Program Families in Scientific Computing

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Outline

1. Why Program Families in Scientific Computing (SC)?
2. Proposed Methodology
3. Multipurpose Tool: A Mesh Generator Generator
4. Specific Physical Model: A Family of Virtual Material Testing Laboratories

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?

- 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

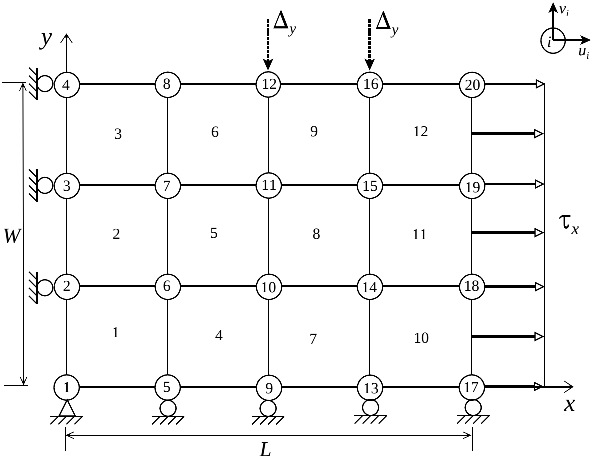
Proposed Methodology

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

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

A Mesh Generator Generator

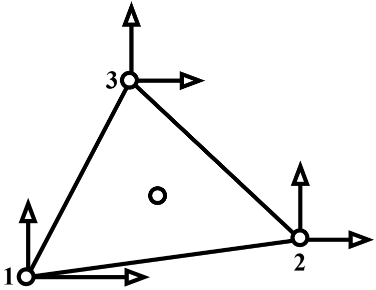


Mesh Generator (MG) Goals

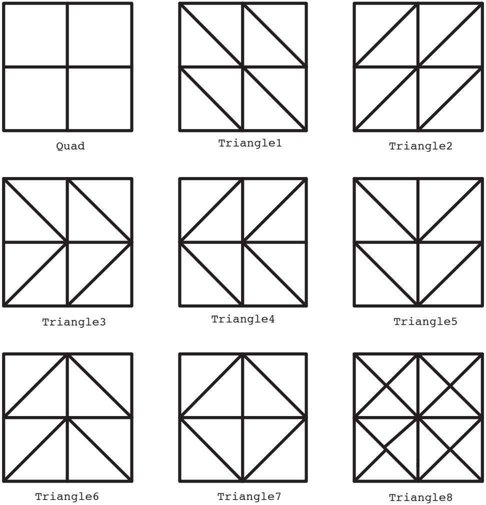
- G1 Input spatial domain Ω output a mesh M that covers this domain.
- G2 Transform information on the materials, material properties and the locations of the different materials
- G3 Transform information on the boundary condition types, values and locations
- G4 Transform system information, such as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

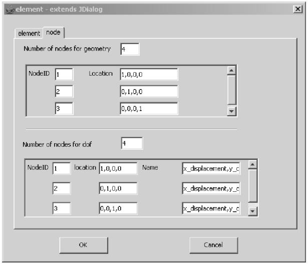


DSL Using XML

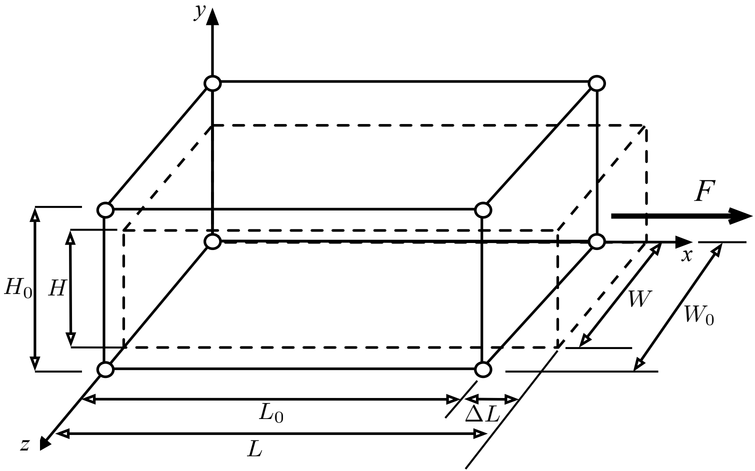
```xml
<elementSet>
    <geometrySpec>
        <shape>triangle1</shape>
        <nodeGeo count="3">
            <node id="1">
                <location>1,0,0</location>
            </node>
            <node id="2">
                <location>0,1,0</location>
            </node>
            ...
      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

Proof of Concept Implementation

- 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

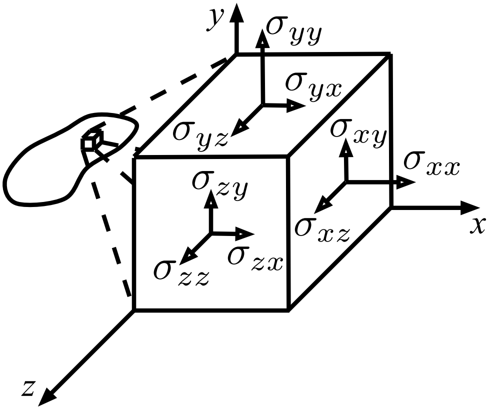


A Virtual Material Testing Laboratory



Goal

Given the deformation history of a material particle, determine the internal stress within the material particle.



Theoretical Model Input

$\sigma_0 : \mathbb{R}^6$

$t_{beg} : \mathbb{R}$

$t_{end} : \mathbb{R}$

$\dot{\epsilon}(t) : \{t : \mathbb{R} | t_{beg} \leq t \leq t_{end} : t\} \rightarrow \mathbb{R}^6$

$mat\_prop\_val : \text{string} \rightarrow \mathbb{R}$

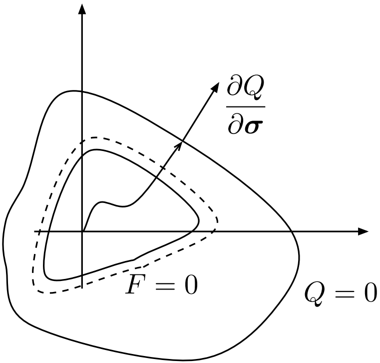
$E : \{x : \mathbb{R} | x \geq 0 : x\}$

$\nu : \{x : \mathbb{R} | 0 < x \leq 0.5 : x\}$

Theoretical Model Output

$\boldsymbol{\sigma}(t) : \{t : \mathbb{R} | t_{beg} \leq t \leq t_{end} : t\} \rightarrow \mathbb{R}^6$ such that

$\dot{\boldsymbol{\sigma}} = \mathbf{D}\left(\dot{\epsilon} - \gamma < \phi(F(\boldsymbol{\sigma}, \kappa)) > \frac{\partial Q(\boldsymbol{\sigma})}{\partial \boldsymbol{\sigma}}\right)$ and $\boldsymbol{\sigma}(t_{beg}) = \boldsymbol{\sigma}_0$



Variabilities

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

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

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

...

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

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

$\langle simulation\text{-}variable\text{-}stress \rangle \rightarrow$ **SigmaXX** | **SigmaYY** | **SigmaZZ** | **SigmaXY** | **SigmaYZ** | **SigmaXZ**

$\langle simulation\text{-}variable\text{-}stress\text{-}macros \rangle \rightarrow$ **Sxx** | **Syy** | **Szz** | **Sxy** | **Syz** | **Sxz** | **Sm** | **J2** | **J3** | **q**

$\langle user\text{-}defined\text{-}constants \rangle \rightarrow \langle string \rangle$

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