# A Literate Approach for Improving the Verifiability, Reusability and Reproducibility of Scientific Computing Software

**Spencer Smith**, Jacques Carette, Dan Szymczak, Steven Palmer

Computing and Software Department
Faculty of Engineering
McMaster University

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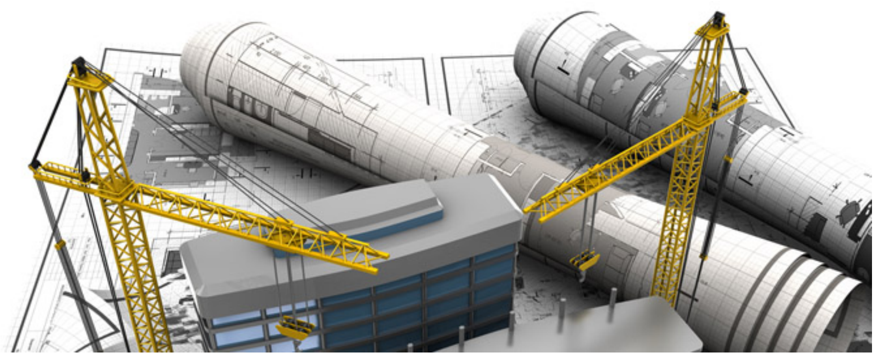
# Abstract

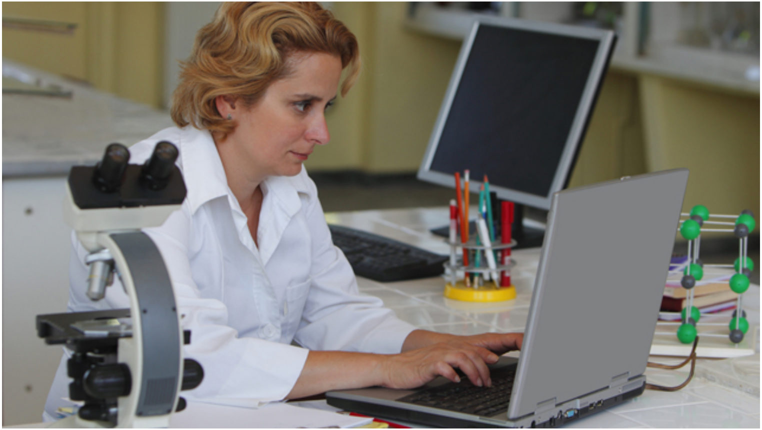
- **Goal** – Improve quality of $\{$SCS$\}$
- **Idea** – Adapt ideas from SE
- **Document Driven Design**
  - Good – improves quality
  - Bad – “manual” approach is too much work
- **Solution**
  - Capture knowledge
  - Generate all things
  - Avoid duplication
  - Traceability
- **Showing great promise**
  - Significant work yet to do
  - Looking for examples/partners

# Scope: Large/Multiyear

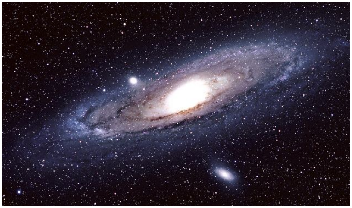


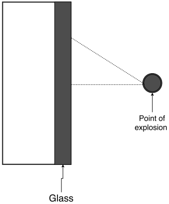
# Scope: Program Families

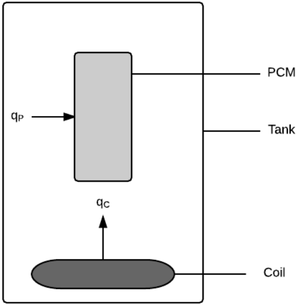
# Scope: End User Developers

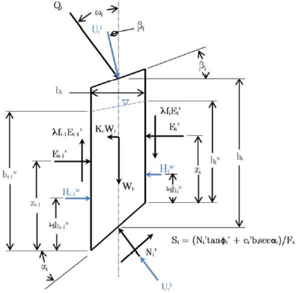


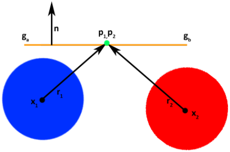
# Scope: Physical Science

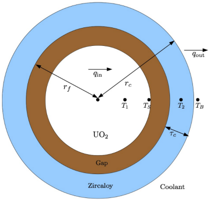




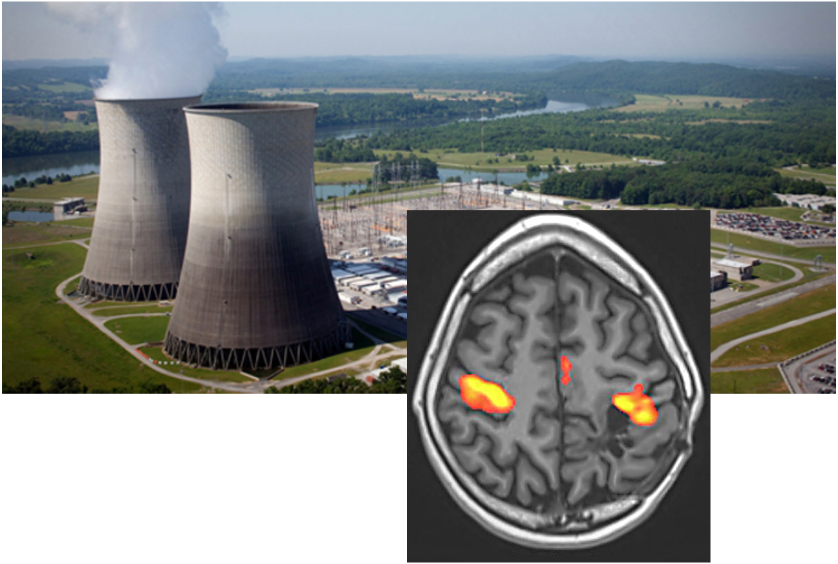



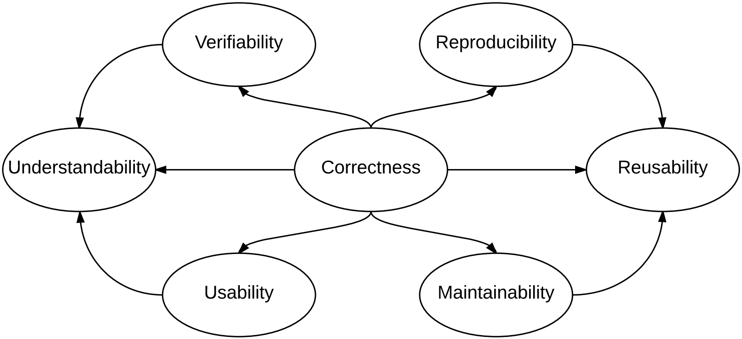



# Motivation: Safety

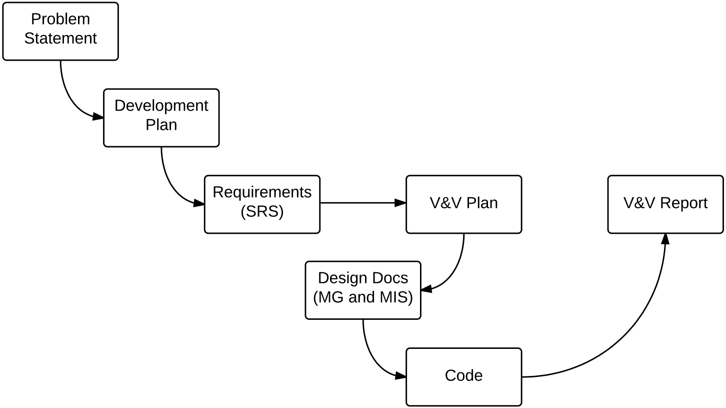


# Motivation: (Re)certification

# Motivation: Improve Quality



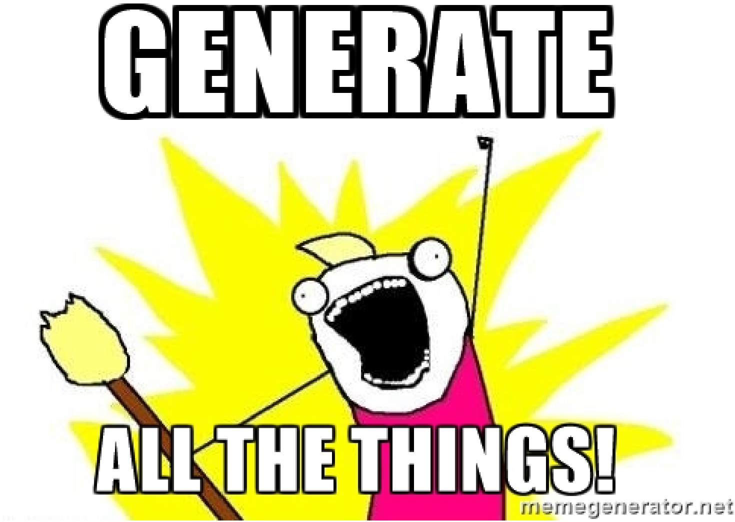
# “Faked” Rational Design Process




SWHS example at https://github.com/smiths/swhs

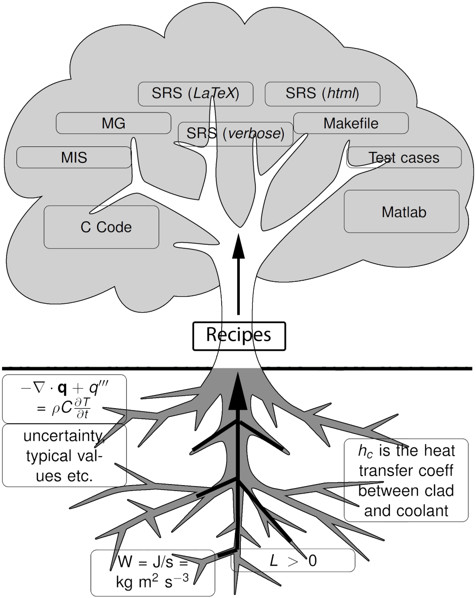
# The Challenge

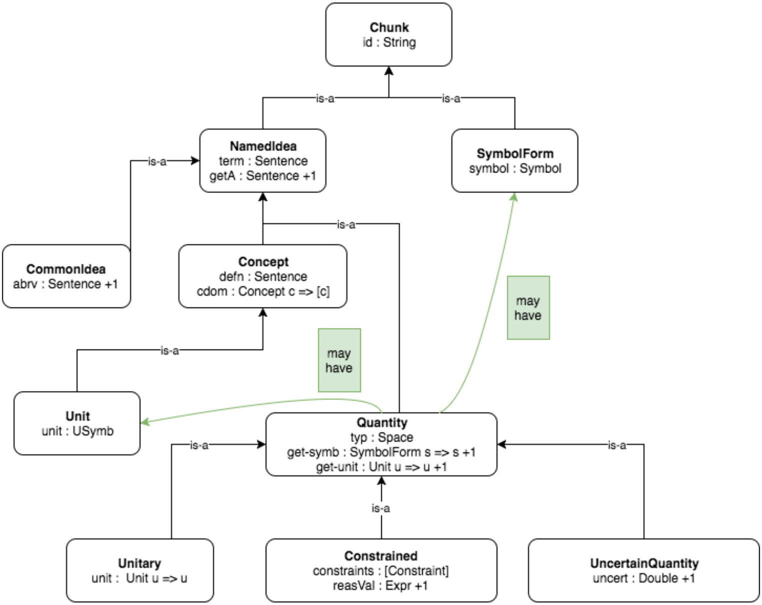
- Documentation provides advantages
  - Improves verifiability, reusability, reproducibility, etc.
  - From Parnas (2010)
    - easier reuse of old designs
    - better communication about requirements
    - more useful design reviews
    - etc.
  - New doc found 27 errors (Smith and Koothoor, 2016)
  - Developers see advantage (Smith et al., 2016)
- But documentation is felt to be ...
  - Too long
  - Too difficult to maintain
  - Not amenable to change
  - Too tied to waterfall process
  - Reports counterproductive (Roache, 1998)
- **The Solution?**


GENERATE
ALL THE THINGS!
memegenerator.net

# Knowledge Capture

# Drasil


SRS (*LaTeX*)
SRS (*html*)
MG
SRS (*verbose*)
Makefile
MIS
Test cases
C Code
Matlab
Recipes
$-\nabla \cdot \mathbf{q} + q''' = \rho C \frac{\partial T}{\partial t}$
uncertainty, typical values etc.
$h_c$ is the heat transfer coeff between clad and coolant
W = J/s = kg m$^2$ s$^{-3}$
$L > 0$


Chunk
id : String
is-a
is-a
NamedIdea
term : Sentence
getA : Sentence +1
SymbolForm
symbol : Symbol
is-a
is-a
CommonIdea
abrv : Sentence +1
Concept
defn : Sentence
cdom : Concept c => [c]
may have
may have
is-a
Unit
unit : USymb
Quantity
typ : Space
get-symb : SymbolForm s => s +1
get-unit : Unit u => u +1
is-a
is-a
is-a
Unitary
unit : Unit u => u
Constrained
constraints : [Constraint]
reasVal : Expr +1
UncertainQuantity
uncert : Double +1

# $J_{tol}$ in SRS.pdf

| **Refname** | **DD:sdf.tol** |
|---|---|
| Label | $J_{tol}$ |
| Units | |
| Equation | $J_{tol} = \log\left(\log\left(\frac{1}{1-P_{btol}}\right)\frac{\left(\frac{a}{1000}\frac{b}{1000}\right)^{m-1}}{k\left((E*1000)\left(\frac{h}{1000}\right)^2\right)^m * LDF}\right)$ |
| Description | $J_{tol}$ is the stress distribution factor (Function) based on Pbtol<br>$P_{btol}$ is the tolerable probability of breakage<br>$a$ is the plate length (long dimension)<br>$b$ is the plate width (short dimension)<br>$m$ is the surface flaw parameter<br>$k$ is the surface flaw parameter<br>$E$ is the modulus of elasticity of glass<br>$h$ is the actual thickness<br>$LDF$ is the load duration factor |

# $J_{tol}$ in SRS.tex

```
\noindent \begin{minipage}{\textwidth}
\begin{tabular}{p{0.2\textwidth} p{0.73\textwidth}}
\toprule \textbf{Refname} & \textbf{DD:sdf.tol}
\phantomsection
\label{DD:sdf.tol}
\\ \midrule \\
Label & $J_{tol}$
\\ \midrule \\
Units &
\\ \midrule \\
Equation & $J_{tol}$ = $\log\left(\log\left(\frac{1}{1-P_
    {btol}}\right)\frac{\left(\frac{a}{1000}\frac{b
    }{1000}\right)^{m-1}}{k\left(\left(E*1000\right)\left
    (\frac{h}{1000}\right)^{2}\right)^{m}*LDF}\right)$
\\ \midrule \\
Description & $J_{tol}$ is the stress distribution factor
     (Function) based on
              Pbtol\newline$P_{btol}$ is the tolerable
                 probability of breakage ...
\end{minipage}\\
```

## $J_{tol}$ in SRS.html

```
<a id="">
<div class="equation">
<em>J<sub>tol</sub></em> = log(log(<div class="fraction">
<span class="fup">
1
</span>
<span class="fdn">
1 &minus; <em>P<sub>btol</sub></em>
</span>
</div>)<div class="fraction">
<span class="fup">
(<div class="fraction">
<span class="fup">
<em>a</em>
</span>
<span class="fdn">
1000
</span>
</div><div class="fraction">
...
```

# $J_{tol}$ in Python

```
def calc_j_tol(inparams):
    j_tol = math.log((math.log(1.0 / (1.0 - inparams.
        pbtol))) * ((((inparams.a / 1000.0) * (inparams.b
         / 1000.0)) ** (inparams.m - 1.0)) / ((inparams.k
         * (((inparams.E * 1000.0) * ((inparams.h /
        1000.0) ** 2.0)) ** inparams.m)) * inparams.ldf))
        )
    return j_tol
```

# $J_{tol}$ in Java

```
public static double calc_j_tol(InputParameters inparams)
    {
        double j_tol = Math.log((Math.log(1.0 / (1.0 -
            inparams.pbtol))) * ((Math.pow((inparams.a /
            1000.0) * (inparams.b / 1000.0), inparams.m -
             1.0)) / ((inparams.k * (Math.pow((inparams.E
             * 1000.0) * (Math.pow(inparams.h / 1000.0,
            2.0)), inparams.m))) * inparams.ldf)));
        return j_tol;
    }
```

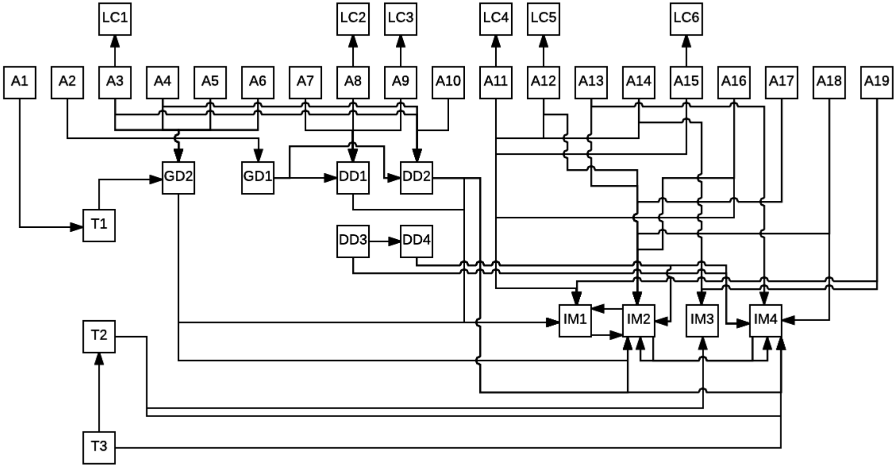
## $J_{tol}$ in Drasil (Haskell)

```
stressDistFac = makeVC "stressDistFac" (nounPhraseSP
  $ "stress distribution" ++ " factor (Function)") cJ

sdf_tol = makeVC "sdf_tol" (nounPhraseSP $
  "stress distribution" ++
  " factor (Function) based on Pbtol")
  (sub (stressDistFac ^. symbol) (Atomic "tol"))

tolStrDisFac_eq :: Expr
tolStrDisFac_eq = log (log ((1) / ((1) - (C pb_tol)))
  * ((Grouping (((C plate_len) / (1000)) * ((C
     plate_width) / (1000)))) :^
  ((C sflawParamM) - (1)) / ((C sflawParamK) *
  (Grouping (Grouping ((C mod_elas) * (1000)) *
  (square (Grouping ((C act_thick) / (1000)))))
  )) :^ (C sflawParamM) * (C loadDF))))

tolStrDisFac :: QDefinition
tolStrDisFac = mkDataDef sdf_tol tolStrDisFac_eq
```

# $J_{tol}$ without Unit Conversion

```
tolStrDisFac_eq :: Expr
tolStrDisFac_eq = log (log ((1) / ((1) - (C pb_tol)))
  * ((Grouping ((C plate_len) * (C plate_width))) :^
  ((C sflawParamM) - (1)) / ((C sflawParamK) *
  (Grouping ((C mod_elas) * (square (C act_thick)))) :^ (
      C sflawParamM) * (C loadDF))))
```

# Traceability Graph



# Verifiability

| Var | Constraints | Typical Value | Uncertainty |
|---|---|---|---|
| $L$ | $L > 0$ | 1.5 m | 10% |
| $\rho_P$ | $\rho_P > 0$ | 1007 kg/m$^3$ | 10% |

$$E_W = \int_0^t h_C A_C (T_C - T_W(t))dt - \int_0^t h_P A_P (T_W(t) - T_P(t))dt$$

- If wrong, wrong everywhere
- Sanity checks captured and reused
- Generate guards against invalid input
- Generate test cases
- Generate view suitable for inspection
- Traceability for verification of change

# Reusability

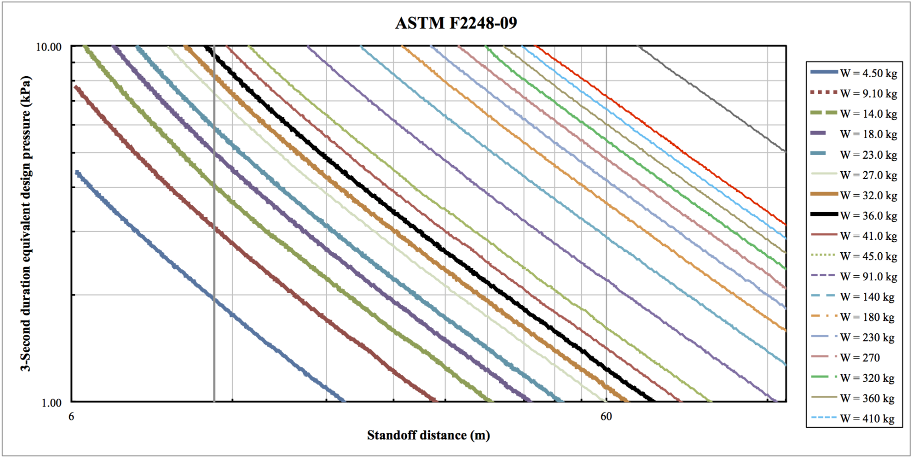
- De-embed knowledge
- Reuse throughout document
  - Units
  - Symbols
  - Descriptions
  - Traceability information
- Reuse between documents
  - SRS
  - MIS
  - Code
  - Test cases
- Reuse between projects
  - Knowledge reuse
  - A family of related models, or reuse of pieces
  - Conservation of thermal energy
  - Interpolation
  - Etc.

# Reproducibility

- Usual emphasis is on reproducing code execution
- However, Ionescu and Jansson (2012) show reproducibility challenges due to undocumented:
    - Assumptions
    - Modifications
    - Hacks
- Shouldn't it be easier to independently replicate the work of others?
- Require theory, assumptions, equations, etc.
- Drasil can potentially check for completeness and consistency

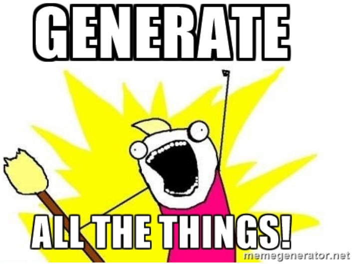

NO
SILVER

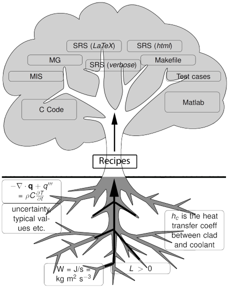
# Future Work


ASTM F2248-09
10.00
1.00
6
60
3-Second duration equivalent design pressure (kPa)
Standoff distance (m)
W = 4.50 kg
W = 9.10 kg
W = 14.0 kg
W = 18.0 kg
W = 23.0 kg
W = 27.0 kg
W = 32.0 kg
W = 36.0 kg
W = 41.0 kg
W = 45.0 kg
W = 91.0 kg
W = 140 kg
W = 180 kg
W = 230 kg
W = 270
W = 320 kg
W = 360 kg
W = 410 kg

# Drasil Framework for LSS

- SCS has the opportunity to lead other software fields
- Document driven design is feasible
- Requires an investment of time
- Documentation does not have to be painful
- Develop/refactor via practical case studies
- Ontology may naturally emerge



# References I

Cezar Ionescu and Patrik Jansson. Dependently-Typed Programming in Scientific Computing — Examples from Economic Modelling. In *Revised Selected Papers of the 24th International Symposium on Implementation and Application of Functional Languages*, volume 8241 of *Lecture Notes in Computer Science*, pages 140–156. Springer International Publishing, 2012. doi: 10.1007/978-3-642-41582-1_9.

David Lorge Parnas. Precise documentation: The key to better software. In *The Future of Software Engineering*, pages 125–148, 2010. doi: 10.1007/978-3-642-15187-3_8. URL `http://dx.doi.org/10.1007/978-3-642-15187-3_8`.

# References II

Patrick J. Roache. *Verification and Validation in Computational Science and Engineering*. Hermosa Publishers, Albuquerque, New Mexico, 1998.

W. Spencer Smith and Nirmitha Koothoor. A document-driven method for certifying scientific computing software for use in nuclear safety analysis. *Nuclear Engineering and Technology*, 48(2):404–418, April 2016. ISSN 1738-5733. doi: http://dx.doi.org/10.1016/j.net.2015.11.008. URL `http://www.sciencedirect.com/science/article/pii/S1738573315002582`.

# References III

W. Spencer Smith, Thulasi Jegatheesan, and Diane F. Kelly. Advantages, disadvantages and misunderstandings about document driven design for scientific software. In *Proceedings of the Fourth International Workshop on Software Engineering for High Performance Computing in Computational Science and Engineering (SE-HPCCE)*, November 2016. 8 pp.