Assessing the Impact of MDE and Code Generation on the Sustainability of Scientific Computing Software: A Research Proposal

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Abstract

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Contents

1 Introduction

Without dramatic intervention, our collective confidence in Scientific Computing Software (SCS) is due for a catastrophic collapse. We are increasingly trusting ever more complex and ambitious computations, but our software foundations are built on sand. Areas of concern include nuclear safety analysis and computational medicine. Successfully building such software requires communication between software developers and experts from multiple domains. Collaboration is difficult at the best of times, and is made worse because developers favour handcrafted solutions over adapting software engineering processes, methods and tools (Faulk et al., 2009). Handcrafted solutions do not account for the inevitable changes in requirements, design and implementation. The twin challenges of changing requirements and inadequate documentation conspire to make computational results notoriously difficult to reproduce, especially in the important endeavour of one researcher independently replicating the results of another (Smith, 2018). Inadequate traceability within documentation means recertification of previously certified engineering software is as expensive and time consuming as the original certification exercise, because of a lack of explicit, effort reducing, traceability information.

Quality of SCS improved through documentation. SCS developers do not always value documentation, but grants such as, NSERC's CRDPJ 447533-13, have allowed me to demonstrate its value and to provide techniques to improve its quality. For instance, Smith et al. (2015) shows that the quality of statistical software for psychology is generally improved when developed using the structured CRAN (Comprehensive R Archive Network) process and tools, versus an ad hoc process. Smith and Koothoor (2016) highlights

the value of proper documentation by redeveloping nuclear safety analysis software. Twenty seven (27) worrisome documentation problems were found, including incompleteness, ambiguity, inconsistency, verifiability, modifiability, traceability and a lack of abstraction. A redevelopment experiment with five existing projects (Smith et al., 2016a) enabled the code owners (as ascertained through interviews) to clearly see the value of documentation. However, mirroring other studies (Carver et al., 2007), the code owners felt documentation takes too much time.

One promising approach to avoid the impending collapse is to use a Model Driven Engineering (MDE) where MDE is an engineering approach that exploits structured representations (metamodels for abstract syntax, and constraints to capture static semantics) to automate repetitive, tedious and error prone tasks. In particular, code generation. approach together with code generation. Citation supporting this idea. My research will dramatically reduce the cost of developing reliable, reproducible and re-certifiable software by: i) creating infrastructure for a knowledge base of scientific and computing models; and, ii) writing explicit "recipes" that weave together this knowledge to generate theoretical models, design documents, code, test cases and build scripts. The generator will render to multiple languages, such as html, LaTeX, RTF for documentation and Python, Java, C, and Matlab, for code. One source of knowledge, with rules for transformation, means completeness, consistency and traceability can be achieved by construction. Moreover, these qualities can be maintained as requirements are modified, design decisions are changed, documentation standards are varied, and software is recertified. The knowledge will be built up incrementally. New projects will reuse existing knowledge and expand as necessary.

Scientists are awakening to the critical importance of SCS sustainability, as evidenced by the success of Software Carpentry and the Software Sustainability Institute, but the current solutions are not bold enough. Although valuable, we need more than studies of developers, training sessions and project support tools. *We need transformative change (enabled by creating new tools for knowledge capture and document/code generation) where documentation, design and verification are expected for all SCS.*

- background and context

- problem statement and research question - research question: What ideas (if any) from Drasil and Drasil procedures are perceived by graduate students and end user developers with improving software quality and productivity - for long lived (safety related?) projects

roadmap of document

2 Literature Review

roadmap of this section

2.1 Current State of Practice for SCS Development

- how currently done, qualities of interest, add sustainability

The SCS community is finally realizing that current practices are not sustainable. Faulk et al. (2009) observe, "growing concern about the reliability of scientific results based on ... software." Embarrassing failures have occurred, like a retraction of derived molecular protein structures (Miller, 2006), false reproduction of sonoluminescent fusion (Post and Votta, 2005), and fixing and then reintroducing the same error in a large code base three times in 20 year (Milewicz and Raybourn, 2018). A recent report on directions for SCS research and education states: "While the volume and complexity of [SCS] have grown substantially in recent decades, [SCS] traditionally has not received the focused attention it so desperately needs ... to fulfill this key role as a cornerstone of long-term collaboration and scientific progress" (Rüde et al., 2018). Estimates suggest that the number of released faults per thousand executable lines of code during a given program's life cycle is at best 0.1, and more likely 10 to 100 times worse (Hatton, 2007).

Although reproducibility is the cornerstone of the scientific method, until recently it has not been treated seriously in software (Benureau and Rougier, 2017). Fortunately, in recent years multiple conferences, workshops and individuals are calling for dramatic change (Bailey et al., 2016). The need for action is highlighted by a study of 402 computer systems papers - only 48.3% of the code was both available and compilable (Collberg et al., 2015). (Drasil addresses this problem because as programming languages evolve the code renderers in Drasil can be updated.) Reproducibility problems are even more extreme when the goal is replicability. A third party should be able to repeat a study using only the description of the methodology from a published article (Benureau and Rougier, 2017). However, replicability is rarely achieved, as shown for microarray gene expression (Ioannidis et al., 2009) and for economics modelling (Ionescu and Jansson, 2012). Drasil addresses completeness and ambiguity problems, since it emphasizes capturing

and documenting all of the required knowledge, including derivation of equations and rationales. Crick et al. (2014) point out potential roadblocks for reproducibility, including page length constraints and differing detail needs depending on the audience. Again Drasil addresses these concerns because the recipes used to generate the documentation can be tailored to the level of detail required.

Although scientists recognize the seriousness of their SCS problems, their corrective steps are too incremental. For instance, a recent proposal for the future of High Energy Physics (HEP) software Stewart et al. (2017) uses words like sustainability, maintainability and reproducibility, but is almost completely silent on how these qualities are to be achieved. The proposal mentions developing new and improved algorithms (including parallel computing and machine learning), programming tools, recruitment and training, but there is little on documentation, design or verification techniques (other than unit testing). Similarly, a recent proposal on future directions for SCS research and education (Rüde et al., 2018) recognizes the desperate need for change, but then only suggests training on project management tools, open sharing and ethics. *Incremental change is not adequate; we need transformative change.*

Thankfully SCS leaders recognize that an interdisciplinary approach provides the path forward. They believe that the solution to SCS quality problems is applying, adapting and developing SE methods, tools and techniques. However, typical software processes are a barrier to progress. "To break the gridlock, we must establish a degree of cooperation and collaboration with the [SE] community that does not yet exist" (Faulk et al., 2009). "There is a need to improve the transfer of existing practices and tools from ... [SE] to scientific programming. In addition, ... there is a need for research to specifically develop methods and tools that are tailored to the domain" (Storer, 2017). *This tailored research will require individuals, like myself, that have a multidisciplinary background.*

2.2 MDE and Code Generation

DSLs and code/document generation provide a transformative technology for documentation, design and verification (Johanson and Hasselbring, 2018; Smith, 2018). DSLs allow scientists their preferred approach of focusing on science not software (Kelly, 2007). A generative approach removes the maintenance nightmare of documentation duplicates and near duplicates (Luciv

et al., 2018), since knowledge is only captured once and automatically transformed as needed. Code generation has previously been applied to improve SCS (Whaley et al., 2001; Veldhuizen, 1998; Püschel et al., 2001). Carette and Kiselyov (2011) shows how to generate a family of efficient, type-safe Gaussian elimination algorithms. FEniCS (Finite Element and Computational Software) (Logg et al., 2012) uses code generation when solving differential equations. Unlike previous work on SCS code generation, Drasil will focus on generating all software artifacts (requirements, design etc.), not just code.

Szymczak et al. (2016) removes excuses for avoiding documentation by providing transformative SCS development technology. Drasil provides an infrastructure for knowledge capture and document/code generation. Jacques Carette and I, along with our students, have developed a prototype (available on GitHub), implemented via Domain Specific Languages (DSLs) embedded in Haskell. Drasil already generates requirements documentation and code for several case studies, including simulating the temperature of a solar water heating system, glass breakage and two-dimensional game physics. The full documentation (requirements, design etc), code and test cases have been created manually for each case study. These manual case studies (many from Smith et al. (2016a)) provide the 'gold standard' against which Drasil is tested. All of these artifacts are available publicly. The generation techniques for Drasil began to take shape during my work on generating geometric data structures and functions (Carette et al., 2011).

2.3 Empirical Methods for Software Engineering

empirical software engineering paper, case study paper

3 Research Design and Methodologies

roadmap - fit the different pieces together

3.1 State of the Practice

A survey of existing SCS software will identify patterns, find opportunities for improvement and identify candidate program families for future implementation. The survey will require developing terminology and a classification

system to answer such questions as: What are the current best practises? What software packages are reused and why these packages? What do practitioners look for in the tools that support their work?

To achieve objective S2, a measurement template, possibly using pairwise comparisons of quality metrics between software packages, will be developed for assessing the quality of the documentation, code, test cases and development processes for existing SCS program families. The quality measurement template will be used to assess the quality of approximately 30 different SCS families. About half of the families will be model oriented and the other half tool oriented. Additional details on best practices will be collected by students interviewing code owners. Based on preliminary discussions, Dr. Jeffrey Carver from the University of Alabama and some of his colleagues may also participate in collecting interview data. Once all the surveys and interviews are completed, a meta-analysis will draw conclusions for each domain and between domains. Knowing the state of practice for family development will highlight which domains are using best practices that should be emulated in LSS.

The plan here is to return to the task of measuring/assessing the state of software development practice in several scientific computing domains. We will update the work that was done previously for domains such as Geographic Information Systems Smith et al. (2018a), Mesh Generators Smith et al. (2016b), Seismology software Smith et al. (2018d), and Statistical software for psychology Smith et al. (2018c). We could return to these domains and/or introduce new domains. Potential domains/collaborators are listed in the subsections.

MEng students will be asked to assess the state of practice in each domain. Last time each student measured two domains, so we would start off with this model again. If the scope becomes large enough, we might switch to one domain per student.

In the previous project, we measured 30 software projects for each domain. With the increased scrutiny required in this re-boot, we won't likely be able to measure the details on this high a number of software projects. We may still start with 30 software examples in each domain, but then use some criteria to create a shorter sub-list for detailed measurement. The details of how to proceed here would be determined and documented in the measurement protocol.

In the previous state of practice assessing exercise, a series of questions and simple metrics was devised to measure the quality of the documentation

and adherence to best software development practices. The new project will critically assess the previous set of questions and revise as necessary. In addition, the following data will be collected/developed for each domain:

- Characterization of the functionality provided by the software in the domain. What services does each member of the domain provide? Ideally this information would be summarized in a commonality analysis document. The document will summarize the domain software via its commonalities, variabilities and parameters of variation.
- Usability testing of each software in the domain. Specific metrics for assessing usability still need to be researched, but measures that involve the time to complete a task and the users overall impression would be considered.
- Collect empirical software engineering related data, such as the number of files, number of lines of code, cyclomatic complexity, number of open issues, etc. As a starting point for tool support, HubListener (https://github.com/pjmc-oliveira/HubListener) could be used.
- Collect at least one empirical measure of the quality of the documentation - the number of lines of documentation. [Has anyone previously looked at this metric?]

The above data will be combined to rank the software in the domain. The specifics are yet to be determined, but in the past the Analytic Hierarchy Process proved helpful in this.

Key to the success of this exercise will be to involve and engage a partner for each state of practice project. In the previous effort we didn't involve domain experts with the rationale of excluding potential bias, but this advantage is not worth not being able to evaluate the functionality/usability of the software. Moreover, not having an expert makes publication more difficult, since there is no one to advice on how best to approach journals and publishers. The domain expert will be asked to help in the following ways:

- Review the protocol for assessing/measuring quality. This same protocol will be used in each domain.
- Provide their expertise on potential publication. Specifically, they will recommend a suitable journal and act as the corresponding author for any paper submissions.

- Provide an authoritative list of domain software, possibly augmented by existing on-line lists.
- Provide some assistance from their own team of supervised students to facilitate software testing and domain characterization. Assessing the functionality and measuring usability will require an individual with domain knowledge. Multiple measurements will be necessary to have confidence. The measurements will likely take a few hours over a few days of time from each student volunteer.

There is no budget for this project, but the student volunteers will be considered co-authors in the resulting paper. Having them as co-authors also means that ethics approval should not be necessary.

GitHub will be used to coordinate the work of the large team of people that will be involved in this project. In addition to the project record left on GitHub, the final data will be exported to Mendeley.

Potential collaborators/domains are listed in the following subsections.

3.2 Medical Imaging

Medical imaging and analysis software (Dr. Michael Noseworthy).

3.3 Climate Modelling Software

Climate modelling software (Dr. Zoe Li or Dr. Xander Wang).

3.4 Computational Medicine

Extraction of 3D geometries from medical images (Dr. Zahra Motamed).

3.5 Finite Element Analysis

Finite element solvers and/or mesh generators (Dr. Dieter Stolle). Potential software includes FeNiCS, MOOSE, FreeFEM++, Dolphin, etc. Install the packages and use them to do something non-trivial.

3.6 Psychology Software

Statistics software for psychology (Dr. Karin Humphreys).

3.7 Chemical Engineering Software

Li Xi (https://www.eng.mcmaster.ca/chemeng/people/faculty/li-xi).

3.8 Geographic Information Systems

Geographic Information Systems (Jason Brodeur and/or Patrick DeLuca).

3.9 Solidification and Casting Software

Solidification and casting software (Dr. André Phillion).

3.10 Quantum Chemistry Software

Quantum chemistry software (Dr. Paul Ayers).

3.11 Impact of MDE on SCS

roadmap

3.12 Fitting Drasil into the Scientific Software Development Process

Scientists generally use an approximation of agile methods for their software development. In addition, documentation is generally not emphasized. How should Drasil be fit into the scientific software development process? The Drasil process should encourage an early intensity of thought and effort, but at the same time, it shouldn't require waterfall development. Drasil supports frequent chance and incremental development, but where should developers start and how should the work proceed? How does one create an almost empty project in Drasil and then borrow from existing knowledge and create new knowledge? This project could start with something like the task described in **??**.

Drasil process should move importance of requirements and domain analysis earlier in the process. The quality of the resulting software depends on the quality of the requirements. As is known from historical data, the greatest return on investment is at the requirements state (Boehm papers). Unfortunately, developers don't like requirements. Quite possibly they don't like the

intensity of thought that is necessary to get the requirements right. Inspection techniques, such as task based inspection (Kelly et al) hold promise for getting the scientist to think deeply at an earlier stage in the development process.

3.13 etc.

Experimentally Determine Appropriate Documentation Template: The best approach for documenting requirements and design is an open question. Drasil could be used to attempt to address this question. Different recipes for documentation could be developed and compared. Some comparison could be automated between the documents, such as empirical measures of their quality (Section **??**). Other measures would require some kind of usability experiments.

Empirical Measurement of Documentation: Considerable effort has been invested into developing metrics, like cyclomatic complexity, to attempt to quantify code quality, but no measures (as far as I know) exist for quantifying the quality of documentation. (Khedri does have some work with Bhahati (sp?) Sanga that quantifies the connectivity of the documentation via the traceability graph.) Likely the reason that effort has not been invested to quantifying the quality of documentation is that is not represented formally. With Drasil much of the documentation is formal. This should facilitate automatic measures of documentation quality, or at least metrics that might be correlated with quality.

Measuring the Impact of Drasil on Developing Scientific Software: This project is challenging to design, but would be HUGE if we were successful. We assume that Drasil will improve the quality of scientific software and the efficiency of its production, but data to back this up would go a long way to convincing the scientific community. Experiments where a given project is developed in parallel by two independent teams come to mind, but this would be expensive, and difficult to control. Some additional thought, and resources, are necessary here. If we could do a project where the scientist, or a student under their supervision, is a true partner in the development, we might get more convincing anecdotal evidence.

To quantify the quality of the generated documentation, measures of information compression will be used. The measure will be based on the length of the (family of) generated documentation, code and test cases, compared to the length of the generator itself. Our measure will be based on the Minimum

Description Length (MDL) Principle, which states that "the more we are able to compress the data, the more we have learned about the data" (Grünwald, 2004). Another important measure will be whether the generated documentation achieves reproducibility. The proposed measure is reproducibility depth (Soergel, 2014). A depth of 1 means that an independent researcher can start from the generated code and calculate the same results. Achieving deeper reproducibility will mean the same results can be calculated for an independent researcher starting with the design documentation. Each higher measure gets further from the source code, until the highest depth (replicability), which starts from the requirements and leads to identical (within acceptable error) results.

3.14 Impact of Assurance Cases for Building Confidence

Some SCS needs to be verifiably safe. We will achieve this by building a safety assurance case. An assurance case is an explicit structured argument pertaining to specific properties, such as trustworthiness

Assurance cases have potential to be used in SC to improve our collective confidence in the developed software Smith et al. (2018b). Further work is necessary to demonstrate the value of assurance cases, but they certainly hold promise. Drasil could go a long way to supporting development of assurance cases. Some potential Drasil related support ideas include the following:

- Automatic generation of visual depiction of the assurance case from the goals, claims, evidence etc.
- Automated reporting of missing evidence, incomplete arguments, etc.
- Coordination of requirements, design decisions, etc. Assurance cases use the same information as recommended in "document driven" design, but the traceability and connection between the data is even more important. A tool like Drasil could go a long way in facilitating the presentation and navigation of an assurance case.

Assurance cases in Drasil could potentially go beyond the scientific context. For instance, they could also incorporate safety cases for control systems. This could potentially be of interest to McSCert.

3.15 Impact of Computational Variability Testing

This activity supports objective S3. The applicant's students will apply LSS and code generation to Computational Variability Testing (CVT), using the example of a family of finite element programs. As proposed by the applicant, CVT uses code generation to build confidence in the generated code in an analogous way to the use of grid refinement studies. Grid refinement looks at how the solution changes by varying the run-time parameter of grid density and comparing the results to theoretical expectations. CVT, on the other hand, can generate code to "refine" build time parameters, such as order of interpolation, or degree of implicitness. These parameters can be systematically varied and the results compared against the expected trend. Varying computational variabilities is not a new idea, but it is only recently that the option has become available of coupling this with code generation, so that the validity of an entire program family can be assessed at the same time. The experimentation with CVT will initially use the FEniCS package (Logg et al., 2012) for elliptical partial differential equations to compare elements with different orders of interpolation to verify that the convergence to the solution agrees with the theoretical expectations.

Design and Documentation For Family of Data Fitting Algorithms: The fitting used in GlassBR and in SFS (Software for Solidification) could be made much more generic. We could have a family of fitting algorithms that could be used in any situation where fitting is required. A proper commonality analysis of this domain could potentially show the potential design decisions that bridge between the requirements and the design. In the SFS example many different fitting routines were tried. If the experiments could have been done easily via a declarative specification, considerable time would have been saved. If the experiments are combined with automated testing and "properties of a correct solution" the human involvement could be reduced, so that we have partially automated algorithm selection.

4 Implications and Contributions to Knowledge

We are currently putting too much trust in SCS. Examples such as nuclear safety analysis and computational medicine show the significance of SCS for health and safety. Although SCS developers do excellent work, we do not

currently have enough checks and balances in place for full confidence. More should be expected for documentation, design and testing. Fortunately, SE offers techniques, like DSLs and code generation, that can be employed to not only improve SCS quality, but also reduce development costs. Now is the time for change. SCS practitioners have recognized problems with the status quo and multidisciplinary researchers are needed to bridge the gap between SE and SCS.

Codifying medical, biomechanical and computational knowledge is challenging, but success will completely transform the development of safety-related software in medicine, science and engineering. MDE will remove the drudgery of generating and maintaining documentation, code, test cases and build environments, enabling scientists to focus on science, engineers to focus on engineering and medical professionals to focus on medicine. MDE will detect inconsistencies between models via inter-model consistency constraints. As a consequence, mistakes like inconsistent units or assumptions cannot occur. MDE will raise the bar so that we can expect an explicit argument for safety, not just code that we are expected to blindly trust. With the right up-front investment of knowledge capture, we can have software that is long lived because the stable knowledge is separated from the rapidly changing modelling assumptions and design decisions.

5 Research Schedule

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