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 [5, 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 [7] found 27 errors in an existing software project when creating new documentation. Developers have become aware of these advantages of documentation [6].

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 [5]

The Solution?

Drasil – a framework, utilizing a knowledge-based approach to software development, proposed in a position paper [8]. 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).

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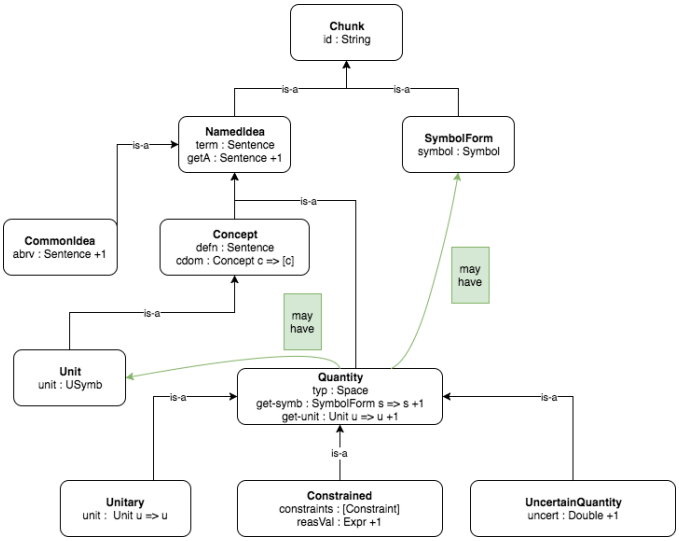

Figure 1: Drasil chunk hierarchy

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 have 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

Drasil's design is based around three main components:

(1) Knowledge capture mechanisms (*Chunks*)
(2) Artifact generation language(s) (*Recipes*)
(3) Knowledge-base (*Data.Drasil*)

Chunks are the primary knowledge-capture mechanism. There are many flavours of chunk (as shown in Figure 1). The most basic chunk is simply a piece of data with an id. From there, all other chunks can be created. For example, a *Quantity* is a *NamedIdea* (a chunk containing an id, as well as a term which represents the idea and a potential abbreviation for that term) which also has a *Space* (integer, boolean, vector, etc.), and symbol representation/units (if applicable).

We can think of chunks as our building blocks of knowledge; they are the ingredients to be used in our *Recipes*. Our language of recipes is a Domain-Specific Language (DSL) embedded in Haskell which is used to define what we would like to generate, and in what order. A small snippet of recipe language code for our Software Requirements Specification (SRS) can be seen in Figure 2. This code is used to generate the *Reference Materials* section of our SRS, which contains an introduction followed by the table of units, table of symbols, and table of abbreviations and acronyms subsections.

The document generation language is highly abstracted, but allows for a fairly high degree of customization. Drasil also contains a code-generation language integrating GOOL [**?**] – a Generic Object-Oriented Language – which can generate code in a number

```
mkSRS :: DocDesc
mkSRS = [RefSec (RefProg intro
        [TUnits,
        tsymb [TSPurpose, SymbOrder],
        TAandA])]
        ...
```

Figure 2: The reference material section for an SRS written in Drasil's Document Language

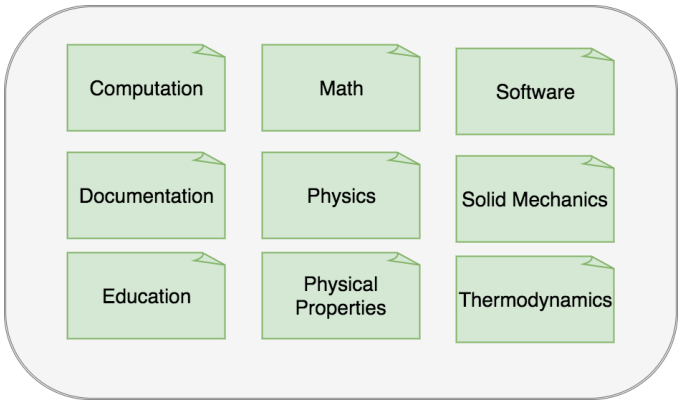

Figure 3: Data.Drasil knowledge domains

of different target languages including Python, Lua, and C++. We will discuss code generation in more depth later on.

Finally, there is the knowledge-base for Drasil (located in Data.Drasil). We are creating a database of reusable scientific knowledge that can be applied across a number of different applications across multiple domains. As the Drasil framework grows, we hope to continue to expand this database into an ontology of scientific information for a number of disciplines. See Figure 3 for an example of some of the domains in which we have started to capture knowledge.

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 [6].

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.

Refname	DD:sdf.tol
Label	J_{tol}
Units	
Equation	$J_{tol} = \log\left(\log\left(\frac{1}{1-P_{btol}}\right)\frac{\left(\frac{a}{1000}\frac{b}{1000}\right)^{m-1}}{k\left((E*1000)\left(\frac{h}{1000}\right)^2\right)^m * LDF}\right)$
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 4: J_{tol} from GlassBR Requirements

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.

Progressive development of Drasil is achieved by not only looking for new features that must be implemented, but also through a cyclic approach towards improvement. This approach relies on finding new (extractable) patterns in the framework through refactoring, de-embedding and extracting knowledge from the example materials, and reducing knowledge duplication by capturing it in a highly reusable way.

4 A PRACTICAL EXAMPLE (GLASSBR)

GlassBR is a piece of software used in Civil Engineering to predict whether or not a slab of glass will be able to withstand a given blast without breaking. It has two classes of input: glass geometry and blast type. Each of these input classes has a number of fields (glass type, dimensions, TNT equivalent factor, standoff distance, etc.) used as input to the simulation. Also, a tolerable probability of breakage is given by the user.

The output of GlassBR is whether or not the glass slab is considered safe. This is based on a probability that is calculated through interpolation being compared to the tolerable probability.

To understand the Drasil implementation, we will follow one specific piece of knowledge through from requirements to code. We intend to show how this knowledge is captured and used in Drasil to produce our software artifacts (documentation and code).

Let us start by taking a look at a data definition for the tolerable stress distribution factor (J_{tol}) from GlassBR. Figure 4 shows the Drasil-generated TeX version of the data definition for J_{tol}, however we can also generate the documents in HTML. This figure is part of the requirements for the GlassBR software, and as such, we will eventually need code (like that in Figure 5) that can be used to calculate J_{tol}. We can generate this code as well! Not only that, but thanks to the incorporation of GOOL we can also generate Java, Lua, etc.

The source knowledge for generating both the documentation and the code has been captured using chunks as shown in Figure 6.

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%

The value of J_{tol} is calculated from the expression tolStrDisFac_eq , which is part of the tolStrDisFac chunk.

Notice there is actually an error in the code and documentation. We should not be dividing by 1000 in a number of places. Luckily, with one quick change to tolStrDisFac_eq (shown in Figure 7), we have corrected the error in our knowledge-base. Thus, after re-running the generator, our code and documentation has now been fixed and remains consistent.

We have similarly captured all of the knowledge pertaining to GlassBR in chunks. This knowledge can be assembled and extracted in different ways to produce a multitude of views, i.e. our artifacts, including the SRS. For a sense of what we can generate from this knowledge, see the table of contents for the currently generated GlassBR SRS (Figure 8). Again, our documents can be generated in TeX and/or HTML for more flexibility. Both contain automated internal references.

Another thing to note in our SRS is that the traceability information between definitions, assumptions, theories, and instance models is automatically generated, including the traceability graph shown in Figure 9.

5 QUALITY IMPROVEMENTS

Throughout Drasil's development lifecycle, we have already noticed a number of non-trivial quality improvements to the software examples being re-developed. These improvements come in a wide range of areas, but for the sake of brevity we will focus on certifiability, reusability, and reproducibility.

5.1 Certifiability

Certifying (or re-certifying) software can be a lengthy and expensive process where a single error can cause the software to fail the certification process. Consider the following equation from our solar water heating example which states that energy must be conserved:

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

This is trivial for a human to check, and writing code to check it during the software execution is also very simple. However, it is still time-consuming and should it ever need to change, it would require developers to make a number of modifications to many artifacts in the future.

Thanks to Drasil's knowledge-capture mechanisms, we can capture the above equation in one place, thus any changes can be made very quickly. Not only that, but sanity checks (such as ensuring constraints on inputs) can also be captured and reused (see Table 1). Capturing that information also delivers a wider array of advantages, including:

```
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
```

Figure 5: Python code to Calculate $J_{\mathbf{tol}}$

```
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 ((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 6: Drasil (Haskell) code for $J_{\mathbf{tol}}$ Knowledge

```
tolStrDisFac_eq :: Expr
tolStrDisFac_eq = 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))))) :^
  (C sflawParamM) * (C loadDF))))
```

Figure 7: Modified Drasil (Haskell) code for $J_{\mathbf{tol}}$

- Generate guards against invalid input automatically
- Generate certain test cases automatically
- Generate views suitable for inspection

We can also see that it is extremely easy to trace changes and verify that they are correct, thanks to our one-source, generative approach.

We have also touched on one of the greatest advantages which was implied earlier: *If there is an error somewhere, it is wrong everywhere.* This may seem like a disadvantage, but ensuring every artifact contains the same errors means there is a much greater chance of those errors being spotted. In our experience, many examples of software include code that does not match the design (due to hacks, last-minute changes, etc.), and an error which could hamper certification efforts can fly under the radar.

For (re-)certification purposes, we want to be able to find any and all errors, trace them to their source, and fix them quickly. Drasil has shown great promise in that respect.

5.2 Reusability

Reusability is a core tenet of ours for Drasil's development. This can be seen most obviously in the knowledge-capture mechanisms we have created.

Consider the following software artifacts typically found in a rational, design process for software development [4]:

- Software Requirements Specification (SRS)
- Module Interface Guide (MIS)
- Source Code
- Test cases

Within these artifacts, there is a lot of duplication of specific knowledge related to the software being designed. Knowledge from the SRS will appear, possibly transformed, throughout each of the other artifacts. We seek to de-embed specific knowledge from within any specific artifact to easily reuse it throughout them all. This knowledge includes, but is not limited to:

- Scientific Knowledge
- Models
- Units
- Symbols
- Descriptions
- Traceability information

Reusing knowledge across artifacts in one software project is already incredibly useful, however, we have taken it a step further. Drasil allows us to reuse between projects. We can reuse a family of related models, or reuse pieces of knowledge from a given domain as necessary. Consider the vast number of software that rely on interpolation, or must ensure conservation of thermal energy. We can capture this knowledge once and reuse it through all of these projects.

1 Reference Material 3
1.1 Table of Units 3
1.2 Table of Symbols 3
1.3 Abbreviations and Acronyms 4

2 Introduction 5
2.1 Purpose of Document 5
2.2 Scope of Requirements 5
2.3 Characteristics of Intended Reader 6
2.4 Organization of Document 6

3 Stakeholders 6
3.1 The Client 6
3.2 The Customer 6

4 General System Description 6
4.1 User Characteristics 7
4.2 System Constraints 7

5 Scope of the Project 7
5.1 Product Use Case Table 7
5.2 Individual Product Use Cases 7

6 Specific System Description 8
6.1 Problem Description 8
6.1.1 Terminology and Definitions 8
6.1.2 Physical System Description 10
6.1.3 Goal Statements 10
6.2 Solution Characteristics Specification 10
6.2.1 Assumptions 10
6.2.2 Theoretical Models 12
6.2.3 General Definitions 13
6.2.4 Data Definitions 13
6.2.5 Instance Models 17
6.2.6 Data Constraints 18

7 Requirements 19
7.1 Functional Requirements 19
7.2 Non-Functional Requirements 21

8 Likely Changes 21

Figure 8: Table of Contents for Generated SRS for GlassBR

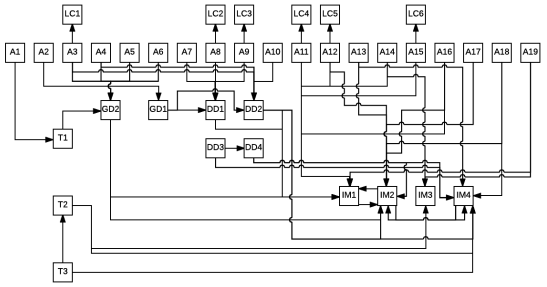

Figure 9: Traceability Graph

We have already begun using knowledge across projects with great results. Our two implementations of the solar water heating systems have a vast amount of overlap in the requisite knowledge, except for the phase change material, which is not present in one of the examples.

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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