# Commonality Analysis of Families of Physical Models for use in Scientific Computing

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# Outline

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# Motivation

- Requirements documentation of physical models
  - 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

# Background

- Program family idea since the 1970s (Dijkstra, Parnas, Weiss, Pohl, ...) - variabilities are often from a finite set of simple options
- Families of algorithms and code generation in SC (Carette, ATLAS, Blitz++, ...) - not much emphasis on requirements
- Previous work on requirements for SC
  - Template for a single physical model
  - Template for a family of multi-purpose tool
- Need a requirements template for a family of physical models

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2. Introduction: a) Purpose of the Document b) Scope of the Family c) 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) Assumptions e) Theoretical Models f) Derived Quantities
5. Variabilities
6. Dependence Graphs
7. Sample Family Members
8. References

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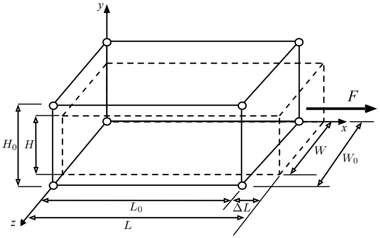
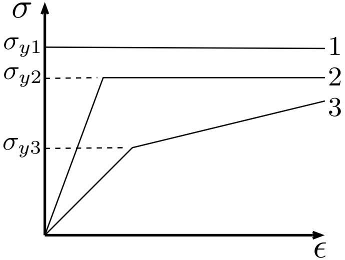
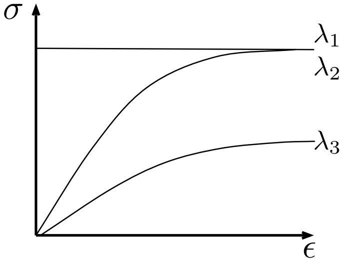
# A Family of Material Models

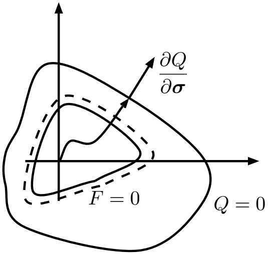


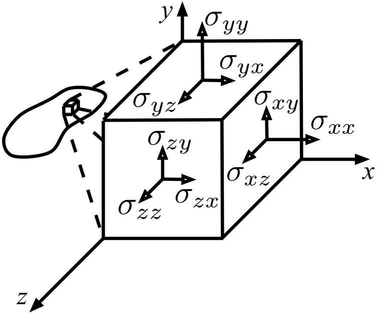
# Terminology Definitions

| 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: | $\dot{\epsilon} = \dot{\epsilon}^e + \dot{\epsilon}^{vp}$ 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: | $\boldsymbol{\sigma}_0$ : tensor2DT (StressU) (Pa)<br>$t_{begin}$ : $\mathbb{R}$ (t) (s)<br>$t_{end}$ : $\mathbb{R}$ (t) (s)<br>$\dot{\epsilon}(t)$ : $\{t : \mathbb{R} \mid t_{begin} \leq t \leq t_{end} : t\} \rightarrow$ tensor2DT (1/t) (1/s)<br>$mat\_prop\_val$ : string $\rightarrow \mathbb{R}$<br>$E$ : $\mathbb{R}^+$ (StressU) (Pa)<br>$\nu$ : poissonT (dimensionless) |

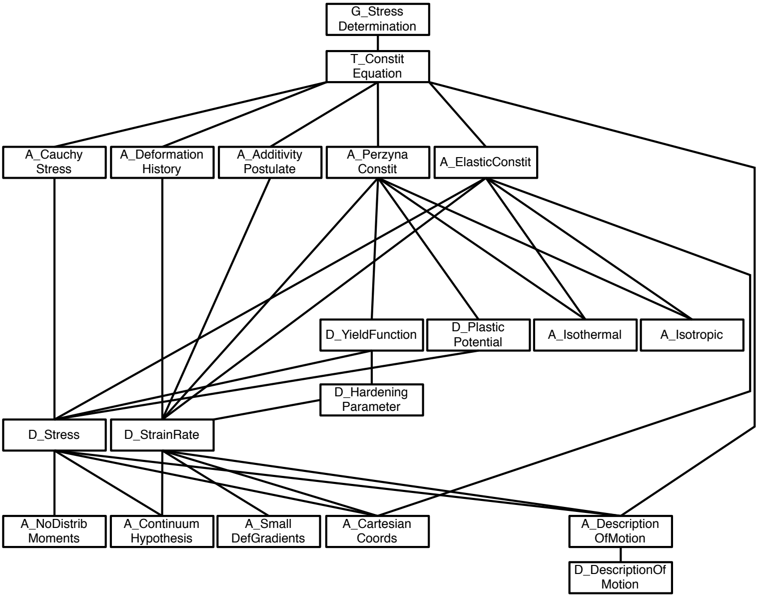
# Theoretical Model Continued

| Label: | T_ConstitEquation |
|---|---|
| Output: | $\boldsymbol{\sigma}(t) : \{t : \mathbb{R} \mid t_{begin} \leq t \leq t_{end} : t\} \rightarrow$ tensor2DT 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 $\boldsymbol{\sigma}(t_{begin}) = \boldsymbol{\sigma}_0$, the components of $\boldsymbol{\sigma}$ have the units of StressU (Pa) |
| Derive: | The governing differential equation is found by first solving for $\dot{\epsilon}^e$ 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 |

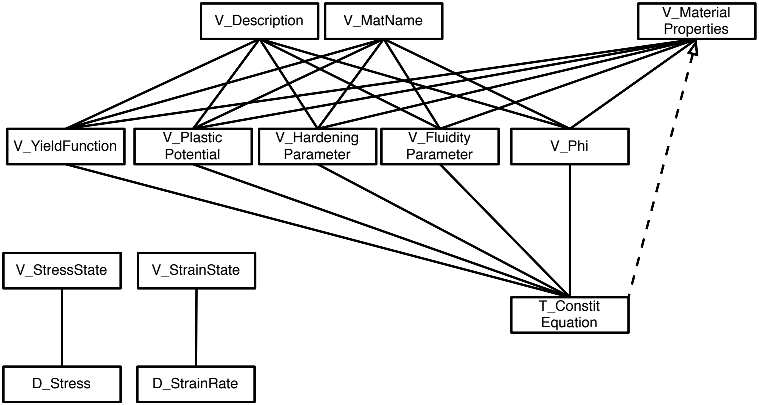
# Variabilities

- $F = F(\boldsymbol{\sigma}, \kappa) : \mathbb{R}^6 \times \mathbb{R} \rightarrow \mathbb{R}$
- $Q = Q(\boldsymbol{\sigma}) : \mathbb{R}^6 \rightarrow \mathbb{R}$
- $\kappa = \kappa(\boldsymbol{\epsilon}^{vp}) : \mathbb{R}^6 \rightarrow \mathbb{R}$
- $\phi = \phi(F) : \mathbb{R} \rightarrow \mathbb{R}$
- $\gamma : \mathbb{R}$
- *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 | $\phi = F^{\frac{m}{n}}$ (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. ...” |

# 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