

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

Fall 2017

## 04 Requirements Continued

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# Requirements

- Administrative details
- Questions?
- License and copyright
- 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
- Updates to SRS template
- Commonality analysis should start from SRS template

# Administrative Details: Deadlines

|                          |         |                 |
|--------------------------|---------|-----------------|
| <b>Problem Statement</b> | Week 02 | Sept 15         |
| SRS Present              | Week 04 | Week of Sept 25 |
| SRS                      | Week 05 | Oct 4           |
| V&V Present              | Week 06 | Week of Oct 16  |
| V&V Plan                 | Week 07 | Oct 25          |
| MG Present               | Week 08 | Week of Oct 30  |
| MG                       | Week 09 | Nov 8           |
| MIS Present              | Week 10 | Week of Nov 13  |
| MIS                      | Week 11 | Nov 22          |
| Impl. Present            | Week 12 | Week of Nov 27  |
| Final Documentation      | Week 13 | Dec 6           |

# Questions?

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

# 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

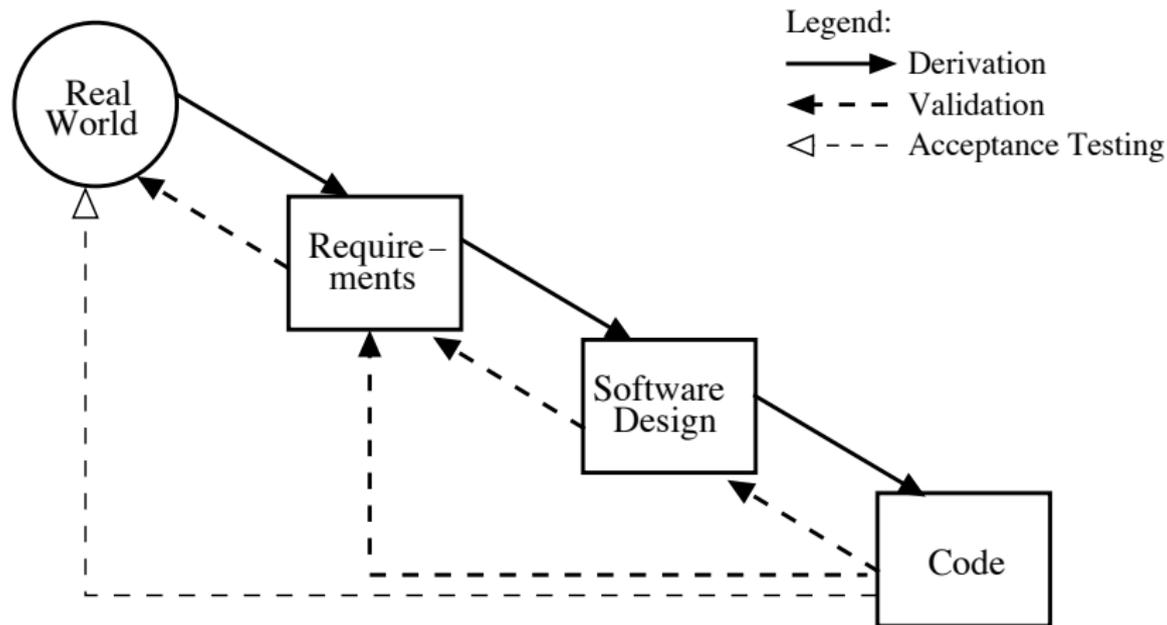
# Developing Scientific Computing Software

- 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

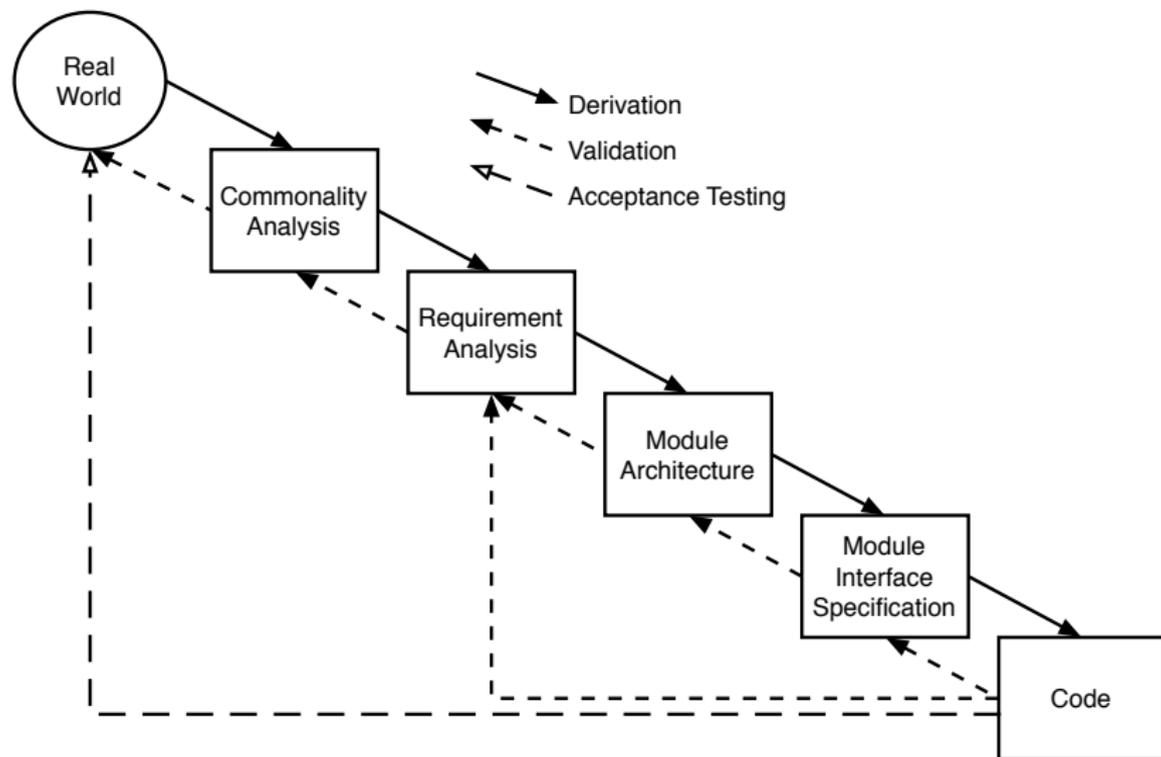
# Outline of Discussion of Requirements

- 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



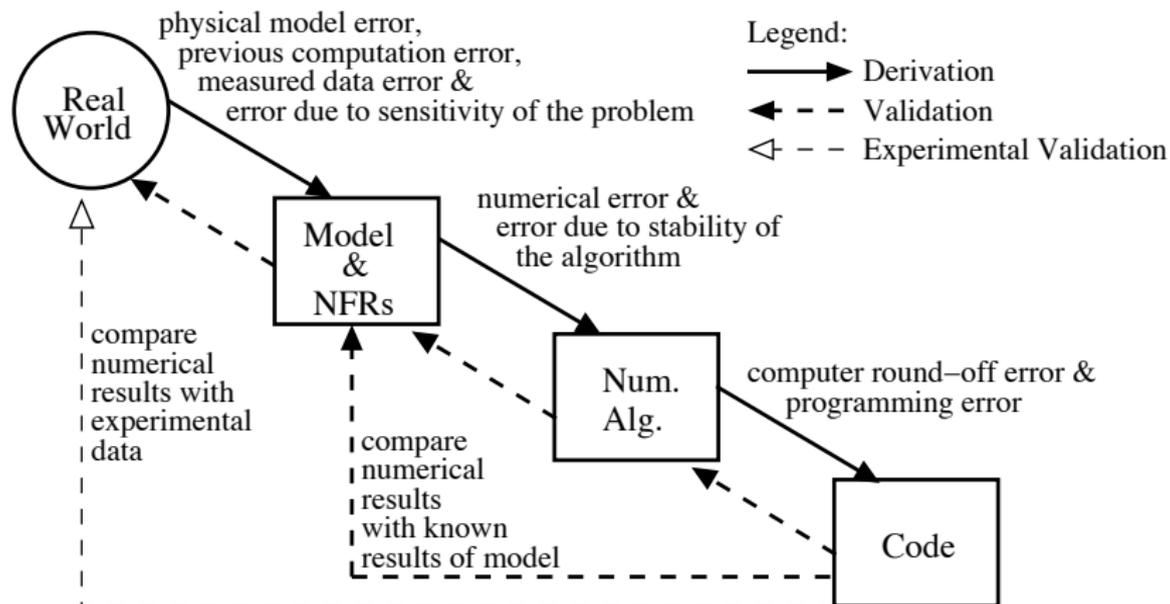
# Sometimes Include Commonality Analysis



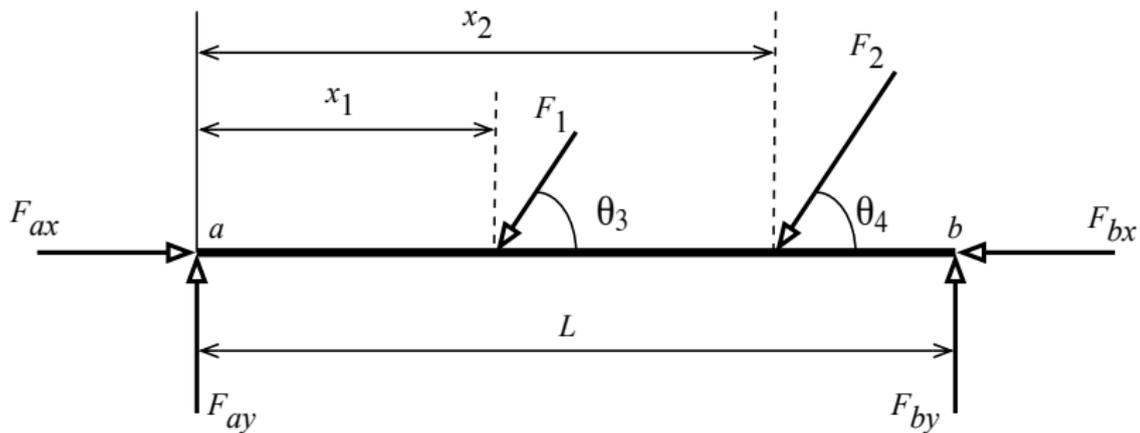
# Software Requirements Activities

- 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

|   |  |
|---|--|
| $S_{unkF} \notin \mathbb{P}_3$  | -  |
| $S_{unkF} = \{\textcircled{F}_{ax}, \textcircled{F}_{bx}, \textcircled{F}_{ay}\}$ | -  |
| $S_{unkF} = \{\textcircled{F}_{ax}, \textcircled{F}_{ay}, \textcircled{F}_1\}$    | $x_1 \neq 0$<br>$\wedge \theta_3 \neq 0$<br>$\wedge \theta_3 \neq 180$ |
|   | otherwise  |

$H_2$

|   |                                     |
|---|-------------------------------------|
| $H_1$   |                                     |
| $S_{GET} = S_{sym} - S_{unkF}$  | $S_{GET} \neq (S_{sym} - S_{unkF})$ |
| $(ErrorMsg' = InvalidUnknown) \wedge ChangeOnly(ErrorMsg)$  | <b>FALSE</b>                        |
| $ErrorMsg' = NoSolution \wedge ChangeOnly(ErrorMsg)$  |                                     |
| $F'_{ax} = \frac{-\cos \theta_3 F_2 x_2 \sin \theta_4 + \cos \theta_3 F_{by} L + F_2 \cos \theta_4 x_1 \sin \theta_3 + F_{bx} x_1 \sin \theta_3}{x_1 \sin \theta_3}$<br>$\wedge$<br>$F'_{ay} = -\frac{F_2 x_2 \sin \theta_4 - F_{by} L - F_2 \sin \theta_4 x_1 + F_{by} x_1}{x_1 \sin \theta_3}$<br>$\wedge F'_1 = \frac{-F_2 x_2 \sin \theta_4 + F_{by} L}{x_1 \sin \theta_3} \wedge ChangeOnly(S_{unkF})$ |                                     |
| $(ErrorMsg' = Indeterminant) \wedge ChangeOnly(ErrorMsg)$   |                                     |

$G$

# 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   |
| $\theta_3$ | <i>Real</i> | $-\infty < \theta_3 < +\infty$ | $0 \leq \theta_3 \leq 180$  | IN   |
| $\theta_4$ | <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.<br>Sys.<br>/Goal | Data<br>/Model | Assumption |     |     |     |     |     |     |     |     |     | Model     |     |
|-----------------------|----------------|------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----------|-----|
|                       |                | A1         | A2  | ... | A4  | ... | A8  | A9  | A10 | ... | A14 | <b>M1</b> | ... |
| <b>G1</b>             | <b>T1</b>      | ✓          |     | ... |     | ... | ✓   | ✓   |     | ... |     | ✓         | ... |
| <b>G2</b>             | <b>T2</b>      | ✓          |     | ... |     | ... | ✓   | ✓   |     | ... |     |           | ... |
| <b>G3</b>             | <b>T3</b>      | ✓          |     | ... |     | ... |     | ✓   | ✓   | ... |     |           | ... |
|                       | <b>M1</b>      |            | ✓   | ... |     | ... |     |     |     | ... |     | ✓         | ... |
| 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

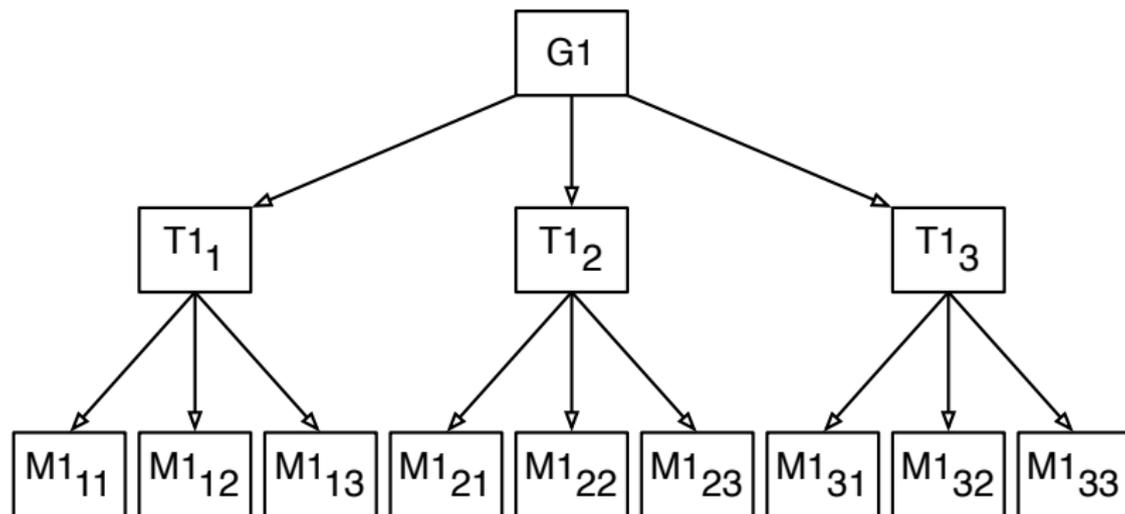
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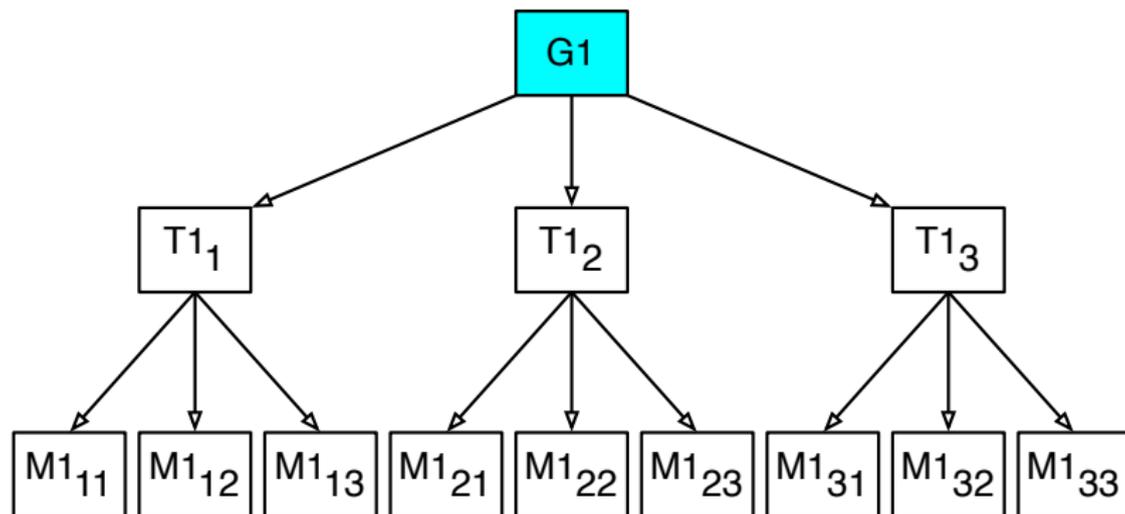
# Excerpts from Specific System Description

- 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

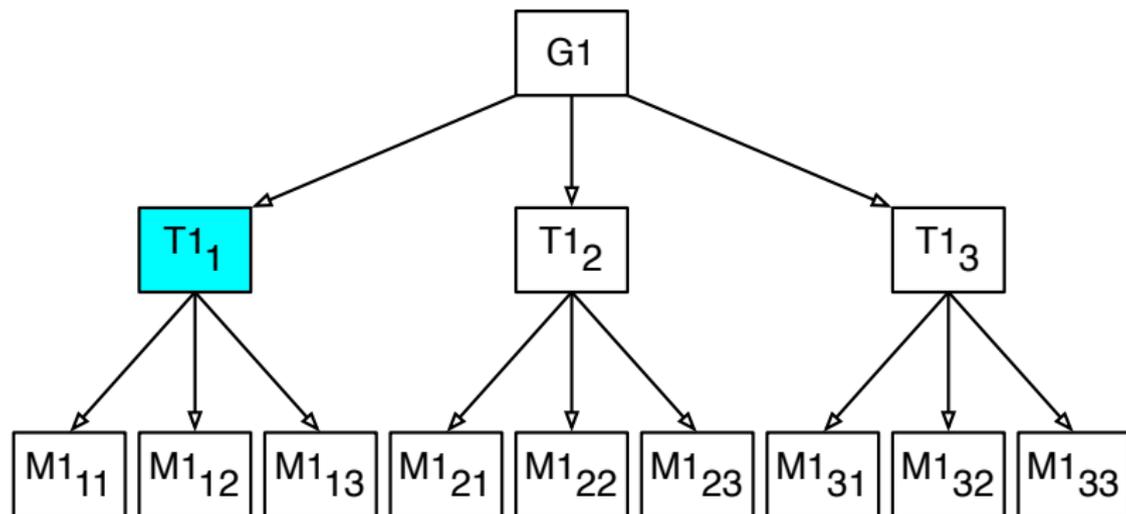


# Refinement from Abstract to Concrete



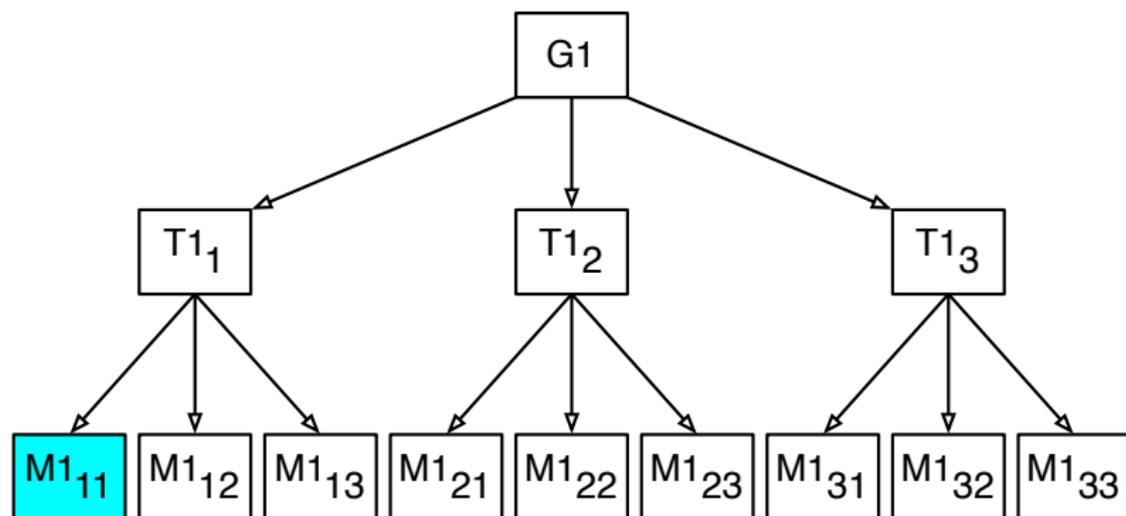
**G1**: Solve for unknown forces

# Refinement from Abstract to Concrete



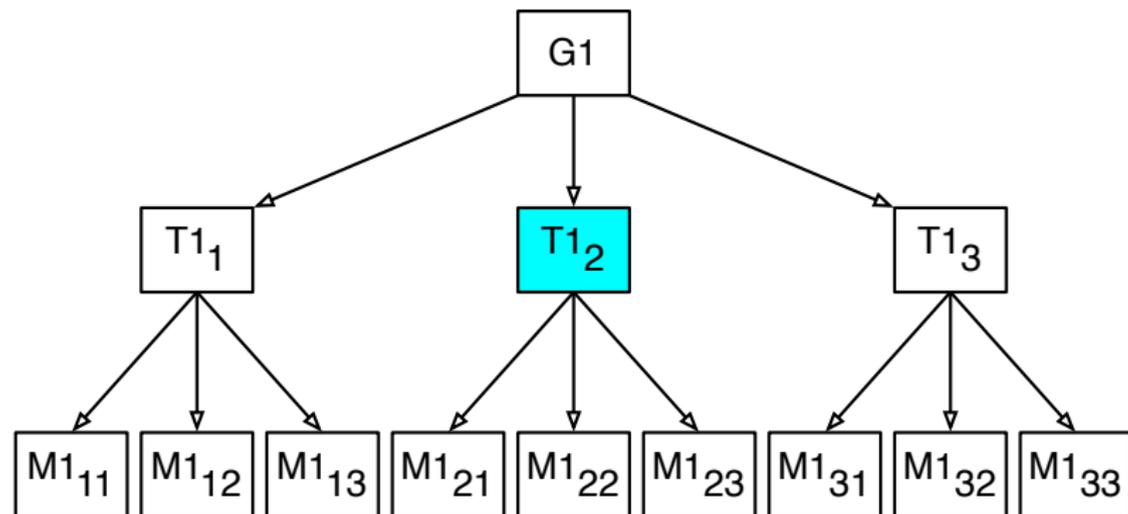
$$(\mathbf{T1}_1) \begin{cases} \sum F_{xi} = 0 \\ \sum F_{yi} = 0 \\ \sum M_i = 0 \end{cases}$$

# Refinement from Abstract to Concrete



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

# 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
- **T3<sub>1</sub>**:  $\frac{d^2y}{dx^2} = \frac{M}{EI}$ ,  $y(0) = y(L) = 0$
- **T3<sub>2</sub>**:  $y$  determined by moment area method
- **T3<sub>3</sub>**:  $y$  determined using Castigliano's theorem
- **M3<sub>11</sub>**:  $y = \frac{12 \int_0^L (\int_0^L M dx) dx}{Eeh^3}$ ,  $y(0) = y(L) = 0$

# 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)

# Specification Qualities

- What are the important qualities for a specification?

# Specification Qualities

- The qualities we previously discussed (usability, maintainability, reusability, verifiability etc.)
- Clear, unambiguous, understandable
- Consistent
- Complete
  - ▶ Internal completeness
  - ▶ External completeness
- Incremental
- Validatable
- Abstract
- Traceable

Summarized in [2, 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?

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  - ▶ 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  $\sigma$ 
  - ▶ 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 matrices
- Common sense suggests traceability improves maintainability
- Shows consequence of change
- Minimizes cost of recertification
- Additional advantages
  - ▶ Program comprehension
  - ▶ Impact analysis
  - ▶ Reuse

# 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.

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A new requirements template for scientific computing.

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*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.