

Status of reproducibility and open science in hep-lat in 2021

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As a fully computational discipline, Lattice Field Theory has the potential to give results that anyone with sufficient computational resources can reproduce, going from input parameters to published numbers and plots correct to the last byte. After briefly motivating and outlining some of the key steps in making lattice computations reproducible, this contribution presents the results of a survey of all 1,229 submissions to the hep-lat arXiv in 2021 of how explicitly reproducible each is. Areas where LFT has historically been well ahead of the curve are highlighted, as are areas where there are opportunities to do more.

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1. Introduction

There has been increasing pressure from many sides in recent years to embrace the principle of open science, and to ensure that data analyses are reproducible. As the software used to analyse data has become increasingly complex, it has become less and less feasible to unambiguously explain in a traditional journal publication exactly what steps were carried out, to the point that another researcher could reproduce them. As enabling this is one of the key aims of academic publication, this trend poses a clear problem, which research funders, journals, and others are looking to address.

As a purely computational field, Lattice Field Theory (LFT) stands to be more severely affected than most fields. However, LFT is also one of the very early adopters of many principles of Open Science. The latter fact, specifically the ubiquitous use of freely-available preprints for written publications, has enabled the work presented here: an analysis of all 1,229 submissions to the arXiv [1] preprint server in the hep-lat category in 2021, to assess where the field is strong and where there remain opportunities for improvement.

2. Terminology

In this work, *reproducible* is used as defined by the Turing Way project [2]: that given the same data, another researcher can repeat the same analysis and obtain the same results. This definition may seem trivial at first glance, as it seems obvious that the same analysis on the same data should give the same result; however, it is a prerequisite of the more challenging concepts of *replicability* (being able to apply the same analysis to fresh data and obtain the same results), and *robustness* (being able to apply different analyses to the same data and obtain compatible conclusions).

Since the mapping from human languages to programming ones is not one-to-one, for any non-trivial software then access to the code is an essential part of reproducibility. Similarly, for data beyond those that can be presented in a handful of tables, access to the raw data is also needed. Removing the possibility for human error is another way to improve reproducibility; every manual step in a process is a place that could be done inconsistently (either within a work, or between the original work and attempts to reproduce it). The primary purpose of computers is to automatically perform repeated tasks in a consistent way, so encoding manual workflows in software significantly reduces the possibility for human error, and where errors do creep into code, then they can be inspected and discovered after the fact.

Open science is the movement that all research—including not only publications, but also physical samples, data, software, and other outputs—should be accessible to all by default (barring specific ethical or legal constraints, for example when working with private personal data). Theoretical particle physics pioneered the use of open-access preprints for publications, and remains a leading field—in many disciplines preprints are still seen by many as a novelty. (For example, in a survey of 3759 researchers [3], 46% of respondents in medical and health sciences had never viewed or downloaded a preprint, and 63.6% of the same cohort had never authored one.)

Data and software published openly can (and should) be FAIR: specifically, *findable*, *accessible*, *interoperable*, and *reusable*. This is a separate consideration to the data being made available publicly—data that will never leave a research group still benefits from new researchers to the group being able to easily find it, and conversely it is entirely possible to share data in un-FAIR ways.

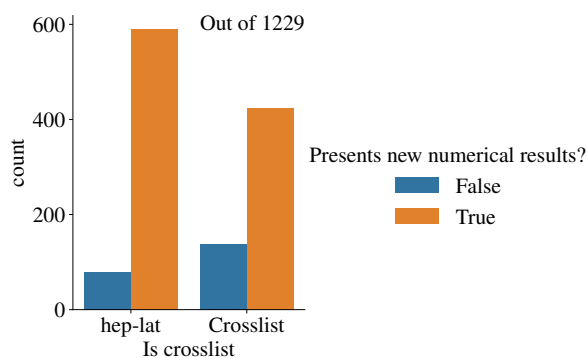


Figure 1: Breakdown of submissions to the hep-lat arXiv in 2021 indicating whether they had hep-lat as their primary arXiv or were crosslists, and whether they presented new numerical results.

Making data and software FAIR increases the uses that others can make of it, and hence makes it more valuable.

3. Survey results

The 1,229 submissions to the hep-lat arXiv (including those cross-listed into the category) were surveyed for some aspects affecting the reproducibility of the work done. The questions were answered based on a combination of full-text search for relevant keywords and a brief skim read of the contents. The complete survey data, and the analysis scripts used to prepare the plots presented here, are released separately [4]. The analysis was performed using Python [5], pandas [6], Matplotlib [7], and seaborn [8], via a Jupyter Notebook [9].

Following the principle of findability, and that a paper should include sufficient information to be able to reproduce it without hunting elsewhere, information not included in the preprint was not considered when completing the survey. This excluded information added in published manuscripts but not updated on the arXiv, and also excluded information that could be found by digging through a collaboration’s website.

Figure 1 shows an initial breakdown of the submissions; a small majority had hep-lat as their primary category, with the remainder being cross-lists. A substantial majority of both cases—1013 in all—included numerical results (e.g. a plot that was not merely schematic, or numbers with uncertainties not quoted from another publication); it is this subset that will be the focus of the remainder of the analysis.

Since one step towards reproducibility is to specify the software used, an initial question to ask is what proportion of submissions do this. As a baseline, this is compared with the proportion of submissions that acknowledge the use of a high-performance computing (HPC) facility. These are of similar difficulty—adding one or two sentences—and fulfil a similar purpose, in demonstrating the utility of the software/facility and ensuring that its development or activities continue to be funded. Figure 2 presents the breakdown of submissions for these questions. The vast majority of submissions presenting new numerical results with hep-lat as the primary arXiv (referred to hereafter as *hep-lat numerical submissions*) acknowledge the use of an HPC facility. However,

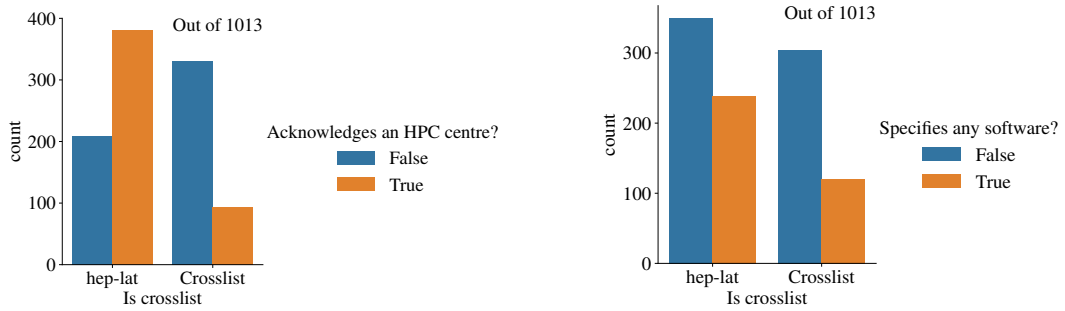


Figure 2: Breakdown of whether submissions to the hep-lat arXiv in 2021 that included new numerical results acknowledged an HPC resource (left panel) or specified any of the software used to generate their results (right panel).

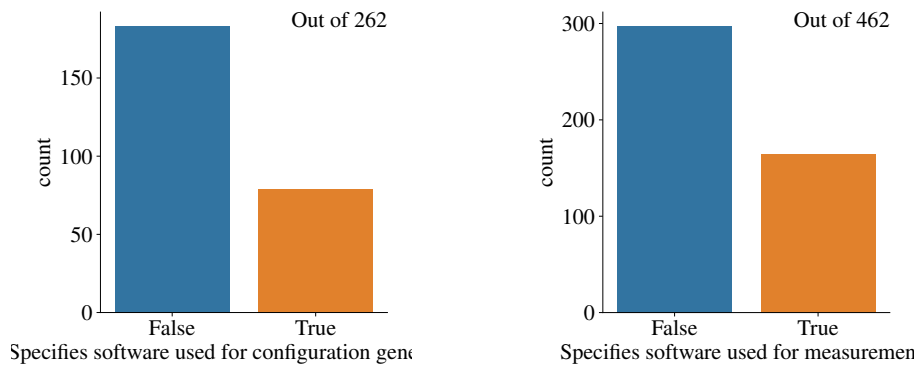


Figure 3: Breakdown of whether submissions to the hep-lat arXiv in 2021 that generate new field configurations (left panel) or measure observables on field configurations (right panel) specify the software that was used to do this.

fewer than half of hep-lat numerical submissions specify or acknowledge any of the software used. This is potentially the simplest change for authors to make; while citing software isn’t sufficient to ensure reproducibility if custom code has been written, it significantly reduces the barrier while also recognising software developers’ contributions to the research.

The survey takes a relatively reductive view towards categorising the work done in LFT: it is assumed that a typical piece of work may generate field configurations using a Monte Carlo-like algorithm, may compute observables on such configurations (generated as part of the same work or otherwise), and will do some kind of statistical analysis on data resulting from one or both of the previous two steps. (Alternative approaches including tensor networks and quantum simulation have their software effort considered in the “analysis” category; their count is sufficiently small that this is not considered to introduce significant bias.)

Generation of configurations is the most computationally expensive activity in LFT, and the associated software suites have had corresponding amounts of effort put into ensuring they are robust and efficient. Steps taken to ensure the reproducibility of generation include having deterministic seeded random number generators, and having detailed log files and storing metadata in configura-

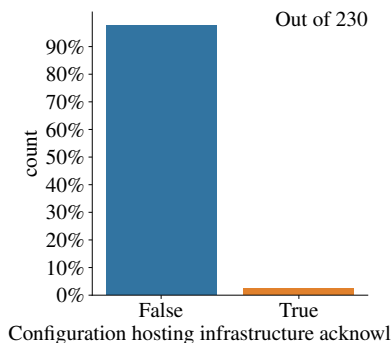


Figure 4: Plot showing the proportion of submissions to the hep-lat arXiv in 2021 making use of existing gauge configurations that acknowledge the infrastructure used to host and serve them.

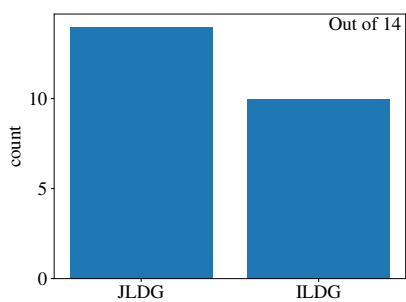


Figure 5: Breakdown of the infrastructure acknowledged by those submissions in Fig. 4 that do acknowledge hosting infrastructure.

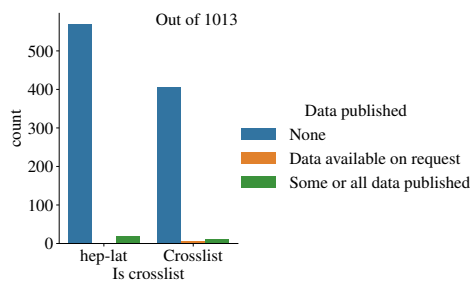


Figure 6: Breakdown of submissions to the hep-lat arXiv in 2021 that publish any of the data they generate.

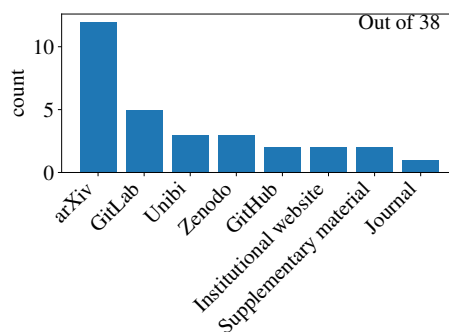


Figure 7: Breakdown of the repositories used to host data published by the authors of the submissions indicated in Fig. 6. Unibi is the institutional repository of the University of Bielefeld.

tions recording what version of a piece of software was used and on what machine. Computation of observables from these ensembles is typically the next most expensive activity, and frequently uses some of the same software infrastructure.

Figure 3 shows the proportion of submissions that specify the software used for each of these activities. Less than one in three of the 262 submissions generating new configurations specified the software, and a slightly larger proportion of the 462 submissions measuring observables on configurations did.¹ Given that due to differences in normalisations and other undocumented conventions, running two different codes with the same parameters can give differing results, this is a barrier to reproducibility of this effort.

Where configurations are not generated as part of the work, they must be obtained from somewhere. This may be a collaborations own storage, or publicly-available ensembles may be used. In either case storage infrastructure must be used, and in the latter case a facility for finding

¹In each case, some of the software specified was toolkits such as Grid [10] and Chroma [11], where significant amounts of additional code (e.g. XML or C++) is needed to perform the work being reported; this additional code was not typically found to be shared or specified.

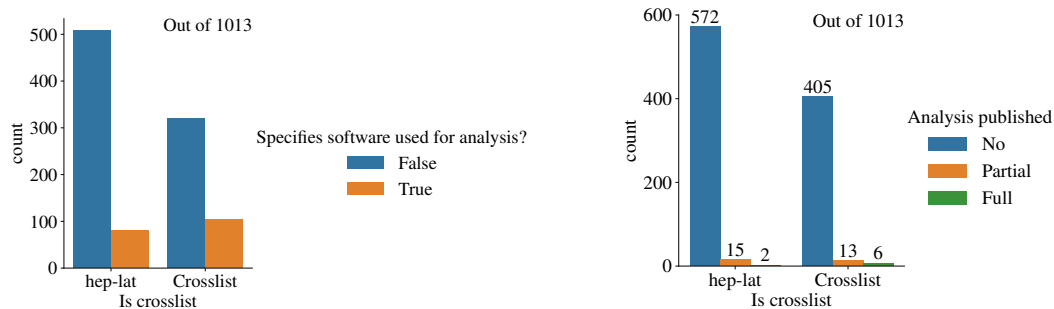


Figure 8: Breakdown of submissions to the hep-lat arXiv in 2021 that generate new numerical results that specify any of the software used for the analysis of the data presented (left panel), and those that publish the full or partial software workflow for this analysis (right panel).

and sharing the configurations. The International Lattice Data Grid (ILDG) provides schemas and specifications for such services, which have been deployed in a number of Regional Grids (RGs). This was a very early example of FAIR data sharing not only in LFT but in all of academia; it in fact pre-dated the coining of the “FAIR” acronym itself. Being the first in the space has however meant that tooling development in the surrounding world has moved on, and left the ILDG tooling unmaintained. Only 14 of 230 submissions using existing configurations acknowledge the hosting and sharing infrastructure used (Fig. 4), all of which acknowledge the Japan Lattice Data Grid (Fig. 5), reflecting the dormant state of the ILDG project and the RGs. Working groups have now however resumed work on ILDG to modernise it, with the support of new funding, as discussed in ILDG’s joint contribution [12].

Publications can also share data other than field configurations. Typically being smaller in size, these require less infrastructure so can be shared with generally-available data repositories such as CERN Zenodo. An advantage of using such a repository over using a regular code or web hosting service is that they will typically provide a persistent identifier (PID) such as a Digital Object Identifier (DOI), which gives a reference that will not change over time (e.g. when a researcher changes their GitHub username, or institution), and a commitment to remain available in the moderately long term (unlike services such as GitLab, which recently announced older repositories would be made unavailable after a period of inactivity, with only a few weeks’ notice²). Sharing data in this format, rather than relying on tables in a PDF file, makes collating data from multiple sources and re-using it in other work significantly easier, and removes the significant likelihood of errors occurring when transcribing data. Figure 6 illustrates that this is not yet common practice in LFT, while Fig. 7 shows a significant reliance on code hosting services like GitHub and GitLab that do not provide persistent identifiers or a guarantee of longevity. The phrase “data available on request” is commonly used in some areas of science where sharing of data is required by publisher policy but authors have not prepared it; in some cases this has led to significant delays in access to data as requests are ignored [13]. This phrase has yet to catch on in LFT.

The final part of the survey considers the data analysis of LFT data, i.e. the process that takes in the data produced from configurations on HPC facilities and outputs the plots and tables shown

²This decision was later overturned due to public outcry, but there is no barrier to the situation occurring again.

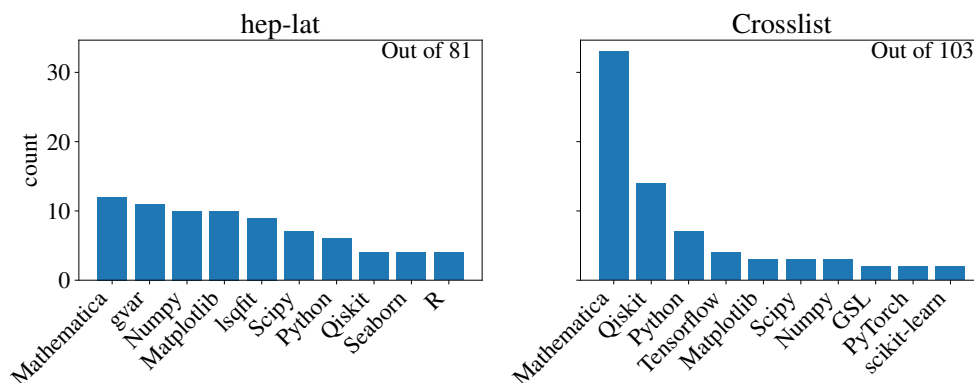


Figure 9: Breakdown of the top ten specific pieces of analysis software referred to by submissions to the hep-lat arXiv in 2021 that acknowledged such software.

in the submissions. Many areas of experimental science have reproducibility efforts, and these have experimental facilities in place of deterministically-generated field configurations, and take measurements on these facilities that are not expected to give machine-precision identical results when repeated; the reproducibility effort focuses on ensuring that the data from experimental measurements always gives the same numerical results once analysed. As discussed above, encoding these procedures into software and sharing that software is the only feasible way to do this unambiguously.

Figure 8 illustrates that fewer than one in six hep-lat numerical submissions specified any of the software used. The most popular tools referred to are shown in Fig. 9; most are programming languages or frameworks rather than computation-specific tools. Also shown in Fig. 8 is that only two of these submissions included the workflow allowing another researcher to fully reproduce the analysis performed. This represents a significant opportunity for growth. A parallel survey, the initial results of which are reported in a separate contribution [14] indicates that significantly more work is enabled by workflows that are at least partially automated; publication of these would significantly boost the reproducibility of the data analysis phase of LFT computations.

4. Conclusions

While LFT has in many cases been at the forefront of open science, being one of the first disciplines to embrace open-access preprints and being ahead of its time with FAIR data for field configurations, there are some areas that suffer from a “first-mover disadvantage” where work is ongoing to realign with more modern tooling, and others where there is an opportunity to learn from the example of other disciplines.

Some low-hanging fruit to improve the reproducibility of publications include specifying and acknowledging publicly-available software that has enabled the research presented, and making existing software workflows available (and citing them in work that uses them). Taking manual processes and automating them so they can be published is more challenging, in particular doing so in a way that can be run end-to-end without intervention. There is work to be done to write tools that

will enable this to be done more easily; this work will be informed by a parallel survey of individual researchers' practices in this area, whose initial results are reported in a separate contribution [14].

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