Position Paper: A Knowledge-Based Approach to Scientific Software Development

Dan Szymczak, Spencer Smith and Jacques Carette

Computing and Software Department
Faculty of Engineering
McMaster University

SE4Science, May 16, 2016
Knowledge-Based Doc Driven Design (DDD)

1. Position
2. DDD Benefits
3. Challenges for DDD
4. Solution – Knowledge Based Approach (KBA)
   Addresses Challenges
   Benefits
5. Feasibility (Introducing Drasil)
6. Future Work
7. Conclusions
Knowledge-Based DDD

- DDD leads to high quality SCS
- Knowledge Based Approach
  - Facilitates DDD
  - Provides benefits
Benefits of DDD

- Improve qualities
  - Verifiability
  - Maintainability
  - Reusability
  - Reproducibility
- Better communication
- How and Why to Fake It (Parnas and Clements, 1996)
Reasons “Manual” DDD is Unpopular

- Up front requirements are challenging
- Rapid change for numerical algorithms
- Information duplication
- Synchronization headaches between artifacts
- Perceived over-emphasis on non-executable artifacts
Knowledge Based Approach

• Capture knowledge
• From one “source” recipes to generate artifacts
• Automated
• Inspired by Knuth’s Literate Programming
How Addresses Challenges

- Supports changing requirements and design
  - Generation
  - Automated traceability
- Supports duplication
  - Knowledge is entered once, generated/transferred
  - Eases maintenance
  - If incorrect, incorrect everywhere
- Non-executable artifacts are generated
## Verifiability

<table>
<thead>
<tr>
<th>Var</th>
<th>Constraints</th>
<th>Typical Value</th>
<th>Uncertainty</th>
</tr>
</thead>
<tbody>
<tr>
<td>$L$</td>
<td>$L &gt; 0$</td>
<td>1.5 m</td>
<td>10%</td>
</tr>
<tr>
<td>$D$</td>
<td>$D &gt; 0$</td>
<td>0.412 m</td>
<td>10%</td>
</tr>
<tr>
<td>$V_P$</td>
<td>$V_P &gt; 0$</td>
<td>0.05 m³</td>
<td>10%</td>
</tr>
<tr>
<td>$A_P$</td>
<td>$A_P &gt; 0$</td>
<td>1.2 m²</td>
<td>10%</td>
</tr>
<tr>
<td>$\rho_P$</td>
<td>$\rho_P &gt; 0$</td>
<td>1007 kg/m³</td>
<td>10%</td>
</tr>
</tbody>
</table>

- Sanity checks captured and reused
- Generate guards against invalid input
- Generate test cases
# Reusability

<table>
<thead>
<tr>
<th>Number</th>
<th>T1</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Label</strong></td>
<td>Conservation of energy</td>
</tr>
<tr>
<td><strong>Equation</strong></td>
<td>$-\nabla \cdot \mathbf{q} + q''' = \rho C \frac{\partial T}{\partial t}$</td>
</tr>
<tr>
<td><strong>Description</strong></td>
<td>The above equation gives the conservation of energy for time varying heat transfer in a material of specific heat capacity $C$ and density $\rho$, where $\mathbf{q}$ is the thermal flux vector, $q'''$ is the volumetric heat generation, $T$ is the temperature, $\nabla$ is the del operator and $t$ is the time.</td>
</tr>
</tbody>
</table>
Usability

- As simple as possible, but not simpler (Einstein)
- Usability challenges for general purpose SCS
  - Complex, confusing
  - Generic symbols and terminology
- Generate apps suited to specific scientific and engineering needs
- Finite element software example
Reproducibility

- Knowledge is explicitly stored for the future
- Recipes can be used to regenerate any artifacts
- Recipes include build instructions
Software Certification

- Recertification can be expensive and time consuming
- Change propagates through documentation
- Traceability and maintainability
- Recipes help with changing documentation standards
Drasil Framework Design

- **Chunk** *(name)*
- **Concept** *(description)*
- **Quantity** *(symbol)*
- **Unit** *(unit)*

**Unital**
SRS for $h_g$ and $h_c$

Spencer Smith

May 15, 2016

1 Table of Units

Throughout this document SI (Système International d’Unités) is employed as the unit system. In addition to the basic units, several derived units are employed as described below. For each unit, the symbol is given followed by a description of the unit with the SI name in parentheses.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>m</td>
<td>length (metre)</td>
<td></td>
</tr>
<tr>
<td>kg</td>
<td>mass (kilogram)</td>
<td></td>
</tr>
<tr>
<td>s</td>
<td>time (second)</td>
<td></td>
</tr>
<tr>
<td>K</td>
<td>temperature (kelvin)</td>
<td></td>
</tr>
<tr>
<td>mol</td>
<td>amount of substance (mole)</td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>electric current (ampere)</td>
<td></td>
</tr>
</tbody>
</table>
Example Recipe

```plaintext
srsBody = srs [h_g, h_c] "Spencer Smith" [s1,s2]
s1 = Section (S "Table of Units") [intro, table]
table = Table
  [S "Symbol", S "Description"] (mkTable
    [((\x -> Sy (x ^. unit)),
      (\x -> S (x ^. descr)) ] si_units)
intro = Paragraph (S "Throughout this ...")
```
Reusable Chunks

\[
\text{metre}, \text{second}, \text{kelvin} :: \text{FundUnit}
\]
\[
\text{metre} = \text{fund "Metre" "length (metre)" } \text{"m"}
\]
\[
\text{second} = \text{fund "Second" "time (second)" } \text{"s"}
\]
\[
\text{kelvin} = \text{fund "Kelvin" "temperature (kelvin)" } \text{"K"}
\]
The $h_c$ Chunk

$$h_c = \frac{2k_c h_b}{2k_c + \tau_c h_b}$$

\[
\begin{align*}
\text{h}_c\_\text{eq} &:: \text{Expr} \\
\text{h}_c\_\text{eq} &= \frac{2 \ast (\text{C k}_c) \ast (\text{C h}_b)}{(2 \ast (\text{C k}_c) + (\text{C tau}_c) \ast (\text{C h}_b))}
\end{align*}
\]

\[
\begin{align*}
\text{h}_c &:: \text{EqChunk} \\
\text{h}_c &= \text{fromEqn } "\text{h}_c" \\
&"\text{convective heat transfer coefficient between clad and coolant}\" \\
&(\text{sub h c) heat transfer h_c_eq}
\end{align*}
\]
Next Steps

- Generate more artifact types
- Generate different document views
- More types of information in chunks
- Use constraints to generate test cases
- Implement larger examples
Conclusions

- SCS has the opportunity to lead other software fields by leveraging its solid existing knowledge base
- DDD is feasible with a knowledge-based approach
- Documentation for QA and software certification does not have to be painful, expensive or time consuming
- Drasil will be developed via practical case studies