

Electronic Supplementary Information for 3D Printing Crystallographic Data Piecemeal for Post-Printing Construction

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1 Details of Supplementary Information

This PDF contains a series of tutorials for the techniques outlined in the main paper, a flowchart outlining the and the various choices that must be made, as well as some tables giving additional details of the work performed. In addition to this there are a series of video tutorials showing these techniques being performed. Finally, the final, successful versions of each 3D printing file is also available in the ESI.

2 Detailed instructions for colour coding and exporting 3D printable files from Mercury

The first step to printing crystallographic data is to convert the data from a crystallographic data file to a 3D printing file. The main procedure we use for this is via Mercury, and that is the procedure we outline here. This is due to the fact that, as far as we know, Mercury is the only crystallographic software to support exporting colour information, which makes the cutting much easier in most cases. However, there is nothing inherent in the connectors that demands the use of Mercury, so the export features of Chimera or PyMol or other software can be used instead and coupled with the technique in Section 5.

This procedure is adapted from that used previously to print either ball and stick or ellipsoidal data from Mercury.^{1,2}

First open the CIF file in question in Mercury.

Second, alter the structure shown on screen to match what you want to print by hiding sections you don't want to print (hydrogen atoms, counterions, etc.) and generating parts you do want to print with short contacts, hydrogen bonds, or specific contacts. How to expand a structure in this manner is beyond the scope of this ESI, and will be familiar to people who have used Mercury before. However, it is advised to do this as little as possible, as Mercury has a tendency to overlaying multiple cylinders on top of one another for its bonds when you do this, which can make printing difficult. The better option, if possible, is to click the "Packing" switch at the bottom of the screen and use the following instructions to edit down your structure from that.

Remove any parts you do not want to print, either by using the *Show/Hide*→*Hide Atoms* right-click command, or the *Delete this Molecule* right-click command. The structure to be printed must be one continuous unit; that is, when it is finished printing it must be one single physical object: For example, you can't print two parts of a non-coordinating anion/cation pair, though you could export each piece to a separate 3D printing file.

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Third, the structure must have physically meaningful dimensions for printing. Go to the *Manage Styles* . . . drop down list and select the “3D print” setting (This assumes you want to use the default “3D Print” style in Mercury, and that they have not been changed³).

Fourth, colour the atoms to separate them into the units you want to print. Note: This is much easier if all the connectors are oriented into the same print plane, or perpendicular to the print plane. Another way of thinking of this: Draw an imaginary cube around each subunit you plan on printing. Every connector should be directly pointing at one of the faces if possible. If this is not possible, continue as normal, placing as many of the connectors as possible to align with the print direction, and see Section 6. If none of the connectors can be aligned in this manner, colouring the structure is unnecessary and can add complications, as the cuts will be put in manually. Instead set the structure to be monocoloured, and export the file as outlined below (either STL or WRL files can be used from here on since colour won't matter in this case), and consult section 6. Now colour the atoms you want to group into a subunit the same colour. This can be done by selecting the atoms you wish to colour, then using the right-click command *Colours* and then selecting the colour you desire. Note that the *Lasso Atoms* tool can make selecting atoms much faster.

Finally, once you have all the subunits coloured as you desire, go to *File*→*Print in 3D* . . . Set the file format to “VRML (colour)”, the output directory to wherever you want the file saved and click print. A Virtual Reality Markup Language (VRML, or *.WRL file) will be generated in that directory. Next use the software of your choice to separate the coloured parts

3 Separating the parts into separate files

The next step in most structures is to separate the parts by colour so that you have two (or more) pieces to add the connectors to.

There are two ways to separate the parts into colours. Most of the work for this paper was done with Magics as outlined in Section 3.2, due to existing expertise with that software. However, due to the cost of that software package serving as a potential limitation on the adoption of this technique, an investigation was undertaken and it was found that the colour separation can be done just as well using MeshLab, though MeshLab (Section 3.1) does not have the same features for repairing structural issues as Magics. There are other tools to repair 3D printed files, though their use falls outside our area of expertise, and given how rapidly this area is developing, we thought investigating this better left to the reader.

3.1 Procedure for using MeshLab to separate parts by colour

The open source and gratis software MeshLab from the Visual Computing Laboratory, the Istituto di Scienza e Tecnologie dell'Informazione and the Consiglio Nazionale delle Ricerche can be used to separate parts by colour. This procedure was tested with MeshLab_64bit_fp v2016.12.⁴

First, import the VRML file into MeshLab. Then use the *Filters* Menu, submenu *Color Creation & Processing* [sic] and select *Transfer Color: Face to Vertex* [sic] and press *Apply*.

Then, for each coloured, section go to the *Filters* Menu, submenu *Selection* and select *Select Faces by Color* [sic]. Click on the block of colour next to *Color To Select* [sic], which will open the “Pick a Color” [sic] window. Click the *Pick Screen Color* [sic] button, and click on the specified subunit. If there are any similar colours on the structure (such as red and orange), adjust the “Variation from” values downwards to ensure that only the clicked colour is selected. Click *Apply*. If multiple colours are highlighted when you click *Apply*, press the *Default* button and press *Apply* again to unselect everything (assuming you didn't use black as a colour, since it is the default. If you did, then find a colour totally unlike anything you used and select that.) Adjust the “Variation from” values downwards and try again.

Then open the *Filters* menu again, submenu *Mesh Layer*, and select *Move selected faces to another layer*. This will create a new layer that can be separately saved to a STL or VRML file with the *Export Mesh As...* command in the *File* menu.

3.2 Procedure for using Magics to separate parts by colour

This procedure is written for Materialise's *Magics* (v19.0.1.11) and may need to be adapted to other versions of the software.

First open your file: *File*→*Import Part*.

Second: Separate your part by colours: *Tools*→*Split Part by Color* [sic].

Third: Unload any parts you do not want to print by right clicking on the part and selecting the "Unload Selected Parts" option (It looks like a green cube with a red x in the lower right hand corner. If in doubt, a tooltip will pop up after a second or two.)

Fourth: Save each part to the hard drive with a descriptive name. This procedure generates a lot of similar files, and it is easy to confuse them. This is done by selecting the part you want and right-clicking on it. The save icon looks like a 3.5" floppy disk with a green cube in the lower right hand corner. For those who don't know what a floppy disk is, it is the standard save icon with a green cube in the lower right hand corner. There is a bug in this version of *Magics* that causes it to save everything in VRML files as 100x smaller than they are. This can lead to detail being lost, and eventually the file will not load correctly, due to the small size of the objects within it being approximated as zero. Therefore, after this point, the authors use STL files to avoid this bug. VRML files do have a much smaller file size however, and can be used if the structure is resized to be 100x larger before saving (Control-R to open the rescale menu).

Fifth: Unload all but one part as the fixing commands only work on one part at a time.

Sixth: Go to *Fixing*→*Fix Wizard* or press Control-F. This opens the Fix Wizard. It should be noted that this order of operations was developed and found to be reasonably reliable with structures imported from Mercury.⁵ Run the Diagnostics tool by pressing *Update* with all the checkboxes except for "overlapping triangles detected" and "intersecting triangles detected" checked. These two flaws have been found to rarely impede successful printing and fixing them often leads to damage to the structure so they are either ignored, or left until last. Ignore the suggested order and go to *Shells*, **not** *Noise Shells*, in the right-hand menu. Select the *Automatic Fixing* option and inspect the damage to the structure. This will work most of the time, as long the structure was not repaired **before** being separated into parts: however it may not work for more complicated structures with overlapping bits. The various methods of fixing this are somewhat beyond the scope of this tutorial, but I suggest playing around with the options, finding small, almost non-existent, shells and removing them first, then try automatic fixing again. Either way, after every fix, examine the structure for damage and use the undo command if there is any damage (Control-Z, the same as in a word processor). If that doesn't work, try playing around with the other fixes. Go back to the diagnostics page and update the list of errors. The automatic fixing of the shells should have removed most or all of the remaining errors. Go through any remaining flaws starting with Normals one by one, again checking for damage to the structure each time. At this point you might as well try the "overlapping triangles detected" and "intersecting triangles detected" options, though be careful, as they often lead to damage to the structure. Once the structure is fully repaired, save it as a new file, again, as either an STL or VRML but avoiding the shrink by a factor of 100 VRML bug if it is present in your version of the software. Close this part, open the next part you wish to print, and repair it in the same manner. Repeat this for each part, then move on to importing them into the CAD editor of your choice to add the pegs and slots.

4 Adding connectors to the parts using Solidworks

Now that the structure has been separated into multiple parts, the connectors can be added.

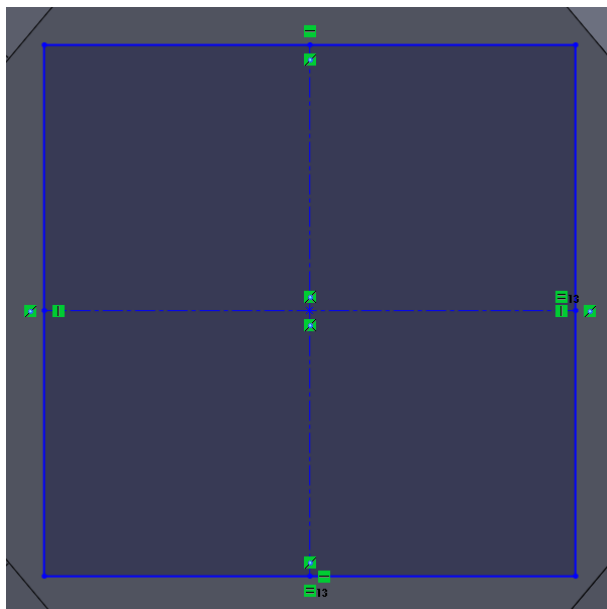
These instructions are a general outline, rather than the more specific steps for Meshlab and Magics. This is due to the fact that there is a wide variety of CAD software available that could be used for this step, and there are likely more efficient ways to reach the same results. Additionally, a large number of closely related tasks must be done, and it would be impractical to list every one step by step. However, to aid in demonstrating this task, several video tutorials have been included to help illustrate the steps.

4.1 A simple square connector

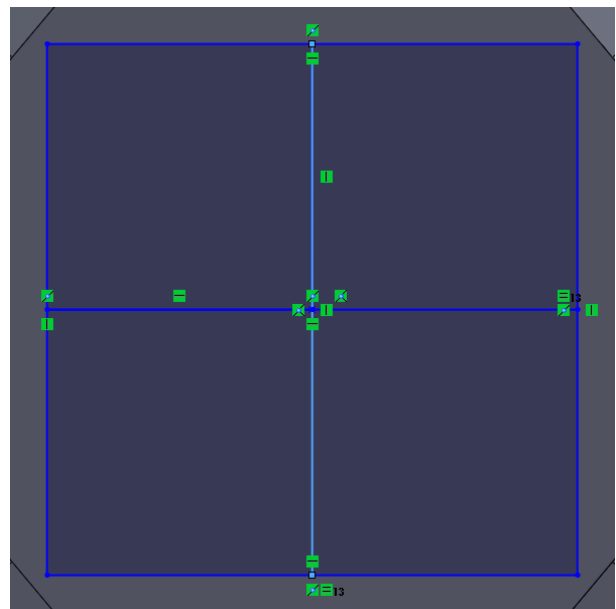
Open the STL or VRML structure in Solidworks and make sure it imported as a solid and not a surface. If it imported as a surface, the repair features can usually be used to correct this. Sometimes you will need to re-export it from Mercury as the other type of file format, or scale the file to twice or half size to get Solidworks to accept it as a solid and not a surface.

Then a sketch must be placed on the flat surface of the face of the bond. In the best case scenario, the face will be a single surface and have the centre of that surface at 0,0 or marked with a point. In this case, use that point as the centre of your connector. If none of these things are true, see subsection 4.2 for the workaround.

Once you have your centre point, use that as a basis for a square of appropriate size. Now go to the *Features* tab and use either the *Extruding Boss/Base* (for a peg) or *Extruded Cut* (for a slot).



(1a) The primary square without anything removed: It has 4-fold rotational symmetry.



(1b) Draw two lines connecting the midpoints of the opposite sides of the primary square. Now you have the centre of the square marked.

4.2 If Solidworks does not provide you with a clean surface or does not mark the centre point

This section details several complications that you may come across while using Solidworks. It is hard to explain these problems if you haven't encountered them, so they are demonstrated in the attached video tutorials.

If the centre point is not marked (most of the time), it can be located using the line tool. The software

uses polygons to approximate cylinders, thus leading to the faces at the end of the bond being polygons instead of circles. Use the line tool to draw lines between opposite vertices of the polygon until you have determined the centre of the polygon. Then use the point tool to mark the centre of the surface and draw the connector based on that. If you get an ugly mess of intersecting shapes, simply ignore it. Most of the time it will not impact the sketch. If inserting a slot into that surface leaves a remnant, simply trace the relevant portion of the connector onto the problematic surface and add another slot on that surface.

4.3 Removing rotational symmetry

As outlined in the paper, when assembling structures it is convenient to remove rotational symmetry from the connectors to avoid errors when assembling the structure. However, this can lead to errors during the design stage, which are harder to fix, though we hope software support will remove this problem.

This design of rotational-symmetry free connectors is created by ‘subtracting’ squares from the main shape to form the connector into the desired shape. There are two ways to do this.

One is to manually determine an appropriate size and draw a square of that size starting at the corner of the connector. This works quite well if the sides of the primary square forming the connector are an even integer value, and the direction of the connector matches the natural way Solidworks wishes to align your square.

If neither of these are the case (for example, if you want to use a connector for which the primary square has a side of 3.141 mm, or if you are finding it difficult to draw a square in that orientation using Solidworks) there is a simple method to place consistently sized squares within your primary square. Solidworks will let you attach lines to the midpoints of other lines, and this can be used to divide your connector up into smaller squares. This technique is demonstrated in Figures 1a through 3b.

5 Using Solidworks to cut structures at arbitrary points

If the software you are using (such as Chimera or PyMol) does not output coloured files, then Solidworks can be used to cut them at arbitrary points. As shown in Section 6, this can also be used to help with the printing of troublesome structures that don’t have a way of aligning the bonds with or parallel to the print tray.

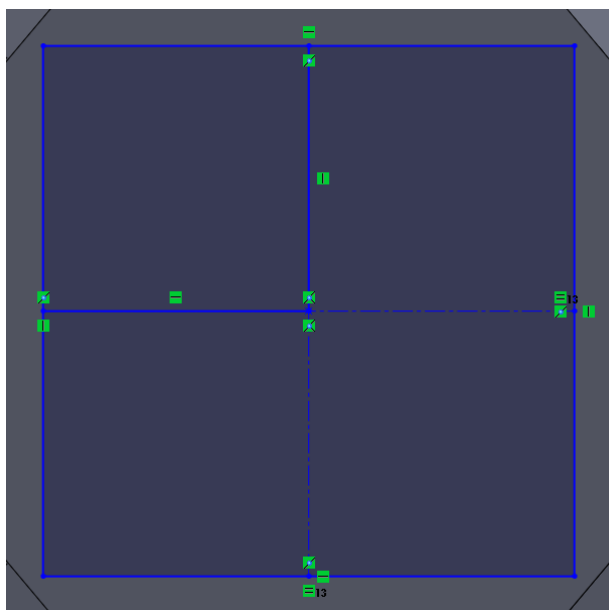
To do this, first make one of the reference planes (“Front Plane”, “Top Plane”, and “Right Plane” in the left-hand tree) visible. This is done by right clicking on the plane and selecting the appropriate option from the popup menu.

While there is not a specific video tutorial for this, it is shown as part of the video tutorial for adding connectors to structures whose bonds do not align with the print tray.

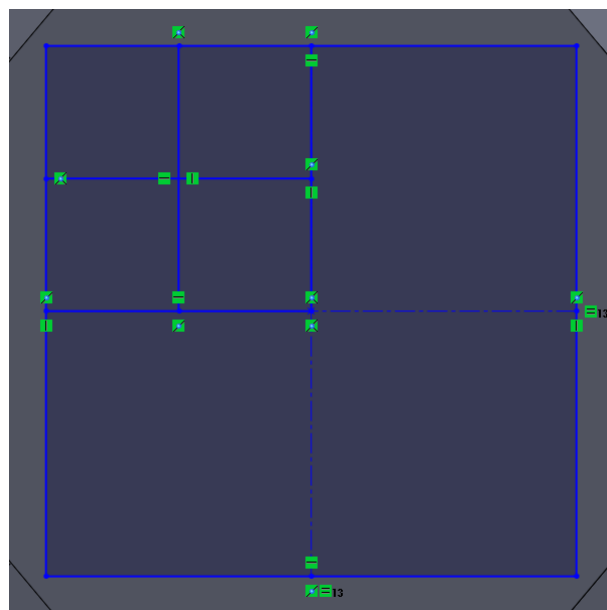
Go to the *Features* menu → *Reference Geometry* to add a plane at the appropriate point. The easiest way to do this is to offset the new plane from one of the reference planes (and this is the only way the authors done it), but it is possible to use up to three reference items to position the plane exactly as you wish.

Select your new plane, then select *Insert* → *Cut* → *With Surface*. Select the direction you wish to delete. If this leaves more than one unconnected object, you will get a popup asking which to save. Select the one you want and save it. Then press the undo button (or press control-Z if on Windows), and repeat the cut, but this time save the other object. You now have two files, each with one of the objects you need to add a connector to.

This description may have to be adapted to more complex situations, such as that shown in Section 6, but the general principles are the same.



(2a) You also have divided the square into quarters. This will let you use the *Trim Entities* tool to remove the walls of the primary square to make an L-shaped connector. If you require more complicated connectors, draw lines from the midpoint of the sides of the primary square to the centre, overlapping the lines you just drew. This will let you repeat this process, by using the midpoints of these new lines to further subdivide the squares. In this diagram the lines connecting one side to the other have been removed to highlight the new lines, but this is not needed in normal practice.



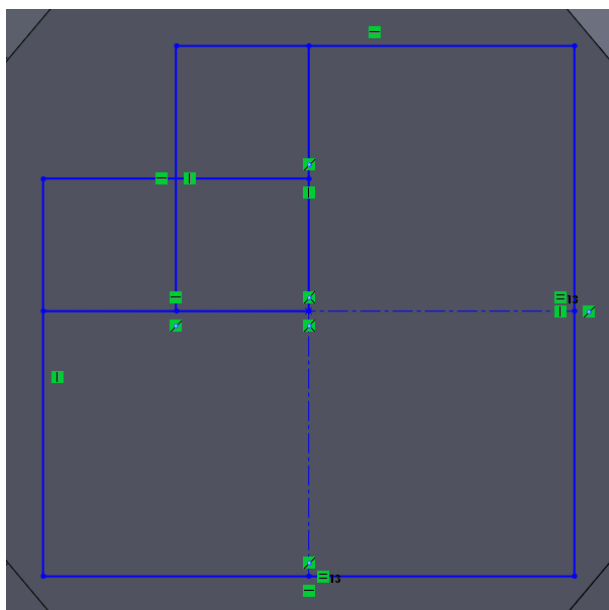
(2b) If a connector other than the basic L shape is needed, this process can be repeated. Divide the quadrants of the primary square themselves into quadrants using the midpoints of the lines drawn in Figure 2a.

6 Printing structures whose bonds do not align with the print tray

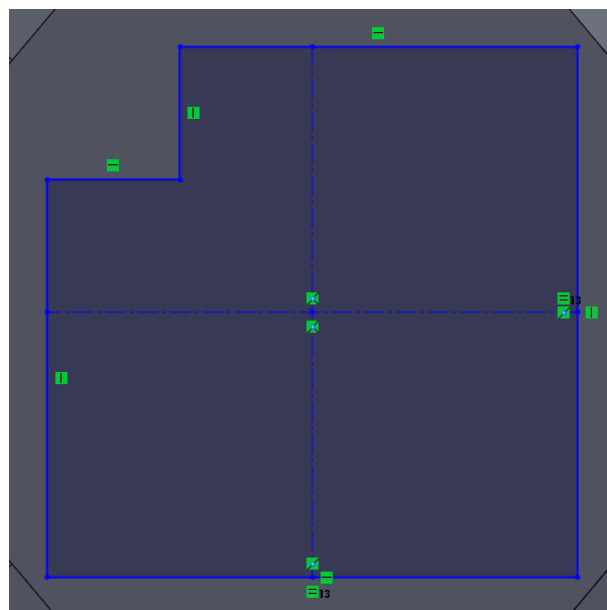
While this does not seem necessary for printing with commercial print services such as Shapeways (based on very limited testing, please don't discover this isn't true in a way that costs you a lot of money), with the printers we have access to, we have found that the connector must be either parallel or perpendicular to the print tray, or the slot and peg deform. This is relatively easy with most d-block complexes (octahedral and square planar geometries lend themselves to this quite well), MOFs that have cubic unit arrangements, polymers that contain aromatic rings and similar. However, complex natural products, main body compounds, minerals, more geometrically complex MOFs such as the UiO series, and f-block compounds often have geometries that do not lend themselves to right-angled alignments. To get around this, we have developed a technique that does not require bonds to be cut perpendicular to the bond angle. While it has some drawbacks, including requiring more labour and sometimes the use of glue, it produces a robust and pleasing final product.

This explanation is rather complicated, and possibly best explained by the video tutorial also included as part of the electronic supplementary information for this paper. However, a best effort has been made to outline the broad strokes of the procedure using *Solidworks*, trusting that the general method can be adapted to the software of the user's choice. This section will make heavy use of the technique outlined in 5.

The general principle is to use planes to cut through the bonds so that all the connectors are at a good angle for printing. This means that the angles of the connectors will no longer be perpendicular to the angles of the bonds. I will be using RaF_2 , which adopts the fluorite structure, as an example, and thus



(3a) Now you can remove sixteenths with the the *Trim Entities* tool until you have an appropriate shape. You could further subdivide the sixteenths, but that would be too small to print at the sizes and with the printers our tests have been done with.



(3b) You will need to remove unneeded lines until Solidworks shades the interior (Compare the blue shading in this figure with the lack of shading in 3a). Then the *Extruding Boss/Base* or *Extruded Cut* tool can be used to add the desired peg or slot.

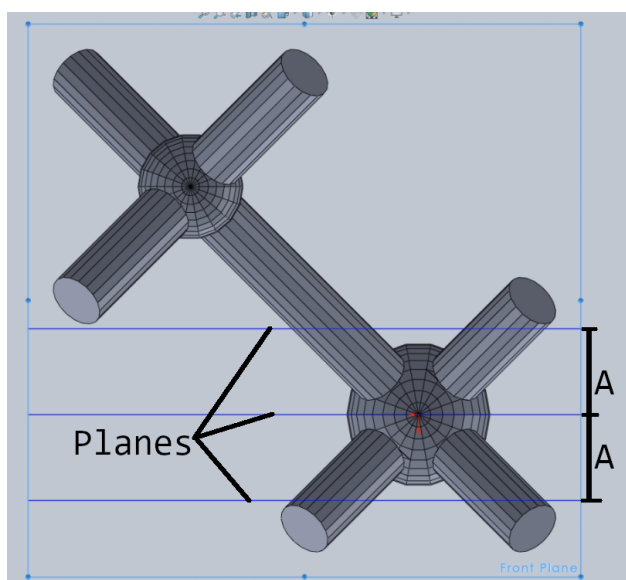


Figure 4 Diagram of placing the planes around radius in RaF_2 . Note the planes are equidistant from the centre of the radius atom.

will have an atom as the centre of my printable unit. However, this technique could be done with larger assemblies as well, with molecules, moieties, or proteins.

To start, create a plane bisecting the bonds on one side of the atom or molecule in question. In a symmetric system such as RaF_2 you will then want to place a plane on the other side of the atom, molecule or moiety in question, equidistant from the centre, so that the bonds are cut to the same length. In asymmetric systems, you don't have to worry about keeping the bonds the same length.

Now place similar planes around the other object. You will likely have a gap between the two, as

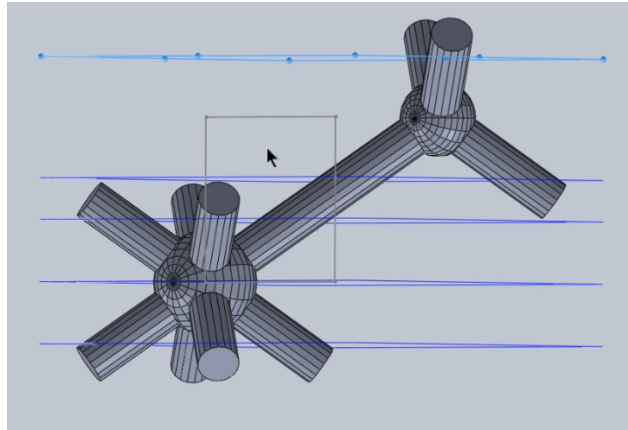


Figure 5 Only four of these planes are needed for cuts: The other serves as a reference. The square is used to measure the distance from the centre of the fluorine atom. Note that since the bonds do not extend far enough, it is not possible to get a clean cut on all the bonds with a single plane between the radius and fluorine. A spacer was used for this reason.

shown in Figure 5. Lines or squares can be used to ensure the planes are equidistant from the centre of the object in question.

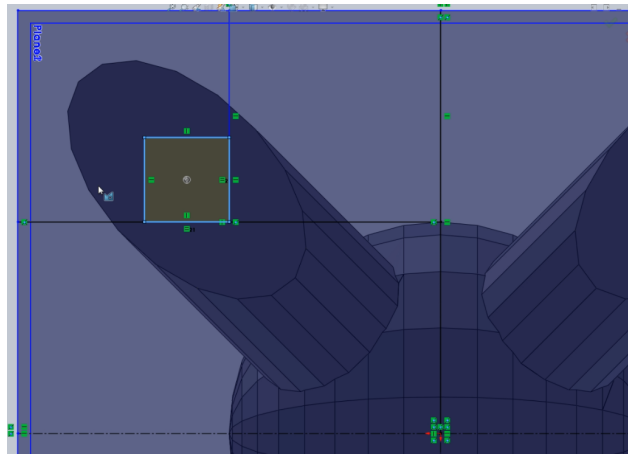
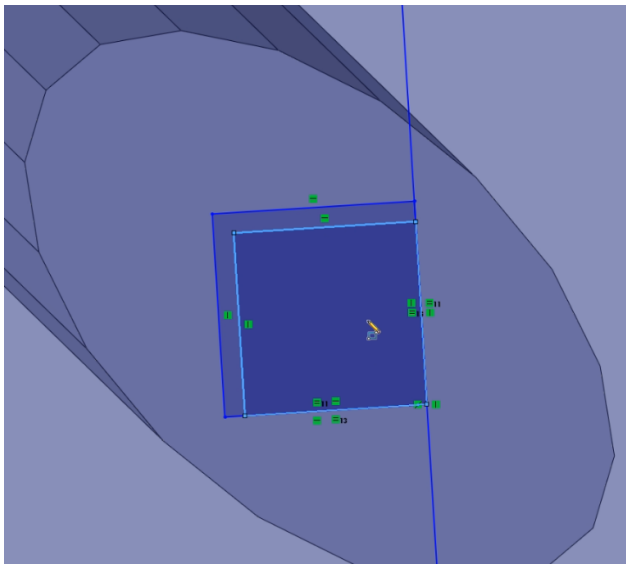


Figure 6 Using a large square centred at the origin as a reference point.

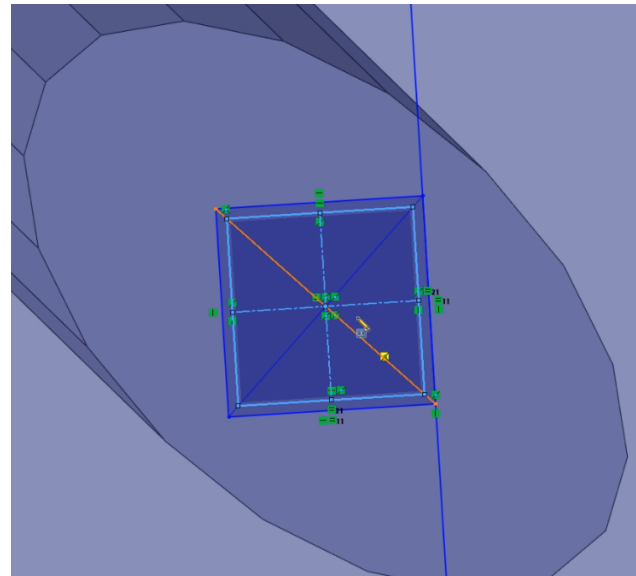
Now cut along the plane as outlined in Section 5. Save each object as a separate file, including one for the spacer.

Now the more complicated part is adding a connector to each of these parts such that they perfectly match. This is done as in Section 4; however, it is complicated by the fact that the surfaces you are placing the connectors on will not be circles, but ellipses. There is one trait of *Solidworks* that we can take advantage of: since all three parts were formed from one file, they share an identical coordinate system. Therefore, the authors can draw a big square on the plane used to form the cut, centred at the origin. Then the authors place each connector at a fixed distance from the closest two walls, and they will be at the same point. For example, draw an x by x square, and place each connector in the centre of each quadrant. Then you can draw the same square on the next part, and place the connectors in the same place.

However, note that you have to make sure the centre of each connector is located at the same place, and not the corners. For example, in Figure 6 the lower right corner is used as the reference point, which



(7a) The results of aligning both the peg and slot to the same corner.



(7b) It is not hard to properly centre a square within another square, to correct for a corner used as a reference point.

if used for both the slot and peg would result in the situation shown in Figure 7a. If both the peg and the slot are aligned in this way, there will be too much clearance along two sides, and none along the other two. This can be avoided, even if the corner is the simpler reference point, by aligning an identical square, then placing the centre of the peg at the centre of the slot.

Since this method places multiple objects to be extruded⁶ on the same sketch, all of them must be extruded at the same time. This can be done by starting to extrude one as normal, then holding down shift and clicking each other part of the sketch to be extruded. The only limitation to this I have found is that it limits you to all pegs or all slots at once. This means that you'll have to create a second sketch on the same plane if you want to mix pegs and slots on the same side of the part.

Since the coordinate system is shared by all three parts, it is valuable to use the Make Assembly feature (under “File” → “Make Assembly From Part...”) to check your work. Add all the parts to the assembly (“Assembly” panel, “Insert Components”), to make sure they align properly. Then use the “Interference Detection” feature (Under the “Evaluate” menu) to check that all of your pegs fit into your slots.

7 Details of Experiments and Tools Used

Table 1 Summary of Software Used

Software	Version	Creator	Licence
Mercury Magics	Multiple versions v19.0.1.11	Cambridge Crystallographic Data Centre Materialise	Gratis–Closed Source Commercial
Solidworks	Educational Edition (Academic Year 2017–2018/2017 SP3.0)	Dassault Systèmes	Commercial
MeshLab	MeshLab_64bit_fp v2016.12	Visual Computing Laboratory, Istituto di Scienza e Tecnologie dell’Informazione and the Consiglio Nazionale delle Ricerche	Free (GPL3.0)
ZEdit Pro Insight	v1.1 v10.6 Build 4739	Z Corporation Stratasys	Commercial Commercial

Table 2 Index of structures printed

Part	Print location	Printer	Plastic
Copper Pyrazine Dicyanoaurate			
Au(CN) ₂ ^α			
White	Shapeways	Unknown	Versatile Plastic—Natural Finish
Red	Shapeways	Unknown	Versatile Plastic—Processed Finish
Gray [sic]	Shapeways	Unknown	Professional Plastic—Standard Finish
Black	Shapeways	Unknown	Professional Plastic—Standard Finish
Translucent	Shapeways	Unknown	Fine Detail Plastic—Smooth Finish
Bronzed-Silver	Shapeways	Unknown	Steel—Polished Finish
Bronze	Shapeways	Unknown	Steel—Polished Finish
Blue	Document Solutions	Stratasys Fortus 250mc	ABSplus P430 and SR-30 Support
Copper Pyrazine ^α			
White	Shapeways	Unknown	Versatile Plastic—Natural Finish
White	Shapeways	Unknown	Fine Detail Plastic—Smooth Finish
Blue	Document Solutions	Stratasys Fortus 250mc	ABSplus P430 and SR-30 Support
Entire Repeat Unit ^β	Document Solutions	Stratasys Fortus 250mc	ABSplus P430 and SR-30 Support
Entire Network ^γ	Document Solutions	Stratasys Fortus 250mc	ABSplus P430 and SR-30 Support
Sodium Chloride	Document Solutions	Stratasys Fortus 250mc	ABSplus P430 and SR-30 Support
Sodium Chloride ^δ	Private Individual	Ender 3	Value PLA 1.75 Yellow
NaCl with failed connector shapes			
Triangular connectors	Document Solutions	Stratasys Fortus 250mc	ABSplus P430 and SR-30 Support
Merged Circular connectors	Document Solutions	Stratasys Fortus 250mc	ABSplus P430 and SR-30 Support
Squares unaligned to plane	Document Solutions	Stratasys Fortus 250mc	ABSplus P430 and SR-30 Support
RaF ₂ ^ε	Document Solutions	Stratasys Fortus 250mc	ABSplus P430 and SR-30 Support
RaF ₂ ^ε	SFU Engineering	Stratasys Fortus 250mc	ABSplus P430 and SR-30 Support
Phthalocyanine ^ζ	Document Solutions	Stratasys Fortus 250mc	ABSplus P430 and SR-30 Support
Phthalocyanine ^{ζ,η}	Document Solutions	Stratasys Fortus 250mc	ABSplus P430 and SR-30 Support

^α Mistake in rotation of the connectors prevented construction of a repeating structure.

^β Unknown flaw in structure led to failed prints twice, despite repairing the structure with all software available.

This is unrelated to the main techniques outlined in the paper, as it isn't near any of the connectors.

^γ Network printed in a distorted manner due to problem with heating sensor.

Before photography, network was knocked off the shelf and broke. It snapped several more times during repairs.

It was eventually glued back into suitable condition for photography, though the distortion could not be corrected.

^δ Printed and assembled by an secondary school student.

^ε These two print runs were combined into one model.

This was the only structure in which glue was needed to hold the connectors together.

^ζ The ligands are slightly incorrect. The two THF ligands should be mirror images of one another.

However, the author decided to create this structure while recording a demonstration.

As a result, this symmetry operation was not noticed, and a single THF was printed twice.

^η A communication error resulted in a print run where the model was printed unaligned to the tray.

8 Flow charts outlining procedures

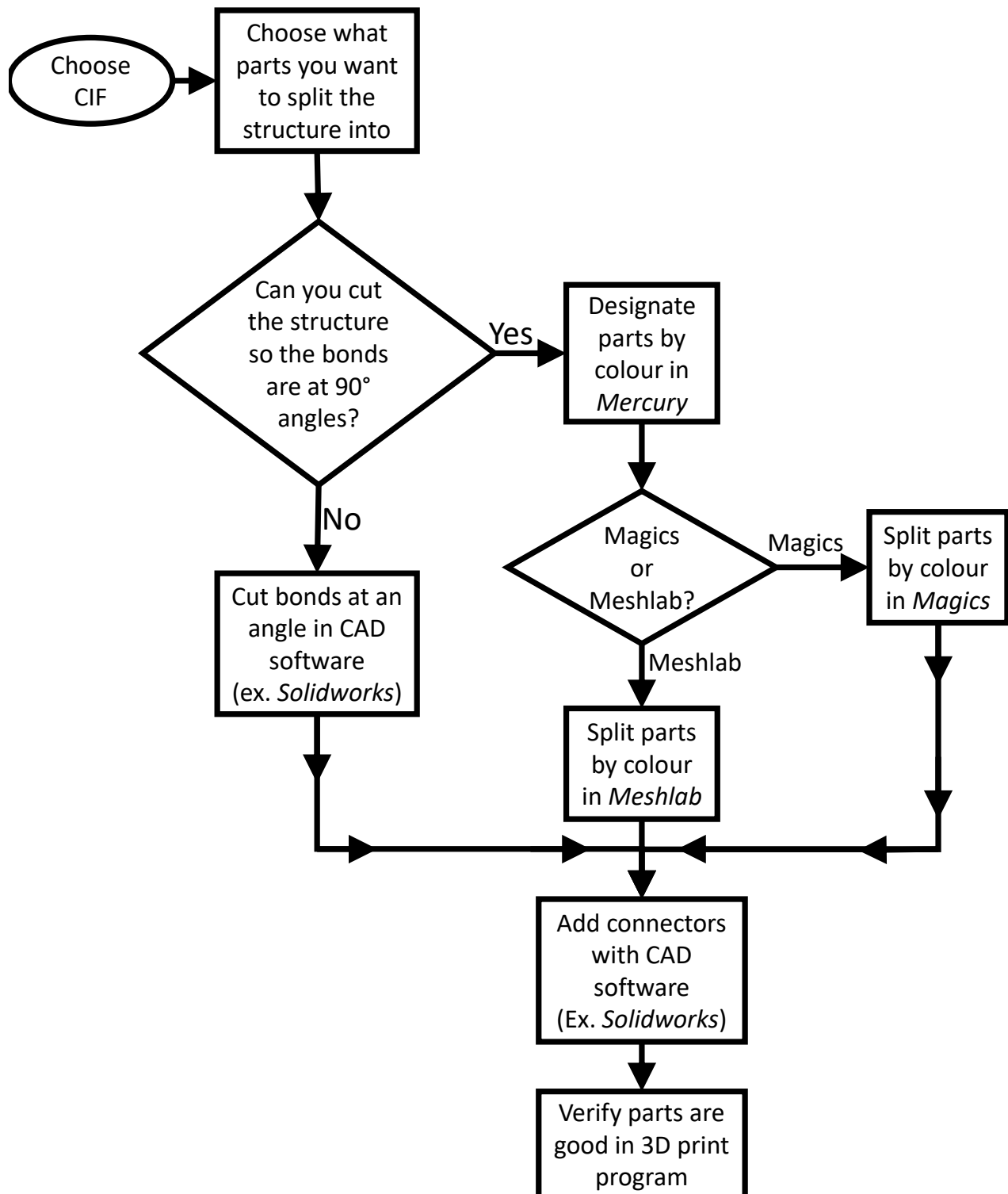


Figure 8 Flowchart aligning what software is needed in what order.

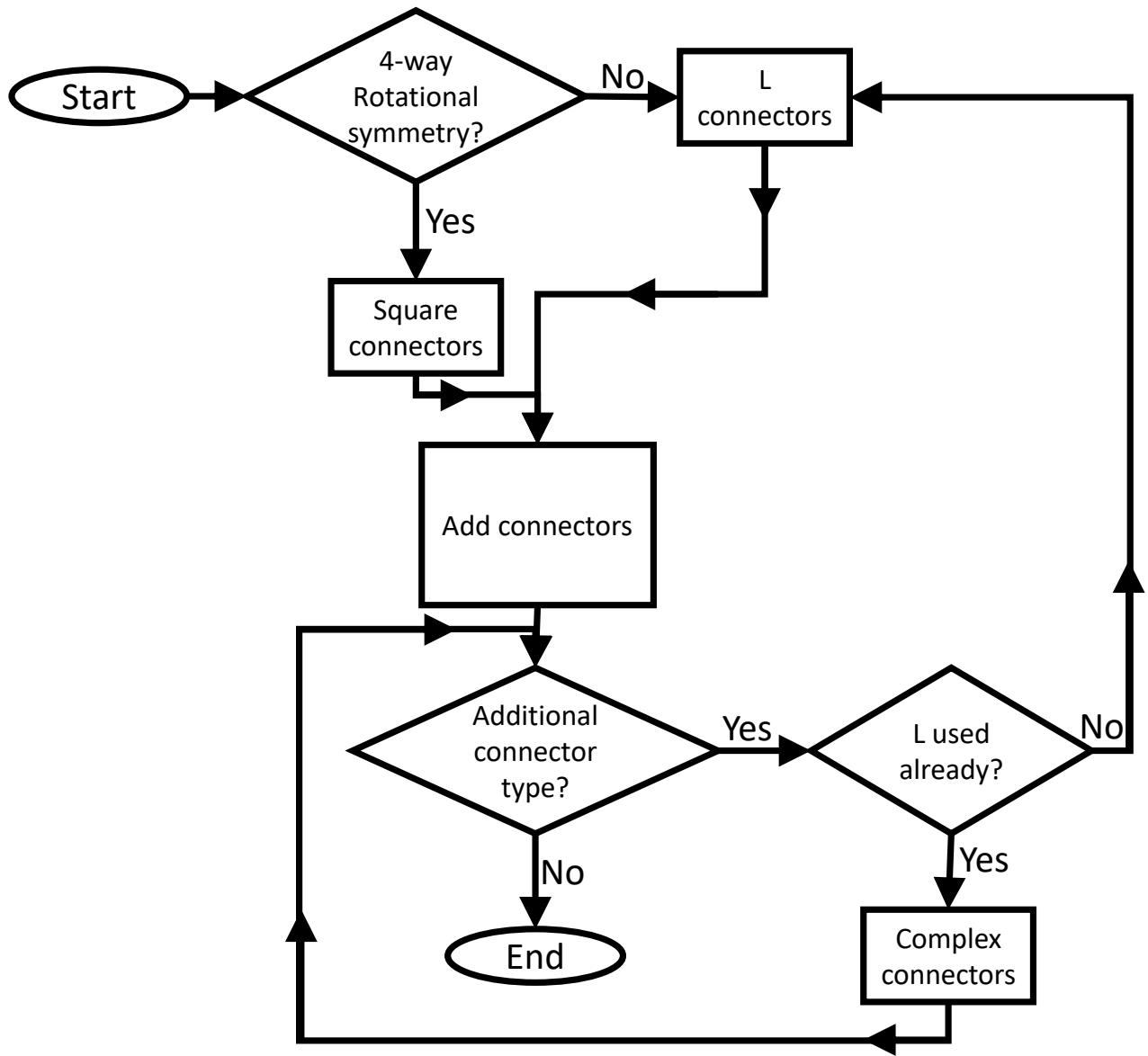


Figure 9 Flowchart aligning what connectors should be used.

9 Other print runs not featured in the paper

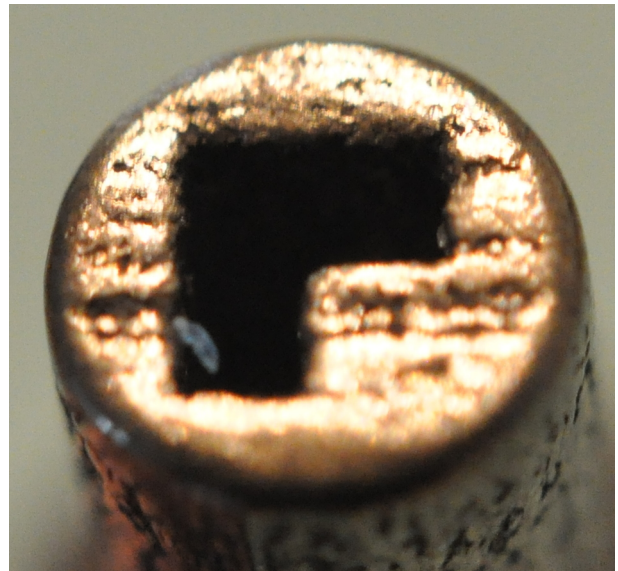
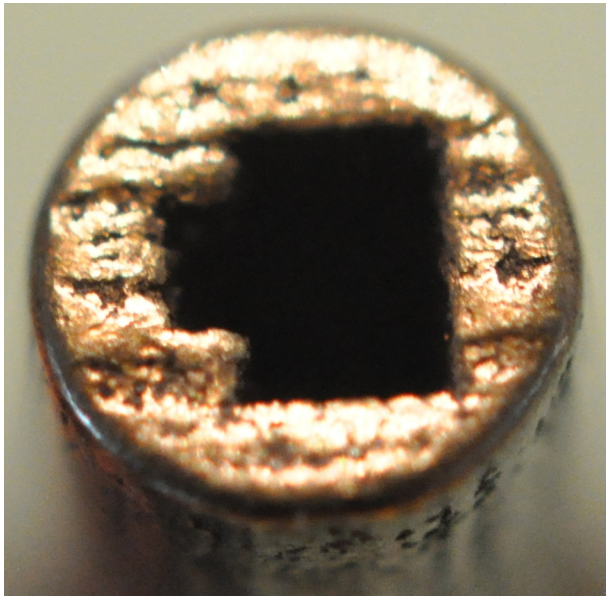


Figure 10 In addition to being too heavy to use, the metal parts from Shapeways came out a slightly different size and would not connect to the plastic parts. However, the cuts were nice and crisp, so we suspect that a totally metal print run should be possible, though budget constraints prevented us from testing this hypothesis.

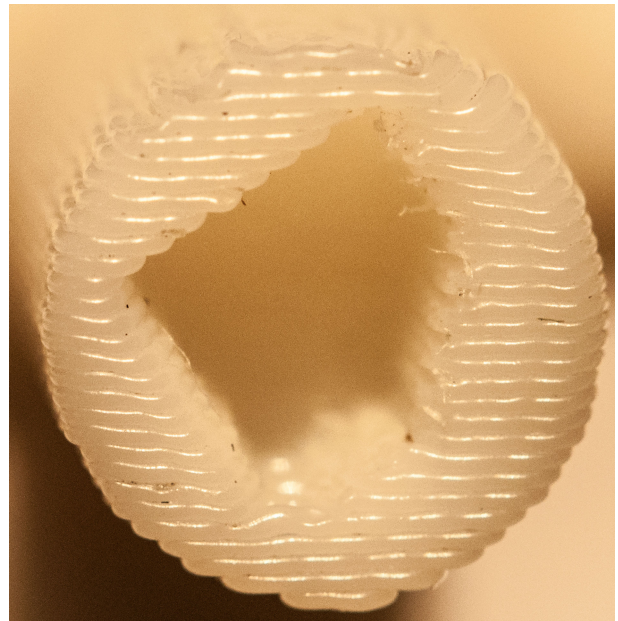
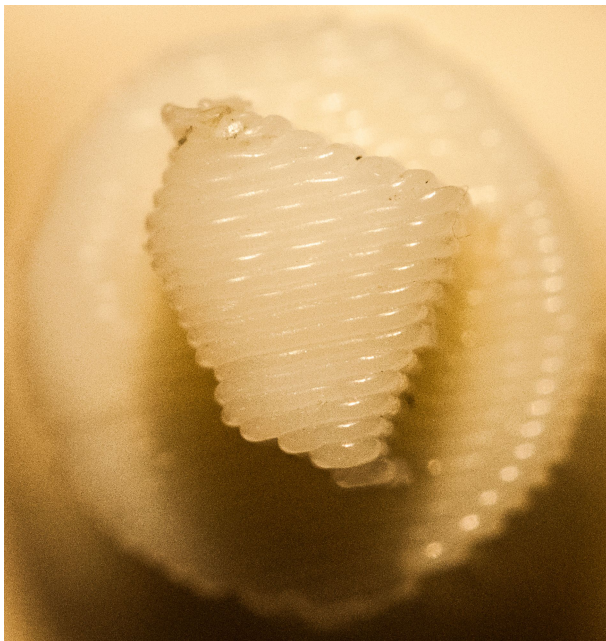


Figure 11 A failed attempt to remove symmetry using cuts at a 45-degree angle.

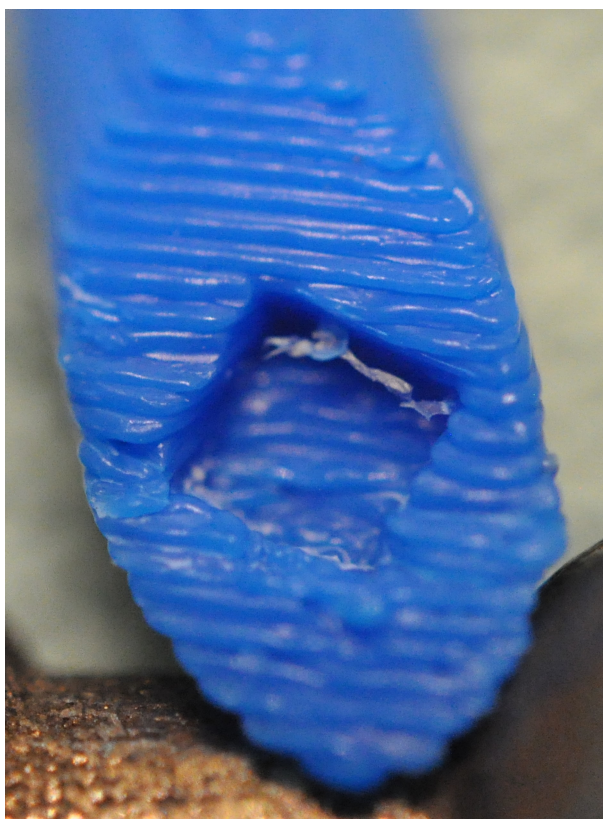


Figure 12 Despite being printed on the same model printer, note the difference between this and the other image of a slot. In this case the item was printed line by line: In the ones printed with SFU physics a more vector approach was obviously used. Despite this both parts were compatible and combined into a single object.

Notes and references

- [1] P. A. Wood, A. A. Sarjeant, I. J. Bruno, C. F. Macrae, H. E. Maynard-Casely and M. Towler, *CrystEngComm*, 2017, **19**, 690–698.
- [2] M. L. Brown, K. Van Wieren, H. N. Taylor, D. Hartling, A. Jean and N. Merbouh, *CrystEngComm*, 2018, **20**, 271–274.
- [3] If they have been changed, the default sizes are *Stick Settings*. . . → *Stick Radius* = 0.2, and *Ball & Stick Settings*. . . *Atom Size*: Non-metals = 0.25, Metals = 0.25, Bond Radius = 0.2.
- [4] P. Cignoni, M. Callieri, M. Corsini, M. Dellepiane, F. Ganovelli and G. Ranzuglia, Eurographics Italian Chapter Conference, 2008. DOI: 10.2312/LocalChapterEvents/ItalChap/ ItalianChapConf2008/129-136.
- [5] However, while preparing this manuscript, a structure exported from PyMol was fixed for a colleague working on an otherwise unrelated project, and it was found to need a different sequence of repairs. Therefore, even more than the rest of these instructions, this section should be taken as guidelines that worked for us, and other combinations of software and structure may need a different order of repairs or manual tweaking to render them watertight and printable.
- [6] This is the terminology Solidworks uses, not to be confused with the physical extrusion process used in 3D printing.