# Digging Deeper Into the State of the Practice for Domain Specific Research Software

Spencer Smith<sup>1</sup>[0000-0002-0760-0987] and Peter Michalski<sup>1</sup>

McMaster University, 1280 Main Street West, Hamilton ON L8S 4K1, Canada smiths@mcmaster.ca

http://www.cas.mcmaster.ca/~smiths/

**Abstract.** To improve the productivity of research software developers we need to first understand their development practices. Previous studies on this topic have collected data by surveying as many developers as possible, across a broad range of application domains. We propose to dig deeper into the state of the practice by instead looking at what developers in specific domains create, as evidenced by the contents of their repositories. Our methodology prescribes the following steps: i) Identify the domain; ii) Identify a list of candidate software; iii) Filter the list to a length of about 30 packages; iv) Collect repository related data on each package, like number of stars, number of open issues, number of lines of code; v) Fill in the measurement template (the template consists of 108 questions to assess 9 qualities (including the qualities of installability, usability and visibility)); vi) Rank the software using the Analytic Hierarchy Process (AHP); vii) Interview developers (the interview consists of 20 questions and takes about an hour); and, viii) Conduct a domain analysis. The collected data is analyzed by: i) comparing the ranking by best practices against the ranking by popularity; ii) comparing artifacts, tools and processes to current research software development guidelines; and, iii) exploring pain points. We estimate the time to complete an assessment at 173 person hours. The method is illustrated via the example of Lattice Boltzmann Solvers, where we find that the top packages engaged in most of recommended best practices, but still show room for improvement with respect to providing API documentation, a roadmap, a code of conduct, programming style guide and continuous integration.

**Keywords:** research software  $\cdot$  software quality  $\cdot$  empirical measures  $\cdot$  software artifacts  $\cdot$  developer pain points  $\cdot$  Lattice Boltzmann Method

#### 1 Introduction

Research software is critical for tackling problems in areas as diverse as manufacturing, financial planning, environmental policy and medical diagnosis and treatment. However, developing reliable, reproducible, sustainable and fast research software is challenging because of the complexity of physical models and the nuances of floating point and parallel computation. The critical importance of research software, and the challenges with its development, have prompted

multiple researchers to investigate the state of development practice. Understanding the creation of research software is critical for devising future methods and tools for reducing development time and improving software quality.

Previous studies on the state of the practice for research software have often focused on surveying developers [7,13,16]. Although surveys provide valuable information, they are limited by their reliance on what developers say they do, rather than directly measuring what they actually do. Therefore, we propose a state of the practice assessment methodology that investigates the work products developers create by digging into the software repositories they create.

Although other studies [6,27] mine research software repositories to estimate productivity, code quality and project popularity, the other studies focus on automation and on code related artifacts. To gain deeper insight, at the expense of taking more time, we will relax the automation requirement and use manual investigation where necessary. We will also expand our assessment beyond code to include other artifacts, where artifacts are the documents, scripts and code that we find in a project's public repository. Example artifacts include requirements, specifications, user manuals, unit test cases, system tests, usability tests, build scripts, API (Application Programming Interface) documentation, READMEs, license documents, and process documents.

The surveys used in previous studies have tended to recruit participants from all domains of research software. This is what we will call research software in general, as opposed to specific domain software. The surveys may distinguish participants by programming language (for instance, R developers [16]), or by the role of the developers (for instance postdoctoral researchers [12]), but the usual goal is to cast as wide a net as possible. Case studies [2,19], on the other hand, go more in depth by focusing on a few specific examples at a time. For our new methodology, we propose a scope between these two extremes. Rather than focus on assessing the state of the practice for research software in general, or just a few examples, we will focus on one scientific domain at a time. The practical reason for this scope is that digging deep takes time, making a broad scope infeasible. We have imposed a practical constraint of one person month of effort per domain. Focusing on one domain at a time has more than just practical advantages. By restricting ourselves to a single domain we can bring domain knowledge and domain experts into the mix. The domain customized insight provided by the assessment has the potential to help a specific domain as they adopt and develop new practices. Moreover, measuring multiple different domains facilitates comparing and contrasting domain specific practices.

Our methodology is built around 8 research questions. Assuming that the domain has been identified (Section 2.1), the first question is:

RQ1: What software projects exist in the domain, with the constraint that the source code must be available for all identified projects? (Sections 2.2, 2.3)

A person month is considered to be 20 working days (4 weeks in a month, with 5 days of work per week) at 8 person hours per day, or  $20 \cdot 8 = 160$  person hours.

We next wish to assess the representative software to determine how well they apply current software development best practices. By best practices we mean methods, techniques and tools that are generally believed to improve software development, like testing and documentation. As we will discuss in Section 2.4, we will categorize our best practices around software qualities. Following best practices does not guarantee popularity, so we will also compare our ranking to how the user community itself ranks the identified projects.

RQ2: Which of the projects identified in RQ1 follow current best practices, based on evidence found by experimenting with the software and searching the artifacts available in each project's repository? (Sections 2.4)

RQ3: How similar is the list of top projects identified in RQ2 to the most popular projects, as viewed by the scientific community? (Section 4)

To understand the state of the practice we wish to learn the frequency with which different artifacts appear, the types of development tools used and the methodologies used for software development. With this data, we can ask questions about how the domain software compares to other research software.

RQ4: How do domain projects compare to research software in general with respect to the artifacts present in their repositories? (Section 5)

RQ5: How do domain projects compare to research software in general with respect to the use of tools? (Section 6)

RQ6: How do domain projects compare to research software in general with respect to the processes used? (Section 7)

Only so much information can be gleaned by digging into software repos. To gain additional insight, we need to interview developers (Section 2.5), as done in other state of the practice assessments [10], to learn:

RQ7: What are the pain points for developers? (Section 8)

RQ8: How do the pain points of domain developers compare to the pain points for research software in general? (Section 8)

Our methodology answers the research question through inspecting repositories, using the Analytic Hierarch Process (AHP) for ranking software, interviewing developers and interacting with at least one domain expert. We leave the measurement of the performance, for instance using benchmarks, to other projects [9]. The current methodology updates the approach used in prior assessments of domains like Geographic Information Systems [24], Mesh Generators [23], Seismology software [26], and statistical software for psychology [25]. Initial tests of the new methodology have been done for medical image analysis software [3] and for Lattice Boltzmann Method (LBM) software [11]. The LBM example will be used to illustrate the steps in the methodology.

# 2 Methodology

4

The assessment is conducted via the following steps, which depend on interaction with a Domain Expert partner, as discussed in Section 2.6.

- 1. Identify the domain of interest. (Section 2.1)
- 2. List candidate software packages for the domain. (Section 2.2)
- 3. Filter the software package list. (Section 2.3)
- 4. Gather the source code and documentation for each software package.
- 5. Measure using the measurement template. (Section 2.4)
- 6. Use AHP to rank the software packages. (Section 2.4)
- 7. Interview the developers. (Section 2.5)
- 8. Domain analysis. (Section 2.7)
- 9. Analyze the results and answer the research questions. (Sections 3—8)

We estimate 173 hours to complete the assessment of a given domain [22], which is close our goal of 160 person hours.

## 2.1 How to Identify the Domain?

To be applicable the chosen domain must have the following properties:

- 1. The domain must have well-defined and stable theoretical underpinnings.
- 2. There must be a community of people studying the domain.
- 3. The software packages must have open source options.
- 4. The domain expert says there will be at least 30 candidate packages.

## 2.2 How to Identify Candidate Software from the Domain?

The candidate software to answer RQ1 should be found through search engine queries, GitHub, swMATH and scholarly articles. The Domain Expert (Section 2.6) should also be engaged in selecting the candidate software. The following properties are considered when creating the list:

- 1. The software functionality must fall within the identified domain.
- 2. The source code must be viewable.
- 3. The repository based measures should be available.
- 4. The software must be complete.

## 2.3 How to Filter the Software List?

If the list of software is too long (over around 30 packages), then filters are applied in the priority order listed. Copies of both lists, along with the rationale for shortening the list, should be kept for traceability purposes.

1. Scope: Software is removed by narrowing what functionality is considered to be within the scope of the domain.

- 2. Usage: Software packages are eliminated if their installation procedure is missing or not clear and easy to follow.
- 3. Age: Older software packages (age being measured by the last date when a change was made) are eliminated, except in the cases where an older software package appears to be highly recommended and currently in use. (The Domain Expert should be consulted on this question as necessary.)

#### 2.4 Quantitative Measures

We rank the projects by how well they follow best practices (RQ2) via a measurement template [22]. For each software package (each column in the template), we fill-in the rows. This process takes about 2 hours per package, with a cap of 4 hours. An excerpt of the template is shown in Figure 1. In keeping with scientific transparency, all data should be made publicly available.

Summary Information	•						•	
Software name?	DL_MESO	SunlightLB	MP-LABS	LIMBES	LB3D-Prime	LB2D-Prime	laboetie	Musubi
Number of developers	unclear	2	1	unclear	1	1	2	unknown
License?	terms of use	GNU GPL	GNU GPL	GNU GPL	unclear	unclear	GNU GPL	BSD
	Windows, OS X,				Windows,	Windows,		Windows,
Platforms?	Linux	Linux	Linux	Unix	Linux	Linux	Linux	OS X, Linu
Software Category?	private	public open	public	public	public	public	public	public
Development model?	freeware	source	freeware	freeware	freeware	freeware	unclear	freeware
	FORTRAN, C++,	C, Perl,	FORTRAN,				FORTRAN, Wolfram	
Programming language(s)?	Java	Python	Markdown	FORTRAN	С	C, Shell	Markdown	Fortran
Installability								
Installation instructions?	yes	yes	yes	yes	yes	yes	yes	yes
Instructions in one place?	yes	yes	yes	yes	yes	yes	yes	yes
Linear instructions?	yes	yes	yes	yes	yes	yes	yes	yes
Installation automated? Descriptive error	yes, makefile	yes, makefile	yes, makefile	yes, makefile	yes, makefile	yes, makefile	yes, makefile	yes
messages?	yes	ves	no	n/a	n/a	no	n/a	n/a
Number of steps to install?	8	6	6	4	2	4	4	10
Numbe extra packages?	4	4	3	1	2	2	2	5
Package versions listed?	yes	no	no	no	no	no	no	no
Problems with uninstall?	unavail	unavail	unavail	unavail	unavail	unavail	unavail	unavail
Overall impression (110)?	9	7	6	8	7	5	7	8
Surface Reliability	***						***	
Journal Remaining								

Fig. 1. Excerpt of the Top Sections of the Measurement Template

The full template [22] consists of 108 questions categorized under 9 qualities: (i) installability; (ii) correctness and verifiability; (iii) surface reliability; (iv) surface robustness; (v) surface usability; (vi) maintainability; (vii) reusability; (viii) surface understandability; and, (ix) visibility/transparency.

The questions were designed to be unambiguous, quantifiable and measurable with limited time and domain knowledge. The measures are grouped under headings for each quality, and one for summary information (Figure 1). The

summary section provides general information, such as the software name, number of developers, etc. Several of the qualities use the word "surface". This is to highlight that, for these qualities, the best that we can do is a shallow measure. For instance, we do not conduct experiments to measure usability. Instead, we are looking for an indication that usability was considered by looking for cues in the documentation, such as getting started instructions, a user manual or documentation of expected user characteristics.

Tools are used to find some of the measurements, such as the number of files, number of lines of code (LOC), percentage of issues that are closed, etc. The tool GitStats is used to measure each software package's GitHub repository for the number of binary files, the number of added and deleted lines, and the number of commits over varying time intervals. The tool Sloc Cloc and Code (scc) is used to measure the number of text based files as well as the number of total, code, comment, and blank lines in each GitHub repository. At this time our focus is on simple metrics, so we do no need the static analysis capabilities of tools like Sonargraph or SonarCloud.

Virtual machines (VMs) are used to provide an optimal testing environments for each package [23] because with a fresh VM there are no worries about conflicts with existing libraries. Moreover, when the tests are complete the VM can be deleted, without any impact on the host operating system. The most significant advantage of using VMs is that every software install starts from a clean slate, which removes "works-on-my-computer" errors.

Once we have measured each package, we still need to rank them to answer RQ2. To do this, we used the Analytical Hierarchy Process (AHP), a decision-making technique that uses pair-wise comparisons to compare multiple options by multiple criteria [17]. In our work AHP performs a pairwise analysis between each of the 9 quality options for each of the (approximately) 30 software packages. This results in a matrix, which is used to generate an overall score for each software package for the given criteria [23].

#### 2.5 Interview Developers

Several of the research question (RQ5, RQ6 and RQ7) require going beyond the quantitative data from the measurement template. To gain the required insight, we interview developers using a list of 20 questions [22]. The questions cover the background of the development teams, the interviewees, and the software itself. We ask the developers how they organize their projects and about their understanding of the users. Some questions focus on the current and past difficulties, and the solutions the team has found, or will try. We also discuss the importance of, and the current situation for, documentation. A few questions are about specific software qualities, such as maintainability, usability, and reproducibility. The interviews are semi-structured based on the question list. Each interview should take about 1 hour.

The interviewees should follow standard ethics guidelines for consent, recording, and including participant details in the report. The interview process presented here was approved by the McMaster University Research Ethics Board

under the application number MREB#: 5219. For LBM we were able to recruit 4 developers to participate in our study.

#### 2.6 Interaction With Domain Expert

Our methodology relies on engaging a Domain Expert to vet the list of projects (RQ1) and the AHP ranking (RQ2). The Domain Expert is an important member of the assessment team. Pitfalls exist if non-experts attempt to acquire an authoritative list of software, or try to definitively rank software. Non-experts have the problem that they can only rely on information available on-line, which has the following drawbacks: i) the on-line resources could have false or inaccurate information; and, ii) the on-line resources could leave out relevant information that is so in-grained with experts that nobody thinks to explicitly record it. Domain experts may be recruited from academia or industry. The only requirements are knowledge of the domain and a willingness to be involved.

## 2.7 Domain Analysis

For each domain a table should be constructed that distinguishes the programs by their variabilities. In research software the variabilities are often assumptions.

## 3 Measuring and Ranking the LBM Domain

For the LBM example the initial list had 46 packages [11]. To answer RQ1, this list was filtered by scope, usage, and age to decrease the length to 24 packages, as shown in Table 1. This table also shows the domain analysis, in terms of variabilities, for LBM software [11].

To answer RQ2 the 24 LBM packages were ranked for the 9 qualities [11]. For space reasons we will only show the overall ranking in Figure 2. In the absence of information on priorities, the overall ranking was calculated with an equal weight between all qualities. The LBM data is available on Mendeley.

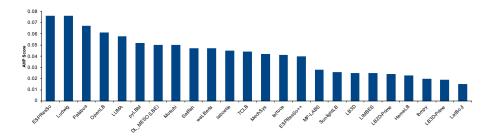


Fig. 2. AHP Overall Score

Name	Dim	Pll	Com Rflx MFl Turb CGE OS					E OS
DL MESO (LBE)	2, 3	MPI/OMP	Y	Y	Y	Y	Y	W, M, L
ESPResSo	1, 2, 3	CUDA/MPI	Y	Y	Y	Y	Y	M, L
ESPResSo++	1, 2, 3	MPI	Y	Y	Y	Y	Y	L
HemeLB	3	MPI	Y	Y	Y	Y	Y	${f L}$
laboetie	2, 3	MPI	Y	Y	Y	Y	Y	${ m L}$
LatBo.jl	2, 3	-	Y	Y	Y	N	Y	${f L}$
LB2D-Prime	2	MPI	Y	Y	Y	Y	Y	W, L
LB3D	3	MPI	N	Y	Y	Y	Y	$\mathbf{L}$
LB3D-Prime	3	MPI	Y	Y	Y	Y	Y	W, L
lbmpy	2, 3	CUDA	Y	Y	Y	Y	Y	L
lettuce	2, 3	CUDA	Y	Y	Y	Y	Y	W, M, L
LIMBES	2	OMP	Y	Y	N	N	Y	$\mathbf{L}$
Ludwig	2, 3	MPI	Y	Y	Y	Y	Y	${ m L}$
LUMA	2, 3	MPI	Y	Y	Y	Y	Y	W, M, L
MechSys	2, 3	-	Y	Y	Y	Y	Y	${ m L}$
MP-LABS	2, 3	MPI/OMP	N	Y	Y	N	N	${ m L}$
Musubi	2, 3	MPI	Y	Y	Y	Y	Y	W, L
OpenLB	1, 2, 3	MPI	Y	Y	Y	Y	Y	W, M, L
Palabos	2, 3	MPI	Y	Y	Y	Y	Y	W, L
pyLBM	1, 2, 3	MPI	Y	Y	N	Y	Y	W, M, L
Sailfish	2, 3	CUDA	Y	Y	Y	Y	Y	M, L
SunlightLB	3	-	Y	Y	N	N	Y	${ m L}$
TCLB	2, 3	CUDA/MPI	Y	Y	Y	Y	Y	${ m L}$
waLBerla	2, 3	MPI	Y	Y	Y	Y	Y	$\mathbf{L}$

Table 1. Features of Software Packages (Dim for Dimension (1, 2, 3), Pll for Parallel (CUDA, MPI, OpenMP (OMP)), Com for Compressible (Yes or No), Rflx for Reflexive Boundary Condition (Yes or No), MFl for Multi-fluid (Yes or No), Turb for Turbulent (Yes or No), CGE for Complex Geometries (Yes or No), OS for Operating System (Windows (W), macOS (M), Linux (L)))

## 4 Comparison to Community Ranking

To address RQ3 we need to compare the ranking by best practices to the community's ranking. Our best practices ranking comes from the AHP ranking (Section 2.4). We estimate the community's ranking by repository stars and watches. The comparison will provide insight on whether best practices are rewarded by popularity. However, inconsistencies between the AHP ranking and the community's ranking are inevitable for the following reasons: i) the overall quality ranking via AHP makes the unrealistic assumption of equal weighting between quality factors; ii) stars are not a particularly good measure of popularity, because of how people use stars and because young projects have less time to accumulate them [28]; iii) and, as for consumer products, there are more factors influencing popularity than just quality.

Table 2 compares the AHP ranking of the LBM package to their popularity in the research community. Nine packages do not use GitHub, so they do not have a star measure. Looking at the stars of the other 15 packages, we can observe a pattern where packages that have been highly ranked by our assessment tend to have more stars than lower ranked packages. The best ranked package by AHP (ESPResSo) has the second most stars, while the ninth ranked package (Sailfish) has the highest number of stars. Although the AHP ranking and the community popularity estimate are not perfect measures, they do suggest a correlation between best practices and popularity.

Name	Our Ranking	Repository Stars	Repository Star Rank	Repository Watches	Repository Watch Rank
ESPResSo	1	145	2	19	2
Ludwig	2	27	8	6	7
Palabos	3	34	6	GitLab	GitLab
OpenLB	4	N/A	N/A	N/A	N/A
LUMA	5	33	7	12	4
pyLBM	6	95	3	10	5
DL MESO (LBE)	7	N/A	N/A	N/A	N/A
Musubi	8	N/A	N/A	N/A	N/A
Sailfish	9	186	1	41	1
•••					
LatBo.jl	24	17	10	8	6

Table 2. Excerpt from Repository Ranking Metrics [11]

# 5 Comparison of Artifacts to Other Research Software

We answer RQ4 by comparing the artifacts that we observe to those observed and recommended for research software in general. While filling in the measurement template (Section 2.4), the domain software is examined for the presence of artifacts, which are then categorized by frequency as: common (more than 2/3 of projects), uncommon (between 1/3 and 2/3), and rare (less than 1/3). The observed frequency of artifacts should then be compared to the artifacts recommended by research software guidelines, as summarized in Table 3.

As Table 3 shows, the majority of LBM generated artifacts correspond to general recommendations from research software developers. Areas where LBM developers could improve include providing: API documentation, a product roadmap, a code of conduct, code style guide, and uninstall instructions.

	[30]	[18]	[1]	[32]	[20]	[8]	[29]	[5]	[14]	LBM
LICENSE README	✓	<b>√</b>	√ √	√ √	<b>√</b>		<b>√</b> ✓	<b>√</b>	√ √	C C
CONTRIBUTIN CITATION	IG	$\checkmark$	$\checkmark$	<b>√</b>	$\checkmark$		$\checkmark$	<b>√</b>	<b>√</b>	U
CHANGELOG		✓		<b>√</b>	$\checkmark$		$\checkmark$	✓	✓	U U
INSTALL					✓		✓	✓	✓	С
Uninstall			,		,			<b>√</b>		R
Dependency List Authors	ī.		✓		<b>√</b>		$\checkmark$	<b>√</b>	$\checkmark$	$_{\mathrm{C}}^{\mathrm{C}}$
Code of Conduc							✓	,	,	
Acknowledgement Code Style Guid		<b>√</b>					√ √	√ √	√ √	R R
Release Info.		✓				✓	✓			U
Prod. Roadmap						<b>√</b>	<b>√</b>	<b>√</b>		R
Getting started User manual			./		$\checkmark$		<b>√</b>	$\checkmark$	$\checkmark$	C U
Tutorials			•				<b>√</b>			Č
FAQ							<b>√</b>	✓	✓	R
Issue Track Version Control		<b>√</b>	<b>√</b>	<b>√</b>	√ √	√ √	<b>√</b> ✓	<b>√</b>	<b>√</b>	$_{\mathrm{C}}^{\mathrm{C}}$
Build Scripts		<b>√</b>	V	<b>∨</b> ✓	<b>√</b>	<b>∨</b> ✓	<b>∨</b> ✓	V	<b>√</b>	C
Requirements		✓				<b>√</b>			✓	
Design Doc. API Doc.		$\checkmark$	$\checkmark$		<b>√</b>		<b>√</b>	<b>√</b>	<b>√</b>	U R
Test Plan		$\checkmark$			<b>v</b>	✓	<b>v</b>	<b>v</b>	<b>v</b>	и U
Test Cases	✓	✓	✓		$\checkmark$	✓	✓	✓	✓	U

**Table 3.** Comparison of Recommended Artifacts in Software Development Guidelines to Artifacts in LBM Projects (C for Common, U for Uncommon and R for Rare)

# 6 Comparison of Tools to Other Research Software

Software tools are used to support the development, verification, maintenance, and evolution of software, software processes, and artifacts [4, p. 501]. To answer RQ5 we summarize tools that are visible in the repositories and that are mentioned during the developer interviews. The tools for LBM are as follows:

**Development Tools:** Continuous Integration (CI), Code Editors, Development Environments, Runtime Environments, Compilers, Unit Testing Tools, Correctness Verification Tools

**Dependencies:** Build Automation Tools, Technical Libraries, Domain Specific Libraries

**Project Management Tools:** Collaboration Tools, Email, Change Tracking Tools, Version Control Tools, Document Generation Tools

Once the data on tools is collected, the use of two specific tools should be compared to research software norms: version control and CI. A little over 10 years ago version control was estimated to be used in only 50% of research software projects [13]. More recently, version control usage rates for active mesh generation, geographic information system and statistical software packages were close to 100% [21]. Almost every software guide cited in Table 3 includes the advice to use version control. For LBM packages 67% use version control. The high usage in LBM software matches the trend in research software in general. CI is rarely used in LBM (3 of 24 packages or 12.5%). This contrasts with the frequency with which CI is recommended in guidelines [1,5,29].

# 7 Comparison of Processes to Other Research Software

The interview data on development processes is used to answer RQ6. This data should be contrasted with the development process used by research software in general. The literature suggests that scientific developers naturally use an agile philosophy [2,19], or an amethododical process [10]. Another point of comparison is on the use of the frequently recommended peer review approach [8,14,30].

The LBM example confirms an informal, agile-like, process. The development process is not explicitly indicated in the artifacts. However, during interviews one developer (ESPResSo) told us their non-rigorous development model is like a combination of agile and waterfall. A loosely defined process makes sense for LBM software, given the small self-contained teams. One of the developers (ESPResSo) also noted that they use an ad hoc peer review process.

## 8 Developer Pain Points

To answer RQ7 and RQ8, we ask developers about their pain points and compare their responses to the literature [31,16]. Pain points to watch for include: cross-platform compatibility, scope bloat, lack of user feedback, dependency management, data handling concerns, reproducibility, and software scope.

An example pain point noted for LBM is a lack of development time. Small development teams are common for LBM software packages (Figure 1). Lack of time is also highlighted by other research software developers [16,15,31].

## 9 Threats To Validity

The measures in the measurement template [22] may not be broad enough to accurately capture some qualities. For example, there are only two measures of surface robustness. Similarly, reusability is assessed by the number of code files and LOC per file, assuming that a large number of relatively small files implies modularity. Furthermore, the measurement of understandability relies on 10 random source code files. It is possible that the 10 files that were chosen to represent a software package may not be representative.

Another risk is missing or incorrect data. Some software package data may have been missed due to technology issues like broken links. Some pertinent data may not have been specified in public artifacts, or may be obscure within an artifact or web-page. For the LBM example, the use of unit testing and CI was mentioned in the artifacts of only three (ESPResSo, Ludwig, Musubi) packages. However, interviews suggested a more frequent use of both unit testing and CI in the development processes. Given that we could not interview a representative for every project, to keep the measures consistent we did not modify our initial repository inspection based CI count.

# 10 Concluding Remarks

To improve the development of research software, both in terms of productivity, and the resulting software quality, we need to understand the current state of the practice. An exciting strategy to approach this goal is to assess one domain at a time, collecting data from developer interviews and digging deeply into their code repositories. By providing feedback specific to their domain, the developer community can be drawn into a dialogue on how to best make improvements going forward. Moreover, they can be encouraged to share their best practices between one another, and with other research software domains.

We have outlined a methodology for assessing the state of the practice for any given research software domain based on a list of about 30 representative projects. In addition to interviews, we use manual and automated inspection of the artifacts in each project's repositories. The repository data is collected by filling in a 108 question measurement template, which requires installing the software on a VM, running simple tests (like completing the getting started instructions (if present)), and searching the code, documentation and test files. Using AHP the projects are ranked for 9 individual qualities (installability, correctness and verifiability, reliability, robustness, usability, maintainability, reusability, surface understandability, visibility/transparency) and for overall quality. Perspective and insight is shared with the user community via the following: i) comparing the ranking by best practices against an estimate of the community's ranking of popularity; ii) comparing artifacts, tools and processes to current research software development guidelines; and, iii) exploring pain points via developer interviews. Using our methodology, spreadsheet templates and AHP tool, we estimate (based on our experience with using the process) the time to complete an assessment for a given domain at 173 person hours.

For the running example of LBM we found that the top packages engaged in most of recommended best practices, including examples of practising peer review. However, we did find room for improvement with respect to providing API documentation, a roadmap, a code of conduct, programming style guide, uninstall instructions and CI.

In the future, we would like reduce measurement time down by increased automation. We would also like to conduct a meta-analysis, where we look at how different domains compare to answer new research questions like: What lessons from one domain could be applied in other domains? What differences exist in the pain points between domains? Are there differences in the tools, processes, and documentation between domains?

#### References

- Brett, A., Cook, J., Fox, P., Hinder, I., Nonweiler, J., Reeve, R., Turner, R.: Scottish covid-19 response consortium. https://github.com/ScottishCovidResponse/ modelling-software-checklist/blob/main/software-checklist.md (August 2021)
- Carver, J.C., Kendall, R.P., Squires, S.E., Post, D.E.: 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. pp. 550-559. IEEE Computer Society, Washington, DC, USA (2007). https://doi.org/http://dx.doi.org/10.1109/ICSE.2007.77
- 3. Dong, A.: Assessing the State of the Practice for Medical Imaging Software. Master's thesis, McMaster University, Hamilton, ON, Canada (September 2021)
- 4. Ghezzi, C., Jazayeri, M., Mandrioli, D.: Fundamentals of Software Engineering. Prentice Hall, Upper Saddle River, NJ, USA, 2nd edn. (2003)
- van Gompel, M., Noordzij, J., de Valk, R., Scharnhorst, A.: Guidelines for software quality, CLARIAH task force 54.100. https://github.com/CLARIAH/ software-quality-guidelines/blob/master/softwareguidelines.pdf (September 2016)
- Grannan, A., Sood, K., Norris, B., Dubey, A.: Understanding the landscape of scientific software used on high-performance computing platforms. The International Journal of High Performance Computing Applications 34(4), 465–477 (2020). https://doi.org/10.1177/1094342019899451
- Hannay, J.E., MacLeod, C., Singer, J., Langtangen, H.P., Pfahl, D., Wilson, G.: How do scientists develop and use scientific software? In: Proceedings of the 2009 ICSE Workshop on Software Engineering for Computational Science and Engineering. pp. 1–8. SECSE '09, IEEE Computer Society, Washington, DC, USA (2009). https://doi.org/10.1109/SECSE.2009.5069155
- Heroux, M.A., Bieman, J.M., Heaphy, R.T.: Trilinos developers guide part II: ASC softwar quality engineering practices version 2.0. https://faculty.csbsju.edu/mheroux/fall2012\_csci330/TrilinosDevGuide2.pdf (April 2008)
- Kågström, B., Ling, P., Van Loan, C.: Gemm-based level 3 blas: High-performance model implementations and performance evaluation benchmark. ACM Transactions on Mathematical Software (TOMS) 24(3), 268–302 (1998)
- 10. Kelly, D.: 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. pp. 299–310. CASCON '13, IBM Corp., Riverton, NJ, USA (2013), http://dl.acm.org/citation.cfm?id=2555523.2555555
- 11. Michalski, P.: State of The Practice for Lattice Boltzmann Method Software. Master's thesis, McMaster University, Hamilton, Ontario, Canada (September 2021)
- 12. Nangia, U., Katz, D.S.: Track 1 Paper: Surveying the U.S. National Postdoctoral Association Regarding Software Use and Training in Research. pp. 1-6. Zenodo (Jun 2017). https://doi.org/10.5281/zenodo.814220
- 13. Nguyen-Hoan, L., Flint, S., Sankaranarayana, R.: A survey of scientific software development. In: Proceedings of the 2010 ACM-IEEE International Symposium

- on Empirical Software Engineering and Measurement. pp. 12:1–12:10. ESEM '10, ACM, New York, NY, USA (2010). https://doi.org/10.1145/1852786.1852802
- Orviz, P., García, Á.L., Duma, D.C., Donvito, G., David, M., Gomes, J.: A set of common software quality assurance baseline criteria for research projects (2017). https://doi.org/10.20350/digitalCSIC/12543
- 15. Pinto, G., Steinmacher, I., Gerosa, M.A.: More common than you think: An indepth study of casual contributors. In: 2016 IEEE 23rd International Conference on Software Analysis, Evolution, and Reengineering (SANER). vol. 1, pp. 112–123 (2016). https://doi.org/10.1109/SANER.2016.68
- Pinto, G., Wiese, I., Dias, L.F.: How do scientists develop and use scientific software? an external replication. In: Proceedings of 25th IEEE International Conference on Software Analysis, Evolution and Reengineering. pp. 582–591 (Feb 2018). https://doi.org/10.1109/SANER.2018.8330263
- 17. Saaty, T.L.: The Analytic Hierarchy Process: Planning, Priority Setting, Resource Allocation. McGraw-Hill Publishing Company, New York, New York (1980)
- 18. Schlauch, T., Meinel, M., Haupt, C.: DLR software engineering guidelines (Aug 2018). https://doi.org/10.5281/zenodo.1344612
- Segal, J.: When software engineers met research scientists: A case study. Empirical Software Engineering 10(4), 517–536 (Oct 2005). https://doi.org/10.1007/s10664-005-3865-y
- 20. Smith, B., Bartlett, R., Developers, x.: xsdk community package policies (Dec 2018). https://doi.org/10.6084/m9.figshare.4495136.v6
- 21. Smith, W.S.: Beyond software carpentry. In: 2018 International Workshop on Software Engineering for Science (held in conjunction with ICSE'18). pp. 1–8 (2018)
- 22. Smith, W.S., Carette, J., Michalski, P., Dong, A., Owojaiye, O.: Methodology for assessing the state of the practice for domain X. https://arxiv.org/abs/2110.11575 (October 2021)
- 23. Smith, W.S., Lazzarato, A., Carette, J.: State of practice for mesh generation software. Advances in Engineering Software 100, 53–71 (Oct 2016)
- 24. Smith, W.S., Lazzarato, A., Carette, J.: State of the practice for GIS software. https://arxiv.org/abs/1802.03422 (Feb 2018)
- 25. Smith, W.S., Sun, Y., Carette, J.: Statistical software for psychology: Comparing development practices between CRAN and other communities. https://arxiv.org/abs/1802.07362 (2018), 33 pp.
- 26. Smith, W.S., Zeng, Z., Carette, J.: Seismology software: State of the practice. Journal of Seismology **22**(3), 755–788 (May 2018)
- 27. Sood, K., Dubey, A., boyana norris, McInnes, L.C.: Repository-Analysis of Open-source and Scientific Software Development Projects (2 2019). https://doi.org/10.6084/m9.figshare.7772894.v2
- 28. Szulik, K.: Don't judge a project by its github stars alone. https://blog.tidelift.com/dont-judge-a-project-by-its-github-stars-alone (December 2017)
- 29. Thiel, C.: EURISE network technical reference. https://technical-reference.readthedocs.io/en/latest/ (2020)
- 30. USGS: USGS software planning checklist. https://www.usgs.gov/media/files/usgs-software-planning-checklist (December 2019)
- 31. Wiese, I.S., Polato, I., Pinto, G.: Naming the pain in developing scientific software. IEEE Software pp. 1–1 (2019). https://doi.org/10.1109/MS.2019.2899838
- 32. Wilson, G., Bryan, J., Cranston, K., Kitzes, J., Nederbragt, L., Teal, T.K.: Good enough practices in scientific computing. CoRR abs/1609.00037 (2016), http://arxiv.org/abs/1609.00037