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

Fall 2019

06 Program Families Continued

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Program Families Continued

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

Administrative Details

- Marking scheme for SRS
  - You should be able to see it in Avenue
  - Do NOT submit on Avenue

Administrative Details: Report Deadlines

SRS	Week 06	Oct 7
System VnV Plan	Week 08	Oct 28
MG + MIS	Week 10	Nov 25
Final Documentation	Week 14	Dec 9

- 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, please ask
- Two days after each major deliverable, your GitHub issues will be due
- Domain expert code due 1 week after MIS deadline

Administrative Details: Presentations

SRS Present	Week 05	Week of Sept 30
Syst. VnV Present	Week 07	Week of Oct 21
MG + MIS Syntax Present	Week 9	Week of Nov 4
MIS Semantics Present	Week 11	Week of Nov 18
Unit VnV or Impl. Present	Week 12/13	Week of Nov 28

- Informal presentations with the goal of improving everyone's written deliverables
- Domain experts and secondary reviewers (and others) will ask questions (listed in Repos.xlsx file)

Administrative Details: Presentation Schedule

- SRS (or CA) Present
  - **Monday: Deema, Sharon, Bo**
  - **Thursday: Sasha, Colin, Zhi**
- Syst V&V Plan Present
  - Monday: Deema, Peter
  - Thursday: Sharon, Ao
- MG + MIS Syntax Present
  - Monday: Deema, Bo
  - Thursday: Colin, Sasha
- MIS Syntax + Semantics Present
  - Monday: Zhi, Peter
  - Thursday: Sharon, Ao
- Unit VnV Plan or Impl. Present
  - Monday: Bo, Sasha, Colin
  - Thursday: Zhi, Peter, Ao

Questions?

- Questions about SRS?
- Questions about CA?
- Any questions on the SRS Checklist?
- Questions about presentations?
- Questions about tools (git, GitHub, LaTeX)?

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 $\}$

- Algorithms are not listed, but they could be
- If they were, they would be in a separate table, to show they are design variabilities

Is SC Suited to a Program Family Approach?

Based on criteria from Weiss [2, 32, 33, 14, 31]

- 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

CA Template From [22]

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. Requirements (added to template)
7. Traceability Matrix

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 (scope) time
  - Compile/generation 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, (moved to separate document)
7. Other System Issues:
8. Traceability Matrix

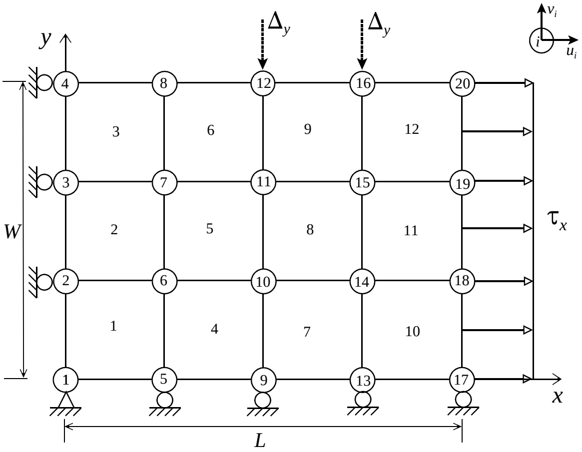
NFRs

- 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) [21]
  - 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 [12, 24, 23]. Alternate approach in [6, 20, 3, 4, 5]

- 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. $\Omega \approx \cup(K|K\epsilon\tau : K)$, 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

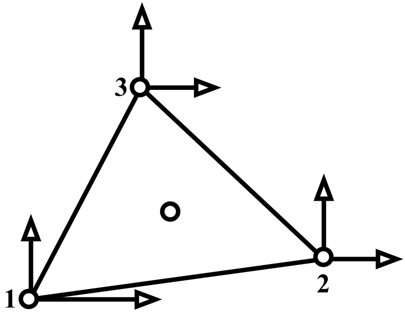
Item Number	C1
Description	A mesh generator discretizes a given computational domain (closed boundary Ω) into a covering up of a finite number of simpler shapes.
Related Variability	V6, V8, V12, V14, V15, V16, V17, V18
History	Created - May 7, 2004

Mesh Generator (MG) Goals

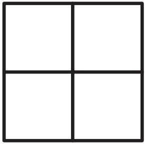
- G1 Input spatial domain Ω output a mesh M that covers this domain.
- G2 Transform information on the materials, material properties and the locations of the different materials
- G3 Transform information on the boundary condition types, values and locations
- G4 Transform system information, such as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

Element Variability

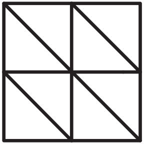
Location of nodes: sequence of LocationT
Number of dof at nodes: sequence of $\mathbb{N}$
LocationT = tuple of (L_1 : natT, L_2 : natT, L_3 : natT)
natT $= \{\ s : \mathbb{R} | 0 \leq s \leq 1 : s\ \}$



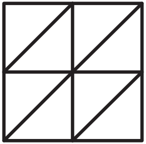
Local Topology Variability



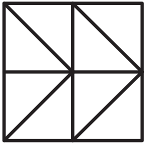
Quad



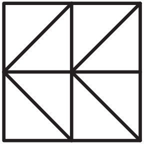
Triangle1



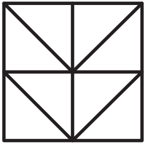
Triangle2



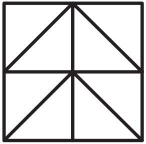
Triangle3



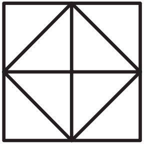
Triangle4



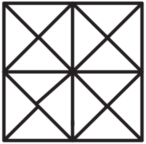
Triangle5



Triangle6



Triangle7



Triangle8

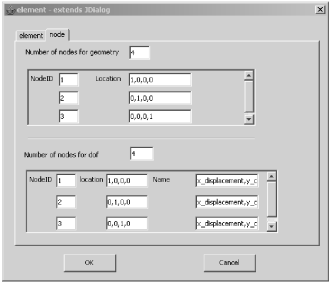
DSL Using XML

```
<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 [8, 27]

- 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



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

NFR for Correctness (for VnV Plan)

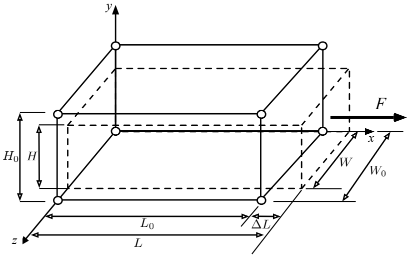
- Create test cases with known solutions
  - Assume A and x, calculate b
  - Given A and b calculate x^* and compare to the assumed x
- Comparison with Matlab
- Comparison with NAG library
- Where possible compare solution to interval arithmetic solution
- Experiments to describe how accuracy changes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

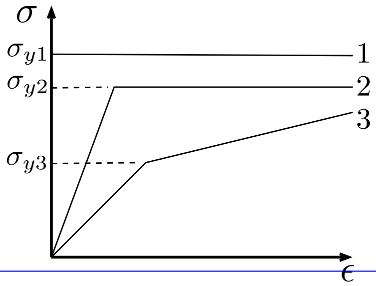
Connection to Design

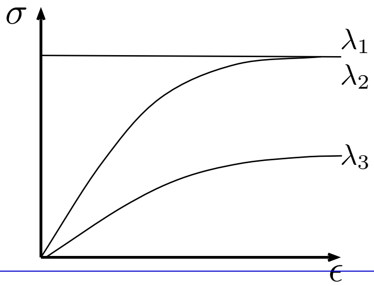
- Abstract requirements to concrete design decisions
- Reuse existing packages within the program family
- Summarize existing software by the parameters of variation and binding time
- If functional requirements match, then use NFRs
  - AHP to compare each design against each of the NFRs
  - Contribution 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 [11, 27, 28, 10, 29, 16]

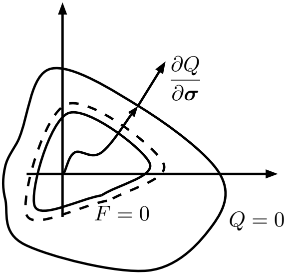






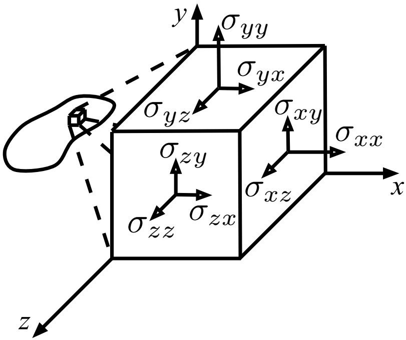
Terminology Definitions

Label:	D_YieldFunction
Symbol:	$F = F(\boldsymbol{\sigma}, \kappa)$
Type:	(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:	$\dot{\boldsymbol{\epsilon}} = \dot{\boldsymbol{\epsilon}}^{e} + \dot{\boldsymbol{\epsilon}}^{vp}$ with the following types and units $\dot{\boldsymbol{\epsilon}}$: tensor2DT (1/t) (1/s) $\dot{\boldsymbol{\epsilon}}^{e}$: tensor2DT (1/t) (1/s) $\dot{\boldsymbol{\epsilon}}^{vp}$: tensor2DT (1/t) (1/s)
Descrip:	The total strain rate ($\dot{\boldsymbol{\epsilon}}$) is assumed to decompose into elastic ($\dot{\boldsymbol{\epsilon}}^{e}$) and viscoplastic ($\dot{\boldsymbol{\epsilon}}^{vp}$) 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:	$\boldsymbol{\sigma}_0$: tensor2DT (StressU) (Pa) t_{begin} : $\mathbb{R}$ (t) (s) t_{end} : $\mathbb{R}$ (t) (s) $\dot{\epsilon}(t)$: $\{t : \mathbb{R} \mid t_{begin} \leq t \leq t_{end} : t\} \rightarrow$ tensor2DT (1/t) (1/s) mat_prop_val : string $\rightarrow \mathbb{R}$ E : $\mathbb{R}^+$ (StressU) (Pa) ν : poissonT (dimensionless)

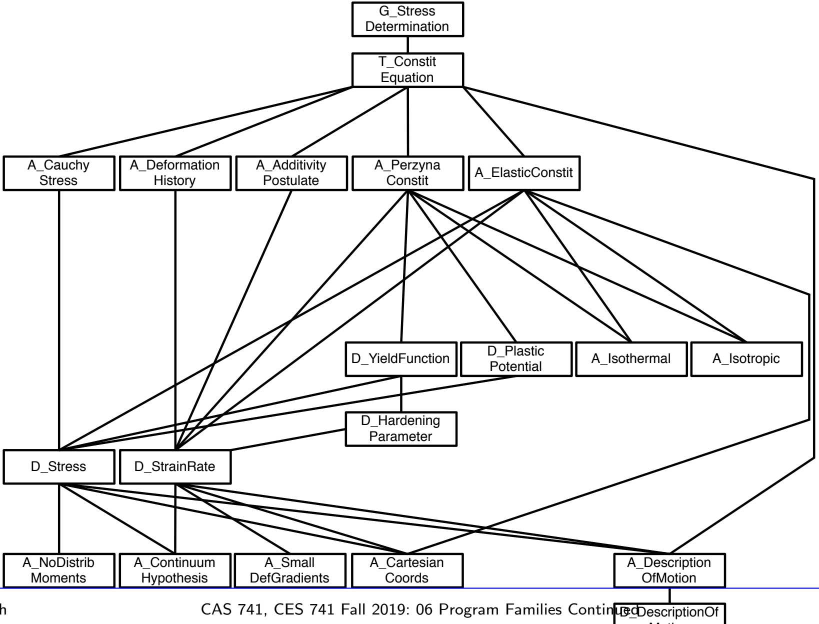
Theoretical Model Continued

Label:	T_ConstitEquation
Output:	$\boldsymbol{\sigma}(t) : \{t : \mathbb{R} \| t_{begin} \leq t \leq t_{end} : t\} \rightarrow$ tensor2DT such that $$\dot{\boldsymbol{\sigma}} = \mathbf{D}\left(\dot{\boldsymbol{\epsilon}} - \gamma < \varphi(F(\boldsymbol{\sigma}, \kappa)) > \frac{\partial Q(\boldsymbol{\sigma})}{\partial \boldsymbol{\sigma}}\right)$$ and $\boldsymbol{\sigma}(t_{begin}) = \boldsymbol{\sigma}_0$, the components of $\boldsymbol{\sigma}$ have the units of StressU (Pa)
Derive:	The governing differential equation is found by first solving for $\dot{\boldsymbol{\epsilon}}^e$ 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

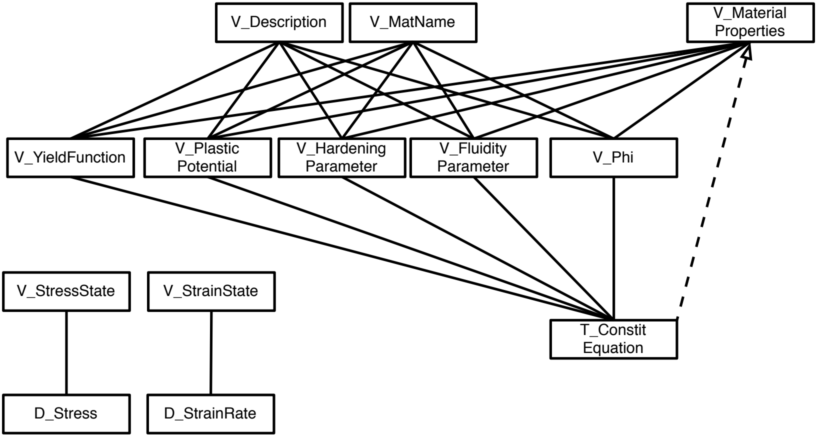
Variabilities

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

Dependency Graph



Dependency Graph Between Commonalities and Variabilities



Example

Label:	E_StrainHardening
V_MatName	*name* = "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	*mat_prop_names* = {"*A*", "*m*", "*n*" }, where the type of the material properties are ...
V_Description	*descript* = "This constitutive equation combines a power-law viscoelastic material with a strain hardening (softening) material. ..."

Code Generation

- Specify variabilities
- Symbolically calculate terms needed by numerical algorithm, including $\frac{\partial Q}{\partial \boldsymbol{\sigma}}$, $\frac{\partial F}{\partial \boldsymbol{\sigma}}$, 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

$\langle expression \rangle \to \langle number \rangle |$
$(\langle expression \rangle)|$
$\langle expression \rangle \hat{}\langle expression \rangle |$
$\langle expression \rangle * \langle expression \rangle |$

...
$\langle simulation\text{-}variable\text{-}F \rangle | \langle user\text{-}defined\text{-}constants \rangle$
$\langle simulation\text{-}variable\text{-}F \rangle \to$ **Kappa**$| \langle simulation\text{-}variable\text{-}stress \rangle | \langle simulation\text{-}variable\text{-}stress\text{-}macros \rangle$
$\langle simulation\text{-}variable\text{-}stress \rangle \to$ **SigmaXX**|**SigmaYY**|**SigmaZZ**|**S**
SigmaYZ|**SigmaXZ**
$\langle simulation\text{-}variable\text{-}stress\text{-}macros \rangle \to$ **Sxx**|**Syy**|**Szz**|**Sxy**|**Syz**|**Sxz**|**Sm**|**J2**|**J3**|**q**
$\langle user\text{-}defined\text{-}constants \rangle \to \langle string \rangle$

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

References I

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