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

Fall 2017

21 Artifact Generation

Dr. Spencer Smith

Faculty of Engineering, McMaster University

November 21, 2017

McMaster University

Artifact Generation

- Administrative details
- Feedback on VnV
- Questions?
- Artifact generation (Drasil)

Administrative Details

- For final documentation, make sure you have **addressed and closed** all open issues
- MIS Marking Scheme
  - Not all of the spec has to be formal
- Course evaluation
  - Nov 23 to Dec 7
  - https://evals.mcmaster.ca

Administrative Details: Deadlines

MIS	Week 12	Nov 29
Impl. Present	Week 12	Week of Nov 27
Final Documentation	Week 13	Dec 6

Administrative Details: Presentation Schedule

- Impl. Present
  - **Tuesday: Alexander S., Steven, Alexandre P.**
  - **Friday: Jason, Geneva, Yuzhi**
- Can present anything related to the implementation
  - Code
  - Tools used
  - Testing
  - As always it is fine to show work in progress
  - Good to bring questions to the class

Feedback on VnV Plan

- Explicit web-link to your GitHub repo
- Reference your SRS document
- Explicitly state programming language
- Very nice to have explicit cross-references between documents. Keep information up to date using make
- Do not postpone decisions, be specific
- Outputs are unlikely to be an exact match for expected, instead summarize the error for all tests
- Define what you mean by error, especially if the output is a sequence
- Avoid unnecessary repetition, summarize similar tests in a table, distinguished by variabilities

VnV Feedback Continued

- Spell check! Proof read!
- Great to see usability tests, but need more information on how tests will be run. For instance, what specific task will they be asked to perform?
- Great to see code walkthroughs, but need more detail
- Provide enough information that the reader can easily verify your test cases, especially the expected output
- **Write as if someone else will be doing the testing**

Questions?

- Questions about MIS

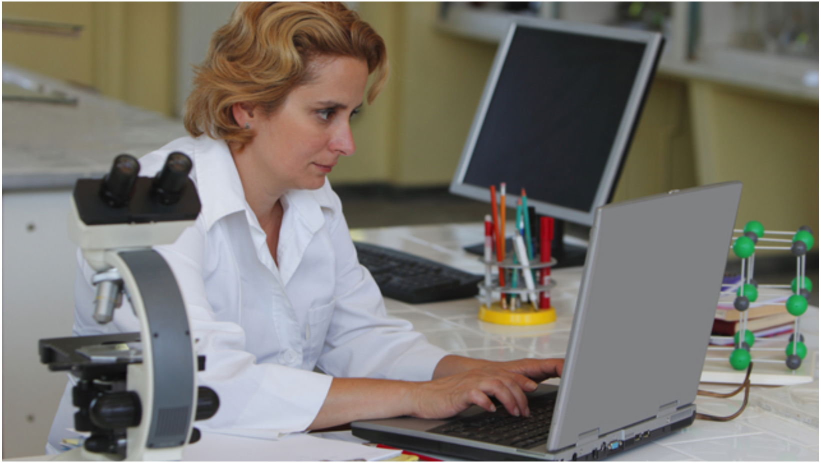
Abstract

- **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

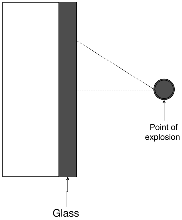
Scope: Large/Multiyear

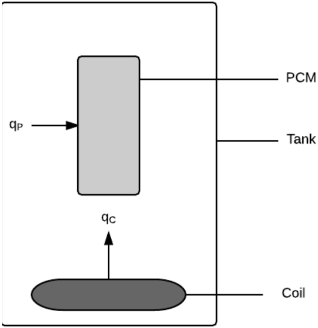
Scope: Program Families

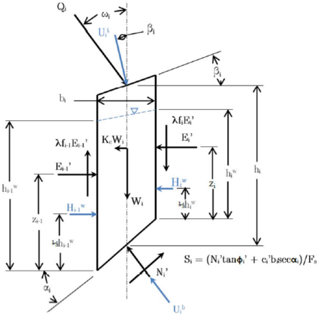
Scope: End User Developers

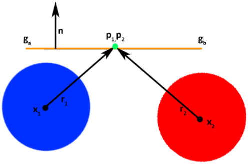


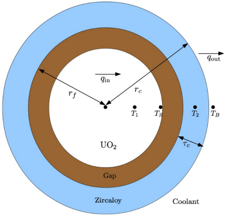
Scope: Physical Science



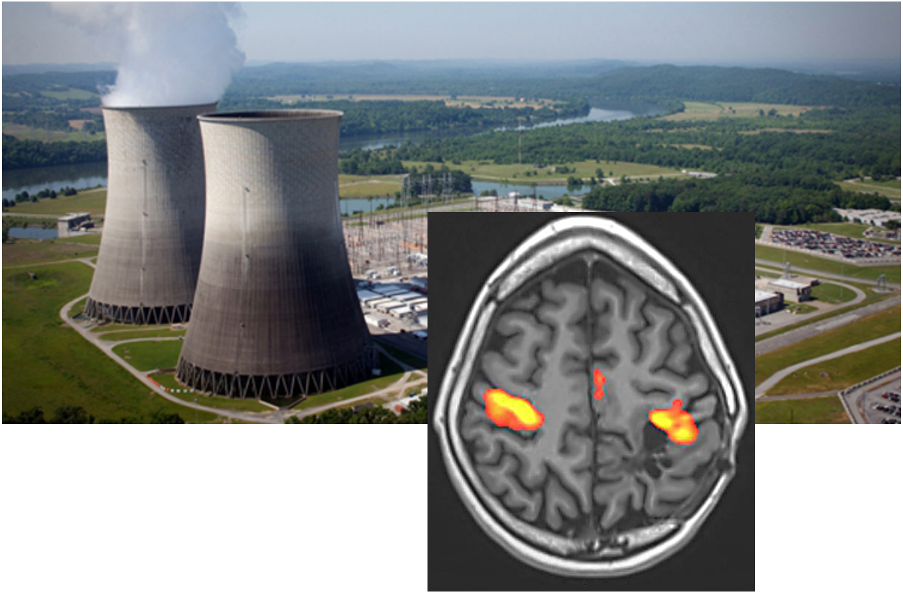






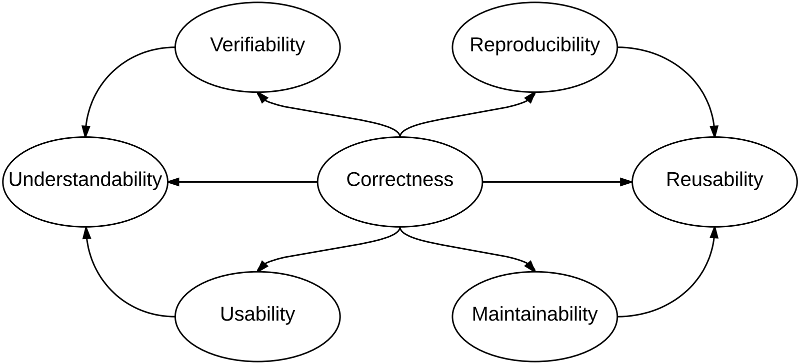


Motivation: Safety



Motivation: (Re)certification

Motivation: Improve Quality



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	✗	✓	✗	✗	✗

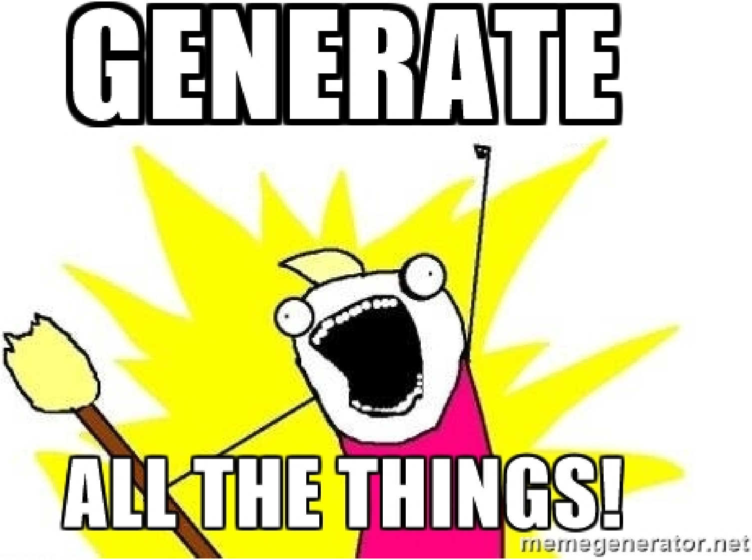
Perceived Advantages from Participants

- 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)

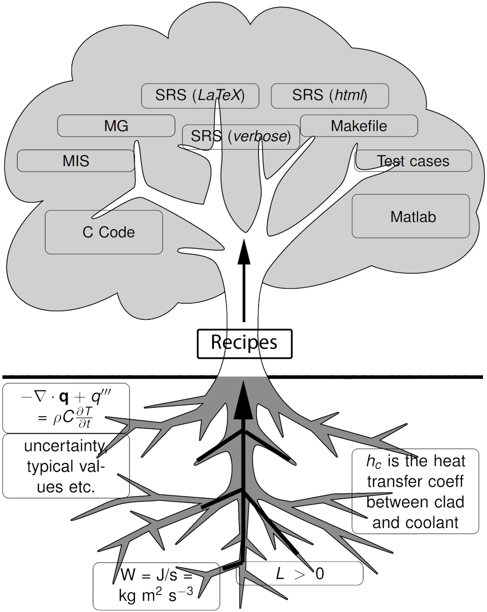
- SRS is too long
- SRS is not necessary
- DDD will not work in reality, since needs upfront requirements
- Too much SE jargon
- Difficult without a team of people
- Too difficult to maintain
- Not amenable to change
- Too tied to waterfall process
- Reports counterproductive [10]

The Solution?

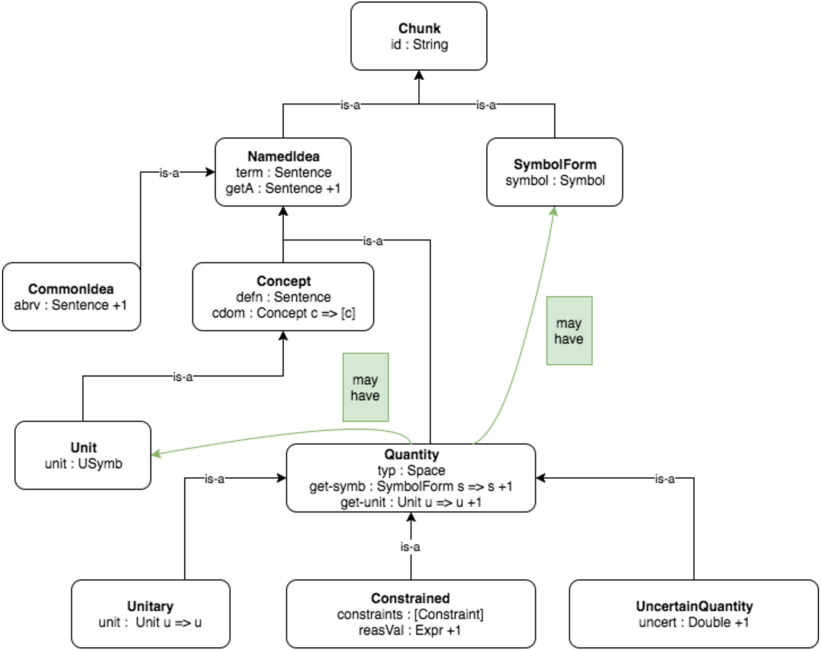

GENERATE
ALL THE THINGS!
memegenerator.net

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
is-a
CommonIdea
abrv : Sentence +1
Concept
defn : Sentence
cdom : Concept c => [c]
may have
is-a
may have
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)

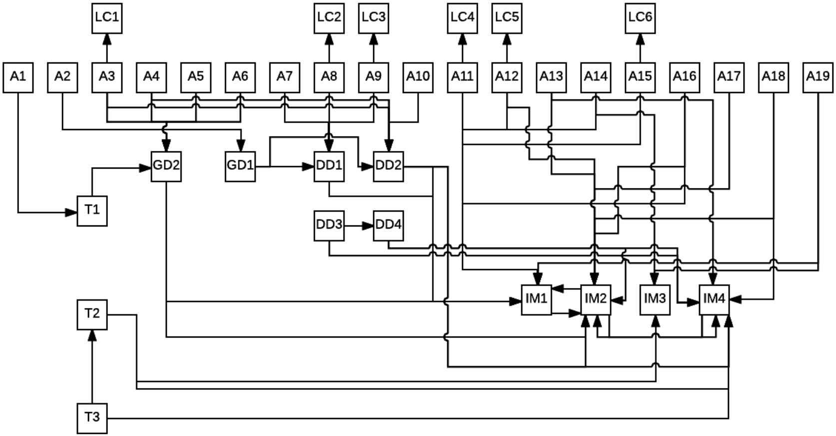
```
stressDistFac = makeVC "stressDistFac" (nounPhraseSP
  $ "stress distribution" ++ " factor (Function)")
     cJ
sdf_tol = makeVC "sdf_tol" (nounPhraseSP $
  "stress distribution" ++
  " factor (Function) based on Pbtol")
  (sub (eqSymb stressDistFac) (Atomic "tol"))

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

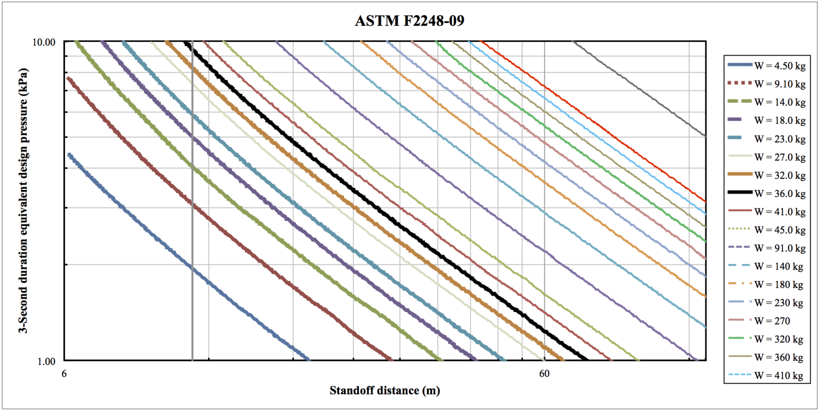
$$R_1^{\mathrm{code}} = \frac{f}{8\pi k_{\mathrm{AV}}} + \frac{1}{2\pi r_f h_g} \tag{1}$$

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

- 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
SILVER

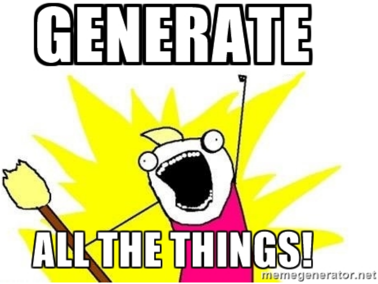
Future Work

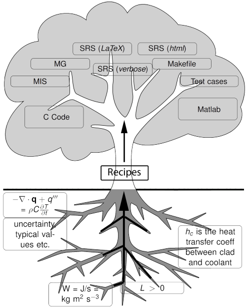


ASTM F2248-09
10.00
1.00
6
60
3-Second duration equivalent design pressure (kPa)
Standoff distance (m)
W = 4.50 kg
W = 9.10 kg
W = 14.0 kg
W = 18.0 kg
W = 23.0 kg
W = 27.0 kg
W = 32.0 kg
W = 36.0 kg
W = 41.0 kg
W = 45.0 kg
W = 91.0 kg
W = 140 kg
W = 180 kg
W = 230 kg
W = 270
W = 320 kg
W = 360 kg
W =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





References I

Jeffrey C. Carver, Richard P. Kendall, Susan E. Squires, and Douglass E. Post.
Software development environments for scientific and engineering software: A series of case studies.
In *ICSE '07: Proceedings of the 29th International Conference on Software Engineering*, pages 550–559, Washington, DC, USA, 2007. IEEE Computer Society.

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*

References II

Computer Science, pages 140–156. Springer International Publishing, 2012.

Diane Kelly.
Industrial scientific software: A set of interviews on software development.
In *Proceedings of the 2013 Conference of the Center for Advanced Studies on Collaborative Research*, CASCON '13, pages 299–310, Riverton, NJ, USA, 2013. IBM Corp.

Diane Kelly.
Scientific software development viewed as knowledge acquisition: Towards understanding the development of risk-averse scientific software.
Journal of Systems and Software, 109:50–61, 2015.

References III

Diane Kelly and Rebecca Sanders.
The challenge of testing scientific software.
In *Proceedings of the Conference for the Association for Software Testing*, pages 30–36, 2008.

Diane F. Kelly.
A software chasm: Software engineering and scientific computing.
IEEE Software, 24(6):120–119, 2007.

Zeeya Merali.
Computational science: ...error.
Nature, 467:775–777, 2010.

References IV

Steven J. Owen.
A survey of unstructured mesh generation technology.
In *INTERNATIONAL MESHING ROUNDTABLE*, pages 239–267, 1998.

David Lorge Parnas.
Precise documentation: The key to better software.
In *The Future of Software Engineering*, pages 125–148, 2010.

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

References V

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.

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.

References VI

Gregory V. Wilson.
Where's the real bottleneck in scientific computing? Scientists would do well to pick some tools widely used in the software industry.
American Scientist, 94(1), 2006.