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

Fall 2017

05 Program Families DRAFT

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Program Families

- 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

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 ...

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 [12, 18]

Background

- Program family idea since the 1970s (Dijkstra, Parnas, Weiss, Pohl, ...) - variabilities are often from a finite set of simple options [16, 17, 14]
- Families of algorithms and code generation in SC (Carette, ATLAS, Blitz++, ...) - not much emphasis on requirements [8, 33, 29, 6]
- Work on requirements for SC
  - Template for a single physical model [25, 24]
  - Template for a family of multi-purpose tool [21, 23, 22]
  - Template for a family of physical models [28, 27, 15]

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 [1, 31, 32, 13, 30]

- 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

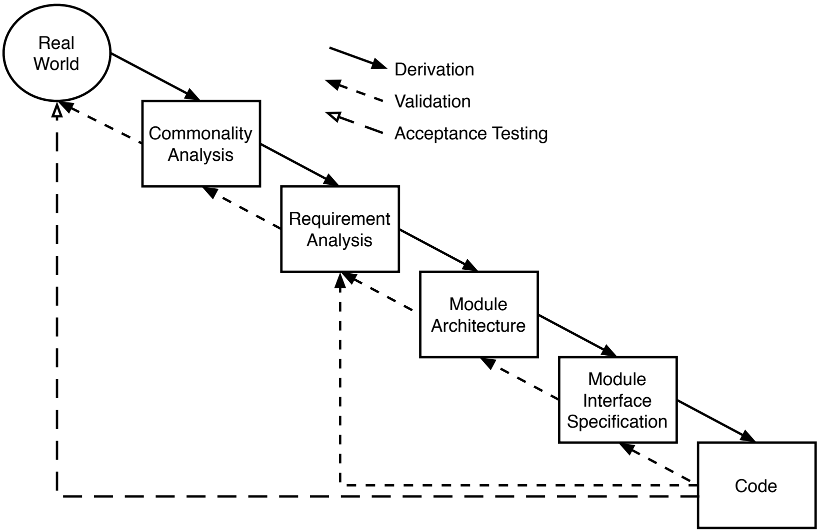
Challenges

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

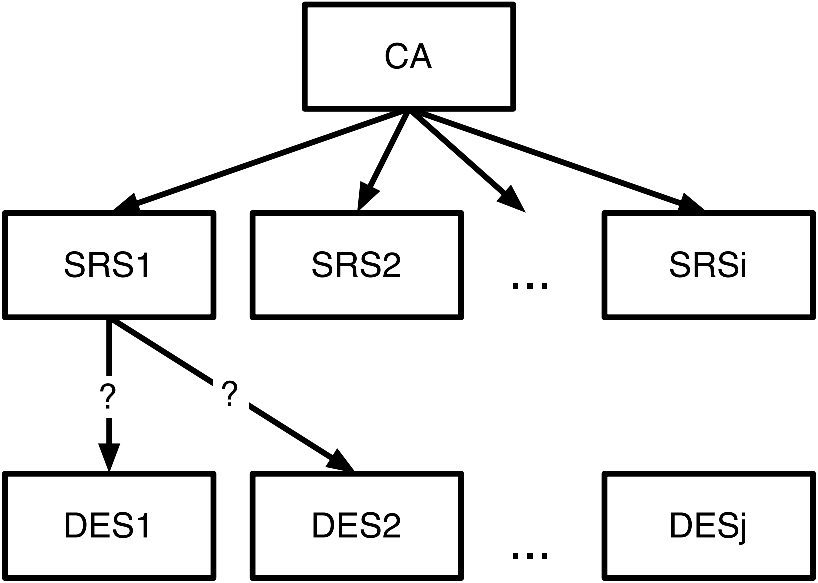
Challenges (Continued)

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

Overview of Process



CA to SRS to Design



Proposed Methodology

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

Commonality Analysis Template

From [21]

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

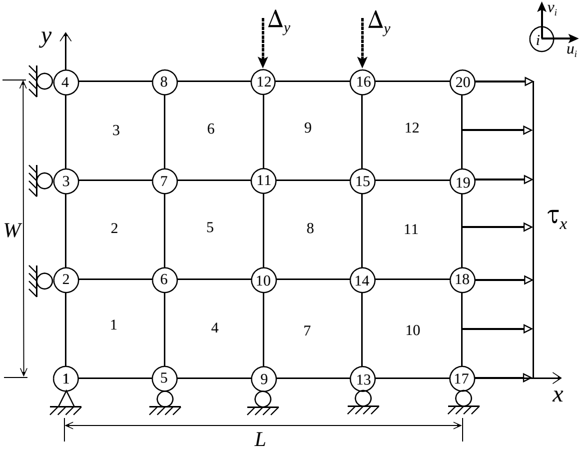
NFRs

- 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) [20]
  - 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 [11, 23, 22]. Alternate approach in [5, 19, 2, 3, 4]

- 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

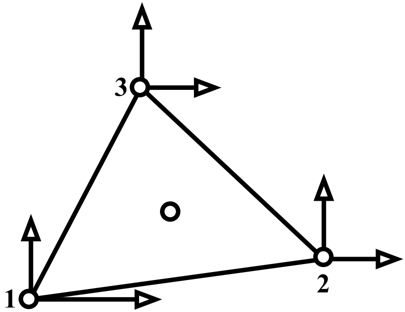
Item Number	C1
Description	A mesh generator discretizes a given computational domain (closed boundary Ω) into a covering up of a finite number of simpler shapes.
Related Variability	V6, V8, V12, V14, V15, V16, V17, V18
History	Created - May 7, 2004

Mesh Generator (MG) Goals

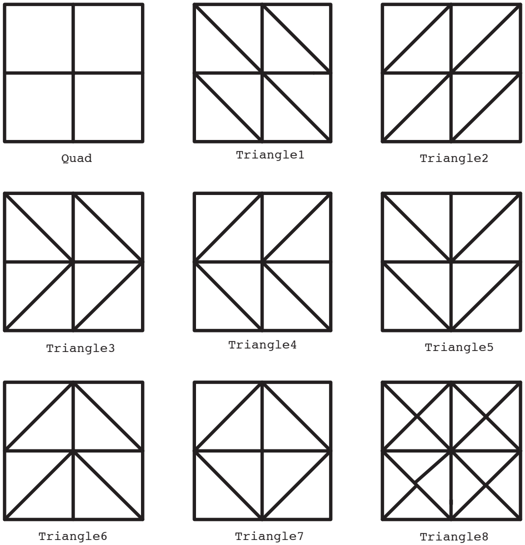
- G1 Input spatial domain Ω output a mesh M that covers this domain.
- G2 Transform information on the materials, material properties and the locations of the different materials
- G3 Transform information on the boundary condition types, values and locations
- G4 Transform system information, such as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



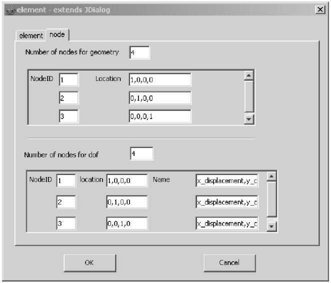
DSL Using XML

```
<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 [7, 26]

- 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 [21]

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 $b \in span(A)$
3. No solution if A is singular and $b \notin span(A)$

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 $\mathbb{R} \cup \{-\infty, \infty, \mathit{undef}\}$

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

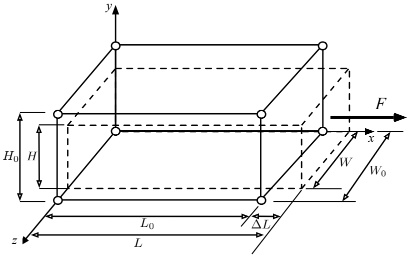
- Create test cases with known solutions
  - Assume A and x, calculate b
  - Given A and b calculate x^* and compare to the assumed x
- Comparison with Matlab
- Comparison with NAG library
- Where possible compare solution to interval arithmetic solution
- Experiments to describe how accuracy changes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

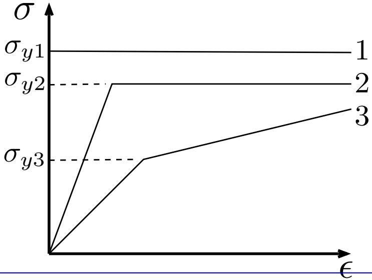
Connection to Design

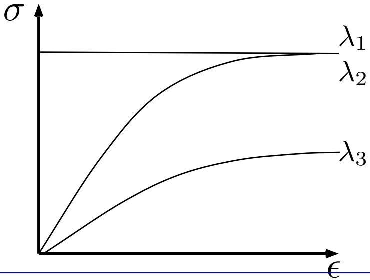
- Abstract requirements to concrete design decisions
- Reuse existing packages within the program family
- Summarize existing software by the parameters of variation and binding time
- If functional requirements match, then use NFRs
  - AHP to compare each design against each of the NFRs
  - Contribution 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 [10, 26, 27, 9, 28, 15]

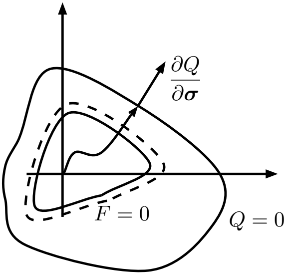






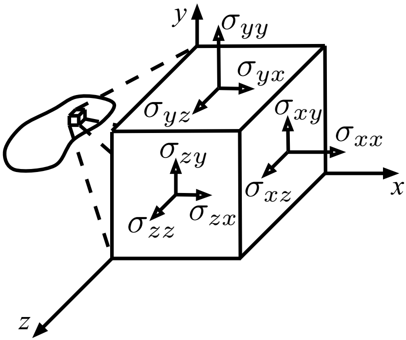
Terminology Definitions

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)

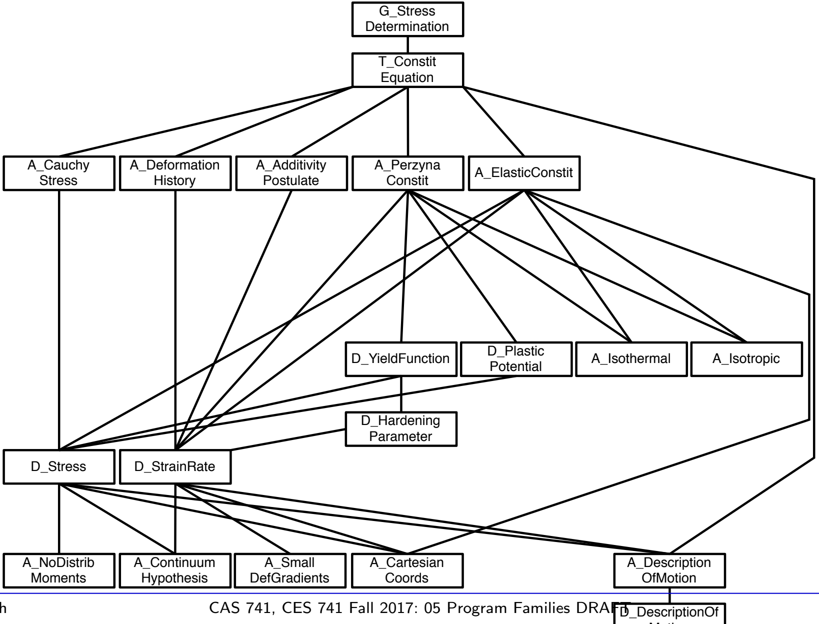
Theoretical Model Continued

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

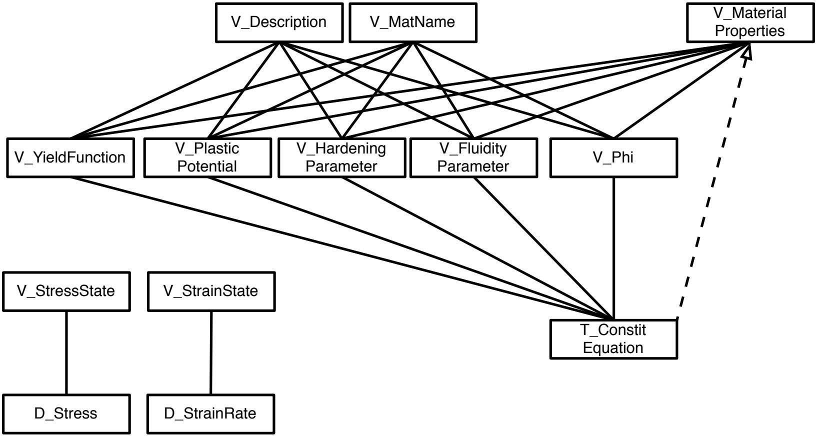
Variabilities

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

Dependency Graph



Dependency Graph Between Commonalities and Variabilities



Example

Label:	E_StrainHardening
V_MatName	$name =$ "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*$\rangle \rightarrow \langle$*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*$\rangle \rightarrow$ **Kappa**|$\langle$*simulation-variable-stress*$\rangle$|$\langle$*simulation-variable-stress-macros*$\rangle$
$\langle$*simulation-variable-stress*$\rangle \rightarrow$ **SigmaXX**|**SigmaYY**|**SigmaZZ**|**SigmaXY**|**SigmaYZ**|**SigmaXZ**
$\langle$*simulation-variable-stress-macros*$\rangle \rightarrow$ **Sxx**|**Syy**|**Szz**|**Sxy**|**Syz**|**Sxz**|**Sm**|**J2**|**J3**|**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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