CAD we share? Publishing reproducible microscope hardware.

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Here we discuss barriers to reproducibility of microscopes and related hardware, along with best practices for sharing novel designs using Computer-Aided Design (CAD). We hope to start a fruitful community discussion on how instrument development, especially in microscopy, can become more open and reproducible, ultimately leading to better, more trustworthy science.

Introduction

Microscopy has often been at the heart of new biological discoveries, and as cutting-edge experiments become more complex, so as the new microscopes required to image them. This has led to rapid growth in interdisciplinary collaborations to develop novel instruments. Increasingly, this has been done using reusable building blocks.

Many scientists successfully use Computer-Aided Design (CAD) software to design custom parts, assemble setups from their components, and render graphics. However, these detailed and reusable designs are rarely archived openly. In recent years, funders and publishers have formulated extensive guidelines and policies on data and software sharing in the context of Open Science [1][2][3]. Conversely, hardware development and its publication lack suitable standards to ensure completeness and quality of the design that is shared, even though such standards are available [4][5]. Indeed, there is often no requirement to share hardware designs at all. The usual practice of including a parts list and rough schematic in Supplementary Material is frequently incomplete and insufficient to reproduce the instrument without extensive involvement of the original authors. We believe the community of researchers, journals, and grant bodies should start treating design files as Research Data.

In this paper, we discuss how CAD and improved publication of design files can make the scientific process more open, reproducible, and valuable. Using and properly sharing CAD file accelerates dissemination of scientific knowledge, allows reproducibility at lower cost, permits its reuse and improvement, and so promotes innovation in the rapidly evolving field of biological imaging. Here we start the conversation about this vision, the associated difficulties, and how to overcome them.

Reproducible hardware with CAD

Reproducing a novel scientific instrument can be a lengthy process. First, specific off-the-shelf components must be obtained, and any custom-made parts must be fabricated. Then, the component parts must be assembled into a complete instrument. Finally, it must be aligned, commissioned, and put into use. With the advent of rapid prototyping technologies such as 3D printing and on-demand machine shop services, scientists are increasingly adopting these tools in research [6][7][8][9]. A CAD can describe both custom-made and commercially available parts and assemble these parts into complete instruments (Fig. 1). This is a convenient way to create and share the manufacturing instructions for custom parts, an accurate bill of materials describing off-the-shelf parts, and information about how the components fit together into a complete instrument.

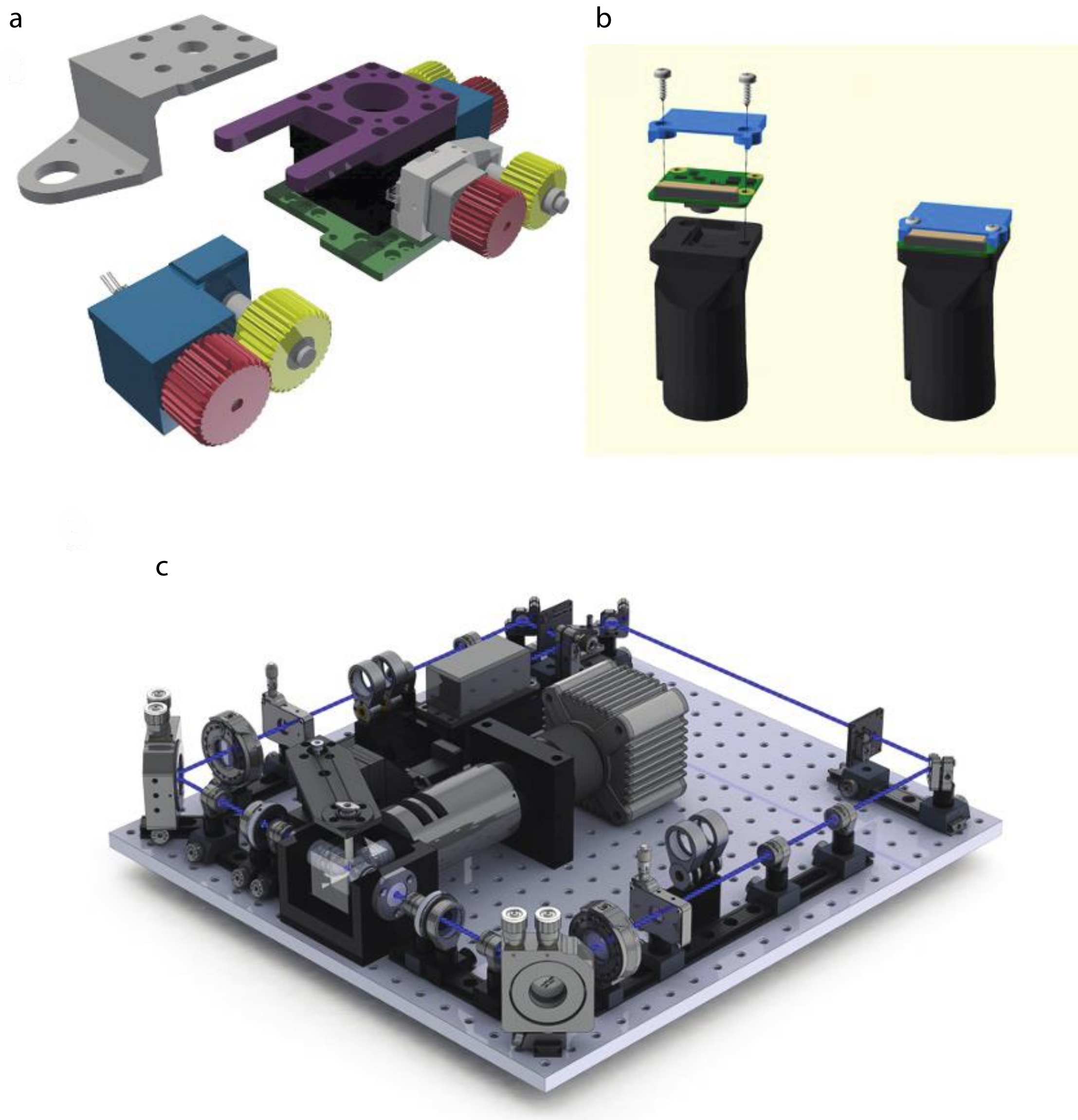

Figure 1. CAD helps produce dimensionally accurate images and assembly instructions. (a) A mechanical assembly including custom parts from the UC2 toolbox modelled in Autodesk Inventor. (b) Assembly of the OpenFlexure optics module, rendered using OpenSCAD. (c) an assembled OpenSPIM showing beam path, modelled with SolidWorks. Figure a,b) are recreated under CC-BY 4.0 license.

A complete set of CAD files can provide most of the information required to reproduce a design of a hardware part or system, though usually a comprehensive set of assembly instructions is also required. A CAD file that is not shared, or is shared only in an inaccessible format, makes reproducibility difficult and costly. Improving the design may then require the part to be re-created from scratch in suitable format (an inefficient and time-consuming process). It is crucial that design files linked to published works are archived in long-term repositories with stable links such as digital object identifiers (DOIs).

CAD behind closed doors

The use of 3D schematics to present protocols, workflow and instrument designs is commonplace and supported by the emergence of specialized journals and social platforms such as Nature Methods, JOVE, HardwareX and Journal of Open Hardware. These visually appealing schematics spark interest and provide useful conceptual understanding. A short survey of Nature Methods papers (2009-2020) reveals that the majority of publications do employ some form of CAD but crucial files are missing, particularly photographs and CAD files (Figure 2). More than half of the papers present CAD renderings, but do not attach original files to the publication. This is not a technical accessibility issue, as 5 out of 50 papers do provide extensive files in the Supplemental Data section.

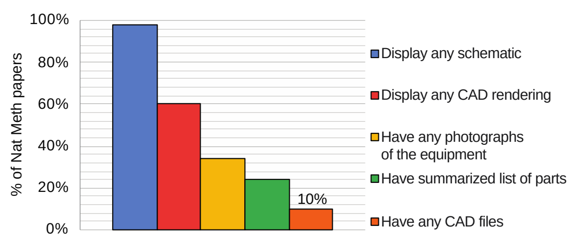

Figure 2. Design of hardware is under-shared in publications. Survey of microscopy-related publications in Nature Methods that include any amount of information related to design of the experimental setup. Many publications use CAD by-products (renderings), but few publications present any CAD files. When files are made available, the formats are very inconsistent. Source data

Hardware design is data

Requiring existing CAD files in their original, editable format as well as exported formats that are easier to view or print will not create undue burden, but instead increase value to the readers and allow higher degrees of reproducibility, improvements, and adaptability. In our opinion, a design that is presented but not properly shared suggests a conflict of interest that ought to be declared; it suggests that the manuscript is promoting a product that is (or will be) commercialized without allowing full scrutiny and reproduction of the science. This is inconsistent with policies on data and code, which already require a statement linking to original files, or explaining why this is not done. Not every hardware design uses CAD, and so editable CAD files may not exist - but where they do exist, sharing them ought to be the default course of action.

CAD file formats

There are many different CAD systems, each with its own native file format, and very few are inter-compatible (see online repository https://github.com/HohlbeinLab/OpenMicroscopy [10]). Most of these are commercial products with expensive licenses, meaning a given institution rarely has access to all of them. This creates a huge barrier to collaboration between institutions or companies and can result in researchers losing access to their own work when they take a new position. Some cloud-based CAD platforms are now available, often at no cost but with no guarantee of future accessibility. Open-source CAD solutions are also available, which are free from restrictive license terms, but currently offer a less polished user experience. Manual technical drawings are an alternative to CAD, and if used correctly can convey information that is just as complete. However, a skilled draftsperson is needed to produce them, and subsequent modifications can be more difficult. It is also more difficult than with CAD to check whether a design is properly constrained and self-consistent.

Most CAD packages allow parametric modeling, where the final 3D object is described in terms of meaningful dimensions and geometric constraints. Typically, 2D “sketches” or technical drawings are used to define geometry that is then converted to 3D, and both the sketches and the operations to make a 3D model are retained (Fig. 3). Alternatively, primitive 3D shapes can be combined in different ways to build up a more complex model. In either approach, the editable CAD file has much more information than the final shape, as the relationships between different dimensions, and the sequence of operations required, must be retained to change the design effectively.

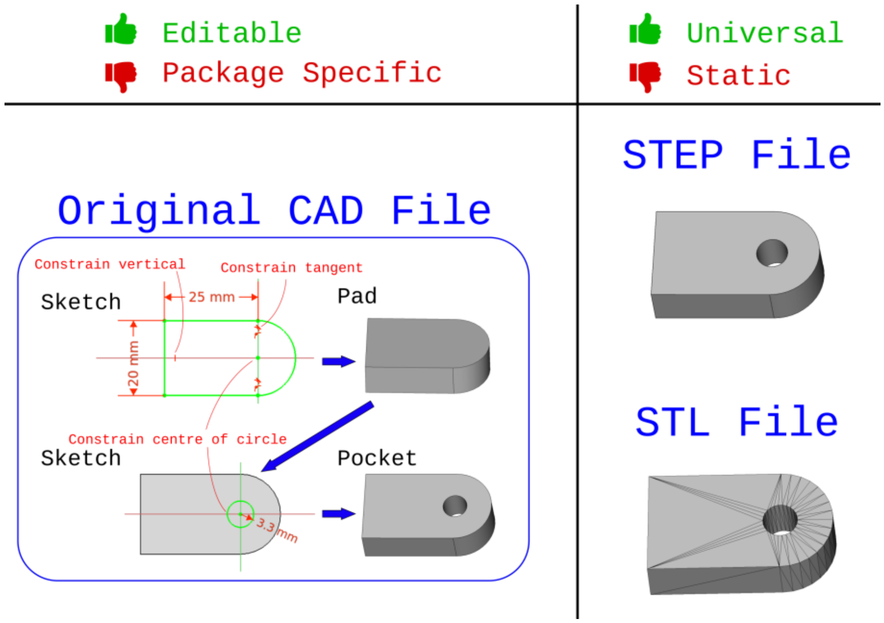

Figure 3. CAD file formats offer a trade-off between compatibility and editability. Native file formats are specific to particular CAD packages but preserve full parametric control and editability. STEP and STL files preserve shape, but not design constraints and parameters.

Custom parts are exported from the CAD package into a transfer format that can be interpreted by a CNC (Computerized Numerical Control) machine or 3D printer. These files allow interoperation of different systems, but lack the parametric information needed for meaningful editing. The *de facto* standard for 3D printed parts is an STL file (STereoLithography), where the model is represented by a triangular mesh that can be viewed or printed but is hard to modify. STEP files (Standard for the Exchange of Product Data; [11]) can preserve assembly arrangement and material properties such as the color of parts, can accurately represent complex 3D objects including curved faces, and can be edited more easily than STL meshes. Many CAD packages have reverse engineering tools which allow STEP and STL files to be edited. This editing, however, is limited in scope since the original design constraints are lost.

Most CAD packages can export technical drawings for manual machining, and these often preserve more of the original design constraints. Good technical drawings can also make it easier for others to design accessories or incorporate a piece of apparatus into another experiment. However, reconstructing the editable CAD model based on drawings is a laborious process.

A universal parametric CAD format would solve a great many technical issues, not only for microscopy but for many fields in industry and in academia. For now, the best solution is to include both the proprietary, native CAD file and as many exported formats as is possible and appropriate for a particular design, including renderings and technical drawings. As with data, it is always important to document the files, which are the originals and which are generated, and to ensure any information not contained within the CAD files is properly documented.

Constructing assemblies with off-the-shelf parts

Optical supply companies such as ThorLabs, Newport, Edmund Optics, McMaster-Carr and recently also the microscopy manufacturer Olympus provide CAD models of their components. This allows designers to check compatibility, preservation of optical axes, and physical constraints before purchasing and building a system. It also allows for the design of specific parts ahead of assembly (e.g. adapters with specific threads). This may be done with only main details of the part, such as rough outline and main openings, but can also go further, adding specific optical elements such as mirrors and lenses to see how the housing will accommodate them, or designing and planning for every screw. A CAD model can even be used to simulate or optimize a system's optical performance [12][13][14].

Creating a virtual assembly can save time and reduce wasted effort procuring incompatible parts, as well as making it easier to share precise designs. Automatically generated bills of materials can make it much easier to obtain all the parts for a system, and exported images make publication-ready informative figures (Figure 4). Assemblies can be represented using many of the CAD formats described previously, and the same recommendation applies: both the native files and appropriate transfer formats (including bill of materials) should be archived as part of a complete design.

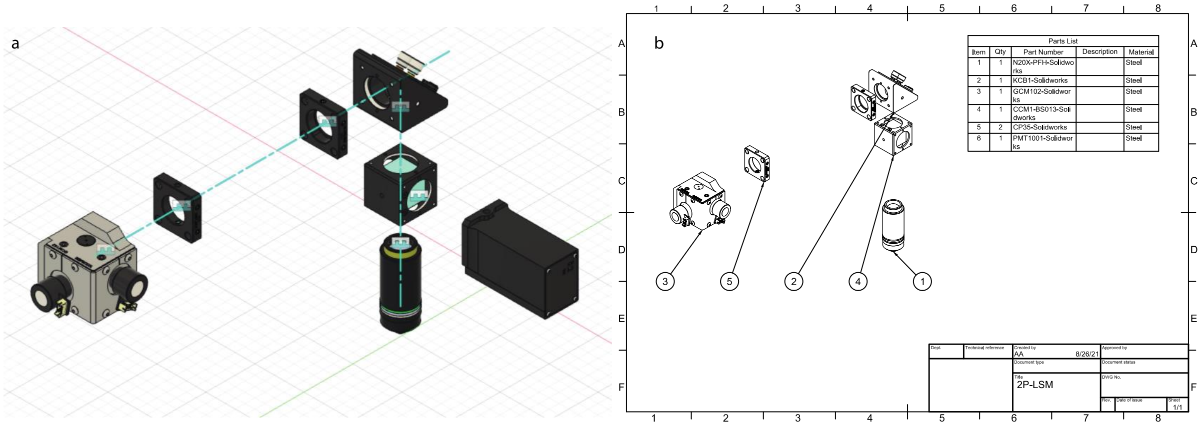

Figure 4. Virtual assembly of setups from commercial parts allows design, rendering, and sharing. (a) Virtual assembly can quickly create an instrument from off-the-shelf parts. Distances and angles can be precisely set, and conflicts checked and avoided early in design. (b) Technical drawings and bills of materials are generated from the model.

Intellectual property and commercialization

Software and data are now routinely archived openly in support of published research, and funders usually require a statement detailing access arrangements and justifying any restrictions on sharing as part of each publication. Moreover, many universities and institutions have established policies regarding open science policies often related to government guidelines and funders. Hardware designs, however, are often handled quite differently [15].

Universities typically require researchers to allow their IP office to “protect” promising technologies with invention disclosures or patents, so that the institution can attempt to license future use of the work. Patents are one way to publicly communicate an idea, protecting that idea from being patented by another entity, but filing is expensive and takes months, and thus is usually delayed until a strong business case can be made. If a novel instrument is to be patented, designs cannot be openly shared until patents are filed. However, sharing a design openly creates “prior art”, therefore acting like a patent to stop other entities patenting the design. This saves both the cost and time of registering a patent, but the researcher must usually obtain the University’s agreement to share designs without patenting them. Often this means publications of designs are delayed and the use of this data in conferences, job interviews, etc. is limited unless a Non-Disclosure Agreement (NDA) has been signed. Consequently, a great many hardware designs are neither patented nor shared openly. Patents (even if they are never exploited) are often counted when evaluating researchers, this provides an incentive for individual scientists to opt for patenting a design, even when open sharing of a design would provide many of the same benefits more quickly and cheaply.

There is a need for clarity on the cost-benefit rationale of this patent-by-default approach as well as the relationship between public funding of research and the IP system in financed institutions: the software community has demonstrated that commercialization and openness are not opposed [16]. Companies such as the open source pipetting robot Opentrons [17] and the 3D printer manufacturer Prusa [18] who release their entire hardware and software sources suggest that a rethink is taking place in industry as to the importance of patents for hardware products. Hardware requires resources and *know-how* to produce, especially for scientific instruments, and thus customers are usually willing to pay for a quality product from the original manufacturer even if it could be legally supplied by another company. Suppliers of optomechanical parts and even companies that sell microscopy hardware are starting to provide detailed design files for easier adaptation [19], recognizing that this improves their product and is good for business. The possibility of building an active community of users and developers holds great potential for long-term customer relations.

Most journals provide a "conflict of interest" section for authors to disclose financial relationships relevant to their work. It is commonly accepted that hardware designs may not be shared due to patent and licensing concerns, but this is often not stated explicitly and so is not considered in the review process. Failing to disclose full hardware designs is detrimental to the reproducibility and credibility of an experiment, and a paper describing a novel, proprietary instrument blurs the distinction between advertising and research - a factor that we argue should be noted by editors and reviewers when deciding to accept such a work and declared as a conflict of interest. It is also important that the authors familiarize themselves with rules of their funders and institutions. Requiring a statement justifying why designs are not shared fully, as is already done for code and data, would provide an incentive to researchers and universities to decide to either patent or release instrument designs, rather than keeping them a secret.

Resources and guidance

Our primary recommendation for researchers sharing a new hardware design is to include both the original, native CAD file and all appropriate transfer formats, drawings, and bill of materials information, in a permanent archive associated with the publication (DOIs, University data archives, or other stable repositories). Detailed guidance on structuring and sharing a hardware project are available from Open Hardware Makers [20] or OSHWA [4]. As an example, established open projects such as OpenSPIM [21], UC2 [22], OpenFlexure [23], and MesoSPIM [24] aim for documentation that links STL files, native CAD files and assembly tutorials to maintain easy replication. One can publish a design on available platforms including accessible wiki solutions [25], hardware-specific platforms that include viewers for common formats [26][27][28], and software-focused platforms [29][30] allowing extensive, custom automation [31]. A well formulated list of metadata to include is given by the Open KnowHow specification [32]. Most of these platforms do not offer permanent archival or DOIs, so we recommend archiving a snapshot of the design with Zenodo or another permanent repository.

Conclusions

When building new experimental setups, we follow design process. Computer-aided design (CAD) allows better and faster engineering, and can make the design of experimental setups open, reproducible, and adaptable. Making these files available will lead to faster, more consistent, and more reproducible biological experiments. However, nowadays while CAD is an essential tool for designing and presenting new hardware, not every researcher fully utilizes these benefits due to lack of training, complexity of tools, or absence of guidelines. In the case of published works primarily describing a novel instrument design, the time is ripe to establish a culture of best practice to improve the reproducibility of this work. We see how reproducibility and openness create new scientific communities that work together, so sharing and documentation of designs ensure that projects stay alive in the long-term, even if the original creators are no longer involved and offer the advantage of decentralized data collection and evaluation.

There are technical barriers to sharing designs fully. CAD files are usually either proprietary, restricting their usefulness to researchers with access to specific commercial packages, or incomplete, describing a final shape but not the design constraints required to edit it. The goal of fully interoperable CAD files is a long way off, and while promising open software exists, it is unlikely to replace proprietary systems soon. However, sharing both the native files and the appropriate transfer formats and documentation is a reasonable solution that can be implemented immediately.

Organizational barriers and deterrents are more difficult to mitigate. University policies on intellectual property are at odds with the principles of Open Science, often resulting in valuable designs being neither shared nor commercialized. We argue that treating hardware designs in the same manner as software or data, specifically requiring an explanation in the paper if designs are not fully shared, is an important action that journals and funders can take to help drive a shift in culture and policy.

Even small changes made by the scientific community can realize the benefits of sharing CAD files in a manner compatible with Open Science. Editors and reviewers should scrutinize works that claim to share designs but omit crucial files, or even better enforce proper file sharing and policies as is already done for data. Researchers can use guidelines like OSHWA's [4] and workshops like the Open Hardware Makers [20] to document hardware effectively. Ultimately, it is essential that global standards for CAD are developed, and become part of good scientific practice, so that curating design files is considered as important for the reproducibility of experiments as documenting biological protocols. International frameworks should better document how to use existing repositories, where essential design files will be stored for longer than a grant lifetime. Ideally, global funding schemes should create the basis for the development of open-source yet professional CAD packages that allow scientists to share reproducible results regardless of restrictive licenses or financial situations. Because we believe that the community of researchers, journals, and grant bodies should start treating design files as research data.

Data and Code Availability Statement

Data presented in Figure 2 available in Supplemental Data file and GitHub repository https://github.com/HohlbeinLab/OpenMicroscopy (https://doi.org/10.5281/zenodo.6406820)

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Author Contributions

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Competing Interests Statement

Authors declare no competing interests

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