

DENSITY-BASED TOPOLOGICAL OPTIMIZATION OF 3D-PRINTED CASTS FOR FRACTURE TREATMENT WITH FREEFEM SOFTWARE

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3D printed plastic casts can be used for healing bone fractures. The main requirements for these cases are: they should be light, require little printing time, have good mechanical properties, and ensure proper skin ventilation. We present a density-based topology optimization algorithm for obtaining optimal cast shapes that fulfil these requirements. The algorithm uses a linear stress model and simplified boundary conditions to model the contact problems. The cast shapes were optimized against the influence of several sharp corners. The parametric studies showed that the mass of optimized casts was reduced by 20 %–25 % in comparison with original industrial casts, and the printing time is reduced by 1.4–1.7 h for the largest cast. A major model drawback is the use of 3D numerical volume to model the density distribution. The density distribution should be homogenized across the cast layer. The overhang problem should also be addressed. We also suggest that the cast producers collect more experimental data on the cast breakages for a better calibration of the numerical model.

Keywords: 3D printing, medical casts for bone fractures, topology optimization.

1. INTRODUCTION

3D printing is used to print plastic casts for medical treatment of bone fractures, in particular forearm fractures [1], [2]. 3D-printed plastic casts have significant advantages over traditional plaster casts – they are lightweight, and they can have complex geometries that fit the patient’s arm and have holes that enhance skin ventilation (see Fig. 1). Important considerations in the production of 3D printed casts are the mass and printing time of the cast, which determine its production costs and its mechanical durability.

A leading producer of 3D printed casts in Latvia is CastPrint Ltd. Currently, Cast-

Print Ltd uses the following method to produce 3D printed casts. A scanned 3D surface of a patient’s arm is sent to Cast-Print Ltd. An operator of the company cuts the scanned surface into two parts and cuts large holes in them. Then a special algorithm generates a triangular mesh with thick connections on the rest of the surface area. After that the surface is extruded to obtain the final 3D shape of the cast; four connectors are added to bind both cast halves together, and then the cast is 3D printed (see Fig. 1) using polylactic acid (PLA plastics) as the material.

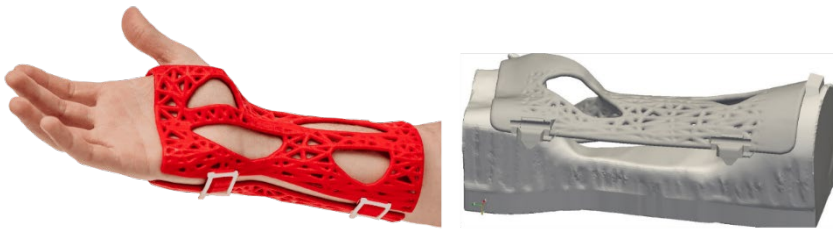


Fig. 1. Examples of original, unoptimized 3D printed casts produced by CastPrint Ltd. Left: a cast on a patient’s arm (promotional materials of CastPrint Ltd). Right: A cast part placed on a lower test fixture for mechanical testing (numerical 3D surface meshes).

Such an approach allows obtaining casts with good skin ventilation, but it has two main deficiencies. First, the large amount of manual work is tiresome for operators and causes mistakes during the shape creation. Second, mechanical durability of the cast is not considered when the shapes and positions of the holes are chosen. An alternative approach would be to use a topology optimization algorithm which would choose holes that would minimize the stresses forming in the cast under different applied loads and would also minimize the mass of plastics used in the production. Therefore, a study

was needed to examine whether the topology optimization could be used to generate lighter casts with at least the same mechanical strength as the casts obtained by the original approach and whether the topology optimization could be incorporated in an automated production line in which 3D cast shapes would be generated with a minimum input from operators.

Numerical modelling was used to determine optimal cast geometry in the past. A very simple approach was used in [1], where the authors considered three different hole patterns for a cast, calculated stress

distributions for two different loads for each pattern and determined the best pattern by comparing maximum stresses and displacements. A powerful two-step topology optimization algorithm was used in [3], [4]. In the first step, the cast surface was meshed with a coarse mesh (100–200 cells) using Voronoi tessellation. The cell sizes were iteratively adjusted to minimize a temperature-based sensitivity comfort functional. In the second step, holes were cut in the cells, and a new finer mesh was constructed. A series of mechanical stress simulations was carried out for a given applied force load, in which the local thickness of the cast was iteratively varied until the local stress values dropped below a predefined maximum level. It seems that the interaction between the cast and the arm tissue was not considered. In [5], a density-based topology optimization algorithm, also known as SIMP (solid isotropic material with penalization, see also [6], [7]), was used to optimize compression casts. The mechanical stresses in the casts were modelled using a thin plate model, which allowed to reduce the mesh size. The authors optimized the cast geometry against the pressure exerted by compressed tissues of patient's extremities. Interaction with external objects was not used in the optimization.

This paper presents an optimization algorithm for the geometry of forearm healing casts which is also based on the density-based topology optimization algorithm (SIMP). The development of the model is the result of collaboration between Cast-

Print Ltd, the Institute of Numerical Modelling, where the model was developed, RTU HPC Center, which provided the computer resources for simulations, and the Institute for Mechanics of Materials, which carried out mechanical tests of original and optimized casts. The model was developed in the frame of a project to design an automated production chain for 3D-printed casts, which would be implemented in the production line of CastPrint Ltd. To reduce costs, the algorithm was implemented via opensource software such as *FreeFEM*, [8], and *python* scripts.

The optimization algorithm consists of two parts: a simplified model for stress simulations, in which interactions with external objects are modelled via simplified boundary conditions, and the topology optimization algorithm that uses the stress simulation results. Due to practical considerations, the project set a limit to the duration of an optimization simulation per cast (one hour). For this reason, several series of simulations were performed to determine whether it was feasible to satisfy this limit, what simplifications should be done in the model for this purpose, and what the optimum values of the model parameters were that could be used for a wide range of casts. Below, a brief description of the optimization model is given, and the results of parametric simulation studies are shown and discussed. The results of mechanical testing of original and optimized 3D printed casts are also presented.

2. MODEL DESIGN AND BOUNDARY CONDITIONS

2.1. Model for Stresses

A 3D-printed cast (Fig. 1) consists of two separate parts connected with four con-

nectors that fix it on the patient's arm. Modelling an interaction of such a cast with an

external object requires, in general, a solution of dynamic contact problems between at least four objects (the arm, the two cast parts, and the object), which could also involve non-linear deformations. Solving such a problem is practically unfeasible, given the time limit set by the project.

To make simulations practical, the stress model was significantly simplified. First, a linear stress model is used under the assumption that the linear model can predict at least the positions of the regions with high stresses. If the cast shape is optimized against the stresses obtained with the linear model, the optimized shape would still work for stronger, non-linear stresses provided that the qualitative distribution of the

stress maxima remains the same. Second, an equation for steady-state stresses σ^{ij} is solved:

$$\nabla \sigma^{ij} = 0, \quad (1)$$

where the gravity force is discarded due to its small importance. In the weak formulation, this equation can be rewritten as

$$\oint f^i \tilde{u}_i ds - \iiint \sigma^{ij} \tilde{\varepsilon}_{ij} dv = 0, \quad (2)$$

where $\tilde{u}_i$ are test functions in the form of a displacement field, $\tilde{\varepsilon}_{ij}$ is a deformation tensor formed from $\tilde{u}_i$, and f^i is the force density field that describes the interaction between the cast and the external world.

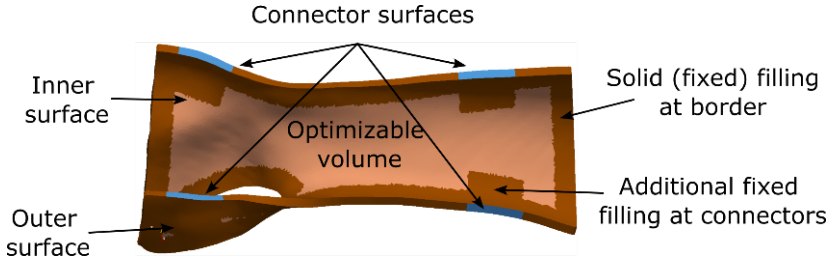


Fig. 2. Numerical representation of one half of a 3D printed cast.

In principle, f^i is not known and is obtained together with σ^{ij} by solving the contact problem. However, to speed up the simulation time, the contact problem is significantly simplified. The stress equation is solved separately for each half of the cast. The interaction of a cast half with the surrounding environment occurs on three surfaces (see Fig. 2): the outer surface can interact with external objects, the inner surface interacts with the arm, and the interaction with the other half of the cast is modelled on four connector surfaces. The contact problem for each of these surfaces is modelled via a special simplified bound-

ary condition.

On the outer surface, the cast can interact with large external objects such as walls or table edges, but modelling such interactions is difficult. For example, a wall can be modelled as a plane surface, but one must ensure a correct plane orientation that does not cut through the cast. It seems that interactions with large objects require proper modelling of the contact problem, which would be too cumbersome and time consuming. For this reason, interactions with large objects were not modelled. Instead, interactions with small, sharp objects are considered.

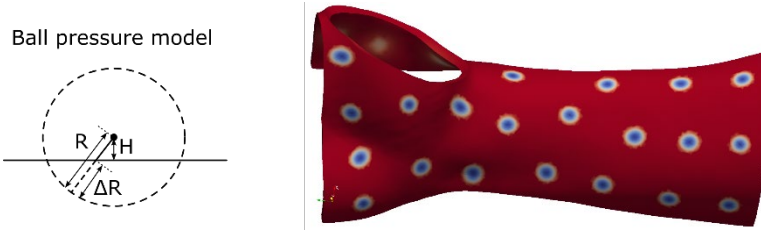


Fig. 3. Left: the parameters of the ball pressure model. Right: an example of ball position distribution on a cast half.

The influence of a small object can be modelled as a pressure distribution on a small area of the outer surface. The pressure has its maximum in the centre of the area, and it decreases to zero at the area boundary. Since the exact details of such a pressure distribution are not important, the following simplified model is used. A point on the outer surface is chosen. A ball with the radius R is drawn at the height H above the point (see Fig. 3). The applied pressure distribution is calculated as $p = A_{ball}\Delta R$ for the outer surface points inside the ball (ΔR is defined as shown in Fig. 3). The pressure distribution outside the ball is zero.

Several impact positions are modelled in the simulations. The stress equation is solved for each position, and the simulation results are averaged before using them in

the topology optimization model. The exact statistics of the impact distribution on the outer surface is not known, so it is assumed that it is homogeneous, and the ball positions are spread out evenly across the outer surface (see Fig. 3) by using a special algorithm.

Due to pressure concentration, the topology optimization algorithm places material around the ball impact points and forms holes between them. Thus, by changing the number of impact points, one can influence the distribution and size of the holes to some extent. A major drawback of this approach is that the hole distribution is heavily dependent on the impact positions. By choosing different initial ball positions, one can obtain a completely different hole distribution.

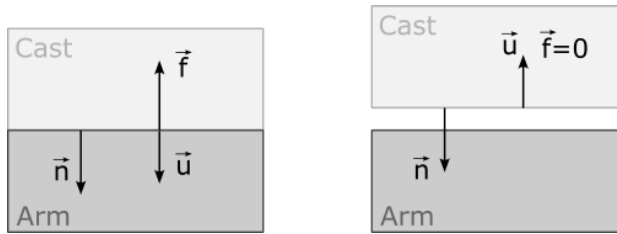


Fig. 4. Qualitative model of forces acting on the inner surface. Left: the pushback from the arm when the cast is pressed into it. Right: no forces when there is an air gap.

For the inner surface, it is assumed that when the cast is pushed against the arm (the normal component of the inner surface displacement $u_n > 0$), the arm pushes back with a force density that is proportional to

u_n (see Fig. 4). However, if $u_n < 0$, an air gap forms between the arm and inner surface, and there is no force acting on the inner surface. Mathematically this is described by the following boundary condition:

$$\vec{f} = -H(u_n)A_{skin}u_n\vec{n}, \quad (2)$$

where $\vec{n}$ is the normal of the inner surface,

A_{skin} is a constant, and $H(u_n)$ is the Heaviside step function.

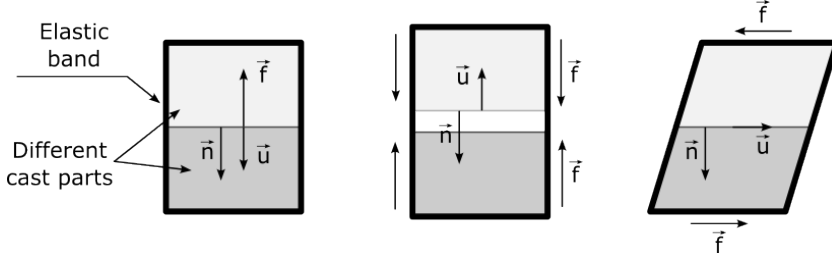


Fig. 5. A model for the contact problem between the connectors of the two cast halves.

The model for the contact problem on the connector surfaces is more complex (see Fig. 5). The cast halves are bound to each other by elastic bands that are put on the connectors (see Fig. 1). The connectors themselves are not modelled. Instead, there are four connector surfaces on the surface of each cast half (see Fig. 2), where the connectors will be placed in the post-processing stage. The forces arising in the interaction between the connectors are modelled as force density distributions on the con-

connector surfaces. It is assumed that a normal force acts on the connector surface when it is pushed against the other cast half. A normal force is also created by the elastic band when an air gap develops between the connectors (it is also possible that the connectors are locked to each other). The elastic band also creates a tangential force when a cast part slips tangentially against the other part. Thus, the following boundary condition is applied on the connector surfaces:

$$\vec{f} = -\left(A_{soft} + H(u_n)(A_{hard} - A_{soft})\right)u_n\vec{n} - A_{soft}\vec{u}_\tau, \quad (3)$$

where A_{soft} , A_{hard} are constants, and $\vec{u}_\tau$ is the tangential $\vec{u}$ component. The tangential term ensures the numerical stability of the solution.

A series of mechanical tests of the 3D printed casts were carried out (see Fig. 1). To compare the results of the mechanical test to the stress simulations and validate the chosen model, the model described above is modified to model the test conditions. The upper fixture in the tests was a cylinder. The interaction with it is modelled via a surface pressure distribution calculated as:

$$p_{cyl} = A_{cyl}\Delta R_{cyl}, \quad (4)$$

where ΔR_{cyl} was calculated as a difference between the cylinder radius and the distance of an outer surface point to the cylinder axis. The pressure on the points that lay outside the cylinder is set to zero. Such a model can be justified by the fact that only a small part of the cylinder touched the cast part. Zero force density is applied to the connectors, and the boundary condition for the inner surface is modified to:

$$\vec{f} = -H(u_n)(A_{skin}u_n\vec{n} + A_{skin,friction}\vec{u}_\tau)F_{groove,mask}, \quad (6)$$

where $A_{skin,friction}$ is an artificial friction coefficient introduced for numerical stability, and $F_{groove,mask}$ is a mask function, which models the groove on the fixture. $F_{groove,mask}$ is set to zero, if the inner sur-

face points lie above the groove of the bottom fixture. It is also set to zero for holes in the cast. Otherwise, the value of this function is one.

2.2. Topology Optimization Algorithm

Due to the complex geometry of the 3D printed casts, a density-based topology optimization algorithm is used for the cast optimization, because it does not change the simulation mesh. The applied algorithm is based on a 2D topology optimization algorithm for a cantilever, which was implemented as a *FreeFEM* script in [9]. This model was rewritten and expanded to use it for optimization 3D printed casts and to make it run on parallel processors.

The core concept of the density-based topology optimization algorithm is a scalar field h , which determines the material distribution in the cast ($h = 0$ means no material and $h = 1$ means fully filled). The material properties are calculated as functions of the field h . For example, the level of material filling at a given point in the cast volume is calculated by using a smooth approximation to the Heaviside step function $H(t, \beta)$, which is defined as

$$H(t, \beta) = \frac{1/2(\tanh \beta/2 + \tanh \beta(t - 1/2))}{\tanh \beta/2}, \quad (7)$$

where β determines the sharpness of the transition area between the holes and fully filled areas. The β value is increased incrementally (every fifth iteration in the script), so that a very sharp material distribution is obtained at the end of the simulation. The total volume of a cast is calculated as the integral:

$$V = \iiint H(h, \beta) dv. \quad (8)$$

The material properties (the Lamè coefficients) are also defined as functions of h :

$$\lambda = \lambda_0 \zeta(H(h, \beta)), \quad (9)$$

$$\mu = \mu_0 \zeta(H(h, \beta)), \quad (10)$$

where λ_0 and μ_0 are the actual material prop-

erties of the plastic, and $\zeta(t)$ is defined as:

$$\zeta(t) = e_{rs} + (1 - e_{rs})t^3, \quad (11)$$

where $e_{rs} = 0.001$ ensures that holes have non-zero material properties. All material properties are isotropic; the anisotropy caused by the 3D printing technology is ignored.

The optimal cast topology is obtained by iteratively modifying the field h to minimize the functional:

$$J(h) = \iiint \sigma^{ij} \varepsilon_{ij} dv + e_{ll} \left(\frac{V - V_t}{V_0} \right)^2. \quad (12)$$

The first term represents the total deformation energy. Minimizing it reduces the stresses in the cast and the risk of the cast

breaking. The second term is a penalty function that forces the solution to converge to a target material filling level V_t/V_0 , where V_0 is the whole simulation volume, and V_t is the desired material amount. e_{ll} is a scaling

coefficient for the penalty term, the value of which is determined in the parametric studies.

The deviation δh that minimizes J is calculated in each iteration step as:

$$\delta h = -k \left(-\frac{\partial \sigma^{ij}}{\partial h} \varepsilon_{ij} + \frac{2e_{ll}(V - V_t)}{V_0^2} \frac{\partial H}{\partial h} \right) F_{opt}, \quad (13)$$

where k is the step. The step size is adjusted to the rate of change of the function J . The stress derivative is calculated as:

$$\frac{\partial \sigma^{ij}}{\partial h} = \frac{\partial \lambda}{\partial h} I(\varepsilon) \delta^{ij} + 2 \frac{\partial \mu}{\partial h} \varepsilon^{ij}. \quad (14)$$

F_{opt} is a special mask function that is used to exclude certain areas of the cast from the optimization. For example, it was required that holes should not reach the borders of the cast parts, so a 5–10 mm wide zone of continuous material is created at the borders (see Fig. 2). This zone is enlarged to 20 mm at the connectors.

A known problem of the topology optimization is the checker-board instability, in which material properties can change from filled to hole in neighbouring mesh cells. To avoid this, δh distribution is smoothed by solving the equation:

$$\alpha^2 \Delta \delta h^* = \delta h^* - \delta h, \quad (15)$$

where α is the smoothing scale. The smoothed deviation δh^* is added to the h field. The same smoothing algorithm is applied to the h field before the calculation of the material properties.

3. RESULTS AND DISCUSSION

3.1. Numerical Implementation

The iterative topological optimization algorithm was implemented as a script for the finite element program *FreeFEM* [8]. The equations for the stresses and smoothing operators are expressed in their weak forms; the Laplacian operator and gradients are expressed via the first order derivatives $\partial_x, \partial_y, \partial_z$, the discretization schemes of which are implemented in *FreeFEM*. *FreeFEM* uses only tetrahedron meshes for volume discretization.

The *FreeFEM* script forms a part of the software that was developed for an automatic generation of 3D printable cast

shapes. The generation of a printable cast (Fig. 6) begins by scanning the surface of a patient's arm and splitting the scanned surface into two parts, which is done already by CastPrint Ltd in the case without topological optimization. A special *python* script reads the scanned surfaces and remeshes them with *gmsh* program [10] to obtain a homogeneous surface mesh with ~ 1.5 mm cell size. The 3D tetrahedron mesh is obtained by extruding the surface mesh by 4 mm (the cast thickness). The *python* script also defines all necessary boundary surfaces and sets the region with fixed filling.

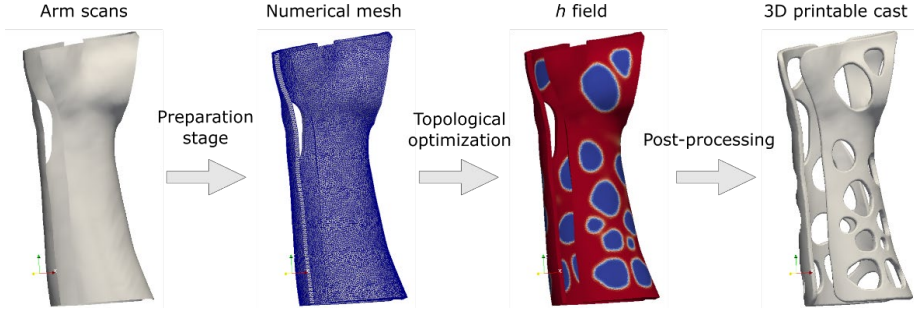


Fig. 6. Outline of generation of 3D-printable casts from scanned patient arms.

After the generation of the numerical mesh, the python script reads numerical parameters and physical property values of the model and launches a parallelized simulation on an HPC cluster. The result of the simulation is the distribution of the h field (Fig. 6). In the post-processing, the h field is averaged across the cast layer, and a 3D surface distribution of the averaged h field is obtained. *mmg* software [11] is used to

cut out holes along the $h = 0.5$ isolines of the averaged field, after which the mesh is extruded again, and sharp corners and edges are rounded. The post-processed 3D cast geometry can be printed after adding connectors manually. All simulations are carried out on the RTU HPC Center computer cluster. Typically, a simulation is run on 24 to 36 processors.

3.2. Results of Parametric Studies

A series of simulations was performed in the parametric studies of the optimization model to determine the optimal parameter values that would be valid for different types of casts. Arm scans of five different persons, labelled from P1 to P5, were used in the simulations: four adults and a child (P3). Table 1 lists the obtained model parameter values and applied material properties of the PLA plastics.

For the PLA plastics, the Young's modulus $E = 2.9$ GPa is used as a representative value, see [12]. The PLA plastics material is assumed to be isotropic; however, the casts are 3D printed by fusing together heated PLA filaments, layer by layer, and the casts tend to break apart along the fusion lines in the mechanical tests. This suggests that the PLA material in the casts could have anisotropic properties, but this problem is ignored in the current model.

The ball radius and height above the outer cast surfaces were kept constant in the simulations. Their values guarantee that the ball pressure areas are small in comparison with the cast dimensions. In principle, the value of the ball pressure scale could be estimated if characteristic parameters of the interaction of the patient with sharp corners were known. However, our stress model is quasi-linear, and a solution u_i obtained for some A_{ball} value can be scaled by a positive number k to obtain a solution for increased pressure value kA_{ball} . Correspondingly, deformation energy density scales as k^2 . Therefore, if an optimized topology (i.e., the h field distribution) is obtained for some A_{ball} and e_{ll} values, we should be able to obtain the same h distribution for kA_{ball} and k^2e_{ll} values. Since the h field is the solution, and u_i is only an intermediate

help value, we decided to use an arbitrary $A_{ball} = 3 \text{ GPa/m}$ value in all simulations.

(This value corresponds to about 150 N pressure created by the ball.)

Table 1. Parameter Values Used by the Topology Optimization Model

Parameter	Value	Parameter	Value
Young's modulus, E	2.9 GPa	A_{ball}	3 GPa/m
Poisson's coefficient, ν	0.36	Ball radius R	10 mm
Cell size	1.5 mm	Ball height H	8.75 mm
Iteration number	80	Ball position density	1600 m ⁻²
e_u	1.5 J	A_{skin}	1 MPa/m
α	5mm	A_{skin} for mechanical tests	100 MPa/m
Filling level V/V_0	0.75	A_{hard}	100 GPa/m
β	0.75..12	A_{soft}	10 GPa/m
k	0.0005..0.2	$A_{skin, friction}$	1 MPa/m

In the final scripts used in the production line, only the first order finite elements are used on a one-layer mesh. The first order elements, however, are very imprecise, and simulations with the second order finite elements were also conducted. The simulations with the second order finite elements produced significantly higher displacements and stresses for the same applied bound-

ary conditions. To compare the optimization results, the ball pressure scale A_{ball} was reduced for the second order elements. The obtained distributions of the h field for the first and second order finite elements are compared in Fig. 7. There are general similarities between the solutions, but the second order finite elements produced additional holes in the middle section.

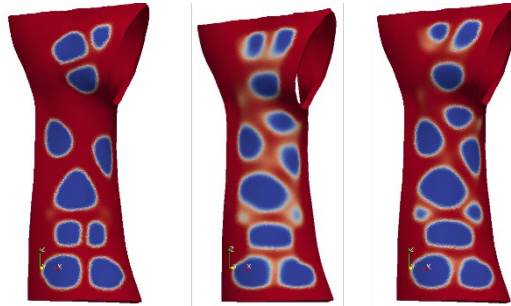


Fig. 7. Topologically optimized shapes of the cast P4. Simulations with $A_{skin} = 1 \text{ MPa/m}$. Left: simulation with first order finite elements, $A_{ball} = 3 \text{ GPa/m}$. Middle and right: simulations with the second order finite elements and $A_{ball} = 1.2 \text{ GPa/m}$ and $A_{ball} = 2 \text{ GPa/m}$. Filling level $V_t/V_0 = 0.70$.

Table 2 shows the approximate times required by simulations for the largest and smallest casts with different finite element orders. The simulations with the second order elements require 5–8 more time than the first order elements, and they can last

several hours for the largest cast. This makes the use of the second order finite elements completely impractical for this project. For this reason, all simulation results below are obtained with the first order elements.

Table 2. Comparison of Simulation Times for the Largest (P1) and Smallest (P3) Casts for Different Finite Element Orders

Number of processors	P1, 1 st order	P1, 2 nd order	P3, 1 st order	P3, 2 nd order
24	0.9 h	7.2 h	0.3 h	1.5 h
36	0.7 h	5.1 h	0.2 h	1.1 h

Similar conclusions can be made about the mesh size. Using more than one layer in the mesh would increase the simulation time beyond the acceptable one-hour limit. Our experience showed that the 1.5 mm cell size for the surface mesh was also optimal.

Convergence of the h field (see Fig.

8) shows that the solution practically converges after about 81 iterations. The h field distribution slightly fluctuates from iteration to iteration; for this reason, all simulations are run for a fixed number of 81 iterations in the production scripts.

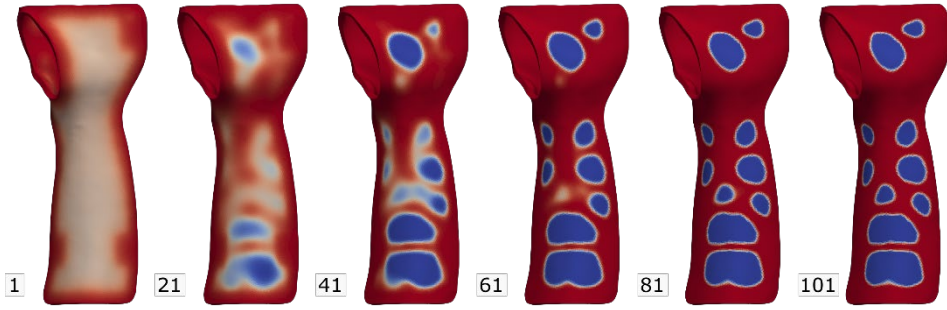


Fig. 8. Convergence of field h at different iterations. Topological optimization of P1. Target material filling level $V_t/V_0 = 0.75$, $e_{ll} = 1.5$ J, $A_{skin} = 1$ MPa/m.

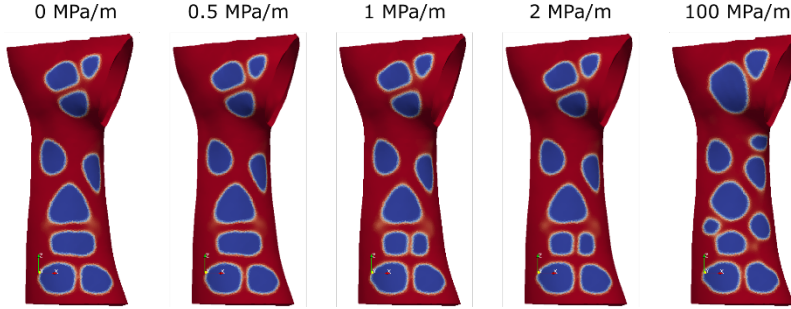


Fig. 9. Dependence of the h field distribution on A_{skin} for the cast P4. Filling level $V_t/V_0 = 0.70$. Basic values for other parameters.

The value of the elastic arm response A_{skin} is estimated as ~ 2 MPa/m from the data in [13]. However, there is an additional sheet of soft material between the cast and arm to prevent their direct contact. Therefore, a smaller value $A_{skin} = 1$ MPa/m was chosen as its basic value. A series of simulations

with different A_{skin} values was performed to determine its influence (see Fig. 9). The calculated h field distributions remain practically the same for $A_{skin} = 0 \dots 2$ MPa/m, which suggests that the arm influence is small. Significant h field changes can be observed when very large A_{skin} values are used.

It is difficult to estimate the value of the A_{hard} coefficient due to the complex shape of the cast. $A_{hard} = 100$ GPa/m was chosen as its basic value, which corresponded to the elastic response of about 30 mm thick plastic layer. It was assumed that A_{soft} was ten times smaller than A_{hard} . A series of simulations with ten times smaller A_{hard} and A_{soft} was carried out (see Fig. 10). The simulation results show a significant change

in the h field distribution both when A_{hard} and A_{soft} are changed. It seems that the connectors are major limiters for the movement of the casts, and the stress distribution is more sensitive to the A_{hard} and A_{soft} values. Therefore, the values of A_{hard} and A_{soft} could be potentially improved further by building a more precise model for the reaction of the cast to the forces on the connector surfaces.

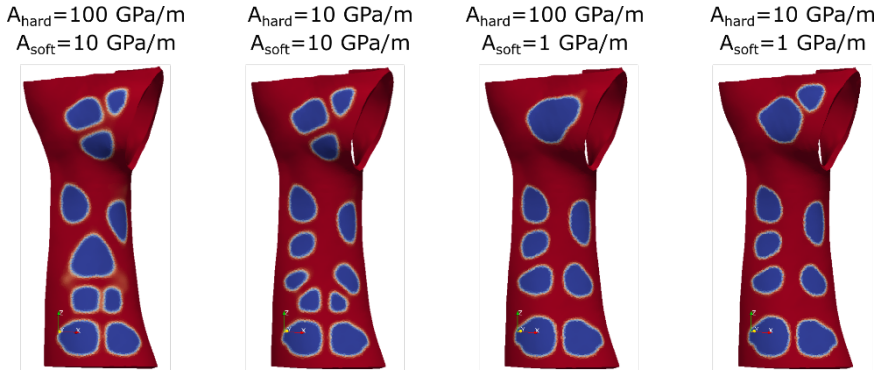


Fig. 10. Dependence of the h field distribution on A_{hard} and A_{soft} for the cast P4. Filling level $V_t/V_0 = 0.70$. Basic values for other parameters.

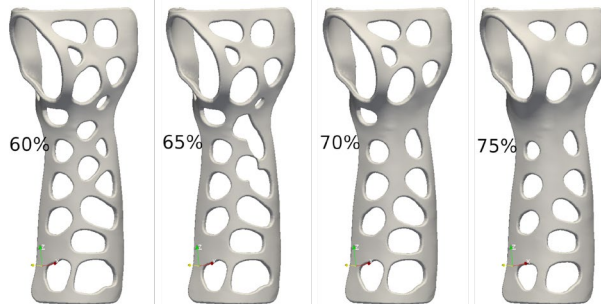


Fig. 11. Topologically optimized P1 shapes for different filling levels. The shape for 65 % filling level shows abnormalities: development of overhangs and a thin connection between two large holes in the middle of the cast.

The optimum material filling level for the casts was estimated to be $\sim 0.70..0.75$. With such fillings, the printing time of the P1 cast is reduced by 1.4..1.7 h (compared to 10.5 h which is required by the original cast), and its mass is reduced by 20 %–25 %, (see Table 3). More mass and printing time could be reduced when lower

filling levels were used (60 %–65 %). However, such casts are mechanically weaker (see Table 4) and have a greater risk of the development of material overhangs which 3D printers cannot print (see Fig. 11). Similar mass reduction is achieved for the P3 cast (see Table 5).

Table 3. Estimated Masses and Printing Times for the P1 Cast; Comparison between the Original Design of CastPrint Ltd and Optimized Designs with Different Target Filling Levels

Parameter	Original	Optimized, 0.60	Optimized, 0.70	Optimized, 0.75
Mass	208 g	139 g	148 g	160 g
Printing time	10.5 h	8.4 h	8.75 h	9.1 h

The parameter e_{ll} determines the weight of the deviation of the cast filling level from the set target value in the optimization functional (12). Increasing e_{ll} allows obtaining solutions where the actual filling level is closer to the target value. However, at very large e_{ll} , the convergence of the solution worsens, and h field fluctuations increase.

The hole boundaries can also become diffused. The results of numerous simulations have shown that $e_{ll} = 1.5$ J is an optimal value that guarantees reasonably small deviations (by few percent) of achieved filling levels from their target values for casts of different sizes (see Fig. 12).

Table 4. Maximum Values of the von Mises Stress σ_{vM} and Deformation Energy $\sigma^{ij}\varepsilon_{ij}$ in the Area around the Palm Base of the Cast P3. Simulation Results for Different Filling Levels

Filling level, V/V_0	0.60	0.65	0.70	0.75
Maximum of σ_{vM}	63.3 MPa	62.8 MPa	59.5 MPa	59.1 MPa
Maximum of $\sigma^{ij}\varepsilon_{ij}$	0.113 MJ/m ³	0.105 MJ/m ³	0.077 MJ/m ³	0.076 MJ/m ³

Table 5. Estimated Masses and Printing Times for the P3 Cast; Comparison between the Original Design of CastPrint Ltd and Optimized Design

Parameter	Original	Optimized, 0.65
Mass	102 g	75 g
Printing time	5 h	4.5 h

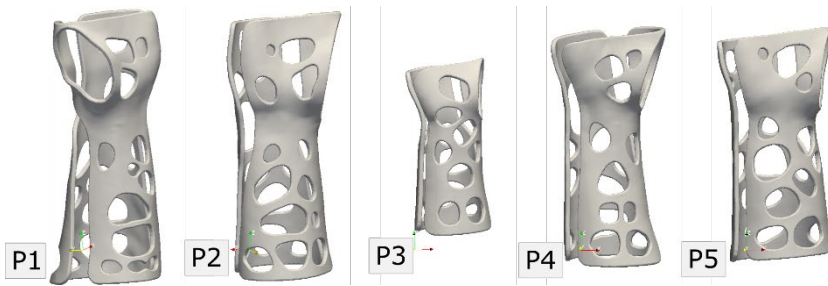


Fig. 12. Optimized 3D-printable cast geometries for five test patients. Target material filling level $V_t/V_0 = 0.70$, $e_{ll} = 1.5$ J, $A_{skin} = 1$ MPa/m.

An important parameter that determines, for example, the hole size is the smoothing scale α . It is suggested in [9] that

α should be about the size of the mesh cell. In our case, the optimum value of $\alpha = 5$ mm is approximately the same as the thickness

of the cast (4 mm). Smaller α values can cause layering of the plastic material in the cast (i.e., a local change of the thickness). A possible solution to the layering problem which would also allow using smaller α was to use a 3D surface mesh to model the h

field distribution (i.e., to use the same material properties across the layer). The material properties would have to be mapped to the 3D volume, and the stress simulations in the 3D volume would have to be mapped to the surface.

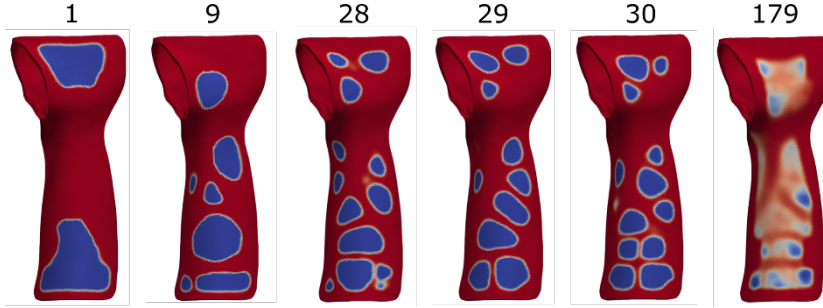


Fig. 13. h field distributions in the P1 cast obtained for different number of ball positions. Basic values for other parameters with the filling level $V_t/V_0 = 0.70$.

A special parametric study was carried out to determine the optimal number for the ball positions (Fig. 13). The number should be large enough to properly model the impact statistics. However, if the number of positions is large, it also increases the sim-

ulation time, and, for very large numbers, the h field distribution becomes diffuse. The optimum value for ball position density is estimated to be 1600 m^{-2} which corresponds to 20–30 positions per cast half for adults.

3.3. Results of Mechanical Tests

Samples of 3D printed casts were tested in ZwickRoell Z100 TEW material testing machine in a custom fixture that allowed bending of a cast perpendicularly to the fixture (see Fig. 14). The upper test support was a 60 mm diameter cylinder. The lower test fixture was a copy of patient's arm with the middle section hollowed out to allow free movement of the sample during the bending test. Both fixtures were made of 3D-printed high-performance polyether-based thermoplastic polyurethane filament, which smoothed the distribution of the applied force in a larger area.

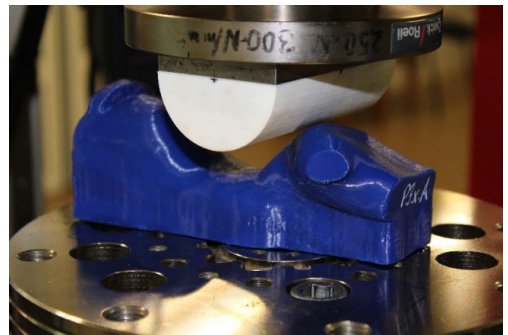


Fig. 14. The cylindrical upper test support together with a lower test fixture for the P3 cast in the ZwickRoell Z100 TEW material testing machine.

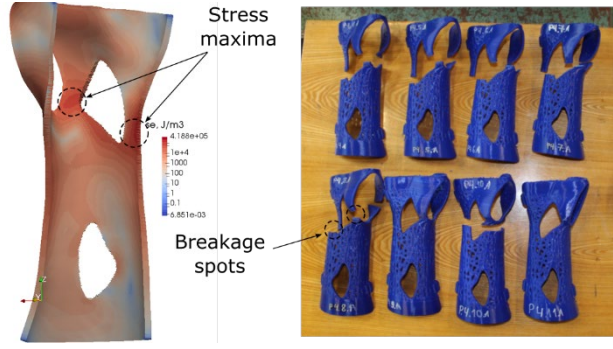


Fig. 15. Left: simulated deformation energy density distribution in original P4 casts in mechanical testing facility. Right: P4 casts broken in mechanical tests.

In the first batch of experiments, original CastPrint casts were tested. The test results for the P4 cast showed that the casts typically broke at specific spots at the palm base (Fig. 15). To validate our linear stress model, a numerical model of the original cast P4 was developed in which the major holes of the cast were modelled. The model parameters (for example, A_{skin}) were adjusted to fit the simulation results to the available data from the tests – the maximum bending of the cast was 6 mm at 100 N force. The cast deformations at the 6 mm bending are most likely nonlinear; however, the breaking spots correspond well to the calculated maxima of the deformation energy density $\sigma^{ij}\epsilon_{ij}$ (see Fig. 15). There-

fore, it seems that the linear stress model can still predict correctly critical stress concentrations against which the cast geometry should be optimized.

In the second test, a topologically optimized P3 cast, obtained with $A_{skin} = 100$ MPa/m and target filling level 0.65, was printed and tested. The test showed that the average breakage force for the optimized cast (635 N) was about 1.5 times higher than for original casts (431 N) (see Fig. 16), even though the optimized casts are 25 % lighter. Thus, the topological optimization could potentially increase the mechanical strength of the casts, but more tests were required for a more definite claim.

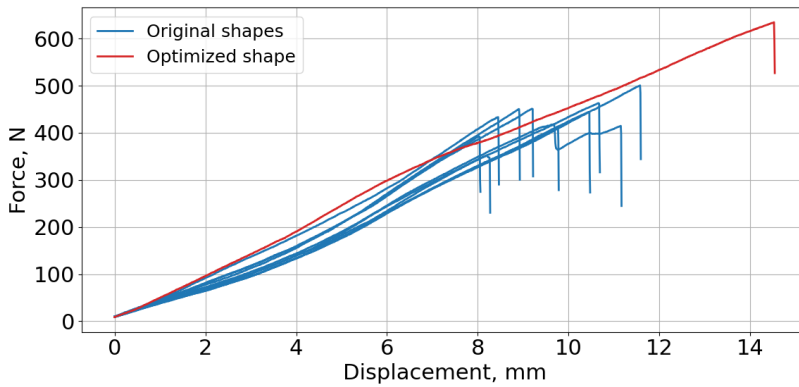


Fig. 16. Results of mechanical tests for the cast P3. Maximum displacement of the casts during bending versus applied forces. Comparison between ten 3D printed casts with the original shapes of CastPrint Ltd and the one optimized shape.

3. 4. Implications of the Results: Discussion

We have shown that the density-based topology optimization can be used to build a software program that produces a 3D-printable cast geometry from a scan of a patient's arm in less than an hour, which fulfils the project requirements. The parametric studies have also shown significant problems with our approach. The model requires significant simplification of the contact problem and can only use the first order finite elements, which makes the simulation results imprecise. To use more precise second order elements, one must speed up simulations ~5 times.

Using a 3D volume mesh is also a significant drawback of the model. It allows layering of the material, which can be solved only by using a very large smoothing parameter. It seems that the thin plate model used by [5] is more advantageous, because it automatically solves the layering problem and requires smaller meshes.

Our simulation results depend significantly on the parameters for the connectors, which means that additional modelling is required to better estimate the values for these parameters. A more general problem is that the interaction of the cast with large

objects such as walls is ignored. Perhaps, the current model with many ball positions could be replaced by a model with few interactions with large objects, but this requires the actual statistics of the interactions of the cast with external objects.

A significant and unsolved problem in the current model is the overhang formation. Here, the model based on the hollowed Voronoi tessellation [4] shows significant advantage, because it allows controlling the shapes and positions of the holes.

The current model also considers only the constant thickness casts. It might be more advantageous to make the cast thicker in places where it breaks more often. For this purpose, we suggest that CastPrint Ltd. collect information about actual breakings that occur during the exploitation of the casts. Such information can also be used to calibrate the boundary conditions for the model and to determine whether the mechanical tests replicate well the conditions of the actual use. Finally, more mechanical tests with different casts and more loads should be conducted to make more definite conclusions about the optimization quality.

4. CONCLUSIONS

The results of numerical modelling have showed that a density-based topology optimization model can be used to optimize the shapes of 3D-printed casts. The shapes are optimized against multiple loads created by small balls placed at different places on the cast to model the statistics of the cast interactions with sharp corners. The interaction between both cast halves and between the cast and the arm are also modelled. However, the numerical model requires signifi-

cant simplifications to make it practical for industrial applications. The contact problems must be significantly simplified, and the first order finite elements must be used.

The simulation results have demonstrated that the mass of the optimized casts is reduced by 20 %–25 % in comparison with the original casts of CastPrint Ltd. The printing time for the largest cast is reduced by 1.4–1.7 h which exceeds the time spent on the simulations. Similar time reduction

is obtained for the smallest cast. These are significant improvements in the cast production from the industrial point of view. The created optimization model has been implemented in the cast production line, and it can be used to generate 3D-printable cast shapes.

The conducted mechanical tests on the smallest cast have shown that it may be more durable than the original cast of Cast-Print Ltd. However, only one optimized cast sample has been tested, which is insufficient to make any definite conclusions. More mechanical tests with a larger variety of mechanical loads should be conducted in the future.

The simulation results show that using a 3D numerical volume to model material distribution in the cast is a drawback, and

the material distribution should be homogenized across the cast layer (this could be done, for example, by using a thin plate model). The problem of material overhangs should also be addressed in the future model versions. The anisotropy of the plastic material properties caused by the production process should be considered, too.

Finally, the cast interactions with other types of external objects should be considered (for example, walls). A significant problem here is the lack of experimental data on the interactions of the casts with external objects. We suggest that the cast producers collect more data on the breakages of the cast during their exploitation, which could help in developing better boundary conditions for the numerical model.

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REFERENCES

1. Ranaldo, D., Zonta, F., Florian, S., & Lazzaro, J. (2023). A Facile, Semi-Automatic Protocol for the Design and Production of 3D Printed, Anatomical Customized Orthopedic Casts for Forearm Fractures. *Journal of Clinical Orthopaedics and Trauma*, 42, 102206.
2. Lin, H., Shi, L., & Wang, D. (2015). A Rapid and Intelligent Designing Technique for Patient-Specific and 3D-Printed Orthopedic Cast. *3D Printing in Medicine*, 2 (1), 4.
3. Zhang, X., Fang, G., Dai, Ch., Verlinden, J., Wu, J., Whiting, E. & Wang, Ch. (2017). Thermal-comfort design of personalized casts. In *UIST '17: Proceedings of the 30th Annual ACM Symposium on User Interface Software and Technology* (pp. 243–254). ACM, New York, USA.
4. Rao, C., Tian, L., Yan, D.-M., Liao, Sh., Deussen, O. & Lu, L. (2019). *Computer Aided Geometric Design*, 71, 130–141.
5. Zhang, Y., & Kwok, Tsz. (2019). Customization and Topology Optimization of Compression Casts/Braces on Two-Manifold Surfaces. *Computer-Aided Design*, 111, 113–122.
6. Sigmund, O., & Maute, K. (2013). Topology Optimization Approaches. *Structural and Multidisciplinary Optimization*, 48, 1031–1055.
7. Bendsoe, M. P. (1989). Optimal Shape Design as a Material Distribution Problem. *Structural Optimization*, 1, 193–202.
8. Hecht, F. (2012). New Development in FreeFem++. *Journal of Numerical Mathematics*, 20, 251–265.

9. Bonnetier, E., & Dapogny, C. (n.d.). *Optimization of a Cantilever Beam with Density-Based Topology Optimization Algorithm. An Introduction to Shape and Topology Optimization*. Available at <https://membres-ljk.imag.fr/Charles.Dapogny/coursoptim.html>
10. Geuzaine, C., & Remacle, J.-F. (2009). Gmsh: A 3-D Finite Element Mesh Generator with Built-in Pre- and Post-Processing Facilities. *International Journal for Numerical Methods in Engineering*, 79, 1309–1331.
11. Balarac, G., Basile, F., Bénard, F. P., Bordeu, F., Chapelier, J.-B., Cirrottola, L., ... & Zakari, M. (2022). Tetrahedral Remeshing in the Context of Large-Scale Numerical Simulation and High Performance Computing. *MathematicS In Action*, 11 (1), 129–164.
12. Pszczółkowski, B., Nowak, K.W., Rejmer, W., Bramowicz, M., Dzadz, Ł., & Gałęcki, R. (2022). A Comparative Analysis of Selected Methods for Determining Young's Modulus in Polylactic Acid Samples Manufactured with the FDM Method. *Materials*, 15, 149.
13. Van Kuilenburg, J., Masen, M. A., & van der Heide, E. (2012). Contact Modelling of Human Skin: What Value to Use for the Modulus of Elasticity? *Proc IMechE Part J: J. Engineering Tribology*, 227 (4), 349–361.