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

Fall 2020

Artifact Generation

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November 27, 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?

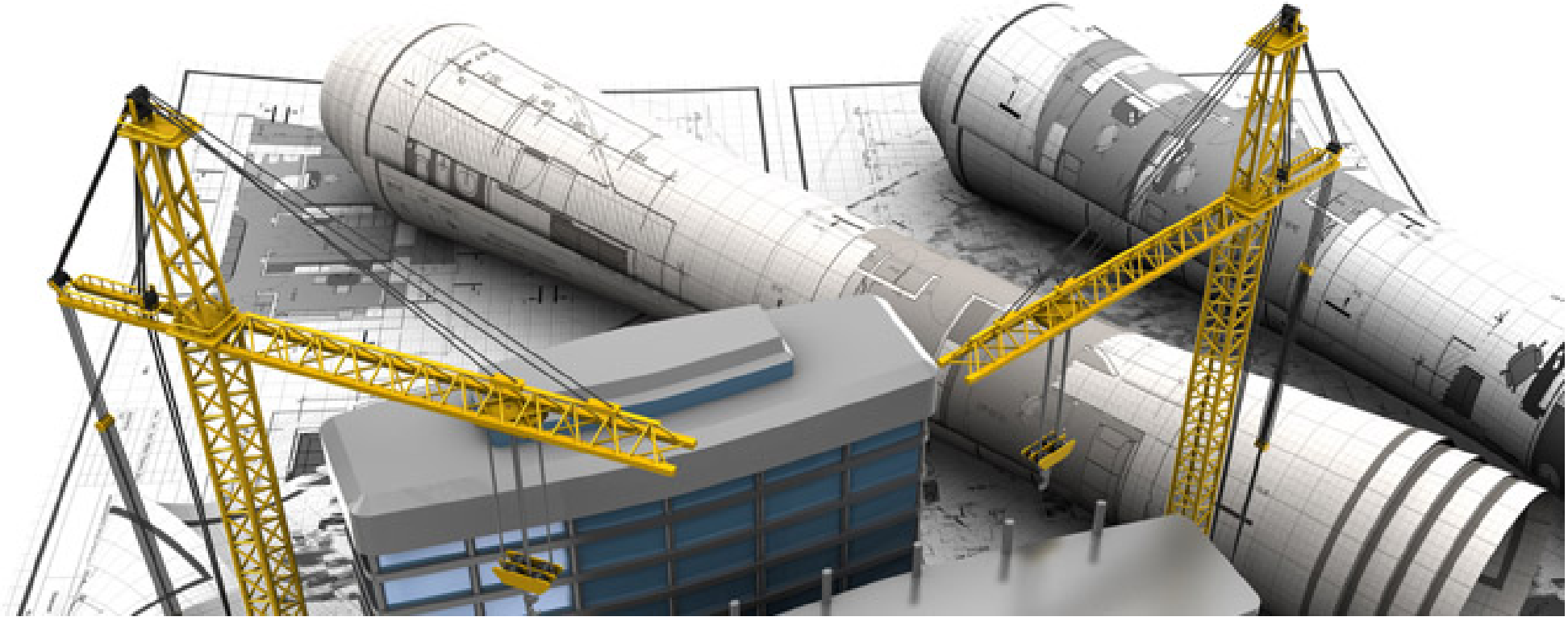
Implementing Your MIS

- 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

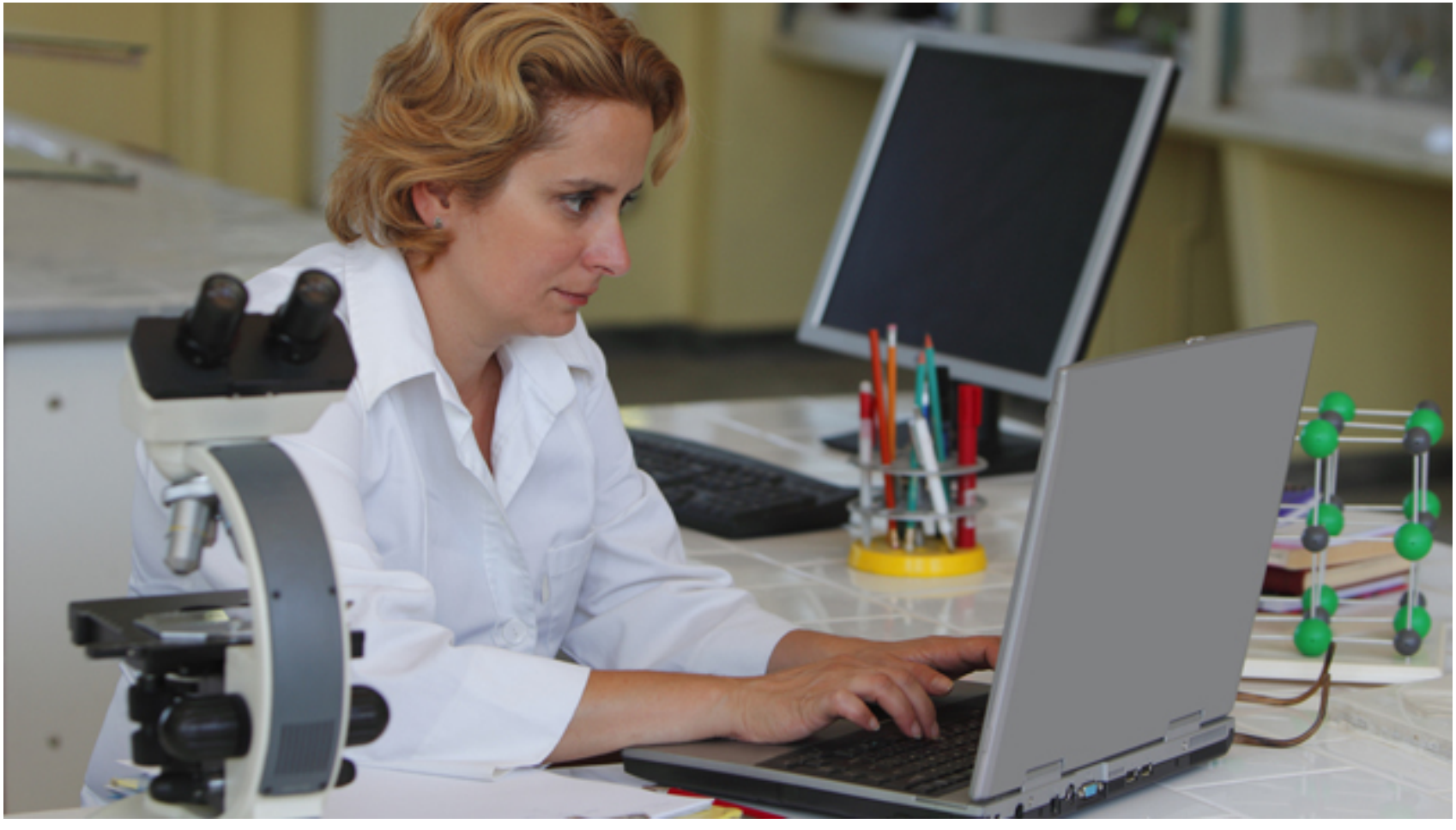
- **Goal** – Improve quality of SCS
- **Idea** – Adapt ideas from SE
- **Document Driven Design**
  - Good – improves quality
  - Bad – "manual" approach is too much work
- **Solution**
  - Capture knowledge
  - Generate all things
  - Avoid duplication
  - Traceability
- **Showing great promise**
 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

Scope: Large/Multiyear

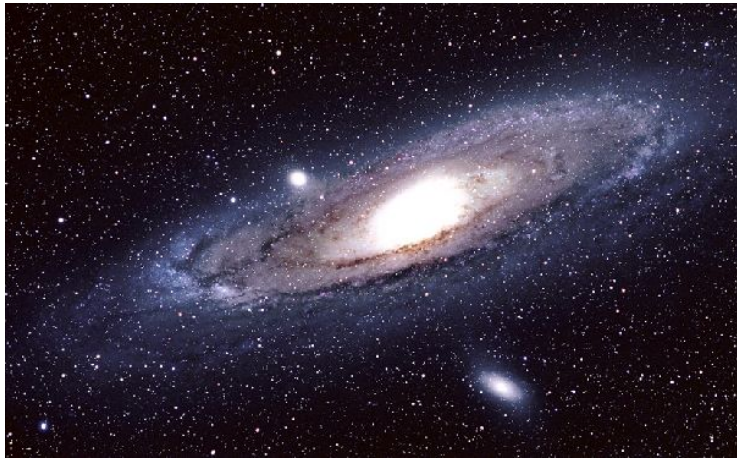


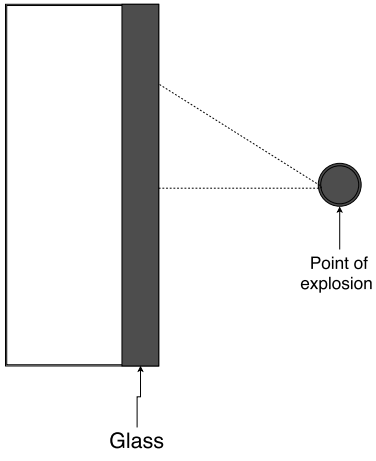
Scope: Program Families

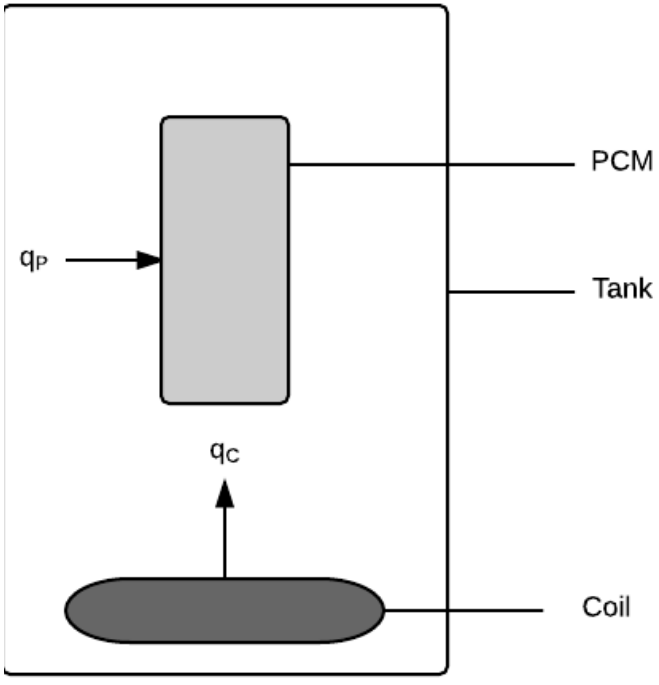
Scope: End User Developers

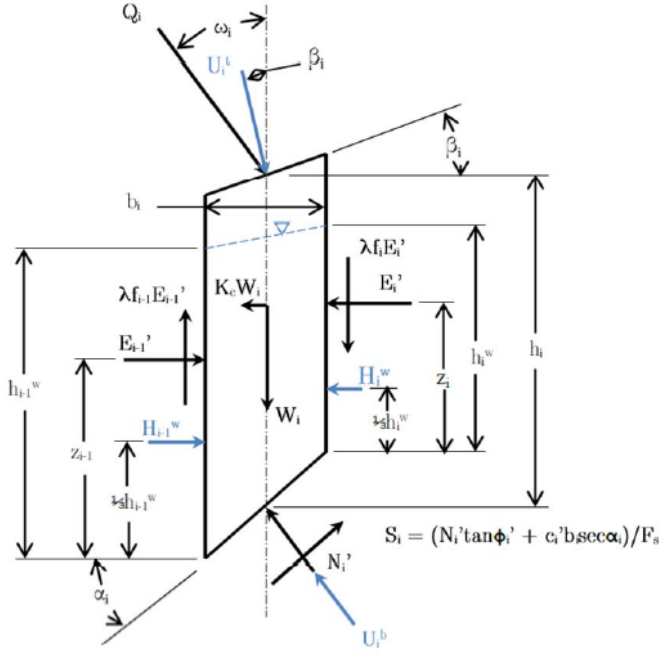


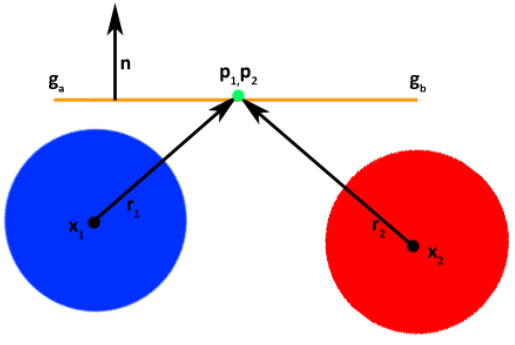
Scope: Physical Science

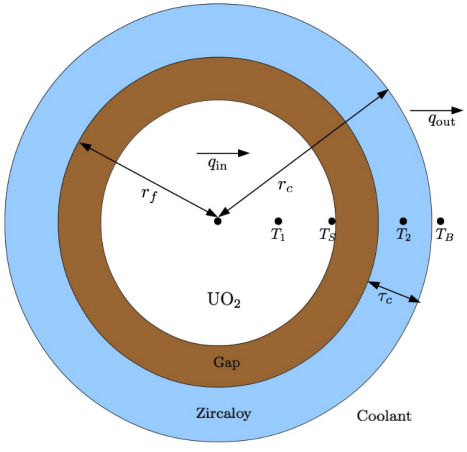




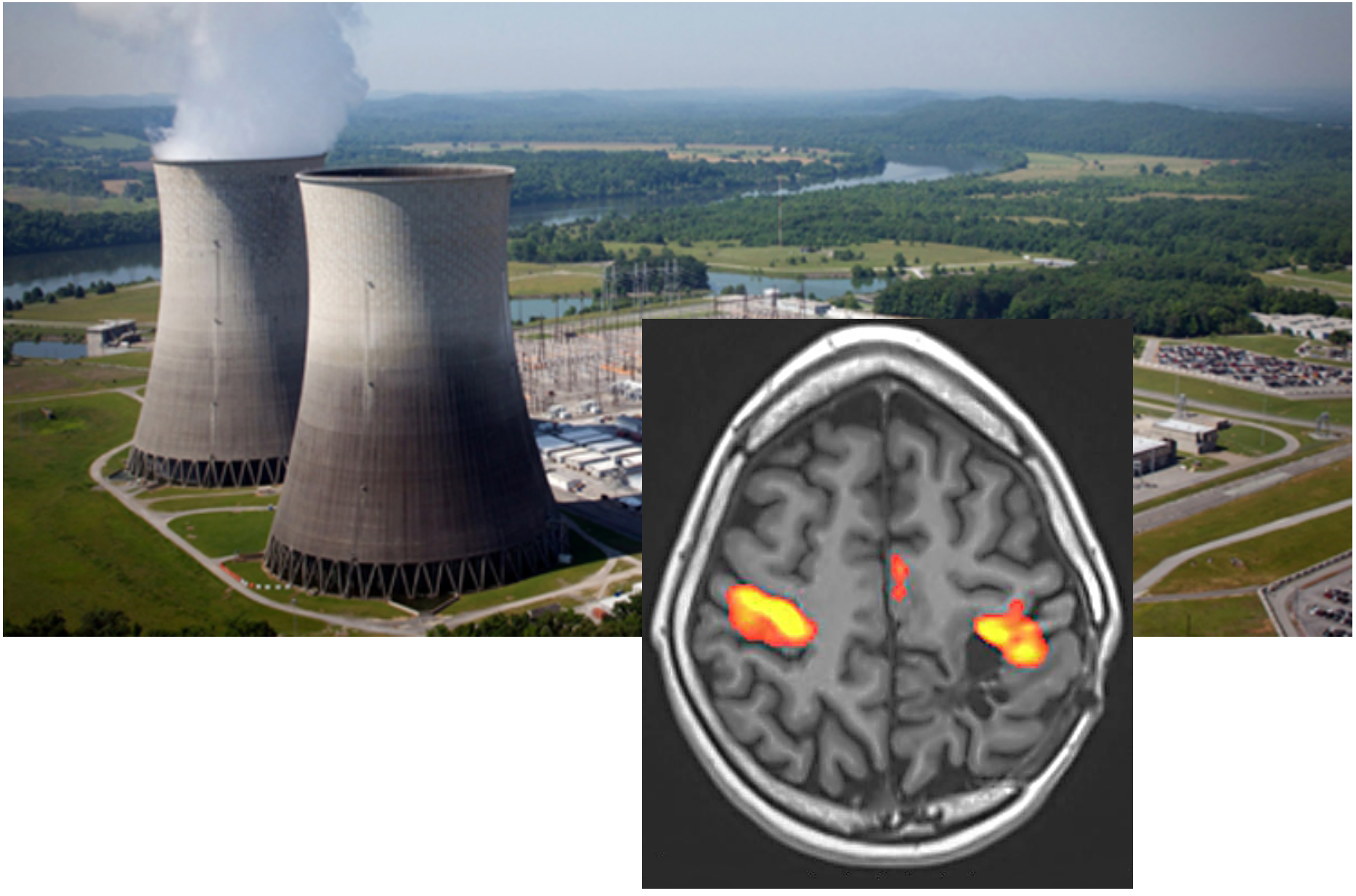






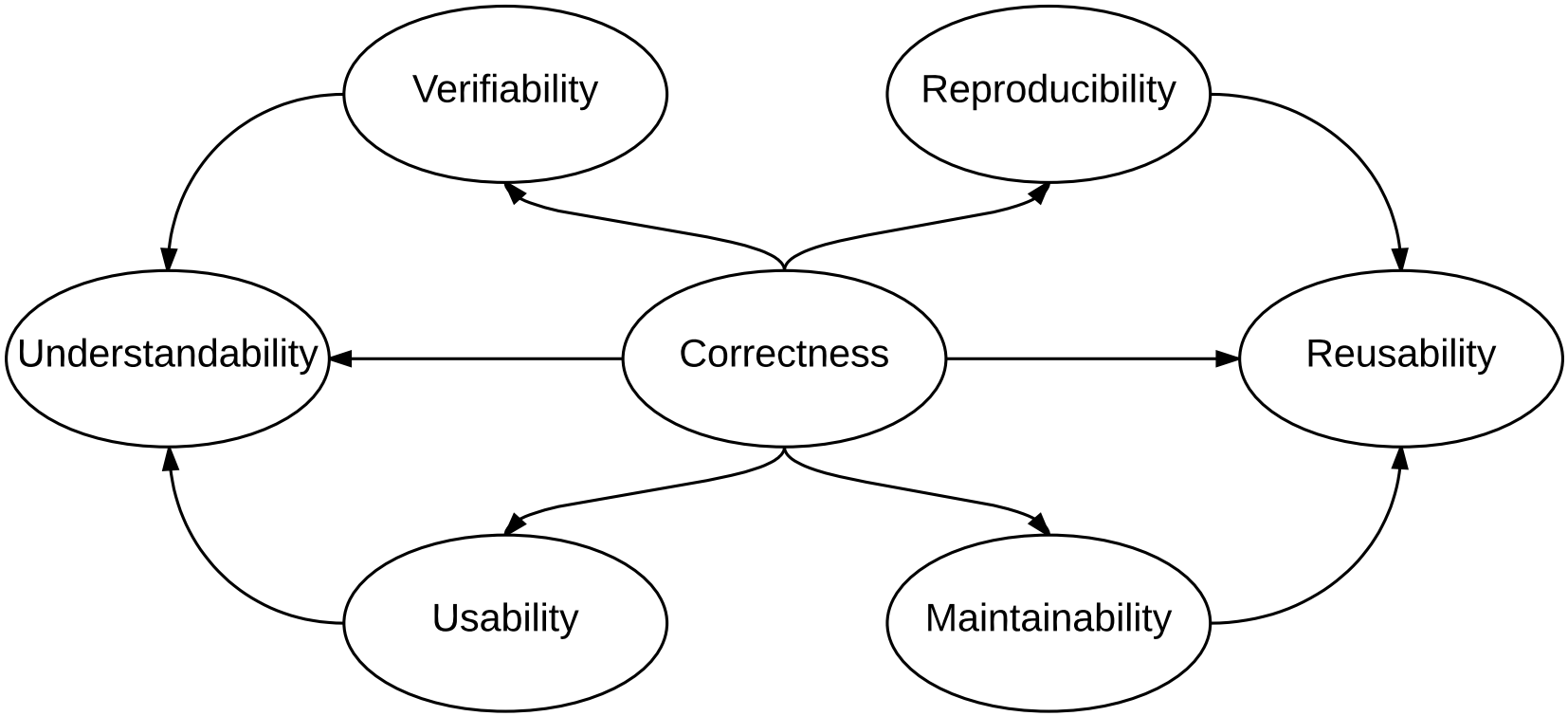


Motivation: Safety



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	✗	✓	✗	✗	✗

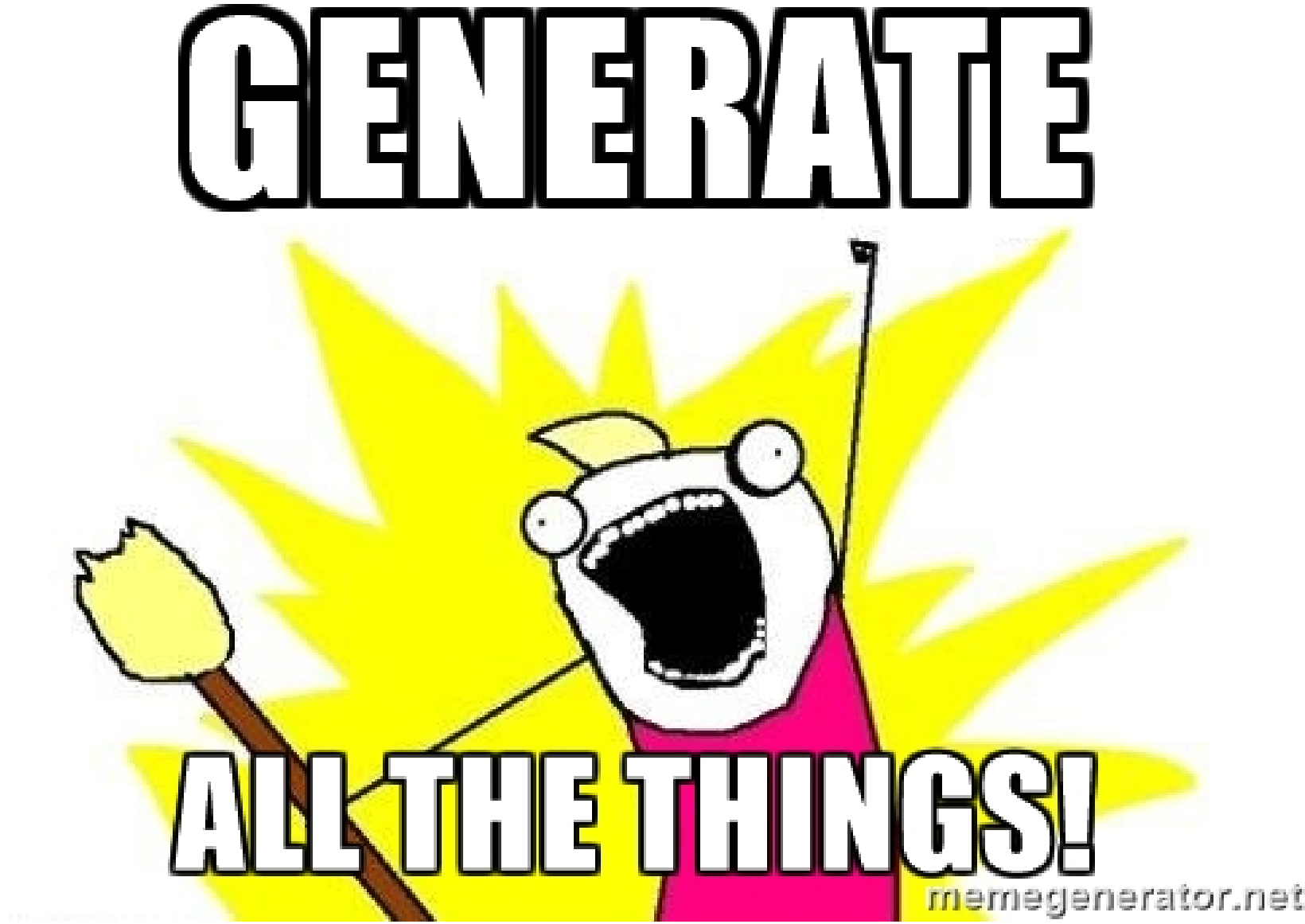
Perceived Advantages from Participants

- 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)

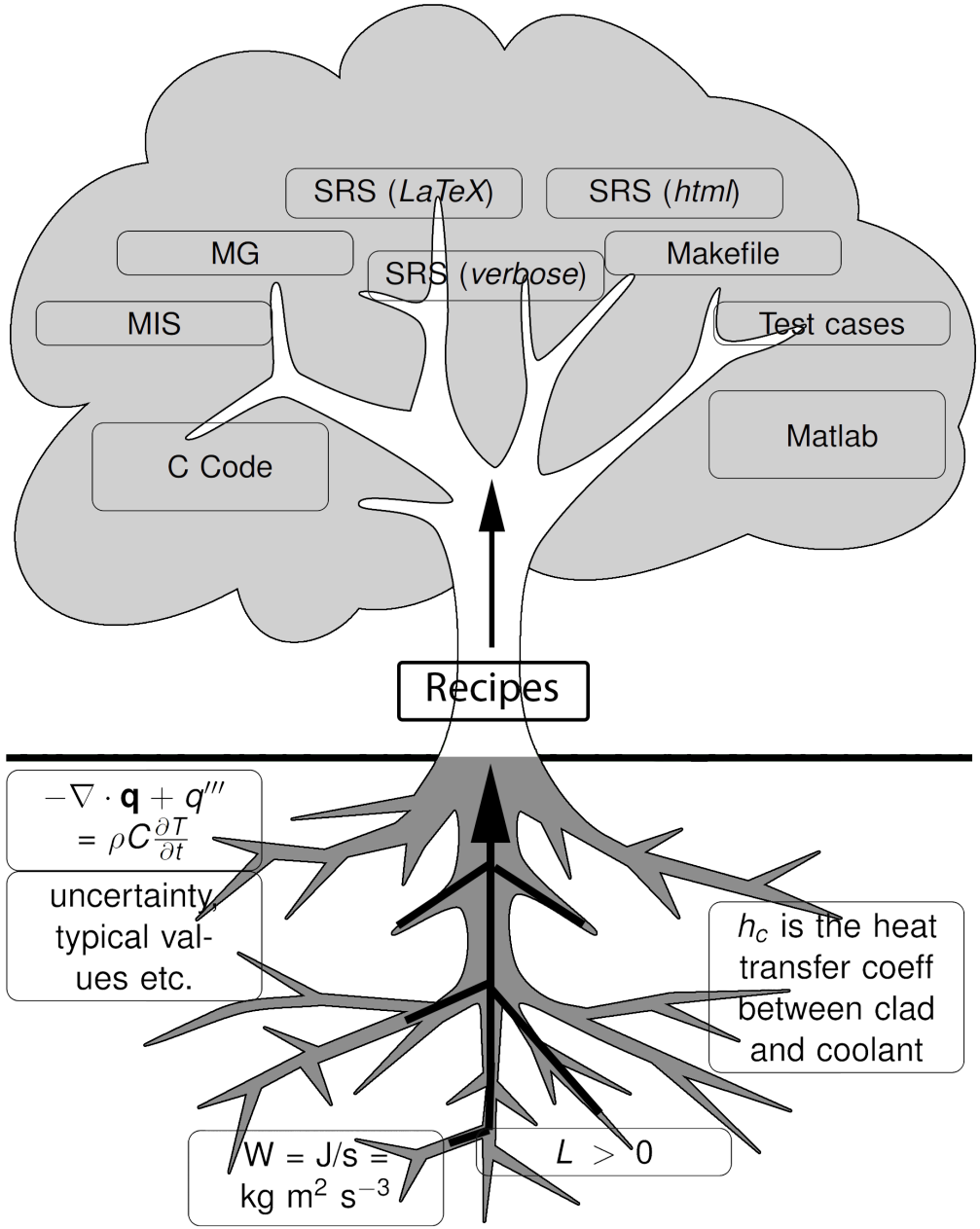
- SRS is too long
- SRS is not necessary
- DDD will not work in reality, since needs upfront requirements
- Too much SE jargon
- Difficult without a team of people
- Too difficult to maintain
- Not amenable to change
- Too tied to waterfall process
- Reports counterproductive [10]

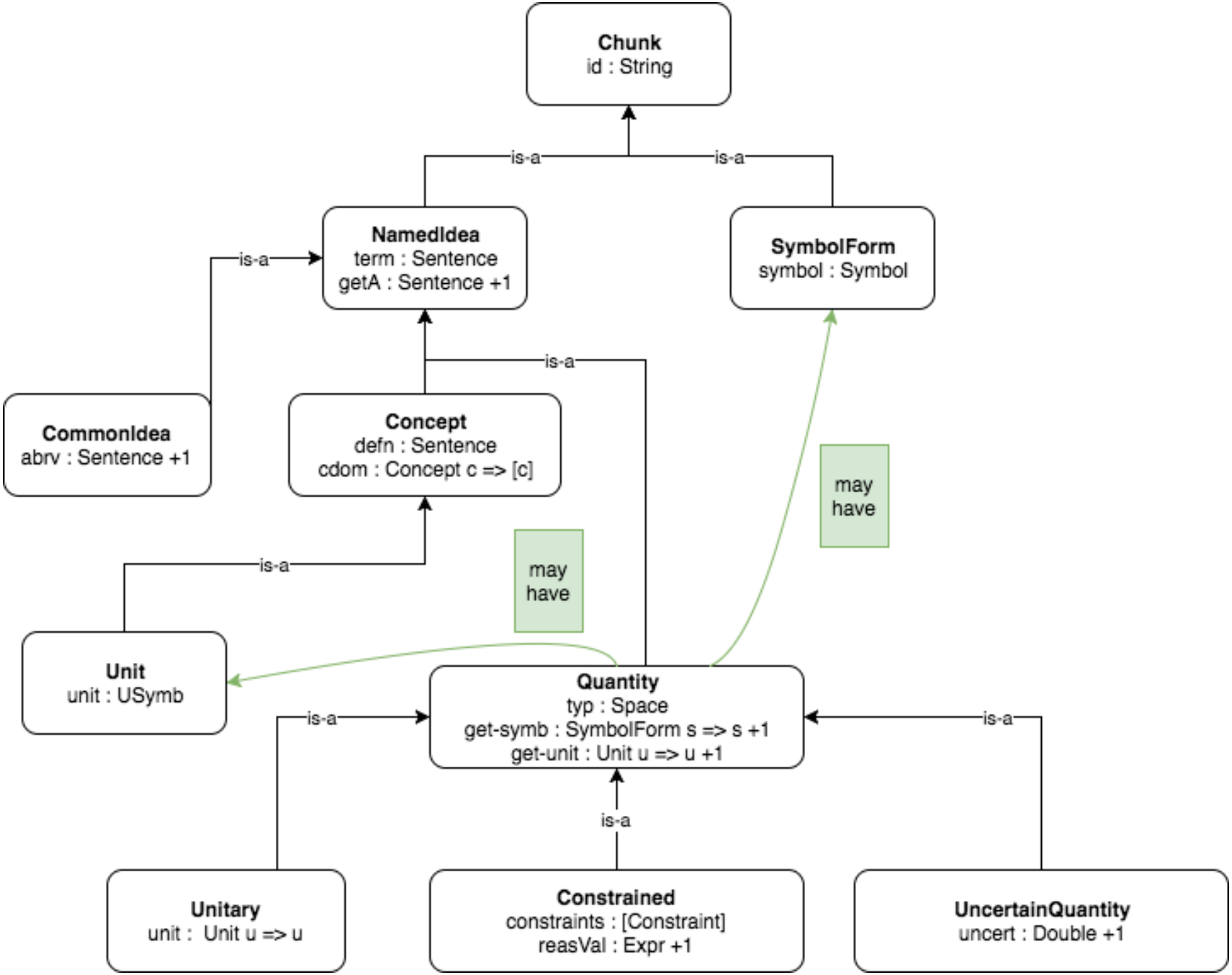
The Solution?


GENERATE
ALL THE THINGS!
memegenerator.net

Knowledge Capture

Drasil


SRS (*LaTeX*)
SRS (*html*)
MG
SRS (*verbose*)
Makefile
MIS
Test cases
Matlab
C Code
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
CommonIdea
abrv : Sentence +1
is-a
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	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	J_{tol} is the stress distribution factor (Function) based on Pbtol P_{btol} is the tolerable probability of breakage a is the plate length (long dimension) (m) b is the plate width (short dimension) (m) m is the surface flaw parameter ($\frac{\mathrm{m}^{12}}{\mathrm{N}^7}$) k is the surface flaw parameter ($\frac{\mathrm{m}^{12}}{\mathrm{N}^7}$) E is the modulus of elasticity of glass (Pa) h is the actual thickness (m) 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
```

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)

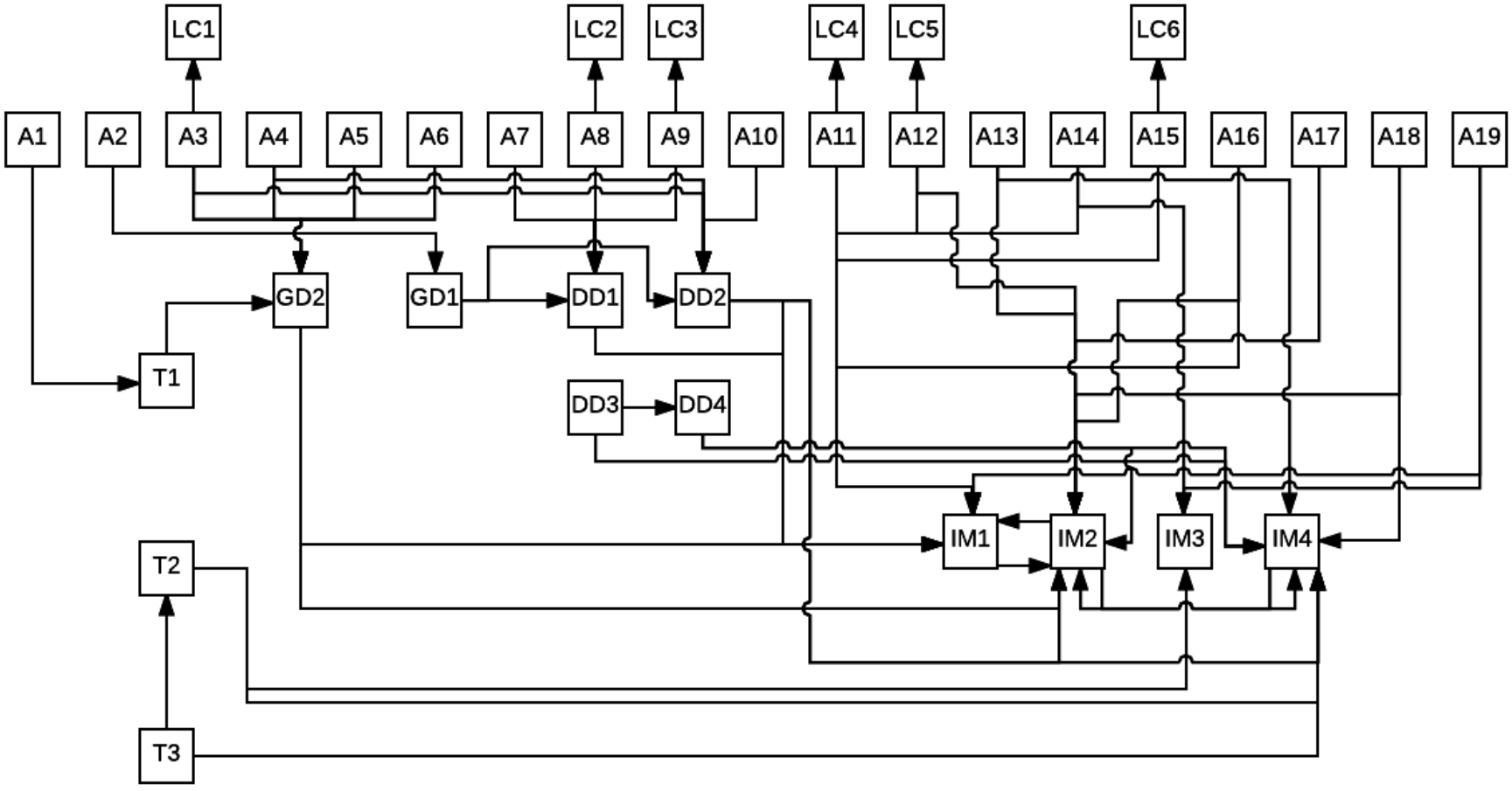
```
stressDistFac = makeVC "stressDistFac" (nounPhraseSP
  $ "stress distribution" ++ " factor (Function)")
      cJ
sdf_tol = makeVC "sdf_tol" (nounPhraseSP $
  "stress distribution" ++
  " factor (Function) based on Pbtol")
  (sub (eqSymb stressDistFac) (Atomic "tol"))

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 +:+ pbTolUsr)
```

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	$-\nabla \cdot \mathrm{q} + q''' = \rho C \frac{\partial T}{\partial t}$
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 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]

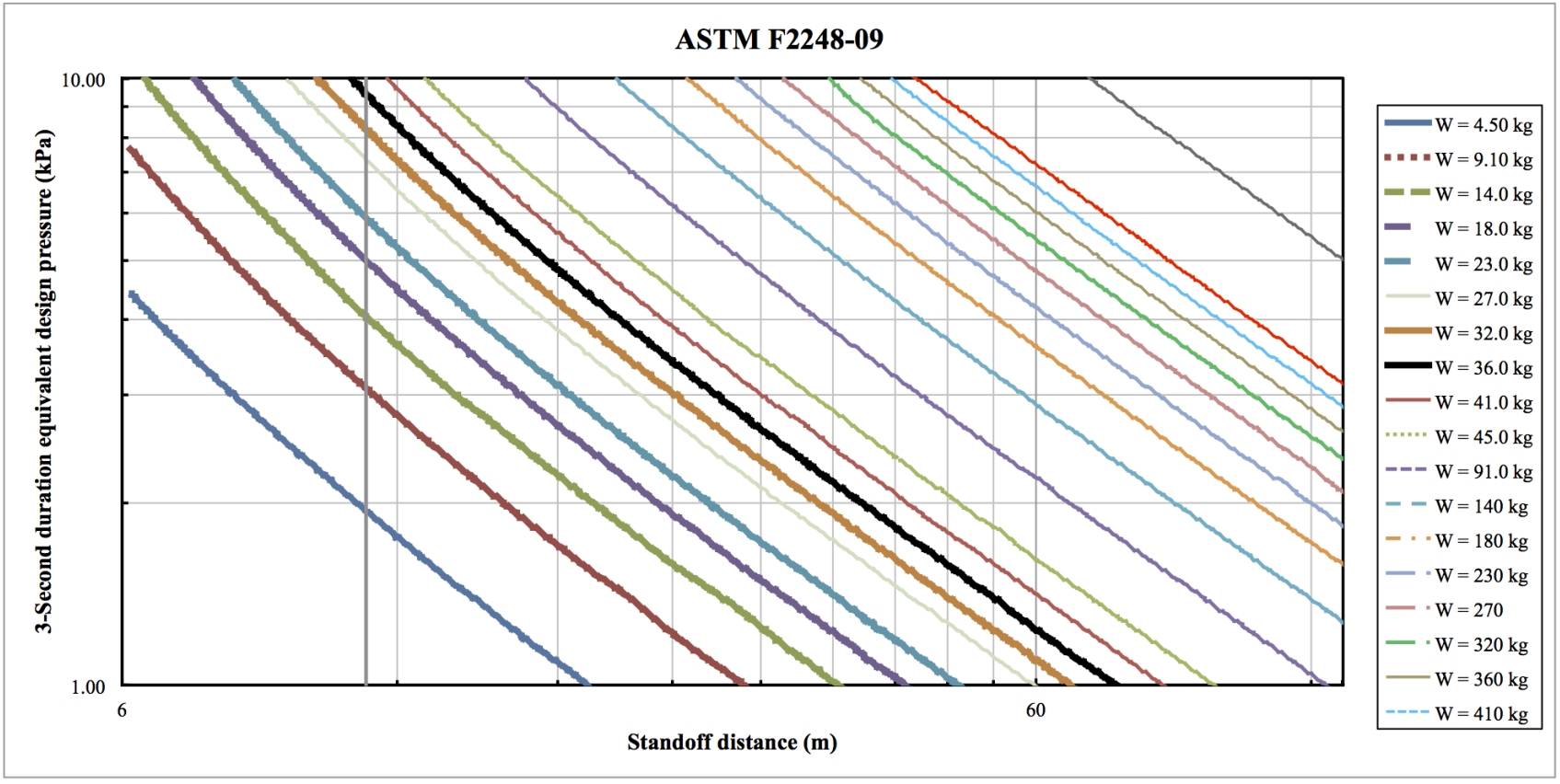
$$R_1^{\text{code}} = \frac{f}{8\pi k_{\text{AV}}} + \frac{1}{2\pi r_f h_g} \tag{1}$$

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

- 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

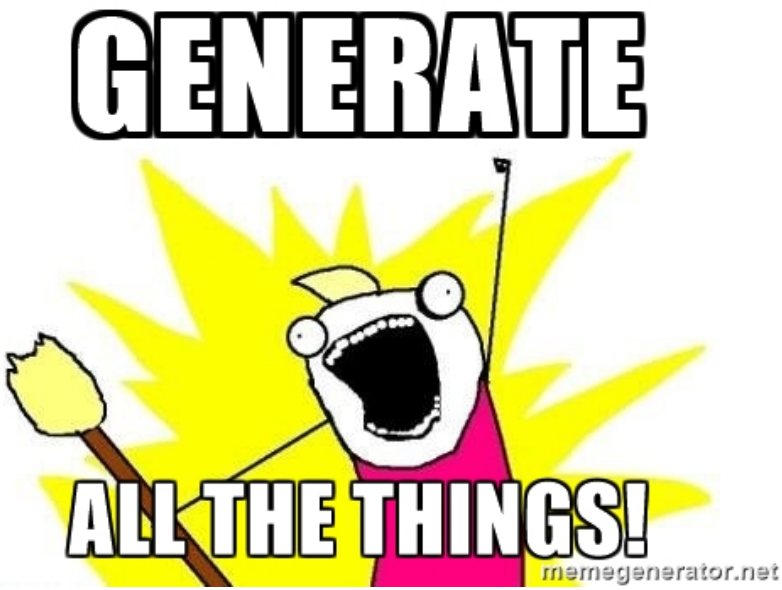
NO

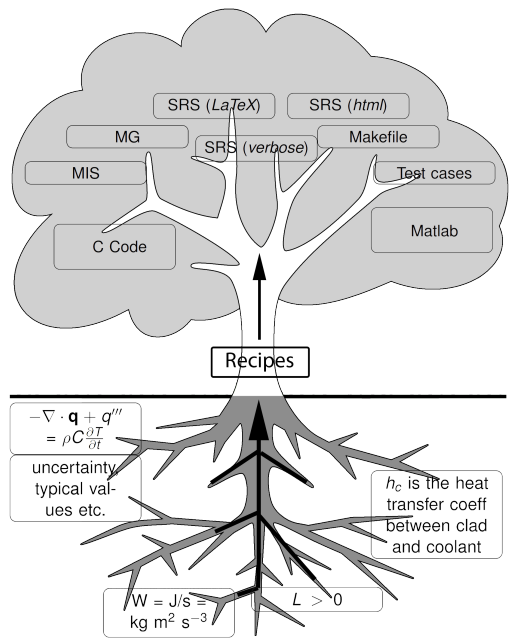
Future Work


ASTM F2248-09
10.00
1.00
3-Second duration equivalent design pressure (kPa)
6
60
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
- Open source Drasil here





Drasil Links

- Drasil on GitHub
- Design Language for Code Variabilities in Chapter 6 of Brook's thesis
- Drasil Generated Examples
- Drasil Haddock Documentation
- Package Dependency Graph (at the bottom of the page)

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References V

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