# McMaster University
# Department of Computing and Software

# Proposal for Thesis Research in Partial Fulfillment of the Requirements for the Degree of Doctor of Philosophy

Title: Literate Software and the Drasil Framework

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**Abstract**

The current state of Scientific Computing software development leaves room for improvement. There is a need for improved software quality, more consistent use of software engineering practices, and reduced information duplication. As it stands, information duplication creates a number of problems. Traceability is hard to achieve as finding the source of a piece of information is difficult among the possibilities. Over time this impacts the maintainability of a piece of software, as developers may not be able to track down the source of a problem. Also, with many duplicated information sources, it makes creating documentation more tedious, reducing a developer's desire to produce and maintain high-quality documentation. I want to facilitate the improvement of qualities (maintainability, traceability, reproducibility, etc.) across all artifacts of a piece of software. I believe a knowledge-based approach, which borrows ideas from literate programming, and involves a larger short-term investment from developers is the first step to improving software as a whole. I am creating a framework (Drasil) to facilitate this approach, focusing on avoiding knowledge duplication, while improving traceability and automating as much of the development process as possible. I believe with the proper tools for automation we can ensure good software engineering practices are followed (regardless of the developer's background) and improve the overall quality of software.

# Contents

# 1 Introduction

Scientists and engineers rely heavily on models that share common mathematical/scientific knowledge. These are shared, in textbook form, across many projects. However, when it comes to implementing software, this information is then duplicated for each project, as well as being duplicated within the project (in requirements, design documents, code and tests, for example). It should be possible to capture this knowledge once, and then re-use it, first within the same project but in different views (documents/contexts), then across many projects. I want to create a system that deals with this issue of information duplication, especially for the knowledge contained in scientific models.

As it stands, information duplication can have a direct impact on qualities such as maintainability, traceability, verifiability, and reproducibility. Consider a project containing (at least) these four software artifacts: Software Requirements Specification (SRS), design document, source code, and a testing document. As the project evolves, some of the knowledge contained within it will inevitably change due to changing requirements, new design decisions, technical or resource limitations, etc. Updating the software artifacts to reflect these changes is tedious; a developer must trace their way through each of the artifacts to ensure new information has been added (new requirements and/or design decisions), the change does not cause conflicts, and any assumptions made or test cases to be used are still applicable (or are appropriately removed/updated).

Now consider a software project with more artifacts: each change to the knowledge becomes even more tedious to propagate. It is not uncommon for developers to lack the resources or motivation to update each artifact to accommodate every minor change.

As artifacts in a software project begin to fall out of sync with each other, the qualities of the project as a whole suffer. Consider traceability: if the artifacts in a software project are inconsistent with each other, how can one accurately analyze a change or validate a requirement? On a similar note, how easy is it to maintain a system if one cannot track where a problem came from?

I think the first step to improving software as a whole is to improve each of the software artifacts. To that end, I would like to expand the ideas of literate programming (which I will discuss more in-depth in Section 2.2). Specifically, I want to keep the idea of *chunks* and expand its application to not only code snippets, but the fundamental knowledge underlying a piece of software. I believe capturing this knowledge will be paramount to creating a new, so-called "knowledge-based" approach to software development.

As improving all software is too broad of a target, I will be focusing on well-understood domains. I believe this is a necessary restriction because a knowledge-based approach will require a thoroughly well-understood background to facilitate the requisite knowledge capture. To that end, I will focus specifically on the domain of Scientific Computing (SC). SC has a very rich, well-understood background, which has already been documented in incredible detail. Also, in many cases, SC developers are scientists first and lack a strong software engineering background. It is my hope that my approach will be well-suited to SC

developers as it will allow them to focus on the science.

I am not creating any individual new ideas. Instead, I want to combine ideas that have existed for some time and use them in a novel way. That is where the idea of a knowledge-based approach to literate software comes from. Not only do I want to create better software using a process similar to literate programming, but I want to ensure that process will cover all necessary software artifacts.

To that end, I believe a tool will be necessary to facilitate my approach. A framework known as "Drasil" is currently in development and will be explained in Section 4.

# 2 State of the Art

To pursue this line of research, first one needs to understand the history of research in several closely-related areas. Since I will be focusing on the improvement of SC software, the obvious starting point would be to look at the current state of SC software development and its challenges. Also, as I am intending to expand the ideas of literate programming, it is necessary to delve into sufficient depth on LP and why it has not been widely adapted as yet, as well as any attempts to expand or build upon it. Finally, with the idea of long-term maintainability, full traceability, and reproducibility in mind, I would be remiss if I did not look into the field of reproducible research.

## 2.1 Current State of SC Software Development

In many instances of SC software development, the developers are the scientists. These developers tend to put the most emphasis on their science instead of good software development practices [13]. Rigid, process-heavy approaches are typically considered unfavourable to these developers [4]. We see the developers choose to use an agile philosophy [1, 4, 6, 28], an amethododical [11], or a knowledge acquisition driven process [12] instead.

There are several clear problems with the current state of SC software development. The first, fairly obvious problem is that knowledge reuse is not being utilized to the fullest extent possible. As an example, a survey [21] showed that of 81 different mesh generator packages, 52 generated triangular meshes. Now that in itself may not show a lack of knowledge reuse, however, looking deeper we see that 37 of those packages used the same Delaunay triangulation algorithm for generating those meshes. There is no reason that the exact same algorithm should be implemented 37 separate times when it could simply be reused.

Another problem in SC software development is the lack of understanding of software testing. More than half the scientists developing SC software lack a good understanding of software testing [18]. It is in such a bad state that quality assurance has "a bad name among creative scientists and engineers" [26, p. 352], not to mention the very limited use of automated testing [22].

It should be obvious that some of these issues could be solved through the use of certain tools. However, it should be noted that tool use by SC software developers is also very limited, especially the use of version control software [36].

Not everything about SC software development today is a negative. For example advanced techniques like code generation have been quite successful in SC. Some generation examples that come to mind are FEniCS [17], FFT [14], Gaussian Elimination [3], and Spiral. The focus of generation techniques, thus far, have been solely on one software artifact: the source code. Focusing solely on code is a disadvantage to SC software developers as the value of documentation, as well as a structured (or rational) process, have been repeatedly illustrated [31, 32, 33, 34].

## 2.2 Literate Programming

The LP methodology introduced by Knuth changes the focus from writing programs that simply instruct the computer on how to perform a task to explaining (*to humans*) what we want the computer to do [15].

Developing literate programs involves breaking algorithms down into *chunks* [10] or *sections* [15] which are small and easily understandable. The chunks are ordered to promote understanding, a "psychological order" [24] if you will. They do not have to be written in the same order that a computer would read them. It should also be noted that in a literate program, the code and documentation are kept together in one source. To extract working source code, a process known as *tangle* must be run on the source. A similar process known as *weave* is used to extract and typeset the documentation from the source.

There are many advantages to LP beyond understandability. As a program is developed and updated, the documentation surrounding the source code tends to be updated simultaneously. It has been experimentally found that using LP ends up with more consistent documentation and code [29]. Having consistent documentation has its own advantages while developing or maintaining software [9, 16]. Similarly, there are many downsides to inconsistent documentation [16, 35]. Keeping both of those in mind we can see that more effective, maintainable code can be produced when (properly) using LP [24].

Even with all of the benefits of LP, it has not been very popular [29]. Though it has not been popular, there are still several successful examples of LP's use in SC; two that come to mind are VNODE-LP [20] and "Physically Based Rendering: From Theory to Implementation" [23]. The latter being a literate program as well as a textbook. Shum and Cook discuss the topic of LP's lack of popularity and present the idea that it comes from a couple of main issues: dependency on a particular output language or text processor, the lack of flexibility on what should be presented/suppressed in the output.

Many attempts to address the issues with LP's popularity have focused on changing or removing the output language or text processor dependency. Many new tools were developed such as: CWeb (for the C language), javadoc (for Java), DOC++ (for C++), Doxygen (for multiple languages), noweb (programming language independent), and more. The development of new tools led the

introduction of many new features including, but not limited to, a "What You See Is What You Get" (WYSIWYG) editor [7], phantom abstracting [29], and even movement away from the "one source" idea [30].

While these tools did not bring LP into the mainstream [25], they did help drive the understanding behind what exactly LP tools must do. Although LP is not yet mainstream, we can see it becoming more standardized in certain domains (for example: Agda, Haskell, and R support LP).

## 2.3 Literate Software

A combination of LP and Box Structure [19] was proposed as a new methodology called "Literate Software Development" (LSD) [2]. Box structure can be summarized as the idea of different views (ex. system specifications, design, code) which are abstractions that communicate the same information in different levels of detail, for different purposes.

LSD was developed with the intent to overcome the disadvantages of both LP and box structure. It was intended to overcome LP's inability to specify interfaces between modules, the inability to decompose boxes and implement the design created by box structures, as well as the lack of tools to support box structure [5].

The framework developed for LSD, "WebBox", expanded LP and box structures in a variety of ways. It included new chunk types, the ability to refine chunks, the ability to specify interfaces and communication between boxes, and the ability to decompose boxes at any level. However, literate software (and LSD) remain primarily code-focused with very little support for creating other software artifacts.

## 2.4 Reproducible Research

Being able to reproduce results is fundamental to the idea of good science. Reproducible research has been used to mean embedding executable code in research papers to allow readers to reproduce the results described [27].

Combining research reports with relevant code, data, etc. is not necessarily easy, especially when dealing with the publication versions of an author's work. As such, the idea of *compendia* were introduced [8] to provide a means of encapsulating the full scope of the work. Compendia allow readers to see computational details, as well as re-run computations performed by the author. Gentleman and Lang proposed that compendia should be used for peer review and distribution of scientific work [8].

Currently, several tools have been developed for reproducible research including, but not limited to, Sweave, SASweave, Statweave, Scribble, and Org-mode. The most popular of those being Sweave [27]. The aforementioned tools maintain a focus on code and certain computational details. It is my hope that the Drasil framework will one day surpass these tools due to its ability to simplify the creation of all software artifacts.

# 3 Research Objectives and Approach

## 3.1 Objectives

Looking at the current state of SC software development, there are many areas for improvement particularly the need for applying better software engineering practices and improving knowledge reuse. The simplest approach for improving development would be to get better developers, which is not necessarily feasible for SC software. Software engineering education is not typically part of an SC developer's background, and having software engineers develop SC software is problematic because the software engineers typically lack the necessary domain knowledge. Domain experts require tools that simplify the software engineering process so they can do things the "right" way. My first objective, therefore, is to simplify the software development process by allowing scientists to focus on the science.

My second objective is to increase software qualities (maintainability, traceability, reproducibility, verifiability, reusability, etc.) in SC software. The first step toward this improvement is to better understand the fundamental scientific background underlying said software. As such I will be focusing on understanding and capturing that knowledge.

My third objective, a natural progression from the second, is better overall software artifacts (requirements and design documents, source code, etc.). It is a worrying trend that software artifacts tend to fall out of sync with each other over time, so ensuring they remain consistent is a means to improve.

Furthermore, developers should not need to spend large swaths of time updating and maintaining their software. I would like to automate as much of the software development process as possible. Automation will also allow developers to avoid some classical software mistakes such as duplication, previously mentioned in the survey by Owen [21]. It will also ensure reproducibility as, if done right, anyone will be able to automatically create and run the same software easily.

## 3.2 Approach

To meet my objectives I am using a combination of existing ideas, which I have dubbed a *knowledge-based* approach to software development. First off, I want to expand and use ideas from LP. Namely, the brilliant idea of chunks, however, it should be expanded to represent encapsulated knowledge. If the knowledge behind an underlying concept can be properly encapsulated, then it can easily be reused and duplication can be avoided.

Knowledge encapsulation should be done at the specification level instead of the code level. It will include assumptions, derivations, equations, etc. and from there it is a fairly simple and straightforward process to get a code representation. Specifically, the high-level knowledge can be used for the automatic generation of code.

The standard LP style helps to increase consistency in documentation, but

it does not go far enough. It is easy for a developer to update the code and/or documentation, however, there is no way to ensure that when the code is changed the documentation is also updated accordingly. I want to ensure that all artifacts are updated any time there is a change (no matter how trivial) with trivial effort.

This automatic updating is achieved through generation. The idea is to have a standard generator which uses *recipes* for the creation of artifacts. Each recipe essentially defines a different view of our knowledge-base (chunks). Since each recipe represents a different software artifact and pulls appropriate knowledge from reusable chunks, the artifacts will remain consistent and fully traceable; finding the source of a piece of information will be trivial. All artifacts will be updated automatically any time the generator is run, thus ensuring consistency is maintained. Also, giving anyone access to the recipes and chunks used will allow them to reproduce a piece of software.

I am currently taking a practical, example-driven approach to create a framework (called *Drasil*) to exemplify this knowledge-based approach to software development. Thus far, the implementation of Drasil has been guided by some small and fairly specific case studies. However, I plan to continue expanding the framework through the use of larger, more varied case studies. More information regarding Drasil can be found in the next section.

# 4 Current Work and Preliminary Results

## 4.1 The Drasil Framework

Drasil is currently being implemented as a combination of embedded Domain Specific Languages (eDSLs) in Haskell. I have currently implemented six eDSLs as follows:

1. Expression language – A simple expression language that allows us to capture knowledge relating to equations and mathematical operations. It includes operations such as addition, multiplication, derivation, and exponentiation among others.

2. Expression layout language – A micro-scoped language for describing how expressions should appear. Expressions may need to use a variety of inline layout modifiers (subscripts, superscripts, etc.) to be properly displayed.

3. Document layout language – A macro-scoped language for describing how large-scale layout objects (tables, sections, figures, etc.) should appear.

4. C Representation Language – A DSL for representing parts of the C programming language inside the Drasil framework. This allows the generator to produce working C code.

5. LaTeX Representation Language – A DSL for representing LaTeX code inside of Drasil. As with the C representation, it is used by the generator to produce working LaTeX code.

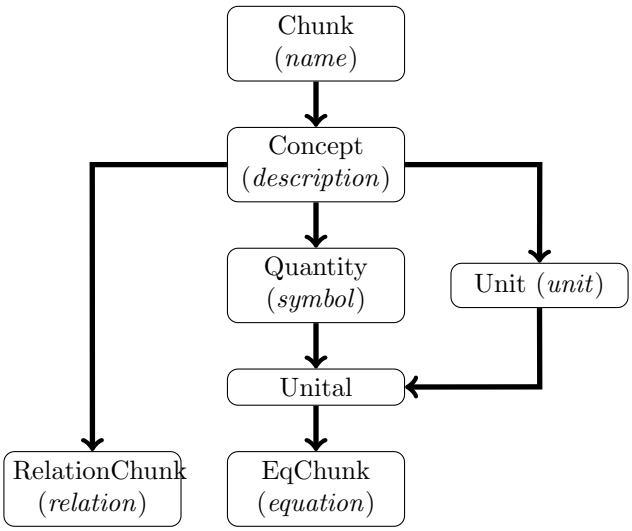


Figure 1: Our current chunk design (parentheses indicate newly added knowledge)

6. HTML Representation Language – A DSL for representing HTML within Drasil. Similar to the other representation languages as it is used by the generator to produce working HTML.

With these eDSLs it is easy to encapsulate knowledge, create recipes, and generate required artifacts.

When it comes to chunks, they come in several varieties. You can see a hierarchy of chunk types in Figure 1.

Each new chunk in the hierarchy adds to the knowledge encapsulated within it. The most basic *Chunk* represents a named piece of information. A *Concept* adds a description to the named information, and so on.

*Unital* chunks are somewhat special as they do not add any new information in and of themselves, they act as a combination of a *Quantity* (concept with a symbolic representation) and a *Unit*. They are quantities with units.

*Equation* chunks continue to expand on *Unital* chunks by allowing us to capture equations for calculating quantities. In a similar vein are *Relation* chunks, which allow us to relate two pieces of knowledge to each other.

Now that knowledge has been encapsulated it is time to do something with it. This is where the recipes, mentioned earlier, come into play. Writing a recipe requires using three of the previously mentioned eDSLs – the expression, expression layout, and document layout languages. I will go into more detail on writing and using recipes in the next section.

Finally, the last piece of the implementation is the generator. The remaining three representation languages are specific to the generator. The generator

| **Number** | **DD2** |
|---|---|
| Label | $h_c$ |
| Units | $ML^0t^{-3}T^{-1}$ |
| SI Units | $\frac{\text{kW}}{\text{m}^2\text{°C}}$ |
| Equation | $h_c = \frac{2k_c h_b}{2k_c + \tau_c h_b}$ |
| Description | $h_c$ is the convective heat transfer coefficient between clad and coolant<br>$k_c$ is the clad conductivity<br>$h_b$ is the initial coolant film conductance<br>$\tau_c$ is the clad thickness |

Figure 2: Data definition for $h_c$ from the fuel pin SRS

interprets the recipes and creates intermediary representations of artifacts using the representation languages, then pretty-prints the results.

## 4.2 Using Drasil

For this section I will touch on two case studies that I have used to motivate the development of Drasil. The first is a simplified version of a Software Requirements Specification (SRS) for a fuel pin in a nuclear reactor [31] and the second is a SRS for a solar water heating tank.

Let's start by looking at a single term from the fuel pin SRS: $h_c$. This term represents the convective heat transfer coefficient between the clad and coolant. We can see the data definition for this term in Figure 2.

From the data definition, we can glean interesting knowledge. First off there is the name of the concept, its description, the symbol representing it, its SI units, and its defining equation. All of this information can be encapsulated into an EqChunk with ease as shown in Figure 3. Note that the units for $h_c$ are defined in a piece of common knowledge known as `heat_transfer`.

The SI Units are a great example of common knowledge. The SI Unit library contains all seven base SI units and several different derived units (for example degrees Celsius, which are derived from Kelvin). The seven fundamental base SI units implemented in Drasil can be seen in Figure 4.

From the captured knowledge and common knowledge, it is now possible to start putting together a document using recipes. A small portion of the recipe for the simplified fuel pin SRS can be seen in Figure 5. Currently the recipes are fairly clunky and rely heavily on Haskell, but in the future this will be improved. However, even with the current recipes we can see that the output from the generator (Figure 6) is exactly what we want. Note: the output I am showing is from the HTML version being generated, the TeX version looks

```
h_c_eq :: Expr
h_c_eq = 2*(C k_c)*(C h_b) /
  (2*(C k_c) + (C tau_c)*(C h_b))

h_c :: EqChunk
h_c = fromEqn "h_c"
 "convective heat transfer coefficient
    between clad and coolant"
 (sub h c) heat_transfer h_c_eq
```

Figure 3: The $h_c$ chunk in Drasil

```
metre, second, kelvin, mole, kilogram, ampere, candela :: FundUnit
metre    = fund "Metre"    "length (metre)"                "m"
second   = fund "Second"   "time (second)"                 "s"
kelvin   = fund "Kelvin"   "temperature (kelvin)"          "K"
mole     = fund "Mole"     "amount of substance (mole)"    "mol"
kilogram = fund "Kilogram" "mass (kilogram)"               "kg"
ampere   = fund "Ampere"   "electric current (ampere)"     "A"
candela  = fund "Candela"  "luminous intensity (candela)" "cd"
```

Figure 4: The seven fundamental SI Units in Drasil

(almost) identical to the original SRS.

Already several advantages of using Drasil and a knowledge based approach are obvious. First off, there are no inconsistencies in the knowledge both within and across artifacts. Manually copying knowledge is no longer necessary, and we can easily trace where a piece of knowledge came from. Should anything need updating, the updates will automatically propagate throughout the artifacts when the generator is run. We also have completely reusable knowledge (for example: the SI Units) and the use of recipes supports design for change. As long as knowledge is captured properly, it is as simple as changing a configuration file to change the software.

```
srsBody = srs [h_g, h_c] "Spencer Smith" [s1,s2,s3]

s1 = Section (S "Table of Units") [intro, table]

table = Table
 [S "Symbol", S "Description"] (mkTable
   [(\x -> Sy (x ^. unit)),
    (\x -> S (x ^. descr)) ] si_units)

intro = Paragraph (S "Throughout this ...")
```

Figure 5: A portion of our simplified SRS recipe

**Table of Units**

Throughout this document SI (Système International d'Unités) is employed as the unit system. In addition to the basic units, several derived units are employed as described below. For each unit, the symbol is given followed by a description of the unit with the SI name in parentheses.

| Symbol | Description |
|---|---|
| m | length (metre) |
| kg | mass (kilogram) |
| s | time (second) |
| K | temperature (kelvin) |
| mol | amount of substance (mole) |
| A | electric current (ampere) |
| cd | luminous intensity (candela) |
| °C | temperature (centigrade) |
| J | energy (joule) |
| W | power (watt) |
| cal | energy (calorie) |
| kW | power (kilowatt) |

Figure 6: Section 1 of the generated SRS (HTML version)

One advantage that may seem like a disadvantage (but is not) is that of pervasive bugs. Thanks to the full traceability and reuse of knowledge, a single bug will be reproduced anywhere that piece of knowledge is necessary. This improves the odds of finding it and makes it simple to fix. A single change should update all of the artifacts and remove the bug.

There are a few disadvantages to using the knowledge based approach with Drasil. The most obvious is the inability to include local hacks. Any human-modified generated file will lose its modifications the next time the generator is run.

Finally, creating common-knowledge libraries is fairly difficult as it requires a domain expert to be involved.

# 5 Work Plan and Next Steps

A full schedule of my work plan can be found in Table 1. There are still many features I would like to add to Drasil as well as improvements to the overall implementation. Currently anticipated additions and changes (in no particular order) are as follows:

- Encapsulate more types of information in chunks. Some of the next additions should be physical constraints and reasonable values.

- Use constraints to generate test cases.
- Implement much larger examples.
- Generate code in more languages. Specifically MATLAB is the next planned output language implementation.
- Generate more artifact types. As it stands, the current recipes only create requirements documents or code. New recipes should be included to cover design documents, test cases, build instructions, user manuals, and more.
- Generate different document views. This is partially implemented in the requirements document recipe by allowing simplified or verbose data descriptions. The ability to simplify parts of the document that are unnecessary for a target audience should be expanded.
- Create an external syntax for Drasil.

Over the summer (2016), three undergraduate students will be working on translating existing implementations of large examples into Drasil implementations. It is my hope that this experiment will provide insight on any lacking features of Drasil, as well as how well the new approach works. A second PhD student will also be joining the project over the summer. His first task will involve implementing a large example and helping to expand Drasil.

Table 1: A detailed work schedule for the next twenty-eight months

| | |
|---|---|
| Summer 2016 | Summer student experiment. Implement multiple (3-4) large examples using Drasil, updating the framework as new needs for features arise.<br>Write up results of experiment as a paper and submit to SEHPCCSE'16. |
| Fall 2016 | Overhaul the Drasil back-end to solidify necessary features and redesign parts of the implementation.<br>Finish PhD course requirements.<br>Meet with Ernie from OPG. |
| Winter 2016 | Implement external syntax for Drasil.<br>Write a paper for ICSR (International Conference on Software Reuse).<br>Write a journal paper for Automated Software Engineering. |
| Spring 2017 | Re-evaluate current Drasil implementation for usability. Work on making it as user-friendly as possible.<br>Submit a paper to Onward!<br>Submit a paper to ASE (International Conference on Automated Software Engineering)<br>Meet with committee. |
| Summer 2017 | Write a paper.<br>Attempt to get summer students for second round of experimentation.<br>Write a journal paper detailing results. |
| Fall 2017 | Meet with Ernie from OPG.<br>Update Drasil and perform a final evaluation. |
| Winter 2017 | Begin writing up full PhD Thesis. |
| Spring 2018 | Complete first draft of thesis and send to supervisors for comments.<br>Complete first round of edits. |
| Summer 2018 | Complete final thesis draft before defense. Make any necessary revisions to the thesis and submit it. |

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