Software development practices in academia: a case study comparison

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Abstract

Academic software development practices often differ from those of commercial development settings, yet only limited research has been conducted on assessing software development practises in academia. Here we present a case study of software development practices in four open-source scientific codes over a period of nine years, characterizing the evolution of their respective development teams, their scientific productivity, and the adoption (or discontinuation) of specific software engineering practises as the team size changes. We show that the transient nature of the development team results in the adoption of different development strategies. We relate measures of publication output to accumulated numbers of developers and find that for the projects considered the time-scale for returns on expended development effort is approximately three years. We discuss the implications of our findings for evaluating the performance of research software development, and in general any computationally oriented scientific project.

Keywords: scientific software, research software engineering, development practices, software evaluation

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1. Introduction

Computational simulation and analysis have become integral parts of scientific research in many disciplines. Research using large scale simulations is often a collaborative effort among scientists and engineers, and tends to require the combined use of multiple software packages developed by different groups. These efforts often involve a range of algorithmic fields such as discretization, mesh generation/pre-processing, domain decomposition, scalable algebraic solvers, statistical analysis, and visualisation. Given this reliance on software from multiple groups and specialities, it is important that the user of the software has confidence that the outcome of the computation is an accurate proxy for the system being modelled and that it delivers reproducible results. A rigorous quality assurance system, which helps deliver accuracy and reproducibility, is a common requirement for software deployment in industry, and it is increasingly recognised as an essential practice for scientific software development. Software engineering approaches form part of a quality assurance system, and may include methods such as waterfall, prototyping, iterative and incremental development, spiral development, rapid application development, and extreme programming [7, 27, 37, 28].

Software development practices in academia differ from those in the commercial sector. In the authors' experience, this is in part due to the relatively small and transient development teams found in academic settings, to project-focused development, and to the fact that academics are incentivized to attract funding and create publications, and usually care less about financial profit than commercial development. In addition, academic software development is rarely performed by full time code developers, and if so, these members are typically hired on short-term contracts with a focus on a specific subset of the code. Most scientific software is developed by researchers such as PhD students and PDRAs (post-docs) who split their time between code development and research activity. This dichotomy has led to a somewhat reluctant and heterogeneous adoption of rigorous software engineering practices in academic contexts. A survey conducted by Hannay et al. [18] reveals that developers of scientific software rely mostly on education from peers and self-study, and they have relatively little formal training in software engineering. Moreover, Hannay et al. found that scientists tend to rank standard software engineering practices higher when they work on larger software projects. Heroux et al. [19] list a number of software practices which they believe would be easy to adapt and would benefit most scientific software development teams. They also note that in the project under consideration, some practices were only applied to particularly challenging sections of code and relied on check-lists to make repetitive development and release operations less error-prone. Jalali and Wohlin [22] investigate the adoption of agile practices in distributed software engineering and find that similar problems in distributed development have been reported in multiple articles, possibly pointing to a need to better interpret the context of different experiences in software development. Recently, Naguib et al. [30] note fundamental differences between software in academia and in industry, i.e., academic software is more engineered to achieve high accuracy and stability, and less so to achieve comprehensibility, maintainability, and extensibility. Joppa et al. [23] have surveyed the attitude towards scientific software among species distribution modelers, and they find the "troubling trend" that scientists tend to make choices based on scientifically misplaced factors (e.g., the popularity of the software-based journal publication, while the software itself has not been formally been peer-reviewed). They concluded that learning from and acting on efforts in scientific software development will form an integral part of delivering models and software that meets high scientific standards.

In this work, we investigate development practices for four open-source scientific codes; Chaste² [36, 29], HemeLB³ [26, 16, 15, 31], Fluidity⁴ [33, 13, 6], and ESPResSo⁵ [25, 2]. These are codes with which the authors have had development roles, allowing us to analyse certain aspects of the development process which would not be accessible otherwise. In our investigation we review the evolution of the applied practices over the life-time of the codes and relate them to changes in the development team. We also discuss typical practices, such as agile methods with test driven development and code review, to what extent they have proven effective and have required modifications over time. Furthermore, we analyse the output in terms of publications generated using respective software packages in relation to other factors. In particular, we explore how invested effort in software development, and adopted practises, translate to scientific outputs. To the best of our knowledge, the impact of software development practices on scientific publication output has not been investigated systematically before,

²Chaste: http://www.cs.ox.ac.uk/chaste/

³HemeLB: https://github.com/UCL/hemelb

⁴Fluidity: http://fluidityproject.github.io/

⁵ESPResSo: http://espressomd.org/

and our analysis based on the four study cases is the first account in this direction. Our findings indicate a need to take software development efforts specifically into account when evaluating the output of science projects that rely on dedicated software development.

The remainder of this paper is organised as follows; in Section 2 we introduce the four case studies, along with their specific development practises. In Section 3, we present the methods used to collect the data on development practices, development team and code size and publications, and in Section 4 we discuss the changes in development practices over time. Finally, in Section 5 we investigate the relationship between code output and expended development effort.

2. Case Studies

2.1. Development, test, and profiling practices

We briefly summarise the development practices encountered in the four scientific software projects considered in this work. The purpose here is not to give a comprehensive overview of software engineering techniques, but to describe the specific practices that are applied in the case studies investigated below. The encountered practices also mirror the prevalent tension between the organizational culture in academia and the needs of sustainable software development and maintenance. In the authors' experience, long-term development efforts are sometimes hampered by short-term funding decisions which typically do not adequately reflect the potential impact of sustainable scientific software. The development and testing practices applied in the studied scientific software projects thus reflect specific ways chosen by the respective teams to overcome the aforementioned obstacles.

Development tools

The first step towards sustainable software development typically is the adoption of tools for version control and release management, automated build systems, and continuous integration tests. While this is arguably a rudimentary approach to software engineering, it can nevertheless lead to considerable improvements in the maintenance of scientific software.

Version control, or revision control, is used to keep track of all the modifications made to components of the software project over time. Revisions can be reviewed, compared, merged and restored whenever it becomes necessary at a later stage of the project. Version control systems allow members of the development team to work on the same files simultaneously, and provide mechanisms to resolve conflicts that arise from concurrent changes. A variety of modern revision control systems are available as free software, for example, Mercurial⁶, SVN⁷, and Git⁸.

Due to the heterogeneity of modern computing systems and software environments, compiling source code and linking to the necessary libraries has become an increasingly involved and time-consuming task. Build management tools such as the GNU Autotools⁹ or CMake¹⁰ provide a remedy by offering automated generation of the necessary steps of the build process, thus enabling developers to provision their software package on a variety of different hard- and software platforms.

Continuous integration [10] involves automated and periodic execution of unit tests and functional tests, ideally on a variety of platforms to ensure ease of deployment and correctness of the software on different platforms.

Scientific software often aims for HPC applications where parallel performance is of critical importance. Hence performance tuning and analysis are essential elements of the software development process. Whereas such aspects are typically not addressed by conventional software engineering strategies, it becomes increasingly obvious that scientific codes require performance profiling to be an integral part of the development and testing process. The Tuning and Analysis Utilities (TAU) [38] are an example of instrumentation and measurement techniques that are useful for regular and automated performance regression tests, which can be referred to as "continuous profiling".

Agile methods

Agile software engineering provides a set of lightweight software development techniques which are well suited for scientific software projects due to the flexibility offered and a close connection between development and usage aspects.

One specific agile methodology referred to in this work is derived from 'eXtreme programming' [3] comprising test-driven development and pair programming. Test-driven development involves writing a failing test for a de-

⁶https://mercurial.selenic.com

⁷http://subversion.apache.org/

⁸https://git-scm.com/

⁹http://www.gnu.org/software/autoconf/

¹⁰http://www.cmake.org/

sired functionality, prior to implementing any source code. Functionality is then added to the source code until the test passes. This ensures a good degree of test coverage for the code. In this work we distinguish between unit tests and functional tests. Unit tests cover small units of the code, for example individual classes and methods, while functional tests are more involved scripts that use the code as a black box to verify correctness of a certain functionality. The latter can also be useful to identify sudden regressions in overall accuracy. Pair programming [5, 40] is a form of code review in which two developers simultaneously work on the same code, and workstation. One developer writes code and the other reviews it. This helps to capture errors efficiently and also helps less experienced developers learn the code and development practices.

Another agile methodology that is adopted partially in one of the case studies is *Scrum* [37]. A key element of scrum are the basic development units called sprints. Sprints involve a planned program of work that is then implemented by the developers during a period of a week up to a month, followed by a review process. The main objective of a sprint is completion of the work into a deployable state, including tests and documentation of the implemented features.

2.2. Scientific software projects

Chaste

Chaste (Cancer Heart and Soft Tissue Environment) is a suite of objectoriented C++ libraries for simulating multiscale processes in biology. Chaste
has been in development, primarily at the University of Oxford, since 2005.
There are two main applications for Chaste: the first comprises a cardiac
simulation package which provides a way to use electrophysiology models in
tissue simulations using high performance computing. This package has for
example been used to predict a 2-lead human body surface electrocardiogram
(ECG) and its changes following drug administration [41]. The second application is a multiscale cell based modeling framework which allows the user
to develop simulations of multiple interacting cells using a variety of agentbased methods including: cellular automata, cell-centre-based (on and off
mesh), cell vertex and cellular Potts models. This framework has primarily
been used for studying cancer in the intestinal crypt, including a representation of cell mechanics (see e.g., [39, 32, 9]). For further applications see the
overview paper by Mirams et al. [29].

At present, Chaste contains approximately 500,000 lines of C++ code, with seven regularly (defined in the Methods section) committing developers. The development team primarily consists of academic researchers (PhD students, post-docs and research fellows), with dedicated developers occasionally hired on a per-project basis. The development team primarily aim to apply elements of Agile methods and eXtreme programming. The rationale for the application of these methods in Chaste is described in Pitt-Francis et al. [35], along with a detailed description of each method.

HemeLB

HemeLB is an open source lattice-Boltzmann simulation environment which has been largely developed by PhD students and post-doctoral researchers at University College London. It has been used to model flow in both cerebral arteries [21] and in retinal vasculature [4], and it has six regularly committing developers as of 2015. The code was first developed in 2005. From 2010 onward, it was extended with a host of new features and refactored into a more systematic structure thereby improving its clarity, accuracy and performance. This effort included the analysis of performance characteristics in great detail [16, 15] and the comparison of the accuracy of several boundary conditions and collision kernels [31]. Current efforts on HemeLB focus on improving the load balancing of the code, embedding support for deformable particles, and enhancing the inflow and outflow conditions [21]. The software is currently in use across about half a dozen institutions, primarily in the United Kingdom.

At present, HemeLB contains approximately 180,000 lines of code, written largely in heavily object-oriented and sophisticated C++, though some of the auxiliary tools have been written in Python. The development team uses Scrum and employs test-driven development including unit testing and functional testing within continuous integration.

Fluidity

Fluidity [33, 13, 34, 6] is a general purpose, multiphase computational fluid dynamics code capable of numerically solving the Navier-Stokes equation and accompanying field equations on arbitrary unstructured finite element meshes in one, two and three dimensions. It is primarily developed at Imperial College London and has been in development since 1999. Fluidity is used in a number of different scientific areas including geophysical fluid dynamics [6], computational fluid dynamics, ocean modeling and man-

tle convection (e.g., [33, 20]). Fluidity's partial differential equation simulator employs various finite element and finite volume discretization methods on unstructured anisotropic adaptive meshes. The software is parallelized using MPI/OpenMP and is capable of scaling to tens of thousands of processors [17, 24]. Other useful features are a user-friendly GUI and a Python interface which can be used to validate the user input, calculate diagnostic fields, set prescribed fields or user-defined initial and boundary conditions.

At present, Fluidity consists of approximately 500,000 lines of code, with 12 regularly committing developers. The developers employ test-driven development [12], and the development team is currently integrating TAU [38] in the agile development process. This serves to obtain performance feedback for each revision of the code.

ESPResSo

ESPResSo (Extensible Simulation Package for Research on Soft Matter [25, 2]) is a highly versatile software package for performing many-particle molecular dynamics simulations, with special emphasis on coarse-grained models as they are used in soft matter research [14, 8]. Its development started in 2001 at the Max Planck Institute for Polymer Research, Mainz, Germany. Since 2010 the ESPResSo project is maintained at the Institute of Computational Physics, University of Stuttgart, Germany. ESPResSo is commonly used to simulate systems such as polymers, colloids, ferro-fluids and biological systems, for example DNA or lipid membranes. ESPResSo also contains a unique selection of efficient algorithms for treating Coulomb interactions [1, 11]. More recently, several grid based algorithms such as lattice Boltzmann and an electro-kinetic solver have been implemented as well. ESPResSo is free, open-source software published under the GNU General Public License (GPL). It is parallelized using MPI and CUDA and can be employed on desktop machines, convenience clusters as well as on supercomputers with hundreds of CPUs/GPUs. The flexibility of the software is enhanced through a Tcl and Python interface, which allows the user to specify bespoke simulation protocols.

At the time of writing, ESPResSo consists of approximately 220,000 lines of code with 24 regularly committing developers. The contributors are distributed all over the world and the adoption of software engineering practices depends largely on individual commitment. The successful maintenance of ESPResSo relies on the use of software development tools, e.g., version control, an automated build system, and continuous integration.

3. Methods

We collected data for the number of developers and lines of code using the version control systems of each software. We retrieved this data from http://www.openhub.net for Chaste, HemeLB and ESPResSo (the project names there are respectively Chaste, HemeLB and ESPResSo_MD) and from legacy version control databases in the case of Fluidity (and partially for ESPResSo). We distinguish between three types of developers for each project. "Full Time Developers" are people hired specifically to develop the software full-time, "Frequet Research Developers" are researchers who have made more than one commit per month, and "Occasional Research Developers" are researchers who have made less than one commit per month, but have made more than one commit in a given year. This data was collected from 2005 onwards for Chaste and HemeLB, from 2006 onwards for Fluidity, and from 2001 onwards for ESPResSo.

We assessed the development practices based on our experience working with the respective codes (JMO and JG with Chaste, DG with HemeLB, XG with Fluidity and US with ESPResSo) and in consultation with the other members of the respective development teams. We categorised practices as being: i) regularly or strictly applied, ii) occasionally or partially applied or iii) rarely or not applied. We opted for generic descriptions that allow general changes in development practices to be identified over time and with changes in the size of the development team, without being overly prescriptive.

The number of publications are based on the number of publications that could be identified to be directly using the code within a calender year, with the aim of reflecting a publication list that a code's website may display. For Chaste and Fluidity a publication list was available on the code's website. For HemeLB and ESPResSo, the publications were identified through literature searches on Google Scholar and Web of Science, followed by manual inspection to filter out irrelevant results. For ESPResSo, the filtering resulted in between 50%-75% of the Google search results actually being included in the publication count. The number of publications was collected from 2005 onwards for Chaste and HemeLB (only data from 2006 onwards is shown below), from 2006 onwards for ESPResSo and Fluidity.

4. Results

4.1. Development Practices

The adopted development practices in relation to the size of the development teams are shown for the four case studies in Figure 1. Green glyphs correspond to regularly or strictly applied practices, amber to occasionally or partially applied and red to rarely or not applied practices.

Figure 1(a) shows the change in practices for Chaste. The development team of Chaste strongly emphasises software engineering practices [35], and aims to apply a consistent set of engineering practices at all times. The only practice that sometimes is not applied in full is pair programming. In smaller development teams, pair programming can become challenging as there are fewer experts at hand and it can be difficult to find suitable programmers for a specific pair programming task. However, code written by a single developer is often reviewed by another developer before being added to the repository.

Figure 1(b) shows the change in practices for HemeLB. The development team of HemeLB is considerably smaller than those of the other applications and comprises many contributors with a relatively short stay in the team. When several new members joined in 2010 and 2011, the development team was able to adopt a range of well-known engineering practices. Nevertheless, the presence of a large legacy code-base has resulted in various parts not being fully test-covered to this day. In 2014, the development team shrank considerably which resulted in a more loose application of the Scrum system, while many of the testing and development practices are maintained to ensure continued code stability.

Figure 1(c) shows the change in practices for Fluidity. Fluidity is developed and maintained by a large and distributed development team. Besides one constantly hired full time developer since 2006, the Fluidity development team has constantly more than dozens "Frequent Research Developers" until 2011. From 2011 on wards, the "Frequent Research Developers" start turn to "Occasional Research Developers" as the result of Fluidity getting mature. Since 2006, the Fluidity developers start to adapt the automated test-driven development approach, this including systematic unit and functional testing, and continuous integration.

Figure 1(d) shows the change in practices for ESPResSo. ESPResSo has a relatively large development team. Besides a core team of three research

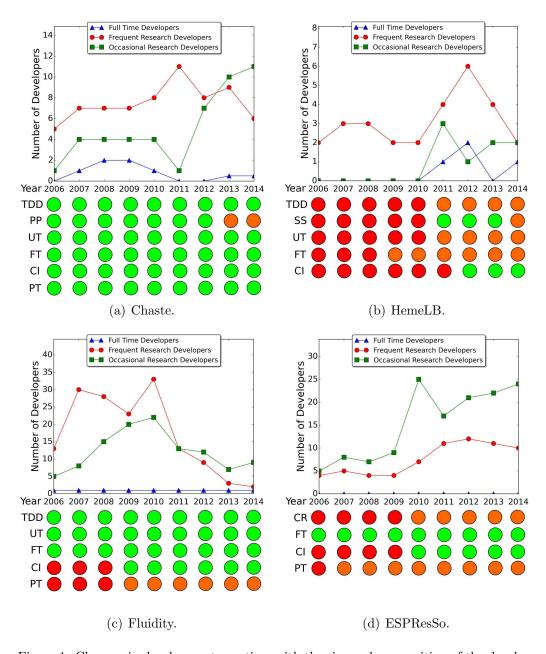


Figure 1: Changes in development practices with the size and composition of the development teams over the last nine years of development. Key: TDD-Test Driven Development; PP-Pair Programming; UT-Unit Testing; FT- Functional Testing; CI-Continuous Integration; PT-Profiling Testing; SS-Scrum Sessions; and CR-Code Review. Green corresponds to 'always applied', amber is 'partially applied' and red is 'rarely or never applied'.

developers, there is a considerable number of regular contributors and "remote" developers. In addition, the research group that maintains ESPResSo relocated twice since the first release. Therefore, it has proven difficult to install consistent software engineering practices, and the extent to which engineering principles are applied depends strongly on personal commitment of the individual developers. Generally, the ESPResSo developers aim to cover every feature by at least one functional test, and since 2010 continuous integration is employed.

4.2. Developer Input and Output

It is interesting to investigate the publication output of research software packages in relation to development effort. Figure 2 shows the number of published papers, code size and the number of active developers ("Frequent Research Developers" and "Full Time Developers") for each year from 2006 to 2014. Where applicable, we also provide information on the number of help tickets raised as a reflection of code development and use.

For the case of Chaste (Fig. 2(a)) the number of active developers has been reasonably constant. The number of publications per active developer largely increased over the first four years, decreasing thereafter. The number of tickets raised shows a behaviour similar to the number of publications.

For the case of HemeLB (Fig. 2(b)) the code base size has been closely linked to the size of the development team. In addition, increases in the size of the development team and the introduction of a ticketing system in 2011 are followed by a delayed increase in the number of publications.

For Fluidity in (Fig. 2(c)) the code size has been closely related to the active developers and the publications, the code size become more stable when the actively developers and publications goes down.

For ESPResSo (Fig. 2(d)) the number of active developers has increased considerably between 2009 and 2011, while the number of publications has remained roughly constant. This is in part a consequence of a considerable number of PhD theses and Faraday discussions that were written in 2009 and 2010, prior to the increase in developers. Therefore, the data points in these years lie higher and subsequently screen the increase expected based on the number of active developers.

4.2.1. Development Effort and Publications

In order to investigate the impact of software development efforts, we analyze the publication output in relation to the accumulated development

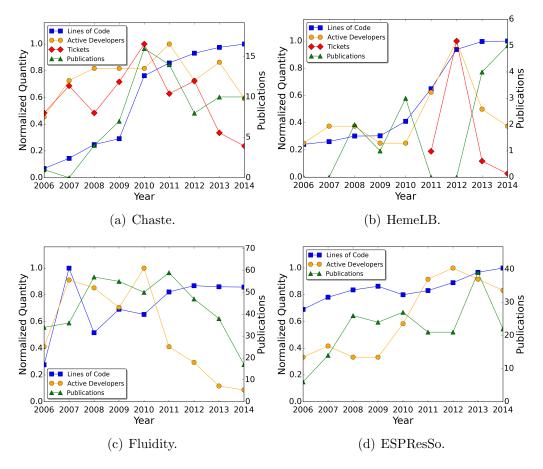


Figure 2: Changes in the size of the development team, code base, number of submitted tickets, and publications over the last nine years of development.

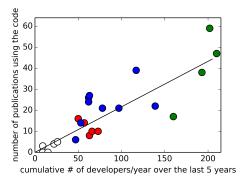
effort. In Fig. 3, we present the number of publications in a given year as a function of the cumulative number of developers over the last last five years (a) and three years (b), respectively, for the four case studies. The scatter plots show that an increased commitment to software development efforts, as measured by number of developers, results in more publications based on these software packages. We performed a linear regression resulting in a slope of $y = 0.71 \times x$ for the five year data and $y = 0.49 \times x$ for the three year data. Both regressions have P < 0.0001, although the regression on the three year data resulted in a higher R-value (R = 0.86) than the one on the five year data (R = 0.78). Note that in Fig. 3 we included the maximum number of data points available in each case study, which varies between the software packages due to the different time span for which developer and publication data was collected (see Sec. 3 for details).

We have also related the number of publications in a given year to the number of developers in each of the five preceding years, respectively, and performed a similar regression analysis for all five relations with results as shown in Tab. 1. We find that there is a strong effect of the number of developers on the number of publications which only levels off after three years. In other words, the software development efforts of our case studies reveal a lasting impact which can not be appropriately reflected by measuring publication output on a short term basis. The full merit of a software project may thus not be accessible until at least three years after the conclusion of development.

A number of factors have not been taken into account here, such as the impact of the venues of each publication (e.g., Chaste publications tend to be less numerous, but quite highly cited) and the exact effort invested by individual developers (i.e., all contributors are treated at equal value in this assessment). In order to address the latter, we have also performed the analysis using a weighting system for development effort (1.0 for full-time developers, 0.5 for researcher-developer, and 0.25 for occasional developers) which resulted in an outcome very similar to the un-weighted assessment shown here.

5. Discussion

We conducted and compared four case studies of software development practices in academia, and analysed the adoption of software engineering practices, the development effort invested, and the publication output over



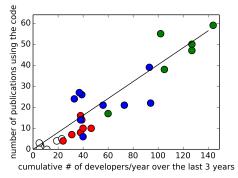


Figure 3: Scatter plot of the number of publications in a given year as a function of the cumulative number of developers in the preceding five years (left) and three years (right). Data points are plotted for Chaste (red), HemeLB (in white), Fluidity (green) and Espresso (blue). The black lines are the result of a linear regression on the data sets.

Table 1: Relation of historical development effort to publication output shown for individual years, ranging from the first year prior to publication (first data row) to the fifth year prior to publication. For each year we report the slope of the correlation found (in publications per active developer that year) in the second column, and the obtained P-values, R-values and standard errors respectively in the third, fourth and fifth column.

Years ago	slope	P-value	R-value	stderr
1	1.11	1.7e-11	0.879	0.11
2	1.07	4.2e-10	0.884	0.10
3	0.99	3.8e-8	0.824	0.13
4	0.71	3.0e-4	0.652	0.17
5	0.73	2.1e-3	0.607	0.21

a period of at least nine years. We find that the publication output of the four scientific codes correlates strongest with the development effort invested in the three years prior to publication, and that each of these years of effort appear to contribute equally to the publication output. The correlations become noticeably weaker when we compare the publication rate with the development effort invested four or five years earlier.

Based on our results, we conclude that the four considered software projects should ideally have been reviewed three years after development efforts have been concluded. This conclusion may be inconvenient given that performing a final scientific review three years after the conclusion of a research project can be impractical, in particular since a large number of academic software development grants are less than three years in duration. In fact even the initial efforts of shorter projects cannot be fully assessed by the final review if the evaluation takes place directly upon the conclusion of such a project. There are several ways to mitigate this problem. Firstly, by funding software projects for at least 3 years reviewers can accurately assess the scientific publication impact of the initial efforts at the time when the project finishes. Secondly, review panels could choose to base their review not directly on peer-reviewed publications, but take into consideration important preliminary components, such as new documented code features, simulation data sets and preprints or paper drafts. Thirdly, for long-running development on academic software, reviewers could choose to limit their review of the project at hand to the technical aspects, and judge the academic software on its scientific potential in a wider context, taking into account the publication impact of preceding comparable projects.

Although development effort invested in these projects have resulted in a publication boost, many of the resultant publications do not feature the original developers as (prominent) authors. For example, two major contributors to HemeLB only featured on a single first-author paper each, after investing three years of development effort. Similarly, a developer contributed the lattice Boltzmann implementation to ESPResSo which has enabled a host of subsequent publications of other authors directly using this code. Therefore, the correlations we presented can not (and must not) be used to assess individual contributions to the publication output, or to the software more generally.

Indeed, publication numbers only partially describe the impact of an individual developer or even a short-term project effort, as they indirectly reflect more fundamental impact, such as technical quality, ease-of-reuse and the presence of valuable new features (these metrics are arguably more difficult to quantify, measure and compare). In addition, although we find these correlations for our four case studies, a much larger investigation is required to assess the relationship between invested development effort and scientific impact for academic software in general.

In terms of adopted software development practices we find that, in particular for HemeLB and ESPResSo, new practices are typically adopted when a development team has recently increased in size. In the case of HemeLB and Chaste, the application of individual practices was slightly reduced when the respective development teams became smaller, but this effect seems to be more limited. More generally, software development practices, once first

applied, appear unlikely to be abandoned later on. This could indicate a high level of satisfaction from the development team regarding the adoption of these practices. While a larger study will be required to assess the efficacy of software engineering practices in computationally oriented research communities in general, our study indicates that the use of software engineering principles improves the quality of the research software and leads to a concomitant increase of the publication output.

Acknowledgements

The authors would like to thank: Dr. Tim Greaves, Dr. Matthew Piggott and Dr. Gerard Gorman for help with data collection and interpretation of the Fluidity software package; the Chaste development team for discussions regarding data collection for the Chaste package; and Axel Arnold and Olaf Lenz for valuable discussions regarding collection and interpretation of data for the ESPResSo software package. This work was spawned as a collaborative project during the first 2020 Science & Software Sustainability Institute Paper Hackathon which took place in Flore, Northamptonshire, United Kingdom in September 2014. This work has been funded by the Computational Horizons in Cancer (CHIC) project under EU FP7 grant agreement number 600841 (JG), the CRESTA project under EU FP7 grant agreement number 287703 (DG,US), and the UK Engineering and Physical Sciences Research Council under grant numbers EP/I017909/1 (www.2020science.net, DG,JG,JMO) and EP/I034602/1 (US).

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