQRL Report 1, Software Quality Research Laboratory, McMaster University, January 2002.

References IV


John McCutchan.
A generative approach to a virtual material testing laboratory.
Master's thesis, McMaster University, Hamilton, ON, Canada, September 2007.


David Parnas.
On the design and development of program families.
IEEE Transactions on Software Engineering, SE-2(1):1–9, 1976.


David L. Parnas.
Designing software for ease of extension and contraction.
IEEE Transactions on Software Engineering, pages 128–138, March 1979.

References V

K. Pohl, G. Böckle, and F. van der Linden.
Software Product Line Engineering: Foundations, Principles, and Techniques.
Springer-Verlag, 2005.

W. Spencer Smith.
Systematic development of requirements documentation for general purpose scientific computing software.
In *Proceedings of the 14th IEEE International Requirements Engineering Conference, RE 2006*, pages 209–218, Minneapolis / St. Paul, Minnesota, 2006.

References VI

W. Spencer Smith and Chien-Hsien Chen.
Commonality analysis for mesh generating systems.
Technical Report CAS-04-10-SS, McMaster University, Department of Computing and Software, 2004.
45 pp.

W. Spencer Smith and Chien-Hsien Chen.
Commonality and requirements analysis for mesh generating software.
In F. Maurer and G. Ruhe, editors, *Proceedings of the Sixteenth International Conference on Software Engineering and Knowledge Engineering (SEKE 2004)*, pages 384–387, Banff, Alberta, 2004.

References VII

W. Spencer Smith and Nirmitha Koothoor.
A document-driven method for certifying scientific computing software for use in nuclear safety analysis.
Nuclear Engineering and Technology, 48(2):404–418, April 2016.

W. Spencer Smith and Lei Lai.
A new requirements template for scientific computing.
In J. Ralyté, P. Ågerfalk, and N. Kraiem, editors, *Proceedings of the First International Workshop on Situational Requirements Engineering Processes – Methods, Techniques and Tools to Support Situation-Specific Requirements Engineering Processes, SREP'05*, pages 107–121, Paris, France, 2005. In

References VIII

conjunction with 13th IEEE International Requirements Engineering Conference.

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.

References IX

W. Spencer Smith, John McCutchan, and Jacques Carette.
Commonality analysis of families of physical models for use in scientific computing.
In *Proceedings of the First International Workshop on Software Engineering for Computational Science and Engineering (SECSE 2008)*, Leipzig, Germany, May 2008. In conjunction with the 30th International Conference on Software Engineering (ICSE).
8 pp.

References X

W. Spencer Smith, John McCutchan, and Jacques Carette.
Commonality analysis for a family of material models.
Technical Report CAS-17-01-SS, McMaster University, Department of Computing and Software, 2017.

Todd. L. Veldhuizen.
Arrays in Blitz++.
In *Proceedings of the 2nd International Scientific Computing in Object-Oriented Parallel Environments (ISCOPE'98), Lecture Notes in Computer Science*. Springer-Verlag, 1998.

References XI


D. Weiss and C.T.R. Lai.
Software Product Line Engineering: A Family-Based Software Development Process.
Addison-Wesley, 1999.


David M. Weiss.
Defining families: The commonality analysis.
Submitted to IEEE Transactions on Software Engineering, 1997.


David M. Weiss.
Commonality analysis: A systematic process for defining families.
Lecture Notes in Computer Science, 1429:214–222, 1998.

References XII


R. C. Whaley, A. Petitet, and J. J. Dongarra.
Automated empirical optimization of software and the ATLAS project.
Parallel Computing, 27(1–2):3–35, 2001.