Template Engine Applied to Rapid Modeling

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Outline

• Introduction
  – Current application
  – Benefits

• Template Engine Capabilities
  – Workflow-based
  – Interactive
Introduction

• Templates are applied to everything
  – Presentations, Reports, Papers, Emails, webpages, etc. all originate from **formal** templates
  – Where are you using templates?
  – How frequently do you use templates that are **informal**?
    • E.g., Copy an existing file with the structural components to update it to your new needs.

• Benefits are numerous
  – Provides consistency
    • Parts in a template don’t need to be reproduced
  – Jumpstarts work
  – Encapsulates knowledge
    • Best practices
  – Consolidates input
Prevalence In Nuclear Modeling

- Why are formal templates not more prevalent?
- Specific applications have template-like constructs
  - E.g., MCNP’s REPEATED STRUCTURE, SCALE’s ALIASES
  - Pro
    - consolidates specific application (e.g., MCNP, SCALE) input
  - Cons
    - requires user have application specific and best practice knowledge
    - requires application specific software feature development
      - May not be consistently available throughout the application

- How to increase prevalence?
  - Develop template engine
    - What capabilities are needed?
Existing Use

• SCALE 6.2
  – Input model sampling for UQ analysis
  – In-document pattern evaluation capability within the Fulcrum user interface

• Used Nuclear Fuel-Storage, Transportation & Disposal Analysis Resource and Data System (UNF-ST&DARDS)
  – Streamline analysis workflow
  – Enables data-driven application input creation
Template Engine Capabilities

• Placeholder
  – Find a named-variable and substitute its value
  – Oldest and simplest construct

• Expressions
  – Find a parameterized expression, evaluate it and substitute its value
  – More complex more powerful

• Pattern repetition
  – Repeat a parameterized section as a function of data
  – Non-obstructive loop construct for repeating patterns of input

• Data-driven
  – Allows incorporation of templates into application workflows
Primary Goals

• Provide users an interactive templating construct
  – Placeholders to keep input consistent
  – Reduce redundancy via consolidated patterns
  – Allow users to request substitution/expansion on demand
  – Facilitates user-driven template

• Provide data-driven reusable templating construct
  – Separate application input format from analysis data
  – Allow reuse of data with different application input templates
Example 1 - Placeholder

• Enhances readability and maintainability

'gbc-32 - be buc 4/50; subtask 1.a.iii.2
'.
gbc-32 - be buc 4/50; subtask 1.a.iii.2
'fuelr=<fr=0.3922>, gapr=<gr=0.4001>,
'cladr=<cr=0.4572>, axialh=<ah=20.32>
'hpitch=<hp=0.6299>
read geom
unit 1
cylinder 101 1 <fr> <ah> 0
cylinder 401 1 <gr> <ah> 0
cylinder 201 1 <cr> <ah> 0
cuboid 301 1 <hp> -<hp> <hp> -<hp> <ah> 0
unit 2
cylinder 102 1 <fr> <ah> 0
cylinder 402 1 <gr> <ah> 0
cylinder 202 1 <cr> <ah> 0
cuboid 302 1 <hp> -<hp> <hp> -<hp> <ah> 0
unit 3
cylinder 103 1 <fr> <ah> 0
cylinder 403 1 <gr> <ah> 0
cylinder 203 1 <cr> <ah> 0
cuboid 303 1 <hp> -<hp> <hp> -<hp> <ah> 0
unit 4
cylinder 104 1 <fr> <ah> 0
cylinder 404 1 <gr> <ah> 0
cylinder 204 1 <cr> <ah> 0
cuboid 304 1 <hp> -<hp> <hp> -<hp> <ah> 0
unit 5
cylinder 105 1 <fr> <ah> 0
cylinder 405 1 <gr> <ah> 0
cylinder 205 1 <cr> <ah> 0
cuboid 305 1 <hp> -<hp> <hp> -<hp> <ah> 0
Example 2 - Expressions

• Expressions can be used to determine numerical values at runtime

• Example calculates $^{234}\text{U}$, $^{236}\text{U}$, and $^{238}\text{U}$ based on formulas provided in Polaris manual

```
' enrichment=<enr=4.8>
read comp

uo2 101 0.96 293 92234 <u234=0.007731*enr^1.0837>
     92235 <enr>
     92236 <u236=0.0046*enr>
     92238 <100-u234-enr-u236> end

...
```

• Variables u234 and u236 will be available for subsequent use

• Numerical value substituted for $^{238}\text{U}$ weight percent, but not available for later use since no variable was defined
Example 3 – Pattern Repetition

- Significantly consolidate input
- Facilitates enhanced fidelity

```
gbc-32 - be buc 4/50; subtask 1.a.iii.2
' fuelr=<fr=0.3922>, gapr=<gr=0.4001>,
' cladr=<cr=0.4572>, axialh=<ah=20.32>
' hpitch=<hp=0.6299>
read geom
unit 1
cylinder 101 1 <fr> <ah> 0
cylinder 401 1 <gr> <ah> 0
cylinder 201 1 <cr> <ah> 0
cuboid 301 1 <hp> -<hp> <hp> -<hp> <ah> 0
unit 2
cylinder 102 1 <fr> <ah> 0
cylinder 402 1 <gr> <ah> 0
cylinder 202 1 <cr> <ah> 0
cuboid 302 1 <hp> -<hp> <hp> -<hp> <ah> 0
unit 3
cylinder 103 1 <fr> <ah> 0
cylinder 403 1 <gr> <ah> 0
cylinder 203 1 <cr> <ah> 0
cuboid 303 1 <hp> -<hp> <hp> -<hp> <ah> 0
unit 4
cylinder 104 1 <fr> <ah> 0
cylinder 404 1 <gr> <ah> 0
cylinder 204 1 <cr> <ah> 0
cuboid 304 1 <hp> -<hp> <hp> -<hp> <ah> 0
```
```
#for( n=1; n <= axialc; n=n+1)
unit <n>
cylinder <100+n> 1 <fr> <ah> 0
cylinder <400+n> 1 <gr> <ah> 0
cylinder <200+n> 1 <cr> <ah> 0
cuboid  <300+n> 1 <hp> -<hp> <hp> -<hp> <ah> 0
#endfor
```
Example 4 – Data-Driven Workflow

- Separate data from input template
- Facilitates UNF-ST&DARD workflow
  - Database to template parameter set to application input

<table>
<thead>
<tr>
<th>id</th>
<th>u235 wtpt</th>
<th>fuelr</th>
<th>gapr</th>
<th>cladr</th>
<th>pitch</th>
<th>height</th>
<th>npins</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3.81</td>
<td>0.48</td>
<td>0.49</td>
<td>0.56</td>
<td>1.48</td>
<td>370.10</td>
<td>14</td>
</tr>
<tr>
<td>2</td>
<td>3.49</td>
<td>0.41</td>
<td>0.42</td>
<td>0.48</td>
<td>1.26</td>
<td>350.25</td>
<td>17</td>
</tr>
<tr>
<td>3</td>
<td>4.20</td>
<td>0.41</td>
<td>0.42</td>
<td>0.48</td>
<td>1.26</td>
<td>350.25</td>
<td>17</td>
</tr>
<tr>
<td>4</td>
<td>4.20</td>
<td>0.39</td>
<td>0.41</td>
<td>0.45</td>
<td>1.26</td>
<td>364.25</td>
<td>17</td>
</tr>
</tbody>
</table>

Critical Safety

SCALE/KENO

MCNP

Thermal Hydraulics

COBRA-SFS

...
Example 5 – Data-Driven Model Perturbation

- Single fuel pin unit cell specified in KENO input
- Position of each rod is sampled uniquely using loop construct

```plaintext
#for(i=1; i<=1170; i=i+1)
  unit <10000+i>
    ' bottom end plug
    cylinder 3 1  0.5588 1.27 0 origin 0 0
    cylinder 5 1  0.6350 1.27 0 origin 0 0
    cuboid 10 1  0.842 -0.842 0.842 -0.842 1.27 0
  
  unit <20000+i>
    ' fueled section
    cylinder 1 1  0.5588 91.44 0 origin 0 0
    cylinder 6 1  0.6350 91.44 0 origin 0 0
    cuboid 9 1  0.842 -0.842 0.842 -0.842 91.44 0
  
  unit <30000+i>
    ' clad top end plug
    cylinder 2 1  0.5588 0.48 0 origin 0 0
    cylinder 4 1  0.6350 0.48 0 origin 0 0
    cuboid 10 1  0.842 -0.842 0.842 -0.842 0.48 0
  
  unit <40000+i>
    ' top end plug
    cylinder 2 1  0.6350 4.6 0 origin 0 0
    cuboid 10 1  0.842 -0.842 0.842 -0.842 4.6 0
#endfor
```

```plaintext
#for(i=1; i<=1170; i=i+1)
  ' sample displacement
  read variable[displacement_<i>_042_001]
    distribution=normal
    value = 0  stddev = 0.0054
    minimum = -0.207  maximum = 0.207
    cases = Case1 end
end variable

  read variable[theta_<i>_042_001]
    distribution=uniform
    value = 0  minimum = 0  maximum = 6.2831853
    cases = Case1 end
end variable

  ' calculate displacement in (x,y) - apply to origin
  read variable[displacement_x_<i>_042_001]
    distribution=expression
    expression = "displacement_<i>_042_001 * cos(theta_<i>_042_001)"
    cases = Case1 end
end variable

  read variable[displacement_y_<i>_042_001]
    distribution=expression
    expression = "displacement_<i>_042_001 * sin(theta_<i>_042_001)"
    cases = theta_<i>_042_001 end
end variable
#endfor
```
Example 5 – Data-Driven Model Perturbation

75 realizations, looped to make animation
Summary

• Templating is not a new concept, but has generally been implemented previously within specific codes
  – MCNP pstudy
  – SCALE PRISM

• Going forward, the TemplateEngine will provide a powerful, code-agnostic capability to process input

• Facilitates automation of model construction based on existing data
  – UNF-ST&DARDS

• Enables construction of more complicated models with looping constructs

• Combination could enable much more realistic modeling for complicated systems