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

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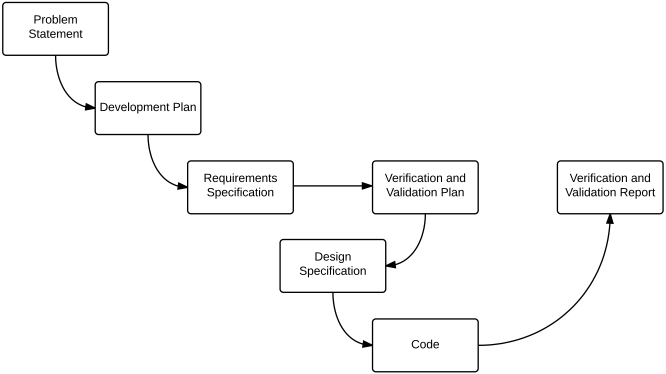
Knowledge-Based Doc Driven Design (DDD)

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/transformed
  - Eases maintenance
  - If incorrect, incorrect everywhere
- Non-executable artifacts are generated

Verifiability

Var	Constraints	Typical Value	Uncertainty
L	$L > 0$	1.5 m	10%
D	$D > 0$	0.412 m	10%
V_P	$V_P > 0$	0.05 m^3	10%
A_P	$A_P > 0$	1.2 m^2	10%
ρ_P	$\rho_P > 0$	1007 kg/m^3	10%

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

Reusability

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

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

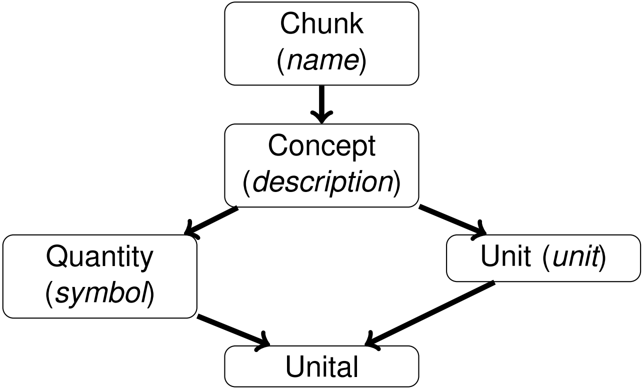
Reproducibility

- Knowledge is explicitly stored for the future
- Recipes can be use 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



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.

Symbol	Description
m	length (metre)
kg	mass (kilogram)
s	time (second)
K	temperature (kelvin)
mol	amount of substance (mole)
A	electric current (ampere)

Example Recipe

```
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

```
metre, second, kelvin :: FundUnit
metre  = fund "Metre"  "length (metre)"           "m"
second = fund "Second" "time (second)"            "s"
kelvin = fund "Kelvin" "temperature (kelvin)"     "K"
```

The h_c Chunk

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

```
h_c_eq :: Expr
h_c_eq = 2*(C k_c)*(C h_b) /
  (2*(C k_c) + (C tau_c)*(C h_b))

h_c :: EqChunk
h_c = fromEqn "h_c"
 "convective heat transfer coefficient between
    clad and coolant"
   (sub h c) heat_transfer h_c_eq
```

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