

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

Fall 2017

06 Program Families Continued

Dr. Spencer Smith

Faculty of Engineering, McMaster University

September 20, 2017



Program Families Continued

- Administrative details
- Questions?
- License and copyright
- Motivation
- Proposed Family Methods
- Family of Mesh Generators
- Family of Linear Solvers
- Family of Material Behaviour Models

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
- Presentations
 - ▶ VGA by default, ask if need adapter
 - ▶ Can you my laptop

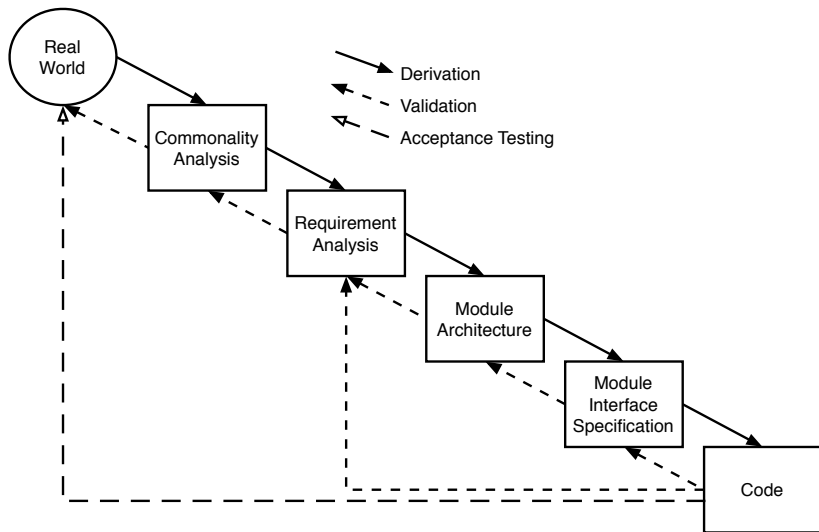
Administrative Details: Deadlines

Problem Statement	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

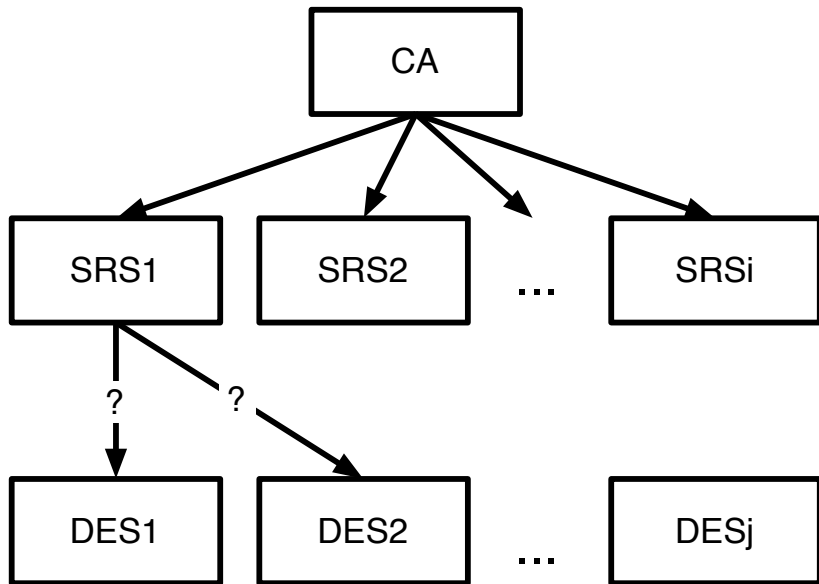
Questions?

- Questions about ...

Overview of Process



CA to SRS to Design



Proposed Methodology

1. Identify family of interest
 - ▶ Specific physical model?
 - ▶ Multipurpose tool?
2. Commonality Analysis (CA)
 - ▶ Terminology
 - ▶ Commonalities
 - ▶ Variabilities
 - ▶ Parameters of variation
 - ▶ Binding time
3. Domain Specific Language (DSL)
4. Generation of family members

CA Template From [12]

1. Reference Material: a) Table of Contents b) Table of Symbols c) Abbreviations and Acronyms
2. Introduction: a) Purpose of the Document b) Organization of the Document
3. General System Description: a) Potential System Contexts b) Potential User Characteristics c) Potential System Constraints
4. Commonalities: a) Background Overview b) Terminology Definition c) Goal Statements d) Theoretical Models
5. Variabilities: a) Input Assumptions b) Calculation c) Output
6. Traceability Matrix
7. References

Abstract Requirements

- Appropriate level of abstraction by refining from goal to theory to input assumptions
- A goal is a functional objective the software should achieve:
G1: Find the roots of an equation
- Goals are refined into theoretical models:
T1: Given a function $f(x)$ and an interval $\{x | x_{lower} \leq x_{upper}\}$, return the points where $f(x) = 0$
- Introduce simplifying assumptions to allow theoretical model to be solved:
VA1,2: $f(x)$ is continuous on the interval and/or $f(x)$ has at least one sign change on the interval

Abstract Requirements (Continued)

- Each variability has an associated parameter of variation and a binding time
 - ▶ Specification time
 - ▶ Compile time
 - ▶ Run time

Capture Existing Knowledge

- Systematic consideration from general to specific
- Communication between experts
- Standard template allows comparison
- Convenient framework for summarizing existing literature
- Eventually a library of requirements documentation
- CA refined by a family of SRSs

System Requirements Specification (SRS)

- Based on IEEE Standard 830 and Volere requirements specification template
- Sections from CA are refined in SRS
- “Potential” descriptions are made specific
- Variabilities are set
- Binding times are set

SRS Template

1. Reference Material
2. Introduction
3. General System Description
4. Specific System Description: a) Background Overview, b) Terminology Definition, c) Goal Statements d) Theoretical Models, e) Assumptions, f) Data Constraints, g) System Behaviour
5. Non-functional Requirements: a) Accuracy of Input Data, b) Sensitivity of the Model, c) Tolerance of Solution, d) Performance, ... i) Portability,
6. Solution Validation Strategies,
7. Other System Issues:
8. Traceability Matrix

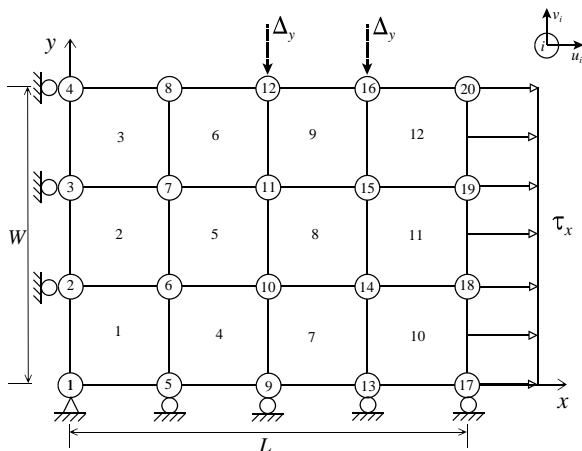
NFRs

- Rather than absolute quantification of NFRs, use relative comparison between other program family members
- Specify requirements in big O notation
- Relative importance between NFRs using Analytic Hierarchy Process (AHP) [11]
 - ▶ Addresses challenge of comparing attributes that are measured in different (or hard to quantify) units
 - ▶ Series of pair-wise comparisons between attributes
 - ▶ 1 for equal importance, 3 for moderately strong importance, ..., 9 for extreme importance

Validatable Requirements

- Relative comparison between programs is a validatable requirement
- Focus on a posteriori description, rather than a priori specification
- Solution validation strategies
 - ▶ Solve using different techniques
 - ▶ Identify benchmark test problems
 - ▶ Test cases built starting from assumed solutions (Method of Manufactured Solutions)
 - ▶ Partially validate for a simpler subset where the solution is known

Mesh Generating Software



Commonality Analysis for a Mesh Generator

From Chen's work [8, 14, 13]. Alternate approach in [4, 10, 1, 2, 3]

- Terminology
 - ▶ requirement
 - ▶ structured mesh, ...
- Commonalities
 - ▶ discretization
 - ▶ input from user is required, ...
- Variabilities
 - ▶ shape of elements
 - ▶ coordinate system used, ...
- Parameters of variation
 - ▶ line, triangle, quadrilateral, tetrahedral, hexahedral
 - ▶ Cartesian, polar, spherical, ...

Definition of a Mesh

Let Ω be a closed bounded domain in \mathbb{R} or \mathbb{R}^2 or \mathbb{R}^3 and let K be a simple shape, such as a line segment in 1D, a triangle or a quadrilateral in 2D, or a tetrahedron or hexahedron in 3D. A mesh of Ω , denoted by τ , has the following properties:

1. $\Omega \approx \cup(K | K \in \tau : K)$, where \cup is first closed and then opened
2. the length of every element K , of dimension 1, in τ is greater than zero
3. the interior of every element K , of dimension 2 or greater, in τ is nonempty
4. the intersection of the interior of two elements is empty

Example Commonality

Item Number	C1
Description	A mesh generator discretizes a given computational domain (closed boundary Ω) into a covering up of a finite number of simpler shapes.
Related Variability	V6, V8, V12, V14, V15, V16, V17, V18
History	Created - May 7, 2004

Mesh Generator (MG) Goals

- G1 Input spatial domain Ω output a mesh M that covers this domain.
- G2 Transform information on the materials, material properties and the locations of the different materials
- G3 Transform information on the boundary condition types, values and locations
- G4 Transform system information, such as numerical algorithm parameters

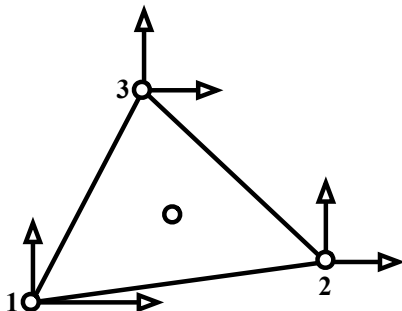
Element Variability

Location of nodes: sequence of LocationT

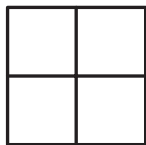
Number of dof at nodes: sequence of \mathbb{N}

LocationT = tuple of $(L_1 : \text{natT}, L_2 : \text{natT}, L_3 : \text{natT})$

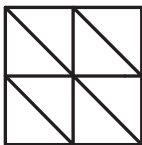
$\text{natT} = \{ s : \mathbb{R} \mid 0 \leq s \leq 1 : s \}$



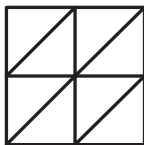
Local Topology Variability



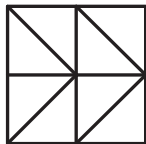
Quad



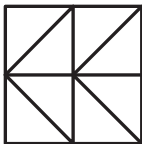
Triangle1



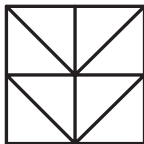
Triangle2



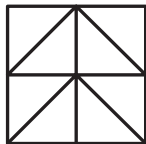
Triangle3



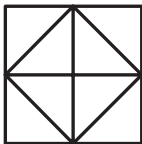
Triangle4



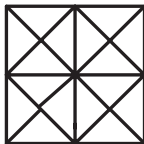
Triangle5



Triangle6



Triangle7



Triangle8

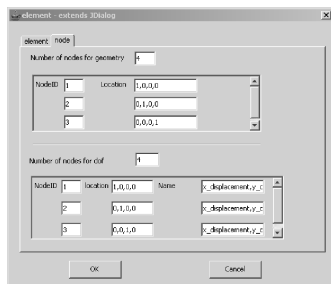
DSL Using XML

```
<elementSet>
  <geometrySpec>
    <shape>triangle1</shape>
    <nodeGeo count="3">
      <node id="1">
        <location>1,0,0</location>
      </node>
      <node id="2">
        <location>0,1,0</location>
      </node>
      ...
    </nodeGeo>
  </geometrySpec>
</elementSet>
```


Proof of Concept Implementation

From Cao's work [5, 15]

- XML document that customizes a Java object
- The Java object customizes the general purpose MG as it is loaded
- General purpose MG
 - ▶ All variabilities bound at run-time
 - ▶ Corresponds to an empty XML specification



Linear Systems of Equations

$$Ax = b$$

Commonality analysis presented in [\[12\]](#)

Goal and Theoretical Model

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

T1: Given 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 $b \in \text{span}(A)$
3. No solution if A is singular and $b \notin \text{span}(A)$

Variabilities for Input Assumptions

Variability	Parameter of Variation
Allowed structure A	Set of { full, sparse, banded, tridiagonal, block triangular, ..., Hessenberg }
Allowed definiteness A	Set of { not definite, positive definite, ..., negative semi-definite }
Allowed class of A	Set of { diagonally dominant, Toeplitz, Vandermonde }
Symmetry assumed?	boolean
Possible values for n	set of \mathbb{N}
Possible entries in A	set of \mathbb{R}
...	...

Variabilities for Calculation

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 }

Variabilities for Output

Variability	Parameter of Variation
Destination for output x	Set of { to file, to 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 $\mathbb{R} \cup \{-\infty, \infty, \textit{undef}\}$

Analytic Hierarchy Process

- Example 1
 - ▶ Embedded real-time system for digital signal processing
 - ▶ $n = 10$
 - ▶ A is assumed to be Toeplitz

	Speed	Accuracy	Portability	Priority
Speed	1	3	5	0.64
Accuracy	1/3	1	3	0.26
Portability	1/5	1/3	1	0.11

Solution Validation Strategies

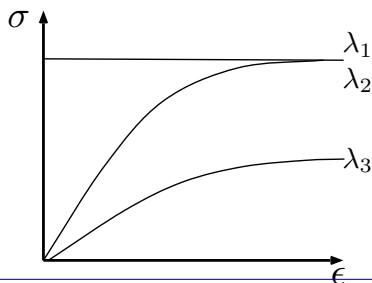
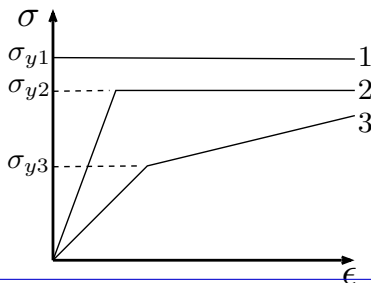
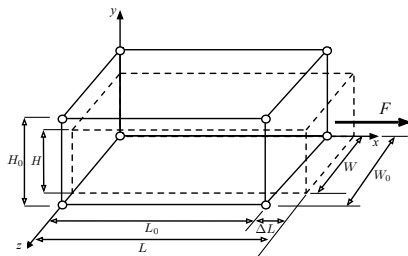
- Create test cases with known solutions
 - ▶ Assume A and x , calculate b
 - ▶ Given A and b calculate x^* and compare to the assumed x
- Comparison with Matlab
- Comparison with NAG library
- Where possible compare solution to interval arithmetic solution
- Experiments to describe how accuracy changes with increasing condition number

Connection to Design

- Abstract requirements to concrete design decisions
- Reuse existing packages within the program family
- Summarize existing software by the parameters of variation and binding time
- If functional requirements match, then use NFRs
 - ▶ AHP to compare each design against each of the NFRs
 - ▶ Contribution of each NFR for each design alternative is found by multiplying the contribution of each alternative to the given NFR with the corresponding priority of that NFR
 - ▶ Sum the contributions
 - ▶ The highest overall score is the “winning” alternative

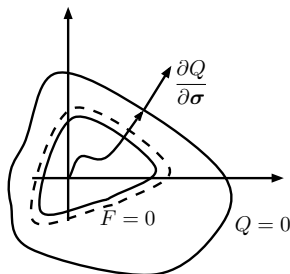
A Family of Material Models

From McCutchan's work [7, 15, 16, 6, 17, 9]



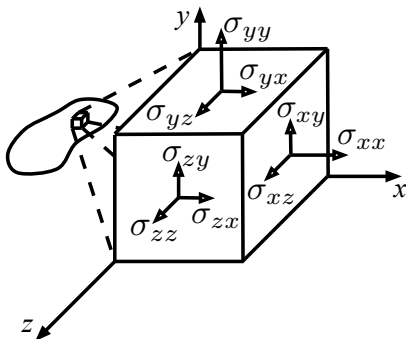
Terminology Definitions

Label:	D_YieldFunction
Symbol:	$F = F(\boldsymbol{\sigma}, \kappa)$
Type:	$(\text{tensor2DT} \times \mathbb{R}) \rightarrow \mathbb{R}$
Related:	D_Stress, D_HardeningParameter
Sources:	...
Descrip:	The yield function defines a surface $F = 0$ in the six dimensional stress space ...



Goal Statement

Label:	G_StressDetermination
Descrip:	Given the initial stress and the deformation history of a material particle, determine the stress within the material particle.
Refine:	T_ConstitEquation



Assumptions

Label:	A_AdditivityPostulate
Related:	D_StrainRate
Equation:	$\dot{\epsilon} = \dot{\epsilon}^e + \dot{\epsilon}^{vp}$ with the following types and units $\dot{\epsilon}$: tensor2DT (1/t) (1/s) $\dot{\epsilon}^e$: tensor2DT (1/t) (1/s) $\dot{\epsilon}^{vp}$: tensor2DT (1/t) (1/s)
Descrip:	The total strain rate ($\dot{\epsilon}$) is assumed to decompose into elastic ($\dot{\epsilon}^e$) and viscoplastic ($\dot{\epsilon}^{vp}$) strain rates.
Rationale	This is a standard assumption for elastoplastic and elastoviscoplastic materials. The appropriateness of this assumption is born out by the success of theories built upon it.
Source:	[6, page 339]; [7, page 181]

Theoretical Model

Label:	T_ConstitEquation
Related:	A_CauchyStress, A_DeformationHistory, A_PerzynaConstit, A_AdditivityPostulate, A_ElasticConstit, A_DescriptionOfMotion, V_MaterialProperties
Input:	$\sigma_0 : \text{tensor2DT (StressU) (Pa)}$ $t_{begin} : \mathbb{R} (t) (s)$ $t_{end} : \mathbb{R} (t) (s)$ $\dot{\epsilon}(t) : \{t : \mathbb{R} t_{begin} \leq t \leq t_{end} : t\} \rightarrow$ $\text{tensor2DT (1/t) (1/s)}$ $mat_prop_val : \text{string} \rightarrow \mathbb{R}$ $E : \mathbb{R}^+ (\text{StressU}) (\text{Pa})$ $\nu : \text{poissonT (dimensionless)}$

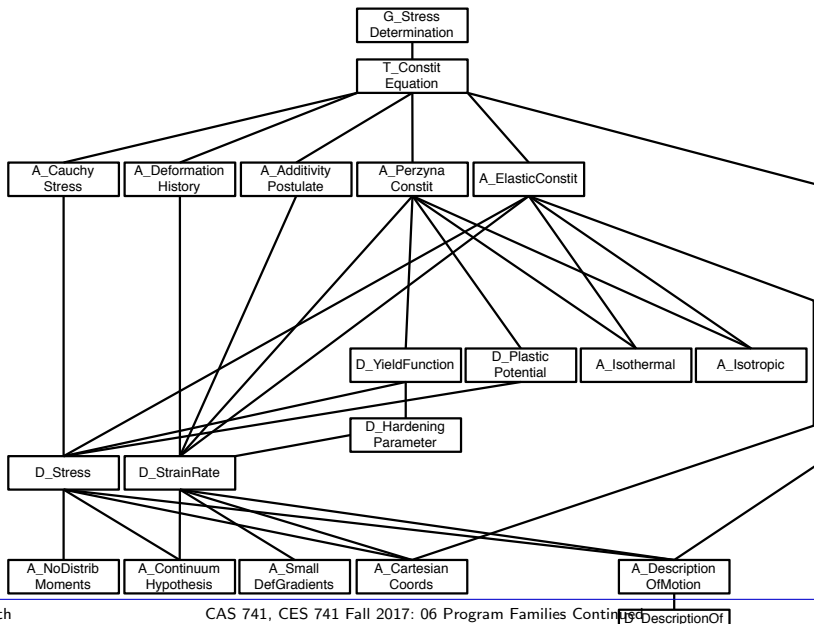
Theoretical Model Continued

Label:	T_ConstitEquation
Output:	<p>$\sigma(t) : \{t : \mathbb{R} t_{begin} \leq t \leq t_{end} : t\} \rightarrow \text{tensor2DT}$ such that</p> $\dot{\sigma} = \mathbf{D} \left(\dot{\epsilon} - \gamma < \varphi(F(\sigma, \kappa)) > \frac{\partial Q(\sigma)}{\partial \sigma} \right)$ <p>and $\sigma(t_{begin}) = \sigma_0$, the components of σ have the units of StressU (Pa)</p>
Derive:	The governing differential equation is found by first solving for $\dot{\epsilon}^e$ in A_AdditivityPostulate and then ...
Descrip:	The theoretical model is only completely defined once the associated variabilities (V_MaterialProperties) that define the material have been set. ...
History:	Created — June 14, 2007

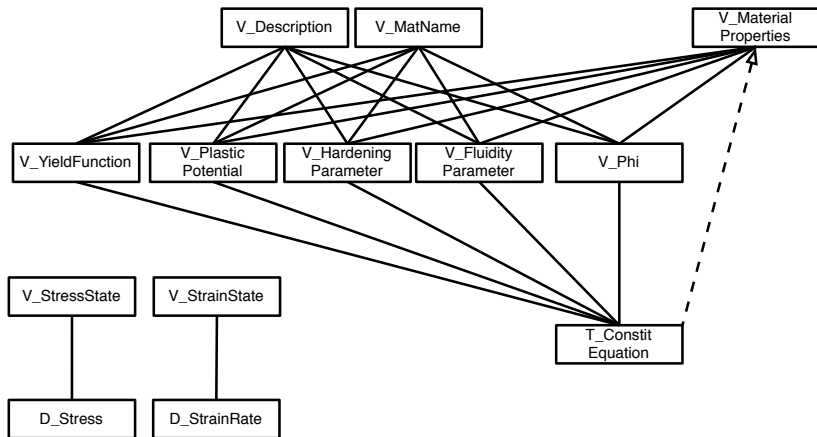
Variabilities

- $F = F(\sigma, \kappa) : \mathbb{R}^6 \times \mathbb{R} \rightarrow \mathbb{R}$
- $Q = Q(\sigma) : \mathbb{R}^6 \rightarrow \mathbb{R}$
- $\kappa = \kappa(\epsilon^{vp}) : \mathbb{R}^6 \rightarrow \mathbb{R}$
- $\varphi = \varphi(F) : \mathbb{R} \rightarrow \mathbb{R}$
- $\gamma : \mathbb{R}$
- *mat_prop_names* : set of string

Dependency Graph



Dependency Graph Between Commonalities and Variabilities



Example

Label:	E_StrainHardening
V_MatName	<i>name</i> = "Strain-Hardening Viscoelastic"
V_YieldFunct	$F = q\kappa^{\frac{n-1}{m}}$ (StressU) (Pa)
V_PlasticPot	$Q = q$ (StressU) (Pa)
V_HardParam	$\kappa = \epsilon_q^{vp}$ (L/L) (m/m)
V_Phi	$\varphi = F^{\frac{m}{n}}$ (StressU $^{\frac{m}{n}}$) (Pa $^{\frac{m}{n}}$)
V_FluParam	$\gamma = nA^{\frac{1}{n}}$ (StressU $^{-m}$ t $^{-1}$) (Pa $^{-m}$ s $^{-1}$)
V_MatProps	<i>mat_prop_names</i> = { "A", "m", "n" }, where the type of the material properties are ...
V_Description	<i>descript</i> = "This constitutive equation combines a power-law viscoelastic mate- rial with a strain hardening (softening) material. ..."

Code Generation

- Specify variabilities
- Symbolically calculate terms needed by numerical algorithm, including $\frac{\partial Q}{\partial \sigma}$, $\frac{\partial F}{\partial \sigma}$, etc.
- Symbolic processing avoids tedious and error-prone hand calculations
 - ▶ Reduces workload
 - ▶ Allows non-experts to deal with new problems
 - ▶ Increases reliability
- Use Maple Computer Algebra System for model manipulation
- Convert math expressions into C expressions using “CodeGeneration”
- Inline into a C++ class defining the material model
- A finite element program can this interface to realize the numerical algorithm

BNF of DSL for F

$\langle expression \rangle \rightarrow \langle number \rangle |$

$(\langle expression \rangle) |$

$\langle expression \rangle ^ \langle expression \rangle |$

$\langle expression \rangle * \langle expression \rangle |$

...

$\langle simulation-variable-F \rangle | \langle user-defined-constants \rangle$

$\langle simulation-variable-F \rangle \rightarrow \mathbf{Kappa} | \langle simulation-variable-stress \rangle | \langle simulation-variable-stress-macros \rangle$

$\langle simulation-variable-$

$stress \rangle \rightarrow \mathbf{SigmaXX} | \mathbf{SigmaYY} | \mathbf{SigmaZZ} | \mathbf{SigmaXY} |$

$\mathbf{SigmaYZ} | \mathbf{SigmaXZ}$

$\langle simulation-variable-stress-$

$macros \rangle \rightarrow \mathbf{Sxx} | \mathbf{Syy} | \mathbf{Szz} | \mathbf{Sxy} | \mathbf{Syz} | \mathbf{Sxz} | \mathbf{Sm} | \mathbf{J2} | \mathbf{J3} | \mathbf{q}$

$\langle user-defined-constants \rangle \rightarrow \langle string \rangle$

Concluding Remarks

- Case studies of applying software engineering methodologies to mesh generating systems and linear solvers
- Appropriate and advantageous to apply program family strategy
- Challenges for software engineers
- General purpose scientific software is best studied as a program family
 - ▶ Variabilities are assumptions about problems that can be handled
 - ▶ Derive requirements from commonality analysis
- Eventually hope for automatic code generation

Concluding Remarks (Continued)

A new methodology for documenting requirements for general purpose scientific computing software

1. Validatable requirements

- ▶ Relative comparison between program family members
- ▶ Focus on description rather than specification
- ▶ Solution validation strategy

2. Abstract

- ▶ Refine goal statement to theoretical model to input assumptions
- ▶ In some cases one may want to turn off input checking
- ▶ Connection to design

Concluding Remarks (Continued)

3. NFRs

- ▶ Relative comparison
- ▶ AHP

4. Capture and reuse

- ▶ Systematic consideration from general to specific
- ▶ CA refined by a family of SRSs
- ▶ CA and SRS summarize existing knowledge and currently available software
- ▶ Standard template allows comparison
- ▶ Convenient framework for summarizing existing literature

Concluding Remarks

- A new template for a family of models of physical phenomena
- Refinement of **Goals** to **Theoretical Models** using **Data Definitions** and **Assumptions**
- **Variabilities** are identified in the Theoretical Model
- A constitutive equation can be written using a (declarative) DSL and the code can be generated
- A DSL has been built, using Maple, for a virtual material testing laboratory

Concluding Remarks

- SC software is a great candidate for development as a program family
- Produce programs that are as special or general purpose as needed
- Improve reusability, usability and reliability
- Potential to improve performance
- A commonality analysis facilitates the design of a DSL
- Symbolic processing and code generation are very useful techniques
- We will return to code generation later

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