

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

Fall 2017

04 Requirements Continued

Dr. Spencer Smith

Faculty of Engineering, McMaster University

September 14, 2018



Requirements

- Administrative details
- Questions?
- Goal statement examples
- Requirements documentation for scientific computing
- A new requirements template
- Advantages of new template and examples
- The new template from a software engineering perspective
- Concluding remarks
- References

Administrative Details

- Add me to your GitHub repos, my GitHub id is smiths
- Assign me an issue to review your problem statements
 - ▶ Clearly state that you would like me to review your problem statement
 - ▶ Include a link to your problem statement
- Do not put generated files under version control
- Create a .gitignore file
- SRS template in blank project folder should be good
- The CA template will be revised soon

Administrative Details: Deadlines

Problem Statement	Week 02	Sept 14
SRS Present	Week 04	Week of Sept 24
SRS	Week 05	Oct 4
Syst. VnV Present	Week 06	Week of Oct 15
System VnV Plan	Week 07	Oct 22
MG Present	Week 08	Week of Oct 29
MG	Week 09	Nov 5
MIS Present	Week 10	Week of Nov 12
MIS	Week 11	Nov 19
Unit VnV or Impl. Present	Week 12	Week of Nov 26
Unit VnV Plan	Week 13	Dec 3
Final Doc	Week 14	Dec 10

Administrative Details: Presentation Schedule

- SRS Present
 - ▶ Wednesday: Jennifer, Yang, Brooks
 - ▶ Friday: Vajiheh, Olu, Karol
- Syst V&V Plan Present
 - ▶ Wednesday: Malavika, Robert, Qirui
 - ▶ Friday: Jian, Hanane
- MG Present
 - ▶ Wednesday: Karol, Malavika, Robert, Qirui, Jian, Hanane
 - ▶ Friday: Vajiheh, Olu, Jennifer, Yang, Brooks
- MIS Present
 - ▶ Wednesday: Malavika, Robert, Qirui
 - ▶ Friday: Jian, Hanane, Jennifer
- Unit VnV Plan or Impl. Present
 - ▶ Wednesday: Yang, Brooks, Vajiheh
 - ▶ Friday: Olu, Karol

Administrative Details: Presentations

- 3 presentations each
- Presentations are about 30 minutes, except for MG, which is 15 minutes
- 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

Questions?

- Questions about project choices?
- Questions about software tools?
- Questions about problem statements?
- Questions about software qualities?

Big Picture View of SRS/CA

- Goal statement(s)
- Inputs and outputs

Goal Statements for SWHS

What are the goal statement for the Solar Water Heating System?

Goal Statements for SWHS

Given the temperature of the heating coil, initial conditions for the temperature of the water and the temperature of the phase change material, and material properties, the goal statements are:

GS1: Predict the water temperature over time.

GS2: Predict the PCM temperature over time.

GS3: Predict the change in the energy of the water over time.

GS4: Predict the change in the energy of the PCM over time.

(Consider using names instead of numbers for labels.)

Goal Statements for GlassBR

Given the dimensions of the glass plane, glass type, the characteristics of the explosion, and the tolerable probability of breakage, the goal statements are:

GS1: Analyze and predict whether the glass slab under consideration will be able to withstand the explosion of a certain degree which is calculated based on user input.

Goal Statements for Game Physics

- G_linear:** Given the physical properties, initial positions and velocities, and forces applied on a set of rigid bodies, determine their new positions and velocities over a period of time (IM-IM_FT).
- G_ang:** Given the physical properties, initial orientations and angular velocities, and forces applied on a set of rigid bodies, determine their new orientations and angular velocities over a period of time. (IM-IM_FR).
- G_dtcCol:** Given the initial positions and velocities of a set of rigid bodies, determine if any of them will collide with one another over a period of time.
- G_Col:** Given the physical properties, initial linear and angular positions and velocities, determine the new positions and velocities over a period of time of rigid bodies that have undergone a collision (IM-IM_C).

Goal Statements for Linear Solver

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

Goal Statements for Linear Solver

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

Problems with Developing Quality Scientific Computing Software

- Need to know requirements to judge reliability
- In many cases the only documentation is the code
- Reuse is not as common as it could be
 - ▶ Meshing software survey
 - ▶ Public domain finite element programs
 - ▶ etc.
- Many people develop “from scratch”
- Cannot easily reproduce the work of others
- Neglect of simple software development technology [5]

Adapt Software Engineering Methods

- Software engineering improves and quantifies quality
- Successfully applied in other domains
 - ▶ Business and information systems
 - ▶ Embedded real time systems
- Systematic engineering process
- Design through documentation
- Use of mathematics
- Reuse of components
- Warranty rather than a disclaimer

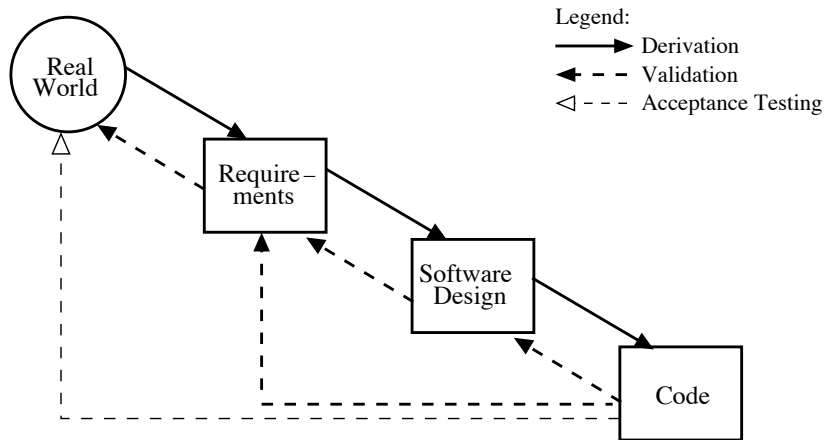
Developing Scientific Computing Software

- Facilitators
 - ▶ One user viewpoint for specifying a physical model
 - ▶ Assumptions can be used to distinguish models
 - ▶ High potential for reuse
 - ▶ Libraries
 - ▶ Already mathematical
- Challenges
 - ▶ Verification and Validation
 - ▶ Acceptance of software engineering methodologies
 - ▶ No existing templates or examples

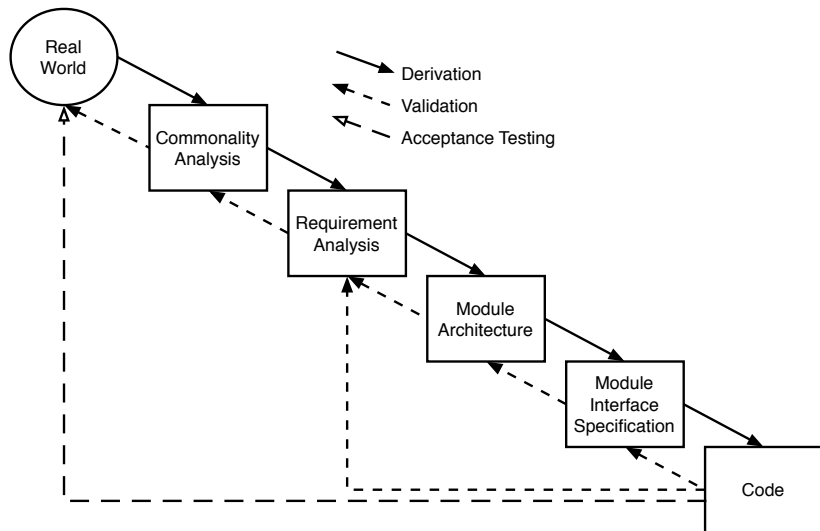
Outline of Discussion of Requirements

- Background on requirements elicitation, analysis and documentation
- Why requirements analysis for engineering computation?
- System Requirements Specification and template for beam analysis software
 - ▶ Provides guidelines
 - ▶ Eases transition from general to specific
 - ▶ Catalyses early consideration of design
 - ▶ Reduces ambiguity
 - ▶ Identifies range of model applicability
 - ▶ Clear documentation of assumptions

A Rational Design Process



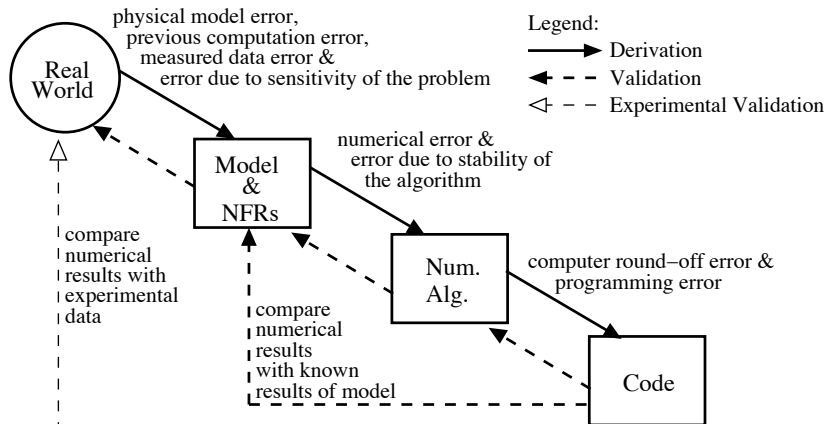
Sometimes Include Commonality Analysis



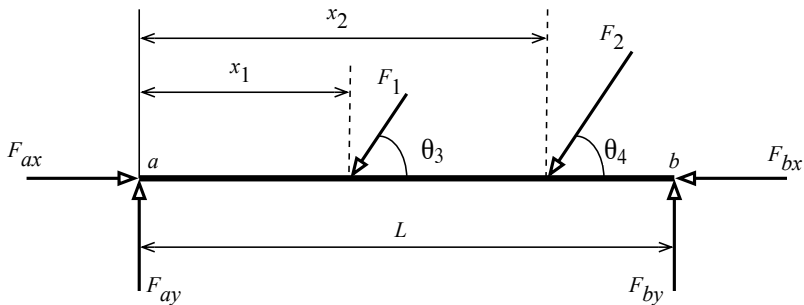
Software Requirements Activities

- A software requirement is a description of how the system should behave, or of a system property or attribute
- Requirements should be 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

Why Requirements Analysis?



Beam Analysis Software



Proposed Template

From [4]

1. Reference Material: a) Table of Symbols ...
2. Introduction: a) Purpose of the Document; b) Scope of the Software Product; c) Organization of the Document.
3. General System Description: a) System Context; b) User Characteristics; c) System Constraints.
4. Specific System Description:
 - 4.1 Problem Description: i) Background Overview ...
 - 4.2 Solution specification: i) Assumptions; ii) Theoretical Models; ...
 - 4.3 Non-functional Requirements: i) Accuracy of Input Data; ii) Sensitivity ...
5. Traceability Matrix
6. List of Possible Changes in the Requirements
7. Values of Auxiliary Constants

Provides Guidance

- Details will not be overlooked, facilitates multidisciplinary collaboration
- Encourages a systematic process
- Acts as a checklist
- Separation of concerns
 - ▶ Discuss purpose separately from organization
 - ▶ Functional requirements separate from non-functional
- Labels for cross-referencing
 - ▶ Sections, physical system description, goal statements, assumptions, etc.
 - ▶ PS1.a “the shape of the beam is long and thin”

Eases Transition from General to Specific

- “Big picture” first followed by details
- Facilitates reuse
- “Introduction” to “General System Description” to “Specific System Description”
- Refinement of abstract goals to theoretical model to instanced model
 - ▶ **G1**. Solve for the unknown external forces applied to the beam
 - ▶ **T1** $\sum F_{xi} = 0, \sum F_{yi} = 0, \sum M_i = 0$
 - ▶ **M1** $F_{ax} - F_1 \cdot \cos \theta_3 - F_2 \cdot \cos \theta_4 - F_{bx} = 0$

Ensures Special Cases are Considered

H_2		H_1	
$S_{unkF} \notin \mathbb{P}_3$	-	$S_{GET} = S_{sym} - S_{unkF}$	$S_{GET} \neq (S_{sym} - S_{unkF})$
$S_{unkF} = \{\odot F_{ax}, \odot F_{bx}, \odot F_{ay}\}$	-	$(ErrorMsg' = InvalidUnknown) \wedge ChangeOnly(ErrorMessage)$	FALSE
$S_{unkF} = \{\odot F_{ax}, \odot F_{ay}, \odot F_1\}$	$x_1 \neq 0$ $\wedge \theta_3 \neq 0$ $\wedge \theta_3 \neq 180$	$ErrorMsg' = NoSolution \wedge ChangeOnly(ErrorMessage)$	
	otherwise	$F'_{ax} = \frac{-\cos \theta_3 F_2 x_2 \sin \theta_4 + \cos \theta_3 F_{by} L + F_2 \cos \theta_4 x_1 \sin \theta_3 + F_{bx} x_1 \sin \theta_3}{x_1 \sin \theta_3}$ \wedge $F'_{ay} = -\frac{F_2 x_2 \sin \theta_4 - F_{by} L - F_2 \sin \theta_4 x_1 + F_{by} x_1}{x_1 \sin \theta_3}$ $\wedge F'_1 = \frac{-F_2 x_2 \sin \theta_4 + F_{by} L}{x_1 \sin \theta_3} \wedge ChangeOnly(S_{unkF})$	
		$(ErrorMsg' = Indeterminant) \wedge ChangeOnly(ErrorMessage)$	
H_2		G	

Catalyses Early Consideration of Design

- Identification of significant issues early will improve the design
- Section for considering sensitivity
 - ▶ Conditioning?
 - ▶ Buckling of beam
- Non-functional requirements
 - ▶ Tradeoffs in design
 - ▶ Speed efficiency versus accuracy
- Tolerance allowed for solution: $|\sum F_{xi}|/\sqrt{\sum F_{xi}^2} \leq \epsilon$
- Solution validation strategies
- List of possible changes in requirements

Reduces Ambiguity

- Unambiguous requirements allow communication between experts, requirements review, designers do not have to make arbitrary decisions
- Tabular expressions allow automatic verification of completeness
- Table of symbols
- Abbreviations and acronyms
- Scope of software product and system context
- User characteristics
- Terminology definition and data definition
- Ends arguments about the relative merits of different designs

Identifies Range of Model Applicability

- Clear documentation as to when model applies
- Can make the design specific to the problem
- Input data constraints are identified
 - ▶ Physically meaningful: $0 \leq x_1 \leq L$
 - ▶ Maintain physical description: PS1.a, $0 < h \leq 0.1L$
 - ▶ Reasonable requirements: $0 \leq \theta_3 \leq 180$
- The constraints for each variable are documented by tables, which are later composed together
- $(\min_f \leq |F_{ax}| \leq \max_f) \wedge (|F_{ax}| \neq 0) \Rightarrow$
 $\forall (FF | @FF \in S_F \cdot FF \neq 0 \wedge \frac{\max\{|F_{ax}|, |FF|\}}{\min\{|F_{ax}|, |FF|\}} \leq 10^{r_f})$

Summary of Variables

Var	Type	Physical Constraints	System Constraints	Prop
x	<i>Real</i>	$x \geq 0 \wedge x \leq L$	$min_d \leq x \leq max_d$	NIV
x_1	<i>Real</i>	$x_1 \geq 0 \wedge x_1 \leq L$	$min_d \leq x_1 \leq max_d$	IN
x_2	<i>Real</i>	$x_2 \geq 0 \wedge x_2 \leq L$	$min_d \leq x_2 \leq max_d$	IN
e	<i>Real</i>	$e > 0 \wedge e \leq h$	$min_e \leq e \leq max_e$	IN
h	<i>Real</i>	$h > 0 \wedge h \leq 0.1L$	$min_h \leq h \leq max_h$	IN
L	<i>Real</i>	$L > 0$	$min_d \leq L \leq max_d$	IN
E	<i>Real</i>	$E > 0$	$min_E \leq E \leq max_E$	IN
θ_3	<i>Real</i>	$-\infty < \theta_3 < +\infty$	$0 \leq \theta_3 \leq 180$	IN
θ_4	<i>Real</i>	$-\infty < \theta_4 < +\infty$	$0 \leq \theta_4 \leq 180$	IN
V	<i>Real</i>	$-\infty < V < +\infty$	-	OUT
M	<i>Real</i>	$-\infty < M < +\infty$	-	OUT
y	<i>Real</i>	$-\infty < y < +\infty$	-	OUT
...

Clear Documentation of Assumptions

Phy. Sys. /Goal	Data /Model	Assumption										Model	
		A1	A2	...	A4	...	A8	A9	A10	...	A14	M1	...
G1	T1	✓		✓	✓		...		✓	...
G2	T2	✓		✓	✓	
G3	T3	✓			✓	✓
	M1		✓		✓	...
PS1.a	<i>L</i>					✓
...

A10. The deflection of the beam is caused by bending moment only, the shear does not contribute.

More on the Template

- Why a new template?
- The new template
 - ▶ Overview of changes from existing templates
 - ▶ Goal → Theoretical Model → Instanced Model hierarchy
 - ▶ Traceability matrix
 - ▶ System behaviour, including input constraints

Why a New Template?

From [3]

1. One user viewpoint for the physical model
2. Assumptions distinguish models
3. High potential for reuse of functional requirements
4. Characteristic hierarchical nature facilitates change
5. Continuous mathematics presents a challenge

Overview of the New Template

- Reference Material
- Introduction: a) Purpose of the Document b) Scope of the Software Product c) Organization of the Document
- General System Description: a) System Context b) User Characteristics c) System Constraints
- Specific System Description: a) Problem Description b) Solution Characteristics Specification c) Non-functional Requirements
- Other System Issues
- Traceability Matrix
- List of Possible Changes in the Requirements
- Values of Auxiliary Constants
- References

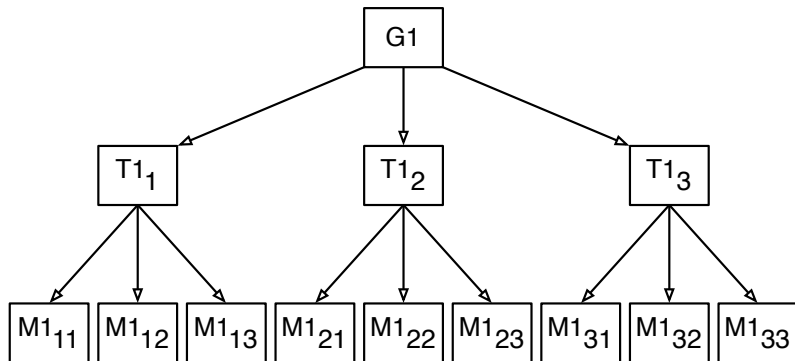
Overview of the New Template

- Reference Material
- Introduction: a) Purpose of the Document b) Scope of the Software Product c) Organization of the Document
- General System Description: a) System Context b) User Characteristics c) System Constraints
- Specific System Description: a) Problem Description b) Solution Characteristics Specification c) Non-functional Requirements
- Other System Issues
- Traceability Matrix
- List of Possible Changes in the Requirements
- Values of Auxiliary Constants
- References

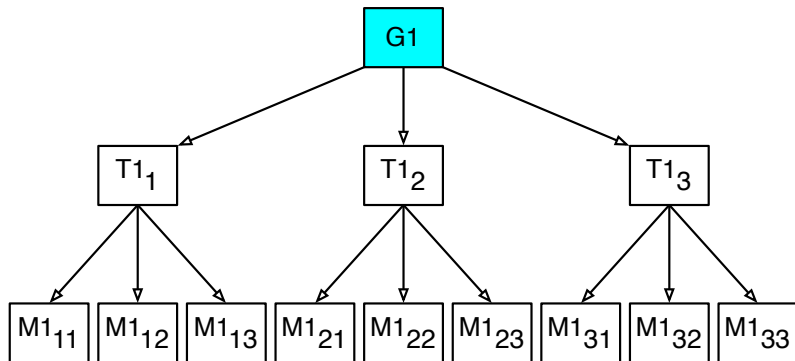
Excerpts from Specific System Description

- Problem Description
 - ▶ Physical system description (**PS**)
 - ▶ Goals (**G**)
- Solution Characteristics Specification
 - ▶ Assumptions (**A**)
 - ▶ Theoretical models (**T**)
 - ▶ Data definitions
 - ▶ Instanced models (**M**)
 - ▶ Data constraints
 - ▶ System behaviour
- Non-functional Requirements
 - ▶ Accuracy of input data
 - ▶ Sensitivity of the model
 - ▶ Tolerance of the solution
 - ▶ Solution validation strategies

Refinement from Abstract to Concrete

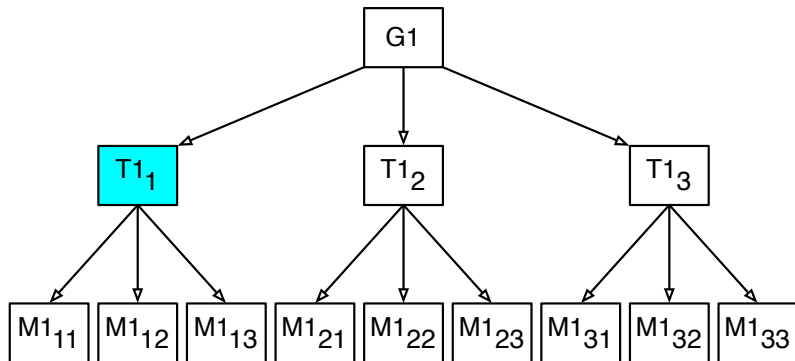


Refinement from Abstract to Concrete



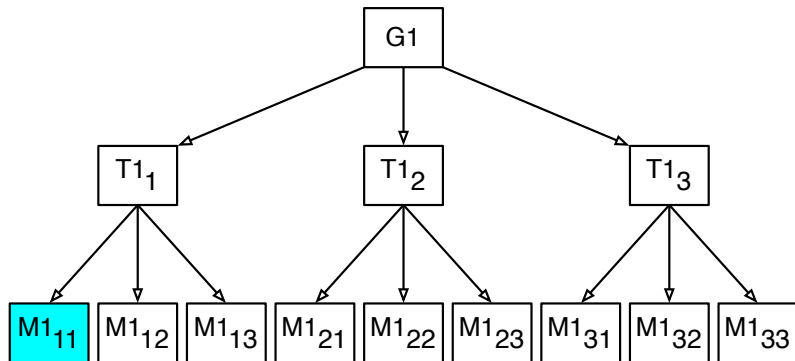
G1: Solve for unknown forces

Refinement from Abstract to Concrete



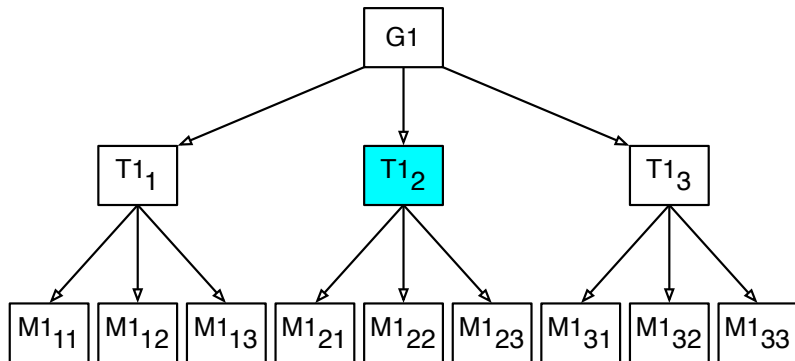
$$(\mathbf{T1_1}) \left\{ \begin{array}{l} \sum F_{xi} = 0 \\ \sum F_{yi} = 0 \\ \sum M_i = 0 \end{array} \right.$$

Refinement from Abstract to Concrete



$$(M1) \quad \begin{cases} F_{ax} - F_1 \cdot \cos \theta_3 - F_2 \cdot \cos \theta_4 - F_{bx} = 0 \\ F_{ay} - F_1 \cdot \sin \theta_3 - F_2 \cdot \sin \theta_4 + F_{by} = 0 \\ -F_1 \cdot x_1 \sin \theta_3 - F_2 \cdot x_2 \sin \theta_4 + F_{by} \cdot L = 0 \end{cases}$$

Refinement from Abstract to Concrete



The virtual work done by all the external forces and couples acting on the system is zero for each independent virtual displacement of the system, or mathematically $\delta U = 0$

Other goals and models

- **G2**: Solve for the functions of shear force and bending moment along the beam
- **G3**: Solve for the function of deflection along the beam
- **T3₁**: $\frac{d^2y}{dx^2} = \frac{M}{EI}$, $y(0) = y(L) = 0$
- **T3₂**: y determined by moment area method
- **T3₃**: y determined using Castigliano's theorem
- **M3₁₁**: $y = \frac{12 \int_0^L (\int_0^L M dx) dx}{Eeh^3}$, $y(0) = y(L) = 0$

Kreyman and Parnas Five Variable Model

- See [\[1\]](#)
- An alternative approach
- Unfortunately the numerical algorithm is not hidden in the requirements specification
- The analogy with real-time systems leads to some confusion

Examples

- Solar Water Heating System
- GlassBR

Summary of Template

- Quality is a concern for scientific computing software
- Software engineering methodologies can help
- Motivated, justified and illustrated a method of writing requirements specification for engineering computation to improve reliability
- Also improve quality with respect to usability, verifiability, maintainability, reusability and portability
- Tabular expressions to reduce ambiguity, encourage systematic approach
- Conclusions can be generalized because other computation problems follow the same pattern of *Input* then *Calculate* then *Output*
- Benefits of approach should increase as the number of details and the number of people involved increase

Summary of Template (Continued)

- A new template for scientific computing has been developed
- Characteristics of scientific software guided the design
- Designed for reuse
- Functional requirements split into “Problem Description” and “Solution Characteristics Specification”
- Traceability matrix
- Addresses nonfunctional requirements (but room for improvement)

References I



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.



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.

References II



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
conjunction with 13th IEEE International Requirements
Engineering Conference.

References III



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.



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.