Progress Report on Drasil: A Framework for Scientific Knowledge Capture and Artifact Generation

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ABSTRACT

abstract here

CCS CONCEPTS

• **Mathematics of computing** → *Mathematical software*; • **Software and its engineering** → *Software development techniques*; *Automatic programming*;

KEYWORDS

scientific computing, software quality, software engineering, document driven design, code generation

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1 INTRODUCTION

Every developer should strive towards creating the highest possible quality software. As scientists, we should be leading the community in this regard as it is our duty to ensure the reusability, reproducibility, and replicability of our work.

Our team is focused on improving the quality of Scientific Computing Software (SCS). We have chosen large, multi-year, multi-developer projects where the end users do much of the development as our target scope. For these projects, we pay particular attention to improving the qualities of reusability, reproducibility, and certifiability. Improving these software qualities is especially important where correctness can have an impact on safety, for example: nuclear safety analysis or medical imaging.

Often considered too high a cost in terms of time and effort for SCS developers, particularly when dealing with rapid changes in development, improved documentation is an important aspect of improving overall software quality. Carver [1] observed that scientists do not view rigid, process-heavy approaches, favourably. SCS developers tend to dislike producing documentation and often consider reports for each stage of software development as counterproductive [4, p. 373].

Well-maintained documentation provides numerous advantages including:

- Improved software qualities
  - Verifiability
  - Reusability
  - Reproducibility
  - etc.
- From Parnas [3]:
  - Easier reuse of old designs
  - Better communication about requirements
  - More useful design reviews
  - etc.

Previous work by Smith & Koothoor [6] found 27 errors in an existing software project when creating new documentation. Developers have become aware of these advantages of documentation [5].

However, documenting software is typically felt to be:

- Too long
- Too difficult to maintain
- Not amenable to change
- Too tied to the waterfall process
- Counterproductive when reporting on each stage of development [4]

The Solution?

Drasil – a framework, utilizing a knowledge-based approach to software development, proposed in a position paper [7]. The goal of the approach is to capture scientific and documentation knowledge in a reusable way, then generate the source code and other software artifacts (documentation, build files, tests, etc).

Work on Drasil has continued steadily since the position paper, as described below. We begin with a brief overview of the design of the Drasil framework in Section 2, then describe its development process to date in Section 3. Following that, we show an example of Drasil in action (Section 4) and the results we've seen to date (Section 5). Finally, we lay out some of the work that still needs to be done (Section 6) before concluding.

2 DESIGN OF DRASIL

- an overview, with an emphasis on the notion of chunks would be good - should mention which DSLs are part of DSL - maybe the ontology figure? - should mention GOOL

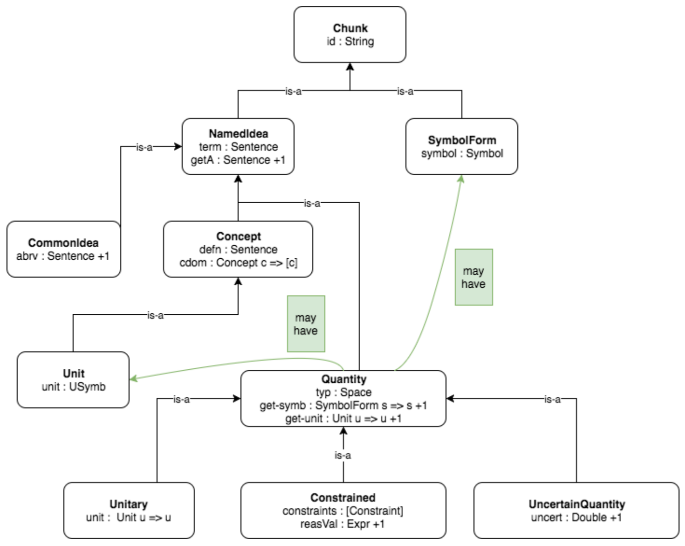

Figure 1: Relationships Between Drasil Classes

3 DEVELOPMENT PROCESS FOR DRASIL

Drasil is being developed using a practical, example-driven process. There are currently five different examples being developed concurrently within (and driving the development of) Drasil:

- Chipmunk2D Game Engine
- Solar Water Heating System Incorporating Phase Change Material (PCM)
- Solar Water Heating System (No PCM)
- Slope Stability Analysis
- Glass Breakage Analysis

These examples overlap with those found in [5].

Our practical design approach allows us the flexibility to prototype without over-designing. As a new feature becomes necessary to continue the implementation of a given example, only then do we design, test, implement, and re-test it. We occasionally implement features we may need in the future, but only in those instances when it is obvious that we are taking the right approach.

The current incarnation of the Drasil framework can be found on GitHub at https://github.com/JacquesCarette/literate-scientific-software. We utilize peer-review of code throughout development to correct missteps early on, and keep an up-to-date issue tracker for any bugs, feature requests, or other "to-do" tasks.

- refactoring - finding patterns - knowledge extraction - reduction of duplication

4 GLASSBR EXAMPLE

- introduce example from Civil Engineering - say what the inputs are to GlassBR and what it calculates - bottom up approach to presentation - start with chunks, build up to SRS, traceability

- start with data definition for Jtol generated by Drasil

Refname	**DD:sdf.tol**
Label	J_{tol}
Units	
Equation	$J_{tol} = \log\left(\log\left(\frac{1}{1-P_{btol}}\right)\frac{\left(\frac{a}{1000}\frac{b}{1000}\right)^{m-1}}{k\left(\left(E*1000\right)\left(\frac{h}{1000}\right)^2\right)^m*LDF}\right)$
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) b is the plate width (short dimension) m is the surface flaw parameter k is the surface flaw parameter E is the modulus of elasticity of glass h is the actual thickness LDF is the load duration factor

Figure 2: J_{tol} from GlassBR Requirements

- figure comes from tex generated by Drasil. Can also generate html. This figure is part of the documentation of the requirements. Eventually need code to calculate Jtol. Can generate code like in the next figure. [this needs to be fit into one column —SS]

```
def calc_j_tol(inparams):
    j_tol = math.log((math.log(1.0/(1.0 - inparams.pbt
* ((((inparams.a / 1000.0) * (inparams.b / 1000.0)) **
    return j_tol
```

Figure 3: Python code to Calculate J_{tol}

- can also generate Java, Lua, etc.

- next show the source file in Drasil. [need to fit in one column —SS]

Now notice a mistake in code - shouldn't divide by 1000 - redo - fixes the mistake everywhere

All of the knowledge on GlassBR can be put together to generate the software requirements specification. Can point to a figure showing the table of contents for the SRS. Explain that it can be generated in tex (pdf) or html.

Part of SRS is automatically generated traceability information between definitions, assumptions, theories and instanced models.

5 QUALITY IMPROVEMENTS

5.1 Certifiability

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

```
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
```

Figure 4: Drasil (Haskell) code for $J_{\mathbf{tol}}$ Knowledge

```
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))))
```

Figure 5: Modified Drasil (Haskell) code for $J_{\mathbf{tol}}$

Table 1: Constraints on quantities Used To Verify Inputs

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

- *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

5.2 Reusability

- De-embed knowledge
- Reuse throughout document
  - Units
  - Symbols
  - Descriptions
  - Traceability information
- Reuse between documents
  - SRS

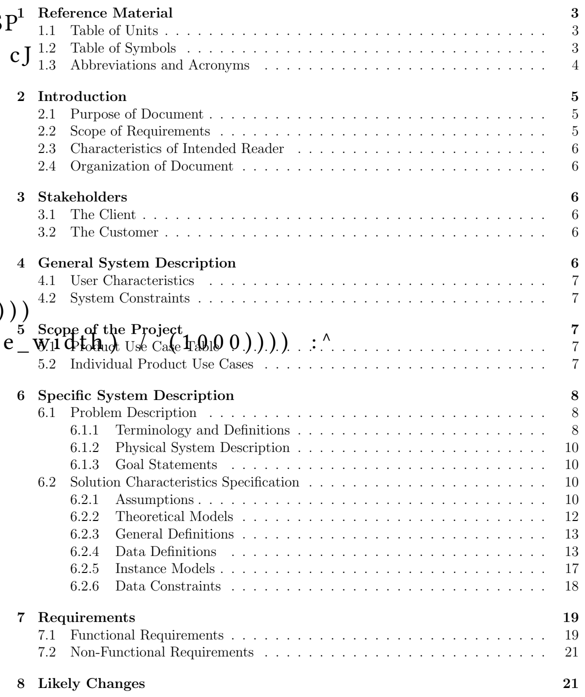

Figure 6: Table of Contents for Generated SRS for GlassBR

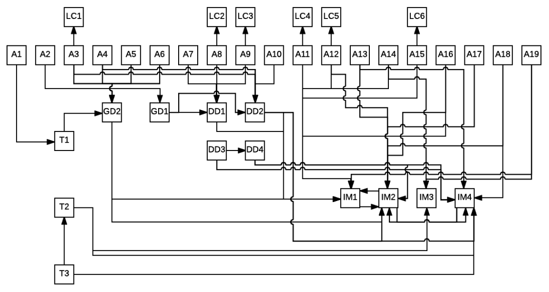

Figure 7: Traceability Graph

  - MIS
  - Code
  - Test cases
- Reuse between projects
  - Knowledge reuse
  - A family of related models, or reuse of pieces
  - Conservation of thermal energy
  - Interpolation
  - Etc.

5.3 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

6 FUTURE WORK

7 CONCLUDING REMARKS

8 ACKNOWLEDGEMENTS

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REFERENCES

[1] Jeffrey C. Carver, Richard P. Kendall, Susan E. Squires, and Douglass E. Post. 2007. 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*. IEEE Computer Society, Washington, DC, USA, 550–559. https://doi.org/10.1109/ICSE.2007.77

[2] Cezar Ionescu and Patrik Jansson. 2012. 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 (Lecture Notes in Computer Science)*, Vol. 8241. Springer International Publishing, 140–156. https://doi.org/10.1007/978-3-642-41582-1_9

[3] David Lorge Parnas. 2010. Precise Documentation: The Key to Better Software. In *The Future of Software Engineering*. 125–148. https://doi.org/10.1007/978-3-642-15187-3_8

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

[5] W. Spencer Smith, Thulasi Jegatheesan, and Diane F. Kelly. 2016. 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)*. 8 pp.

[6] W. Spencer Smith and Nirmitha Koothoor. 2016. A Document-Driven Method for Certifying Scientific Computing Software for Use in Nuclear Safety Analysis. *Nuclear Engineering and Technology* 48, 2 (April 2016), 404–418. https://doi.org/10.1016/j.net.2015.11.008

[7] Daniel Szymczak, W. Spencer Smith, and Jacques Carette. 2016. Position Paper: A Knowledge-Based Approach to Scientific Software Development. In *Proceedings of SE4Science'16 in conjunction with the International Conference on Software Engineering (ICSE)*. In conjunction with ICSE 2016, Austin, Texas, United States. 4 pp.