

CAS 741, CES 741 (Development of Scientific Computing Software)

Fall 2020

Artifact Generation

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November 23, 2020



Artifact Generation

- Start recording
- Administrative details
- Artifact generation (Drasil)

Administrative Details

- Upcoming classes
 - ▶ L20 - Artifact Generation (Today)
 - ▶ L21 - Drasil Demos
 - ▶ L22 – L24 - Implementation and testing presentations

Administrative Details

- For final documentation, make sure you have **addressed and closed** all open issues
- MIS marking scheme on Avenue
- Course evaluation
 - ▶ Wed, Nov 25, 10:00 am to Wed, Dec 9, 11:59 pm
 - ▶ <https://evals.mcmaster.ca>
- MG/MIS Reviews
 - ▶ Assign issues to your domain expert and secondary reviewer
 - ▶ Due two days after assignment (but we can be flexible on this)
- Further Deliverable Reviews
 - ▶ Not part of marking scheme for course
 - ▶ Encouraged to do anyway, maybe as a quid pro quo?

Administrative Details: Report Deadlines

MG + MIS (Traditional) Nov 23

Drasil Code and Report (Drasil) Nov 23

Final Documentation Dec 9

- The written deliverables will be graded based on the repo contents as of 11:59 pm of the due date
- If you need an extension for a written deliverable, please ask
- You should inform your primary and secondary reviewers of the extension
- Two days after each major deliverable, your GitHub issues will be due

Admin Details: Presentation Schedule

- Drasil Project Present (20 min each)
 - ▶ Thurs, Nov 26: Andrea, Naveen, Ting-Yu
- Test or Impl. Present (15 min each)
 - ▶ Mon, Nov 30: John, Salah, Liz, Xingzhi, Leila
 - ▶ Thurs, Dec 3: Shayan, Naveen, Sid, Gaby, Seyed
 - ▶ Mon, Dec 7: Ting-Yu, Xuanming, Mohamed, Andrea, Tiago
- 4 presentations each
- If you will miss a presentation, please trade with someone else

Implementation and Testing Presentations

You can present anything related to implementation or testing

- Show off your code, or as much of it as you have completed
- Unit VnV Plan
- Test case report
- Verification/validation activities
- Demonstrate technology
 - ▶ Continuous integration
 - ▶ Valgrind
 - ▶ Doxygen for API documentation
 - ▶ Etc.
- Drasil presentations - emphasize testing
- Fine to show work in progress
- Good to ask the audience for advice, feedback
- Other ideas are likely fine

Questions?

- Questions on administrative details?
- Questions about Module Guide?
- Questions about upcoming presentation?
- Questions about MIS?
- Other questions?

Implementing Your MIS

- The mapping between the MIS and the code is generally not “term” by “term”
- You do not need to use the mathematical type listed in the spec
- Consider A2 (Allocation to Engineering Programs) for set types
 - ▶ Problem Description
 - ▶ Source Code

Abstract for Artifact Generation Talk

- **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

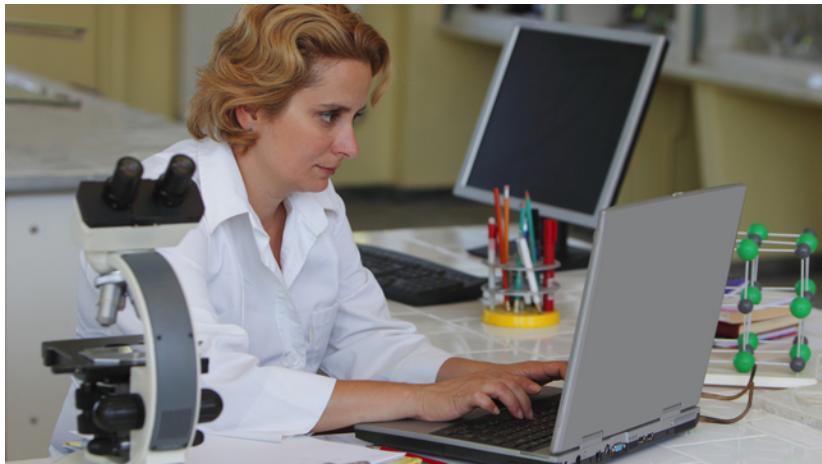
Scope: Large/Multiyear



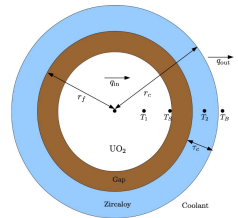
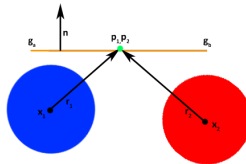
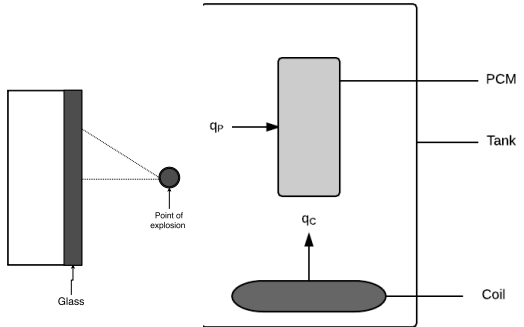
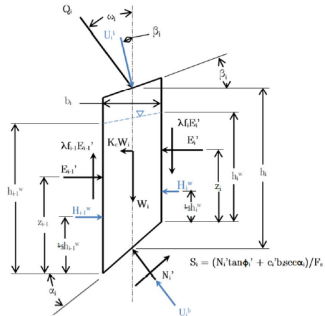
Scope: Program Families



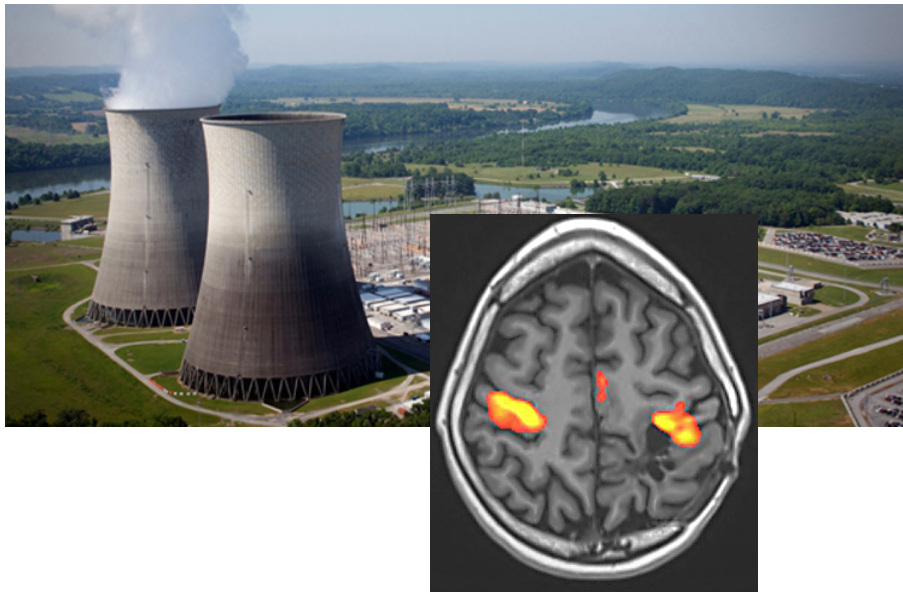
Scope: End User Developers



Scope: Physical Science



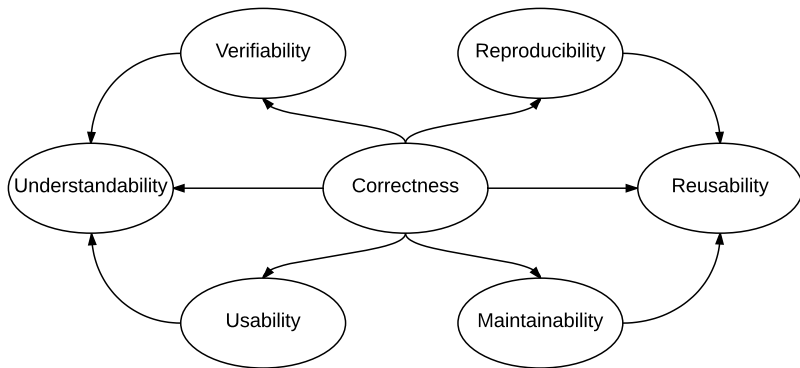
Motivation: Safety



Motivation: (Re)certification



Motivation: Improve Quality



Current Approach

- Agile like [1]
- Amethododical [3]
- Knowledge acquisition driven [4]
- Each stage reports counterproductive [10]
- Limited tool use [13]
- Limited testing of code [5]
- Lack of understanding of testing [7]
- Missed opportunities for reuse [8]
- Emphasis on:
 1. Science [6]
 2. Code

Documentation Advantages

- Improves verifiability, reusability, reproducibility, etc.
- From [9]
 - ▶ easier reuse of old designs
 - ▶ better communication about requirements
 - ▶ more useful design reviews
 - ▶ easier integration of separately written modules
 - ▶ more effective code inspection
 - ▶ more effective testing
 - ▶ more efficient corrections and improvements
- New doc found 27 errors [12]
- Developers see advantage [11]

Study Of Documentation in SC [11]

1. Select 5 small to medium size SCS
2. Interview code owners
3. Redevelop using Document Driven Design (DDD)
4. Interview code owners
5. Analyze responses

Summary of Case Studies

| | LOC | Lng | ND | Ag | SE | Prg | Tst | VC | Bug |
|---------------|------|-----|----|-----|----|-----|-----|----|-----|
| SWHS | 1000 | F77 | 1 | 5 | ✗ | ✓ | ✗ | ✗ | ✗ |
| Astro | 5000 | C | 2 | 10 | ✗ | ✓ | ✗ | ✗ | ✗ |
| Glass | 1300 | F90 | 1 | <1 | ✗ | ✓ | ✗ | ✗ | ✗ |
| Soil | 800 | M | 1 | 5 | ✓ | ✓ | ✓ | ✓ | ✗ |
| Neuro | 1000 | M | 1 | 5 | ✓ | ✓ | ✗ | ✓ | ✗ |
| Acoust | 200 | M | 4 | 2.5 | ✗ | ✓ | ✗ | ✗ | ✗ |

Perceived Advantages from Participants

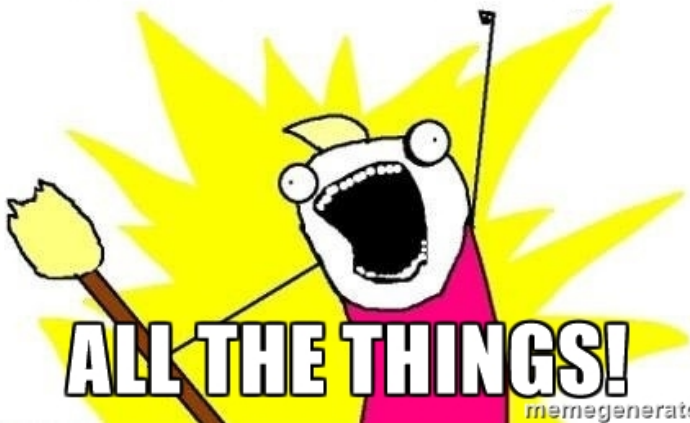
- Documentation of assumptions
- All variables have explicit units
- SRS helpful with new graduate students
- Modules result in more user friendly code
- Traceability between modules and requirements useful
- Better organized code
- Information sharing on design choices
- Detailed record of knowledge capital
- Code is produced to make testing easier

Disadvantages (Perceived and Real)

- SRS is too long
- SRS is not necessary
- DDD will not work in reality, since needs upfront requirements
- Too much SE jargon
- Difficult without a team of people
- Too difficult to maintain
- Not amenable to change
- Too tied to waterfall process
- Reports counterproductive [[10](#)]

The Solution?

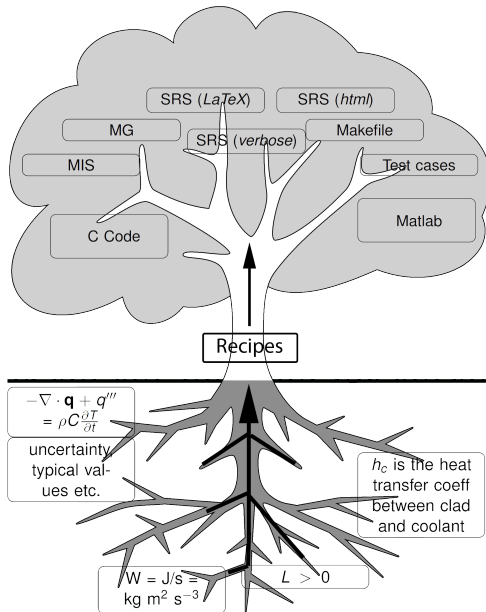
GENERATE

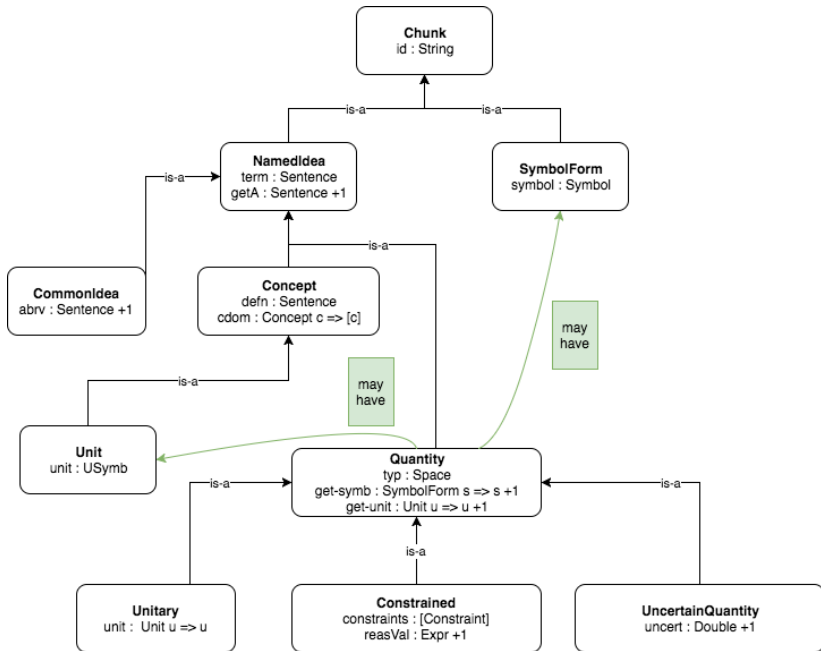


memegenerator.net

Knowledge Capture







J_{tol} in SRS.pdf

| | |
|-------------|--|
| Refname | DD:sdf.tol |
| Label | Stress Distribution Factor (Function) Based on Pbtol |
| Units | Unitless |
| Equation | $J_{tol} = \log \left(\log \left(\frac{1}{1-P_{btol}} \right) \frac{\left(\frac{a}{1000} \frac{b}{1000} \right)^{m-1}}{k \left(\left(E \cdot 1000 \left(\frac{h}{1000} \right)^2 \right) \right)^m \cdot LDF} \right)$ |
| Description | <p>J_{tol} is the stress distribution factor (Function) based on Pbtol</p> <p>P_{btol} is the tolerable probability of breakage</p> <p>a is the plate length (long dimension) (m)</p> <p>b is the plate width (short dimension) (m)</p> <p>m is the surface flaw parameter ($\frac{m^{12}}{N^7}$)</p> <p>k is the surface flaw parameter ($\frac{m^{12}}{N^7}$)</p> <p>E is the modulus of elasticity of glass (Pa)</p> <p>h is the actual thickness (m)</p> <p>LDF is the load duration factor</p> |

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 &  $J_{tol} =$ 

$$\log\left(\log\left(\frac{1}{1-P_{btol}}\right)\frac{\left(\frac{a}{1000}\right)\frac{b}{1000}}{\left(\frac{E*1000}{1000}\right)\left(\frac{h}{1000}\right)^2}\right)^{m*LDF}$$

\\ \midrule \\
Description &  $J_{tol}$  is the stress distribution
factor (Function) based on
```

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>
```

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)

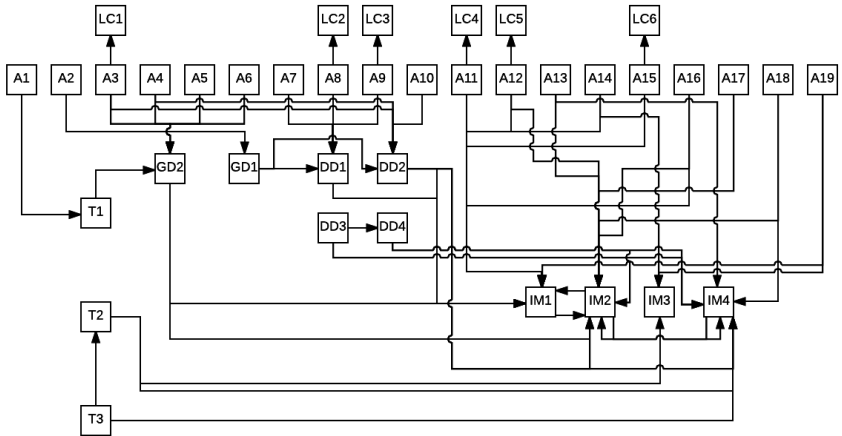
```
stressDistFac = makeVC "stressDistFac" (nounPhraseSP
  $ "stress distribution" ++ " factor (Function)"
  cJ
sdf_tol = makeVC "sdf_tol" (nounPhraseSP $
  "stress distribution" ++
  " factor (Function) based on Pbtol")
  (sub (eqSymb stressDistFac) (Atomic "tol"))

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 lDurFac)))))
tolStrDisFac :: QDefinition
tolStrDisFac = mkDataDef' sdf_tol tolStrDisFac_eq
  (aGrtrThanB ++ hRef ++ ldfRef ++ pbTolUstr)
```

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 (Grouping ((C mod_elas * 1000) *
    (square (Grouping (C act_thick))))) :^
    (C sflawParamM) * (C lDurFac)))))
```

Traceability Graph



Maintainability

- A1: The only form of energy that is relevant for this problem is thermal energy. All other forms of energy, such as mechanical energy, are assumed to be negligible [T1].
- A2: All heat transfer coefficients are constant over time [GD1].
- A3: The water in the tank is fully mixed, so the temperature is the same throughout the entire tank [GD2, DD2].
- A4: The PCM has the same temperature throughout [GD2, DD2, LC1].
- A5: etc.

Verifiability

| Var | Constraints | Typical Value | Uncertainty |
|----------|--------------|------------------------|-------------|
| L | $L > 0$ | 1.5 m | 10% |
| ρ_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

| | |
|-------------|-----------|
| Num. | T1 |
|-------------|-----------|

| | |
|--------------|-------------------------------|
| Label | Conservation of energy |
|--------------|-------------------------------|

| | |
|-----------|--|
| Eq | $-\nabla \cdot \mathbf{q} + q''' = \rho C \frac{\partial T}{\partial t}$ |
|-----------|--|

| | |
|----------------|--|
| Descrip | 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. |
|----------------|--|

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, [2] 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

Smith and Koothoor (2016) [12]

$$R_1^{\text{code}} = \frac{f}{8\pi k_{\text{AV}}} + \frac{1}{2\pi r_f h_g} \quad (1)$$

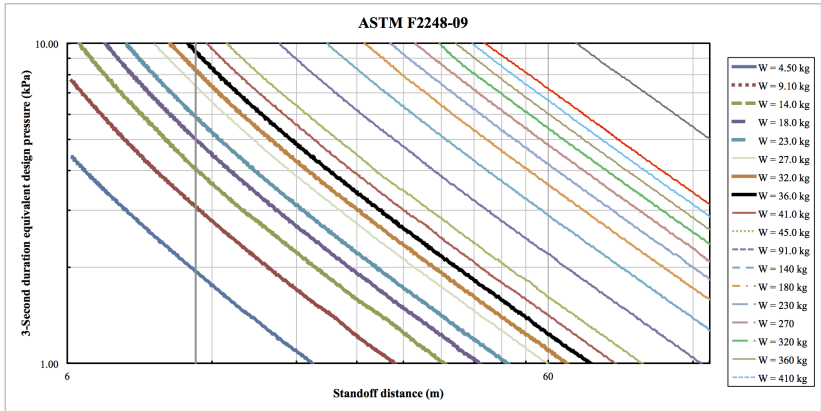
$$R_1^{\text{manual}} = \frac{f}{8\pi k_{\text{AV}}} + \frac{1}{2\pi r_f h_g} + \frac{\tau_c}{4\pi r_f k_c} \quad (2)$$

- Uncovered 27 issues with the previous documentation
 - ▶ Incompleteness (R_{gap})
 - ▶ Inconsistency(r, r_0, h_g)
 - ▶ Verifiability problems (R_1)
 - ▶ Lack of traceability (circuit analogy)
- Advantages of proposed approach
 - ▶ Abstract to concrete
 - ▶ Separation of concerns
 - ▶ Every equation, assumption, definition, model, derivation, source and traceability between them

NO

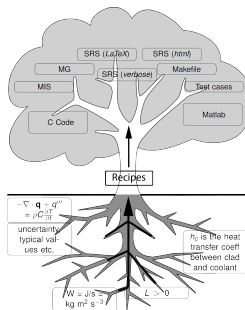
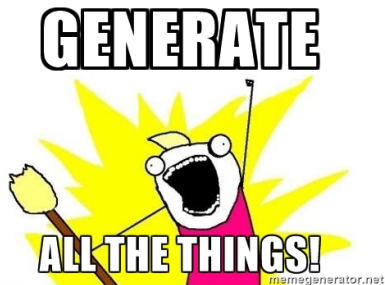


Future Work



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
- Open source Drasil [here](#)



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