3D Printing for Visualisation of the Complex Physical Structures of Agent-Based Simulation Models on Lattices

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ABSTRACT

Visualising the complex emergent spatial structure of large-scale agent-based models is a challenge that is only partially addressed by 3D rendering. We explore the use of 3D printing technology to construct physical artifacts from lattice-oriented models such as the Kawasaki and Potts models in 3D. We describe the problems of support structure, resolution and overhangs in constructing physical 3D print models, and describe our work using additive manufacturing technologies including both both Filament Fabrication and Powder-Bed Fabrication. We experimented with cut away approaches to reveal the complex internal structure of the emergent model configurations and we describe our techniques for generating 3D printable artifacts for models of this nature. We found that powder bed technology enabled quite crisp coloured model components, and present some photographic examples of printed complex model system configurations, showing results of quenching and annealing in stochastic lattice simulations.

KEY WORDS
3d-print; additive manufacture; modelling; simulation; agent-based model; simulations; lattice models.

1 Introduction

Simulating complex systems such as agent-based models can yield great insights into emergent behaviour, and this is enhanced if whole model systems can be visualised to identify spatial structures. Visualising models with graphical rendering technology is a powerful and now well established approach, with virtual reality technologies becoming commodity priced and accessible to wider user groups.

However, being able to examine a physical artifact can also provide significant and different insights into emergent spatial structures and growth properties [35]. In this article we report on experiments with a range of 3D printers and associated technologies to make physical 3D printed constructs from some simulation models such as Kawasaki diffusion model [24] on a lattice and multi species Potts [31] model variants [15, 21] of it.

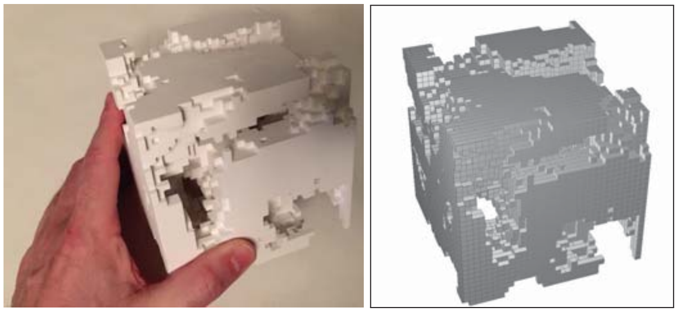

Figure 1: Kawasaki Model rendered in 3D right and photograph of 3d-printed solid model using colour inkjet powder bed fabrication (left).

3D printing technology [19, 34] has developed considerably in recent years [3] and as well as the industrially-priced devices, there are also a range of desktop and consumer priced 3D printers available [8]. It is therefore now much more feasible for researchers to aspire to making representations of their models. We have used both low priced filament extrusion 3D printers as well as more sophisticated devices such as a layered powder bed printer [27]. We describe the relative advantages of both, particularly in the context of detailed spatial structures as can be seen in models such as that shown in Figure 1.

The Kawasaki model is essentially a lattice gas model [30] and is typically studied on a lattice of cells, where each cell is occupied by a different species of atom in for example an alloy [5]. The model is quenched from an initially random pattern and complex striated spatial structures grow during the thermal annealing of the model, following what is known as spinodal decomposition [2, 4, 12, 25].

Although the Kawasaki model "agents" are very simple ones, and their microscopic behaviour of diffusing around the system is largely governed by thermodynamics, this class of model is a good foundation for more sophisticated agent-based models. We experimented with visualising multiple species using 3D printed artifacts as a first step. Colour or embossing of the individual cells in the 3D printed artifact offers potential for making constructs that show off various microscopic properties of such models.

The key area of interest to us for making 3D printed artifacts of models is being able to gain insights into the clusters, components [16] and spatial structures, and for 3D models this primarily involves seeing inside the complex 3D shapes and structures that arise from the models.

In addition to colouring the model cells therefore, we have experimented with omitting some species and leaving them represented as vacancies - either real vacancies or just a visual representation of a particular species. The photographs of model artifacts we have generated show how this approach lets one see inside models that one can hold in one's hand, and examine at length in a way that is still difficult to do with graphical renderings or even with virtual reality technologies.

Computer aided design software packages [32] are also widely available both as proprietary packages but as as open community software packages that can help generate designs for 3D printing. However, our own use of 3D printers is with models that are not generated by design packages, but which are generated by our own software, semi-automatically from out data from our simulations [10].

The key challenge in printing complex simulation models with various physical length scales present is understanding the geometry and physicality of what is possible, given the way that 3D printers work, building up material gradually in sliced layers - and which must be supported and stable during the manufacturing process. We discuss temporary support structural issues [26] and the contributions that different 3D printer approaches can offer to this problem.

We also explore various ways of cutting away parts of the model itself to enable seeing inside the 3D physically printed structures and describe the algorithms and software we have developed to support this, taking data from the lattice cells generated from the simulation code, through to a realisable 3D printable artifact. Missing parts of the model can exacerbate the support structure problem however, and we analyse the tradeoffs that result from the different approaches.

Figure 1 shows a comparison between a Kawasaki model configuration grown in our simulation system, and rendered using 3D graphics (above) and photographed as a 3d-printed solid using inkjet powder bed fabrication (below). The figure shows the key challenge in "seeing inside" the complex emergent structure.

Our article is structured as follows: In Section 2 we give some background to models such as the Kawasaki exchange model, the Potts model ,and the way we use these as representative of more complex Agent-Based models. We give some technical background on 3D printers in Section 3 and in particular describe the filament extrusion and powder bed technologies we used for the work reported in this present article.

We describe our techniques for making appropriately formatted information for driving the printers in Section 4 and present some selected photographic results in Section 5 where we also discuss the relative advantages and disadvantages of the various 3D print technologies and model cut-away approaches. We offer some conclusions and areas for further research and development in Section 6.

2 Lattice Agent-Based Growth Models

Agent-Based Models of interest to us are often simulated on a mesh or lattice, with each cell occupied by a particular agent or species of agent. Generally agents interact with the spatially localised neighbours and the Kawasaki model and its variants provide a good starting point for agent-based models involving spatial movement or rearrangement. Similar models include the Potts variant of Kawasaki (involving an arbitrary number of different agent species, and other systems including: cellular automata like the two state Game of Life model [9], or three-state variant such as the Game of Death [17]. Similar models include simulations of: health systems including disease propagation [14]; predator-prey systems [18]; social segregation systems [13]; materials propagation in gas and oil wells [11].

The Kawasaki model has been described in depth elsewhere, but for completeness we give a brief summary of its properties for 3D print-ability. We consider a spatial (cubic) mesh of length L so that the N = L^3 sites are all occupied by one of Q different states of agent. The simple Kawasaki model has $Q = 2$ and we typically represent these two states as material or vacancy in the 3D printed artifacts.

The model is initialised with a random mixture of the agent species, and since the diffusion model has not a direct physical energy equation to drive it, a stochastic model [29] is used to provide an effective dynamics scheme that drives the model through a quench to a finite temperature followed by an annealing process at that temperature. In practice, the algorithm involves:

- pick a random neighbouring pair of cells;
- compute energy consequences of swapping them;
- Boltzmann probability determines probability of the swap;
- repeat, above.

The pair-wise site swaps emulate an atomic diffusion process very effectively and drives the model from an initial random mixture to a phase separated structure where like species have congregated together [22].

In this present article, we do not study wide temperature variations in this present paper by simple fix on models that have been quenched to half of the characteristic critical temperature of the Kawasaki model. This means we obtain steady growth and large scale complex spinodal structures that are challenging to visualise and understand.

3 3D Print Technologies

There are a range of different 3D print technologies now available including filament extrusion; resin photopolymerisation; powder-based binder jetting; material jetting; and laser sintering. We focused on just two for the work reported in this present paper - filament based extrusion and powder bed ink binder jetting.

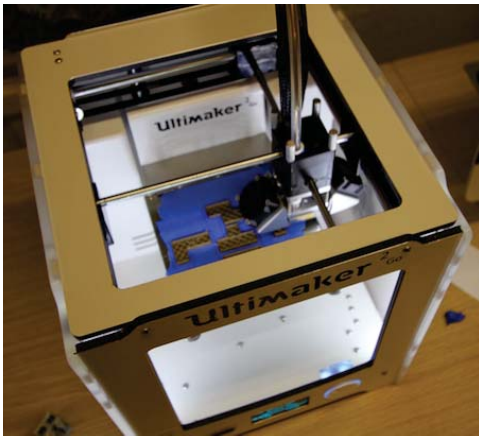

Figure 2: Ultimaker Go Filament-based portable printer showing the horizontal axes of extrusion head movement and the raise-able blue build plate.

The Ultimaker shown in Figure 2 is one of many widely available filament extrusion based 3D-printers. This heats and deposits melted filament that is most commonly made from either the starch based polylactic acid (PLA) or acrylonitrile butadiene styrene (ABS) plastic. It layers melted filament into a heated glass build plate upon which the model is formed and fans on either side of the the heated print heads cool and set the filament. Filament printers are good for prototyping work and they are cheap to run but the materials used are relatively brittle and in the case of PLA, due to the starch based nature of the material, over time it can decompose in the air [28]. The Ultimaker devices we used can only print one colour or sort of material at a time. While they can make cheap prototypes of the structure, it is difficult to introduce any realisation of multiple species of our models.

Figure 3: 3D Systems ProJet 660 Powder Bed Printer; Removing excess powder from printed Kawasaki model cube.

The 3D Systems ProJet 660 seen in Figure 3 uses a gypsum based powder with polymer binding agent as a printing medium, and it spreads a thin layer of this powder across its print bed and then binds it with jetted ink. Layers are built up as it the lowers the print bed and repeats. When the print is complete the printer then heats up the entire print area drying out the powder and the printed model, which remains quite structurally weak and which can easily crumble without cautious handling. The model is transferred to the cleaning section where excess powder is blown off of the model (Figure 3 - right), and which is subsequently submerged in a cyan-acrylate based setting substance. This reacts exothermically and cures the polymer binding agent producing a robust model that can be readily handled safely. The printer uses standard print heads and due to the setting of the powder being done by a fluid the device is able to print models in high resolution and full colour.

All of the 3D-print platforms require data to be fed to them in a particular format, and we discuss this as part of the process of practical model generation.

4 Cellular Model Data Generation

A crucial aspect of facilitating the 3D model artifacts is to interface the simulation code and its data formats with the STL format files used to drive the 3d-printers [20].

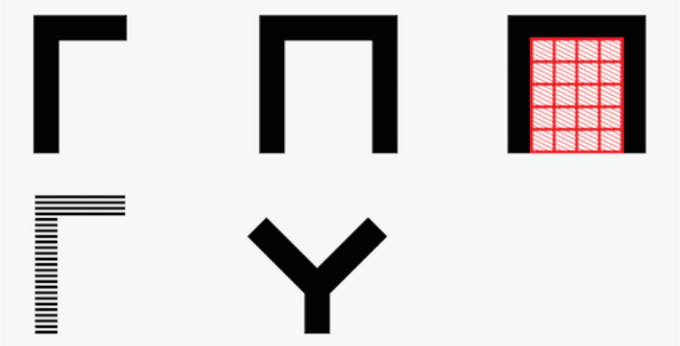

Figure 4: Geometric Support Issues: cantilever or hollow shapes require physical support during print material deposition although temporary support material (shown as red hatched) could be added. The structure is actually being made with horizontal layers or material, and 45 degree slopes are generally feasible, but not appropriate for our models.

Figure 4 illustrates the geometric support issues that are key to being able to feasibly manufacture a particular structure using the various 3D print technologies.

The interface language specifications [23, 33] for modern 3D-printers have evolved over several decades, the most common format is the STereoLithography or Spatial Tessellation Language or STL [6]. This was developed from commercial formats [1] but have similar properties to 3D computer aided design files and with the widespread exchange of graphical object files for games characters and other digital assets, these formats have converged in recent years to a relatively open *de facto* standard [7]. STL files are used by 3d-printers [7] such as the Ultimaker and Form1 to describe the models being loaded on to them. The printer itself generally cannot read STL files directly, and instead the file is first loaded into a slicer program such as Cura. This software will translate the file into something that the printer can read and use telling it how to move the print head this format depends on the brand of printer, the most common is *gcode*. We describe our model data formats and software to convert them to STL in [20].

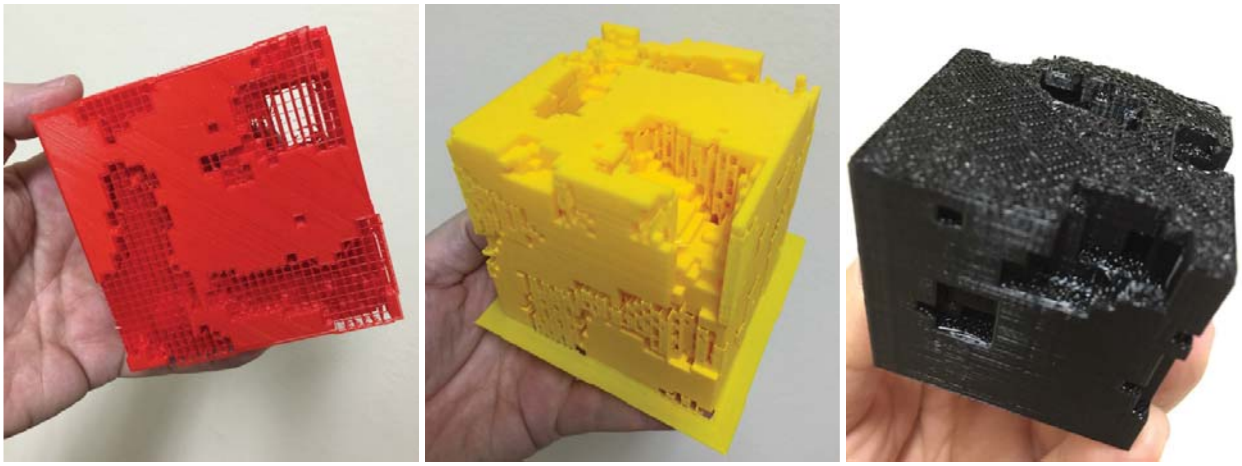

Figure 5: Cube constructs using mono-colour PLA filament and with support structure partially cut away.

5 Selected Results

The first of the Kawasaki models that we attempted to print was that of a simple two state Kawasaki system. The first attempt was done on an "Ultimaker 2 Extended" model and this can be seen in Figure 5, the only way that the print could handle printing the model as with the addition of considerable PLA support structure. This caused problems as it was very difficult to remove all of this structure due to the complexity of the model and the cavernous nature of it, it would not be possible to get into the model to remove this support structure with any practical tools.

Figure 6 shows our attempts at making hollowed out boxes. This uses less material, and is quite rapid on the filament printer - although it can only show one colour at present. We are investigating using an embossing of physical texturing approach to make bas relief surfaces that convey the different species on a filament print. The powder bed manufactured hollow boxes are feasible, although we had to experiment with different box thicknesses in terms of ABM cells, to avoid the physical box structure being too fragile. This approach of making two half-boxes should be useful for making a sequence of solid cube models for illustrating the time evolution, but is not useful for our central goal of seeing inside the physical 3D structures.

To circumvent the support structure problems, we used the powder based 3D printer (ProJet 660) because of the nature of the supporting structure being that of unbounded gypsum based powder it mean the the removal of the support structure was very easy only requiring the use of a air gun even in the complicated cavernous like internal structure of the Kawasaki model. It should also be noted that when the supporting structure was removed unlike with the filament models, caused no damaged to the look of the model. An example of the Kawasaki model print on the Projet 660 is shown in Figure 7 and as can be seen, the model has numerous overhangs and a highly complicated internal structure - which is of course the central challenge for visualisation and physical realisation.

The filament style printers were only capable of represent bi-state models with the 2 state being filled or empty. This meant that model with the need to represent more data states would not be possible on these particular printer. But the project 660 with it capability to print in full colour with the use of standard commercially available print heads could realise much more complex models and example of this can be seen in Figure 8 which show a three state Kawasaki model with the state being that of green, red, and empty. This allow for a much wider range of these complex physical structure to be realised and with the addition of its very easy to remove support structure it even allows for very minimal damage to the model itself.

One highly valuable approach with 3D visualised agent-based models is the ability to look inside of the model at the internal structure, due to the opaque nature of the model being rendered this requires the application of slicing to octant removal the allow for these otherwise unseen aspects of the model the be brought to the light of day and be analysed effectively, giving a much more complete understand one the model its self. This means that in order to avoid the the obfuscation of such aspects of the simulation model when realising the model into a 3D print it is important to be able to print off these slices example of this can be seen in Figure 9 shows both of these figure show the same 4 state Kawasaki model sliced in different ways allowing for the interaction that have occurred inside of the model to be seen.

Figure 10 shows another approach we developed for seeing inside the structure. We remove a whole octant of the cube, so that a cross sectional slide can be inspected, with exposure all the way to the core centre of the simulated model system. This also shows two-dimensional cross-sections through the model, which can of course also be generated as free standing slices.

One solution to the excess supporting structure that we thought of was to slice the model into one cube thick sheets that would allow fore then to be printed off of the printing with and overhangs at all and example of this type of sheet can be seen in figure Figure 11 (left). When doing this we encountered a problem when the sheet grew to a considerable size, that be that as that model would print the corners of it would become detached from the heated glassed build plate and would begin to curl upwards, meaning that they would not be able to be attached to one

Figure 6: Various hollowed out half box cube constructions of single or four cells in thickness. From left: using powder 1 cell thick and 4 thick and using yellow PLA, 1 thick.

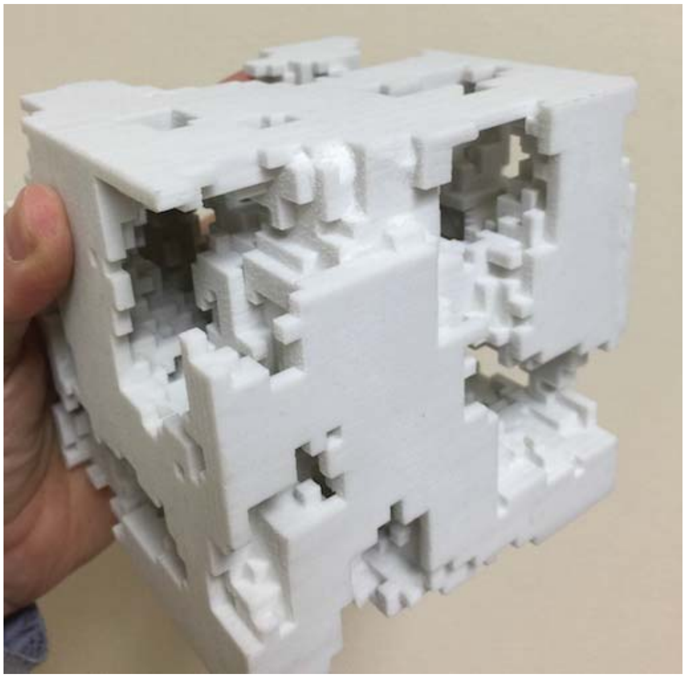

Figure 7: white-q2-sand

another once printed. Figure 11 (right) shows some free standing slices through the model, with just 4 layers of cells rendered. Note that in this particular print, no ink was used to colour the normally hidden faces, so white gypsum powder is exposed on one side.

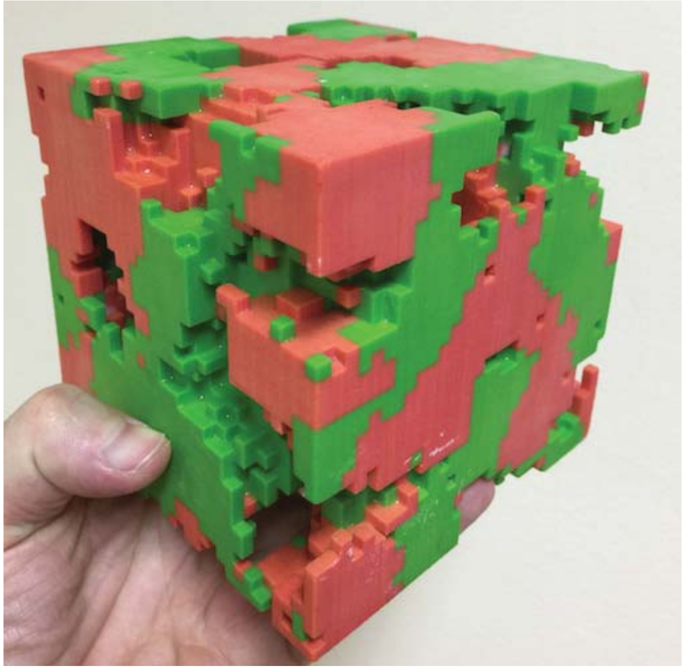

Figure 8: 3-Species Kawasaki model on 32^3 lattice with vacancy species removed as cavities allowing see-through into the internal structure.

6 Conclusion

We have described how we manufactured physical manifestations of the Kawasaki diffusion model using various 3D printing technologies and approaches to see inside the complex emergent structure of the model. Filament based extrusion printers are cheap and adequate for structural prototyping but at the time of writing can not yet effectively print in different colours with in a complex print model, and tend to require the addition of considerable material support structures to make a complex model into a feasible print.

Removing excess support material post-print is a difficult task and typically leads to damage of the near fractal physical structure of some models. Powder-bed 3D print technology with self support from the powder itself is a more feasible approach for complex models with the excess dry powder being relatively simple to blow out of the model's complex interior. There are still limitations on the relative weight the uncured model can self support when removing excess powder.

We have shown how using vacancies, hollowed cores; diagonal

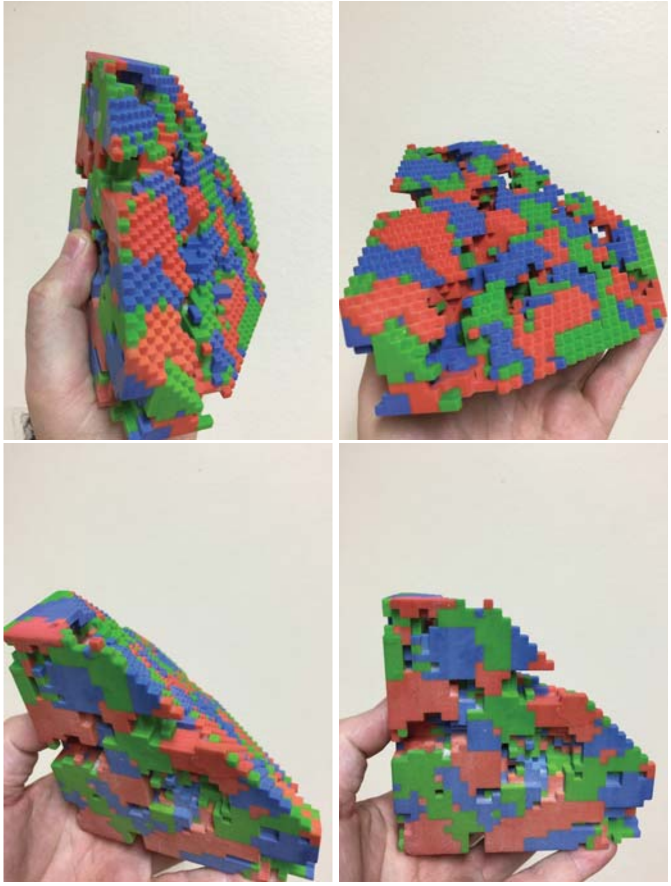

Figure 9: Diagonal Cut-away Views of 4-state model showing interior structure of spinodal interfaces.

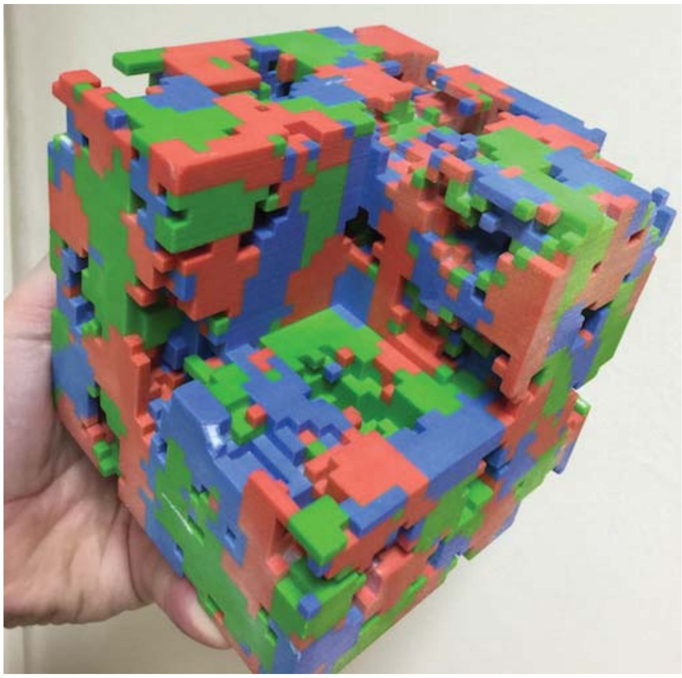

Figure 10: Octant Cut-away View of 4 state model with unprinted vacancies used for the fourth species.

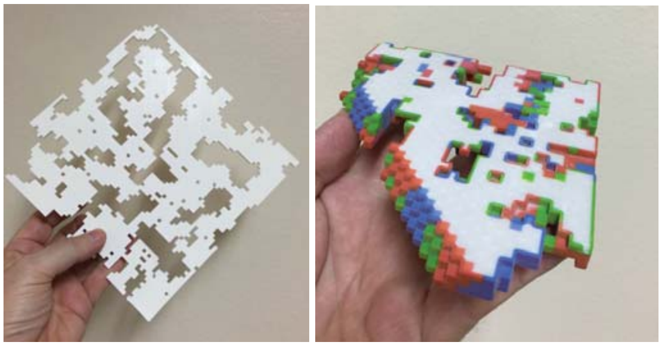

Figure 11: Sheet approach - manufactured by filament extrusion and 1 model layer thick (left) and with powder bed and 4 layer thickness (right).

and octant cut-aways and sheet slicing all give different insights into the interior structure of these 3D models, as well as reducing the amount of physical material used. . We have used simple but inefficient construction techniques that do not economise on the printed materials used for our simulation model artifacts. This is adequate for one-off print runs of scientific models, but there are a number of techniques to make better use of the printer capacity. Managing the cost effectiveness and practical logistics of manufacturing these sort of models is an important area for further research.

The colour capability of the powder bed ink jetted printer opens up considerable possibilities for multi state models with different species. We found that the powder printed models with internal vacancies used for one of the model species was an adequate approach, giving good insights into the complex interior structure of the spinodals formed by the Kawasaki model under annealing.

We believe this approach could be usefully deployed for other and more complex agent-based simulation models. Identifying isolated cluster components of agents and removing them or printing them separately is likely to be useful however to simply the print process and avoid damage to partially cured models.

There is scope for investigation of other 3D manufacturing techniques for making physical artifact realisations. Laser cutting of layered material such as cardboard or wood and plastic and resin printing using photo-polymerisation techniques may also lend themselves well to making models of this sort.

In summary, 3D printing offers a different experience to graphical rendering of complex agent based models. 3D printed artifacts are enduring, can be handled, and viewed from different angles, as well as offering a much more tactile experience, perhaps giving different insights into complex structure formation. We envisage various educational and model demonstration uses for the printed cluster or artifacts from such simulation models. We believe 3d-printing complements 3D graphical rendering for such model visualisation, and that commodity priced 3d-printers will have a significant role to play in analysing such models of complex systems.

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