

**CAS 741 (Development of Scientific Computing  
Software)**  
**Winter 2024**

**Artifact Generation**

Dr. Spencer Smith

Faculty of Engineering, McMaster University

March 22, 2024



# Artifact Generation

- Administrative details
- Finish Assurance Case review
- Artifact generation (Drasil)

# Administrative Details: Report Deadlines

Final Documentation    Week 13    Apr 12

- 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** doc, please ask
- When ready, assign issues to your primary and secondary reviewers
- GitHub issues due two days after assignment deadlines
- From Drasil Code onward, Drasil projects no longer need to maintain traditional SRS

# Administrative Details: Presentations

Unit VnV/Implement    Week 12    Week of Apr 3

- Specific schedule depends on final class registration
- Informal presentations with the goal of improving everyone's written deliverables
- Domain experts and secondary reviewers (and others) will ask questions

# Presentation Schedule

# Presentation Sched Cont'd

- Implementation Present (15 min each)
  - ▶ **Mar 26: Reyhaneh, Waqar, Al, Tanya, Atiyeh**
  - ▶ **Apr 2: Nada, Phil, Xinyu, Fasil, Yi-Leng**
  - ▶ Apr 5: Gaofeng, Morteza, Valerie, Hunter, Ali
  - ▶ Apr 9: Cynthia, Adrian, Yiding, Kim Ying

# Presentation Schedule

- 3 presentations each
  - ▶ SRS everyone
  - ▶ VnV and POC subset of class
  - ▶ Design subset of class
  - ▶ Implementation everyone
- If you will miss a presentation, please trade with someone
- Implementation presentation could be used to run a code review, or code walkthrough

# Questions?

- Questions on administrative details?
- Questions on final documentation?
- Questions on reflection document?
- Questions on final implementation?
- Questions on VnV report?
- Other questions?



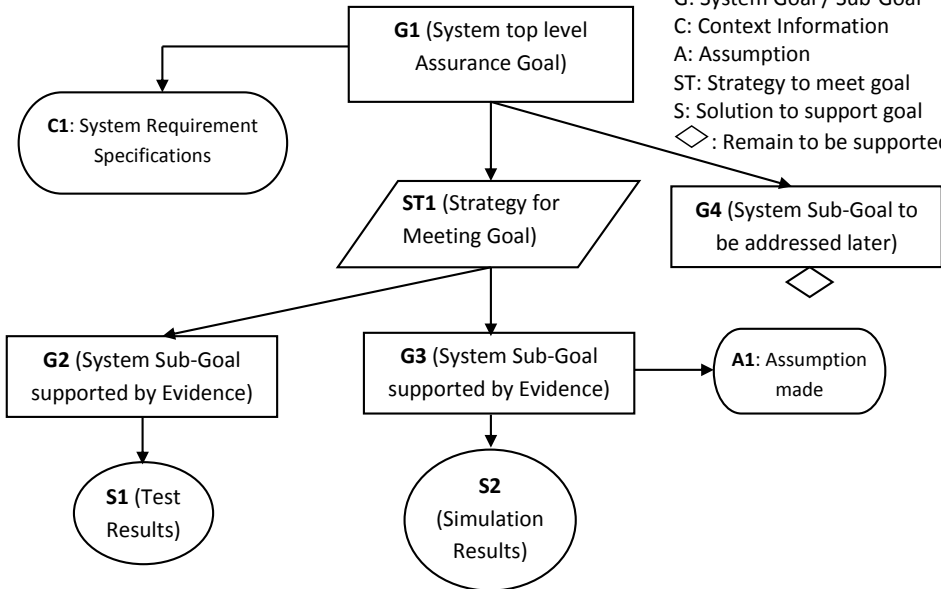
# Assurance Cases in Scientific Computing [14, 13]

- Assurance cases
  - ▶ Organized and explicit argument for correctness
  - ▶ Successfully used for safety critical systems
- Advantages for SC
  - ▶ Engaging domain experts
  - ▶ Producing necessary and relevant documentation
  - ▶ Evidence that can be verified/replicated by a third party
- Example of 3dfim+
  - ▶ No errors found
  - ▶ However
    - ▶ Documentation ambiguities
    - ▶ No warning about parametric statistical model

# Assurance Cases in SC Motivation

- Do we put too much trust in the quality of SCS?
- Are enough checks and balances in place, especially for safety related software?
- Problems with imposing external requirements for certification
  - ▶ External body does not have expertise
  - ▶ SCS developers dislike documentation
- Solution – Assurance Cases by experts
  - ▶ Experts engaged
  - ▶ Relevant documentation
- Current techniques of development and testing still used, but arguments will no longer be ad hoc and incompletely documented

G: System Goal / Sub-Goal  
C: Context Information  
A: Assumption  
ST: Strategy to meet goal  
S: Solution to support goal  
◇ : Remain to be supported



[A] AFNI: tmp/LRtap/mdef3d\_01+ori

[Order: RAI=DICOM]  
 x = -39.500 mm [R]  
 y = 31.500 mm [P]  
 z = 45.500 mm [S]

Xhairs ☒ Multi ☐ X+

Color ☒ green

Gap ☐ 5 ☒ Wrap

Index

Axial ☒ Image ☐ Graph  
 Sagittal ☒ Image ☐ Graph  
 Coronal ☒ Image ☐ Graph

New ☒ Views

BHelp ☒ done

◆ Original View  
 ◆ AC-PC Aligned  
 ◆ Talairach View

Define Markers  
☒ See Markers

Define Overlay  
☒ See Overlay

Define Datamode

Switch Session  
 Switch UnderLay  
 Switch Overlay  
 Control Surface

[A] AFNI: tmp/LRtap/m

Colr  
 Swap  
 Norm

c  
b  
r  
g  
i  
9  
z

pan  
crop

141

left=Right float [2%-98%]

Disp Sav1.ppm Mont Done Rec

[A] AFNI: tmp/LRtap/mdef3d\_01+ori

Colr  
 Swap  
 Norm

c  
b  
r  
g  
i  
9  
z

pan  
crop

135

float [2%-98%]

Disp Sav1.ppm Mont Done Rec

[A] AFNI: tmp/LRtap/m

Colr  
 Swap  
 Norm

c  
b  
r  
g  
i  
9  
z

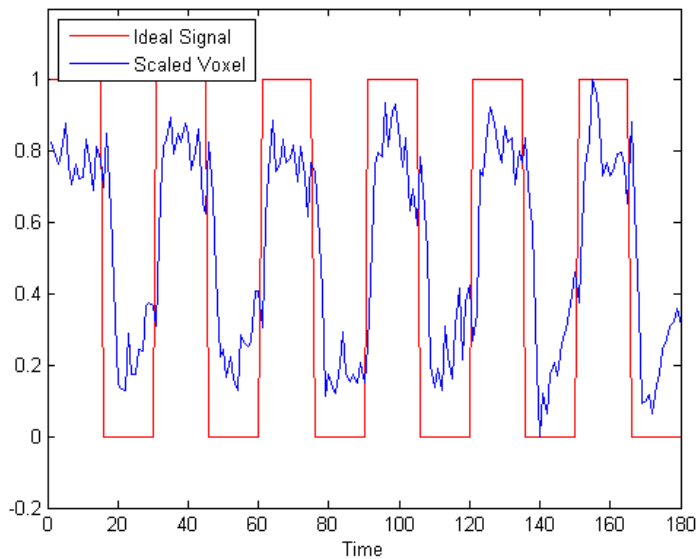
pan  
crop

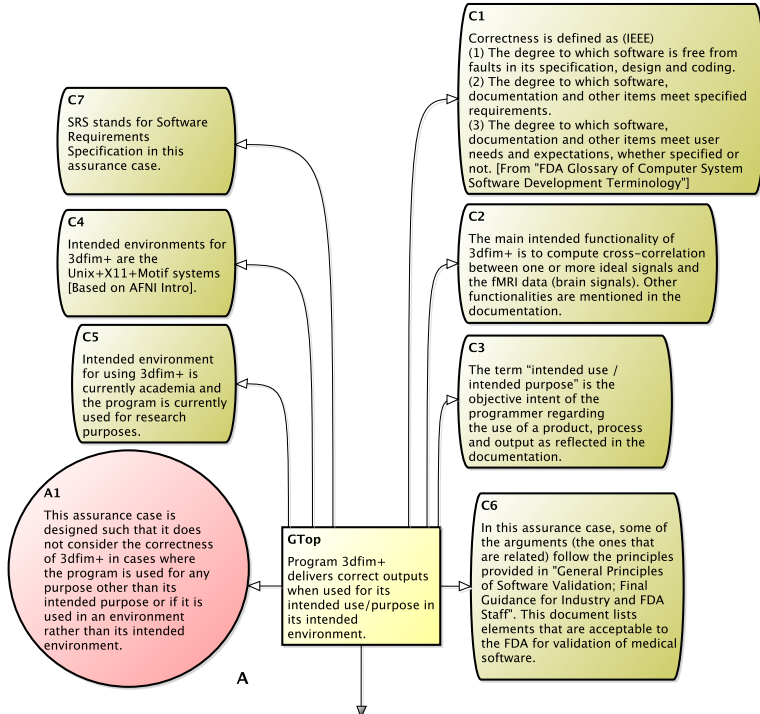
159

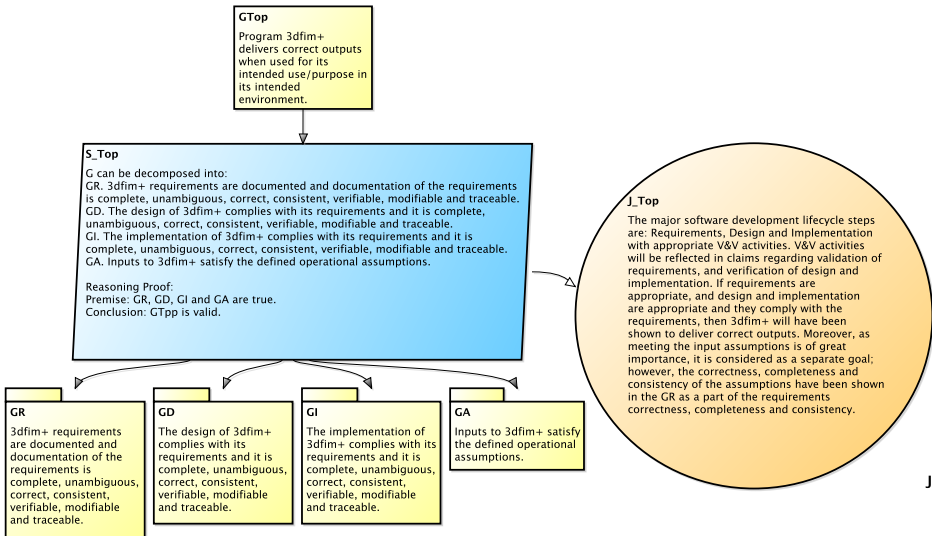
float [2%-98%]

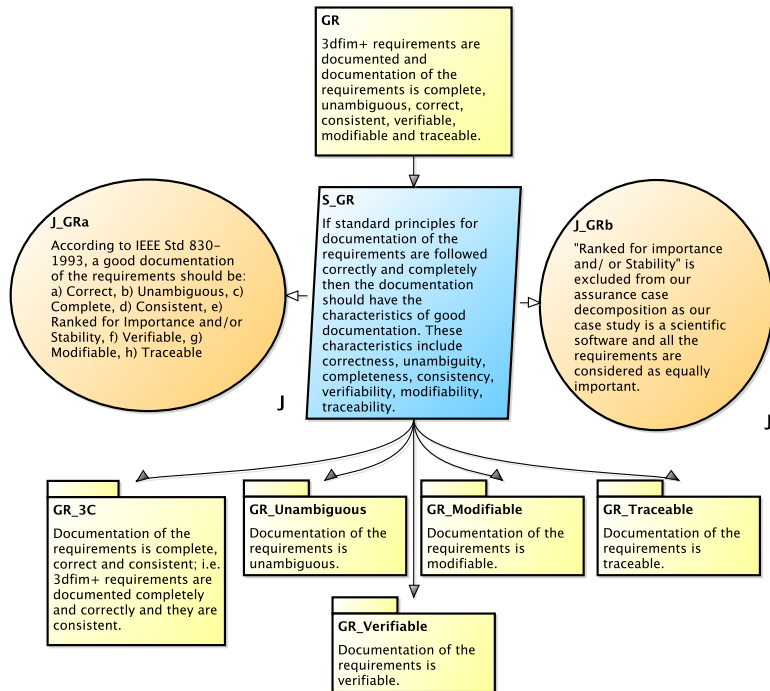
Disp Sav1.ppm Mont Done Rec

Scaled Voxel (23,27,22) and Ideal Signal over time

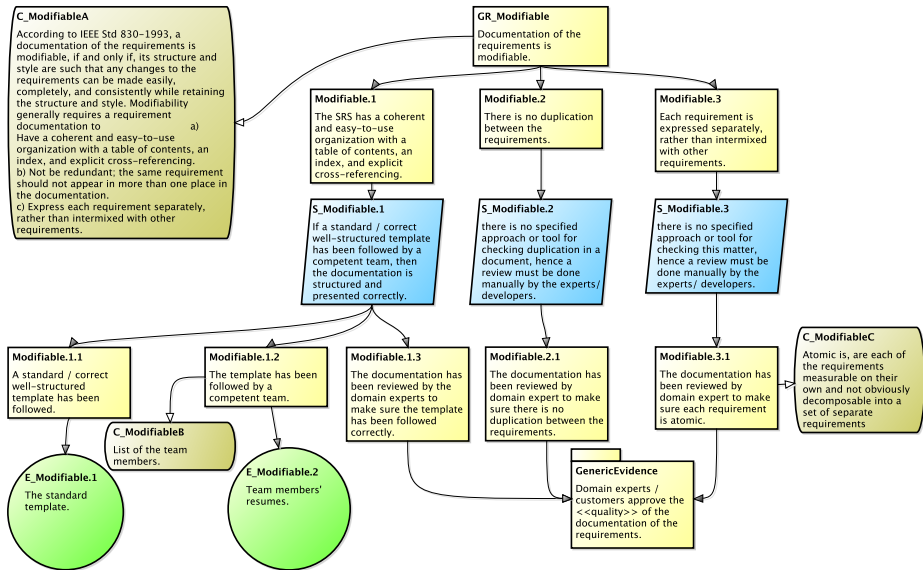


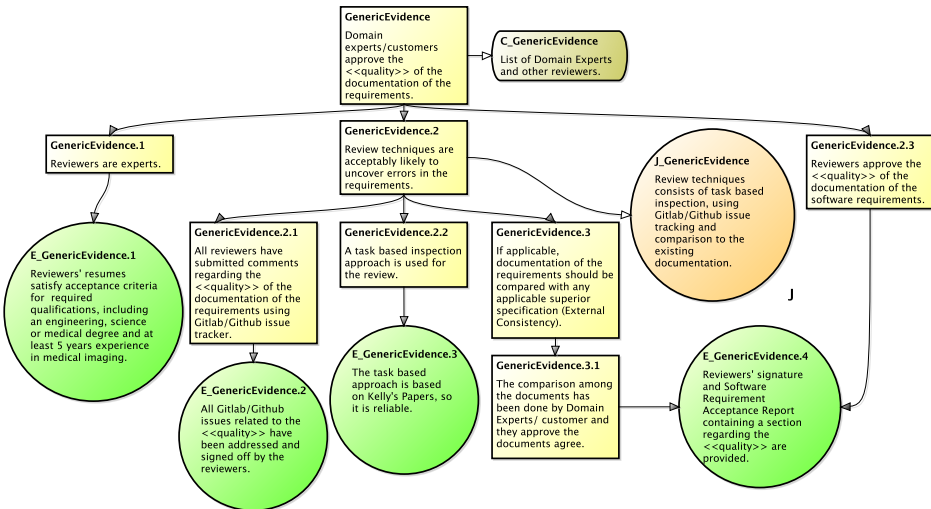


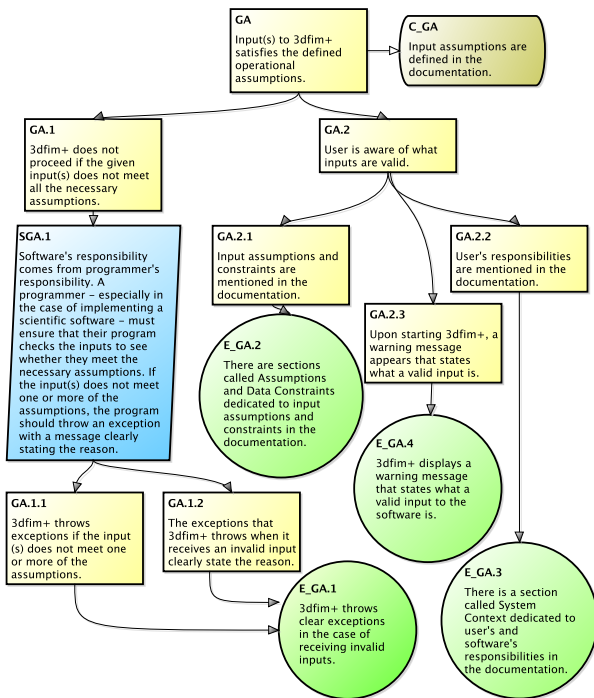












# Proposed Changes to 3dfim+

- No mistakes found in calculations
- Goal of original software was not certification
- Problems found
  - ▶ GR goal not satisfied
    - ▶ Not complete, verifiable, modifiable or traceable
    - ▶ Coordinate system information missing
    - ▶ Ambiguous rank function
  - ▶ Inputs not checked in code
  - ▶ User not informed of their responsibility to use tool with correct statistical model

# Concluding Remarks

- Hopefully motivated assurance cases for SC
- Quality is improved by looking at a problem from different perspectives, assurance cases provide a systematic and rigorous way to introduce a new perspective
- An assurance cases will likely use the same documentation and ideas used in CAS 741
- However, an assurance case can focus and direct efforts right from the start of the project

# 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





## PRODUCT SPECIFICATIONS

The appearance and specifications listed in this manual may vary due to constant product improvements.

**Electrical requirements:** 115 V, 60 Hz

**Min. / Max. water pressure:** 20 - 120 psi (138 - 827 kPa)

ENGLISH

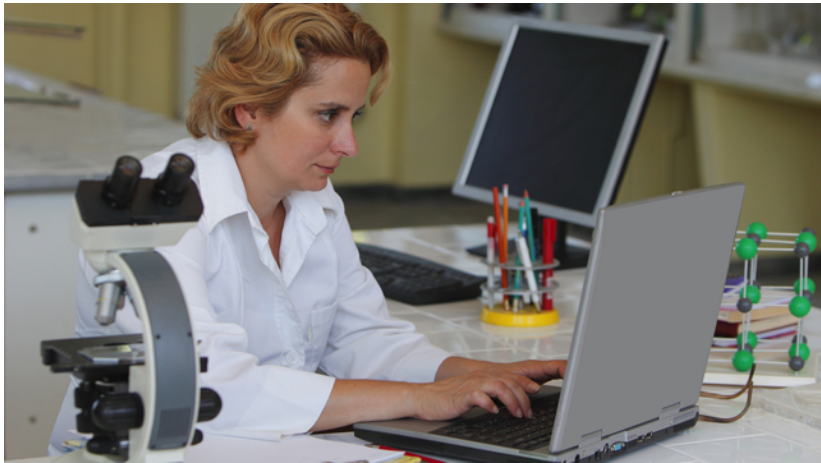
Model	LFCC22426*
Description	Counter-depth, French door refrigerator, bottom freezer
Net weight	243 lb (110 kg)

Model	LFCS27596*
Description	Standard-depth, Door-in-Door French door refrigerator, bottom freezer
Net weight	284 lb (129 kg)

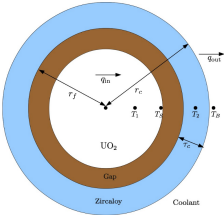
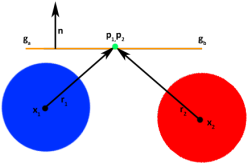
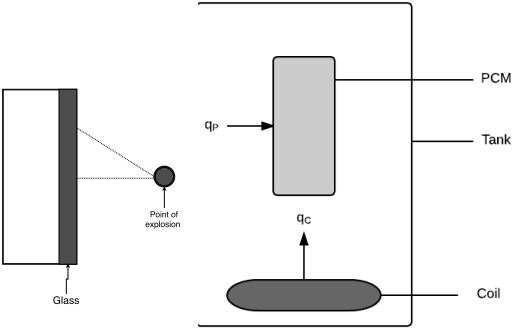
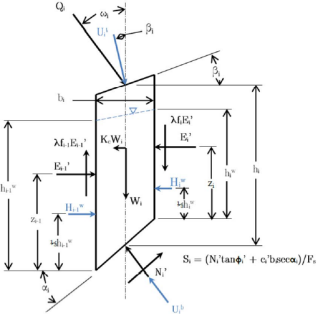
Model	LFCC23596*
Description	Counter-depth, Door-in-Door French door refrigerator, bottom freezer
Net weight	269 lb (122 kg)



## Scope: End User Developers

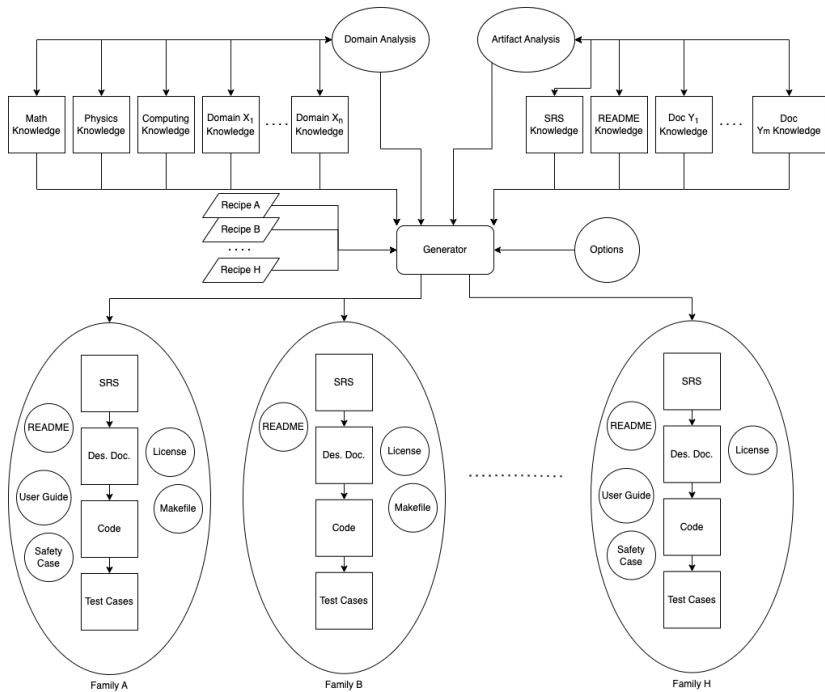


# Scope: Physical Science



# Build on Success of MDSE

- Codify (capture) code and non-code info together
  - ▶ Natural language (text)
  - ▶ Definitions
  - ▶ Assumptions
  - ▶ Rationale, Derivations
  - ▶ Abstract theory
  - ▶ Etc.
- Generate all artifacts from one framework
  - ▶ Requirements
  - ▶ User manuals
  - ▶ Build scripts, dev environment (CI etc)
  - ▶ Assurance case
  - ▶ Code (in different languages)
  - ▶ Test cases
  - ▶ etc.



$$\mathbf{a} = \frac{d\mathbf{v}}{dt} \text{ and } \mathbf{v} = \frac{d\mathbf{p}}{dt}$$

$$\mathbf{F} = m\mathbf{a}$$

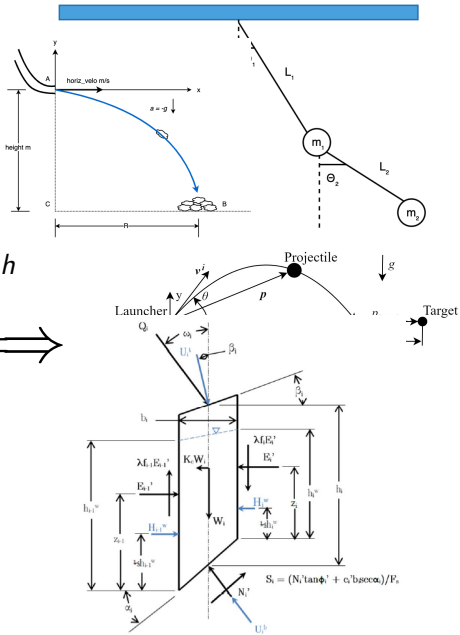
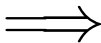
$$m \frac{d\mathbf{v}}{dt} = m\mathbf{g} - c\mathbf{v}$$

$$g = 9.8m/s^2 \text{ or } g = 32.2ft/s^2$$

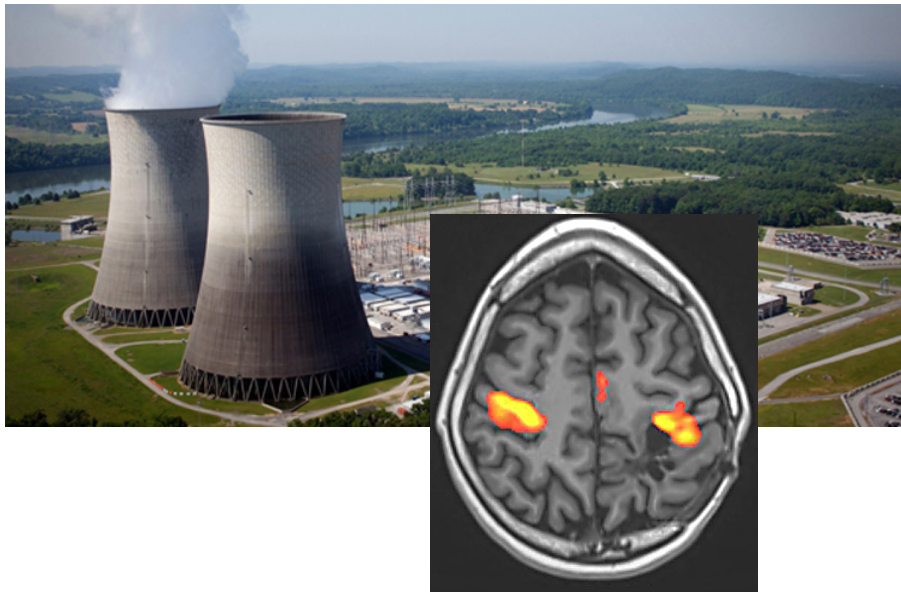
$$y_{n+1} = y_n + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)h$$

$$\sigma_{ij} = D_{ijkl}\epsilon_{kl}$$

coordinate system



## Motivation: Safety

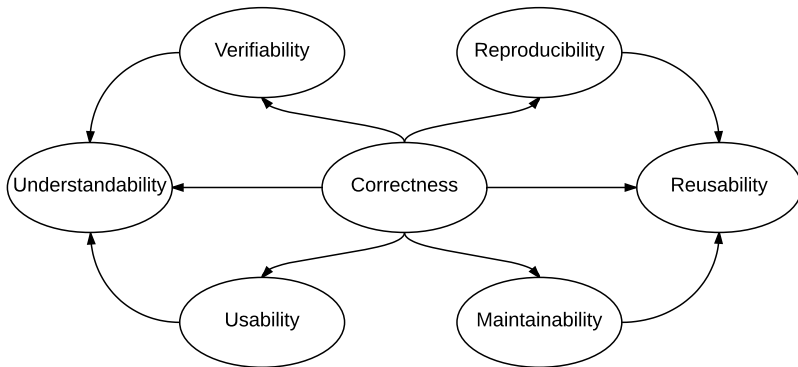




Motivation: (Re)certification



# Motivation: Improve Quality



# Current Approach

- Agile like [1]
- Amethododical [3]
- Knowledge acquisition driven [4]
- Each stage reports counterproductive [10]
- Limited tool use [16]
- 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
<b>SWHS</b>	1000	F77	1	5	✗	✓	✗	✗	✗
<b>Astro</b>	5000	C	2	10	✗	✓	✗	✗	✗
<b>Glass</b>	1300	F90	1	<1	✗	✓	✗	✗	✗
<b>Soil</b>	800	M	1	5	✓	✓	✓	✓	✗
<b>Neuro</b>	1000	M	1	5	✓	✓	✗	✓	✗
<b>Acoust</b>	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?



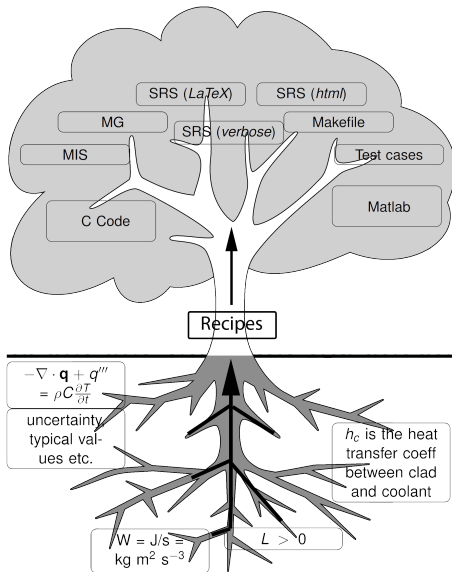
# GENERATE

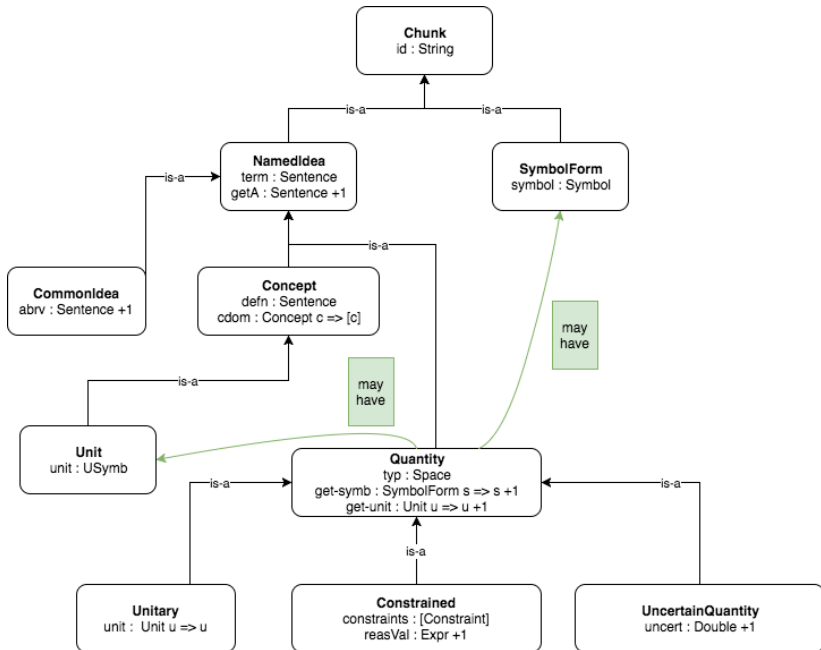


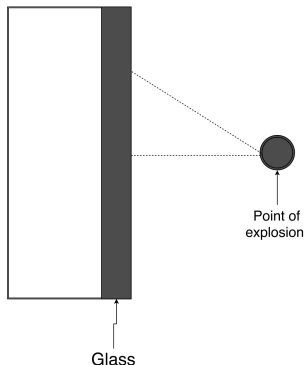
memegenerator.net

# Knowledge Capture









Given

- dimensions of glass plane
- glass type
- explosion characteristics
- tolerable breakage probability

Predict whether the glass will withstand the explosion

## Drasil Inputs:

- Program Name: GlassBR
- Authors: Nikitha K and Spencer S
- Symbols: tolerable load ( $\hat{q}_{tol}$ ), Risk of failure ( $B$ ), ...
- Assumptions: Load duration factor constant,
- Data definitions: relation for  $B$ , ...
- Design decisions:
  - Modularity (input module),
  - Implementation Type (Program),
  - Logging (Yes),
  - Input Structure (Bundled),
  - Constant Structure (Inlined),
  - Constant Rep (Constants),
  - Real Number Rep (Double),
  - ...

## Drasil Inputs:

- Program Name: GlassBR
- Authors: Nikitha K and Spencer S
- Symbols: tolerable load ( $\hat{q}_{tol}$ ), Risk of failure ( $B$ ), ...
- Assumptions: Load duration factor constant,
- Data definitions: relation for  $B$ , ...
- Design decisions:
  - Modularity (input module),
  - Implementation Type (Program),
  - Logging (Yes),
  - Input Structure (Bundled),
  - Constant Structure (Inlined),
  - Constant Rep (Constants),
  - Real Number Rep (Double),
  - ...

/glassbr  
/Website/GlassBR\_SRS.html  
/Website/GlassBR\_SRS.css  
/SRS/bibfile.bib  
/SRS/Makefile  
/SRS/GlassBR\_SRS.tex  
/SRS/GlassBR\_SRS.pdf  
/src/python  
/src/python/README.md  
/src/python/InputParameters.py  
/src/python/Calculations.py  
/src/python/Makefile  
/src/python/doxConfig  
...

...  
/src/java/GlassBR/Calculations.java  
/src/java/Makefile  
/src/java/README.md  
...  
/src/cpp/GlassBR  
/src/cpp/ReadTable.cpp  
/src/cpp/InputFormat.hpp  
/src/cpp/Calculations.cpp  
...  
/src/swift/Calculations.swift  
...  
/src/csharp/Control.cs  
...



/glassbr  
/Website/GlassBR\_SRS.html  
/Website/GlassBR\_SRS.css  
/SRS/bibfile.bib  
/SRS/Makefile  
/SRS/GlassBR\_SRS.tex  
/SRS/GlassBR\_SRS.pdf  
/src/python  
/src/python/README.md  
/src/python/InputParameters.py  
/src/python/Calculations.py  
/src/python/Makefile  
/src/python/doxConfig  
...

...  
/src/java/GlassBR/Calculations.java  
/src/java/Makefile  
/src/java/README.md  
...  
/src/cpp/GlassBR  
/src/cpp/ReadTable.cpp  
/src/cpp/InputFormat.hpp  
/src/cpp/Calculations.cpp  
...  
/src/swift/Calculations.swift  
...  
/src/csharp/Control.cs  
...

# Software Requirements Specification for GlassBR

Nikitha K and Spencer S

html

## Table of Symbols

$\hat{q}_{\text{tol}}$

$B$

...

## Introduction

... The software, herein called GlassBR, ...

## Assumptions

ldfConstant: LDF is constant, depends on assumed value of  $t_d$  and  $m$ , ...

## Data Definitions

$$B = \frac{k}{(ab)^{m-1}} (Eh^2)^m \text{LDF} e^J$$

...

sBR

$$B = \frac{k}{(ab)^{m-1}} (Eh^2)^m \text{LDF} e^J$$

## GlassBR

Authors: Nikitha K and Spencer S

**How to Run the Program:** In your terminal command line, enter the same directory as this README file. Then enter the following line

```
make run RUNARGS=input.txt
```

**Configuration Files:** SDF.txt, TSD.txt must be in the same directory as the executable to run successfully

Versioning: Python Version 3.5.1

```
...
```

```
build:
```

```
run: build
```

```
python Control.py
```

```
...
```

```
build: GlassBR/Control.class
```

```
...
```

```
GlassBR/Control.class:
```

```
GlassBR/Control.java ...
```

```
javac GlassBR/Control.java
```

```
run: build
```

```
java GlassBR.Control $(RUNARGS)
```

```
...
```

Calculations.py

Calculations.java

```
## \file Calculations.py
# \author Nikitha Krithnan and W. Spencer Smith
# \brief package GlassBR
...
## \file Calculations.java
/**
 * \author Nikitha Krithnan and W. Spencer Smith
 * \para \brief Provides functions for calculating the outputs
 * \para
 * \return */
def func...
    out public static double func_B(InputParameters inParams, double J) throws IOException {
    pri     PrintWriter outfile;
    ...     outfile = new PrintWriter(new FileWriter(new File("log.txt"), true));
    out     outfile.println("function func_B called with inputs: {}");
    ...
    ret     outfile.close();

    return 2.86e-53 /Math.pow(inParams.a * inParams.b, 7.0 - 1.0) *
        Math.pow(7.17e10 * Math.pow(inParams.h, 2.0), 7.0) * inParams.LDF
        * Math.exp(J);
    }
```

$J_{tol}$  in SRS.pdf

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

## $J_{\text{tol}}$ in SRS.tex

...

Label & Stress distribution factor (Function) based on  
Pbtol

\\ \midrule \\

Symbol &  $J_{\text{tol}}$

\\ \midrule \\

Units & Unitless

\\ \midrule \\

Equation & 
$$J_{\text{tol}} = \ln \left( \ln \left( \frac{1}{1 - P_{\text{btol}}} \right) \frac{\left( \frac{a}{1000} - \frac{b}{1000} \right)^m - 1}{k \left( E \cdot 1000 \left( \frac{h}{1000} \right)^2 \right)^m \text{LDF}} \right)$$

\\ \midrule \\

Description & ...

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

```
...
<th>Equation</th>
<td>
\[{J_{\text{tol}}}=\ln\left(\ln\left(\frac{1}{1-{P_{\text{tol}}}}\right) \frac{\left(\frac{a}{1000} \frac{b}{1000}\right)^{m-1}}{k \left(E\cdot 1000 \left(\frac{h}{1000}\right)^2\right)^m \text{LDF}}\right)\]
```



## $J_{tol}$ in Python

```
## \brief Calculates stress distribution factor (Function)
      based on Pbtol
# \param inParams structure holding the input values
# \return stress distribution factor (Function) based on
      Pbtol
def func_J_tol(inParams):
    outfile = open("log.txt", "a")
    print("function func_J_tol called with inputs: {",
          file=outfile)
    print("  inParams = ", end="", file=outfile)
    print("Instance of InputParameters object", file=
          outfile)
    print("  }", file=outfile)
    outfile.close()

    return math.log(math.log(1.0 / (1.0 - inParams.P_bt看ol)
        ) * ((inParams.a / 1000.0 * (inParams.b / 1000.0))
            ** (7.0 - 1.0) / (2.86e-53 * (7.17e10 * 1000.0 *
                (inParams.h / 1000.0) ** 2.0) ** 7.0 * inParams.
                LDF))))
```

## $J_{tol}$ in Java

```
/** \brief Calculates stress distribution factor (
    Function) based on Pbtol
    \param inParams structure holding the input values
    \return stress distribution factor (Function)
        based on Pbtol
*/
public static double func_J_tol(InputParameters
    inParams) throws IOException {
    PrintWriter outfile;
    outfile = new PrintWriter(new FileWriter(new File(
        "log.txt"), true));
    ...
    return Math.log(Math.log(1.0 / (1.0 - inParams.
        P_btoll)) * (Math.pow(inParams.a / 1000.0 * (
        inParams.b / 1000.0), 7.0 - 1.0) / (2.86e-53 *
        Math.pow(7.17e10 * 1000.0 * Math.pow(inParams
        .h / 1000.0, 2.0), 7.0) * inParams.LDF)));
}
```

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

```
tolStrDisFacEq :: Expr
tolStrDisFacEq = ln (ln (recip_ (exactDbl 1 $- sy pbTol))
  'mulRe' (((sy plateLen $/ exactDbl 1000) 'mulRe' (sy
    plateWidth $/ exactDbl 1000))) $^ (sy sflawParamM $-
    exactDbl 1) $/
  (sy sflawParamK 'mulRe' ((sy modElas 'mulRe' exactDbl
    1000 'mulRe'
    square (sy minThick $/ exactDbl 1000))) $^ sy
    sflawParamM) 'mulRe' sy lDurFac)))
```

## $J_{tol}$ without Unit Conversion

```
tolStrDisFacEq :: Expr
tolStrDisFacEq = ln (ln (recip_ (exactDbl 1 $- sy pbTol))
  'mulRe' ((sy plateLen 'mulRe' sy plateWidth) $^ (sy
    sflawParamM $- exactDbl 1) $/
    (sy sflawParamK 'mulRe' ((sy modElas 'mulRe'
      square (sy minThick)) $^ sy sflawParamM) 'mulRe' sy
      lDurFac)))
```

## Drasil Inputs:

- Program Name: GlassBR
- Authors: Nikitha K and Spencer S
- Symbols: tolerable load ( $\hat{q}_{tol}$ ), Risk of failure ( $B$ ), ...
- Assumptions: Load duration factor constant,
- Data definitions: relation for  $B$ , ...
- Design decisions:
  - Modularity (input module),
  - Implementation Type (Program),
  - Logging (Yes),
  - Input Structure (Bundled),
  - Constant Structure (Inlined),
  - Constant Rep (Constants),
  - Real Number Rep (Double),
  - ...

Drasil Source for software to predict whether a plate of glass will break

- Program Name: GlassBR
- Authors: Nikitha K and Spencer S
- Symbols: tolerable load ( $q_{tol}$ ), Risk of failure ( $B$ ), ...
- Assumptions: Load distrib. fact. constant,
- Data definitions: relation for  $B$ ,
- Design decisions:
  - Modularity (input module),
  - Implementing Type (Program),
  - Logging (Yes),
  - Input Structure (Bundled),
  - Constant Structure (minors),
  - Constant Rep (Constants),
  - Real Number Rep (Double) ...

Generate

```

/glassbr
/Website/GlassBR_SRS.html
/Website/GlassBR_SRS.css
/SRS/bibfile.bib
/SRS/Makefile
/SRS/GlassBR_SRS.tex
/SRS/GlassBR_SRS.pdf
/src/python
/src/python/README.md
/src/python/InputParameters.py
/src/python/Calculations.py
/src/python/Makefile
/src/python/doxConfig

...

/src/java/GlassBR/Calculations.java
/src/java/Makefile
/src/java/README.md

...

/src/cpp/GlassBR
/src/cpp/ReadTable.cpp
/src/cpp/InputFormat.hpp
/src/cpp/Calculations.cpp

...

/src/swift/Calculations.swift

...

/src/csharp/Control.cs
    
```

Software Requirements Specification for GlassBR  
Nikitha K and Spencer S

## Table of Symbols

$q_{tol}$   
 $B$

## Introduction

... The software, herein called GlassBR, ...

## Assumptions

Load Constant: LDF is constant, depends on assumed value of  $q_d$  and  $m$ , ...

## Data Definitions

$$B = \frac{k}{(ab)^{m-1}} (Eh^2)^m LDF e^J$$

$$B = \frac{k}{(ab)^{m-1}} (Eh^2)^m LDF e^J$$

## GlassBR

Authors Nikitha K and Spencer S

**How to Run the Program:** In your terminal command line, enter the same directory as this README file. Then enter the following line  
make run RUNARGS=input.txt  
**Configuration Files:** SDF.txt, TSD.txt must be in the same directory as the executable to run successfully  
Versioning: Python Version 3.5.1

```

...

build:
python Control.py
...
    
```

```

build: GlassBR/Control.class
...
GlassBR/Control.class:
GlassBR/Control.java ...
javac GlassBR/Control.java

run: build
java GlassBR.Control $(RUNARGS)
    
```

```

## #file Calculations.py
# \author Nikitha Krithnan and W. Spencer Smith
# \brief Provides functions for calculating the
...
## \brief Calculates risk of failure
# \param inParams structure holding the input v...
# \param J stress distribution factor (Function)
# \return Risk of failure
def func_B(inParams,J):
    outfile = open("log.txt","a")
    print("function func_B called with inputs: ")
    ...
    outfile.close()

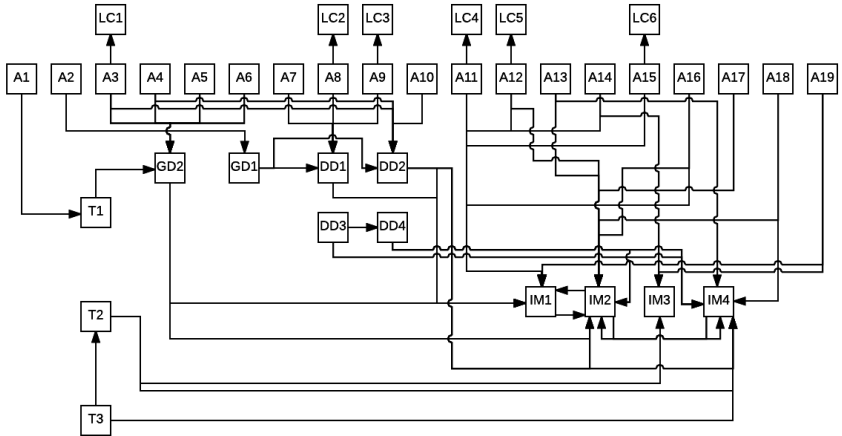
    return 2.86e-53 / ((inParams.a * inParams.b)
inParams.h ** 2.0) ** 7.0 * inParams.LDF * math
    
```

```

package GlassBR;
/** #file Calculations.java
 * \author Nikitha Krithnan and W. Spencer Smith
 * \brief Provides functions for calculating the outputs
 */
public static double func_B(InputParameters inParams, double J) throws IOException {
    PrintWriter outfile;
    outfile = new PrintWriter(new FileWriter(new File("log.txt"), true));
    outfile.println("function func_B called with inputs: {}");
    ...
    outfile.close();

    return 2.86e-53 / (Math.pow(inParams.a * inParams.b, 7.0 - 1.0) *
Math.pow(7.17e10 * Math.pow(inParams.h, 2.0), 7.0) * inParams.LDF
* Math.exp(J));
}
    
```

# 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%
$\rho_P$	$\rho_P > 0$	1007 kg/m <sup>3</sup>	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

---

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 $\rho$ , where $\mathbf{q}$ is the thermal flux vector, $q'''$ is the volumetric heat generation, $T$ is the temperature, $\nabla$ 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]

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

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

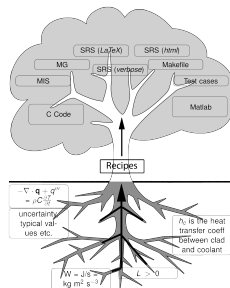
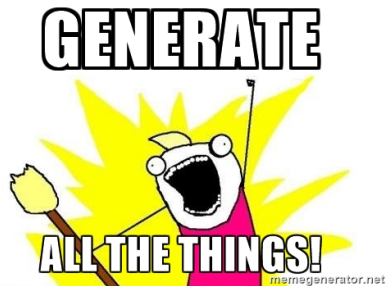
- Uncovered 27 issues with the previous documentation
  - ▶ Incompleteness ( $R_{\text{gap}}$ )
  - ▶ Inconsistency( $r, r_0, h_g$ )
  - ▶ Verifiability problems ( $R_1$ )
  - ▶ Lack of traceability (circuit analogy)
- Advantages of proposed approach
  - ▶ Abstract to concrete
  - ▶ Separation of concerns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

**NO**



# 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 \(at the bottom of the page\)](#)



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

# References II



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.



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.

## References III



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.



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.

# References IV



Patrick J. Roache.

*Verification and Validation in Computational Science and Engineering.*

Hermosa Publishers, Albuquerque, New Mexico, 1998.



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).* In conjunction with SC16: The International Conference for High Performance Computing, Networking, Storage and Analysis, November 2016.

8 pp.

# References V



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.



W. Spencer Smith, Mojdeh Sayari Nejad, and Alan Wassying.

Assurance cases for scientific computing software (poster).

In *ICSE 2018 Proceedings of the 40th International Conference on Software Engineering*, May 2018.

2 pp.



W. Spencer Smith, Mojdeh Sayari Nejad, and Alan Wassying.

Raising the bar: Assurance cases for scientific computing software.

*Computing in Science and Engineering*, 23(1):47–57, February 2020.

# References VI



Muhammad Usman, Muhammad Zohaib Iqbal, and Muhammad Uzair Khan.

A product-line model-driven engineering approach for generating feature-based mobile applications.

*Journal of Systems and Software*, 123:1–32, 01 2017.



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.