

Ollscoil na hÉireann, Corcaigh
National University of Ireland, Cork



Self-Assembling Magnetic Chains for Minimally-Invasive Surgery

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for the degree of
Doctor of Philosophy

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2022

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Declaration

This is to certify that the work I am submitting is my own and has not been submitted for another degree, either at University College Cork or elsewhere. All external references and sources are clearly acknowledged and identified within the contents. I have read and understood the regulations of University College Cork concerning plagiarism and intellectual property.



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Abstract

Minimally-invasive surgery has led to significantly improved success rates and decreased recovery times for surgical procedures, by minimising the access wounds to the patient. This imposes a restriction on any tool used during minimally-invasive surgery. A trade-off between incision size and the number of tools or tool size has to be achieved. The development of tools that change their shape, are able to pass through narrow ports and can assemble into functional forms is therefore desirable. This would decouple the size of the tool during use from the size during deployment. Such reconfiguring tools can be categorised under the engineering field of self-assembly, a process with countless examples in nature.

The principle of self-assembly applied to surgical tools could potentially remove the size limitation a port imposes on the used tool. This work seeks to work toward the development of a general concept of self-assembly to be used in minimally-invasive surgery. The concept proposed in this thesis employs a subcategory of self-assembly, the self-folding chain. The self-folding chains analysed and proposed in this work mimic the process of the protein biosynthesis as it happens on a molecular level in our cells. A chain of magnetic components, linked together by rotational joints, allows for deployment through a long flexible tube and therefore facilitates the application in a range of surgical procedures. Once deployed and free of the confinement of the deployment tube, the magnetic attraction between the chain components in combination with the unique restrictions of the joints cause the chain to fold on itself to a functional device.

Folding was first investigated in a plane where it could be recorded and analysed. The experimental results were tested against simulation and evaluated for their reliability and repeatability. Based on the results, a three-dimensional concept was developed. This concept allows for a uniform magnetic orientation of the folded device and consequently promotes the utilisation of the magnetic properties in surgery. Based on these properties, target applications were chosen in magnetic anastomosis creation and magnetic anchoring. The target scale necessary for use in minimally-invasive surgery places a range of challenges on material and mechanisms used. A prototype of a folding magnetic anastomosis device, which solves the need for an intelligent design of a compliant mechanism, was developed and tested in a pre-clinical study, demonstrating the feasibility of the concept.

Acknowledgements

None of our achievements is ever truly done alone and this work is no exception. I would like to thank Pádraig Cantillon-Murphy for believing in me and allowing me to work on this captivating project. Even when there was hardship, it was a brilliant experience. I want to thank both Pádraig Cantillon-Murphy Murphy and Guangbo Hao for the relentless support as my supervisors. Without them I could not have done this.

I would also like to thank the staff of the Department of Electrical Engineering. Among those, I want to express my gratitude and respect to Mick O'Shea and Tim Power for their workmanship. With their flawless expertise so many experimental setups were made possible. I want to thank them for the trust they put in me, by allowing me independent access to the 3D printing facilities.

Lastly, I would have never finished this body of work without the emotional support of all the friends and colleagues, who I met along the way. The welcoming student community in the power lab made me feel at home from day one and the lunch and coffee breaks were an integral part of my routine. In my peers and colleagues in Tyndall I found friends who encouraged me even through the pandemic and difficult times. Thank you Stefania for bearing with my impossible night shifts of the last months and thank you for all your love and support.

Thank you all.

*To all those who are lost but will never be forgotten,
To all those who have lost someone but can't forget,
In memory of Arne*

List of Publications

Peer Reviewed Journal Papers

1. T. H. Fass, G. Hao, and P. Cantillon-Murphy, "Vectorised Formulation of Newton-Euler Dynamics for Efficiently Computing 3D Folding Chains," *Journal of Mechanism and Robotics*, ASME, 2021, vol. 14, p. 061007.
2. T. H. Fass, G. Hao, and P. Cantillon-Murphy, "Design and Pre-Clinical Evaluation of a Folding Magnetic Anastomosis Device for Minimally Invasive Surgery," *Minimally Invasive Therapy & Allied Technologies*, 2022, accepted subject to revision.
3. T. H. Fass, G. Hao, and P. Cantillon-Murphy, "On Planar Self-Folding Magnetic Chains: Comparison of Newton–Euler Dynamics and Internal Energy Optimisation," *Robotics and Autonomous Systems*, vol. 132, p. 103601, 2020.

Peer Reviewed Conferences

1. Presentation: T. H. Fass, G. Hao, and P. Cantillon-Murphy, "General Concept of Self-Assembling tools for minimally invasive surgery," 26th Annual Conference of the International Society for Computer Aided Surgery (ISCAS), Tokyo, Japan, 2022
2. Presentation: T. H. Fass, G. Hao, and P. Cantillon-Murphy, "Pre-Clinical Evaluation of a Folding Magnetic Anastomosis Device for Minimally Invasive Surgery," *International Society for Medical Innovation and Technology*, Oslo, Norway, 2022.
3. Paper: T. H. Fass, G. Hao, and P. Cantillon-Murphy, "Vectorised Formulation of Newton-Euler Dynamics for Efficiently Computing 3D Folding Chains," *International Conference on Reconfigurable Mechanism and Robotics*, Toronto, Canada, vol. 5, p. 645, 2021.

4. Presentation: T. H. Fass, G. Hao, and P. Cantillon-Murphy, "Self-Assembly in Magnetic Surgery, a Folding Anastomosis Device for Minimally Invasive Surgery," International Congress of Magnetic Surgery, online, Xi'an, China, 2021.
5. Poster: T. H. Fass, G. Hao, and P. Cantillon-Murphy, "Self-Assembling Magnetic Tools for Minimally Invasive Surgery," International Society for Medical Innovation and Technology, Online, USA, 2020.
6. Presentation: T. H. Fass, G. Hao, and P. Cantillon-Murphy, "Self-Folding Magnetic Anastomosis Device," International Congress of Magnetic Surgery, online, Xi'an, China, 2020.
7. Presentation: T. H. Fass, G. Hao, and P. Cantillon-Murphy, "Magnetic Self-Assembling Tool for Minimally Invasive Surgery," Biomedical & Clinical Engineering Association of Ireland, Cork, Ireland, 2019.
8. Poster: T. H. Fass, G. Hao, and P. Cantillon-Murphy, "Self-Assembling Magnetic Chain or Minimally Invasive Surgery," International Society for Medical Innovation and Technology, Heilbronn, Germany, 2019.
9. Presentation: T. H. Fass, and P. Cantillon-Murphy, "Intelligent Magnetics for Surgery 4.0," International Congress of Magnetic Surgery, online, Xi'an, China, 2018.

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Nomenclature

exp.	description		
z	scalar		
$\mathbf{z}$	generalised vector		
$\vec{\mathbf{z}}$	vector in space $\vec{\mathbf{z}} = (z_1, z_2, z_3)$		
$\mathbf{Z}$	matrix		
$\dot{z}$	first derivative by time $\dot{z} = \frac{\partial z}{\partial t}$		
$\ddot{z}$	second derivative by time $\ddot{z} = \frac{\partial^2 z}{\partial t^2}$		
$[\vec{\mathbf{z}}]_x$	cross product matrix $[\vec{\mathbf{z}}]_x = \begin{pmatrix} 0 & -z_3 & z_2 \\ z_3 & 0 & -z_1 \\ -z_2 & z_1 & 0 \end{pmatrix}$		
sym.	description	set	unit
n	number of components in the chain	$\in \mathbb{N}$	
m	mass of a body	$\in \mathbb{R}$	kg
$\mathbf{I}$	inertia of a body	$\in \mathbb{R}^{3 \times 3}$	kg m ²
$\vec{\mathbf{x}}$	position vector	$\in \mathbb{R}^3$	m
$\vec{\mathbf{v}}$	velocity vector $\vec{\mathbf{v}} = \frac{\partial \vec{\mathbf{x}}}{\partial t}$	$\in \mathbb{R}^3$	m/s
$\vec{\mathbf{a}}$	acceleration vector $\vec{\mathbf{a}} = \frac{\partial \vec{\mathbf{v}}}{\partial t}$	$\in \mathbb{R}^3$	m/s ²
$\vec{\mathbf{r}}$	position vector in a rotating system	$\in \mathbb{R}^3$	m
$\vec{\varphi}$	rotation vector	$\in \mathbb{R}^3$	rad
$\vec{\omega}$	angular velocity vector $\vec{\omega} = \frac{\partial \vec{\varphi}}{\partial t}$	$\in \mathbb{R}^3$	rad/s
$\vec{\alpha}$	angular acceleration vector $\vec{\alpha} = \frac{\partial \vec{\omega}}{\partial t}$	$\in \mathbb{R}^3$	rad/s ²
$\mathbf{Q}$	rotation matrix	$\in \mathbb{Q}^{3 \times 3}$	
$\mathbf{W}$	angular velocity cross product matrix $\mathbf{W} = [\vec{\omega}]_x$	$\in \mathbb{R}^{3 \times 3}$	rad/s ²
$\vec{\mathbf{f}}$	force vector	$\in \mathbb{R}^3$	N
$\vec{\tau}$	torque vector	$\in \mathbb{R}^3$	N m
q	point charge magnitude	$\in \mathbb{R}$	A m
$\mathbf{B}$	magnet flux density	$\in \mathbb{R}$	T
$\mathbf{H}$	magnetic field strength	$\in \mathbb{R}$	A/m
$\mathbf{M}$	magnetisation field	$\in \mathbb{R}$	A/m
$\vec{\mathbf{m}}$	magnetisation vector	$\in \mathbb{R}^3$	A/m

Constants			
sym.	value	description	unit
g	$= 9.81$	gravity acceleration on the surface of earth	m/s^2
μ_0	$= 4\pi \times 10^{-7}$	electromagnetic permeability of free space	H/m

Abbreviations

short	full
API	Application Programming Interface
BBS	Benign Biliary Strictures
CPU	Central Processing Unit
DOF	Degree of Freedom
EMA	European Medical Agency
FDM	Fused Deposition Modeling
GJ	gastro-jejunal (between stomach and small intestine)
GPU	Graphical Processing Unit
GUI	Graphical User Interface
JJ	jejuno-jejunal (between two portions of the small intestine)
PLA	Polylactic acid
PP	Polypropylene
PTBD	Percutaneous Transhepatic Biliary Drainage
SIMD	Single instruction, multiple data
STL	Standard Tessellation Language
UCC	University College Cork

1 Introduction

Minimally-invasive surgery (MIS) has revolutionised modern medicine by significantly reducing the invasiveness of procedures and with it improving recovery rate and time compared to open surgery [1]. MIS was first pioneered by interventional clinicians in the 1970s and has been continuously developed and improved since then. Minimising the invasiveness of procedures places unique challenges on the surgeon as well as on the tools used during surgery. Any procedure can be improved with the aim to be completely non-invasive. Surgical procedures are constantly improved. While surgeons improve their techniques, new and improved tools need to be developed to facilitate these new and improved procedures. The tools used are often tailored to a specific class of procedures or are specifically designed for a single procedure. Over the decades a wide range of specialised instruments have been developed to enable and improve minimally-invasive procedures. [2] These tools have to balance a range of requirements. While the tools have to fulfill a certain function such as cutting, manipulating or connecting tissue, they also have to be minimal in size, operable remotely and comply with strict safety standards.

Every tool used in minimally-invasive surgery has to be deployed. The port used to deploy it, typically has to be proportional to the size of the tool. To minimize any incision necessary to create a port, new generations of surgical tools have become smaller and more intelligently designed. However, there is a limit on how small a tool might be before it interferes with its functionality. Depending on the procedure, larger tools would be necessary and a port to deploy the tool has to be significantly larger, resulting in increased invasiveness of the procedure. In such procedures the cavity inside of the body might be pressurised using techniques such as positive pressure ventilation [3]. As such, the cavity often offers sufficient space for larger tools but the size of the incision necessary to deploy these tools would be increasingly

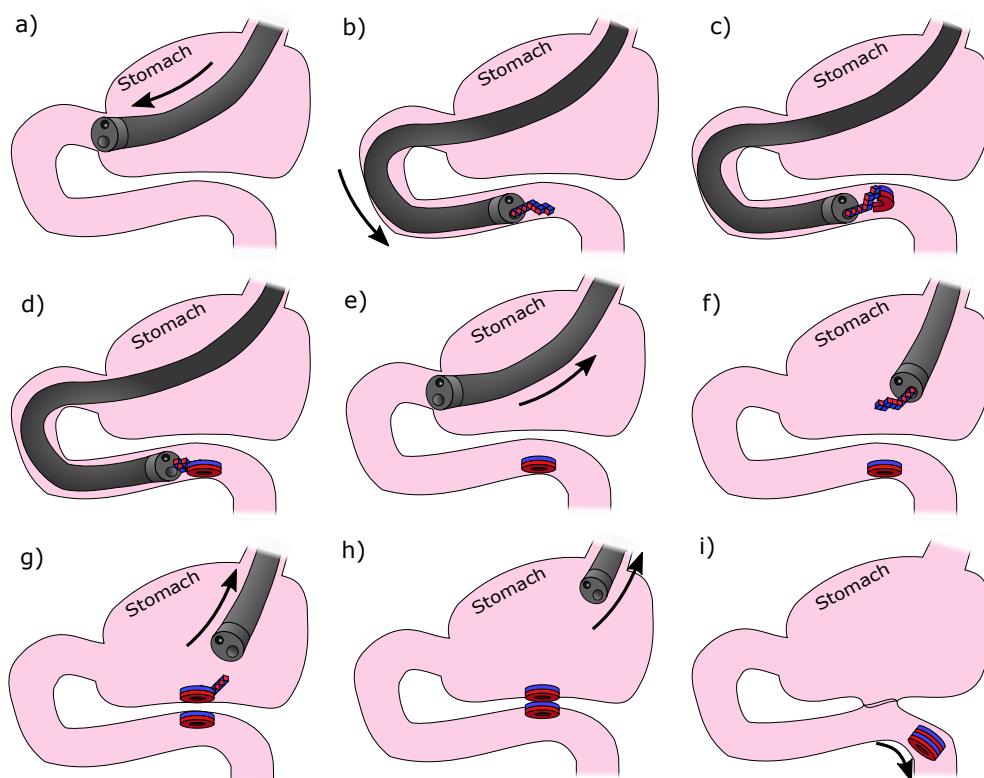


Figure 1.1: Storyboard of a self-reconfiguring magnetic anastomosis device in a gastrojejunostomy. a) positioning of endoscope, b) and c) deployment of first magnetic device, e) repositioning of endoscope, f) and g) deployment of second magnetic device, h) anastomosis is formed due to magnetic compression, i) devices are latched and is expelled via natural processes.

invasive. Recent developments in surgical technology have focused on eliminating the human limits of the surgeon by introducing robotic systems that perform the operation [4]. However, what if we use principles of robotics to improve the tool itself and create reconfigurable surgical tools that transform once deployed, to address one of the limiting factors in minimally-invasive surgery, the port size.

1.1 The Challenges

Devices to be used in minimally-invasive surgery are typically delivered through device channels approximately from 2.4 mm to 9.8 mm in size [5]. In this work we focus on device channels with a diameter of 3.8 mm, as used in endoscopes [6]. In consequence, any mechanism that allows them to change their shape and functionality has to fit into this size for delivery. In this target size scale, the requirements of necessary force output and reliability put a hard stop to many concepts. Depending on the use case, a surgical device might be required to withstand considerable forces. A reconfiguring device is reliant on the hinges that enable the reshaping. In the target scale of millimeters these hinges present the weak spot in most constructions of reconfiguring surgical tools. Even if a device is devised that works at a larger scale at a laboratory the translation to the clinical setting introduces a range of unknown factors that pose additional requirements on robustness and reliability of a device.

A range of theoretical concepts exist in this field, some of which provide specific solutions. Others propose a general concept applicable to a range of possible tools. Translating these concepts into reality poses an immense challenge to production methods, material properties and designed mechanism, as the necessary size requirements are limiting. As a result, very few of the existing concepts have ever been tested in a clinical setting.

1.2 Aim of this Thesis

This thesis seeks to contribute to address the size limitation which the deployment port imposes on the surgical tool and in consequence, allow for improved and novel procedures in minimally-invasive surgery. To this end, a general concept has been developed on how to apply principles of robotics to reconfigure a tool after deployment into a functional shape larger than the

port used to deploy it. The hope is that this thesis may serve as a cornerstone for future surgical tools which can transform their shape to the given need. In its most simple application, this thesis intends to transform a surgical tool from a string that can easily pass through small spaces into simple shapes that can be used in surgery. The developed mechanism and principles used to realise this folding are targeted to be transferable to more complex shapes. Therefore, this thesis aspires to present prototypes that not only demonstrate that a transformation of a surgical tool is possible but also that the concepts proposed in this work are capable of achieving the reliability to allow for their use in a clinical setting and that it is possible to produce the proposed designs. The objectives of this thesis can be summarised in the following points:

- The primary aim is to create a concept to construct self-folding magnetic chains, that can be used as tools in minimally-invasive surgery.
- The concept needs to consider production methods to facilitate the application to tools used in minimally-invasive surgery.
- The concept needs to include necessary software tools to construct and analyse self-folding chains.
- The concept is validated in a range of benchtop experiments and prototypes.

1.3 Thesis Outline

This thesis is structured to offer the reader an informative presentation of the conducted research and the research that has been done in the field. The thesis consists of six main parts; The introduction, the background chapter, the methods, the body of theoretical work, the body of practical work and lastly the conclusion.

Chapter 2 provides all necessary knowledge for a comprehensive understanding of the thesis. This chapter details key knowledge from the various disciplines of minimally-invasive surgery, medical device design, self-assembly and rigid body kinematics. Finally existing technology in the field will be described to establish relevant up to date research.

Chapter 3 details the theoretical concepts that have been developed in

the scope of this PhD. The methods of simulation will be introduced in Section 3.1. In Section 3.4 a novel interpretation of Newton Euler dynamics will be presented, that allows for the efficient computation of rigid body chains. The methods presented in this chapter will be validated in simulation and in comparison to a benchtop experiment of a planar folding chain. The planar folding chain reduces the chain movement to two dimensions to allow for efficient analysis of the underlying folding behaviour.

From there, the investigation of a general concept of self folding magnetic chains will be presented in Chapter 4. This general concept explores underlying folding behaviour and introduces secondary structures analogous to protein folding observed in biology. These secondary structures aid in the construction of magnetic self-folding chains.

Chapter 5 will focus on the specific implementations of the developed theoretical concepts and introduce prototypes that work as a proof of concept. These prototypes will be introduced in order of device complexity. The direct application of the previously secondary structures as an anchor for surgical applications is investigated in Section 5.2. The concept is expanded to a prototype implementing full self-assembly of a three-dimensional device in Section 5.3. Lastly, a proof-of-concept prototype for a folding magnetic anastomosis ring that was tested in a pre-clinical study is documented in Section 5.4.

At the end of each Chapter a summary will be presented. The conclusion of Chapter 6 will put all findings in context and provide an analysis on the work as a whole.

2 Background

This chapter will introduce the necessary knowledge to understand and interpret the findings presented in this thesis. At first the background and concepts of medical devices and guidelines on medical device design will be detailed. The relevant information of chain kinematics and information on self-assembly are presented. Finally, work that has been done in the field and that builds the foundation for this thesis will be detailed to establish the frame of reference for this work.

2.1 Medical Devices

In contrast to open surgery, minimally-invasive surgery seeks to minimise invasiveness of a given procedure by utilising a number of techniques and highly specialised devices, that allow for internal operation through ports. These ports, often named "key holes", might be small incisions or natural orifices. The challenges minimally-invasive surgery needs to overcome to allow the surgeon to operate, are accessibility of the target area and visualisation of the performed operation.

Medical devices are any and all tools that aid in a medical procedure. Due to the application in minimally-invasive surgery these devices have to comply with strict regulations and need to be highly efficient and reliable. An overview on requirements and best practice in medical device design is given in Section 2.1.1. While this work seeks to develop a general concept of self-assembling surgery devices, two primary target procedures and corresponding tools have been selected to act as direct applications and proofs of concept: anastomosis creation and surgical anchoring. Both procedures are detailed in Section 2.1.2.

2.1.1 Medical Device Design

Medical devices have to adhere to strict rules and regulations to be considered safe for use in surgery. The specific rules applying depend on the specific application of the device and the country of use. Due to the location of our research group and associates, the primary consideration in device design are the European *Medical Device Regulations* published by the *European Medicines Agency* (EMA) [7].

The *Medical Device Regulations* classify medical devices into four overarching categories differentiating in the possible risk for the patient:

- Class I: This class contain medical devices that are not used *in vivo* and are completely noninvasive.
- Class IIa: This classification encompasses devices that might be used *in vivo* but are designed to have minimal invasiveness. An example might be a surgical clamp.
- Class IIb: Devices that are *in vivo* but could pose potential harm are classified under this category. An anastomosis device might be classified here.
- Class III: If a Device could be potentially lethal it is classified under this category. Typically devices that are used *in vivo* and rely on electricity or emit heat are in class III such as pacemakers.

The final classification of any medical device is open to interpretation by the EMA and certification granting body. Therefore this work might only specify a targeted classification. The use of magnets to project forces without electrical devices *in vivo* is a significantly safer device design compared to the use of electromagnets or electrical driven motors. The final classification likely depends on the magnitude of projected forces. Devices as they are proposed here might be classified as Class IIa or IIb. Electric potential and forces are not the only risk factor in a medical device. The material used in a device might pose a risk factor to a patient. Any potentially toxic material should be avoided or sealed within medically approved material.

Aside from official regulations, the usability and ergonomics of a medical device has to be considered. The end user of a medical device is a surgeon or their assistants. Best practices in medical device design from [8] have been taken into consideration for the development of the presented prototypes as

well as the European standard for medical device design in *ISO 13485* [9]. While some form of training to use a device can be expected, for a surgical setting the device should be fast and secure to use. This requires a simple, straight-forward use with minimal setup time and a minimal number of steps to use the device. The handle to operate a medical device therefore is of importance, as is the interface for the surgeon and should promote a fast and error free operation [8]. All necessary steps to operate a device should be clearly marked and a handle should be designed to prevent or hinder misuse. Furthermore, a handle to operate the device should feature an ergonomic design. In the medical setting any used device should be designed to offer the possibility of easy and reliable sterilisation.

Lastly devices and appropriate handles should be designed under consideration of existing production methods and facilitate a design that is possible to produce and can be assembled in a minimum of production steps.

2.1.2 Magnets in minimally-invasive Surgery

One of the first applications of magnets in surgery has been described in 1957 by *M. Equen* [10]. The unique ability of magnets to project a force over any non-magnetic barriers such as tissue potentially allows for manipulation without the need for an incision. This principle is used in magnetic anchoring and magnetic anastomosis creation.

Magnetic Anchoring

During a procedure, it often is necessary to move tissue to be able to operate in the necessary areas. A forcep to move the tissue commonly has to have a physical connection to relay the pull force through an additional port. In magnetic anchoring however, a magnet is attached to the tissue, typically via a clip. It then is attracted using an external magnet and as a consequence the target tissue is pulled in the desired direction due to the magnetic forces pulling on the attached magnet. This technology might be used to lift a gastric polyp in an operation as seen in Figure 2.1(a) without the need of an additional port for anchoring.

Figure 2.1 also shows commercially available instances of magnetic anchoring for minimally-invasive surgery. The *Levita Magnetics* technology utilizes a permanent magnet for internal and external magnet. The *Pentax*

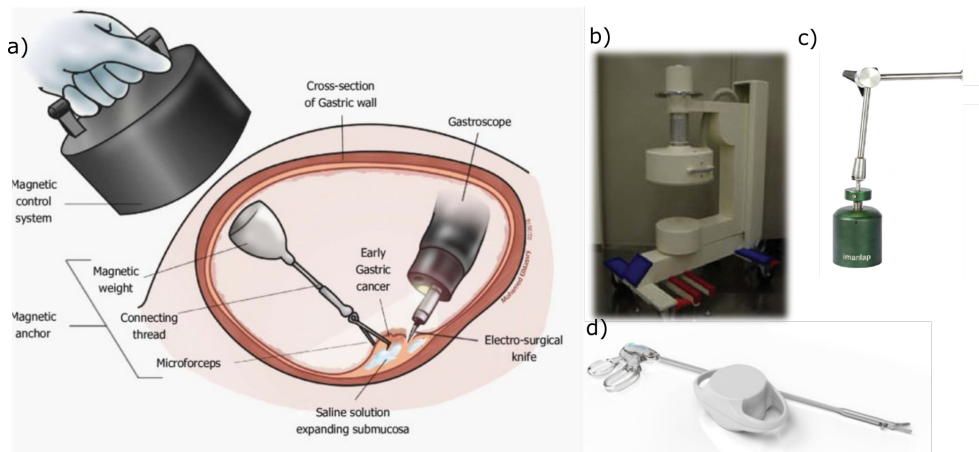


Figure 2.1: a) Working principle of magnetic anchoring devices [11] b) Pentax system, electromagnetic anchoring device [12] c) Magnetic anchoring device from Guillermo Dominguez [13] d) Levita Magnetix, magnetised instruments [14].

System uses an electromagnet as an external magnet. While the permanent magnet is smaller in size, an electromagnet offers significantly more control. The magnet that is deployed internally however is a permanent magnet. A permanent magnet might achieve a better size-to-force ratio and avoids potentially harmful electric currents in devices that are used internally. To project significant forces, the internal magnets have a size of 3mm and consequently have to be deployed through ports of at least the same size. Systems such as the *Levita Magnetix* are deployed at the end of a rigid beam and can not be deployed through flexible catheters or device channels.

Magnetic Anastomosis Creation

Anastomosis creation is a class of procedure where a connection is established between previously unconnected cavities or vessels [16]. Such an artificial connection between parts of the body is called fistula. One of the first documented cases of an anastomosis creation was performed by A. Woelfer in 1881 [2]. These procedures might be used to clear blockages or join organs previously not connected. In general three types of anastomosis creation are differentiated as seen in Figure 2.2 [15]. A common application is in the gastrointestinal tract to treat obesity or cancer where parts of the digestive system is taken out or bridged [2]. Depending on the joined parts of the digestive system these procedures are named as seen in Figure 2.3. For example the Jejunojejunostomy (JJ-anastomosis) where the Jejunum (that is part of the small intestines) is shortened by joining two loops of intestine together. A part of the small intestine (usually containing disease such as cancer) is

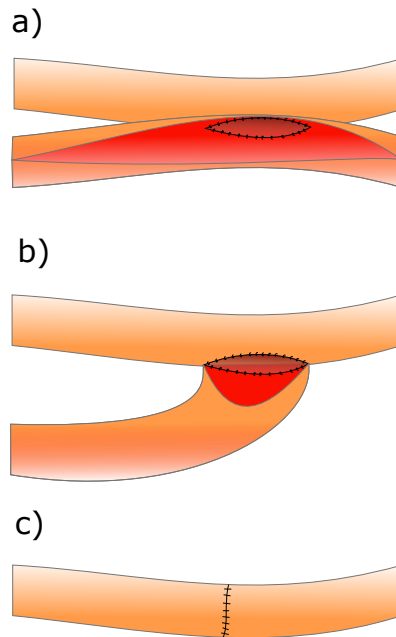


Figure 2.2: a) Side-to-side anastomosis b) side-to-end anastomosis c) end-to-end anastomosis [15].

cut out and the open ends are joined [15]. This might be used to treat obesity or to cut out cancerous parts of the intestine. The anastomosis creation between Stomach and intestine is commonly named as Gastrojejunostomy (GJ-anastomosis). Due to the nature of surgical anastomosis creation, it is highly invasive [17].

In contrast to conventional anastomosis creation, magnetic anastomosis creation does not require cutting, sewing or stapling of tissue and is, in an ideal case, bloodless. Two magnets might be placed in neighbouring parts of the body. The magnetic attraction between the magnets will cause them to couple together over the tissue wall and exert pressure on the tissue that is trapped between them [19]. This pressure will hinder the blood flow into the tissue. As a result, the tissue between the magnets will become necrotic and eventually die off until both magnets contact and an anastomosis is formed, ideally without leakage around the sealed fistula. As this techniques require the tissue to be trapped between the magnets, it is commonly utilised for side-to-side anastomosis or for the clearing of blockages.

One example application of interest to this work is the use of magnetic compression to form a jejunojejunostomy as seen in Figure 2.4. Here the magnets are placed in two parts of the small intestine and will form an anastomosis between them [20]. The successful use of magnetic compression

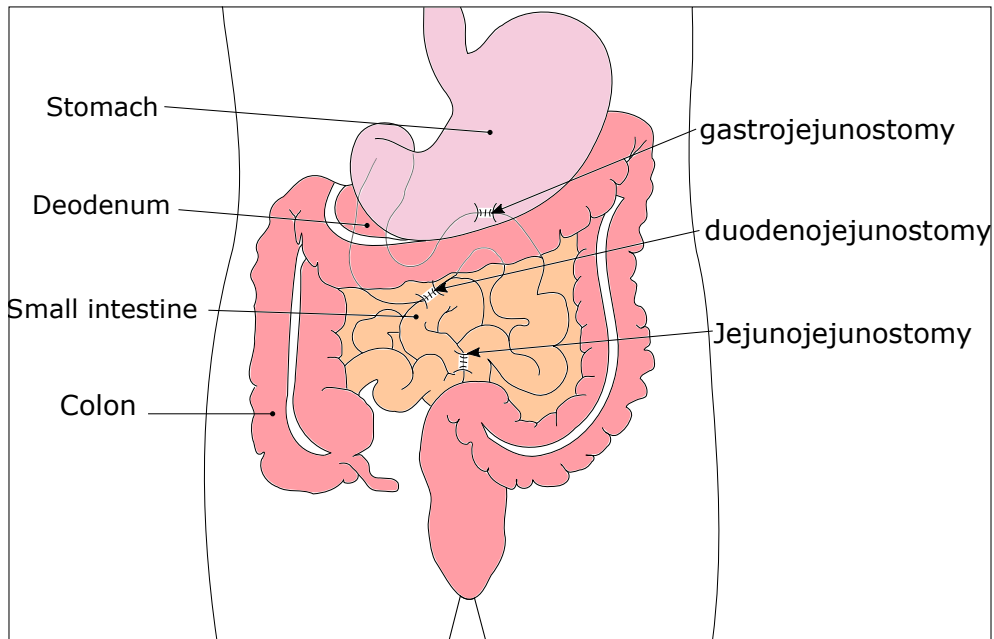


Figure 2.3: Types of anastomosis in gastrointestinal tract [18].

anastomosis has further been shown in GJ-anastomosis [20] and to clear blockages in the bile tree [21]. A study on successful anastomosis creation and the respective pressure and forces on the tissue has been created by *Lambe et al.* [22]. Similarly an estimate of what forces could potentially harm tissue, provides a limit of acceptable force for magnetic anchoring applications. It is noteworthy that these studies show the importance of magnetic force per area (pressure) over simply magnetic force.

Challenges of Magnetic Surgery

A shortcoming of current magnetic technology for surgery is the deployment. Commonly, *in vivo* applications avoid the use of electromagnets to project magnetic forces as the current necessary to run them is potentially harmful to the patient. Instead, permanent magnets are preferred for *in vivo* use for their space efficiency and safety. However a permanent magnet requires a certain size to project sufficient forces and, in case of anastomosis creation, the magnet requires the same diameter as the desired size of the anastomosis. In case of JJ- or GJ-anastomosis this might be up to 23mm [19]. Any such magnet typically requires a port of similar size for deployment, potentially negating the reduced invasiveness gained by the use of magnets.

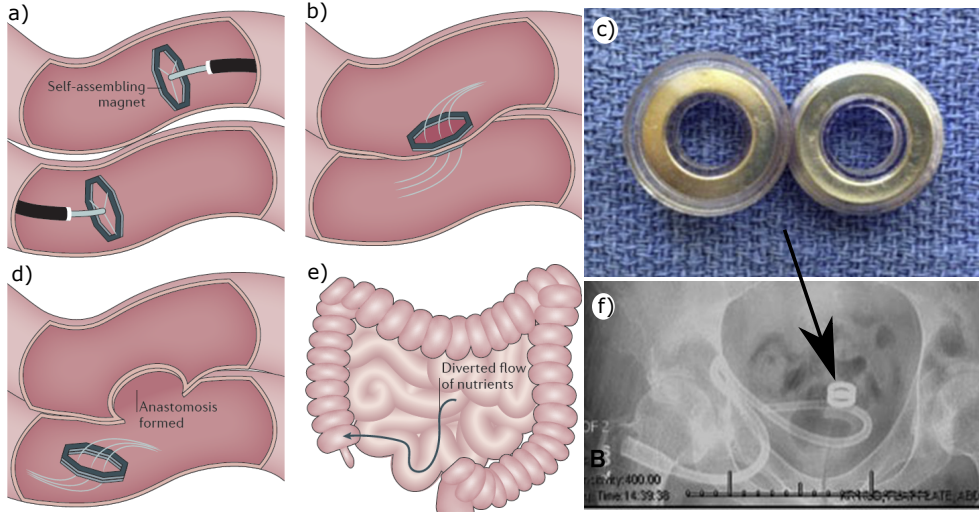


Figure 2.4: a), b), d) and e) Magnetic anastomosis device principle [23]; c) and f) Magnetic anastomosis creation (Magnamosis) on a human [19].

2.2 Magnetism

The desired driving force in the target procedures and in the self-reconfiguration process is magnetism. From children's toys, to fridge magnets, to electric engines, magnets and electromechanical devices are an essential part in modern life. Magnetism is a consequence of the electromagnetic force that is one of the fundamental forces of nature and is capable of projecting forces over a distance much like gravity. This force manifests between electrically charged particles and is expressed in an electromagnetic field defined by *Coulomb's Law*

$$|\vec{f}| = k \frac{q_1 q_2}{d^2} \quad (2.1)$$

where the magnitude of a force between two charged particles $\vec{f}$ is equivalent to the product of the Coulomb constant k and the charges q_1 and q_2 divided by the square of the distance between the particles d [24]. The magnetic potential of an electromagnetic field is described by two closely related vector fields: the magnetic flux density $\mathbf{B}$ and the magnetic strength $\mathbf{H}$. An electromagnet creates an electromagnetic field due to the electric current in a body of metal [25]. The magnetic field generated by a copper wire can be described by *Ampere's Law*

$$\oint_S \mathbf{J} dA = \oint_C \mathbf{H} dl \quad (2.2)$$

where the magnetizing field $\mathbf{H}$ around any closed loop C is equivalent to the current $\mathbf{J}$ integrated over the surface S of the cross section A of a wire [25].

The response of a material with the magnetisation $\mathbf{M}$ under an electromagnetic field can be measured in the magnetic flux $\mathbf{B}$. In linear media, the magnetic flux and magnetic field strength are linked by the electromagnetic vacuum permeability $\mu_0 = 4\pi * 10^{-7}$ H/m and the magnetisation of a material $\mathbf{M}$ via the expression

$$\mathbf{B} = \mu_0(\mathbf{H} + \mathbf{M}) \quad (2.3)$$

In non-magnetic or not magnetised material the magnetisation can be considered zero. It is important to note that the magnetic point charge model and magnetic surface current model for magnetic field are useful mathematical tools, though they have no physical analogue in the way that electrical point charges and surface currents exist in the physical domain. This is due to the absence of a magnetic monopole.

Most magnetic materials consist of magnetic domains within these materials. These domains are regions within a material where the magnetisation is in a uniform direction. The magnetisation of each domain can be expressed in a vector describing the direction of the magnetic field it projects. A non-magnetic material has all of its magnetic domains aligned differently and resulting in a randomly oriented magnetic moment for each domain. In a ferromagnetic material, all of these domains might spontaneously align in the same direction, maximising the net magnetic field of the material [25]. Permanent magnets most commonly consist of ferromagnetic material that has been magnetised by subjecting it to a strong external electromagnetic field. A part of the magnetic charge of a ferromagnetic material is retained in its internal magnetisation $\mathbf{M}$ as remanence after removal of the external electromagnetic field. The relationship between the magnetic field strength of an external magnetic field and the magnetisation of a material can be seen in its magnetisation curve, displayed in Figure 2.5. A hysteresis curve is produced by subjecting a material to an electromagnetic field with varying field strength $\mathbf{H}$ and changing magnetic field direction to continuously flip the magnetisation direction of the material.

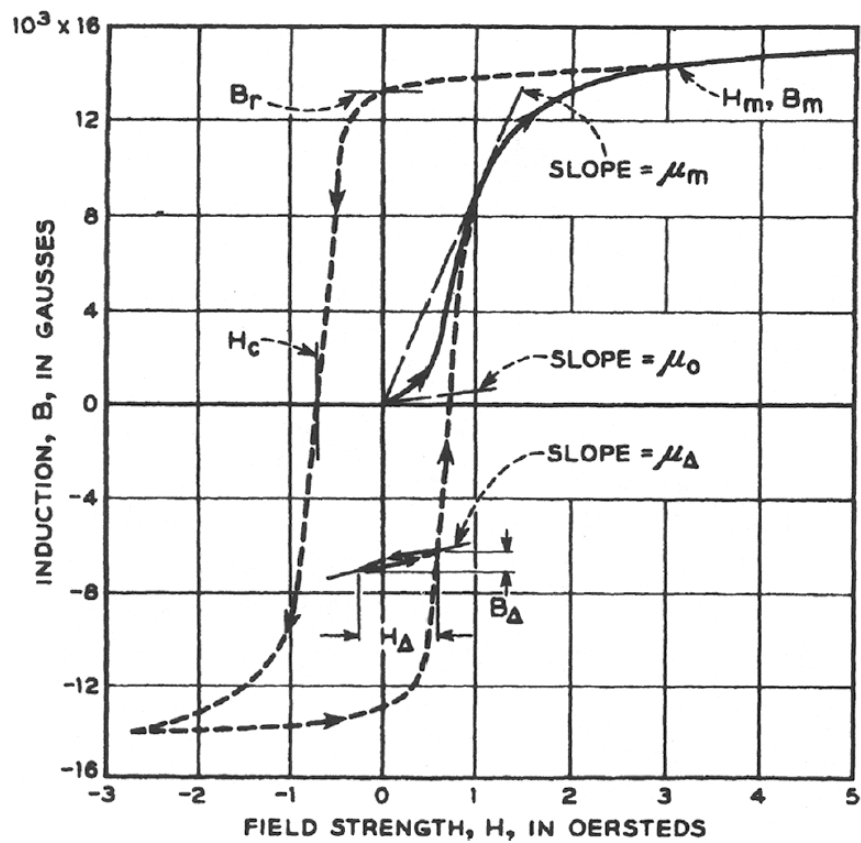


Figure 2.5: Magnetic flux response of ferromagnetic material to an electromagnetic field. Solid line: Magnetisation curve; Dotted line: Hysteresis curve [24].

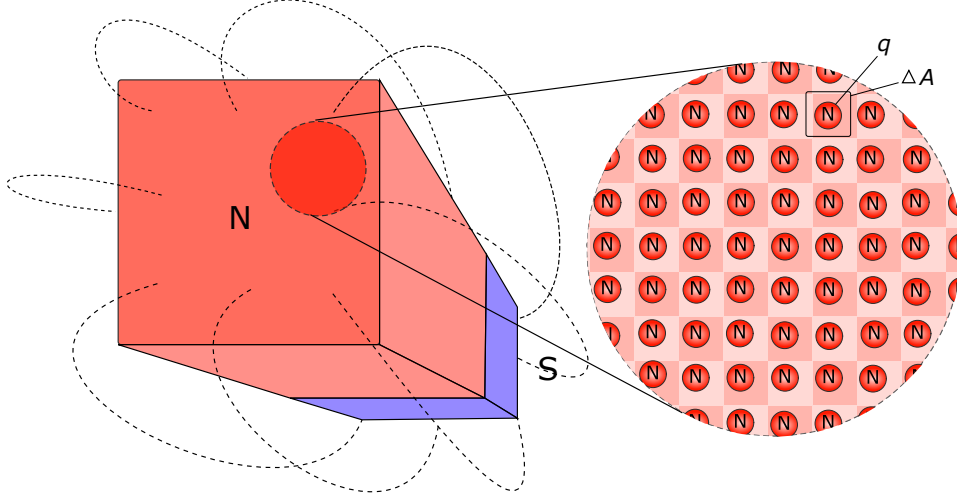


Figure 2.6: Point charges model to approximate the magnetic surface of a beam magnet.

2.2.1 Point Charge Model

While *Coulomb's law* is capable of analytically describing the electromagnetic field that is exerted by a permanent magnet, a numerical solution needs to be found to simulate the underlying physics of complex magnetic systems. Coulomb's Point charge model, describes a magnetic body by discretising finite elements of surface area of a magnet as point charges as seen in Figure 2.6. These point charges are defined by their individual surface charge q [25] that represent the magnetic potential of a finite element of surface area δA equally distributed over each north and south polarised surface. The forces acting between the magnets are approximated by the sum of forces acting between the point charges. The force acting on the k^{th} magnetic point charge with respect to the l^{th} magnetic point charge, with the charges q_k and q_l , is defined by *Coulomb's law* for magnetic charges [25]:

$$\vec{f}_{mag\ kl} = \vec{d}_{kl} \frac{\mu_0}{4\pi} \frac{q_k q_l}{|\vec{d}_{kl}|^3} \quad (2.4)$$

where the $\vec{d}_{kl}$ is the vector from point charge q_k to q_l .

Much like gravity, this is a conservative force, meaning that any work needed to separate magnets is equivalent to the work generated when reversing the separation. As such the magnetic interaction can be characterised by a potential energy. The part of the potential energy that results from magnetic interaction can be approximated by the point charge model as the *Coulomb energy*:

$$U = \sum_k^{n_q} \sum_{l|k \neq l}^{n_q} \frac{\mu_0}{4\pi} \frac{q_k q_l}{|\vec{\mathbf{d}}_{kl}|} \quad (2.5)$$

with U being the *Coulomb* energy of the system, given by the double summation over all n_q point charges in the system and where $|\vec{\mathbf{d}}_{kl}|$ is the distance between the point charges with the indices k and l , and with $k \neq l$.

The point charge q_i is proportional, to the scalar product of the magnetisation $\vec{\mathbf{m}}$ and surface normal $\vec{\mathbf{n}}_i$ divided by the individual area ΔA_i the charge represents.

$$q_i = \frac{\vec{\mathbf{m}} \cdot \vec{\mathbf{n}}_i}{\Delta A_i} \quad (2.6)$$

This model is an adequate approximation of the magnetic properties of a body if the diameter of a surface slice is significantly smaller then the distance to the opposite charge [25].

$$\odot \Delta A_i \ll \mathbf{d}_{kl} \quad (2.7)$$

In this thesis Coulomb's Point charge model is used to model magnetic interaction and to subsequently analyse and predict the folding of magnetic chains. The relationship between $\odot \Delta A_i$ and $\mathbf{d}_{kl}$ is investigated in Section 3.1.2.

2.3 Self-Assembly

This work employs methods of self assembly to construct self reconfiguring chains to be used in minimally-invasive surgery. To date, there is no general definition of self-assembly. What is seen as self-assembly strongly differs depending on the area the term is used in. For example, *Kazuo Hosokawa*, researching in the field of biology, defines self-assembly as

“Viruses and bacterial flagella are constructed automatically out of protein sub-units. This phenomenon is called self-assembly, which is a powerful technique applicable to microfabrication.” [26]

From snowflakes, to galaxies, every self organising system that does not have direct human interaction could be seen as self-assembly. This thesis works within the boundaries of the definition, provided by John A. Palesko, in his book “Self Assembly - The Science of Things That Put Themselves

Together”:

“Self-assembly refers to the spontaneous formation of organized structures through a stochastic process that involves pre-existing components, is reversible, and can be controlled by proper design of the components, the environment, and the driving force.”[27]

If we compare self-assembly with regular assembly, when an object is assembled by an outside intelligence, such as a human or a robot, it is assembled according to the plan of this intelligence. In self-assembly, however, the information of the assembled shape of the system is encoded within the system itself. This is possible as every system always tends to reach its most stable state, namely the state in which it has the least free energy. One of the most intuitive examples is two magnets. Placed apart, in a free space at a certain distance, each will experience a force with respect to the other. Once released the magnets will accelerate toward each other due to the magnetic attraction and eventually the north surface mates with the south surface. In this state, the maximum of force will be necessary to pull them apart again. Therefore the state in which the magnets are mated is already encoded in the system as the state with the minimum potential energy. In any state where the magnets are prevented from mating, a change of environment that allows for the magnets to mate will cause the system to self-assemble.

While this is the most simple example with just two bodies, self assembling systems in nature consist of millions of bodies in complex restrictions that allow for the self-assembly of various structures. Examples of self-assembly might be found everywhere in nature. Possibly most well-known is self-reproduction, a subgroup of self-assembly. A single cell contains the complete information of the organism and a cell is capable to reproduce itself to eventually form a human. While this process is infinitely more complex than two magnets interacting, it relies on similar principles of minimising potential energy. At the center of this process is a less well-known example of self-assembly, protein biosynthesis: a phenomena that functions as a biological role model for the research done in this thesis. A protein is composed of amino acids. Amino acids are large molecules, connected by only one bond to the next amino acid and thus form a chain, like pearls on a string.

These amino acids have various mode of interaction with each other, such as chemical bonds, hydrogen bridges and hydrophobic interactions. These interactions define the internal energy of the molecule, not unlike magnetic interaction between magnets. In this way, the protein composed of a chain of amino acids folds on itself building a functional tool in our body. The specific folding and, thus, the task the protein is able to fulfil in our body, is only encoded in the sequence of different amino acids along the chain of the protein and its interaction with the environment. The sequence of amino acids in proteins is what is encoded in our *DNA* and every process in our body has its origin in the folding of these proteins. This process happens continuously in our body, with an incredible reliability. One of the rare cases where this process decreases in reliability is theorised to be directly linked to neurological degeneration diseases such as Alzheimer and Parkinson [28].

This work employs techniques and proposes devices that mimic the principles of protein folding in a simplified and controllable form. Protein Biosynthesis is a proof that reliable and repeatable self-assembly in a macroscopic scale is possible. In this work existing ways to predict this process of self-folding are discussed, using methods from protein structure prediction. The goal is to construct a system that will self-assemble into the desired shape. To achieve this, a method is required that is capable of predicting the shape a system will self-assemble to. Two methods to conclude to such a prediction are:

- (1) Analysing the dynamics of the system, allowing to predict the steps of movement of all components and follow it to its state of interest.
- (2) Calculating states where the system is in equilibrium and picking the one most likely to occur.

Following the definition of self-assembly from *John A. Palesko* [27], each self-assembling system is defined by:

- *The components*, often referred to as tiles, that form into a larger structure. In every self-assembling system, there are a finite number of component types;
- *The binding force* is the force that binds the components together once they interact;
- *The environment* is critical to a self-assembly process as it imposes boundary conditions, enabling or disabling certain states;

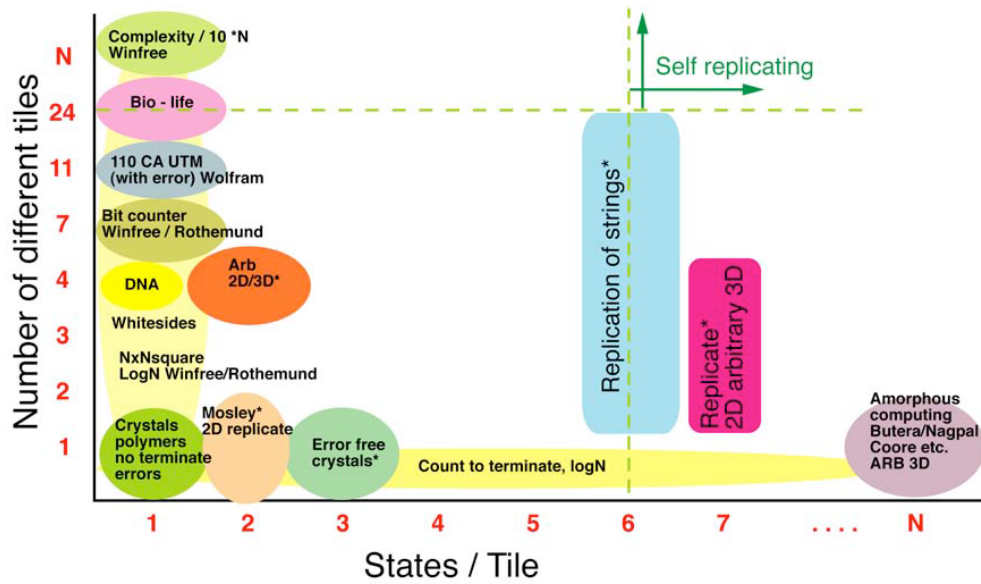


Figure 2.7: Complexity of self-assembling systems. Plotting the number of possible states per tile (component) against the number of different tiles (components) [29].

- *The driving force* is the force that moves the components, ultimately causing them to interact with each other.

The environment is often a difficult factor to determine. In the following, relevant research of self-folding will be defined by these categories. A controlled environment refers to laboratory conditions without any random error, taken into account for the assembling process. Of special importance to this work is the size of the components a self-assembling system is composed of. Magnetic forces are proportional to the magnetic area as seen in Equation (2.6), while mass is proportional to the volume. Thus the ratio of mass to the forces that move these mass might drastically change with the general scale of a self-assembling system.

An exceptional work to mention is the thesis of *Saul Thomas Griffith* [29]. It is one of the most complete works in self-assembly and therefore builds one of the cornerstones of this thesis. In his work he categorizes the different self-assembly systems according to their complexity, as displayed in Figure 2.7. As such, he defines the complexity of a self-assembly system due to the different number of components and the number of states of each component.

In his thesis *Griffith* describes the physical process behind the folding of

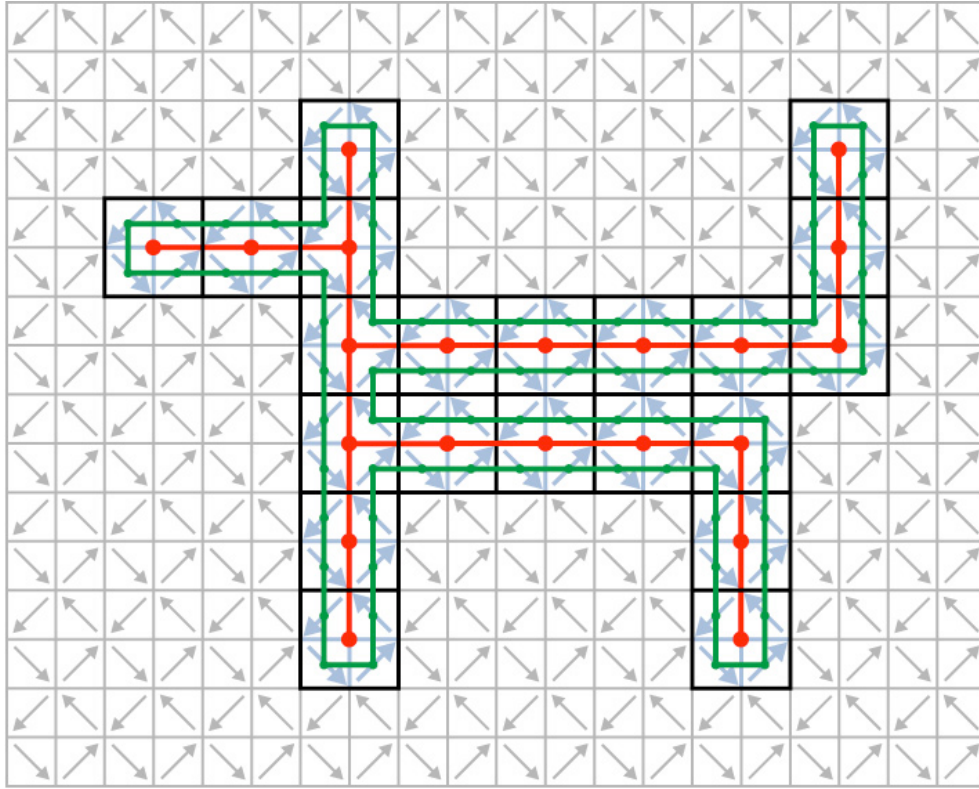


Figure 2.8: 2D folding construction for a dog-shape. Grey: Underlying matrix for folding. Black: Tiles for folding. Green Hamiltonian path. The path a chain of tile elements could take to fold into the specific shape [29].

a chain as well as the path planning for the chain to achieve 3D-structures. Furthermore, he analyses different geometries for components, with respect to their efficiency of filling a three dimensional space. As seen in Figure 2.8 any planar structure can be approximated as long as a *Hamiltonian* path can be planned that visits all components in the shape exactly once. This is equivalently translatable to volumetric shapes [29].

A thorough analysis of the mathematics behind self-assembly, packing and space filling shapes is presented by *Dustin Reishus* [30] and *Leonard M. Adamant* [31]. They also highlight the importance of the complexity of a self assembling system. As an example, consider a system of n cubes. Considering it is important which side of the cube is connecting as well as the orientation, each cube has 6 different states. This results in 6^n different possible states. Brute force solving a system of 100 such cubes is impractical. Intelligent search algorithms exist to find possible folding states more efficiently via the internal energy minimisation method. The chains considered in this work are short compared to most nano-scale self-assembly and this work relies on simple energy minimisation methods based on the potential

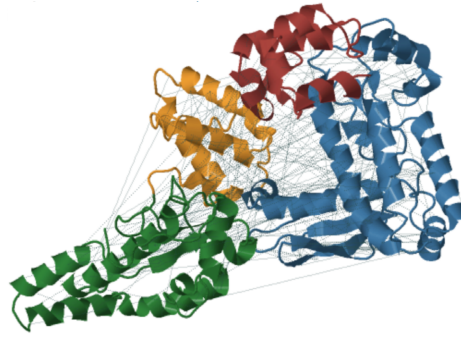


Figure 2.9: Protein folding prediction using *AlephProteinDatabase* [32].

energy described by Coulomb's Law in Section 2.2. On the other hand, a simulation of the folding dynamics is computationally significantly heavier than for long chains as well. Existing methods for the prediction of the folding dynamics are discussed in Section 2.4

2.3.1 Self-Assembly in Nature

This thesis has a great focus on a special subclass of self-assembly: the self-folding of a chain of components. The aforementioned protein bio-synthesis is the classical example that this work seeks to imitate for use in surgery. Therefore this section classifies the protein bio-synthesis, represented in Figure 2.9, under defined categories.

- Type: Component: Amino acid diameter 0.8nm:
- Complexity: n components, 24 states:
- Binding force: Chemical interactions (for example H-bound) and Hydrophobicity:
- Driving force: Charges and Hydrophobicity:
- Environment: Cell environment.

Each amino acid could be seen as a component of the chain that experiences attraction or repulsion from all other elements [33]. As a result of these forces, component along the chain move in a certain direction dictating the folding of the chain. Therefore the protein folding could be understood as a purely kinematic problem. However, with 50 to 27,000 amino acids in one protein and several different forms of attraction between the amino acids, this kinematic problem is far too complex to be computed. Therefore the most common approach is to understand the folding prediction as an

optimisation problem, purely focused on computing and finding a minimal state of energy for the protein. The internal energy is then seen simply as a landscape where the correct minima has to be found. This is achieved by optimizing algorithms such as *Monte Carlo* or *genetic optimization*, aided by cross-referencing with similar known proteins and their folded state. *T. J. Brunette* and *Oliver Brock* make a great effort employing this technique to predict the folding of proteins [32]. Another successfully approach is the use of AI to predict the folding of proteins [34].

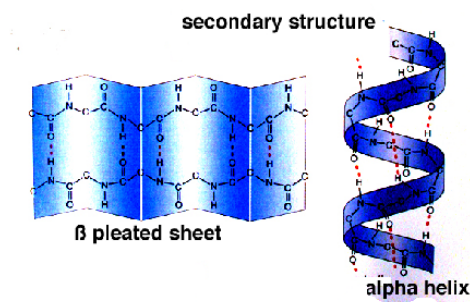


Figure 2.10: Secondary structure of proteins [35].

Of special interest are the repeating patterns in the folding of proteins, resulting in a differentiation of primary, secondary and tertiary structures within one protein. The primary is the chain of amino acids. The tertiary structure is the outer shape of the finished folded protein. The secondary structures however are reoccurring substructures within the protein, called alpha helix and beta sheet. These substructures, seen in Figure 2.10, feature a low internal energy and are therefore favorable for the whole systems internal energy [35]. Identifying possible secondary structures can therefore lead to a simplification in the folding prediction.

Based on this analysis of self-assembly in general a concept of self-reconfiguring magnetic chains is introduced in this thesis. This concept mimics the self-assembling of proteins and primary, secondary and tertiary structures are defined to enable a reliable folding.

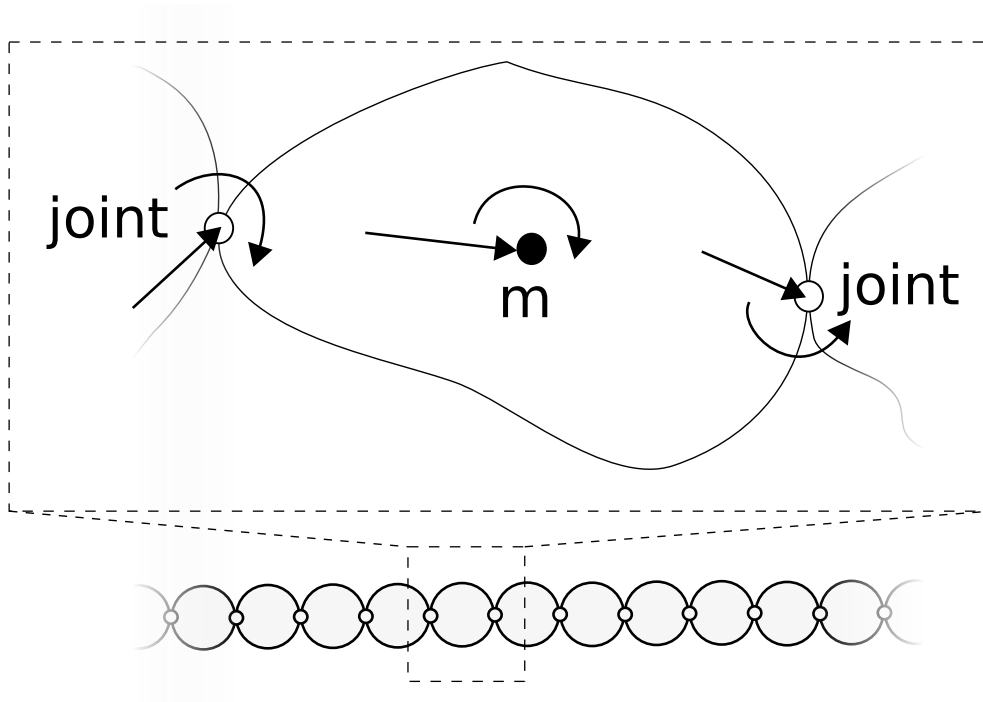


Figure 2.11: Generic component in a chain of solid bodies linked by joints.

2.4 Simulation of MultiBody Chains

This section focuses on methods to compute the dynamics of a folding chain of components in order to predict how each component will move and with it the final folded state. To predict and control this folding process all involved forces have to be understood and a numerical or analytical expression of the underlying physics is necessary. In this section we will introduce the central equations that govern the movement of rigid body chains and describe ways to simulate their behaviour. To achieve this the chain is idealised as a set of rigid bodies linked together by joints.

2.4.1 Dynamics of Rigid Body Chains

The dynamics of a system are commonly characterised by the *Newton-Euler* equation or the *Euler-Lagrange* equation. The *Newton-Euler* equation is based on an equilibrium of forces $\vec{f}$ and acceleration $\vec{a}$ acting on a body with the mass m [36];

$$\sum \vec{f} = m\vec{a} \quad (2.8)$$

and the equilibrium of torques $\vec{\tau}$ and angular acceleration $\vec{\alpha}$ of the same body with inertia I can be described as;

$$\sum \vec{\tau} = I\vec{\alpha} + \vec{\omega} \times I\vec{\omega} \quad (2.9)$$

If all rotation and torque is described around the center of mass, Equation (2.9) is reduced to;

$$I\vec{\alpha} = \sum \vec{\tau} \quad (2.10)$$

These equations describe the connection between the forces acting on a solid body and the acceleration resulting from it as well as the torques acting on a body and the consequent angular acceleration. A link between solid bodies as seen in Figure 2.11 might as well be described by reactive forces that act on a body corresponding to the forces that act on the linked body. To solve a system of multi body chains the forces in the links might be considered unknowns.

The *Euler-Lagrange* equations on the other hand define the kinematics from the potential energy of the system and as such offer a convenient solution for a multi body system. The *Euler-Lagrange* [37] equation (second kind) is expressed as;

$$\frac{\partial}{\partial t} \frac{\partial L}{\partial \dot{\xi}_i} - \frac{\partial L}{\partial \xi_i} = 0 \quad (2.11)$$

where $L = T - V$ is the difference of the kinetic energy T and the potential energy V . ξ_i are the generalised coordinates of the system and $\dot{\xi}_i$ are the generalised velocities. *Silver 1982* [38] attempts a comparison between the *Euler-Lagrange* and the *Newton-Euler* approach and shows that both are comparable in the possible representation of rotation in the system and both may potentially be used recursively to compute the dynamics of a system.

2.4.2 Numerical Computation

While the primary focus of this thesis is the resolution of simulated results for short chains, the simulation of very long chains is investigated in an effort to understand the limits of the proposed concept of self assembling surgery tools. Many numerical approaches that are capable of correctly simulating the self-reconfiguring process governing multi-body chains and rigid body dynamics exist. The differentiating factor between the simulation approaches is the computational effort that results in the time necessary to compute the dynamics. There is a range of factors that change the computational effort, from the programming language chosen to the hardware used. However as

specifically long chains are of interest this thesis focuses on the complexity of a numerical approach and the potential use of specialised hardware that allows for some of these calculations to be processed simultaneously. The complexity describes the relationship between number of components in the chain and the number of computational steps required. The majority of modern *Central Processing Units* (CPU) in computer systems support *Single Input Multiple Data* (SIMD) architectures, a method to compute a limited number of operations at the same time. A *Graphical Processing Unit* (GPU), in contrast, is a hardware specialized in parallel computing and allows for the fast computation of compatible algorithms.

The system dynamics can be efficiently computed recursively with the *Articulated-Body Algorithm* [39] [40]. This algorithm has a complexity of $\sigma(n)$, meaning the number of necessary computations is linear compared to the number of components in the chain. However it is computing the forces in the links, component by component, which relies on the result of the previous component and therefore is computed in sequence. Due to the use of GPU, multi core processors and the SIMD model [41] modern computers can process multiple operations simultaneously and significantly increase computational speed. A different class of algorithm is necessary to utilise this potential for parallel computation architectures, where the independent calculations do not depend on each other's results. The Divide and Conquer algorithm [42] that is based on the Newton-Euler equations allows for some form of parallel computation. Chadaj 2017 [43] presents an implementation of Divide and Conquer for the Hamilton equations and uses parallel computation. These algorithms separate the chain in segments that are computed simultaneously.

Another possibility is the vectorisation of the algorithm, where the dynamics of the system are represented in a set of independent vector equations that allow for the computation of dynamics for all components of the system simultaneously. GPUs and the SIMD model are particularly efficient in regard to vector computations [41]. A. Stokes 1996 [44] and P.C. Müller 1992 [45] describe two vectorised approaches to the *Euler-Lagrange* kinematics. The *Euler-Lagrange* equations have the distinct advantage of deriving the kinematics from the energy of the system and therefore have an estimated complexity of $\sigma(n)$ as well as being expressed in a vector equation as favorable for parallel computation. However as previously discussed the

Euler-Lagrange equations are unfavorable to include complex forces.

2.5 Existing Technology

This work lies at the intersection of medical technology and self-assembly. In this section, existing technology in the field will be highlighted to establish the inspirations this work relied upon. To this end self-assembling robots and the current state of the art in this field is detailed, with mention of possible solutions in magnetism. Finally, research that has been done specifically in the field of self-assembling in medical technology is described.

2.5.1 A Map of Self-Assembly

This section presents specific devices that exist in the field. Influential instances of self-reconfiguring robots are described. Finally recent research of self-assembly and self-reconfiguration in medicine is presented. This seeks to establish a frame of reference and allows for the work presented in this thesis to be compared to the state of the art.

Self-Assembling Robots

The self-assembly of robots represents the most flexible and intelligent branch of self-assembly, as they typically consist of a swarm of only one kind of programmable robotic-component. Therefore, in comparison to crystals or proteins, the assembly information is not encrypted in a formation or sequence of different components but is instead variable in the program of the robots. In conclusion, the concept of complexity is only remotely applicable here. The individual robots with a means of actuation couple together to form larger structures. These systems are also refereed to as "*self-reconfiguring systems*". Yim et al. give a very good overview of current self-reconfiguring robotic systems in their work [46]. That work provides three examples which mark the boundaries and current capabilities, of self-reconfiguring robots. They are classified in Table 2.1.

The fundamental difference of these systems in comparison to proteins or crystals is that the structure the components are building is variable. This means that the very same components are capable of building different structures. To achieve this, every component of the system has to have a means of actuation as well as a means of computing and communication. As a result, the minimal size of the devices is limited by the minimal size

Table 2.1: Self-assembling robots: Individual robots with a means of actuation couple together to form larger structures. Groups: self-organising, self-assembling, self-reconfiguring.

	M-Blocks [47]	Superbot [48]	Mini-Bot [49]
Type:	... dynamic-, programmable self-assembly ...		
Component dimension:	50mm	84mm	20mm
Complexity:	 1 component, infinite states		
Binding force:	magnetism	mechanical	mechanical
Driving force:	momentum	mechanical	mechanical
Environment:	 controlled		

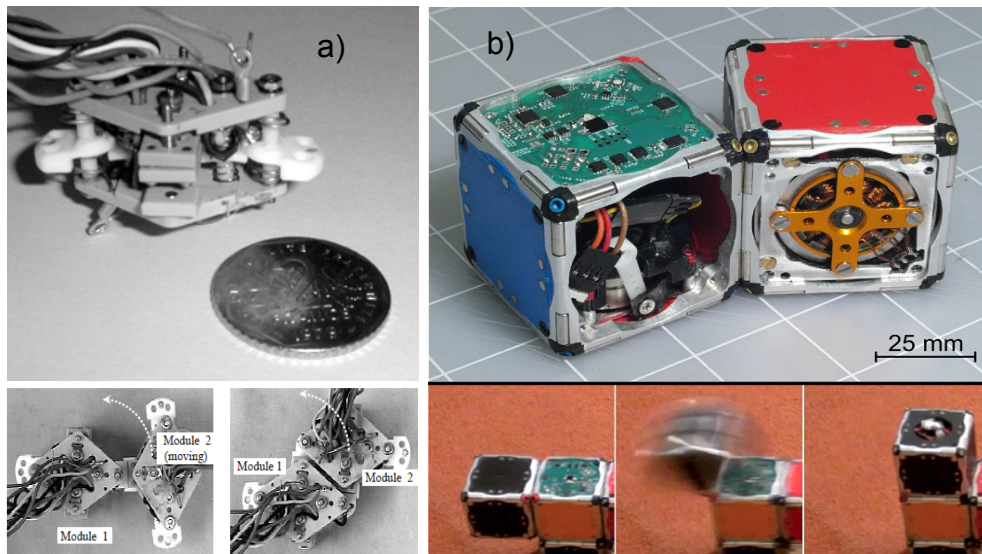


Figure 2.12: a) Smallest modular robot developed by *Yoshida* et al., using memory shape alloy as actuation [49] b) Modular momentum driven robot, developed by *Rus'* group at MIT [47], where robots bind to each other magnetically.

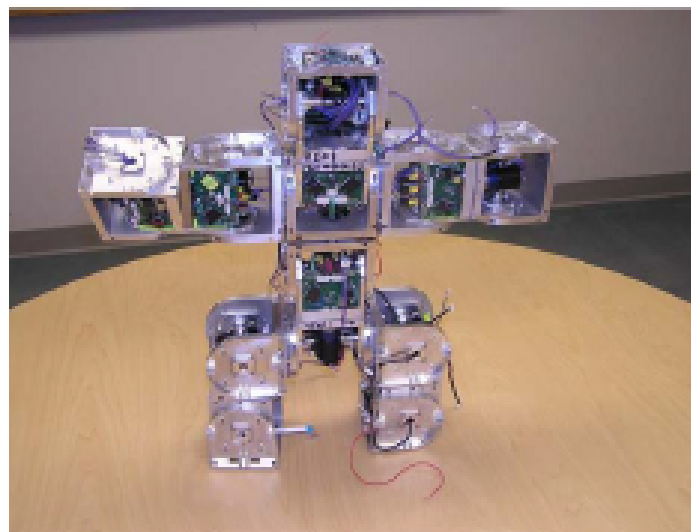


Figure 2.13: Superbot, a modular robot [48].

Table 2.2: Self-reconfiguring robots: Memory material changing its shape for assembly. Belongs to the group of self-folding and origami-robot

	origami-bot[51]	micro gripper[52]	polymer strip[49]
Type:	dynamic-, programmable self-assembly		
Device dimension:	>10mm	2mm	1.5x0.18x3.7mm
Complexity:	 1 component, N states		
Binding force:	-	-	-
Driving force:	thermal	thermal	magnetic
Environment:	controlled		

of their actuators and electronics. The smallest modular robot has the size of a penny and was developed by *Yoshida* et al. [49] and is actuated by electromagnets. It is displayed in Figure 2.12.

Many modular robots use magnetism as their binding force, such as the M-Blocks robot; a robotic system developed by *Rus* et al. from *MIT*, seen in Figure 2.12. Despite its size, its actuation by momentum, using dc motors and its binding, using permanent magnets, is reliable for cubes with respect to each other against gravity. The *Superbot* from *Salemi* et al. [48] is displayed in Figure 2.13. Each component of this modular robot has one degree of freedom and therefore only displays limited ability for movement. However an important study was done on the capability of locomotion of a collective of *Superbot*-components by *Shen* et al. [50]. It displays the capability of a self-assembled system to be used as a tool, in this case locomotion, which exceeds the capabilities of the individual component.

Origami Robots

One of the most elegant and easiest means of self-assembly is the use of memory materials. These materials have the property to change their present shape due to an external trigger. Many researchers exploited this principle leading to a subgroup in the self-reconfiguring robot design. This area is of special interest as the use of memory material allows the minimisation of the self-reconfiguring robot technology.

One well known origami robot uses thermally triggered memory material heated by a circuit printed on the material. It was developed by *Felton* et

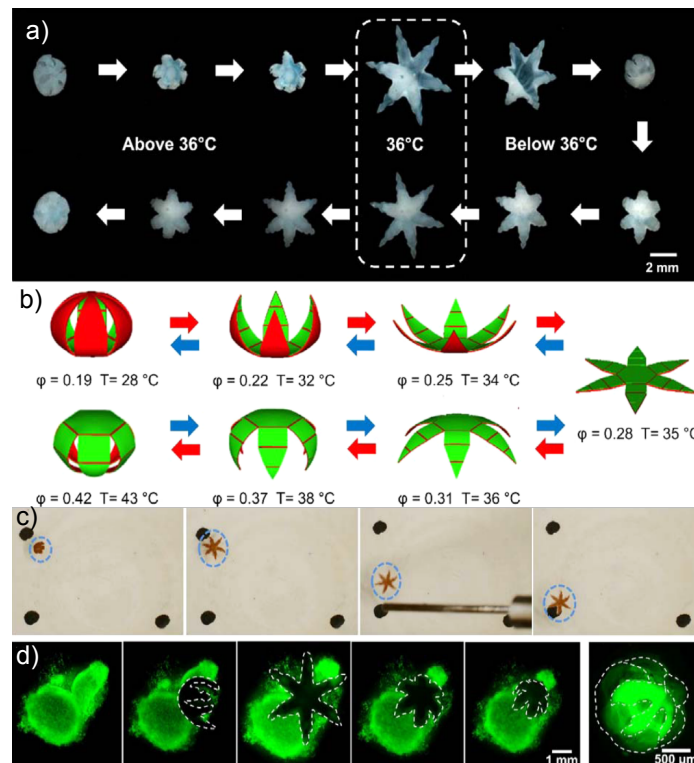


Figure 2.14: Origami micro gripper capable of grabbing a single cell. a) and b) shows the real and simulated working principle. c) and d) show how the gripper attaches to a cell under a microscope. The dashed lines are added to show the gripper [52].

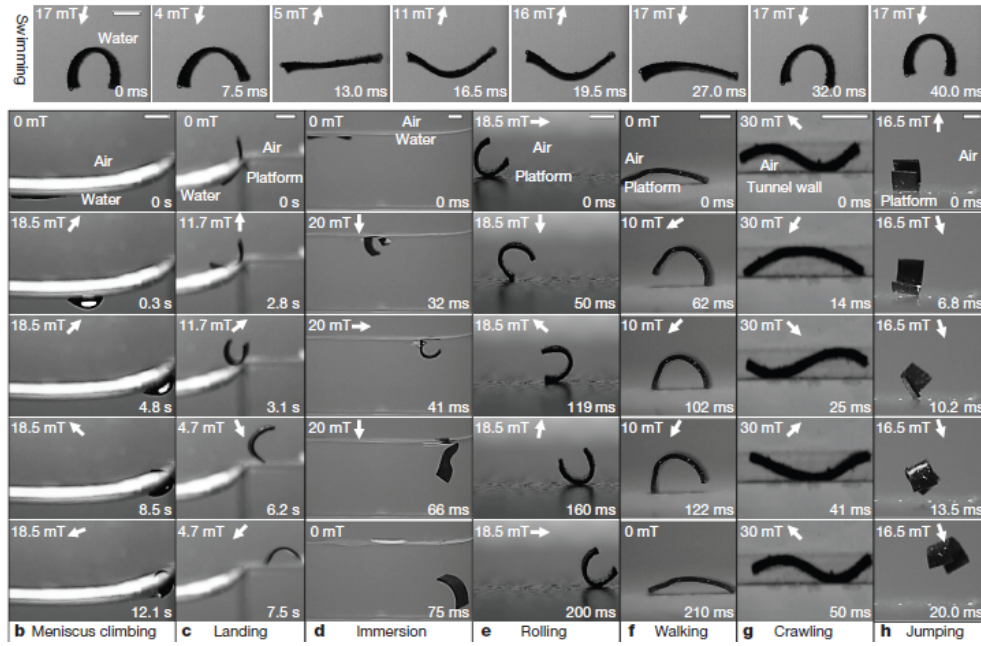


Figure 2.15: Flexible magnetic mini robot [53]. The robot consists of a single polymer strip with magnetic properties. Within a magnetic field the strip bends and is able to preform a wide range of locomotion.

al. [51]. The miniaturisation of this technology is able to act on a cellular level as *Breger* and his team demonstrated, by using memory material to grab a single cell [52]. The micro gripper and how it grabs a cell is displayed in Figure 2.14. This micro gripper highlights an explicit characteristic of thermally triggered self-reconfiguring systems: The cell is grabbed as the cells temperature triggers the folding process. The temperature needs to be lowered to release the cell. This fine control over the temperature might be impractical in some settings. In a surgical setting it is potentially dangerous to alter the body temperature to trigger or reverse a self-reconfiguring process as specified in section 2.1.1.

Hu et al. developed a flexible polymer strip that actuates in an electromagnetic field to be used as a mini robot for locomotion in nearly any terrain [53]. The strip is made of magnetic polymer and is displayed in Figure 2.15.

2.5.2 Soft Magnetics

Among others, the Institute of Solid State Physics of Vienna University of Technology is researching in 3D printable magnets [54]. One embodiment of the technology is a polymer material with embedded ferromagnetic *NdFeB* spheres as seen in Figure 2.16. An additive manufacturing process using this

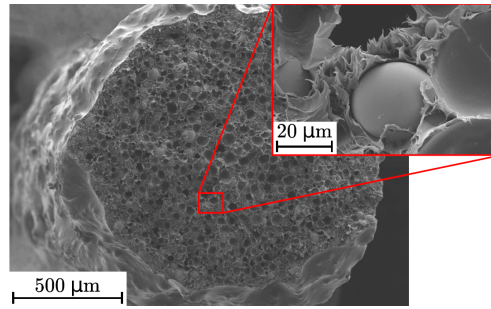


Figure 2.16: Ferromagnetic particles embedded in 3D printable polymer allows the additive manufacturing of any magnetic shape and polarisation [54].

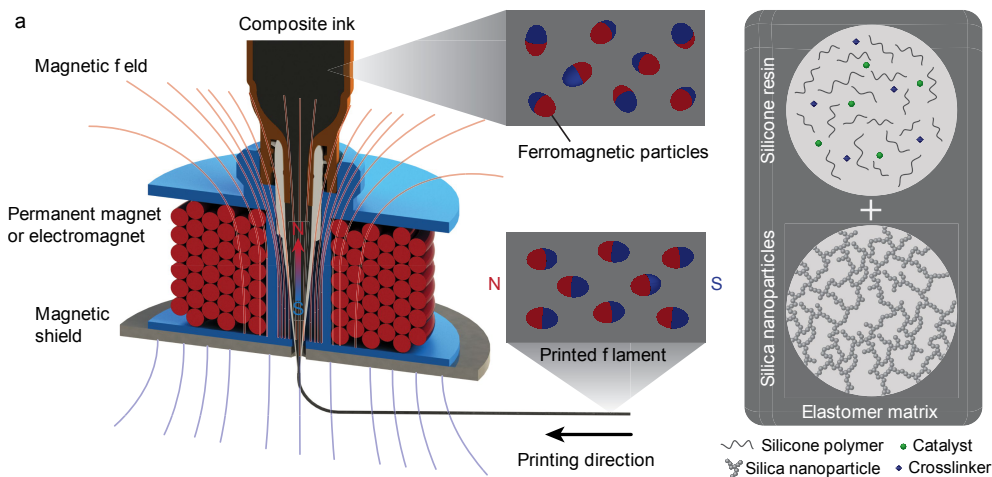


Figure 2.17: Schematics of the nozzle to print polymer with embedded ferromagnetic particles and polarise the material during the printing process [55].

material was developed, magnetising it during the process. This resulted in the permanent magnetic material to be polarized locally. This way the magnetic surface might be structured as desired and build a unique landscape of magnetic poles. The advantage of this technology is the enabling of engineered magnetic interaction. For example, two magnetic surfaces might be produced that only couple together in a specific orientation and might not couple with other magnetic surfaces.

A similar project from *Kima* and *Yuk* uses an elastic polymer for the additive manufacturing process as seen in Figure 2.17 [55]. The result is an elastic material that deforms in a magnetic field as seen in Figure 2.18. This material has great potential for self-assembly, especially considering that with the removal of the magnetic field, the elastic material unfolds. The origami mini gripper [52] and the flexible magnetic mini robot [53], discussed in Section 2.5.1, are two examples of how this technology might be applied in

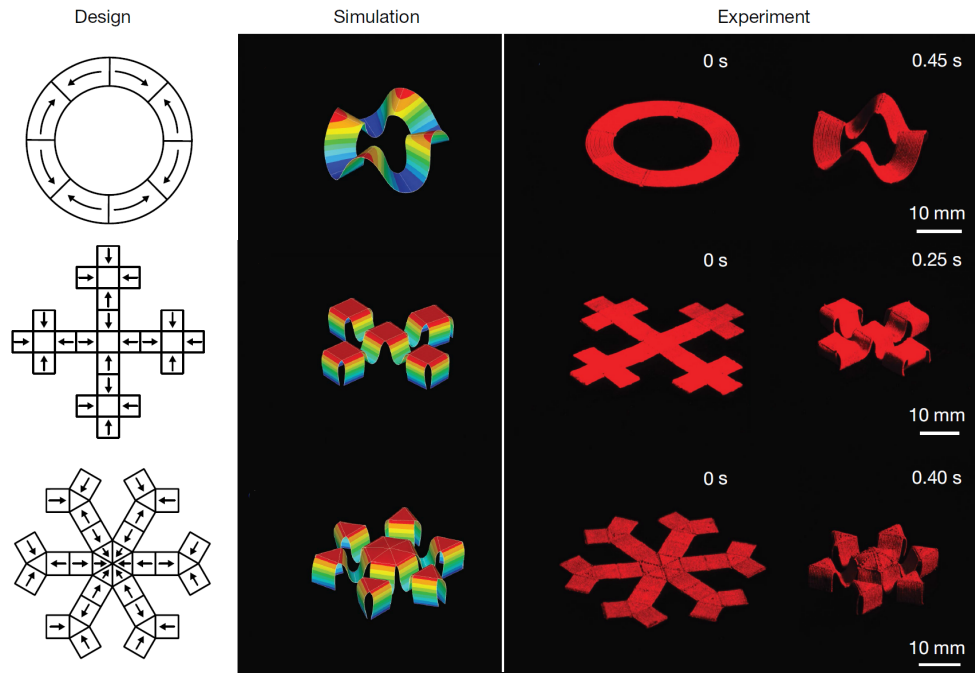


Figure 2.18: Different geometries of elastic magnetic polymer, their simulated and experimental folding inside a magnetic field [55].

a clinical setting.

2.5.3 Reconfiguring Magnetic Medical Devices

The aforementioned examples are applications of self-assembly and self-reconfiguration in robotics. This section focuses on the specific applications of self-folding chains in minimally-invasive surgery. One embodiment in literature is the work of *Cantillon-Murphy*, who developed in cooperation with *GI Windows*, a self-folding magnetic device, for anastomosis creation [56]. Each component of the magnetic chain is linked to the next with a hinge. Inside these components are housed magnets, polarised in different directions as seen in Figure 2.19. This results in an attraction and deflection between the components along the chain. In its compressed state, the chain has a bigger inner tension due to these forces. Once released the chain will order its elements in a square to minimise these tensions and reach a state of minimal inner energy. The classification of the *SAMSEN device* as an example of self-folding magnetic chains, is displayed in Table 2.3. It is particularly noteworthy that in comparison to many examples of self-assembly in nano-scale, the driving and binding-force are the same. As a result simulation of the system is much easier as the system is simpler.

Table 2.3: Self-folding magnetic chains: Magnetic elements of a chain fold due to magnetic coupling between the elements into a unique shape. Counts to the group of self-folding

	<i>SAMSEN Device</i> [57]	<i>Soft-Cubes</i> [58]
Type	 Dynamic self-assembly	
Component:	magnet diameter 5mm	cube diameter 2.5mm magnet diameter 1.5mm
Complexity:	1 component, 2 state	4 components, 2 states
Binding force:	magnetic	elasticity, magnetic
Driving force:	magnetic	elasticity,magnetic
Environment:	in vivo	controlled

The work of *Yim and Sitti* [58] describes a chain where cubic components are composed of soft silicone, seen in Figure 2.20. The chain is produced in the desired folded state, where each element is physically linked to only the two neighbouring elements in the chain. Due to its soft material properties, the shape is easily disassembled and fed as a chain through a small port. Without external forces the chain will self-assemble due to inner stress, back to its original state. The authors compare the folding of silicon soft cubes alone in comparison to cubes with embedded magnets to aid the folding process. Each component has a size of 2.5mm. In their conclusion, the authors propose to further miniaturize the technology to use in minimally-invasive surgery.

Self-assembly presents a great potential for minimally-invasive surgery tools to reconfigure without the need for active actuation. *Hernandez et al.* [59] proposed a device that consists of a number of smaller magnets linked in a chain and will fold after deployment into a ring by connecting the two ends of the string. This concept however poses a tremendous challenge on the construction of the device. The magnetic components in the string need to be linked to their neighbours by rolling hinges to allow for a reliable folding process. Figure 2.21 a) shows an implementation where these rolling hinges are approximated by a backbone. This backbone however offers only a very crude approximation as it needs a certain flexibility to allow for the folding of the ring.

GI Windows proposes a self-folding device with an exoskeleton [59]. Employing self-folding for an anastomosis device excludes any control of the folding mechanism by the surgeon. The capability for anastomosis creation

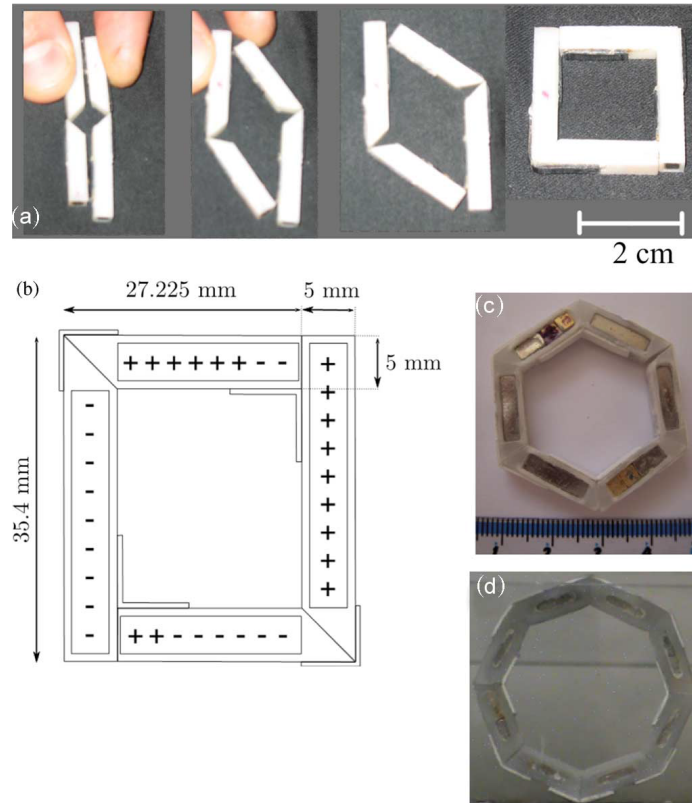


Figure 2.19: SAMSEN Device. Magnetic elements linked together in a chain. Once released they fold into a ring due to the magnetic forces between them. The device is used for magnetic anastomosis creation [57]. a) Folding of the device; b) device schematics, c) and d) hexagonal iteration.

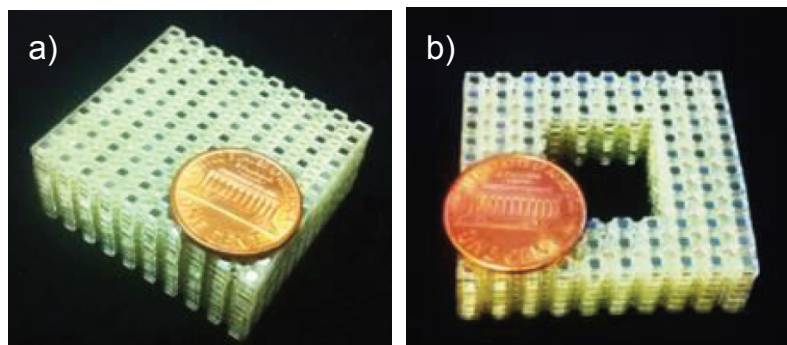


Figure 2.20: Elastomer cubes with embedded magnet to self-assemble to a a) cubic-shape and b) doughnut-shape [58].

of the device depends on the pressure it exerts on the tissue and therefore on the coupling force per unit area. Consequently, a high percentage of the device's surfaces should be magnetic. A maximum of magnetic material in the device is required to ensure an optimal coupling distance and force.

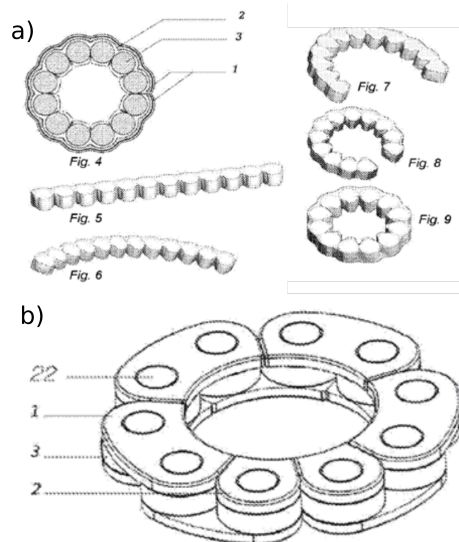


Figure 2.21: Patent design of a folding magnetic anastomosis ring by Hernandez et al. [59].

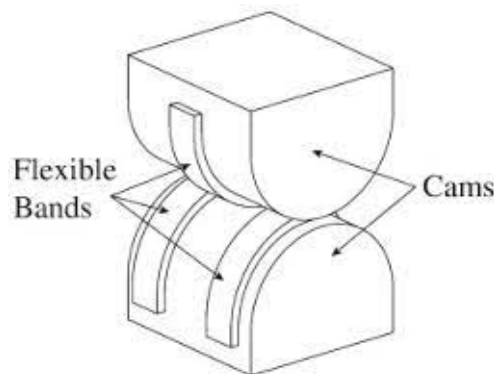


Figure 2.22: Living rolling hinge: Core hinge [60].

Consequently, these hinges need to be minimal in size to allow for a small device and so as to not weaken the magnetic potential of the device. However, the hinges need to be strong enough to resist forces resulting from this magnetic potential. Conventional hinges as seen in Figure 2.21 b) are a suitable solution in a large scale but pose non-trivial challenges to materials and production in a sub-millimetre scale.

Living hinges and compliant designs are widely used in sub millimetre mechanical applications and allow for a variety of different hinge types. The shape of living hinges can vary drastically to accommodate different purposes and link two parts of the same solid body by a hinge. The solution to implement living hinges in Figure 2.21 a) requires an ill-defined backbone. Such a backbone would need to be flexi-

ble to allow the folding but prevent any twisting of the chain. Instead, a compliant rolling hinge would be a specific and concrete solution and allow for a controlled folding of the chain. The *core hinge* [60], displayed in Figure 2.22, presents an elegant solution to implement a compliant mechanism that behaves like a rolling hinge. It consists of two bodies connected by bands or strings. These bands or strings are configured in opposite directions and restrict all relative movement of the bodies but to roll on each other. As

a result, the *core hinge* allows for smooth, low friction rolling between two bodies and is implementable in very small scale.

2.6 Summary

This chapter provides an overview of existing technology in the field of magnetic self-assembling surgery tools. It highlights some of the challenges that arise from the target scale of a tool for minimally-invasive surgery. This scale is derived from the preferred deployment method of a device channel. Device channel diameter ranges from 2 mm to 8 mm. This defines the maximum size of each component in the chain. Programmable self-assembly [61] commonly requires actuators or electronics larger than this. Other programmable self-assembly relies on external fields [53]. It was therefore concluded to create a chain of magnets where the final folding chain is encoded in the sequence of magnetic components as an analogue to protein bio-synthesis. A need in similar technology [59] was identified for the creation of a concept that would be versatile and considers production methods at the target scale.

3 Methods to Analyse Magnetic Chains

This work seeks to expand the existing theory of tools that self-fold from a chain of components into a functional shape. The aim is to create the foundation of a new class of surgical instruments that can fit through small ports to then transform into a functional shape larger than the port used to deploy them. To allow for the passage through small ports, a chain of components is considered one that folds into a range of three dimensional shapes. A force within the chain is necessary to act between the components and cause the chain to fold. However this process needs to be reliable and a set of constructive and software tools is necessary to validate if a folding process is reliable and what possible shape a chain of components can form into. As highlighted in Chapter 2, the two possible approaches to predict the folding of a chain are:

- Simulating the folding dynamics and predicting the movement of a chain of rigid bodies until an equilibrium is reached.
- Analysing the internal energy of the chain in its possible states of equilibrium and predicting the most likely to occur.

This chapter focuses on these two methods and how they are implemented in this work to validate specific folds of a chain of components. To this end Section 3.1 details the mathematical and physical model used to simulate a chain of magnetic components. This model and consequent simulation approaches are validated using a benchtop experiment detailed in Section 3.3. Section 3.2 details the numerical implementation of the model and gives an overview of different simulation tools created in software. The first of these tools is a simulation of chain dynamics using a novel interpretation of *Newton-Euler* equations that is presented in Section 3.4. Another approach is the analysis of internal energy of a folding chain, detailed in Section 3.6.

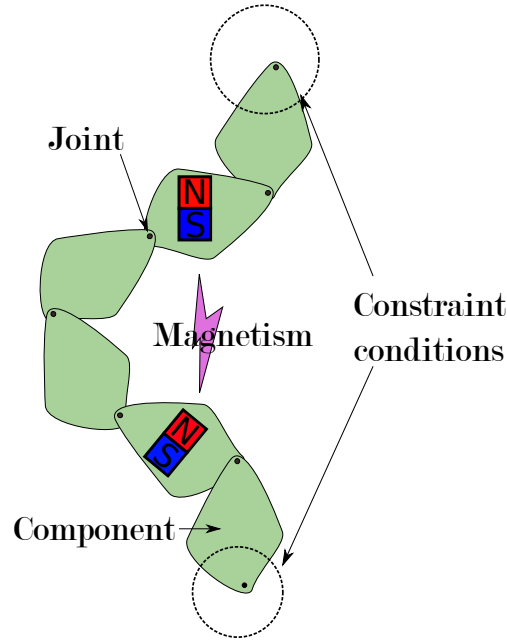


Figure 3.1: Considered attributes of a folding chain.

Finally the presented methods are discussed in Section 3.7.

3.1 Chain Model

The model used to simulate the chain, defines how realistic and flexible the simulation based on the model might be. Therefore this section details the physical and magnetic model as it is applied to a chain of components. However when done on computer systems with finite computing resources the simulation has to implement simplifications to mathematically describe a system and reduce computational effort. The primary assumptions in this work are that the chain is simplified to a set of rigid bodies linked by rotational joints. As seen in Figure 3.1, the considered attributes of a folding chain are the component, the joints linking the component, the magnetic forces between the components and the constraint conditions of the chain.

3.1.1 Kinematic Model

A free-force diagram with all considered forces and geometries of any component within the chain can be seen in Figure 3.2. Each of the joints are defined by at least one degree of freedom (DOF) in relation to the two components they link. As the components are rigid, the shape of the chain is completely defined by the state of the degree of freedom of each joint.

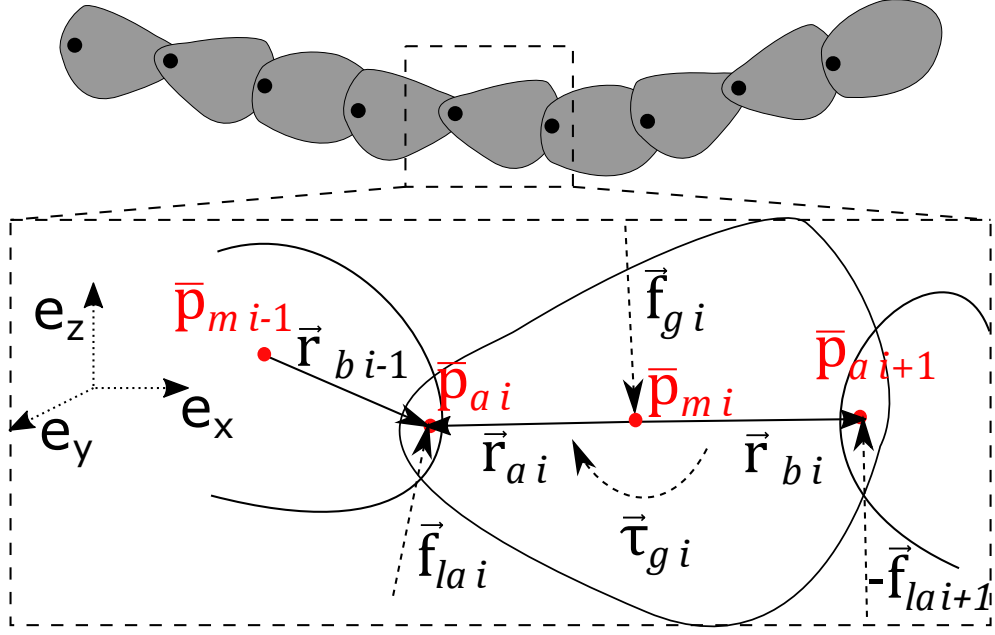


Figure 3.2: Free force diagram of a single chain component.

Each component moves due to the forces it experiences. These forces originate either from the joints that link them to their neighbours and the forces they experience or from external sources. Any component with index i therefore is defined by the properties defined in Table 3.1. All components in the chain with the exception of the first and last component are linked by two joints to the neighboring components in the chain. These joints are defined by relaying forces $\vec{f}_{la,i}$, $\vec{f}_{lb,i}$ and/or torques $\vec{\tau}_{la,i}$, $\vec{\tau}_{lb,i}$ acting on the components. How the forces and torques are relayed depend on the type of joint. A ball joint that is capable of rotating around three axis, for example, relays forces exclusively but not torques. In this case $\vec{\tau}_{la,i} = \vec{\tau}_{lb,i} = 0$. All other forces and torques that are relayed through the joint consequently are of opposite direction, resulting in

$$[\vec{f}_{lb,i}, \vec{\tau}_{lb,i}] = \mathbf{Q}_i \mathbf{L}_i \cdot [\vec{f}_{la,i+1}, \vec{\tau}_{la,i+1}] \quad (3.1)$$

where $\mathbf{L}_i$ is a matrix that defines what forces and torques are transmitted between the components and $\mathbf{Q}_i$ describes the absolute orientation of the component. This work considers 3-DOF rotational joints with

$$\mathbf{L}_{3-dof,i} = [\delta_3, \mathbf{0}] \quad (3.2)$$

where δ_3 is the unity matrix and $\mathbf{0}$ is the zero matrix. This joint transmits all forces but no torque between the components and, as such, models a 3-DOF

Table 3.1: Properties of component with index i

physical properties	
mass	m_i
inertia	I_i
magnetisation	M_i
geometrical properties	
position of center of mass	$\vec{x}_i$
orientation of component	Q_i
relative position of joint a	$r_{la\ i} = \overrightarrow{p_m p_{la}}$
relative position of joint b	$r_{lb\ i} = \overrightarrow{p_m p_{lb}}$
local restraints	
general force acting on center of mass	$\vec{f}_{g\ i}$
general torque acting on center of mass	$\vec{\tau}_{g\ i}$
force applying to joint a	$\vec{f}_{la\ i}$
force applying to joint b	$\vec{f}_{lb\ i}$
torque applying to joint a	$\vec{\tau}_{la\ i}$
torque applying to joint b	$\vec{\tau}_{lb\ i}$
Joint matrix	L_i

rotational joint. The other considered joint type is a 1-DOF rotational joint that only allows rotation around one axis and is modeled with

$$L_{1-dof\ i} = [Q_{axis\ i}, 0] \quad (3.3)$$

where R_{axis} contains the axis of rotation in the component's local coordinate frame. Any external force acting on the chain, such as gravity or forces from magnetic interaction, can be included in the generalised forces $\vec{f}_{g\ i}$ and torques $\vec{\tau}_{g\ i}$ acting on each component.

Constraint Conditions

The first and last component in a chain are only linked to one other component in the chain and thus define the restraint conditions which the chain experiences. We might define three cases of possible constraints for a generalised chain.

- Both endpoints of the chain are free to move.
- One endpoint of the chain is free to move, the other end point is forced to a defined movement.
- Both end point are forced to a defined movement.

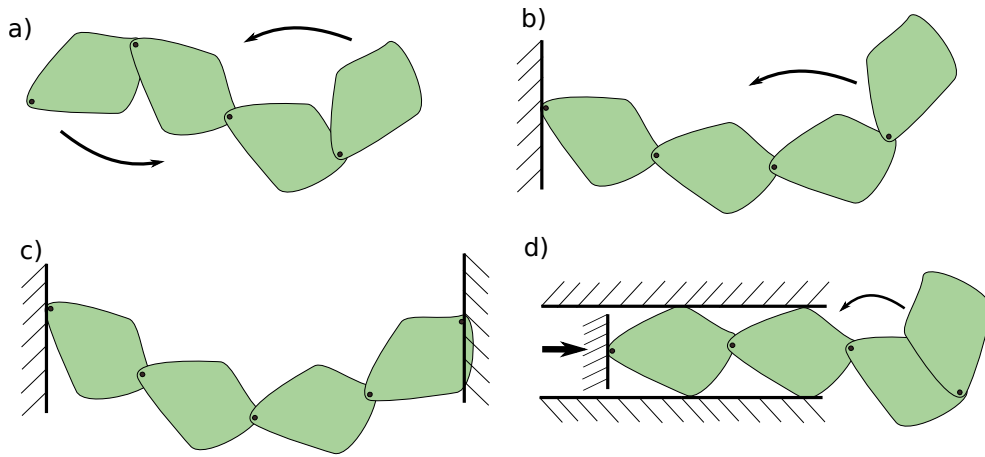


Figure 3.3: Constraint conditions of an idealised chain at deployment with a) both ends free, b) one end constrained, c) both ends constrained and d) component by component folding.

As we analyse a moving folding chain however, the constraints at deployment are of special interest. Considering the desired use case as described in Chapter 2, the chain is designed to be pushed out of a tube or channel. As long as the chain is within the channel it can not fold. Upon exiting the channel, the chain is free of constrictions and self-folds due to magnetic forces acting between the components. If we assume that the process of folding is significantly faster than the chain exits the deployment channel, only one joint at a time will fold in this deployment scenario. Under consideration of the possible constraints, four deployment scenarios are defined, as seen in Figure 3.3.

- a) The chain folds free of constraints
- b) The chain folds while one end is constrained.
- c) The chain folds while both ends are constrained.
- d) The chain fold component by component while being released from the deployment channel.

3.1.2 Magnetic Driving Force

To self-fold the chain as defined in Section 2.3, a driving force acting between the components is required. While a wide range of possible driving forces to enable the self-folding process are possible, as discussed in Section 2.5.1, this work focuses on magnetism as a driving force. Considering the use case in the medical setting as defined in Section 2.1.1, the folding process as initiated by the driving force has to be reliable and safe for clinical

application. To enable a reliable folding process, the driving force has to be predictable and controllable.

Magnetism as a driving force fulfils these criteria. It is safe for clinical application as magnetic forces do not significantly interact with tissue [62]. As shown in Section 2.2, it is possible to model the magnetic forces acting between components and a magnetic chain is controllable to some degree by interacting with extracorporeal magnets [63]. Furthermore this interaction allows the magnetic interaction of multiple devices for procedures such as magnetic anastomosis creation. Finally magnetic forces acting within a self-folding magnetic chain might be seen as an analogue to forces acting during protein biosynthesis and such chains might be seen as micro- or macroscopic to explore observable folding behaviour analogous to nanoscopic protein folding.

Magnetic Model

Section 2.2 describes the Coulomb point charge model that is employed in this thesis to simulate the magnetic interaction between the chain components. This section details the model as it is specifically applied to the magnetic folding chain with different shapes of magnetic components. Each component with index i is assigned a magnet in its local coordinate frame. This magnet is defined by a set of κ_i points that uniformly spread over the surface of the magnet $\mathbf{P}_i = (\vec{p}_{m\ i1}, \dots, \vec{p}_{m\ ij}, \dots, \vec{p}_{m\ i\kappa})$ and corresponding charge $\vec{q}_i = (q_{i1}, \dots, q_{il}, \dots, q_{i\kappa})$. Each magnet is considered to be uniformly polarised in a direction described by the magnetisation vector $\vec{m}_i$. In practice the magnitude of the magnetisation is provided by the manufacturer and can be approximated by measuring the $B_{max\ i}$ field at the surface of the magnet. Equation (2.6) demonstrates that Coulomb's point charge model approximates a magnetic surface with a set of points, where the a charge magnitude depends on the area A_{mag} the charge represents and its inclination $\vec{n}_{il} \cdot \hat{\vec{m}}_i$ to the normalised magnetisation vector $\hat{\vec{m}}_i$ relative to the corresponding surface normal $\vec{n}_{il}$. Therefore we calculate each individual charge as

$$q_{ik} = B_{max\ i} (\vec{n}_{il} \cdot \hat{\vec{m}}_i) \frac{A_{il}}{\kappa_i \mu_0} \quad (3.4)$$

where the surface area represented by an individual charge is approximated as the magnet's total surface area divided by all point charges $A_{il} = A_{mag} / \kappa_i$.

As highlighted in Section 2.2.1, it is important that each surface increment is significantly smaller than the distance to the next magnetic component. However, the higher the point cloud density the higher the computational effort. A study of the ideal point cloud density is made in Section 3.2. The absolute position of each point charge might be updated with

$$\mathbf{P}_i = \mathbf{Q}_i(t)\mathbf{P}_{i0} \quad (3.5)$$

where $\mathbf{P}_{i0}$ is the relative position of all point charges of the component with the index i . Considering Equation (2.4), the force acting on component i now might be computed with

$$\vec{f}_i = \sum_{j=1|i \neq j}^n (\vec{P}_j - \vec{P}_i) \frac{\mu_0}{4\pi} \frac{\vec{q}_i \vec{q}_j}{|\vec{P}_j - \vec{P}_i|^3} \quad (3.6)$$

Similarly the Coulomb energy of the full system can be calculated with

$$U_c = \sum_{i=1}^n \sum_{j=i+1}^n \frac{\mu_0}{4\pi} \frac{\vec{q}_i \vec{q}_j}{|\vec{P}_j - \vec{P}_i|^2} \quad (3.7)$$

3.2 Simulation Tools

To consider the range of approaches to simulate the folding of a magnetic chain or analyse possible folding behaviour, a set of software tools has been implemented. A detailed documentation of the software is provided in Appendix A.5. The full source code is available on *GitHub* [64]. This section introduces the software tools used and extends the kinematic model from section 3.1.1 to a numerical model as it is used for subsequent simulation. As different possibilities of predicting the movement of the chain are investigated in this work, three software tools have been implemented to execute these simulations.

- **Potential Energy Simulation** allows for construction of magnetic chains and offers a toolkit to compute the internal energy torques and forces in specific states. Furthermore it offers tools to investigate these potential energies, forces and torques over a single degree of freedom.
- **Vectorised Newton-Euler (VNE) Simulation** allows for the simulation of kinematic chains and supports the use of GPU's.
- **3D Chain Simulation** offers a toolbox to generate magnetic chains

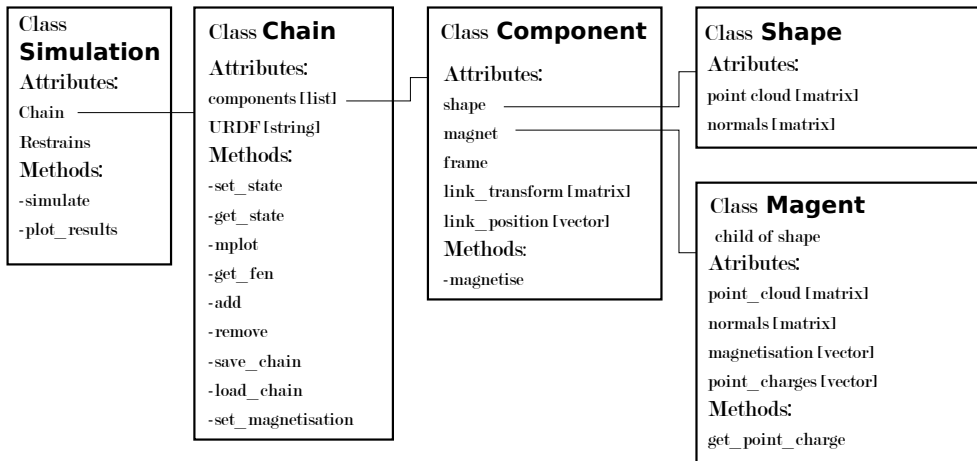


Figure 3.4: Class structure for a kinematic folding chain.

and investigate their folding behaviour via an API to the *PyBullet* physics simulation.

3.2.1 Numerical Model

All simulations have been implemented in the programming language *Python* under the use of vector computation libraries *NumPy* and *CuPy*. An overview of the program structure representing a folding chain can be seen in Figure 3.4, where all classes defining the simulation software are listed with their main features. The top class is the *Simulation* that manages user input to ease chain simulation. The simulation class contains one *Chain* class that in turn is defined by a list of components. Each component in the virtual chain is described by its shape, the magnets and the links to neighboring components. Component shape and magnet shape are defined by the following primitive shapes: box, cylinder or sphere.

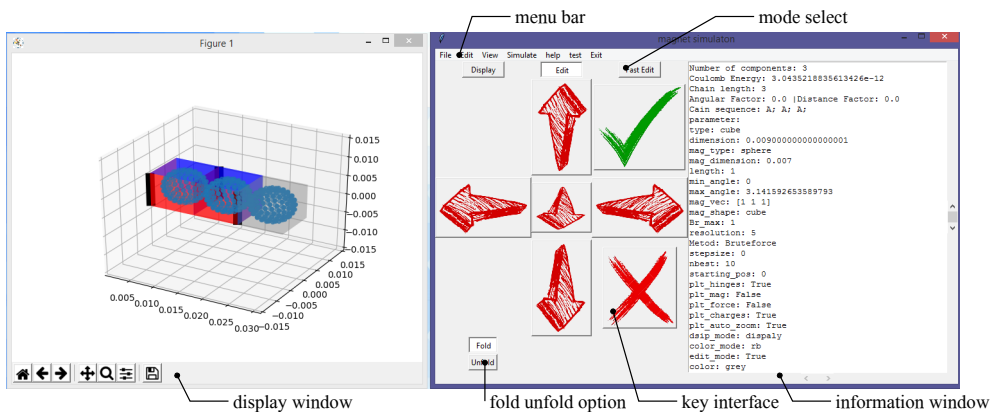


Figure 3.5: Graphical User Interface to construct and test magnetic folding chains.

To interface with the simulation software, a set of methods have been implemented as detailed in Appendix A.5. The primary methods for chain manipulation are:

- **Chain.create** creates a chain object
- **Chain.append** appends a component at the end of the chain
- **Chain.set_state** sets a specific state for all degree of freedom within the chain
- **Chain.get_state** returns the current degree of freedom of each component in the chain
- **Chain.set_mag** sets the magnetic vector of all components according to the the current state
- **Chain.get_mag** returns the relative magnetisation vector of all components
- **Chain.get_fen** computes magnetic forces, torques and potential energies within in the chain based on the Coulomb point charge model.

The software package allows for the construction of a chain in a specific state using *Chain.create*, *Chain.append*, *Chain.set_angle* and *Chain.set_mag*. Once created the software allows one to compare different possible folds with each other as described in *Chain.get_fen*. Furthermore a rudimentary *Graphical User Interface (GUI)* as seen in Figure 3.5 has been implemented using the *tkinter* library. It allows for a limited use of the above methods in a graphical interface for an intuitive construction of chains. Due to time constraints the *GUI* only features cubical components with spherical or cubical magnets.

3.2.2 Magnetic Point Cloud

As detailed in Section 2.2 and 3.1, the magnetic model is based on a discretisation of the magnetic surface as a set of point charges. As such, the algorithm that generates these point charges is of critical importance. A *Standard Tessellation Language (stl)* file, that is capable of representing geometric shapes, features a cloud of points on the surface of said shape. However the *stl*-file format is not designed to have a uniform distribution of point charges over the surface. As Equation (3.4) shows, the individual point charge is dependent on the area it represents. Therefore a uniform spread of point charges is important to ensure a high degree of simulation precision. For this reason, custom algorithms have been implemented to generate the

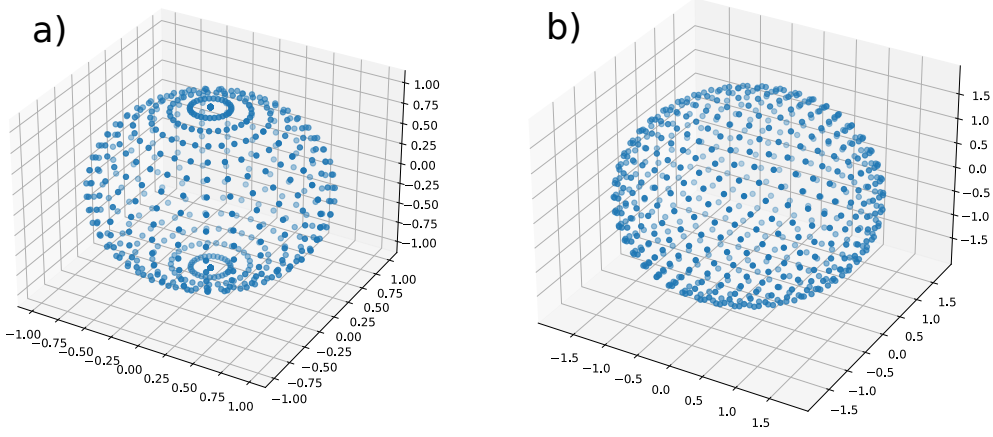


Figure 3.6: Point cloud generated with a) spherical coordinates and b) with the icosphere algorithm.

point cloud for a set of primitive shapes. These primitive shapes are sufficient to simulate most commercially available magnets that come in such shapes.

- **Box:** A grid of points is generated on each surface of the box where all points have an identical distance to each other. The points generated directly on the edge of the surface are rejected to prevent overlapping with adjacent surfaces. Populating each surface this way with k point charges along each axis leads to $6k^2$ number of point charges for a six sided cube.
- **Cylinder:** The cylinder is defined with a round base in e_x and e_y directions and radius r and the height h in e_z direction. The curved surface of the cylinder is populated with points similar to the surface of the box, using cylindrical coordinates. Finally, the top and bottom layer of the cylinder are populated as a rectangular surface and all points with $\sqrt{p_x^2 + p_y^2} \geq r$ are deleted.
- **Sphere:** A sphere with radius r is populated with point charges by creating an icosphere using the *PyMesh* library. A icosphere is a geometric object created from triangle vertices with a nearly uniform spread of points over the surface [65].

Most magnets used in subsequent experiments are round or cylindrical as they are space efficient. To generate the point cloud of a sphere using spherical coordinates would lead to a clustering of points at the pole, as seen in Figure 3.6. To test different algorithms to uniformly generate spherical point clouds, the magnetic interaction between two spherical magnets with rotating point clouds but static magnetic orientation has been simulated. Figure 3.7 shows these forces for point clouds generated by spherical co-

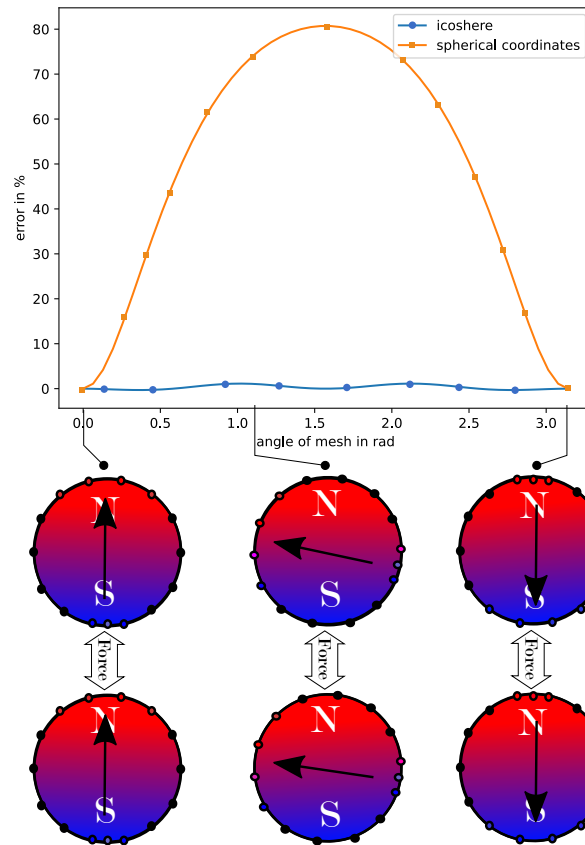


Figure 3.7: Comparison in angular error for spherical generated point cloud versus icosphere algorithm.

ordinates and the icosphere algorithm. It can be seen that the icosphere is nearly independent of the rotation of the point clouds, with a change of 2.1%.

3.2.3 Validation of the Magnetic Model

To validate this simulation model, magnet to magnet interaction has been simulated and compared against experimental results. Magnets have been mounted on polymer spacers to maximise the distance to any potential metal that could interact with the magnets. Magnets and spacers have been placed a *TA HD Plus* Texture analyser from *Stable Micro Systems*, UK. A pull-test, measuring the distance with increasing separation from 1mm to 30mm has been performed. The load-cell measuring the force was calibrated for up to 5kg. To achieve a higher measuring accuracy, two types of axially polarised cylindrical magnets from the supplier *KJ-magnetic*, USA with a grade of N42, have been used.

- **cylinder magnet** height: 1/4 inch = 6.35 mm; diameter: 1/4 inch =

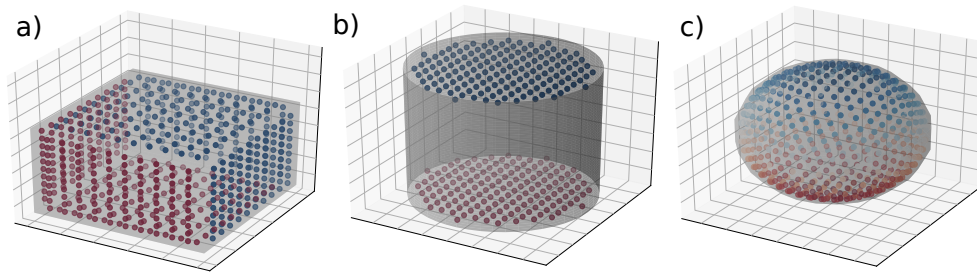


Figure 3.8: Point cloud of primitive shape with box (left), cylinder (middle), sphere (right).

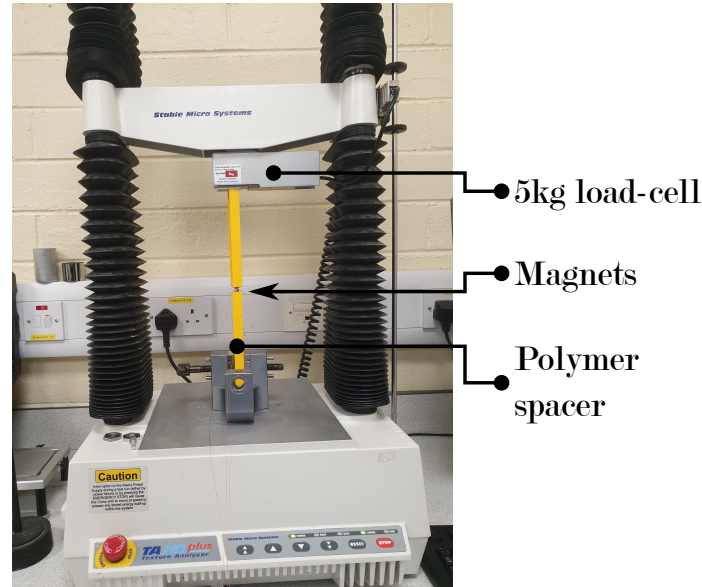


Figure 3.9: Pull-test setup from *Stable Micro Systems*, UK, with a 5 kg load-cell and polymer spacers.

6.35 mm; Br_{max} :1.1T; supplier number D44; results seen in Figure 3.11

- **cylinder magnet** height: $1/8$ inch = 3.175 mm; diameter: $1/2$ inch = 12.7 mm; Br_{max} :1.1T; supplier number D82; results seen in Figure 3.10

The average of five pull tests in comparison to the simulation can be seen in Figure 3.11 and 3.10. For this work we are interested in separation distances in the lower millimetre range. However, the magnets used for the pull tests are larger than the target size for a magnetic device to decrease the measuring error. Therefore we define the separation distance of interest as a function of magnet size to estimate simulation accuracy.

For both magnet types the simulation results can be seen to closely relate to measurement data in a range from 1 mm to 20 mm. Equation (3.6)

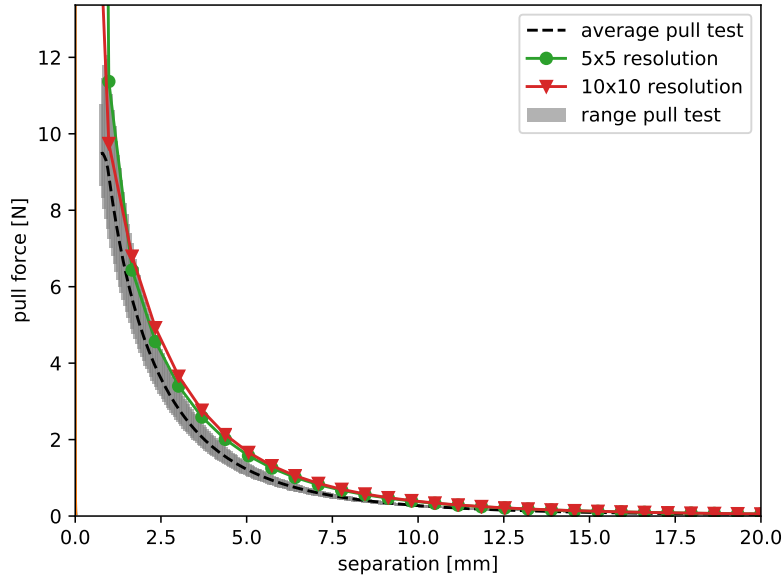


Figure 3.10: Force between two axially polarised disks N42 magnets ($h : 1/8\text{ inch} = 3.175\text{ mm}$ $d : 1/2\text{ inch} = 12.7\text{ mm}$) with experimental results (dotted) and simulation (full).

suggests that the accuracy of the model depends on the distance between magnets in relationship to the area represented by an individual point charge. Therefore computing magnetic forces between smaller magnets with the same number of point charges and in consequence smaller surface area per point charge, is expected to yield accurate results for closer magnetic interaction. As such, it is assumed that the magnetic simulation model adequately simulates magnetic interaction if the magnetic surfaces are approximated with approximately 100 magnetic mono-poles per magnetic surface with an area of $A_{cylinder} \approx 31.17\text{ mm}^2$ and $A_{cylinder} \approx 126.68\text{ mm}^2$ respectively and at a minimal distance of 1 mm. Translated to smaller magnets the same ratio between area per surface charge and separation distance between magnets is assumed. Magnets used in subsequent experiments are as small as 2 mm. A magnet with a diameter of 2 mm and associated surface area of 3.14 mm^2 is expected to be accurately simulated for a minimum separation distance of 0.1 mm.

3.2.4 Featherstone Physics Simulation

The described programmatic representation of folding chains has been used to create a custom *Application Programming Interface (API)* to the *PyBullet* physics engine, that simulates the dynamics of a folding chain using the

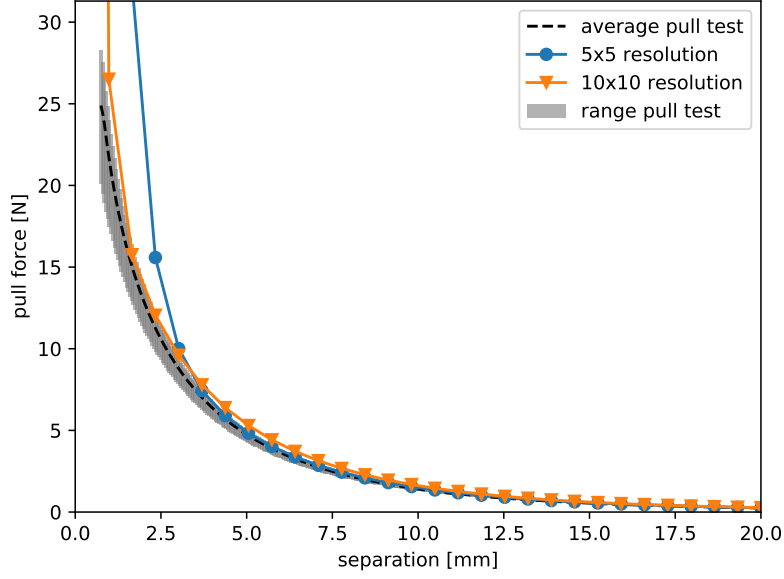


Figure 3.11: Force between two axially polarised cylinders N42 magnets ($h : 1/4 \text{ inch} = 6.35 \text{ mm}$ $d : 1/4 \text{ inch} = 6.35 \text{ mm}$) with experimental results (dotted) and simulation (full).

Featherstone algorithm [66], as seen in Figure 3.12. Furthermore, the *PyBullet* engine features collision handling to simulate different chain component colliding. The *Featherstone* algorithm is suited to simulate any constrain conditions. A chain of components can be constructed using the commands described in Section 3.2.1. A phraser was implemented that translates the constructed chain into *Unified Robot Description Format (urdf)*, a widely used codex to describe multi body robots. Using the *loadURDF* command, the *urdf* file is then read and understood by the *PyBullet* engine. A simulation can be started by using the *Simulation.simulate()* command. The corresponding boundary conditions have to be defined by passing the corresponding flag as an argument, as described in Appendix A.5.

3.3 Benchtop Model

To validate simulations and preliminary investigations of magnetic folding behaviour, a benchtop experiment was implemented in a controllable environment [67]. This experimental setup was designed to test how the magnetic poles need to be implemented to allow for folding as well as to test how reliable the folding is. The benchtop experiment is limited to a planar folding case to investigate folding with reduced complexity and to allow for a convenient visual confirmation of predicted folding behaviour.

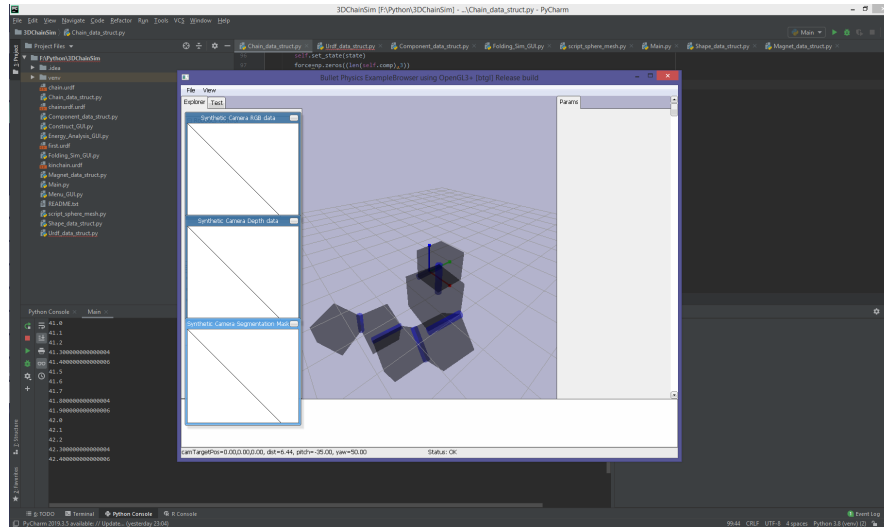


Figure 3.12: Example simulation of a magnetic folding chain using the *PyBullet* physics engine.

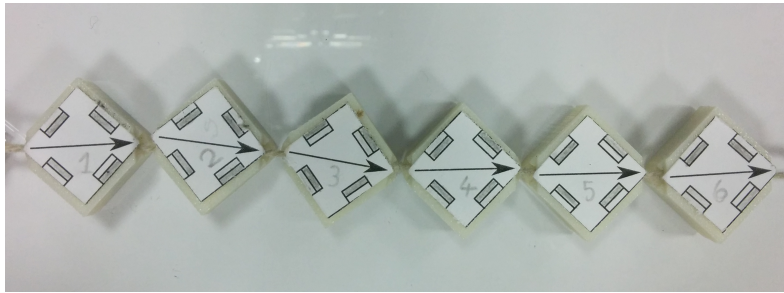


Figure 3.13: Experimental setup of the 2D self-folding magnetic chain.

A prototype of a modular planar magnetic folding chain was implemented for the experimental setup. Each component of this chain has a square casing and is connected to the previous and the next component by a wire as seen in Figure 3.13. A mixed fabric wire with high bending elasticity and a low axial elasticity was chosen to best approximate a revolute joint between the components. The dimension of each component can be seen in Figure 3.14. The casings were designed to allow an exchange of the magnets and approximate the behaviour of an ideal chain. In the present work, the degree of freedom is defined as the angle between each chain component. The chain folds on a flat, low friction surface due to the forces acting between the magnets. All movement is along the surface and is restricted to two dimensions. Gravity is normal to the surface and therefore does not directly influence the folding. Each component contains one magnet on each of the four faces, having either its north or south side closest to the outer face as seen in Figure 3.14.

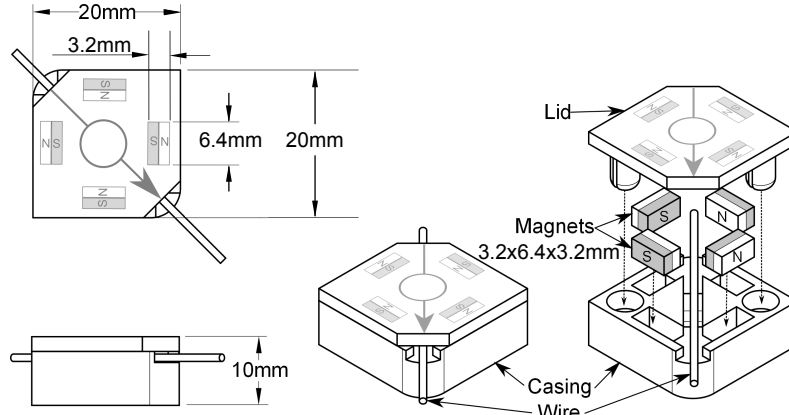


Figure 3.14: Single component of the planar self-folding magnetic chain, investigated in this work, with the orientation of the magnet is displayed on the lid of the casing.

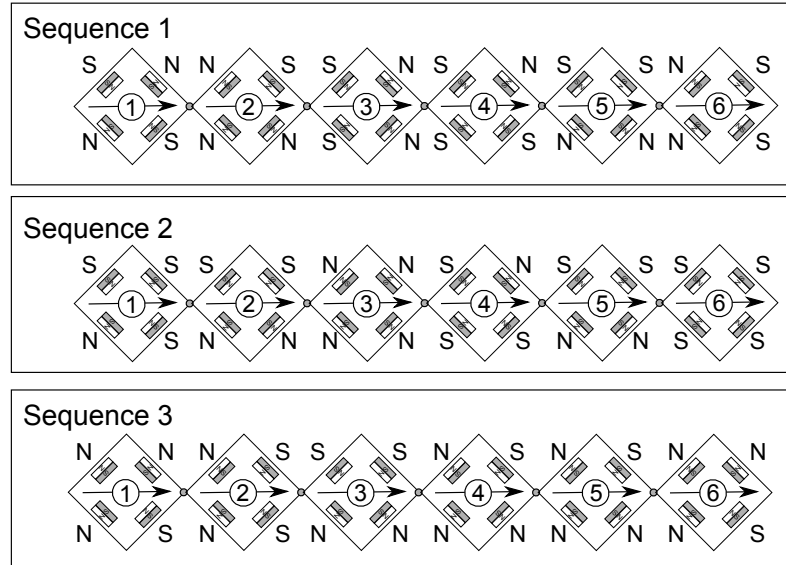


Figure 3.15: Tested sequences of components in 2D self-folding, with "N" and "S" indicate the magnet polarisation relative to outward faces.

The chain is defined by the sequence of casing components and how their magnets are oriented relative to outward faces. For components containing four magnets as seen in Figure 3.14, this results in $2^4 = 16$ different combinations of magnetic orientation in each casing component, resulting in 16^n different sequences of chain components for a chain with n components. This setup allows for an easy implementation of different sequences by manually exchanging the magnets, while the limitation of the movement to a plane increases controllability and allows for a better observation and analysis of the chain movement.

3.4 Dynamics of Magnetic Chains

As both the *Newton-Euler* and the *Euler-Lagrange* methods are capable of describing the dynamics of a chain, it is important to determine which one leads to the computationally more efficient algorithm to accurately compute the dynamics of longer chains. In the presented case of a magnetic folding chain, the degrees of freedom are the folding angles between the chain components. Applying the *Euler-Lagrange* Equation (2.11) directly, the potential energy and therefore the *Coulomb* energy given in Equation (2.5) is derived by all degrees of freedom. *J. Luh 1980* [68] proposed the introduction of pseudo-accelerations to compensate for gravitational forces. However, the forces acting on each component in a self-folding magnetic chain and the potential energy in the system depend on their distance to other components in the chain as seen in Equations (2.4) and (2.5), whereas this distance depends of the folding angles between chain components. The magnetic forces and the potential energy in the presented system dependent on all folding angles defining the system. The resulting equation gets super-linearly¹ more complex with a increasing number of chain components.

3.4.1 Newton-Euler Dynamics for Efficient Computation

This work seeks to analyse the dynamics of folding chains. To make use of parallel computation, a vectorised differential equation was devised that would express angular acceleration of all chain components in the form;

$$\dot{\vec{\omega}} = \mathbf{F}(\vec{\omega}, \vec{f}, \vec{r}) \quad (3.8)$$

where $\mathbf{F}(\vec{\omega}, \vec{f}, \vec{r})$ is the desired function that describes the angular acceleration of all components as a function of angular velocity $\vec{\omega}$, forces acting on the system $\vec{f}$ and system state and geometry $\vec{r}$.

Expressing the dynamics in such a form allows for a convenient implementation with common vector computation libraries, enabling a convenient use of parallel computation architecture, including *SIMD* and *GPU* architectures. The vectorisation library used in this work are *NumPy* and *Cupy*.

¹A super linear function grows faster than a linear function. An example is a quadratic function.

Vectorised Newton Euler

Applying the Newton-Euler Equations (2.8) and (2.10), the dynamics of each individual body is described as:

$$m_i \vec{a}_{mi} = \vec{f}_{gi} + \vec{f}_{ai} + \vec{f}_{bi} \quad (3.9)$$

and

$$\mathbf{I}_i \frac{d\vec{\omega}_i}{dt} + \vec{\omega}_i \times (\mathbf{I}_i \vec{\omega}_i) = \vec{\tau}_{gi} + \vec{r}_{ai} \times \vec{f}_{ai} + \vec{r}_{bi} \times \vec{f}_{bi} \quad (3.10)$$

where $\vec{f}_{ai}$ and $\vec{f}_{bi}$ are the forces acting on the joints induced from the neighbouring components and $\vec{f}_{gi}$ is the generalized force acting on its centre of mass, as seen in Figure 3.2. Therefore $\vec{f}_{bi} = -\vec{f}_{ai+1}$

As $|\vec{r}_{ai}|$ and $|\vec{r}_{bi}|$ are constant in time, the second derivative of $\vec{r}_{ai}$ and $\vec{r}_{bi}$ describes the acceleration of the components around their centre of mass as [69];

$$\vec{a}_{a\perp i} = \frac{\partial^2 \vec{r}_{ai}}{\partial t^2} = \ddot{\vec{r}}_{ai} = \vec{\omega}_i \times (\vec{\omega}_i \times \vec{r}_{ai}) + \dot{\vec{\omega}}_i \times \vec{r}_{ai} \quad (3.11)$$

$$\vec{a}_{b\perp i} = \frac{\partial^2 \vec{r}_{bi}}{\partial t^2} = \ddot{\vec{r}}_{bi} = \vec{\omega}_i \times (\vec{\omega}_i \times \vec{r}_{bi}) + \dot{\vec{\omega}}_i \times \vec{r}_{bi} \quad (3.12)$$

Note that the derivative with respect to time t of any vector $\vec{p}$ is noted as $\frac{\partial \vec{p}}{\partial t} = \dot{\vec{p}}$ and $\frac{\partial^2 \vec{p}}{\partial t^2} = \ddot{\vec{p}}$. The cross product in Equation (3.11) and (3.12) is expressed by defining the skew-symmetric matrices [36];

$$[\vec{r}_{ai}]_X = \begin{bmatrix} 0 & -r_{azi} & r_{ayi} \\ r_{azi} & 0 & -r_{axi} \\ -r_{ayi} & r_{axi} & 0 \end{bmatrix} \quad (3.13)$$

$$[\vec{r}_{bi}]_X = \begin{bmatrix} 0 & -r_{bzi} & r_{byi} \\ r_{bzi} & 0 & -r_{bxi} \\ -r_{byi} & r_{bxi} & 0 \end{bmatrix} \quad (3.14)$$

$$[\vec{\omega}_i]_X = \begin{bmatrix} 0 & -\omega_{zi} & \omega_{yi} \\ \omega_{zi} & 0 & -\omega_{xi} \\ -\omega_{yi} & \omega_{xi} & 0 \end{bmatrix} \quad (3.15)$$

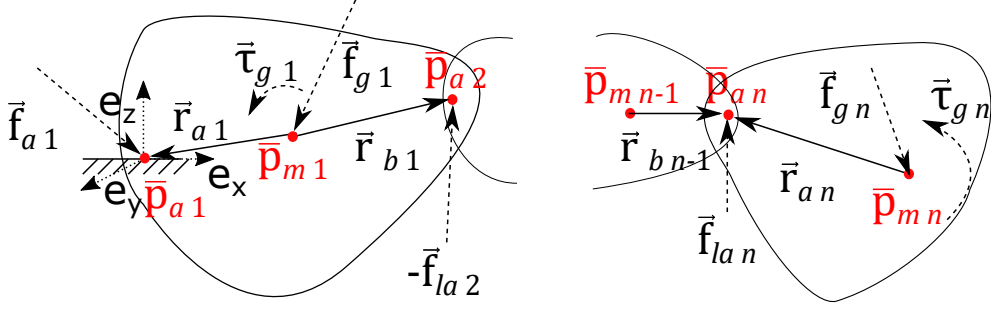


Figure 3.16: Free force diagram of a multi body chain with the first component fixed to the world frame and the last component only connected to the previous component.

As seen in Figure 3.2, the position $\bar{\mathbf{p}}_{mi}$ of the i^{th} component's centre of mass in relation to the previous component's centre of mass $\mathbf{p}_{m-1}$, for all $i \in [2, \dots, n]$, can be described as:

$$\bar{\mathbf{p}}_{mi} = \bar{\mathbf{p}}_{mi-1} + \vec{\mathbf{r}}_{bi-1} - \vec{\mathbf{r}}_{ai} \quad (3.16)$$

As seen in Figure 3.16, Equation (3.16) holds true for the last component $i = n$. For component $i = 1$, this might be expressed under the chosen constraints of one end free and one end fixed to the world frame, as:

$$\bar{\mathbf{p}}_{m1} = -\vec{\mathbf{r}}_{a1} \quad (3.17)$$

Therefore, the acceleration of the centre of mass can be expressed as the second derivative of the position with respect to time for $i \in [2, \dots, n]$

$$\frac{\partial^2 \bar{\mathbf{p}}_{mi}}{\partial t} = \vec{\mathbf{a}}_i = \vec{\mathbf{a}}_{i-1} - \frac{\partial^2 \vec{\mathbf{r}}_{ai}}{\partial t} + \frac{\partial^2 \vec{\mathbf{r}}_{bi-1}}{\partial t} \quad (3.18)$$

and for $i = 1$

$$\frac{\partial^2 \bar{\mathbf{p}}_{m1}}{\partial t} = \vec{\mathbf{a}}_1 = -\frac{\partial^2 \vec{\mathbf{r}}_{a1}}{\partial t} \quad (3.19)$$

Inserting Equation (3.11) and (3.12) into Equation (3.18) as well as expressing the cross product with the respective matrices (3.13), (3.14) and (3.15), the difference in acceleration between component i and $i - 1$ might be expressed as:

$$\begin{aligned} \vec{\mathbf{a}}_i - \vec{\mathbf{a}}_{i-1} = & -[\vec{\omega}_i]_X \cdot ([\vec{\omega}_i]_X \cdot \vec{\mathbf{r}}_{ai}) + [\vec{\mathbf{r}}_{ai}]_X \cdot \dot{\vec{\omega}}_i \\ & + [\vec{\omega}_{i-1}]_X \cdot ([\vec{\omega}_{i-1}]_X \cdot \vec{\mathbf{r}}_{bi-1}) - [\vec{\mathbf{r}}_{bi-1}]_X \cdot \dot{\vec{\omega}}_{i-1} \end{aligned} \quad (3.20)$$

Vectorised Formulation for a Chain of n Components

The primary challenge in formulating a single differential equation is to unify the kinematic Equations (3.9) and (3.10), with the geometrical constraints expressed in Equation (3.18). Momenta resulting from forces in the links as well as Equation (3.18) contain cross products. Cross products are neither commutative nor associative.

These two properties complicate a unification to a single differential equation as there is no inverse to a cross product [70]. Thus the cross product hinders the rearranging of an equation. The same is true if the cross product is represented as a cross product matrix. The cross product matrix is *skew-symmetric* and as such is non-invertible. However the expression

$$a\delta_3 + \mathbf{X} \quad (3.21)$$

with a being a constant, the unity matrix δ_3 and the *skew-symmetric* matrix $\mathbf{X}$, is invertible [70]. This property is utilised in the following under the assumption that the resulting matrices are invertible as subsequently shown for significant cases.

In order to express the whole system in a single equation we define the vectors

$$\begin{aligned} \vec{\mathbf{a}}_s &= [a_{x1}, a_{y1}, a_{z1}, \dots, a_{xn}, a_{yn}, a_{zn}] \\ \vec{\boldsymbol{\omega}}_s &= [\omega_{x1}, \omega_{y1}, \omega_{z1}, \dots, \omega_{xn}, \omega_{yn}, \omega_{zn}] \\ \vec{\mathbf{r}}_{as} &= [r_{ax1}, r_{ay1}, r_{az1}, \dots, r_{axn}, r_{ayn}, r_{azn}] \\ \vec{\mathbf{r}}_{bs} &= [r_{bx1}, r_{by1}, r_{bz1}, \dots, r_{bxn}, r_{byn}, r_{bzn}] \\ \vec{\mathbf{f}}_{as} &= [f_{ax1}, f_{ay1}, f_{az1}, \dots, f_{axn}, f_{ayn}, f_{azn}] \\ \vec{\boldsymbol{\tau}}_{gs} &= [\tau_{x1}, \tau_{y1}, \tau_{z1}, \dots, \tau_{xn}, \tau_{yn}, \tau_{zn}] \\ \vec{\mathbf{f}}_{gs} &= [f_{gx1}, f_{gy1}, f_{gz1}, \dots, f_{gxn}, f_{gyn}, f_{gzn}] \end{aligned} \quad (3.22)$$

Equation (3.20) might now be expressed as;

$$\mathbf{A}\vec{\mathbf{a}}_s = \mathbf{B}\mathbf{W}_s\mathbf{W}_s\vec{\mathbf{r}}_{bs} - \mathbf{W}_s\mathbf{W}_s\vec{\mathbf{r}}_{as} + (\mathbf{R}_{as} - \mathbf{B}\mathbf{R}_{bs})\dot{\vec{\boldsymbol{\omega}}}_s \quad (3.23)$$

With the unity matrix δ_d of dimension d and the block matrices;

$$\mathbf{B} = \begin{bmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} & & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \delta_3 & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \delta_3 & \mathbf{0} & & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ & \vdots & & \ddots & & \vdots & \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \cdots & \delta_3 & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \delta_3 & \mathbf{0} & \mathbf{0} \end{bmatrix} \quad (3.24)$$

$$\mathbf{R}_{as} = \text{diag}([\vec{r}_{a1}]_X, \dots, [\vec{r}_{an}]_X) \quad (3.25)$$

$$\mathbf{R}_{bs} = \text{diag}([\vec{r}_{b1}]_X, \dots, [\vec{r}_{bn}]_X) \quad (3.26)$$

$$\mathbf{W}_s = \text{diag}([\vec{w}_1]_X, \dots, [\vec{w}_n]_X) \quad (3.27)$$

Note that the $\mathbf{0}$ entries in block matrix $\mathbf{A}$ represent zero matrices of dimension 3×3 .

Equivalently the Newton-Euler Equations (3.9) and (3.10) for the system can be expressed as vectorised equations describing the complete system as;

$$\mathbf{M}_s \vec{a}_s = \vec{f}_{gs} + \mathbf{C} \vec{f}_s \quad (3.28)$$

and

$$\mathbf{I}_s \dot{\vec{\omega}}_s + \mathbf{W}_s \mathbf{I}_s \vec{\omega}_s = \vec{\tau}_{gs} + (\mathbf{R}_{as} - \mathbf{R}_{bs} \mathbf{D}) \vec{f}_s \quad (3.29)$$

where the block matrices $\mathbf{M} = \text{diag}([m_1 \delta_3, \dots, m_n \delta_3])$ and $\mathbf{I}_s = \text{diag}([\mathbf{I}_1, \dots, \mathbf{I}_n])$, describe the system properties and $\mathbf{C} = (\delta_{3n} - \mathbf{B}^T) = \mathbf{A}^T$ and $\mathbf{D} = \mathbf{B}^T$, describe the system constraints.

Equations (3.23), (3.28) and (3.29) describe the system dynamics and can be combined in a single equation. This is achieved by substituting the force acting on the joint $\vec{f}_c$ in Equation (3.29) with Equation (3.28) and finally by substituting the acceleration $\vec{a}_c$ with Equation (3.23), resulting in the nonlinear differential equation describing the motion of a chain with n components;

$$\begin{aligned} & (\mathbf{I}_s - \mathbf{R}_D \mathbf{E} \mathbf{R}_B) \dot{\vec{\omega}}_s = \\ & \mathbf{R}_D \left(\mathbf{E} \mathbf{B} \mathbf{W}_s \mathbf{W}_s \vec{r}_{bs} - \mathbf{E} \mathbf{W}_s \mathbf{W}_s \vec{r}_{as} - \mathbf{C}^{-1} \vec{f}_{gs} \right) + \\ & \vec{\tau}_{gs} - \mathbf{W}_s \mathbf{I}_s \vec{\omega}_s \end{aligned} \quad (3.30)$$

For a convenient notation, the matrices $\mathbf{E}$, $\mathbf{R}_D$ and $\mathbf{R}_B$ are defined as

$$\begin{aligned}\mathbf{E} &= \mathbf{C}^{-1}\mathbf{M}_s\mathbf{A}^{-1} \\ \mathbf{R}_D &= \mathbf{R}_{as} - \mathbf{R}_{bs}\mathbf{D} \\ \mathbf{R}_B &= \mathbf{R}_{as} - \mathbf{B}\mathbf{R}_{bs} \\ \mathbf{I}_s &= \mathbf{Q}_s\mathbf{I}_{0s}\mathbf{Q}_s^T\end{aligned}\tag{3.31}$$

3.4.2 Numerical Solution

The non-linear differential Equation (3.30) describes the angular acceleration between the components as a function of angular velocity and their orientation. Solving this equation allows for the accurate simulation of the dynamics of multi-body chains and might be used to predict the folding of magnetic chains or proteins under the defined restraint conditions. Equation (3.30) is solvable if the square matrices $\mathbf{A}$, $\mathbf{C}$ and $(\mathbf{I}_s + \mathbf{R}_D\mathbf{E}\mathbf{R}_B)$ are invertible. For the given constraint conditions $\mathbf{A}$ and $\mathbf{C}$ can be shown to be invertible. The left-hand side of Equation (3.30) $(\mathbf{I}_s + \mathbf{R}_D\mathbf{E}\mathbf{R}_B)$ is shown in simulation to be invertible for significant cases with $|\vec{r}_{ai}|, |\vec{r}_{bi}| > 0$ and $\vec{r}_{ai} \neq \vec{r}_{bi}$. The initial conditions are defined as $\vec{r}_{as}(t=0) = \vec{r}_{as0}$, $\vec{\omega}_s(t=0) = \vec{\omega}_{s0}$, $\vec{r}_{bs}(t=0) = \vec{r}_{bs0}$, with constant matrices $\mathbf{E}$, $\mathbf{B}$, $\mathbf{D}$, $\mathbf{I}_s$, $\mathbf{C}^{-1}$ and time step Δt . The geometry at any given time t then is computed by solving $\vec{r}_{as}(t) = \mathbf{Q}_s(t)\vec{r}_{as0}$ and $\vec{r}_{bs}(t) = \mathbf{Q}_s(t)\vec{r}_{bs0}$.

A reduction of dimension is implemented by defining:

$$\vec{z} = [\mathbf{Q}_s, \mathbf{W}_s]\tag{3.32}$$

$$\dot{\vec{z}} = \left[\mathbf{W}_s\mathbf{Q}_s, \left[\dot{\vec{\omega}}_s \right]_X \right]\tag{3.33}$$

where $\dot{\vec{\omega}}_s$ is calculated solving Equation (3.30) and the system state $\vec{z}(t)$ to a time t can be acquired by integrating Equation (3.33);

$$\vec{z}(t) = \int_{t_0}^t \dot{\vec{z}} dt\tag{3.34}$$

In this work, a fourth degree Runge-Kutta integration $\vec{z}(t + \Delta t) = \text{rk4}(\vec{z}, \dot{\vec{z}}, t, \Delta t)$ [19] is used to integrate Equation (3.33) and simulate the system. The presented algorithm does not consider interaction between components other than in the joint and therefore collision handling has to be implemented by modeling the general forces $\vec{f}_{gs}$ and torques $\vec{\tau}_{gs}$ respec-

tively. $\vec{f}_{gs}$ and $\vec{t}_{gs}$ can model constant forces such as gravity, as well as non-constant forces such as friction, magnetic interaction or collision forces. The non-constant forces are easily integrated by updating $\vec{f}_{as}$ and $\vec{r}_{as}$ with every time step.

3.4.3 Planar Folding Case

Many folding applications occur over just one axis and thus happen in a two dimensional plane. The vectorised interpretation of the *Newton-Euler* equations, presented in Section 3.4.1 might be simplified for such cases by utilising complex numbers. This Section discusses this case and its advantages. As discussed in Section 3.4.1, the primary challenges of unifying Equations (3.9), (3.10) and (3.18) into a single differential equation is the non-invertible cross product. In a planar scenario however, the cross product might be avoided by using complex numbers.

In contrast to the three dimensional case, each component in the chain has one degree of freedom, the folding angle. For ease of trigonometric notation and due to their convenient representation of planar rotations, complex numbers were used to express coordinates and rotations in this work. The *Cartesian* coordinates of the vector $\vec{p} = [p_x, p_y]^t$ are represented by complex numbers of the form $z = p_x + jp_y$, with $j = \sqrt{-1}$. The imaginary and real part of these complex numbers represent orthogonal coordinates in a *Cartesian* coordinate system as shown in Figure 3.2. As in the three dimensional case, the position of each component in the system is dependent on the angles of the components with respect to the world frame. For the i^{th} component, this angle is named ϕ_i . The angles of each component are the degree of freedom of the system, represented by the vector $\vec{\phi} = [\phi_1, \dots, \phi_n]$ defining the whole system at time-point t . Absolute angles were chosen to eliminate the need for coordinate transformations and a direct application of ϕ_i and ω_i into Equation (2.10).

The complex representative of the vector from the link connecting component with indices i and $i - 1$ to the centre of mass of the i^{th} component is labelled r_{li} , as shown in Figure 3.2. r_{ci} represents the complex vector from the i^{th} centre of mass to the link connecting the i^{th} component to the component with the index $i + 1$. Consequently d_i is the complex representation of the vector from one link of the i^{th} component to its other link. As

d_i , r_{li} and r_{ci} , all belong to the same rigid body, where their position and orientation with respect to each other is constant over time, these might be defined as:

$$d_i = |d_i|e^{j\phi_i} = r_{li} + r_{ci} \quad (3.35)$$

$$r_{li} = |r_{li}|e^{j(\phi_i + \beta_{li})} \quad (3.36)$$

$$r_{ci} = |r_{ci}|e^{j(\phi_i - \beta_{ri})} \quad (3.37)$$

where e is *Euler's* number and $j = \sqrt{-1}$. As $|r_{li}|$, $|r_{ci}|$, β_{li} and β_{ri} are constant in time, therefore the first and second derivative of r_{li} , r_{ci} derived by time t are [36]:

$$\frac{\partial r_{li}}{\partial t} = \dot{r}_{li} = jr_{li}\dot{\phi}_i = jr_{li}\omega_i \quad (3.38)$$

$$\frac{\partial r_{ci}}{\partial t} = \dot{r}_{ci} = jr_{ci}\dot{\phi}_i = jr_{ci}\omega_i \quad (3.39)$$

and

$$\frac{\partial^2 r_{li}}{\partial t^2} = \ddot{r}_{li} = jr_{li}\dot{\omega}_i - r_{li}\omega_i^2 \quad (3.40)$$

$$\frac{\partial^2 r_{ci}}{\partial t^2} = \ddot{r}_{ci} = jr_{ci}\dot{\omega}_i - r_{ci}\omega_i^2 \quad (3.41)$$

Similar for the three dimensional case, the position of the i^{th} components centre of mass in relation to the previous components centre of mass, for all $i \in [2, \dots, n]$, can be described as:

$$z_{mi} = z_{mi-1} + r_{ci-1} + r_{li} \quad (3.42)$$

Using (3.41) to twice differentiate (3.42) with respect to time, the corresponding acceleration of the i^{th} centre of mass, for all $i \in [2, \dots, n]$, may be expressed as

$$\begin{aligned} a_{mi} &= \ddot{z}_{mi} = \ddot{z}_{mi-1} + \ddot{r}_{ci-1} + \ddot{r}_{li} \\ &= a_{mi-1} + jr_{li}\dot{\omega}_i - r_{li}\omega_i^2 + jr_{ci-1}\dot{\omega}_{i-1} - r_{ci-1}\omega_{i-1}^2 \end{aligned} \quad (3.43)$$

As seen in Figure 3.16, the component with index 1 is considered to be connected with a rotational joint to the world frame. In conclusion, (3.43) for $i = 1$ may be expressed as

$$a_{m1} = jr_{l1}\dot{\omega}_1 - r_{l1}\omega_1^2 \quad (3.44)$$

Expressed as a vector equation, where every entry corresponds to one component, this leads to

$$\mathbf{A}\vec{a}_m = \mathbf{jR}\dot{\vec{\omega}} - \mathbf{R}\vec{\omega}^2 \quad (3.45)$$

with

$$\mathbf{A} = \begin{bmatrix} 1 & 0 & 0 & .. & .. & .. & 0 \\ -1 & 1 & 0 & & & & : \\ 0 & -1 & 1 & & & & : \\ : & & .. & & & & : \\ : & & & -1 & 1 & 0 & 0 \\ : & & & 0 & -1 & 1 & 0 \\ 0 & .. & .. & 0 & 0 & -1 & 1 \end{bmatrix} \quad (3.46)$$

$$\mathbf{R} = \begin{bmatrix} r_{l1} & 0 & 0 & .. & .. & .. & 0 \\ r_{c1} & r_{l2} & 0 & & & & : \\ 0 & r_{c2} & r_{l3} & & & & : \\ : & & .. & & & & : \\ : & & & r_{cn-3} & r_{ln-2} & 0 & 0 \\ : & & & 0 & r_{cn-2} & r_{ln-1} & 0 \\ 0 & .. & .. & 0 & 0 & r_{cn-1} & r_{ln} \end{bmatrix} \quad (3.47)$$

From *Newton-Euler's* law, the acceleration of the i^{th} component [36], for all $i \in [1, .., n - 1]$, also follows as:

$$m_i a_{mi} = f_{gi} + f_{li} - f_{li+1} \quad (3.48)$$

As the last chain component with index n is considered free and only connected to the previous component as seen in Figure 3.16, (3.48) for $i = n$ might be expressed as:

$$m_n a_{mn} = f_{gn} + f_{ln} \quad (3.49)$$

Equations (3.48) and (3.49) might be expressed as a vector equation as:

$$\mathbf{M}\vec{a}_m = \vec{f}_g + \mathbf{B}\vec{f}_l \quad (3.50)$$

with

$$\mathbf{M} = \text{diag}(m_1, \dots, m_n) = \begin{bmatrix} m_1 & 0 & \dots & 0 \\ 0 & \cdot & & \vdots \\ \vdots & & \cdot & 0 \\ 0 & \dots & 0 & m_n \end{bmatrix} \quad (3.51)$$

$$\mathbf{B} = \begin{bmatrix} 1 & -1 & 0 & \dots & \dots & 0 \\ 0 & 1 & -1 & & & \vdots \\ 0 & 0 & 1 & & & \vdots \\ \vdots & & & \ddots & & \vdots \\ \vdots & & & & 1 & -1 & 0 \\ \vdots & & & & 0 & 1 & -1 \\ 0 & \dots & \dots & \dots & 0 & 0 & 1 \end{bmatrix} \quad (3.52)$$

Solving (3.50) for $\vec{\mathbf{f}}_l$ and (3.45) for $\vec{\mathbf{a}}_m$, leads to the force acting on the joints expressed as:

$$\vec{\mathbf{f}}_l = \mathbf{jB}^{-1}\mathbf{MA}^{-1}\mathbf{R}\dot{\vec{\omega}} - \mathbf{B}^{-1}\mathbf{MA}^{-1}\mathbf{R}\vec{\omega}^2 - \mathbf{B}^{-1}\vec{\mathbf{f}}_g \quad (3.53)$$

As $\mathbf{B}, \mathbf{M}, \mathbf{A}, \vec{\omega}$ and $\dot{\vec{\omega}}$ are real, they can be seen as scalars to the complex matrix $\mathbf{R}$. Therefore the real and complex part of $\vec{\mathbf{f}}_l$ might be expressed as

$$\text{Re}(\vec{\mathbf{f}}_l) = -\mathbf{B}^{-1}\mathbf{MA}^{-1}\mathbf{R}_I\dot{\vec{\omega}} - \mathbf{B}^{-1}\mathbf{MA}^{-1}\mathbf{R}_R\vec{\omega}^2 - \mathbf{B}^{-1}\vec{\mathbf{f}}_{gR} \quad (3.54)$$

$$\text{Im}(\vec{\mathbf{f}}_l) = \mathbf{B}^{-1}\mathbf{MA}^{-1}\mathbf{R}_R\dot{\vec{\omega}} - \mathbf{B}^{-1}\mathbf{MA}^{-1}\mathbf{R}_I\vec{\omega}^2 - \mathbf{B}^{-1}\vec{\mathbf{f}}_{gI} \quad (3.55)$$

with $\mathbf{R}_R = \text{Re}(\mathbf{R})$, $\vec{\mathbf{f}}_{gR} = \text{Re}(\vec{\mathbf{f}}_g)$ and $\mathbf{R}_I = \text{Im}(\mathbf{R})$, $\vec{\mathbf{f}}_{gI} = \text{Im}(\vec{\mathbf{f}}_g)$ being the real and complex part of $\mathbf{R}$ and $\vec{\mathbf{f}}_g$

Analysing the momenta [71] in the i^{th} component we find

$$I_{mi}\dot{\omega}_i = t_{gi} + (-r_{li}) \times f_{li} + r_{ci} \times (-f_{li+1}) \quad (3.56)$$

Considering the restraint condition displayed in Figure 3.16, the force acting on the free link of the last component is zero:

$$f_{ln+1} = 0 \quad (3.57)$$

Considering two vectors with their complex representations:

$$\vec{\mathbf{p}}_1 = [p_{x1}, p_{y1}, 0]^t \Rightarrow z_1 = p_{x1} + j \cdot p_{y1} \quad (3.58)$$

$$\vec{\mathbf{p}}_2 = [p_{x2}, p_{y2}, 0]^t \Rightarrow z_2 = p_{x2} + j \cdot p_{y2} \quad (3.59)$$

the cross product might be written as

$$\vec{\mathbf{p}}_1 \times \vec{\mathbf{p}}_2 = \text{Re}(z_1)\text{Im}(z_2) - \text{Im}(z_1)\text{Re}(z_2) \quad (3.60)$$

Therefore, (3.56), taking (3.57) into account, might be written as

$$\begin{aligned} I_{mi}\dot{\omega}_i = & \tau_{gmi} - \text{Re}(r_{ci})\text{Im}(f_{li+1}) + \text{Im}(r_{ci})\text{Re}(f_{li+1}) \\ & - \text{Re}(r_{li})\text{Im}(f_{li}) + \text{Im}(r_{li})\text{Re}(f_{li}) \end{aligned} \quad (3.61)$$

To satisfy the constraint of the component with the index n being a free end, (3.61) for $i = n$ might be expressed as:

$$I_{mn}\dot{\omega}_n = t_{gmn} - \text{Re}(r_{ln})\text{Im}(f_{ln}) + \text{Im}(r_{ln})\text{Re}(f_{ln}) \quad (3.62)$$

Equations (3.61) and (3.62) expressed as a vector equation might be written as:

$$\mathbf{\Gamma}\dot{\vec{\omega}} = \vec{\mathbf{t}}_{gm} - \mathbf{R}_R^t \vec{\mathbf{f}}_{lI} + \mathbf{R}_I^t \vec{\mathbf{f}}_{lR} \quad (3.63)$$

with $\vec{\mathbf{f}}_{lI} = \text{Im}(\vec{\mathbf{f}}_l)$ and $\vec{\mathbf{f}}_{lR} = \text{Re}(\vec{\mathbf{f}}_l)$ being complex and real part of $\vec{\mathbf{f}}_l$, $\mathbf{R}^t$ is the transpose of $\mathbf{R}$ and:

$$\mathbf{\Gamma} = \text{diag}(I_{m1}, \dots, I_{mn}) = \begin{bmatrix} I_{m1} & 0 & \dots & 0 \\ 0 & \cdot & & \vdots \\ \vdots & & \cdot & 0 \\ 0 & \dots & 0 & I_{mn} \end{bmatrix} \quad (3.64)$$

Substituting (3.54) and (3.55) into (3.63) leads to the nonlinear differential equation describing the motion of a 2D pendulum chain with n components:

$$\begin{aligned} (\mathbf{\Gamma} + \mathbf{R}_R^t \mathbf{E} \mathbf{R}_R + \mathbf{R}_I^t \mathbf{E} \mathbf{R}_I) \dot{\vec{\omega}} = \\ \vec{\mathbf{t}}_{gm} + (\mathbf{R}_R^t \mathbf{E} \mathbf{R}_I - \mathbf{R}_I^t \mathbf{E} \mathbf{R}_R) \vec{\omega}^2 + \mathbf{R}_R^t \mathbf{B}^{-1} \vec{\mathbf{f}}_{gI} - \mathbf{R}_I^t \mathbf{B}^{-1} \vec{\mathbf{f}}_{gR} \end{aligned} \quad (3.65)$$

with the substitution $\mathbf{E} = \mathbf{B}^{-1} \mathbf{M} \mathbf{A}^{-1}$. While not immediately apparent,

the planar expression of the vectorised *Newton-Euler* equation uses matrices and vectors with a length equal to the number of components in the chain. The three dimensional version however uses vectors and matrices which are three times the length and thus is expected to be computationally slower. Considering that many applications can be realised in a planar folding device, this simulation approach might be considerably faster than a full three dimensional simulation.

3.4.4 Validation of the Vectorised Newton Euler Algorithm

Equation (3.30) was applied using the numerical methods described in section 3.4.2 to simulate the dynamics of a chain of components with one end fixed to the world frame and the other end free. All computations were done in Python on a 64Bit Windows computer system with 2.5GHz CPU, 16GB internal memory and a *Nvidia GTX1080* GPU. For a meaningful comparison, the algorithm was applied for a 3D case of a pendulum with a varying number of components. The following system properties have been used for simulation:

$$\begin{aligned}
 m_i &= 0.1 \\
 \mathbf{I}_{0i} &= 4 \cdot 10^{-6} \\
 \mathbf{W}_i(t=0) &= \mathbf{0} \\
 \vec{\mathbf{r}}_{ai0} &= -\vec{\mathbf{r}}_{bi0} = [0, 0, 0.2m]^T \\
 \vec{\mathbf{f}}_{gi} &= m_i [0, 0, -9.807 \text{ m/s}^2]^T \\
 \mathbf{Q}_i(t=0) &
 \end{aligned} \tag{3.66}$$

These conditions represent a hanging chain with a deflection of 25° . A total simulation time of 5 seconds was chosen. In this time, the simulated chain was swinging back and forth a total of 18 times.

The algorithm has been tested by introducing torques resulting from friction as well as introducing magnetic forces between components. However, depending on the complexity to compute the non-constant forces, the performance of the presented algorithm would be altered. Therefore, as this section seeks to analyse the computation time and error of the presented algorithm where gravity is constant, force conservation is assumed in the following simulations.

To estimate the error of the simulation, the internal energy of the system

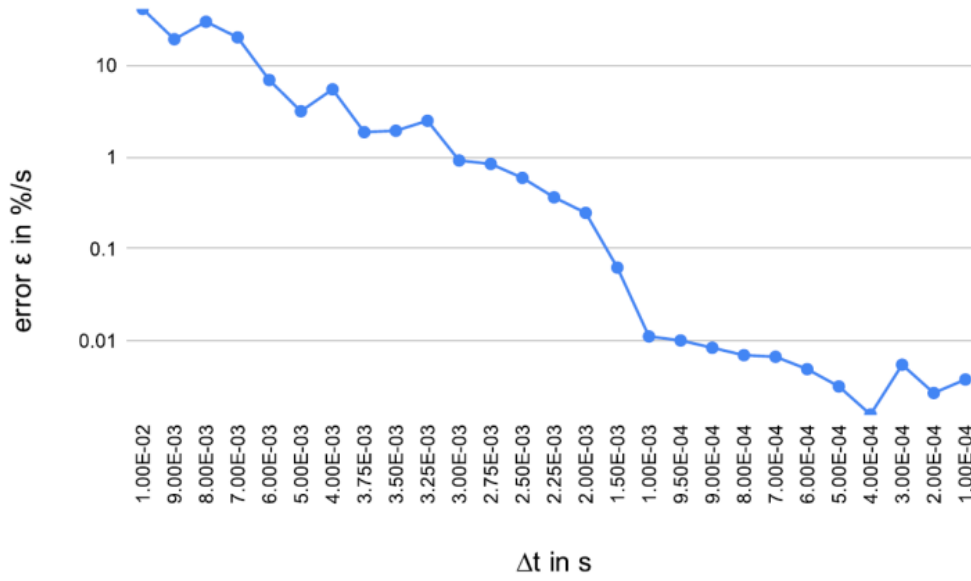


Figure 3.17: Computational error per second of vectorised Newton-Euler equations, on the example of a swinging chain, over integration time step Δt .

was analysed for a chain length of $n = 10$ components, over a simulated time of 5 s, with varying Δt and containing multiple oscillations in which the chains swung back and forth. The results are shown in Figure 3.17

All forces in the implemented simulation are conservative forces. As a result, in an ideal case scenario, there is no change in internal energy $U(t) = T(t) + V(t)$ in the system, where $T(t)$ is the sum of kinetic energy and $V(t)$ is potential energy. Therefore, any change to the internal energy $\|U(t) - U(t_0)\|$ is seen as the error of the numerical simulation. For ease of interpretation, the error displayed in Figure 3.17 is expressed as;

$$\varepsilon = \frac{\text{mean}(\|U(t) - U(t_0)\|)}{U_{\text{total}} \cdot \Delta t} \quad (3.67)$$

The error ε can be interpreted as the average offset from a zero internal energy that can accumulate over a second of simulation, in relation to the total energy available in the system. For the given system, the total available energy can be estimated as the maximum potential energy the system can release $U_{\text{total}} = \max(\|V(t) - V(t_0)\|)$. Figure 3.17 shows that the error ε tends towards zero for small time steps Δt . This leads to the assumption that the error in simulation originates from the chosen numerical integration method, as it is the only part of the simulation that depends on Δt . The presented interpretation of the Newton-Euler equation correctly represents the dynamics of a chain of components under the given constraints.

Furthermore, it leads to the interpretation that for any system fulfilling the constraints, Δt can be chosen to adequately simulate the dynamics of the system.

The parallel Newton-Euler algorithm, however, relies on square matrices with a size of $(3n)^2$ entries. As a result, longer chains might generate matrices which are too large for the memory of the computer to process. This is expected to limit the efficient computation of very long chains depending on the available memory space.

3.5 Comparison to Benchtop Experimental Test

In contrast to the *Euler-Lagrange* algorithm, the consideration of forces in the *Newton-Euler* is more convenient. In the 2D case as it is analysed here, the *Newton-Euler* equations are expressed in their simplified Equations (2.8) and (2.10) and therefore chosen to formulate a single vectorised differential equation describing the dynamics of a planar folding-chain with any number of components and thus allowing for the convenient use of vector computation libraries that are able to utilise the advantages of GPU architecture.

The algorithm was applied to the 2D folding chain with the first component in the chain being fixed to the world frame and analysed for its expected error and energy conservation, as well as compared to motion tracking of the real system. For a realistic comparison, dynamic friction was introduced based on the *Coulomb* friction model of *L. Lazzarotto 1997* [72]. A friction force was introduced to the generalised force equivalent to:

$$\vec{f}_{fric} = -\frac{\vec{v}_m}{|\vec{v}_m|} \mu_f \vec{m}g \quad (3.68)$$

with $\vec{m} = (m_1, \dots, m_i)$.

The friction coefficient of $\mu_f = 0.35$ was adopted using the data of *L. Lazzarotto 1997* [72] and *H.S. Benabdallah 2007* [73]. The static friction in the system was neglected as the dynamic behaviour of the chain was analysed. The folding process of sequence 3, as defined in Figure 3.15, was recorded by a *Hero 4 black* (*GoPro Media Ltd, UK*) camera with a frame rate of 240 frames per second. Position and orientation of each component was detected in each frame, as seen in Figure 3.18 and compared against simulation results.

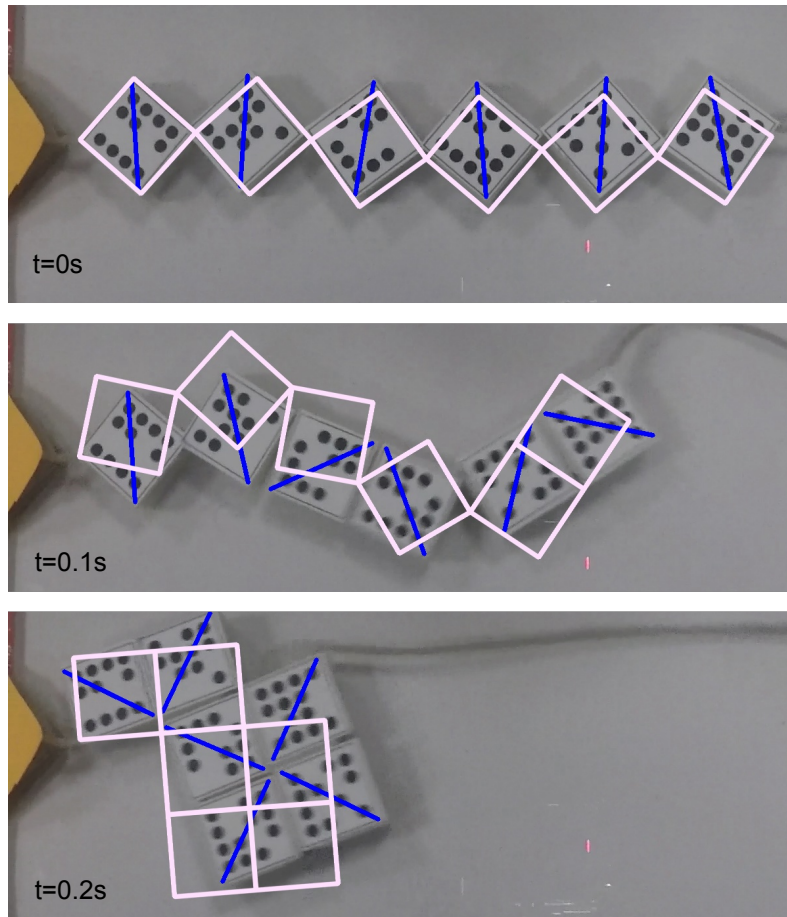


Figure 3.18: Motion tracking footage of different time steps of modified *free-fold* experiment for sequence 3 as defined in Figure 3.15, with overlay dynamic simulation results, with the left chain end fixed in place and the other chain end free. Diagonal lines are produced by motion tracking. Squares display the simulated system response.

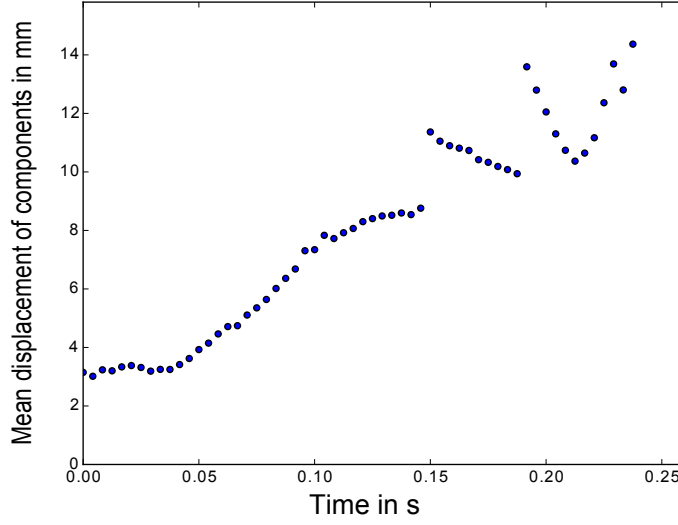


Figure 3.19: Displacement of the centre of mass between simulation and motion tracking of sequence 3 over time, with $\Delta t = (240 \times 5)^{-1}$ s. The *Coulomb* friction coefficient $\mu_f = 0.35$ and charge density of $q_{total} = 17.1892 \text{ C m}^{-3}$.

Figure 3.19 shows the mean displacement between the centre of mass in simulation and the tracked components, with an average displacement over all time steps and components of 8.2 mm. Noticeable are the jumps in the mean displacement due to the previously described collision handling. At time point $t = 0$ s, there is a mean displacement of 3 mm between simulation and experiment as the experimental system only approximated hinges, and the distances between the components is not constant.

Figure 3.20 shows the change of the relative angle between the components in simulation compared to the results of the experimental motion tracking. The simulation predicts the final folded shape correctly, with a difference in angle averaged over all time steps and components of $0.442 \text{ rad} \approx 25.32^\circ$. However as seen in Figure 3.20, there are some differences between the recorded and simulated movement: The order of components to reach a relative angle of $\pm\pi/2$ is different in simulation. In more complex systems, this could cause a significant difference between the prediction and final folding. However, this was not the case for the system investigated in this work.

One possible reason for this error in prediction could be the constructive simplicity of the experimental setup, approximating a system with hinges

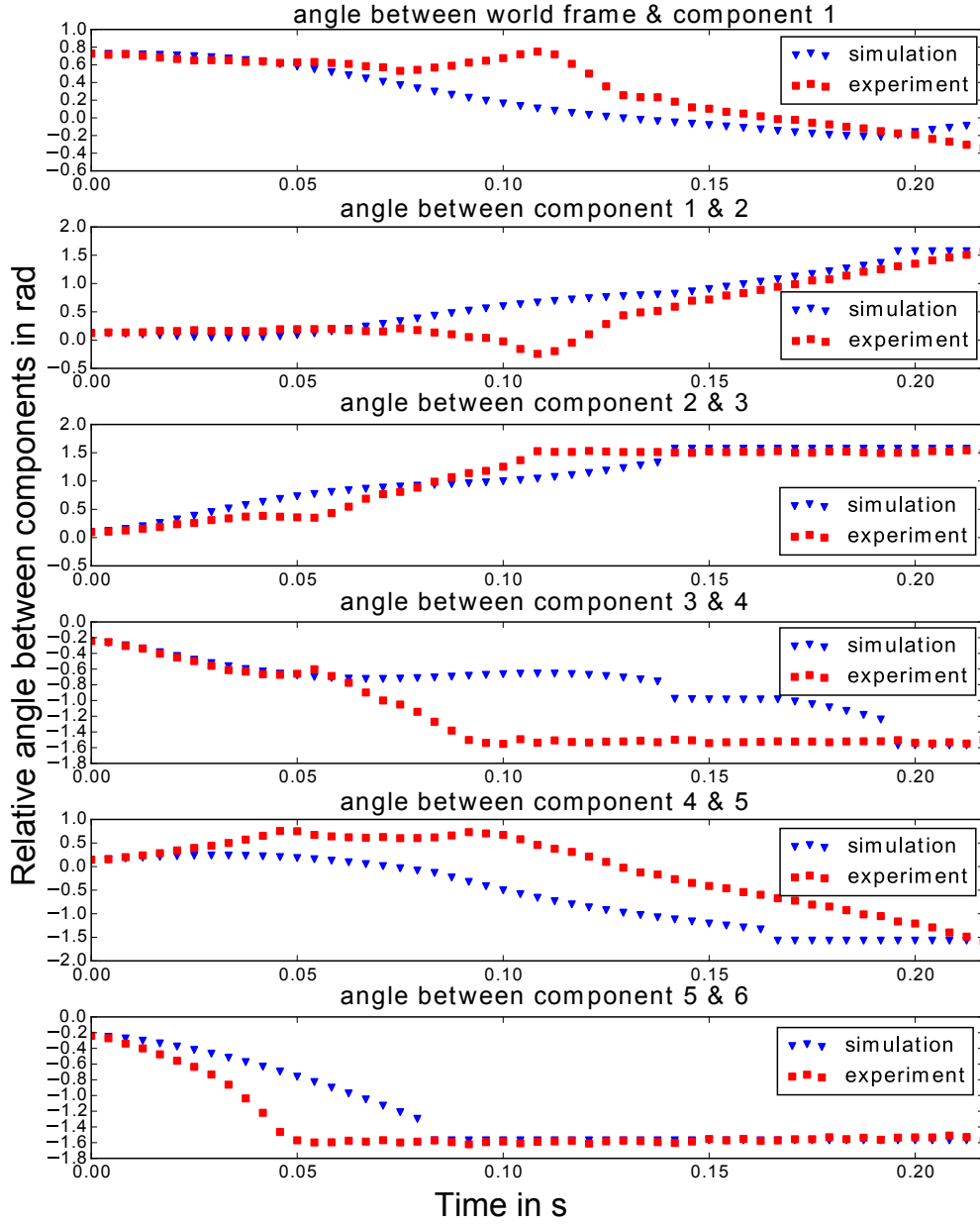


Figure 3.20: Relative angle compared between simulation and motion tracking, with $\Delta t = (240 \times 5)^{-1} \text{ s}$, *Coulomb* friction coefficient $\mu_f = 3.5$ and charge density of $q_{total} = 17.1892 \text{ Cm}^{-3}$.

and the inevitable error associated with manual priming and triggering of the folding process. Another possible explanation is the error introduced by the approximation of the magnetic forces, using the point charge model.

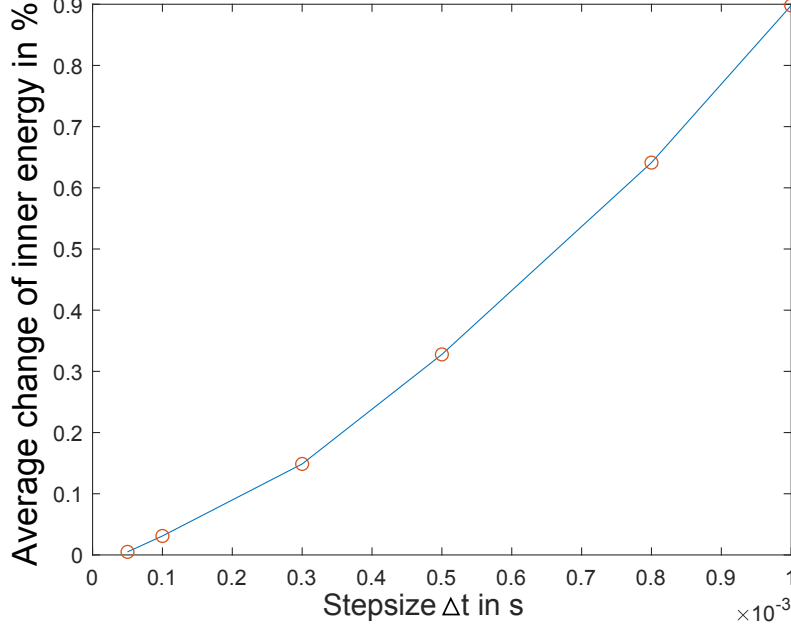


Figure 3.21: Percentage difference in total kinetic and potential energy between two time steps in a pendulum system with 3 components, averaged over 1000 time steps for different time step size Δt .

3.5.1 Computation Time

An algorithm was implemented to improve the computation time and allow for the computation of very long chains.

The algorithm was implemented twice, once using SMID-supported computation of vector equations and once using GPU supported computation. Computation with the *Numpy* library supporting SIMD architecture was compared in its average computation time against computation using the *Cupy* library supporting GPU architecture seen in Figure 3. The CPU calculation using the SMID structure shows a significant rise in computation time for chains with more than 300 components. The presented algorithm uses square matrices with $(3n)^2$ entries. The increase in computation time could be explained by the large matrices for the SMID structure to work efficiently. The GPU computation is slower for small numbers of components compared to the CPU computation. It is assumed that this is due to the overhead created by the implementation of the GPU architecture. However, for $n \geq 100$ components, GPU computation of the chain dynamics clearly takes significantly

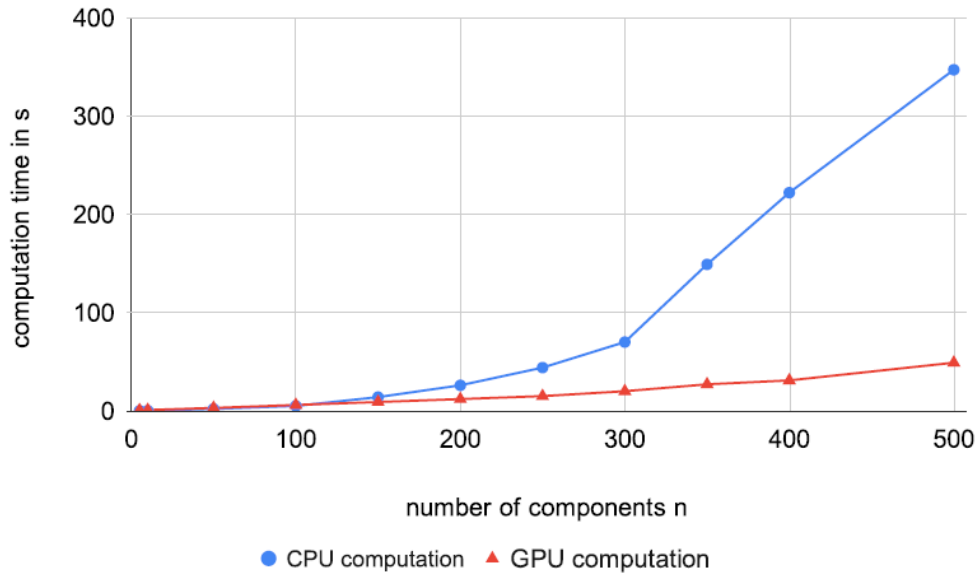


Figure 3.22: Comparison of computation time utilizing SMID architecture (CPU) versus computation utilizing GPU architecture.

less computation time than SMID calculation and displays a near-linear relationship between the number of chain components and computation time.

3.6 Energy Minimisation Folding Prediction

Considering the significant increase in computation time for long magnetic chains, a different method is necessary to predict and analyse possible folding pattern in these cases. Section 2.5.1 described how self assembly is based on the natural process of systems to strive for an equilibrium in internal energy and in the process minimise their internal free energy. This section details how this work seeks to simulate the internal free energy of a folding chain in order to predict possible states it might naturally fold into. Compared to simulating the dynamics of a folding chain where the magnetic forces need to be computed for every time step, the energy analysis method only computes the forces and internal energy for a few select states of the chain. This leads to the energy analysis method being computationally more efficient. The following forces might affect the folding of a chain of magnetic components;

- **Gravity** that expresses itself in a conservative force affecting all components, proportional to their mass [74];
- **Friction**, a non conservative force that is proportional to the relative movement speed;
- **Magnetism** that as seen in Equation (2.4), expresses itself in a con-

servative force field [25];

- **Collision** between components of the chain or with the environment which result in reactionary forces.

We might define the total energy in the system as

$$U = Kin + Pot \quad (3.69)$$

where the kinetic energy Kin is defined by the energy resulting from Velocity U_v of all components, as

$$Kin = U_v = \sum_{i=0}^n \frac{1}{2} m_i \vec{v}_i \cdot \vec{v}_i \quad (3.70)$$

Considering the magnetic forces defined in Equation (3.7) the potential energy might be defined as

$$Pot = U_g + U_c = \sum_{i=0}^n m \vec{g} \cdot \vec{x}_i + \sum_{j=i+1}^n \frac{\mu_0}{4\pi} \frac{\vec{q}_i \vec{q}_j}{|\vec{P}_j - \vec{P}_i|^2} \quad (3.71)$$

where $\vec{g}$ is the gravitational vector and $\vec{q}_i$ and $\vec{q}_i \vec{q}_j$ are the magnitude of the point charged defined by Coulomb's point charge model, detailed in Section 2.2 and 3.1.

Friction and collision will create entropy and as such lower the overall energy of the system. Using this method we can map the conversion of potential energy to kinetic energy and to entropy. Any acceleration of the magnets happens in trade-off with the potential energy. Depending on the case, the potential energy can be expected to steadily decline to its minimal state or to show local maxima and minima. Such local minima might stop the magnets from fully folding together if the kinetic energy in the system is insufficient to overcome the local maxima in potential energy. A fully folded state is when the defined maximum folding angles for the degrees of freedom are reached and thus all components and magnets in the system stop moving in respect to each other. The folding can only be guaranteed if the potential energy is steadily decreased over the analysed degree of freedom. Figure 3.23, shows the potential end kinetic energy while a complex structure of magnets folds.

If the chain folds over multiple degrees of freedom, an analysis of the

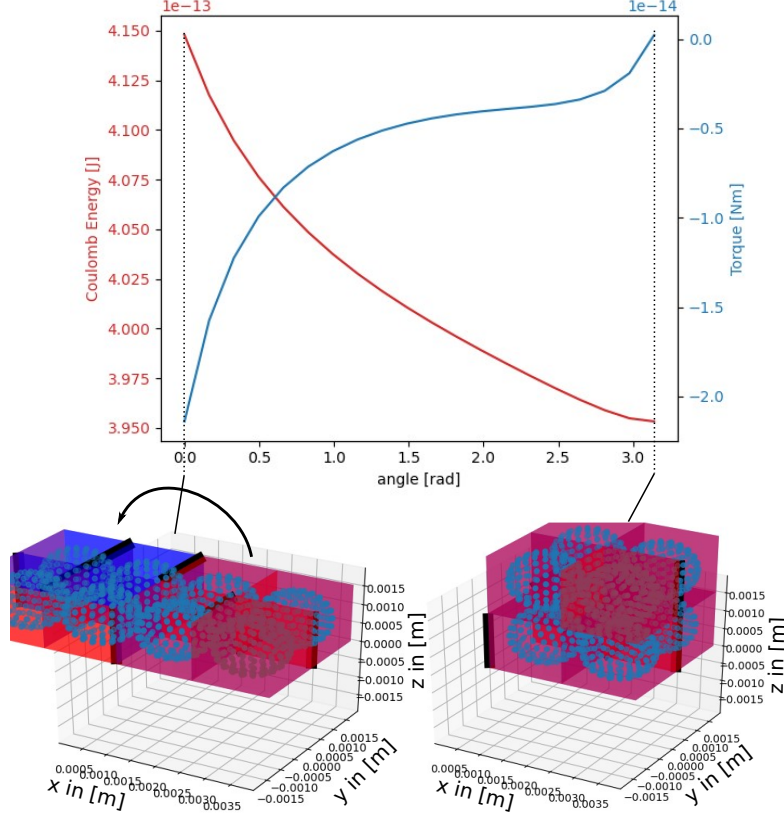


Figure 3.23: Torque and coulomb energy of a folding chain.

potential energy over the degrees of freedom is no longer feasible. However, if we only consider fully folded states, we can compare the potential energy in the possible fully folded states and rate the probability of which is most likely to occur. As we only consider fully folded states, the speed of the components during the folding is unknown, and as such, the friction cannot be estimated. In the presented model, the force which with the friction resists the movement is proportional to the velocity. The energy lost to friction is then equivalent to the work done by this friction which is defined as force multiplied by distance:

$$U_f = \sum_{i=0}^n F_{fric\,i} \cdot |\vec{x}_i - \vec{x}_{0\,i}| \quad (3.72)$$

where $\vec{x}_{0\,i}$ is the initial position of component with index i . A weight function is formulated that estimates the loss of internal energy to friction by setting the friction force constant $F_{fric\,i} = \sigma_f = 0.35$.

$$Pot = U_g + U_c - U_f = \sum_{i=0}^n m\vec{g} \cdot \vec{x}_i - \sigma_f |\vec{x}_i - \vec{x}_{0\,i}| + \sum_{j=i+1}^n \frac{\mu_0}{4\pi} \frac{\vec{q}_i \vec{q}_j}{|\vec{P}_j - \vec{P}_i|^2} \quad (3.73)$$

With this weight function, different possible states of folding of a chain of components can be compared against each other to estimate the most likely to occur without the need for a resource-heavy computation of folding dynamics.

3.6.1 Comparison to Planar Model

The benchtop experiment described in Section 3.3 supports a chain length of up to 6 components. In experiments with more components, the magnets at this scale do not provide sufficient force to overcome surface friction and the folding process does not occur. During the folding process, the *self-folding* chain is assumed to minimise its internal free energy. The chain changes from an unfolded high energy state to a folded low energy state. This low energy state might not be the minimal possible energy of the system but a local minimum. The free energy of the chain is the sum of the kinetic and potential energy. In the folded position, the chain is at rest and the kinetic energy is zero. Therefore, only the potential energy defines the folded states of the chain. However, during the folding process, the inertia of the chain might influence how the fold occurs and which energy minimum is reached. The experimental setup allows for the specific construction of the number and shape of possible folding shapes and the corresponding energy minima. It is of interest what the effect of multiple energy minima has on the reliability of the folding process as well as the possible effect of the chain inertia. Three distinct chain types were investigated to quantify the folding process:

- (1) The chain has multiple stable states, resulting in multiple local minima of the internal free energy;
- (2) The chain has multiple stable states, resulting in local minima of the internal free energy, one of which requires the least possible lateral displacement of the components;
- (3) The chain is constructed to only support one stable state.

A state is considered stable if it is fully folded and no two magnets with the same polarity face toward each other. Therefore, for each chain type case, a representative exemplar of a distinct chain as displayed in Figure 3.15 was built and analysed. This section interprets potential energy simulation results and compares them to results for the planar self-folding chain benchtop model.

Potential Energy Simulation

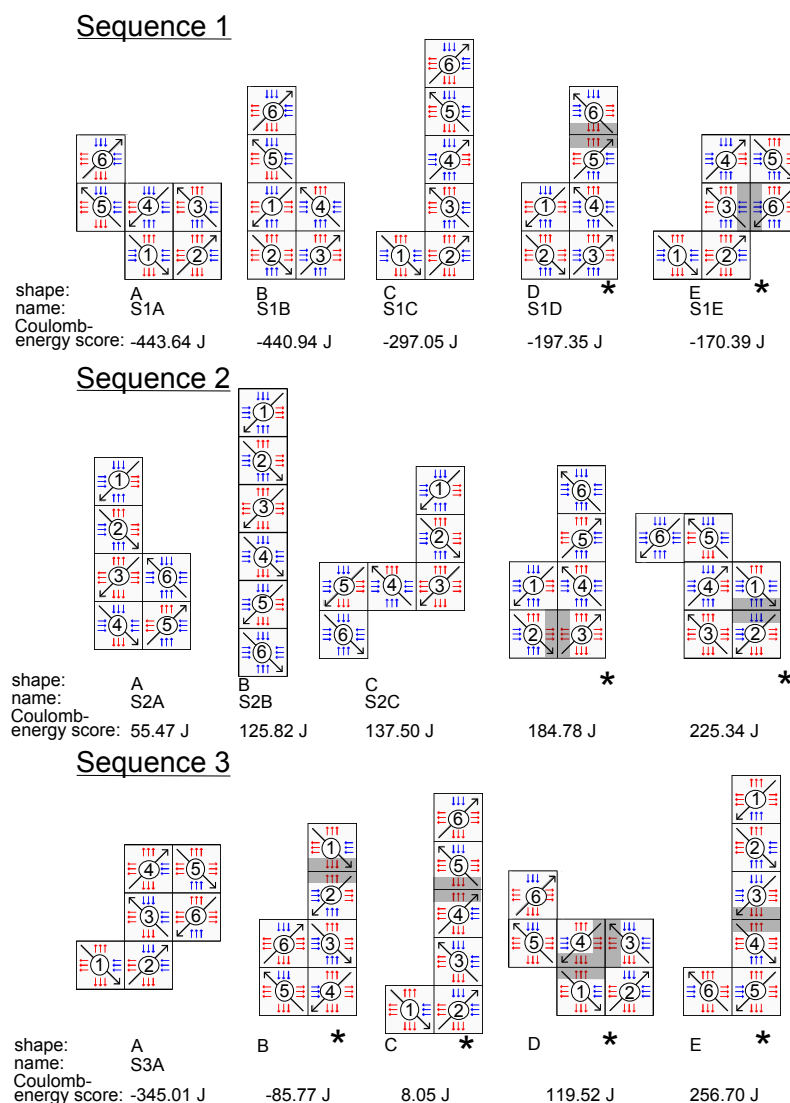


Figure 3.24: *Coulomb* energy minimisation results. Short arrows show the direction of magnetic polarisation. The base of the arrow marks the position of a positive charge, whereas the tip marks the position of a negative charge. Long arrows show chain direction. Folded shapes marked with * contain a conflict, highlighted in the drawing, meaning two surfaces of the same polarisation are in contact with each other.

Figure 3.24 shows the calculated *Coulomb* energy for the 5 folded states with the least *Coulomb* energy, for each chain sequence shown in Figure 3.15. The results show that only sequence 3 provides a single stable folded state. Furthermore, it shows, that sequences 1 and 2 feature more than one possible stable state, with associated local minima which the chain could fold into.

The results show that different sequences can stably fold into the same shape, as S1A and S3A have equivalent outlines, yet different *Coulomb* en-

ergy score results. As Equation (2.5) shows, the potential energy between two equally polarised point charges repelling each other, increases the sum of *Coulomb* energy in the system, whereas two opposite polarised point charges reduce it. The *Coulomb* energy is computed between all point charges, including those point charges that are located in the same component. As the relative distance between point charges in the same component does not depend on the position to other components, these add a sequence-specific constant to the *Coulomb* energy score. As a result, the *Coulomb* energy score of a folded chain might be positive as seen for Sequence 2 and yet represent a stable folding state.

The difference in *Coulomb* energy between S2B and S2A is 55.89% with just one of the relative angles between the components being different. S2B in comparison to S2C has two different angles and a change in *Coulomb* energy of just 8.75%. Therefore the change of *Coulomb* energy is not directly proportional to the change in shape.

The results also support the assumption that, as the *Coulomb* energy of stable foldings decreases, the more faces with opposite polarity are in contact with each other and as a result, the more compact the shape is.

The *tube-fed* simulation shows that the chain under the conditions of a *tube-feed* does not necessarily fold into its global minima of internal free energy. The *tube-feed* energy minimisation prediction results for each sequence are summarised in Table 3.2.

Table 3.2: Component by component energy minimisation results, for the *tube-feed* deployment mode.

energy minimisation simulation	predicted shape
sequence 1; forward	S1A
sequence 1; backward	S1C
sequence 2; forward	S2B
sequence 2; backward	S2B
sequence 3; forward	S3A
sequence 3; backward	S3A

As sequence 3 only supports one possible stable state, it is to be expected that both forward and backward *tube-feed* simulation result in the

shape S3A. Sequence 1 shows different folding shapes depending on deployment direction, as different states might be more favourable depending on deployment direction when only one component at a time folds. However, sequence 2 features multiple stable states but only folds into shape S2B during *tube-feed* simulation. As shape S2B is a straight line of components the calculation of the *Coulomb* energy, component per component, remains constant whether the simulation starts with the first or the last component. The reason for this can be described by comparing shape S2A and S2B. The only difference between these two shapes is the angle between components 4 and 5. The connection between components 3 and 6 gives shape S2A two more magnetic surfaces in contact with each other than all other stable states and, as a result, shape S2A is the global minima of all states of interest of sequence 2. However, in the forward *tube-feed* scenario when the angle between component, 4 and 5 is optimised, component 6 is still in the tube and cannot come in contact with component 3. As a result, a fold in the opposite direction is more favourable. Similarly, the shape S2B is more favourable during the backward *tube-feed* scenario.

The backward *tube-feed* prediction of Sequence 1 suggests that the chain does not necessarily fold into its global minima, depending on the deployment mode. In conclusion, the energy minimisation method might be modified such as in the *tube-feed* prediction to compensate for some deployment modes. However, the internal energy of the system is computed by assuming the system to be static and, depending on the movement speed, the dynamics of the system might cause a fold into an unpredicted minimum of internal energy.

Experimental Results

Figure 3.25 shows the probability of each sequence folding into their defined stable states, or misfolding for each deployment mode as measured in the experimental setup. The final chain fold is considered a misfold when the components come to a halt before the folding process is complete. The folding process is considered complete when all components are in contact with at least one other component (i.e. surface to surface). The only exception to this is outcome S1E, which is the only occurrence of a conflict in a finished folded shape during the experiments. As can be seen, a small gap exists between components 4 and 5 upon completion of the folding.

As shown in Figure 3.25, the experiment fully supports the simulation

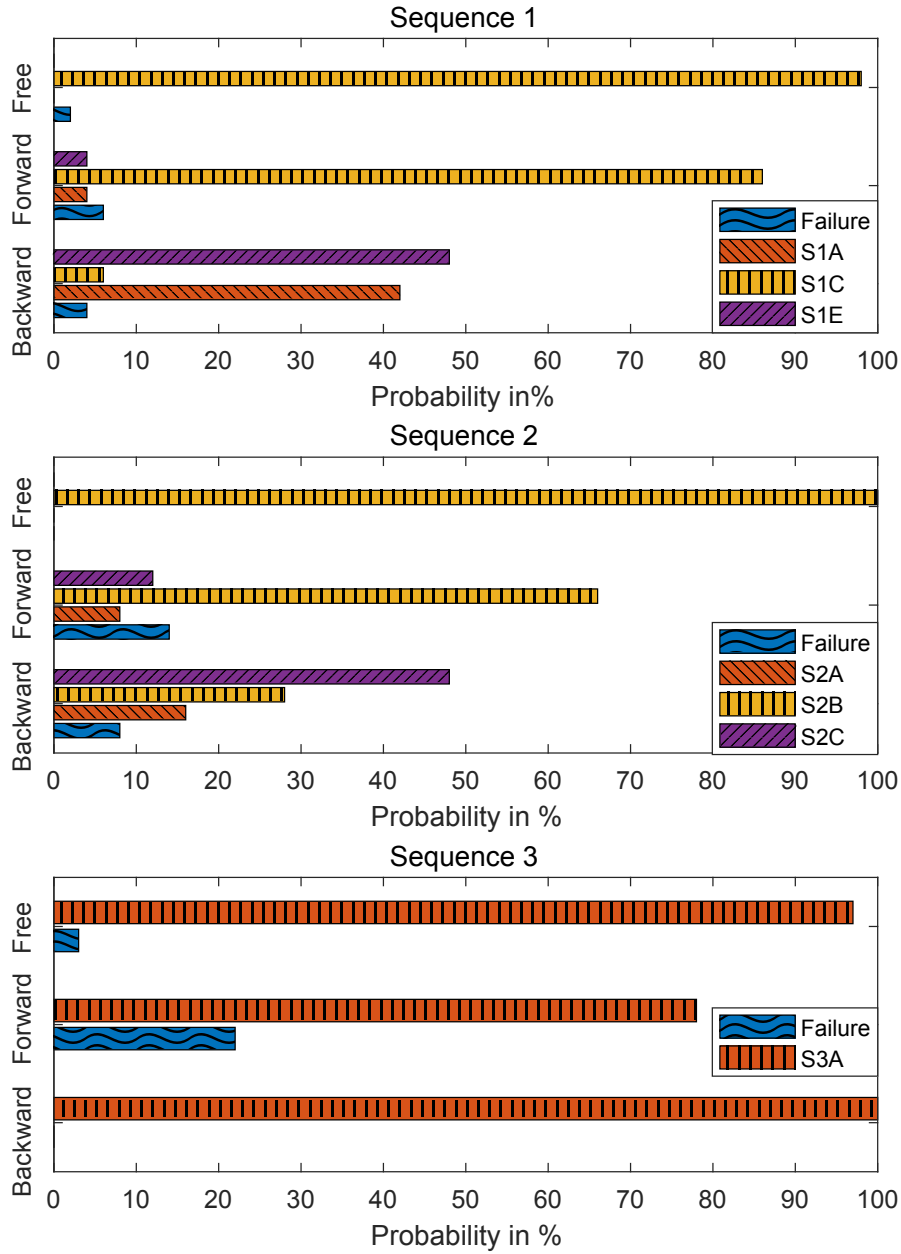


Figure 3.25: Probability of each chain sequence and deployment mode to fold into predicted shapes displayed in Figure 3.24 or misfold, as measured during experiment.

results for sequence 3. Forward *tube-feed* and *free-fold* experiments of sequence 1 and 2 however, have a higher probability to fold into a local minima instead of the global minimum for that sequence. In these cases, the chains fold into the respective shapes with the least lateral movement of the components. While this is predicted by the *tube-feed* simulation for sequence 2, *tube-feed* simulation fails to predict the folding of sequence 1. The backward *tube-feed* experiment for both sequence 1 and 2 show near equal probability of folding for multiple shapes and therefore cannot be compared to prediction.

It is noteworthy that sequences 1 and 2 have high probability to fold into different shapes depending on the deployment modes of the release, whereas sequence 3 preferentially folds into only one shape. All other possible folds of sequence 3 would result in two magnets meeting with the same polarisation and thus repelling each other. Nevertheless, the deployment modes of deployment also have a measurable influence on the probability of a misfold of sequence 3.

In the case of S3A, components 5 and 6 are connected to components 3 and 4. This requires that component 5 is dragging component 6 along during the *free-fold* and forward *tube-feed* experiments. The resulting friction force gives rise to a misfold.

For *tube-feed* systems, the force used to push the chain out of the tube can be seen as a driving force [27] of the system and can promote the fold into a lower or higher internal free energy state. However the direction of deployment of the chain out of the tube also has a significant influence. It follows that only certain driving forces promote some folded shapes. For example, the backwards deployment of sequence 1 gives nearly the same probability to fold into shape S1A as into S1C with a much lower probability to fold into shape S1B compared to the forward deployment.

3.7 Summary

To efficiently analyse and understand the folding of the magnetic chains that are presented in this work, a set of software tools has been implemented. An analysis of the potential energy within the folded system and a simulation of the folding dynamics is included. These software tools have been tested against a benchtop model of a magnetic folding chain. The magnetic model defining the forces that lead to the folding has been validated using experimental data. The simulation algorithms have been tested on prediction reliability and accuracy as well as on computational effort. A novel interpretation of the Newton-Euler dynamics tailored to a chain of rigid components and efficient in parallel computation has been formulated. This algorithm was tested against the benchtop model. It was shown that the calculation of magnetic forces has a super-linear relationship to the number of components in the chain. The simulation of the folding dynamics has to calculate these forces at every time step and is dependent on small time steps for an accurate simulation. Therefore the simulation of folding dynamics proves too

computationally heavy to predict the folding of long chains.

Longer chains might be evaluated in their folding by analysing the potential energy in the system. The proposed software model of a chain allows for a convenient interface and is capable of computing *Coulomb* energy and magnetic forces for specific states of a chain. Different tools for analysis have been implemented for a convenient interface with the software. The software allows the user to construct a chain of magnetic components using various primitive shapes. Furthermore, the user might compute forces and *Coulomb* energy of specific states of the chain to predict which configuration is most likely to occur. The prediction demonstrated a sufficient reliability in a statistical investigation using data from a benchtop.

Investigating the primary deployment method where only one component is expected to fold at a time, the software offers a tool to analyse the potential energy over this one degree of freedom. This was shown to accurately predict folding behaviour and allows for the construction of reliably folding magnetic chains.

4 Applied Reconfiguring Devices

In this chapter the previously established methods of constructing and analysing magnetic folding chains are applied to construct magnetic chains and derive a general concept of self-assembling magnetic chains for minimally-invasive surgery. To test the developed theories and concept, a range of prototypes have been developed. Special focus in this chapter is to put the developed theories to test and to prove that a self-folding device can be deployed in a minimally-invasive setting. Therefore, constructive and material requirements of the magnetic chains have been researched and considered in the development of a general concept for self-folding magnetic chains.

This concept aims to lay a foundation for a toolbox that can be used to create a range of functional shapes to be used in minimally-invasive surgery. The concept is deducted from the most simple application of a self-assembling chain to be reinforced by analysis of gradually more complex folding shapes and finally the definition of possible secondary structures that in turn might be used as building blocks for larger structures.

4.1 General Concept of Self-Reconfiguring Chains for Surgery

This section develops the general concept of self-reconfiguring magnetic chains for minimally-invasive surgery. As highlighted in Chapter 2, self-assembly is a broad concept and refers to a range of processes. To generate a concept that can be used to construct self-assembling tools, a subset of processes enabling a reliable construction has to be defined together with a set of guidelines that simplify the process and provide rules of best practice. Using

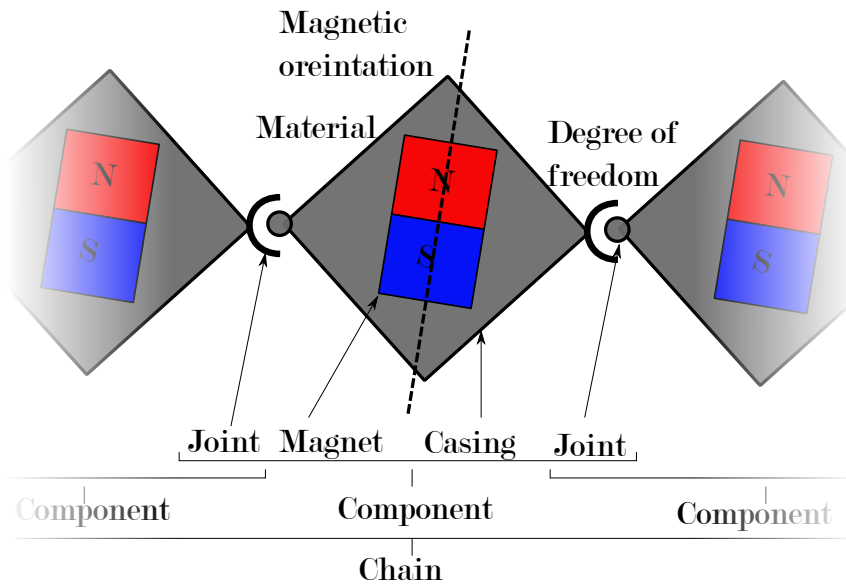


Figure 4.1: Component breakdown of a magnetic folding chain.

this concept and following the guidelines provided in this chapter, a chain of magnetic components might be conceived with a specific sequence of joints and magnetic orientation along the chain, to fold reliably and repeatably into a configuration that can fulfill a function as a tool in minimally-invasive surgery. The prototype model for a self-folding chain is the protein biosynthesis, highlighting the complexity of the underlying challenge. Chapter 3 highlighted the challenges in predicting folding and analysing whether a specific fold is feasible. However preliminary testing made clear that size and material further limits possible concepts.

The primary requirements for a general concept of self-folding magnetic chains to enable the construction of self-assembling tools are to provide:

- a set of construction tools that allow for the construction of a wide range of tools shapes;
- a mechanism to fold these tools from a subset of components arranged in a chain;
- a set of software tools to analyse construction on their folding behaviour and reliability;
- a set of construction rules that allow for a convenient construction of reliably folding tools.

In the following, the components of a magnetic folding chain are analysed, independently and in context of each other. As such, the central features of a folding chain as seen in Figure 4.1 are;

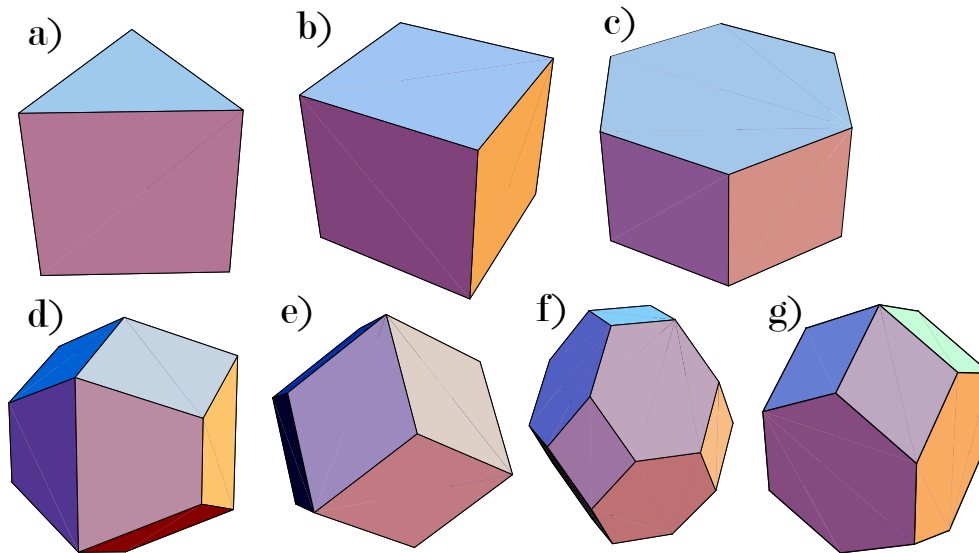


Figure 4.2: Examples of space filling shapes, with a) triangular prism, b) cube, c) hexagonal prism, d) trapezo-rhombic dodecahedron, e) rhombic dodecahedron, f) truncated octahedron, g) elongated dodecahedron [75].

- **The magnet** and its magnetic orientation
- **The casing** that contains the magnets
- **The joint** that connects the components

From there, a general concept of self-folding magnetic chains is formulated.

4.1.1 Building Blocks

To form a three dimensional shape, the individual components have to fit together like puzzle pieces to fill the volume of the shape. Furthermore, if we assume the components to be arranged in a chain, their relative movement is limited and not every shape promotes the folding of a chain in a volumetric structure without holes. Under the assumption that all components have the same basic shape, only a subgroup of component shapes can be considered that fulfill this requirement and fill a volume without a gap in between. Figure 4.2 shows an overview of space filling shapes that satisfy this requirement [76]. Furthermore the assembly is required to fold from the shape of a string into a range of possible shapes. As components are assembled in a chain, any component will be linked by two adjacent points to its neighbours. If there is no possible linking that allows for neighboring components to fold and cover any surface of the component, then the folding chain might not fold into a volumetric shape but leave a hole in the folded structure. Lastly

the components in the chain are linked via joints, allowing for some degree of rotation between components. Therefore the geometry of the components needs to retain its space filling property when rotated over a possible joint axis.

As such, the requirements to the geometric shape of a component are:

- The shape needs to be space-filling to enable an efficient use of available space
- The shape needs to allow the arrangement in a chain and allow the chain to fold, in order to fully fill the available space

To choose a specific shape, the assumption is made that components are linked at the edges of adjacent facets and fold over the edge where they are linked. The triangular prism, the cube and the hexagonal prism all full-fill these requirements and might be assembled in a chain with triangular, square and hexagonal cross sections respectively. Of these, the cube is the most simple solution leading to a homogeneous grid that fills a volume and can fold from a chain into any form. However, considering the use of the assembled grid to be used as a tool, the ability of the grid to resist forces is of importance. A grid formed from triangular prism, cubes or hexagonal prism has at least one common shear plane. Forces in such grids therefore are mostly compensated by the joints and not the bodies the grid is formed from.

Forming a grid out of the other space-filling shapes shows no common shear plane and thus would be expected to have a higher resistance to external forces. However, all but the rhombic dodecahedron consist of varying surface facets. The elongated dodecahedron, for example has rhombic and hexagonal facets. These shapes require a specific orientation in the grid to fit together and fill the space. If folding from a chain, possibly over a one degree of freedom (DOF) joint, the components are required to rotate. Therefore, geometric constraints of shape and joint position can contradict each other. Only the rhombic dodecahedron allows for a versatile folding as all its facets are rhombic in shape. The shapes that satisfy all three requirements are the cube and the rhombic dodecahedron.

4.1.2 Linking the Chain

Considering two magnetic components without any joint or constraint between them, the components will naturally force a orientation of north pole

latching to south pole. To satisfy the requirement of components being assembled in a chain, some form of joint that allows the components to roll or rotate with respect to each other is required. The more possible degrees of freedom (DOF) between components the more possible states a chain might form into. Considering that the desired shape is a singular one, it is beneficial for the folding process to reduce the degrees of freedom in a chain as much as possible and therefore encode the final folding shape as much in the joint configuration as in the magnetic orientation. Under consideration of the target size (in this work a target component size between 10 mm and 2 mm) one DOF rotating hinges have been chosen to connect components.

4.1.3 Magnetic Folding

To fold a chain of magnetic components into a range of shapes, rules for the magnetic polarisation of said components have to be derived that enable this folding. From the preliminary experiment in Chapter 3.3, the conclusion was drawn that a maximum of the components volume should consist of magnetic material to maximise magnetic forces and to maximise the length of a possible magnetic chain. If we consider feasibility of production, only a single magnet might be integrated per component to maximise magnetic forces to other components. Composite magnets created in additive manufacturing could allow for multiple magnetic orientation within the same magnetic component. However, these composite magnets are significantly more expensive than standard magnets and can be significantly weaker if their magnetic domains are not co-linear. Therefore, to favour rapid prototyping, a single magnet with a uniform direction of magnetisation per component was considered in this work. To analyse the folding of a magnetic chain we firstly reduce the folding to its most simplistic case: the folding of two magnetic components in a 2D plane.

Single Axis Folding

To understand the processes of self-folding in a chain of magnetic components, the most simple case is analysed first. The most simple form of the described self-folding is that between two components. Furthermore we assume folding over a single axis of cubical components. As such, the problem might be reduced to a planar folding case. Further considering that the desired mode of folding is for a component to be in full surface contact to its neighbour, a binary system can be defined where cube A might fold to 0° or 90° . Figure 4.3 shows different folding cases between two components

under this simple case. It can be seen that any configuration where the cubes are magnetised from edge to edge, no distinct folding due to magnetic interaction can occur. Case a) and b) in Figure 4.3 results in the magnetic axes of both magnets to be perpendicular to each other and thus having no clear magnetic interaction. While cases c) and d) lead to the alignment of the magnetic axis, the result is either an unstable or bi-stable system. An unstable system means that either of these folding possibilities results in the same magnetic poles in contact with each other and thus repulsion. This likely leads to the magnets maximising their distance to each other. On the other hand, a bi-stable system is such that both folding possibilities result in attraction and are similarly likely to occur.

The same is true for cases e) and f), where the magnetic poles are in the corners of the shape, and the magnetic axis is at angle $\beta_{mag} = 45^\circ$ angle to the edges of the cubes. However, if the magnetic orientation of the components are as seen in g) and h), a specific folding can be enforced. It shows that in these cases, the the magnetic orientation is from corner to corner and in the folded state the magnetic axis of both tiles align. Magnetisation of the component in a direction between the two extremes $0^\circ < \beta_{mag} < 45^\circ$ can be argued to lead to similar but weaker folded results. As such, magnetising the components in the desired folding case shows the same absolute orientation for the magnetic axis of all components in the same direction and a maximum angle, to the surfaces where the components might interact.

This behaviour can be observed during simulation, using the simulation methods described in Chapter 3. The cubes are considered to have a size of $7\text{ mm} \times 7\text{ mm} \times 7\text{ mm}$ and contain a spherical magnet with a diameter of $1/4\text{ inch} = 6.35\text{ mm}$. Figure 4.4 shows the estimated torque and potential energy resulting from the magnetic forces between the components. The potential energy is steadily decreasing over the folding angle. As such it can be concluded that the potential energy is steadily transformed into the system's kinetic energy leading to subsequent angular acceleration of the component. This is further enforced by analysing the torque. The torque is a constant negative, suggesting a continuous torque accelerating the folding in the predicted direction.

Standardised Component

The previous observations are investigated in minimal necessary system size and then extrapolated to more complex systems. The initially considered

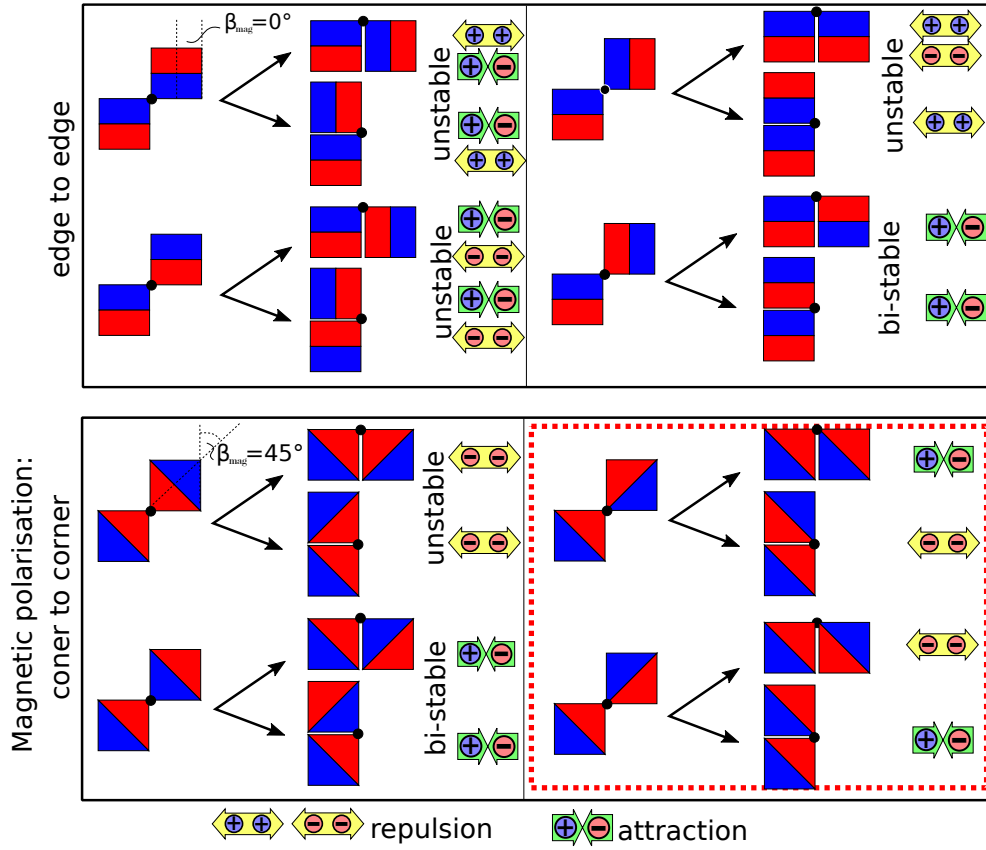


Figure 4.3: Magnetic folding cases between two tiles, with blue indicating the magnetic south pole, red indicating the magnetic north pole, a) to d) magnetisation from edge to edge and e) to f) magnetisation from corner to corner.

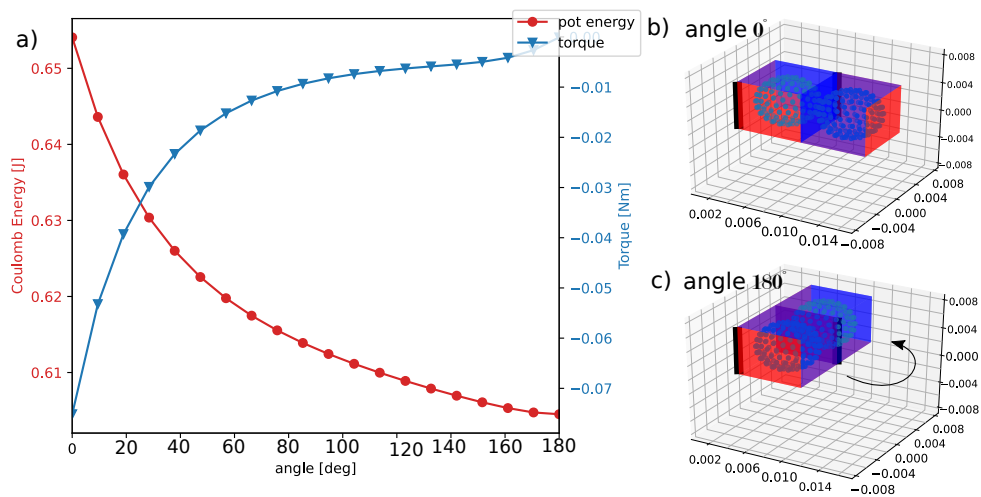


Figure 4.4: Left: Potential energy landscape for a pair of magnetic components. Right: Visualisation of cubical components and magnetic point charges.

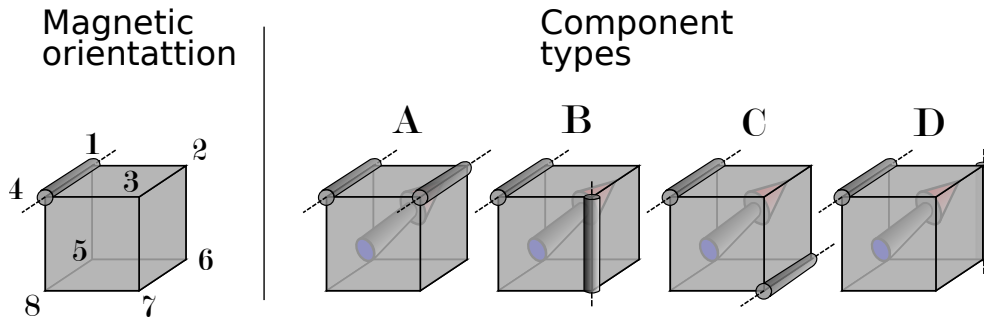


Figure 4.5: Standardised cubic magnetic component, left: Magnetic orientation coded by the corner it point towards, right: types of component joint configuration.

system consists of a chain of cube components, each containing a spherical magnet. During the deployment procedure via a tube or catheter of the same diameter as a single component, the chain can be idealised to be assembled in a beam. Therefore, the initial state of each chain is considered to be a beam. In this state, the four cube components have been defined covering all geometric possibilities of joint combination in a folding chain, as seen in Figure 4.5. As shown, magnetisation from corner to corner allows for a distinct folding between chain components to be enforced. As such, a single component can be characterised by its joint configuration and magnetic orientation. The joint configuration is marked with a letter from A to D while the magnetic orientation is marked by the number of the corner in which the magnetic north pole is located. There are $4 \times 8 = 32$ possible components with combinations of magnetic orientation and hinge position. The hypothesis is analogous to how a sequence of amino acids codes for a specific protein; similarly a specific sequence of these cube components can form any three-dimensional structure that can be discretised in cube sub-shapes. This statement is subsequently investigated.

Magnetic Arrays

Applying this concept to more complex systems, a longer chain of components is analysed and tested for the necessary conditions to fold into an array. From considering a planar folding case, it can be observed how the folding between two components can simply be stacked to form a chain.

Translating this behaviour as depicted in Figure 4.3 to the three dimensional case, the same behaviour can be observed and leads to the formulation of the folding requirements of magnetic arrays;

- The orientation of the magnetic axis of all components has to be

uniform for the final folded structure.

- Each individual magnetic orientation has to be at a maximum angle to all possible contact surfaces.

For a cube component, this results in the magnetic axis to be oriented from one corner of the cube to the opposite corner. Applying these rules to other possible components listed in Section 4.1.1, it becomes clear that not all shapes are capable of fulfilling these criteria. The more complex the shape, such as a dodecahedron, the lower the maximum angle of the magnetisation axis to all possible contact surfaces. A spherical magnet inside the components approximates the ideal polarisation as assumed in Figure 4.3. The closer the component shape is to a sphere, the better this approximation. As such, more round shapes such as the presented dodecahedron are unfavourable for magnetic interaction due to the small angles to the magnetic axis. In summary, the cube is the most versatile space-filling shape for a components casing. While it is structurally not favorable due to a common shear plane in a grid of cubes, it enables a uniform and simple method to construct self-assembling magnetic grids. Other shapes such as the prism and dodecahedron might be used as component shapes in certain cases.

4.1.4 Magnetic Building Blocks

Forming a volumetric structure from a string of components that can act as a tool might require the formation of larger shapes. Comparing the process of magnetic self-folding to its biological prototype model the *protein biosynthesis* it becomes apparent that three main components define the folding Process:

- **The components**, the smallest part of the chain that is linked together to form bigger structures
- **The secondary structures**, that are a set of reoccurring shapes with a high reliability of folding and can be used to simplify the construction of more complex structures.
- **The superstructure**, defining the final folded shape of the chain.

For a graphical understanding, the comparison to the construction of a house is made in Figure 4.6

To ease the construction of such larger shapes, a range of secondary

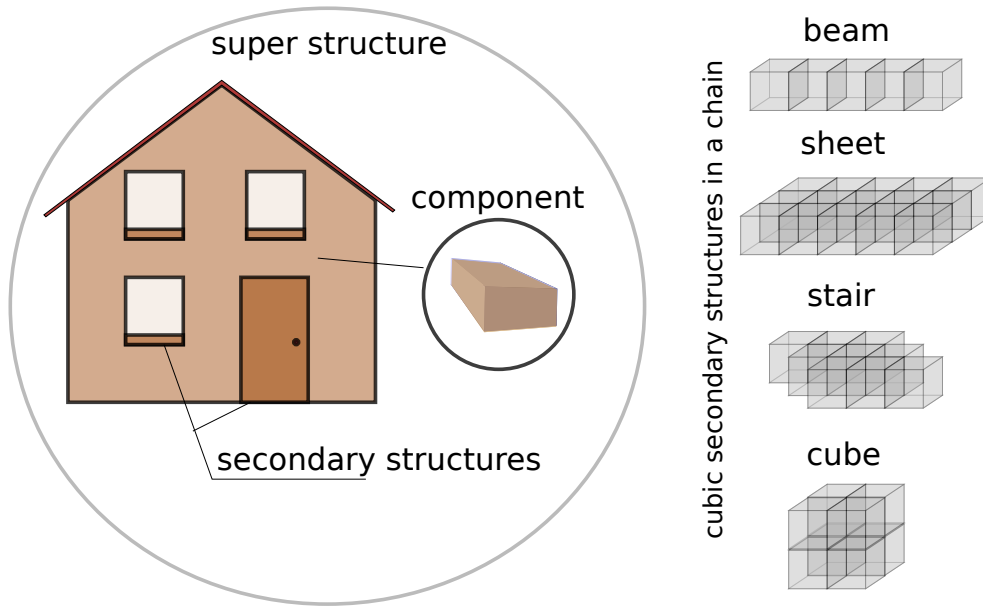


Figure 4.6: Left: example of components, secondary structures and super-structures in analogy with a house. Right: secondary structures of a magnetic chain with cubical components.

structures has been defined. These secondary structures are optimised to fold reliably and and to ease construction of reliably folding tools.

Beam

The assembly of the chain components in a single direction might be called a beam. The chain is designed to fit through a tube or catheter. Considering tool deployment in a clinical setting, this shape is defined to be the standard state of deployment. However there is a possibility that a beam needs to be shaped in a manner that does not fit with this standard state of deployment. Therefore an analysis of potential energy has been conducted to simulate such folding behaviour. Multiple component combination might form a beam. As stated, a beam also is considered to be the initial state of each chain to facilitate deployment through a catheter. Therefore a component combination is required that folds from a beam into a beam. The chain analysed here is a alternating series of type $C1$ and $C2$ cubes and fullfils this requirement. Multiple lengths of chains where tested. The exemplar used here is a chain with the length of $n = 3$ with the sequence $C1 - C2 - C1$; and $n = 10$ with a sequence of b) $C1 - C2 - C1 - C2 - C1 - C2 - C1 - C2 - C1 - C2$. Any length of a chain of this configuration leads to the same result.

The initial configuration where all joints are at folding angle 0° is always considered to be the beam configuration as the chain would be deployed

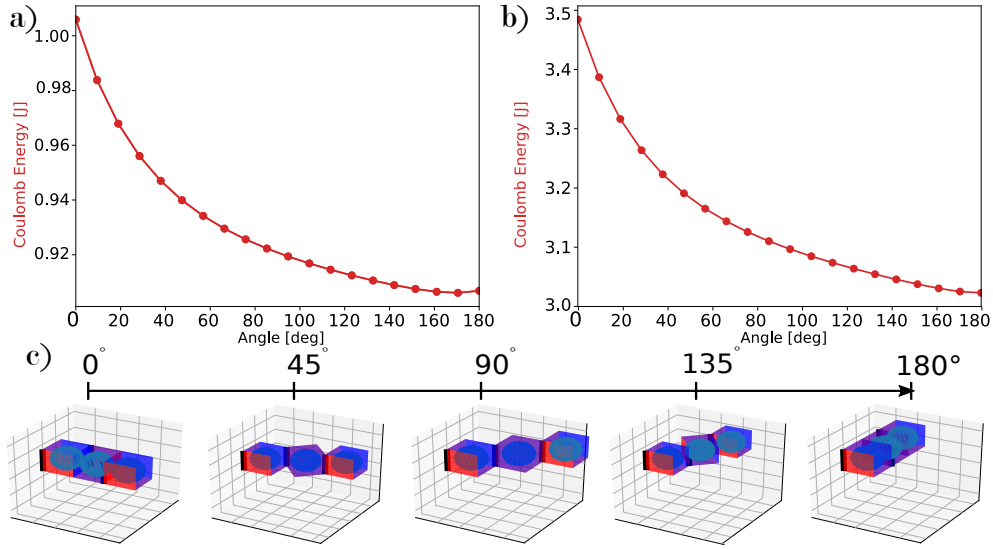


Figure 4.7: Potential energy of simulations folding of a beam of length a) $n = 3$, b) $n = 10$ beam length and c) visualisation of beam folding for $n = 3$.

through a channel or catheter. The final configuration for this sequence is a beam as well. Figure 4.7 shows the potential energy from magnetic interactions when all joints in the system are at the same folding angle at the same time for both $n = 3$ and $n = 10$. The potential energy in the system clearly shows how the final beam shape presents the global minimum of potential energy and can be seen as the favoured state for the chain. Both start and end configurations of the chain can be described as a beam. The only difference is the magnetic orientation of each component. While in the starting configuration this orientation is partially with north and south pole in contact with each other, the final configuration has all magnets oriented in the same direction from one corner of the components to another and thus has a significantly more favorable configuration of the magnets. This shows that the underlying rules of construction hold true in three dimensional space for a beam structure.

It concludes that a beam structure might be seen as a serial addition of single cubes folding. It shows that the same pattern of potential energy and torque can be observed for any length of components in the chain. This leads to the conclusion that the suggested magnetic folding concept allows for a reliable folding of beam structures. To investigate the maximum possible length of a beam structure folding against gravity, the measured component weight of 1.51 g and component diameter of 7 mm is included in the simulation and compared against the simulated torque. The result is a

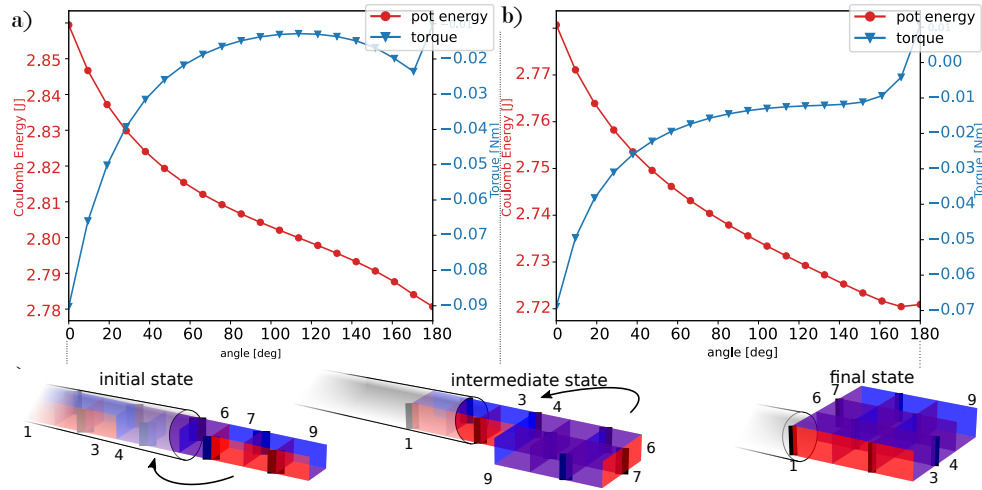


Figure 4.8: Potential energy simulation of the folding behaviour for the sheet secondary structure folding sequentially, with a) folding between component 6 and 7, b) folding between components 3 and 4, c) visualisation of folding.

maximum chain length of $n = 12$ components as a conservative estimation.

Sheet

A beam is a one dimensional structure. It needs to be proven that the postulated rules allow for a folding of volumetric shapes. As an intermediate step, a planar folding structure is investigated. A planar structure is achieved by stacking multiple beams. The analysed chain has a sequence of $Z1 - Z2 - B1 - D1 - Z2 - Z1 - Z2 - B1 - D1 - Z2 - Z1 - Z2 - Z1$, where the Z is a placeholder for any other component. As the initial shape deployed is a beam, it is used here to form a sheet. Following the defined guidelines, a sequence of B -type components is recommended to maximise flexibility of the chain. The $B1 - D1$ sequence folds multiple beams into a sheet.

Considering the length of a chain folding into a sheet structure, it can no longer be assumed that all components fold simultaneously if deployed through a catheter. In this instance, three beams with a length of 3 components are folded into a 3×3 sheet. Therefore the chain has a total of 9 degrees of freedom of which only 2 are used to fold the structure. All other DOF are already in their most stable state as shown with the beam secondary structure. The folding has been simulated under tube deployment conditions. Under this conditions only the joint between the B and D -type components are expected to move. The folding has been simulated in sequence where the first relevant DOF exiting the tube folds and then the second, as seen in Figure 4.10. It can be seen that both plots of potential

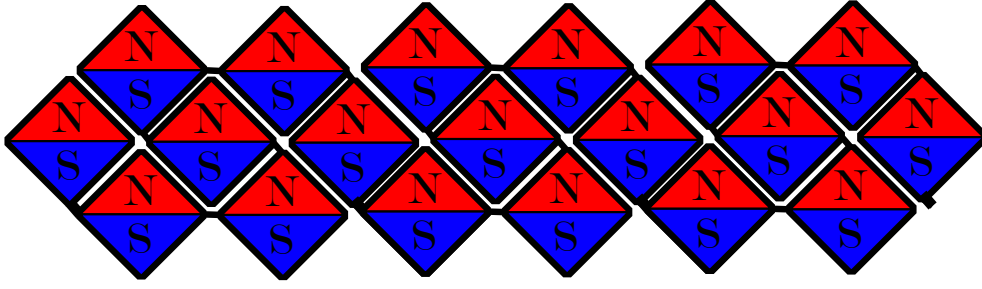


Figure 4.9: Concept of the steps secondary structure with a homogeneous magnetic interface.

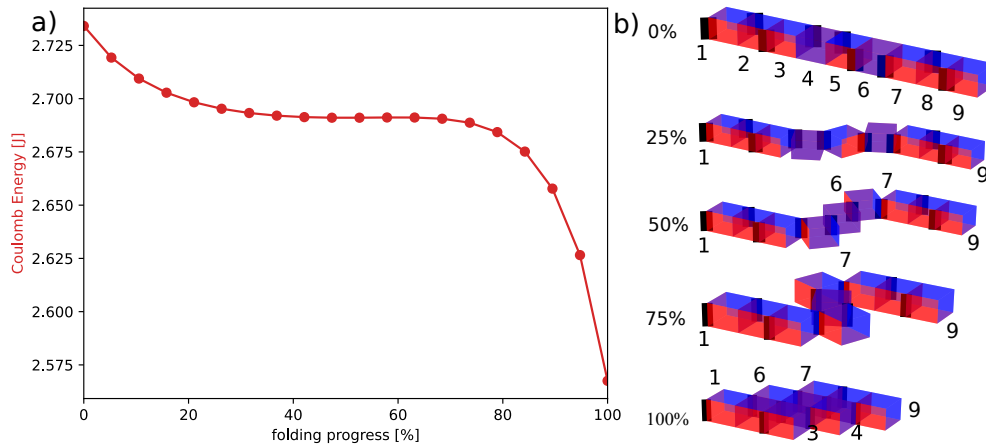


Figure 4.10: Potential energy simulation of the folding behaviour for the steps secondary structure.

energy are consciously decreasing. This leads to the assumption that beams of magnetic components with the suggested magnetic orientation are able to fold reliably into a sheet secondary structure.

Step

Before considering a chain configuration expanding in all three dimensions, a variation of the sheet needs to be discussed, the Step. As magnetic orientation of each component is from corner to corner, the superstructure does not have a natural surface perpendicular to the total magnetic axis. As such, magnetic interaction between the superstructure and another magnetic structure might be limited. However if the cubes can spontaneously self-assemble into a stair structure, as seen in Figure 4.9, a magnetic surface can be formed that is significantly more favorable for magnetic interaction between different bodies. Analysing the potential energy under free-folding release conditions shows that for this shape that the desired shape under the postulated rules of construction is the configuration with the minimum in potential energy and therefore is likely to be spontaneously self-assemble.

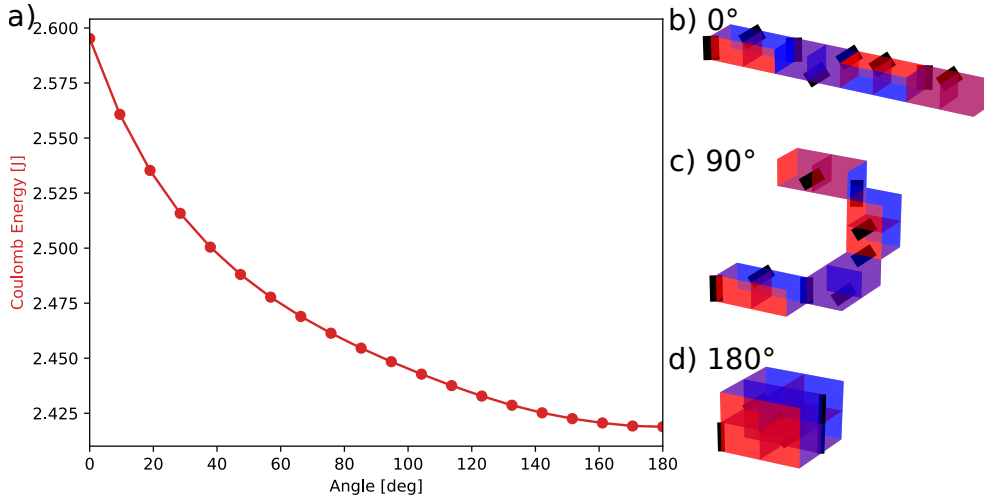


Figure 4.11: Potential energy simulation of the folding behaviour for the cube secondary structure under free fold deployment conditions, with a) potential energy over folding angle and b), c) and d) visualisation of folding process.

However intermediate steps of the folding show minor changes in potential energy. While the shape represents a minimum in potential energy, the fold is expected to have a low folding reliability. The stair effectively is a beam in the natural direction followed by another beam against the natural direction of deployment to form a sheet that is offset by one component. This shape further demonstrates how shapes of beams and sheets can be combined to form more complex structures.

Cube

Lastly it needs to be proven that the proposed rules are capable of forming a volumetric structure. As proof-of-concept, a configuration consisting of $2 \times 2 \times 2$ components has been chosen. The unique feature is that the superstructure itself resembles a cube with the same overall magnetic orientation as its individual components. Thus multiple cubes can form even larger structures. This concept is often described as a voxel [77] and is the volumetric equivalent to a pixel that make up digital pictures. A cube secondary structure might be achieved using the sequence $B7 - B3 - B8 - C5 - A7 - B7 - C1 - Z5$. Figure 4.11 displays the potential energy of such a chain folding into a cube superstructure under free-fold conditions. It is evident how the cube superstructure represents a minimum in potential energy with 2.413 J. This leads to the conclusion that the cube is a possible folding shape for the presented sequence.

As seen in Figure 4.12 a) and b) there is a single way in which all compo-

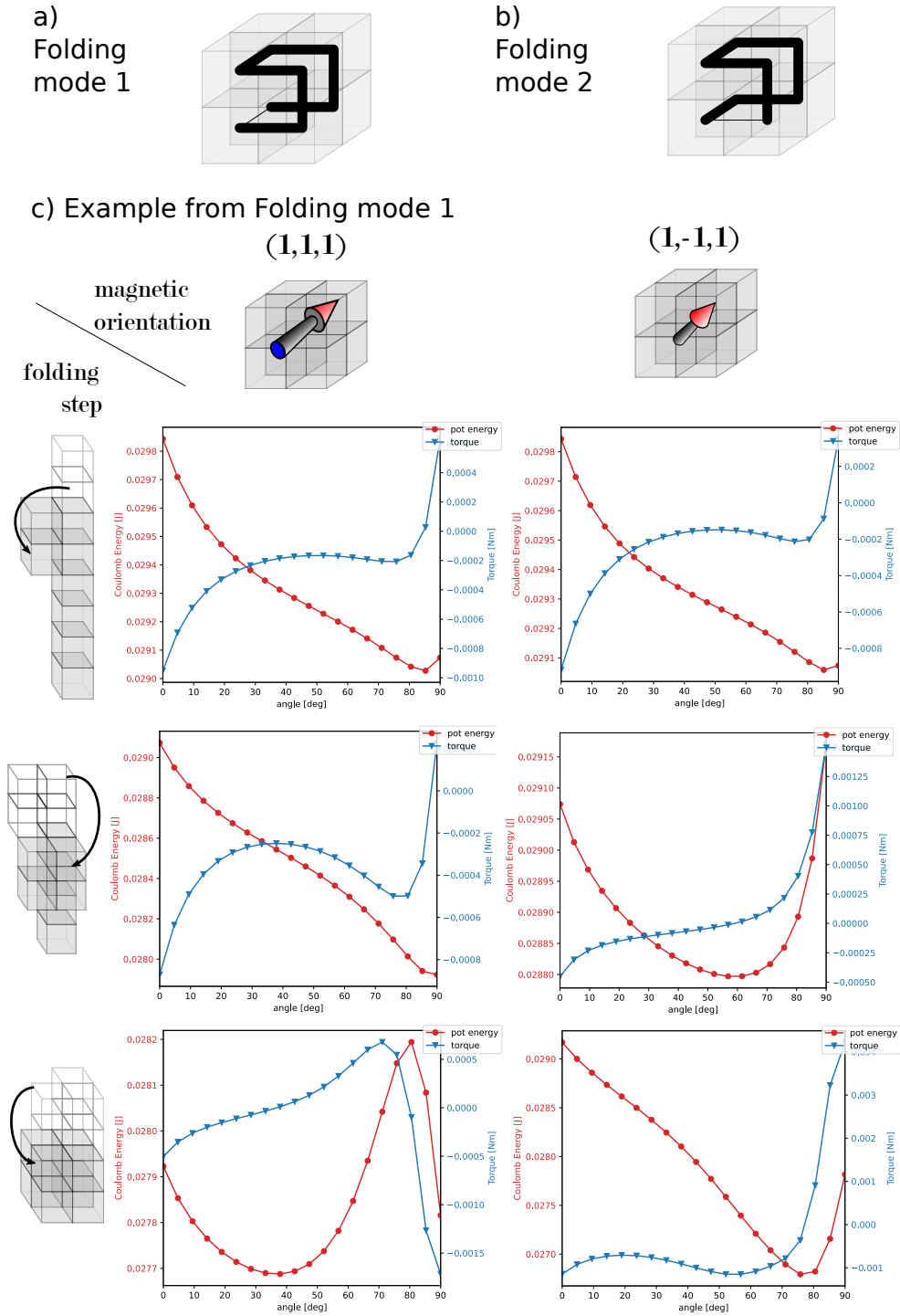


Figure 4.12: a) and b) Possible pattern to fold a cube where the black line tracks the center of connected components and c) shows an example for sequential folding and associated potential energy of folding mode 1.

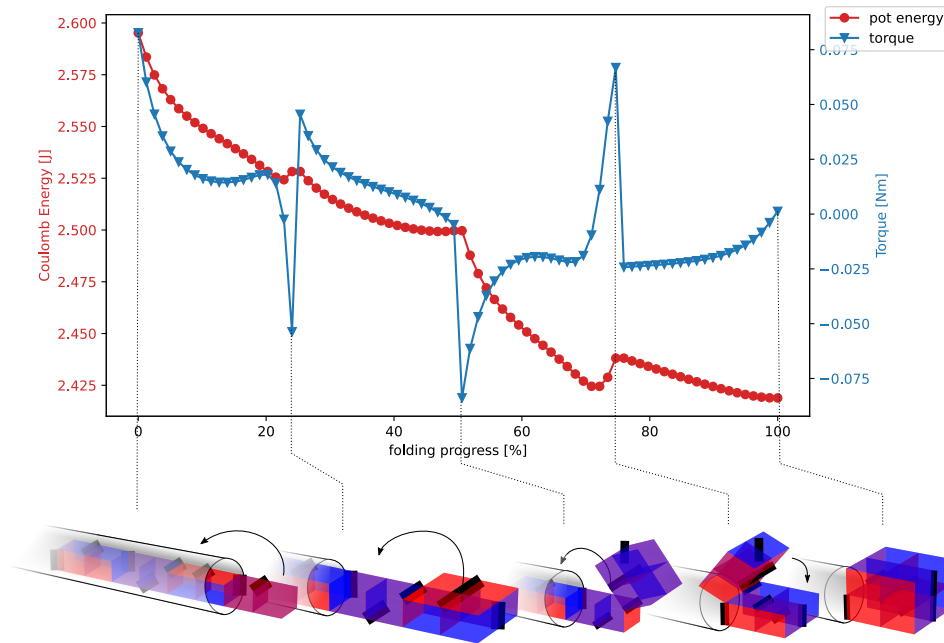


Figure 4.13: Potential energy of selected sequential cube secondary structure folding.

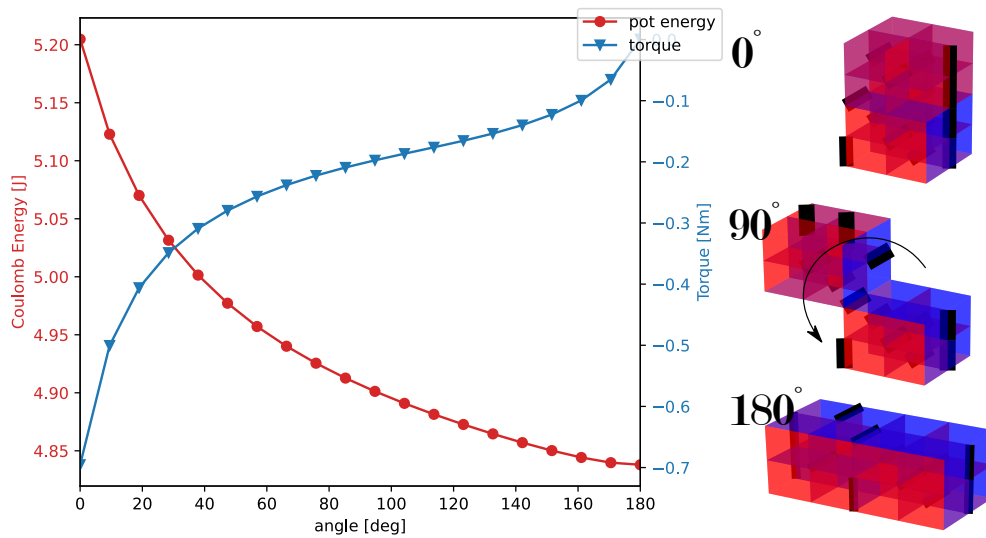


Figure 4.14: Potential energy of two cubic super-structures.

nents of a $2 \times 2 \times 2$ cube can be connected in a chain. The differentiation is where the chain starts and the orientation of magnetisation of the superstructure. If we consider the sequential folding, as with the tube feed deployment condition, the order of deployment also matters. This results in a total of 16 possible folding cases each with 3 to 4 degrees of freedom. The potential energy of all these different cases have been simulated and documented in Appendix A.2. It becomes apparent and is subsequently shown in benchtop experiments that not all of these cases successfully fold into a cube.

Figure 4.12 c) highlights the two distinct scenarios where one leads to a successful fold and the other does not. In the unsuccessful cases it can be observed how the last degree of freedom shows a minima of potential energy at a folding angle of approximately 35° . It is expected that any folding process will halt at this angle. Analysing the magnetic pattern, in relation to the folding pattern a possible conclusion can be drawn. The last parts of the $2 \times 2 \times 2$ cube superstructure folds into a north, with magnets on two sides of it. The energy minimum is potentially created when one of these sides is repelling the last part. However if the magnetic axis of the final shape is going through this last folding part, it can be observed that a full folding would occur. The successful case also features a local energy minimum in its second DOF. This means that half the cube would rest at that angle until the DOF has finished folding. Once that occurs, the case resembles two 2×2 sheets folding on top of each other to form to a cube superstructure. The full process can be seen in Figure 4.13.

Finally, multiple $2 \times 2 \times 2$ cubes can be used to form larger structures. Figure 4.14 shows two $2 \times 2 \times 2$ cubes folding analogous to two single cube components as described in Figure 4.4. Therefore a $2 \times 2 \times 2$ acts the same as a single component, leading to the formation of all listed secondary structures on a larger scale including a $4 \times 4 \times 4$ cube and larger.

4.2 Guidelines to Construct Self-Assembling Magnetic Chains

A self-folding magnetic chain is defined by its component shape and DOF of the joints linking the components. With this information, the chain components can be standardised as outlined in this work for cube components. Viable secondary structures can be investigated to significantly ease con-

struction of possible folding shapes. One of the most viable concepts due to its simplicity is the presented cube component with a one DOF rotational joint. Using this concept, a desired folding shape can be constructed from secondary structures. Folding behaviour can be analysed with the presented tools to estimate possible folding reliability. Specifically analysing the potential energy over single degrees of freedom during the fold allows to estimate the likelihood that folding will occur. The general rules of self-folding magnetic chains that have been defined are;

- A set of magnetic components are linked in a chain by joints. Fewer DOFs for each joint results in fewer possible folding states and thus more reliable folding;
- Each component contains one magnet to maximise magnetic material in the structure. The axis of magnetic orientation should be at a maximum angle to any contact surface with neighboring components;
- The shape of the components has to be space-filling to promote the previous guidelines;
- In the desired folding configuration all components should be magnetised in the same direction;
- Where multiple possible hinge positions can be placed, to increase the flexibility of the chain;

It needs to be considered that the chain is designed to be deployed through a device channel or catheter. A chain passing through a catheter or device channel requires a high degree of flexibility to adapt to possible curvature of the channel. Therefore, hinges should be placed in such a way that the chain is most flexible. Secondary structures have varying degrees of free hinges which do not fold, as they are in their most stable position during deployment. These hinges can be described as passive hinges and might be used to increase the flexibility of the chain by choosing alternating joint positions.

4.3 Summary

It was shown that the presented concept of magnetic self-assembling chains can be used to construct a string of magnetic components that fold into specific shapes. Simulation of a $2 \times 2 \times 2$ cube secondary structure folding has highlighted the challenge to construct a self-folding volumetric structure.

In the case of a volumetric structure, a specific sequence of folding might be necessary that heavily depends on the specific folding shape. For more complex structures it can be challenging to analyse all possible folding sequences that would lead to such a structure. However, it was demonstrated that a set of basic shapes can be defined analogous to the secondary structures of proteins. Using these secondary structures, larger structures can be constructed more easily if they can be constructed from these secondary structures. The defined secondary structures, holding special significance, have been analysed for their folding behaviour. While the steps structure is less reliable to fold and likely needs careful integration in a larger structure, it enables a homogeneous magnetic interface of the device. These secondary structures and possible application in magnetic devices for minimally-invasive surgery are further investigated in bench top experiments in the following chapter.

5 Proof of Concept

The focus of this thesis is the creation of a general concept of self-folding magnetic chains to be used in minimally-invasive surgery. As highlighted in the background Chapter 2, existing approaches to self-folding might not have been qualified for the strict requirements of the surgical setting. Therefore a range of prototypes have been constructed to prove the concept itself and show a possible application in a clinical setting. The secondary structures introduced in Section 4.1.4 have been implemented in benchtop experiments and their folding behaviour was validated. This chapter describes the development of these self-folding magnetic prototypes in Section 5.1. The secondary structures are documented in their respective applications to demonstrate a possible application in minimally-invasive surgery. The self-folding magnetic anchor is documented as an exemplar in Section 5.2 as it represents the application of cube, beam and sheet secondary structures. The stairs secondary structure is applied in a self-folding magnetic anastomosis device, detailed in Section 5.3. Finally, due to limitations in manufacturing, a modified prototype was developed for the explicit application in a pre-clinical study. As such, three significant proofs-of-concept were demonstrated and are described here:

- **The magnetic anchor** demonstrates the possible use of magnetic interaction between a folded magnetic device and an external magnet. To this end, the secondary structure of the cube is implemented to prove the concept of self-folding;
- **The magnetic anastomoses device** is a ring shaped configuration of the self-folding chain and demonstrates the adaptability of the presented concept;
- **The pre-clinical study** implements a modified folding anastomosis ring to prove the feasibility of deployment and application in minimally-invasive surgery;

5.1 Rapid Prototyping

As highlighted in Section 2.5, the production of a magnetic chain on a scale small enough to be deployed in minimally-invasive surgery limits possible concepts of self-assembly. This thesis therefore employed rapid prototyping to not only test the developed concepts but also to find constructive solutions to implement them on the target size scale. To function as self-folding devices, the prototypes were constructed to be a chain of magnetic components. Each component has a direction of magnetisation and is linked by a joint to its neighboring components. The self-folding process is driven by the magnetic interaction between the components. As initial simulations described in Section 4.1 have demonstrated, the maximum feasible chain length is limited by the relation between magnetic forces and chain weight and friction. In the clinical setting, the chain length might be further restricted by environmental factors, such as a lack of space to fold. To enable sufficient magnetic force between components for the self-assembly process, the amount of magnetic material per component is to be maximised.

Cubic $2\text{ mm} \times 2\text{ mm} \times 2\text{ mm}$ magnets made from an aluminum-nickel-cobalt alloy were linked in a chain. A one-DOF hinge between components was approximated by fixing two magnets with adhesive fabric tape as used in medical applications. The tape ensured a low bending resistance but reasonable resistance against twisting. An experimental setup to magnetise the cubes after assembly was constructed. This setup was designed to effectively program a folding shape into a chain of magnets. By magnetizing all magnetic cubes individually after assembly, the final folding shape was adaptable. This was possible as soft magnetic material was used that could be magnetised with relatively small equipment at low currents as opposed to hard magnetic material that require significantly stronger external field strength to magnetize. The full prototype is documented in Appendix A.1. The used soft magnetic material were custom magnets made from a Aluminum-Nickel-Cobalt alloy with an expected remanence of 1 T to 1.2 T [78] (AlNiCo 5 from *Eclipse Magnetics*,UK). The material was chosen to be magnetisable in a benchtop experiment.

These preliminary tests where unsuccessful but revealed two major causes of failure. Firstly, the *AlNiCo 5* magnets are anisotropic and exhibit a significant change in magnetic field strength depending on the direction of magnetisation. However no isotropic magnetic material could be identified that could have created sufficient magnetic force to realistically enable a folding

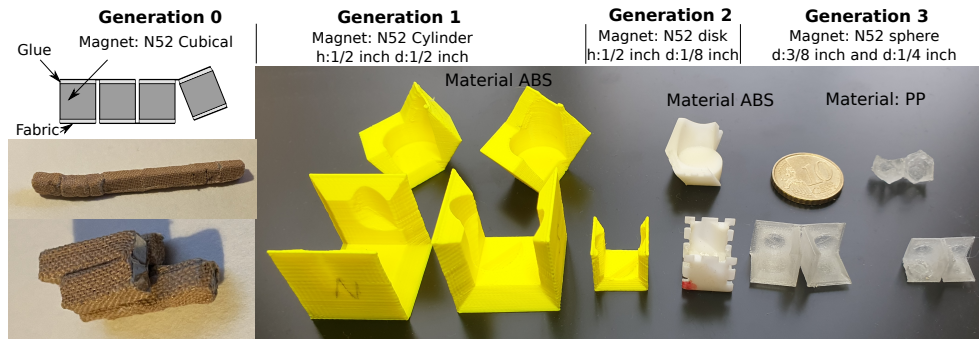


Figure 5.1: Generations of magnetic folding chain prototypes.

process. It followed that a dynamic programming of an assembled chain was unrealistic. Secondly, the medical tape emulating the rotational joints was too weak and was prone to fail. From these initial experiments additional demands on material properties was necessary. To highlight these demands, a selection of milestones in the prototyping process is presented here.

To improve material properties, successive prototypes were separated in the casing, hinges and magnet. The casing and joint are designed from non-magnetic material and are minimised in size to allow a maximum of magnetic material. These casings and joints were produced using additive manufacturing to allow for an investigation of a range of possible constructive solutions. The component then houses a single hard-magnet to ensure a maximum of magnetic potential. For all following investigations, neodymium magnets with grade 52 with a residual flux density between 1.45 T and 1.48 T [79] from (*K&J Magnetics*, USA) were used. Neodymium magnets were selected due to their common availability for permanent magnets and the strong magnetic potential in relation to magnet size. These magnets are fixed in their relative position to the casing. During prototyping, the unique magnet orientation can be chosen relative to the chain component casings. The sequence of the magnetic orientation within the chain enables the self-folding process. A timeline of prototype casings including the above mentioned initial experiments using soft magnets can be seen in Figure 5.1. All consecutive casings have been produced using additive manufacturing technology. Component shapes of cubical and rhombic dodecahedron have been investigated. In these cases, the casings were designed for cylindrical magnets of a diameter and height of 1/2 inch $\approx$ 12.7 mm.

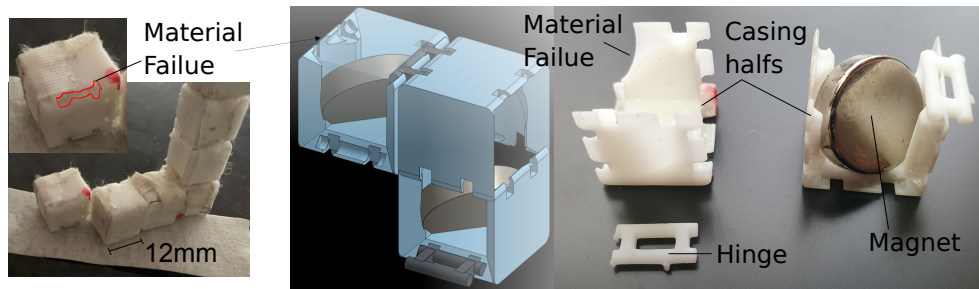


Figure 5.2: Mechanical hinge design, prototype and material failure on the left and construction concept on the right.

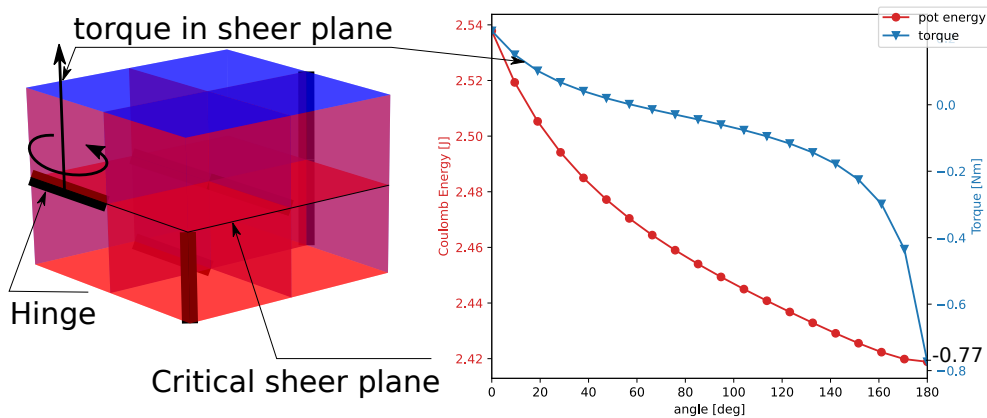


Figure 5.3: Cubical assembly critical shear plane torque.

5.1.1 Conventional Hinges

The first generation of components was designed to investigate casing concepts. Each component casing is divided in two identical half shells that could slide together. The shells were created using Fused Deposition Modeling (FDM) of Acrylonitrile Butadiene Styrene (ABS) and later high-quality Stereolithography (SLA), in an attempt to compensate for material failure.

Simulations documented in Section 4.1.3 have highlighted that the magnetic components experience severe torsion forces due to magnetic interaction and were prone to experience joint failure. Thus a prototype featuring conventional hinges was constructed to investigate folding, restricting any movement outside of a single axis of rotation. The magnets chosen were N52 disk magnets with a diameter of $1/2$ inch = 12.7 mm magnets to maximise magnetic surface and allow for easier simulation. The joints emulated a 1-DOF rotational joint as seen in Figure 5.2.

The housing casing consisted of two halves that could be slid together with the magnet inside. Two connected beams acted as a hinge between two components and could be clipped in between component halves, as seen in

Figure 5.3. The disk magnets were incorporated in the housing such as to provide the full component with an axis of magnetic orientation from corner to corner, following the construction guidelines given in Chapter 4.1. Experiments showed that a grid of this magnetic configuration leads to significant torque between the components. As a grid of cubic magnetic components has multiple shear planes, the hinges are the only structural element to absorb these torques. In consequence, the size of the hinges were maximised without decreasing magnet size. However, in the proposed sequence of folding as well as in a majority of possible folding patterns for a cube, the two halves of the cube are only connected by a single joint. During experiments, this joint was most likely to fail due to fatigue. Using the simulation, the torque around this critical joint was estimated to have a magnitude of 0.77 Nm as seen in Figure 5.3.

As seen in Figure 5.2, the conventional joints are prone to material failure. Most conventional joints rely on a hinge and consist of multiple parts. These parts have to be minimal in size to maximise magnetic material. As such, a trade-off between reducing magnetic material and increasing size and robustness of conventional hinges exists. Considering significant risk of material failure at the centimeter scale, a downsizing of conventional hinges to the millimeter scale to be used in minimally-invasive surgery seems unrealistic.

5.1.2 Living Hinges

Living hinges are made from a single body and rely on local flexibility of the geometry and material. As such, they are easier to reduce in size compared to conventional hinges. However as highlighted in preliminary experiments, the hinges are required to compensate for a significant torque that acts between components. The designed casings, as seen in Figure 5.4, are possible to produce at target scale. Each part is produced by FDM using polypropylene (PP) as material with a 0.1 mm nozzle. PP has the highest maximum elongation of 200% among the available materials for the *Ultimaker* and was therefore best suited for the creation of living hinges. *Ultimaker* PP has a maximum elongation of 200% at break with a 27.1 kJ/m² [80]. Due to these material properties of PP, the thin bridge between component halves acts as a living hinge, approximating a 1-DOF rotational joint.

Thickness of the hinge and the gap between components has been investigated in experiment in the range of 0.1 mm to 0.5 mm. To further maximise magnetic material volume, the casings are designed to house ball magnets.

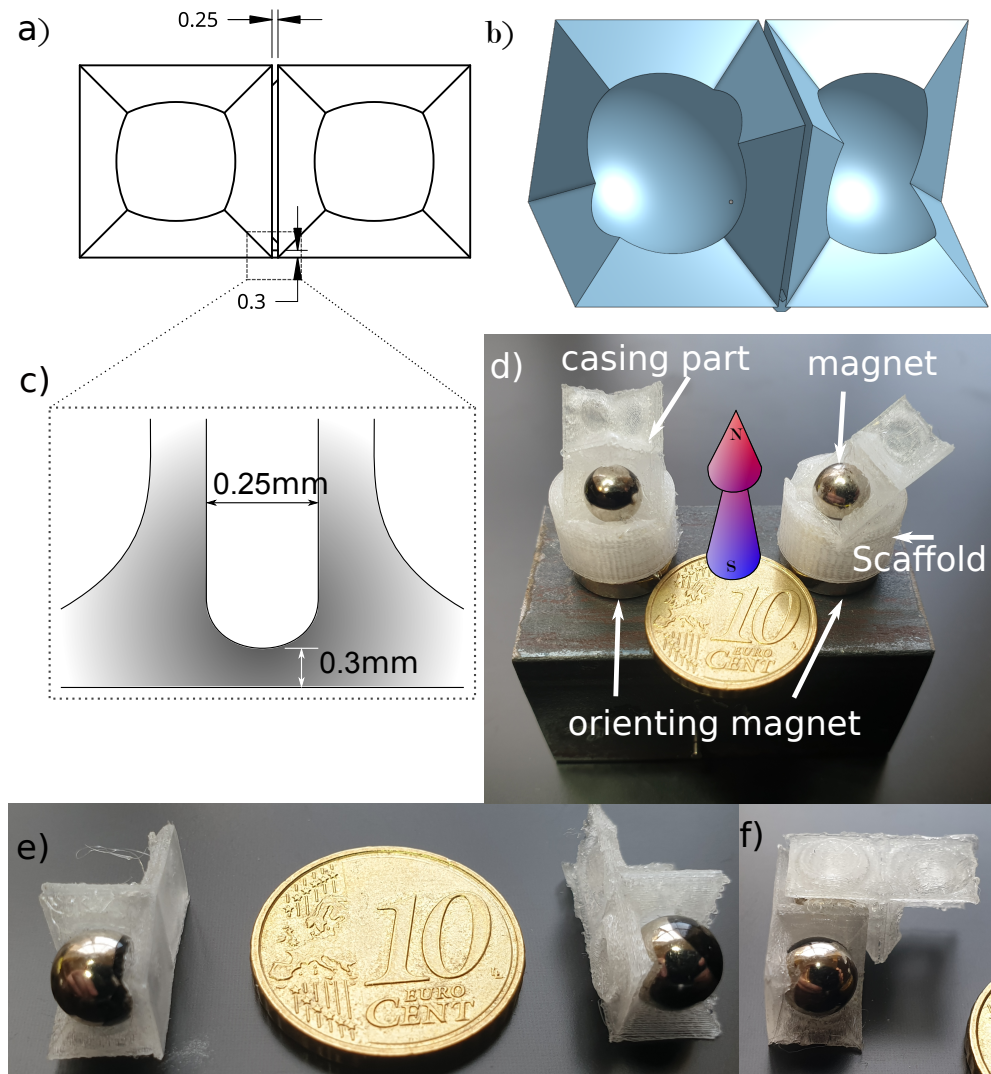


Figure 5.4: Living hinge cube components with a) and b) CAD construction, c) living hinge cross-section, d) manufacturing method, e) and f) benchtop prototype.

Both magnets and casing parts are assembled using cyanoacrylate adhesive. As there is no geometric restriction ensuring the correct orientation of each spherical magnet, correct placement of the magnets is critical. A setup seen in Figure 5.4 was used to correctly orient the magnets. The component part and ball magnet are placed in a scaffold on top of a disk magnet and the ball magnet is fixed using cyanoacrylate adhesive. The disk magnet forces the ball magnet into the correct direction. Each component part is fitted with one magnet. Then the component parts are assembled using adhesive.

5.1.3 Limitations

As shown in Figure 5.1, the size of prototypes has been continuously decreased during the stages of prototyping. However available production methods put a limit on possible miniaturisation of the device. While a living hinge can potentially be produced at very small scales [81], manufacturing by hand has its limits on the possible size a device can be. The available additive manufacturing, using the *Ultimaker 3* (Ultimaker, NE), was optimised to produce at small dimensions. The material used for the living hinges is Polypropylene (PP) *PP* with a 0.1 mm nozzle. A considerable amount of time has been invested to find an optimal printing setup for this combination of material and nozzle. However, while the small nozzle allows the printing of features down to 0.1 mm, a "stringing" of the material could not be fully prevented. Stringing refers to strings of material that are cast during the printing process due to oozing of the nozzle. The strings are removed manually but could limit minimum printing size of some features as it can lead to unwanted connection between parts. Some production artifacts in the form of stringy extrusions from the printed body were not possible to fully remove.

The primary limitation however is the placement and adhering of the magnets. Figure 5.4 shows the manufacturing process where the component halves are placed into scaffolds. External magnets ensure a correct orientation of the ball magnets within the component. One ball magnet is then glued into the component part. This fixes the magnetic orientation of the component. Multiple component parts with magnets can then be assembled via gluing. This process poses some limitations. Firstly, the orientation of the magnet is only ensured via the external magnet during the gluing process. A precise magnetic orientation is difficult to achieve. Secondly, assembly by hand naturally limits down-scaling of the device size and assembly precision. A semi- or fully-automated assembly line could greatly improve both limita-

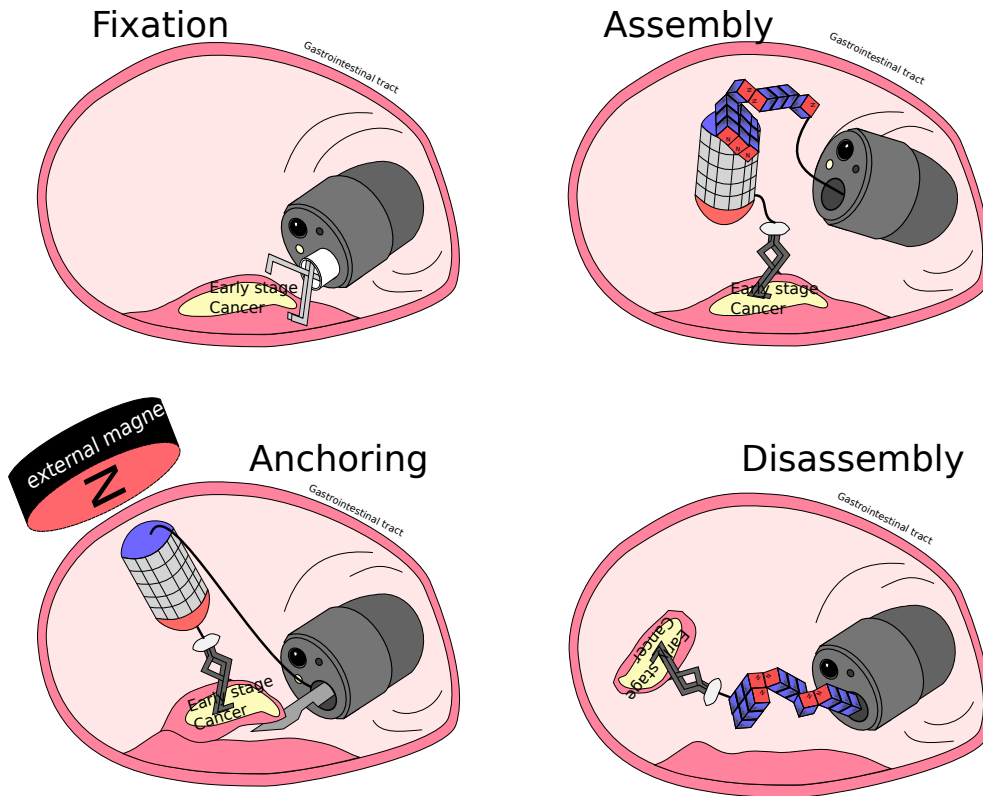


Figure 5.5: Storyboard of a self-folding magnetic anchor used in the example procedure of the removal of gastrointestinal cancer.

tions and allow for the production of prototypes at millimeter scale. While automated manufacturing certainly can achieve the required component size, it was not realistic in the scope of this research, as custom production lines would have been necessary to assemble casing parts and magnets, using adhesive.

5.2 Magnetic Anchors

As one of the target implementations of a self folding magnetic device, the magnetic anchor is designed to lift tissue. Magnetically lifting tissue may enable procedures in inaccessible areas or can be used to remove tissue altogether. Figure 5.5 shows an example application for the removal of gastric cancer. The primary advantage here is that the anchor could be deployed via the device channel of a colonoscope and fold into a shape larger than the device channel to exert meaningful magnetic force in conjunction with an external magnet.

Multiple chains have been constructed and tested to fulfill this purpose.

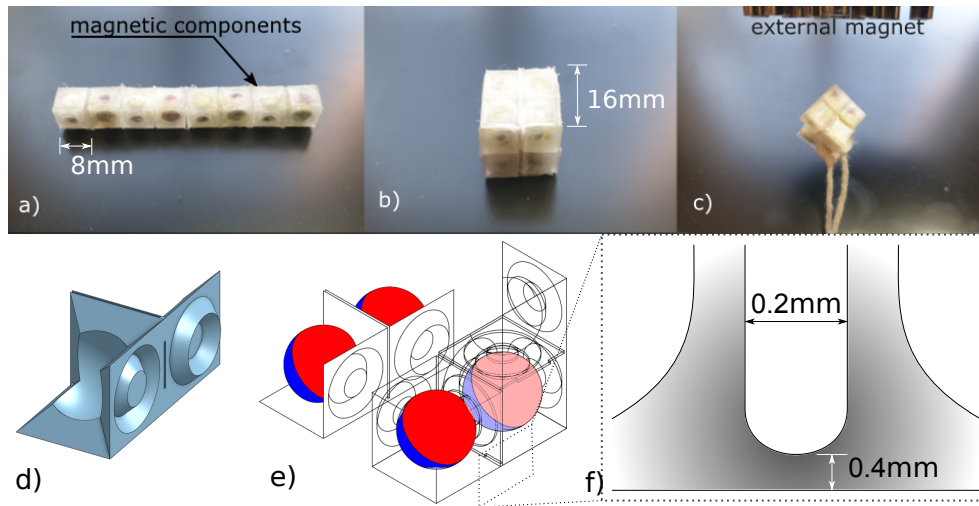


Figure 5.6: Benchtop prototype of a folding magnetic anchor with a) initial configuration, b) folded configuration c) interaction with external magnet, d) component half schematics, e) cubic components concept and f) cross-section of living hinge.

The $2 \times 2 \times 2$ cube proposed in Chapter 4.1.3 represents the most compact shape a self-folding magnetic chain composed of cubical components might take. A cube structure is composed of beam and sheet secondary structures. Therefore, the $2 \times 2 \times 2$ cube superstructure is a proof of concept for the beam, sheet and cube secondary structures, proposed in Section 4.1.1. A cube with the sequence $B7 - B3 - B8 - C5 - A7 - B7 - C1 - Z5$ and magnetic orientation in $(1, -1, 1)$ direction has been used as it was simulated to fold reliably in Figure 4.13. The main dimension of the cube can be seen in Figure 5.6. To address the issue of torsion forces and shear planes, the components have been constructed with a ring relief on the surface, as seen in Figure 5.6. This relief fits into a matching notch on the counterpart and thus breaks the common shear plane and compensates for the torques within the system.

Furthermore the cube was used as a first proof of concept for a self-folding magnetic anchor. The anchor described in Chapter 2.1.2 can be used to lift tissue. For this purpose, it is required to generate sufficient magnetic force in interaction with an external magnet to lift itself and an attached load. Experiments shown in Figure 5.6 c) show that the device is capable of lifting itself. The overall lifting strength is dependent on the external magnet. Disassembly as suggested in the storyboard of Figure 5.5 has been a secondary interest. The cube withstood the forces during experiments when used as a magnetic anchor but disassembled during experiment when sub-

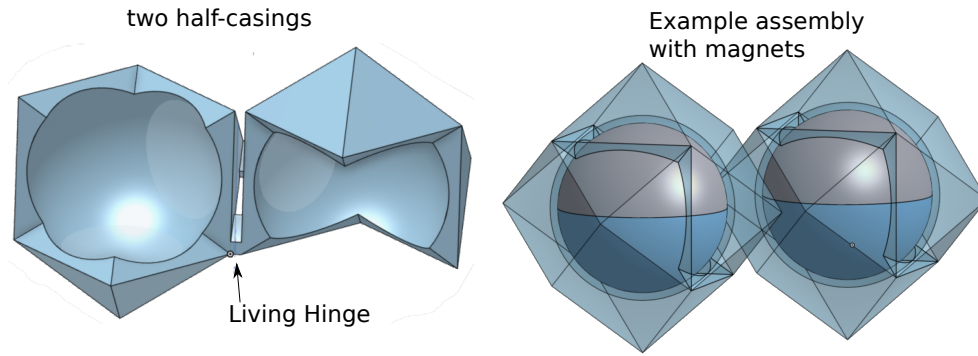


Figure 5.7: Concept of a dodecahedron component with left: half-components and right: example assembly with magnets.

jected to significant force. This might allow for retraction of the device from the body by forcing it back into the deployment port. However the practicality of disassembly when using an endoscope for deployment as suggested could not be tested because the device could not be produced at a scale to fit through a colonoscope's device channel, due to manufacturing limitations described in Section 5.1.3.

During experiment, it could be observed that some sequences would not fully form a cube. Not all of these cases could be attributed to material failure or manufacturing issues. Upon investigating the specific chain sequence, it was found that the last fold of a $2 \times 2 \times 2$ cube could only form if it is in line with the magnetic axis, as predicted in Section 4.1.4.

The production of a prototype in a scale capable of passing through a 3 mm device channel was not achieved due to above mentioned production limitations. However, while the presented prototype is four times this target scale, it demonstrates the ability to form spontaneously into a volumetric structure where all magnets are oriented in the same direction. The projected coupling force of the assembled structures gives reason to believe that the application as a magnetic anchor is feasible.

5.2.1 Other Component Shapes

Alongside the cubical component shape, the rhombic dodecahedron has been considered for the shape of the casing. The basic shape was produced in two half parts and then assembled with a spherical magnets in the center as seen in Figure 5.7. Folding was achieved in small chains with these components. However, volumetric shapes have been difficult to produce due to one of the

faces being parallel to the magnetic axis of the components. Any interaction of components therefore as theoretically analysed in Section 4.1.1, repelled each other. While this validates the underlying theory, it shows that the rhombic dodecahedron is inferior in folding behaviour to the cube. However for planar folding applications it shows that shapes other than the cube can be used to achieve magnetic self-assembly.

5.3 Self Reconfiguring Anastomosis Ring

The concept for self assembling chains described in Section 4.1 was applied to a ring-like structure, to be used as an anastomoses device during surgery. This section details how the developed guidelines can be used to create such a device. A prototype is presented and analysed at the various stages of development. This proof-of-concept demonstrates many of the secondary structures and how they can be applied to overcome design challenges. The challenge that is of concern here is that magnetic anastomoses rings require a magnetic interaction between two rings. The specific workings of magnetic anastomoses devices are detailed in Section 2.1.2.

5.3.1 Premise

One example application of self-folding chains that is of interest to this work is the use of magnetic compression to form a jejunojejunostomy. Here, the magnets are placed in two parts of the small intestine and over time will form an anastomosis between them as seen in Figure 5.8. The magnetic attraction between them causes compression and ultimately necrosis of the tissue in between. Once the anastomosis has formed, the device might be excreted via natural means. To allow for a safe excretion it is crucial that the device is connected in a chain so as to not lose components inside a patients body. For this purpose, the final folded structure needs to fulfill the requirements;

- **I** The folded shape is a ring to create a clean anastomosis;
- **II** The device needs to have a common direction of magnetisation to enable a strong magnetic force to another device;
- **III** The magnetic orientation is along the rings geometrical axis;
- **IV** The device is required to fold reliably;
- **V** The device is deployed through a flexible tube.

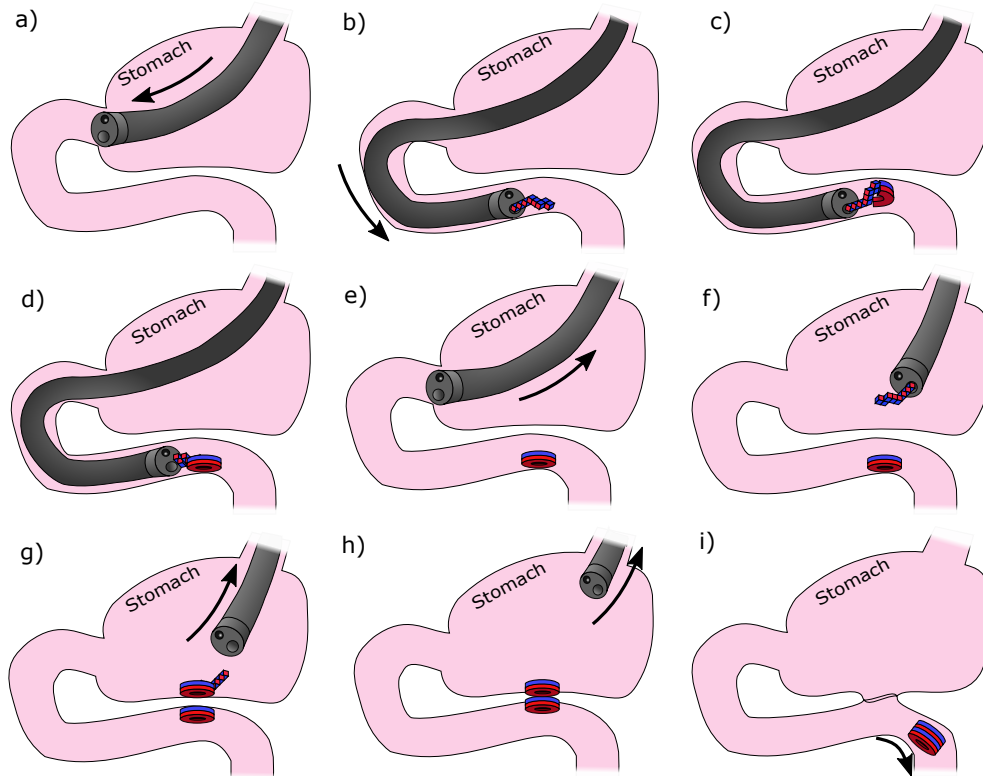


Figure 5.8: Storyboard of jejunojejunostomy using a self-folding device.

A ring shape might only be approximated when using cubical component shapes. However this example shows how the basic shape might be modified to apply to structures that can not be formed from cubes.

5.3.2 Simulated Folding Behaviour

Folding of the device was analysed using the simulations described in Section 3.2. As the required shape can not be acquired from primitive component shapes, the cubical component shape is modified to apply to this scenario.

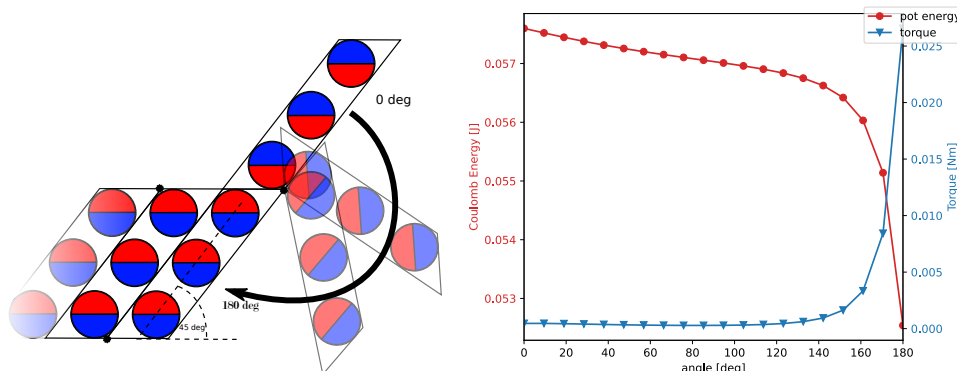


Figure 5.9: Self-folding magnetic ring folding analysis, with (left) folding principle and (right) potential energy and torque in the system.

Each component is considered to house one spherical magnet of diameter 6 mm. Planar folding patterns described in Section 4.1 can be applied to a warped plane. Magnetic anastomoses rings are designed to meet surface-to-surface to exert homogeneous pressure on the tissue between the rings and cause necrosis of the tissue. However, the developed concept of self assembly requires that the magnets are magnetised from edge to edge or corner to corner and therefore do not have a flat contact surface to couple with other magnets and exert homogeneous pressure. This can be solved by using a modified version of the stairs secondary structure, described in Section 4.1. To achieve a continuous stair structure that would wrap around the curved plane, a repeating sequence of $B2 - C3 - D6^*$, introduced in Section 4.1, with a modified casing of $D6$ components was used, noted as $D6^*$. The curvature and diameter of the superstructure ring then depends on the extent that the casing diverges from a cubical component. As the folding is technically planar, the device only shows one pattern of folding, i.e., when the beam secondary structures fold from a string to a sheet. The potential energy and torques associated with this folding can be seen in Figure 5.9. The simulation results support the observed folding behaviour with a strong tendency to assemble in a stairs structure. The modified component $D6$ allows for a single active hinge enabling the folding between two beams into a stairs structure.

5.3.3 Benchtop Self-Assembling Anastomoses Ring

The prototype was manufactured using the methods described in this chapter. Figure 5.10 shows construction details as well as the main dimensions of the prototype. The first prototype was prone to folding error and was too unstable to be realistically used as a magnetic anastomosis device. The cause of this instability was the size of the superstructure. Due to the amount of overall degrees of freedom, the chain was prone to magnetically connect between parts of the structure where it was not intended to. The exact folding was the result of environmental factors, such as gravity and manufacturing errors. As a result, the final folding shape was impossible to predict. The chain is separated into active and passive DOFs. The active are the DOFs that enable the folding between an elongated chain ready to feed through a tube and the desired folding structure of a tool. The passive DOFs provide the flexibility of the chain to allow for the chain to pass through a deployment channel. However it becomes evident that the presented prototype has far more passive DOFs than active. In conclusion, the final folded shape is

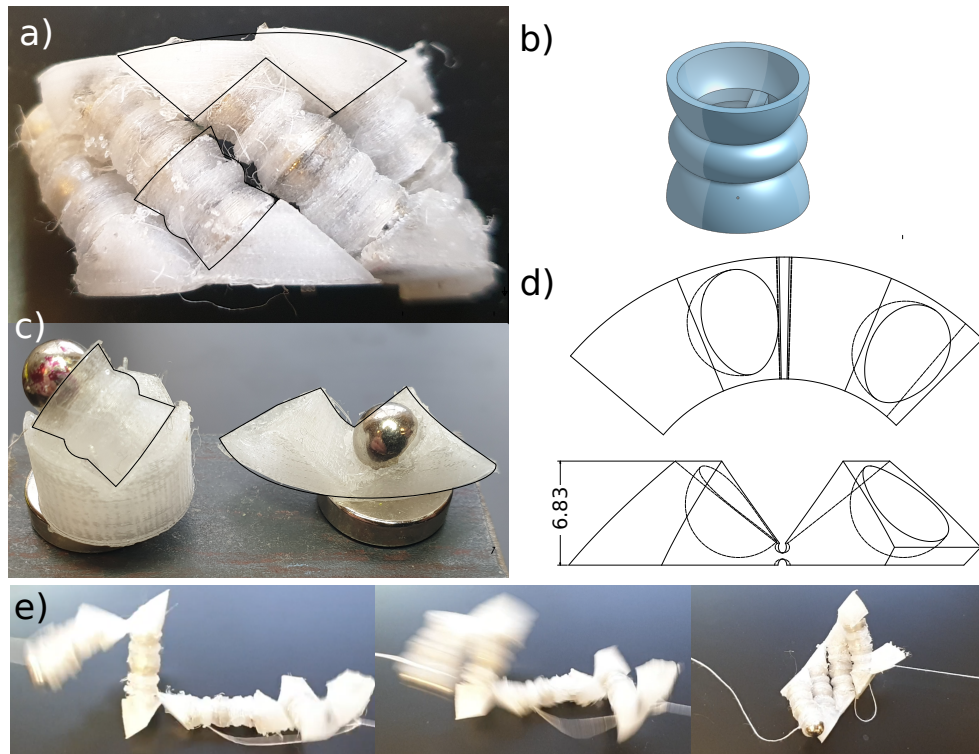


Figure 5.10: Self-folding benchtop, with a) prototype, b) U-joint, c) components, d) corner components and e) folding footage.

primarily defined by hinges that are not supposed to move. However these hinges are prone to significantly change the shape of the device and cause unintended magnetic coupling.

The solution is the introduction of another kind of hinge. While initially only one DOF hinges were considered, the requirements for the passive hinges are significantly different. Hinges used to increase chain flexibility are only required to support a significantly smaller folding angle than hinges used for chain folding. As such, a universal joint (u-joint) classified as a 2 DOF hinge has been designed that permits a limited degree of movement. In this passive hinge, the PP acts as a spring mechanism between components, providing the flexibility for the chain to move through a catheter but does not allow a significant folding angle between components. The hinge was produced using additive manufacturing and can be seen in Figure 5.10. This prototype has less components compared to the previous version to allow for more reliable folding. The prototype is able to spontaneously self-assemble. However, the manual assembly of this prototype is more challenging compared to previous prototypes due to the irregular shape of the components. These components are more complex and have finer features compared to

the cubical components. The quality of additive manufacturing is reduced as a result, as seen with extensive string-like extrusions on the prototype.

Furthermore, experiments showed that the exact magnetic orientation of the sphere in the grid is required to enable the folding process. Extensive trial and error was necessary under the given production methods and the available resources, to produce a half-ring. A full ring was not produced as the primary objective was achieved by analysing the folding process in a benchtop environment. The produced prototype showed the limits of the available production methods and could therefore not be produced in a sufficiently small size to be applied in minimally-invasive surgery. However the prototype was able to show that the spontaneous self assembly of a ring-like structure is possible using the presented concept. Continuing the research and improving the production method promises to lead to a fully self-assembling anastomosis device that can be deployed in minimally-invasive surgery.

5.4 Supported Reconfiguring Anastomosis Ring

Considering the challenges in methods to produce a self-folding chain to be used as a device in minimally-invasive surgery, a supported folding chain was constructed to prove the general feasibility of folding surgery tools. One example application of interest to this work is the use of magnetic compression to form a jejunojejunostomy [20]. Here the magnets are placed in two parts of the small intestine and will form an anastomosis between them. Another possible application is in the treatment of biliary strictures after liver transplant. The use of magnets to treat benign biliary strictures (BBS) was investigated by Yu Li et al. [82]. The use of a folding device could further improve the procedure, as seen in Figure 5.14.

Living hinges, as a subcategory of compliant mechanisms, present a scalable solution to approximate the mechanical behaviour of different hinge types. Living hinges are composed of a singular body and exhibit significant resistance in all movement other than the desired movement due to their partial flexibility [83]. Due to this partial flexibility, it is a challenge to construct the living hinge such that it compensates for the internal and external forces but allows a smooth movement in the desired direction. The self-folding ring design presented in Section 5.3, is a promising candidate for application in minimally-invasive surgery. However, available production methods did

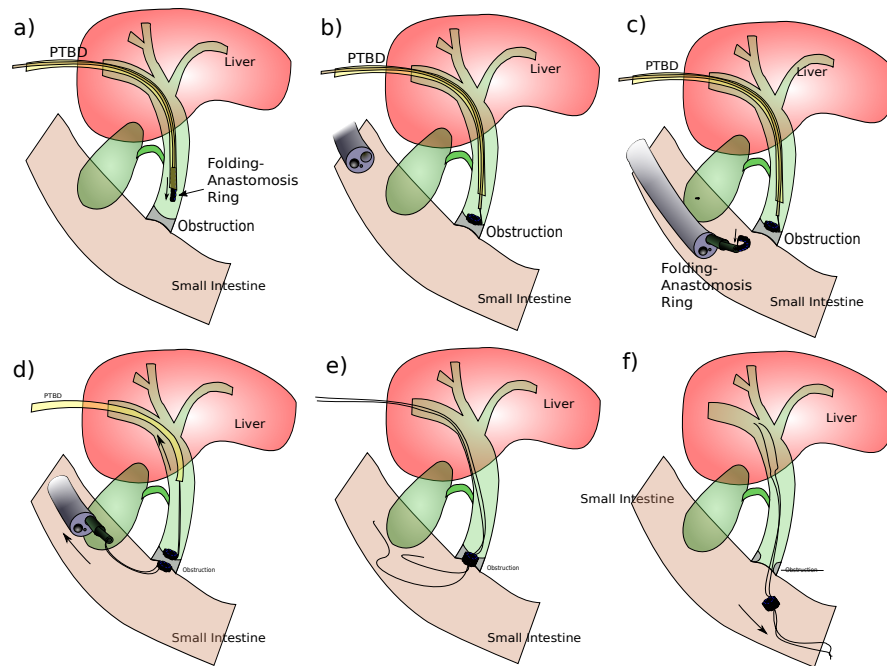


Figure 5.11: Folding magnetic anastomosis device for BBS where a) the liver magnet is deployed via a previously placed percutaneous transhepatic biliary drainage (PTBD) catheter; b) to d) a second device is deployed on the intestine side of the blockage via an endoscope; e) and f) the anastomosis forms and the device can be endoscopically retrieved through the stomach.

not allow for a prototype production on a scale useful for minimally-invasive surgery. To show that a folding device can be used in minimally-invasive surgery, a supported folding ring was developed. A modified version of the core hinge has been used in this work to construct a robust rolling hinge with minimal size. The following sections describes the proposed design of the magnetic folding ring and details the use and deployment procedure of the device in the pre-clinical porcine model. The presented prototype has been developed in an iterative design process relying on end-user feedback. Significant variations of the presented prototype have been explored.

5.4.1 Device Design

In this work, a number of cylindrical magnets are connected by a string or suture woven around them as seen in Figure 5.12. This weaving effectively replicates the core living hinge and allows for the components to roll on each other in a shared plane, while preventing any bending of the chain outside this plane. The direction of magnetisation of the magnets in the chain is in the plane of the chain to ensure maximum magnetic interaction with other devices.

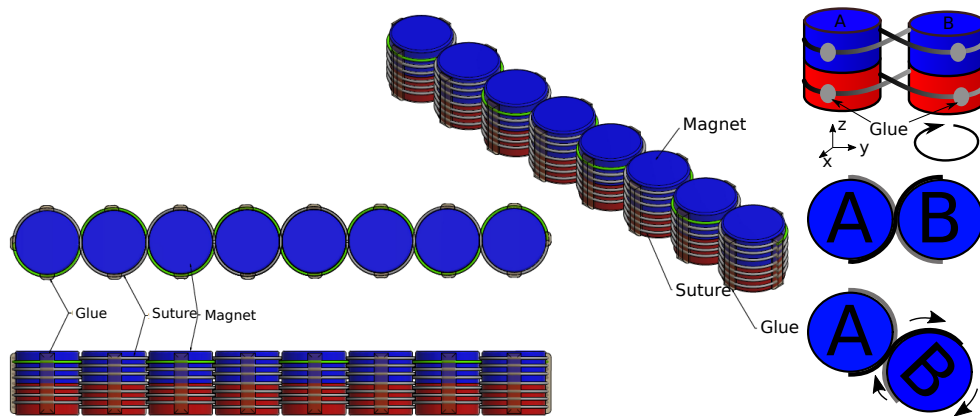


Figure 5.12: Supported magnetic folding device, right: schematics, left: principle of rolling joint.

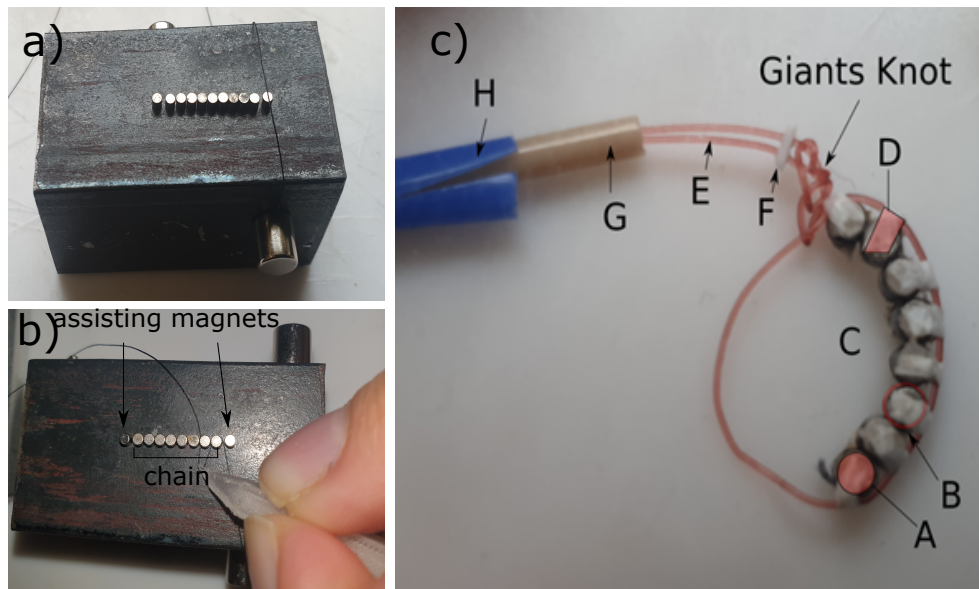


Figure 5.13: Folding magnetic anastomosis device. a) device materials and components. b) and c) winding of suture. d) prototype of a folding magnetic anastomosis device.

Table 5.1: Key design features of the folding magnetic anastomosis device with, relative measurements and measurements of presented prototype iteration.

A	Magnet	Height and diameter $a = 1/16 \text{ inch} = 1.5875 \text{ mm}$
B	Suture	Diameter $b = 0.05 \text{ mm}$
C	Magnetic folding anastomosis device	Length $c = n \cdot a + b(n + 1) \approx 13.2 \text{ mm}$
D	Support sheet, holds the guiding wire in place	Minimal thickness and broadness $< a$
E	Guiding wire, folds the device	Diameter $e = 0.6 \text{ mm}$
F	Spacer, allows for a reliable folding	Thin Disk with diameter $< a$ and two holes with diameter b
G	Pusher, deploys devices out of mantle	Inner diameter $gi \geq 2 \cdot e$ outer $go < hi$; length $gl = hl + c \approx 500 \text{ mm}$
H	Mantle, protects device and tissue	Inner diameter $hi \geq \sqrt{2} \cdot a$ outer ho ; length $hl \approx 1485 \text{ mm}$

Key design features of the device are listed in Table 5.1. The specific configuration of the displayed device features eight magnets that are arranged in a chain. Between these magnets a silk suture is woven around the magnets as seen in Figure 5.13. The silk suture has no significant resistance to bending but a high resistance against elongation. The same suture is woven back and forth between the magnets. The tension of the suture is crucial for successful assembly and was applied manually based on qualitative trial and error. As the suture is crossing itself in an alternating pattern, it prevents any movement but enables rolling of the cylindrical magnets. All magnets are oriented in the same direction as seen in Figure 5.13 (i.e., magnetic north of each magnet is on the same side of the device). As such the magnets repel their direct neighbours and the magnets must be manually forced into this position during the manufacturing process. To keep the magnets in this position, additional external magnets were introduced in proximity to the magnetic chain to counteract the repulsion between the magnets. The forces acting between neighbouring magnets introduce torsion along the chain. However, a total of 8 to 10 layers of suture has proven to be sufficient to allow for the rolling behaviour of the chain and compensate for internal torques and forces to prevent any twisting of the chain. The suture is spot-glued to the flanks of the magnets as seen in Figure 5.12, to prevent displacement of the sutures during use.

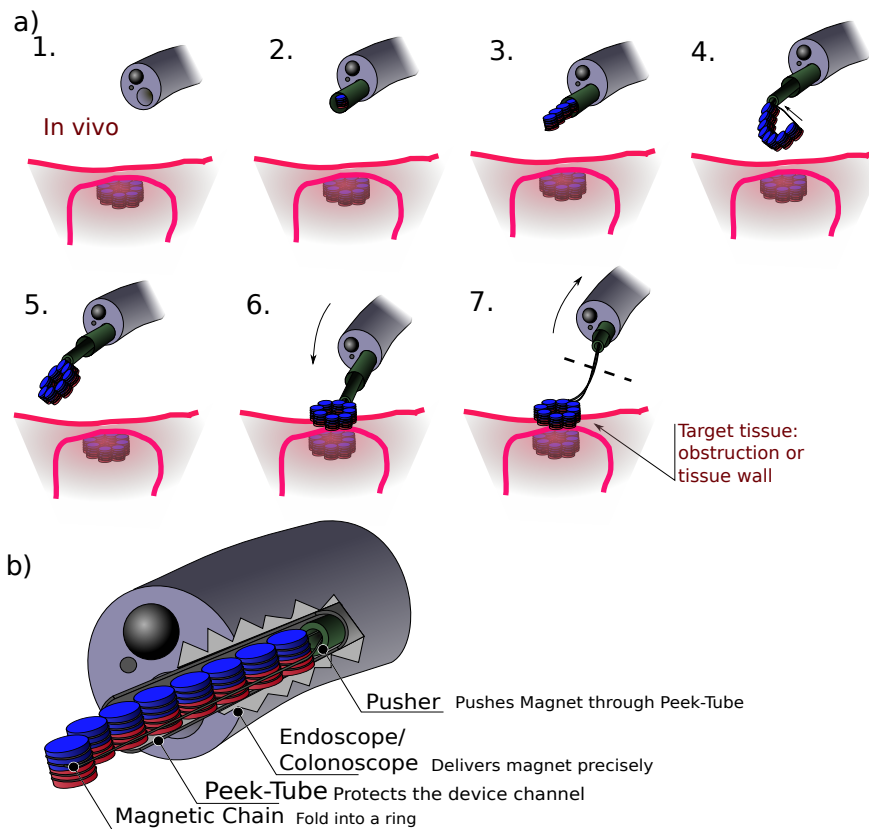


Figure 5.14: Folding magnetic anatomises device story board, with a) general deployment method and b) Device deployment breakout view.

A thin support sheet is glued to the top and bottom of each magnet and acts as a sheet for a guidewire to run through. This guidewire guides the chain of magnets into a ring-like structure by forming a lasso around the magnetic array. This lasso is closed by a giants-knot [84]. The giants-knot forms the nylon wire into a loop in which the device is placed on one side of the knot. The two ends of the nylon wire exit on the other side of the knot. If one end of the wire is pulled relative to the knot, the loop will shrink and force the magnetic device into a ring structure. Once the device is in its ring configuration, the other end of the nylon wire might be pulled. This causes a fastening of the giants-knot and significantly increases the internal friction inside the knot, efficiently locking the loop from opening up again. To support the delivery and deployment, a support structure consisting of a spacer, a handle, two extruded tubing, a pusher and a mantle was constructed as seen in Figure 5.13.

5.4.2 Device Operation

The device is deployed as seen in Figure 5.14 via an instrument port that might be long and flexible, such as an endoscope, colonoscope or catheter. All control over the device is exerted via the handle which operates the pusher, mantle, and nylon strings. The steps to deploy and ready the device are detailed in Appendix A.3 and are summarised in Figure 5.15;

- (I) The mantle containing the device is inserted into the device channel or port;
- (II) The mantle reaches through the device channel and exits at the target area;
- (III) Once the device exits the device channel the device can be readied by pushing the pusher into the mantle by a distance $c+5\% \approx 13.5\text{ mm}$;
- (IIV) Wire end is pulled by a distance c to close the device;
- (IV) Wire end is pulled by approximately $5\%gl \approx 2.5\text{ mm}$ to lock the device. The device can be precisely placed aided by fluoroscopic guidance, X-ray or camera;
- (V) The Pusher G is carefully removed while feeding the wire ends into the pusher;
- (VI) The wire ends are cut to length as required;
- (VII) Mantle H and endoscope or port might be removed.

The dimensions represent the prototype iteration as well as in reference to the variables defined in Table 5.1.

The device is deployed by moving the pusher relative to the mantle. It maybe closed and locked by pulling the respective wire. Finally the pusher and mantle may be removed in sequence.

As outlined in Section 2.1.1, an ergonomic and easy-to-use handle enables surgeons to use the device in the medical setting. An external company was hired to design an ergonomic handle for this work. Unfortunately the resulting product was substandard, both in its practical handling and mechanical functionality. The full report on the handle design can be found in Appendix A.4. A minimal implementation of a handle therefore has been developed as seen in Figure 5.16. This handle allows for a convenient operation of mantle and pusher in steps III, VI and VIII. Furthermore it forces the correct operation sequence between steps III and VI. While the presented

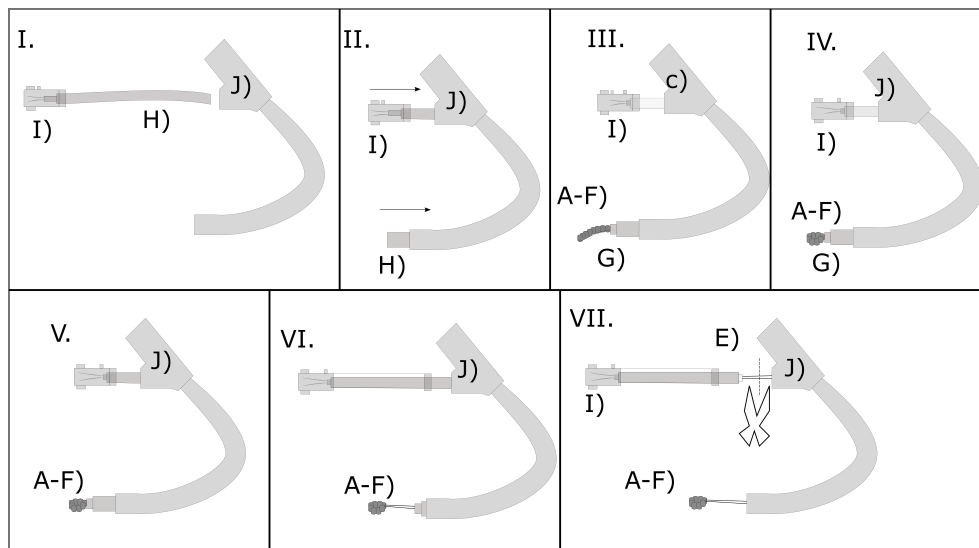


Figure 5.15: Step by step depiction of the deployment process.

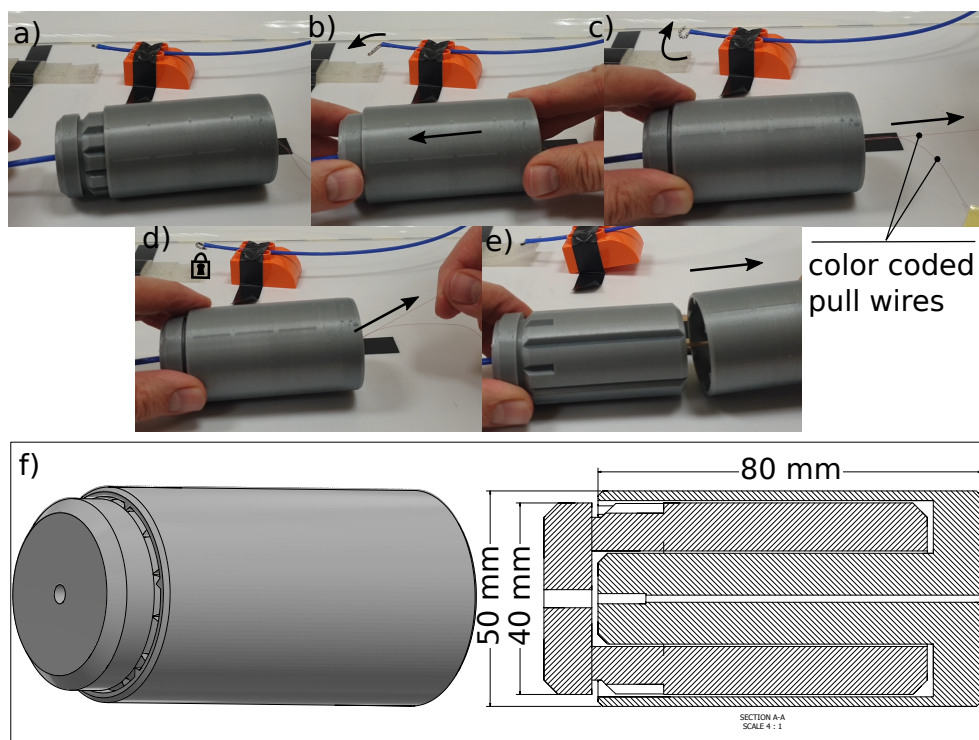


Figure 5.16: Deployment steps of the folding magnetic anastomosis device, with a) initial state, b) deployment of prototype, c) closing the ring, d) locking the ring, e) removal of pusher and f) schematics.

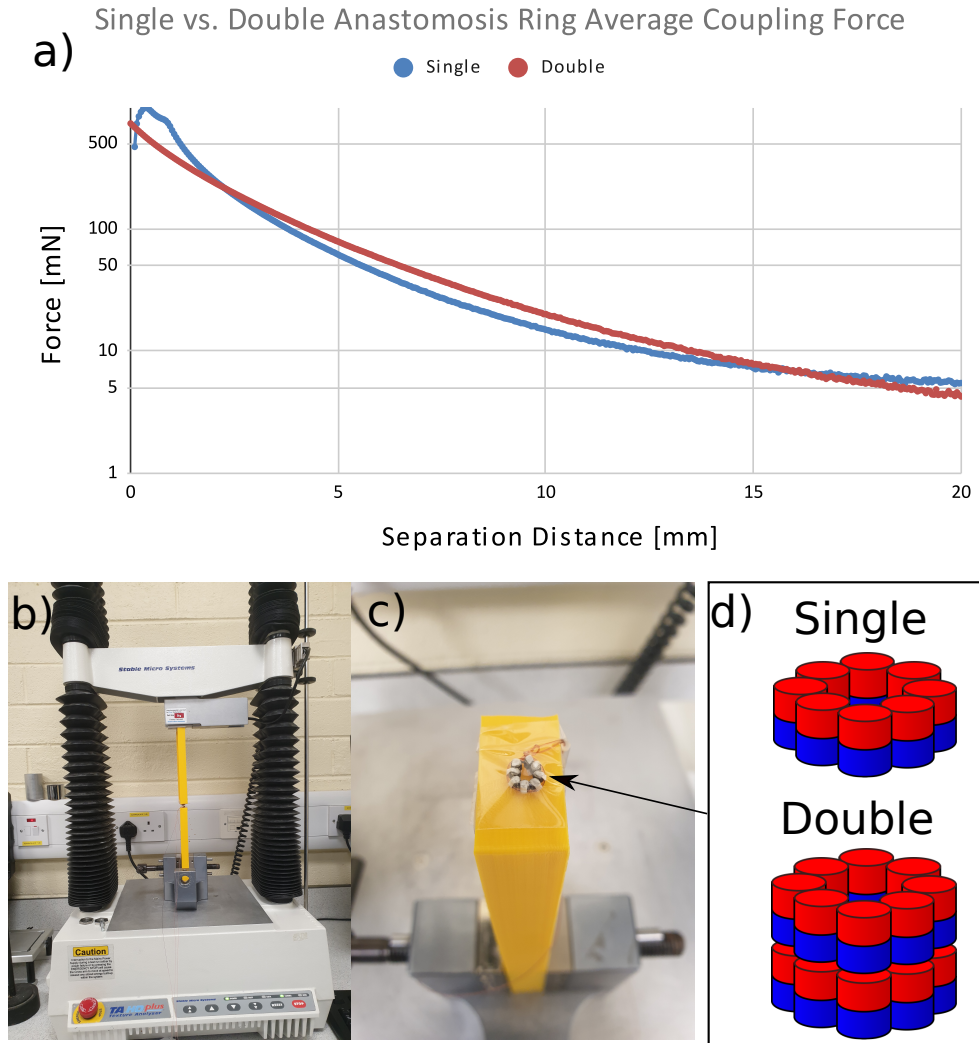


Figure 5.17: Pull test results with single magnetic devices and stacked (i.e. double) magnetic devices, with a) force measurement. b) experimental setup, c) closeup of magnetic device and d) schematics of magnetic device.

handle needs to be improved in ergonomics and form factor, it allows for the operation of the device by instructed surgeons.

5.4.3 Pull Force Estimation

In this work, the folded structure is larger than the port used to deploy it, although each individual magnet is still limited by the port size. Consequently, the coupling force per unit area is limited. Stacking multiple magnets, as seen in Figure 5.17, could potentially increase the coupling force. The coupling force of two coupled magnetic devices as well as the coupling force of four coupled devices where two were stacked on each side was investigated. The associated pull force was investigated with a pull test, where the magnetic devices were positioned in proximity and then pulled apart while the

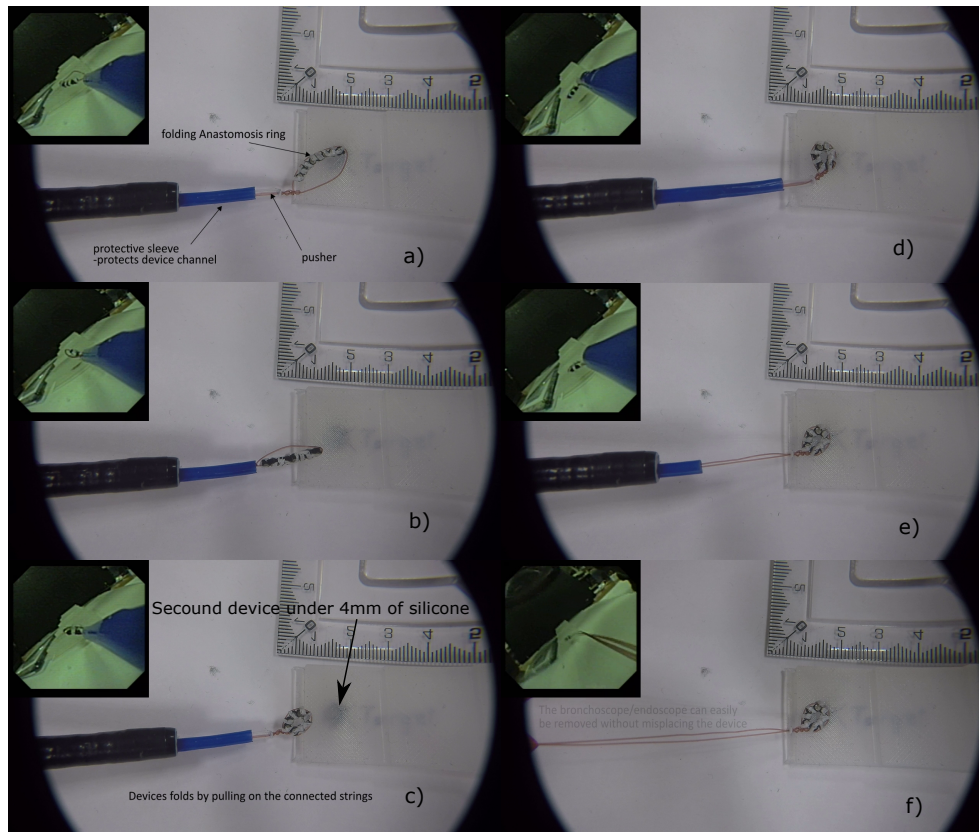


Figure 5.18: Folding magnetic anastomosis device in benchtop experiment a) device overview b) step III c) step IV to V c) step VII d) fully deployed device.

force in pulling direction was measured. To minimize magnetic interaction between the measurement devices, the magnetic folding rings were placed on polymer spacers and had a minimal distance of 100 mm to any nearby metal. To compensate for gravity, it was assumed that the force at a separation distance of 50 mm (where magnetic coupling is no longer evident) is zero and all other data points were zeroed in reference to that.

The measurements show a coupling force and resulting pressure of 137 mN (2231 N/m) to 23.54 mN (382 N/m) for coupling distances of 3 mm to 8 mm for single rings. For stacked rings a force of 154.7 mN (2516 N/m) to 32.96 mN (536 N/m) was recorded. Compared to coupling forces established for successful magnetic anastomosis creation, with forces between 180 mN and 300 mN [22], the forces for single as well as stacked rings is clearly sufficient for anastomosis creation.

5.4.4 Benchtop Experiment

The benchtop tests have been performed with all configurations of the device during the development process to evaluate shortcomings and improvements. The highlighted benchtop experiment in Figure 5.18 is the final configuration of the device and represents the first full deployment under pre-clinical conditions.

The device has been deployed as specified in Section 5.4.2, through an endoscope with a standard device channel diameter of 3.2 mm. Each device was successfully deployed and magnetically coupled over a silicon tissue replacement with a thickness of 6 mm. Experimental estimation of a maximum distance for a successful coupling against gravity was around 19 mm and has been subsequently validated in the pull force measurement. After deployment of the device, the pusher and mantle were removed manually. While removing the pusher, some tugging on the nylon wire can be observed which was addressed in subsequent handle designs as this might displace the device. This tugging contributed to the friction between the pusher and wire when the pusher is removed. After the removal of the pusher, the mantle was removed. The same issue was then observed but with significantly lower force. The effect is due to the different material surfaces in contact and the larger internal diameter of the mantle. A modified deployment procedure has been successfully tested where the device was held in place using the mantle during deployment to address this concern.

The handling of the pull wires and the issues of internal friction during the deployment highlighted the advantages of a handle that allowed for an ergonomic and safe deployment without misplacing the device. The deployment allows for two magnets to be deployed simultaneously or in sequence. If deployed in sequence, the deployment steps are performed independently for each of the magnets. Next the devices are coupled and only then are the mantle and pusher of both devices removed.

5.4.5 Pre-Clinical Study

To evaluate the possible use case of the device in a clinical setting, a cadaveric pre-clinical study has been performed at the *Mater University Hospital* in Dublin. The study was performed by Prof. R. Cahill and Dr. MF. Khanc., as seen in Figure 5.19. A total of three experiments were performed. In all

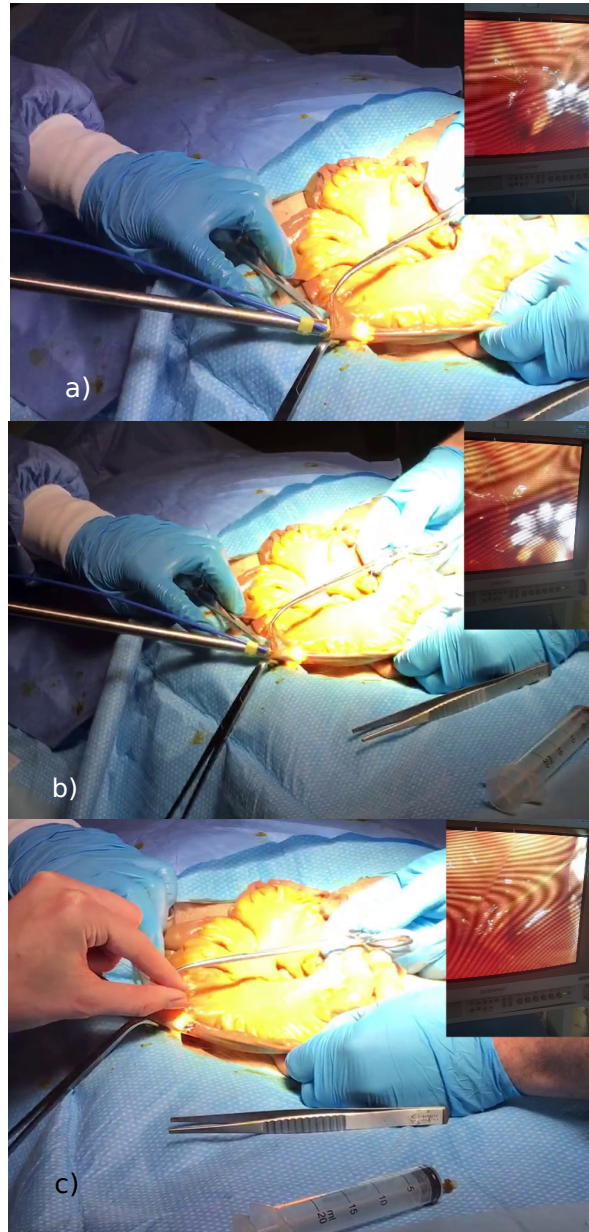


Figure 5.19: Experiment 1: Deployment of a folding magnetic anastomosis device in a cadaveric pre-clinical study preformed at the *Mater University Hospital* in Dublin, with a) device deployment b) folded ring and c) coupling to external device.

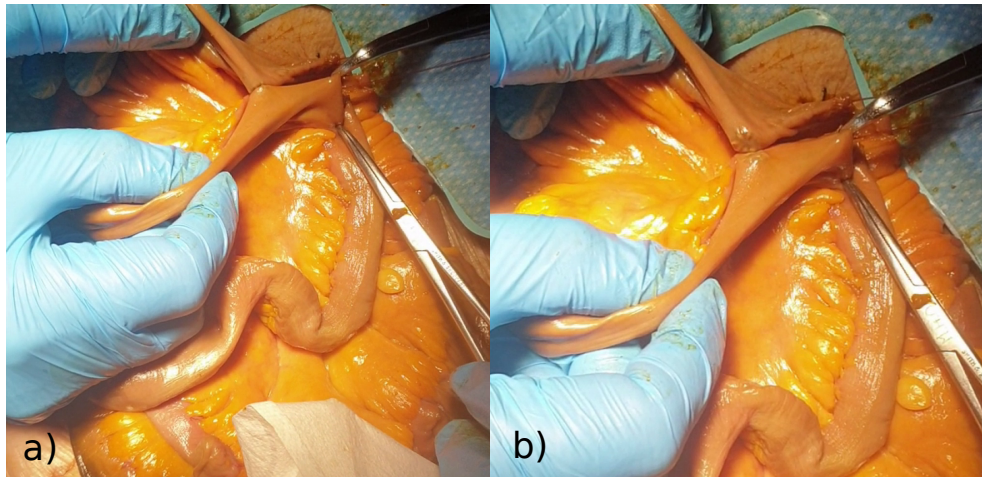


Figure 5.20: Experiment 2: coupling, where folding magnetic anastomosis devices deployed in separate parts of small intestine are repeatedly pulled apart to subjectively estimate the coupling force, with a) devices are in direct contact c) devices are pulled apart.

three cases, the folding magnetic anastomosis device was delivered directly via the mantle H. The mantle was fixed to a laparoscopic camera to ensure visual footage of the folding process inside the abdomen. The objective of this pre-clinical study was to estimate the deployability and folding behaviour under clinical conditions rather than the possible delivery through a device channel which was confirmed in the benchtop tests,

- **Experiment 1:** This experiment was designed to work as a first proof of concept that the device was deployable within the small intestine. The laparoscopic camera together with the mantle was inserted into the small intestine via an incision. The device was deployed via the described deployment procedure with steps I-V, as introduced in Section 5.4.2. A second already deployed magnetic ring was positioned manually outside of the small intestine and a coupling over the singular wall of the small intestine was observed.
- **Experiment 2:** This experiment was designed to prove that the coupling between two neighbouring parts of the small intestine is possible and to subjectively estimate if the coupling force could suffice to form an anastomosis. The mantle and laparoscopic camera were inserted via an incision in a part of the small intestine. The device was deployed following deployment procedure I-V. A second device in the folded state, was inserted via incision into a different part of the small intestine. The second device was placed in the immediate vicinity of the first one and coupled over both walls of the small intestine. Deployment steps

VI to VIII (as seen in Figure 5.15) were executed to leave both devices inside the intestine. The surgeon pulled the coupled parts of the intestine apart repeatedly to subjectively estimate the coupling force and estimated it to be sufficient for an anastomosis creation, as seen in Figure 5.20.

- **Experiment 3:** Building on experiment 2, the objective of this experiment was to objectively quantify the coupling capabilities of the prototype. To that end an incision was introduced between the deployed magnets as seen in Figure 5.21, to simulate an anastomosis. As such, the incision connects the two parts of the intestine and is only sealed by the magnetic coupling force between the two devices. Both parts of the intestine were sealed closed by clamps to the magnetic devices. Coloured liquid was introduced into the sealed area with a 20 ml syringe to an approximate pressure of 2.2 bar [85]. The liquid was observed to pass through the hole between the magnetic devices into the other part of the intestine. No liquid was observed to leak at the intersection of the two magnets.
- **Experiment 4:** The objective of this experiment was to evaluate possible gastrojejunal (GJ) anastomosis creation. A prototype was deployed via incision with a laparoscopic camera into the subject's stomach. Following deployment steps, I to V (as seen in Figure 5.15), the device was deployed, folded and placed close to the stomach wall. A second device was deployed manually via incision into the small intestine. The devices were manually coupled. A coupling of the small intestine magnet assembly to the stomach assembly could be observed. However, upon testing, the coupling force was estimated to be too low by the surgeon for successful GJ anastomosis creation.

Photographic evidence documenting the pre-clinical study can be seen in Figure 5.19. A total of 6 prototypes have been used in the study. Five successful deployments in small intestine and stomach have been documented. A sixth deployment failed due to the wrong sequence in the device deployment procedure, the device was accidentally locked before the magnetic ring was closed. The preliminary testing confirmed successful deployment in the small intestine and a successful coupling over the single intestine wall. Successful deployment and coupling between adjacent parts of the small intestine was observed.

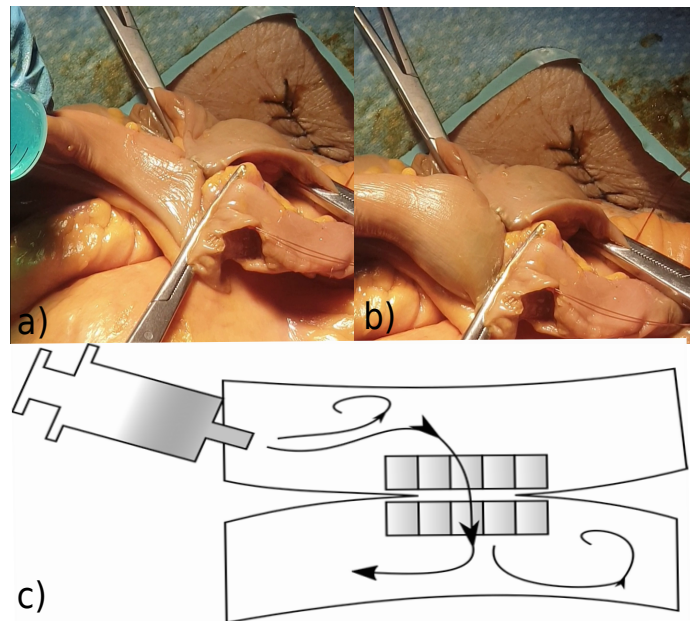


Figure 5.21: Flow test to evaluate sealing force of two coupled folding magnetic anastomosis devices in the small intestine a-b) photographic documentation of the procedure c) schematics.

The coupled magnetic components deployed inside the loops of bowel were pulled apart repeatedly to subjectively estimate the coupling force as seen in Figure 5.20. Our clinical experts estimated it to be sufficient for an anastomosis creation. The coupling force was objectively quantified in the previously described flow test, where a sealed part of the abdomen was pressurised with a liquid to pass through an incision sealed by two magnetic devices. The liquid was observed to pass through the hole between the magnetic devices into the connected part of the intestine. No liquid was observed to leak externally at the intersection of the two magnets.

Coupling between the magnet in the small intestine and that in the stomach could be observed. However, upon testing, the coupling force was estimated to be too low for successful anastomosis.

5.4.6 Scalability

The prototypes have been assembled by hand under a magnifying glass. Accuracy of human assembly places a clear limit on how small the prototype might be and on how thin a structure where the weaving is possible. However, the weaving process itself is a simple repeating motion. Automated weaving exists for hundreds of years and a suitable machine is expected to assemble the weaving significantly faster, more precise and potentially in smaller devices and with more layers than a human possibly could [86].

The weave is fixed with spot gluing that is sub millimetre in size in the current version of the prototype. In a hand assembly process, surface tension is used to have the weave absorb small droplets of liquid glue delivered on the tip of a wood needle. A wood needle was used as non magnetic material was required and wood may be sharpened easily to exhibit sufficiently fine tips. If this process would be automated and a machine would deliver the glue via micro syringes, precision and assembly speed could be significantly improved. The binding of the Giant's Knot and the assembly of pusher and mantle are expected to be more complicated to automate. However, these processes take the least amount of time and precision in the production process and could be performed in post processing by humans, independent of device size.

5.5 Summary

This chapter documented the production of several prototypes and benchtop models, that act as a prove-of-concept for the general concept of magnetic self-assembly, introduced in Chapter 4. The development process of these prototypes has been accompanied by rapid prototyping to find adequate constructive solutions to produce the device at a size useful for applications in minimally-invasive surgery. As a result, it was possible to significantly reduce component size and develop a component construction that might be produced at a scale of 2 millimeters. A modular component system has been developed that allows for the production using additive manufacturing methods at the target scale. However, commercial magnets have been used with the printed component housings. Magnets and housings were joined manually. This manual manufacturing limited the possible downsizing of prototypes to approximately four times target scale. Both the functionality as a magnetic anchor as well as a self-folding magnetic anastomosis ring were proven at this larger scale. Access to additive manufacturing that prints with magnetic polymer compounds might have enabled to print magnetic components without the need for manual assembly. However, collaboration with research groups who have access to such technology [58] has been attempted but has not been achieved.

To demonstrate an application of folding devices in minimally invasive surgery a folding anastomosis ring was developed, where the ring is closed

by a wire. This eliminated the existing issues in production and demonstrates the application of folding devices in minimally-invasive surgery in a pre-clinical study. The design was implemented in a range of manufactured prototypes. The prototypes presented in this work are in the same scale as sufficient for the suggested use case of jejunum-jejunal anastomosis creation. To investigate feasibility of the use of the device during surgical procedures, a number of experiments were conducted.

The benchtop experiments demonstrate that the device can be delivered through the device channel of a bronchoscope with a diameter of 3.2 mm. The results suggest that the delivery of the current device is possible through any flexible tubing such as a catheter channel with a maximum length less than the length of the mantle. In the current prototype iteration this length is 1.5 m. The suggested deployment procedure has proven to be successful if a second device is in place or is deployed simultaneously. The deployment and folding in laboratory conditions is reliable and repeatable despite the low manufacturing precision of manual assembly.

To further investigate the device under clinical conditions, a series of experiments were performed in the scope of a pre-clinical study. The device was successfully deployed multiple times and folded inside the small intestine and stomach. Coupling both between two parts of the small intestine as well as between stomach and small intestine has been achieved. A leakage test demonstrated that the device exerts sufficient force to seal an artificial compression anastomosis of the small intestine. In conjunction with the conducted force measurement, we therefore conclude that the device can provide sufficient magnetic force on each other to be viable to create an anastomosis over short distances. The possible stacking of devices to increase the potential coupling distance has been investigated.

The specific construction of the device is manufacturable at millimetre and potentially sub-millimetre scale. Furthermore, it potentially allows for partial or full automation of the production process. In conclusion, the presented design is qualified to produce cost-efficient folding magnetic anastomosis rings that might be deployed through small ports and fold into rings larger than the port used to deploy them. This suggests a use of the device in minimally-invasive surgery for small distance anastomosis creation in difficult-to-reach areas. Suggested uses are for jejunum-jejunal anastomosis

creation and the treatment of stable cases of benign biliary strictures.

6 Conclusions and Future Work

This work lays the groundwork for self-assembling surgery tools that may loosen the size limitation which the deployment port imposes. This conclusion chapter will summarise the findings of this thesis and discuss the findings in light of the objectives defined in Chapter 1.

6.1 Summary

Chapter 2 provided a summary of existing technology in the field of magnetic self-assembling surgery tools. It highlighted some of the challenges that arise from the target size scale of a tool for minimally-invasive surgery.

Chapter 3 expanded on the existing theory of magnetic folding chains. Two methods to analyse folding chains were explored; simulating the dynamics of a folding chain and computing the potential energy with the chain. A novel interpretation of the *Newton-Euler* equations was developed to efficiently compute the chain dynamics. Software tools that aid in the construction and analysis of magnetic folding chains have been introduced. The software tools presented in Section 3.2.1 enable the analysis of specific folding behaviour. This analysis allows conclusions on the likelihood of a specific fold to occur. A simulation of the chain kinematics to predict the folding from a specific sequence to the final folded shape has been implemented and detailed in Section 3.4.

Chapter 4 developed the concept of a self-folding magnetic chain. The primary driving force is the magnetic interaction between components. An observation was made that two magnetic components might only fold into a specific configuration if the direction of magnetisation is at an angle to the potential contact surfaces of the components. This observation was extended to longer chains and other possible component shapes. The cube was chosen as the initial shape for components. While a matrix of cubes is less resistant to external forces, the component represents the most simple

and versatile application for the given concept. As a result, clear guidelines were developed that would aid in the construction of a self-folding magnetic device.

Chapter 5 detailed the development and testing of prototypes to act as a proof of concept. Two primary applications in minimally-invasive surgery have been implemented in benchtop experiments; the magnetic anchor and the magnetic anastomosis device. These examples have been chosen to highlight the unique property of the introduced magnetic chains to fold into a structure where all magnetic components are polarised in the same direction. This enables a strong magnetic interaction between devices and enables the use as magnetic surgery tools such as anastomosis rings and anchors.

The concept of self-assembling magnetic chains introduced in Chapter 4, results in theory in the correct folding between two components, longer chains might show multiple possible folding shapes that have varying degrees of stability. The potential energy in the system is used to validate the expected folding behaviour. Using this technique, a number of secondary structures for cube components have been defined. Analogous to protein bio-synthesis, these secondary structures reliably form and can add together to compose larger and more complex structures. The exemplar folding behaviour of these secondary structures has been investigated using the analysis of potential energy during the folding behaviour. As such, the concept proved versatile, enabling the reliable folding of small to medium structures.

In conclusion, the presented concept allows for the construction of self-folding magnetic chains that can fold into structures with strong magnetic potential. A set of software tools and guidelines have been developed that ease the construction of functioning tools formed from a magnetic chain. Constructive solutions have been investigated to produce these tools in adequately small sizes to allow for the delivery in minimally-invasive surgery. A promising prototype has been developed that, while not being strictly self-folding, allows for the delivery of tools through a channel smaller than the tool, and has been successfully tested in the pre-clinical setting.

6.2 Contribution to the Field

This thesis analysed folding behaviour of magnetic chains and derived a concept of self-folding magnetic chains. This concept was put to test in various prototypes and was modified to fit different tools to be used in minimally-

invasive surgery. The novel contributions of this thesis are listed in this section.

- *Vectorised interpretation of the Newton-Euler equations:* The dynamics of folding chains have been investigated in this thesis and a novel interpretation of the Newton-Euler equations has been presented in Chapter 3. This interpretation allows for expressing the differential equations that describe the movement of rigid body chains in a single vector equation. Expressing the dynamics of a chain in this manner benefits the use of modern computer architecture such as *Graphical Processing Units* (GPUs) and potentially faster computation of long chain dynamics. The presented algorithm can be applied to some cases of kinematic rigid-body chains. A potential application in the field of protein structure prediction could allow the kinematic simulation of protein folding.
- *Concept for the construction of self-folding magnetic chains:* A novel concept and guidelines to construct self-folding chains was introduced in Chapter 4. This concept was created considering state-of-the-art production methods to produce devices at the millimetre scale, to allow the application in minimally-invasive surgery. Guidelines for constructing self-folding magnetic chains have been defined. At the core of these guidelines is the observation that all components have the same magnetic orientation in the folded configuration. When constructing a chain to fold into a specific shape the magnetic orientation of all components is therefore determined by this requirement. This reduces the complexity of the construction challenge, as only the possible configurations of the chain needs to be optimised.
- *A folding magnetic anastomosis device:* While the concept and introduced solutions in construction theoretically allow for the production at a millimeter scale suitable for the application in minimally-invasive surgery, the manual manufacturing methods limited testing to larger devices. To prove feasibility at the target scale, a supported folding magnetic device was developed. A separate construction was created to specifically address the manufacturing issues and allow for the manufacturing of folding magnetic anatomises rings that could be delivered through a 3 mm device channel of an endoscope. Prototypes of this device were successfully used in a pre-clinical cadaveric study and the possible use of the device as a magnetic anastomosis device used in minimally-invasive surgery was confirmed. The prototype presents a

fully functioning device and deployment mechanism that allows for possible commercialisation. The design of the device allows for a potentially semi- or fully automated production.

6.3 Future Work

The research work presented in this thesis might be expanded on as described in this section.

Expansion on the Vectorised Newton-Euler Equations

The novel interpretation of the *Newton-Euler* equations presented in this thesis is valid for specific restraint conditions. To be applicable in a wider range, when simulating the dynamics of different cases of rigid-body chains, additional restraint conditions need to be explored.

Vectorising the Magnetic Model

The *Coulomb* point charge model was shown to accurately simulate the magnetic interaction between components. However, the model relies on a set of monopole point charges for each component. The magnetic interaction between all point charges in a chain is computed. This requires a significant amount of computational effort, specifically for longer chains. In future, an analytical model could be fitted instead of the *Coulomb* point charge model. This model could return the force between two magnetic bodies $\vec{f}_m$ as a function of their relative distance d_m and orientation φ_m to each other, in the form $\vec{f}_m = \mathbf{F}(d_m, \varphi_m)$. *Coulomb's* point charge model might be used to fit such a function. Expressing the magnetic interaction in this form could greatly reduce the computational effort for specific magnet shapes and potentially allow for a vectorised expression, analogous to the vectorised *Newton-Euler* equations.

Developing the Software Tools

A software environment was developed that allows for the construction and analysis of magnetic self-folding chains. This software environment might be expanded on by creating compatibility with other constructions tools. While some compatibility with standardised data formats such as *Standard Tessellation Language* (STL) and *Unified Robotic Description Format* (URDF) was implemented, these features were not in the focus of this thesis and need to be expanded on. Furthermore, additional shapes and functionalities

to expand the available user interface might be implemented. Lastly, the software tools might be improved by implementing them in a more efficient programming language such as *C++*.

Further Investigation of the General Concept for Self-Folding Magnetic Chains

The developed concept for self-folding magnetic chains has been applied in this thesis for cubic components. Cubic components have been chosen as the most versatile application to fold from a chain into a volumetric structure. However, in Section 5.3 it was shown that variations of these building blocks can allow for the construction of specific tools such as a ring structure. Therefore, other component shapes and variations on these shapes need to be investigated to develop tools tailored for specific applications. This thesis focused on the possible self-assembly process of surgery tools. However, the disassembly of the proposed concept needs to be investigated. This disassembly is expected to be highly dependent on the specific tool shape and different methods of disassembly need to be developed to meet different tool shapes.

Additive Manufacturing of Flexible Magnetic Components

While constructive solutions were found that potentially allow the production of the proposed tools at a sufficiently small scale, the production methods have to be improved to create self-folding devices small enough to fit in an endoscope device channel. The presented prototypes of self-folding magnetic chains are composed of polymer component casings, each containing a magnet. The casings implement the living hinges between components while the magnets provide the magnetic interaction necessary to fold the device. As highlighted in Section 2.5 a flexible magnetic polymer composite material might be used in an additive manufacturing method [63]. As the material is flexible and magnetic it can be used to create the living hinges between components as well as the body of each component. Using this method the chain could be printed in a single process. As no assembly would be required, a production in very small size scales would be possible and as a result the deployment of the printed chain through small ports might be feasible in the future.

Further Clinical Investigation

The presented research on self-folding magnetic surgery tools is still in an early stage. More development has to be done before the first of this new generation of surgery tools might be used on a patient. To this end, a more ergonomic design for the handle has to be developed and further studies. Further corporation with interested surgeons could progress a possible mass production and commercialisation strategy of the technology.

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A Appendix

A.1 Programmable Self-Folding Magnetic Device

This section describes design and benchtop experiments for the first iteration of a programmable self folding device. Ultimately, the experiments were unsuccessful and the notion of a programmable device had to be dropped. The premise of the device is a chain of magnetic components linked by hinges. The specific magnetic orientation of each device can be altered using an external electromagnet. Achieving different sequences of magnetic orientation within the chain the same device can fold into different possible shapes and as such can emulate different functions as a tool. Following the theoretical conclusions from chapter 3, a chain of cubical components was considered and the first most simple implementation. This first prototype was designed to generate first data on feasibility of self-folding chains and programmable self-folding chains as well on practical solutions for the various constructive challenges.

A.1.1 Construction

The chain consists of cubical components each containing a single magnet. Each is a custom magnet from *Eclipse Magnetics*, UK made from the material *AlNiCo 5*. *AlNiCo* is an Aluminum, Nickel and Cobalt Alloy with an expected remanence of 1 T to 1.2 T¹. The magnets have a side length of $2 \times 2 \times 2$ mm. All components are assembled in a chain and linked by medical tape along one of the free sides. The medical tape fabric enables a high stability and was chosen to best approximate a rotational joint between components as seen in Figure A.1. During production, a beam of components is wrapped by the medical tape. By slicing the medical tape at the correct cube intersection, any sequence of hinges can be created along the chain.

Due to the relatively low remanence the magnets can be demagnetised and re-magnetised by subjecting them to a magnetic field stronger than the remanence. The device was designed to be magnetisable in different configurations on demand and therefore programmable. An electromagnet was designed that could produce a sufficient electromagnetic field to re-magnetise the device. The electromagnet had 802 turns turns of 0.71 mm copper wire. The core of the electromagnet was made from five 99.9% pure iron pieces ($25 \times 25 \times 50$ mm). The apparatus was held together by a

¹Website: Eclipse Magnetics, "Magnets Catalogue", last accessed Feb 2022

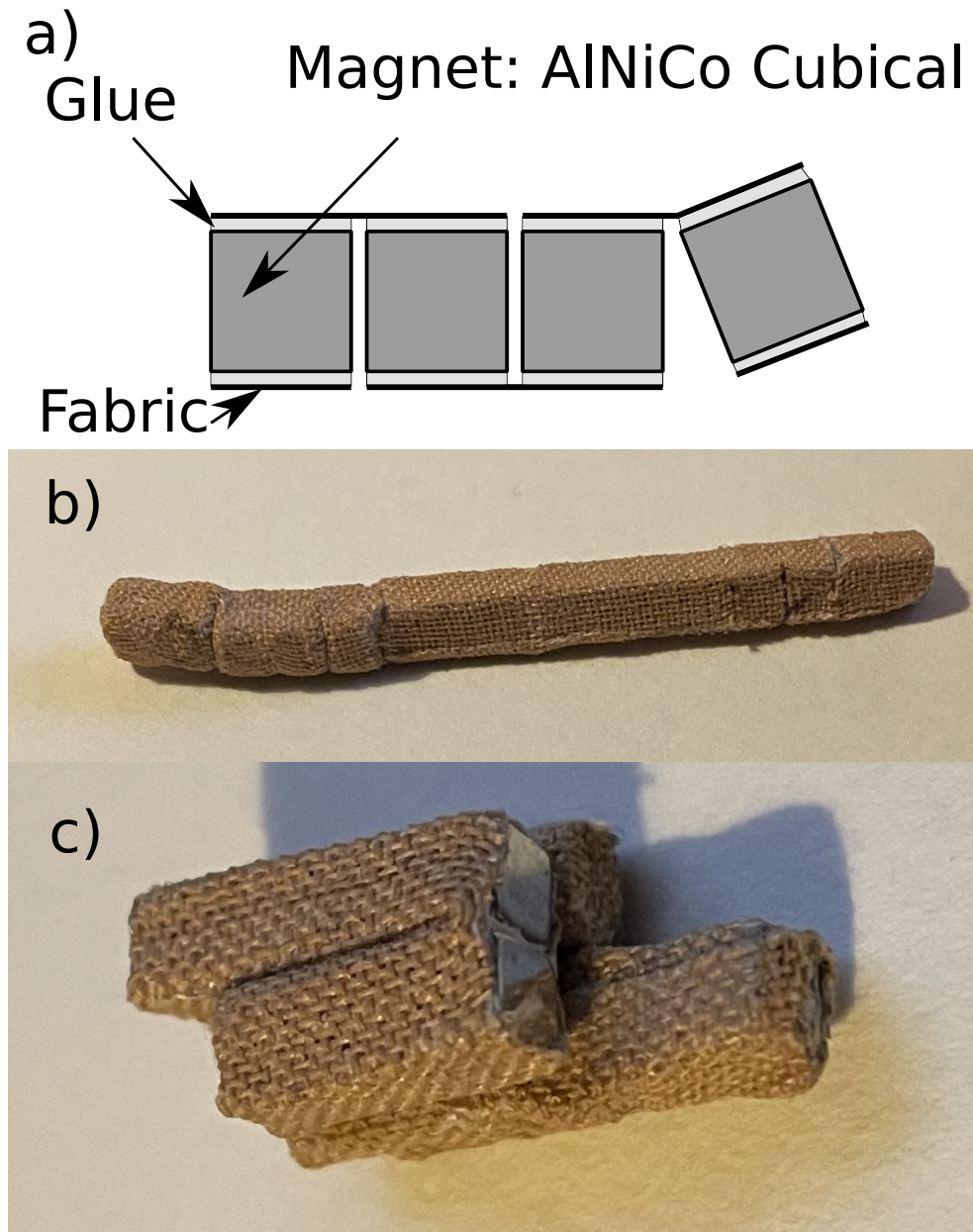


Figure A.1: Programmable self-folding magnetic chain, with a) schematics, b) unfolded state and c) folded state.

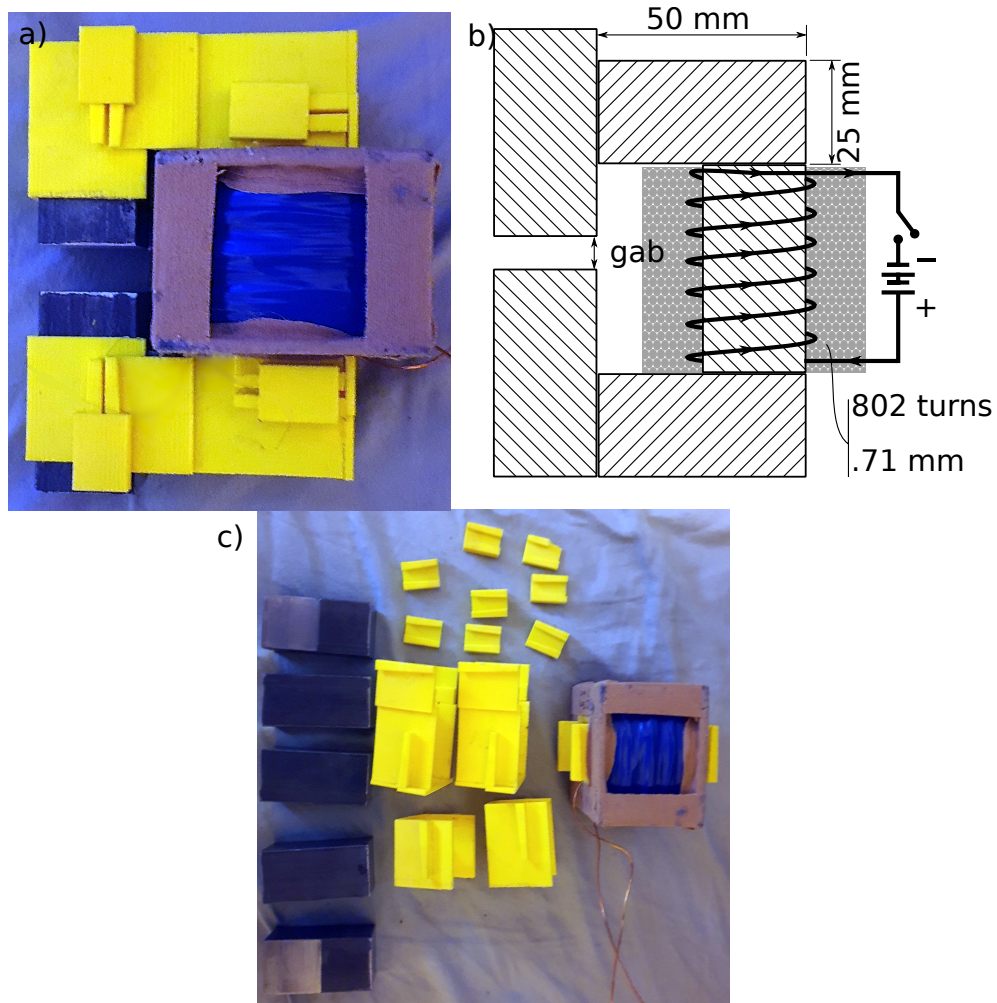


Figure A.2: Electromagnet setup for magnetisation with a) assembled device, b) schematics and c) component overview.

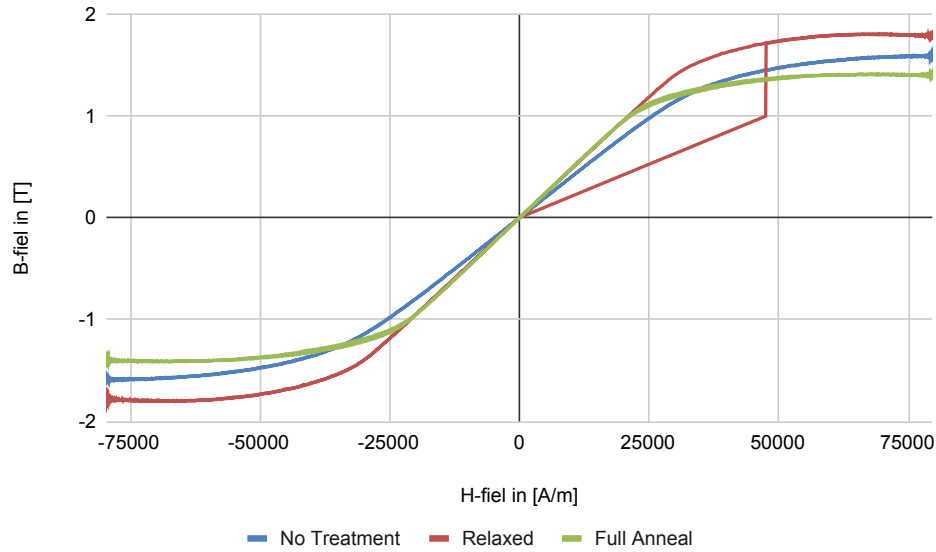


Figure A.3: Magnetic response of pure iron after different stages of annealing, with blue: no treatment, red: relaxed and green: full annealing.

polymer fixture as seen in Figure A.2. The core and fixture were designed to have a variable gap where a strong uniform electromagnetic field could be produced. If the AlNiCo magnets were placed into the gap, it could be possible to permanently change their magnetic orientation.

A.1.2 Tempering of the Core

It was observed that the iron did not exhibit the required electromagnetic permeability to create the field. As a result the iron was tempered to alter its magnetic properties and increase its electromagnetic permeability². An experiment was conducted to find the correct annealing procedure. The 99.9% iron was sliced in samples with dimensions of 25 mm × 25 mm × 1.9 mm. Three samples each were tempered with the following procedures:

- **No treatment:** Baseline sample without annealing;
- **Relaxation:** Heating to 500 Celsius for 30 minutes;
- **Full annealing:** After relaxation, heating to critical temperature 800 C for 4 hours.

The electromagnetic permeability was estimated by measuring the response of the tempered material to external electromagnetic fields. Figure A.3 shows

²Akujärvi, V., Cedell, T., Gutnichenko, O. et al. Evolution of magnetic properties during tempering. *Int J Adv Manuf Technol* 119, 2329–2339 (2022). <https://doi.org/10.1007/s00170-021-08464-7>

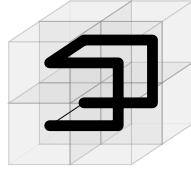
the results of these measurements. The figure shows the magnetic flux density B of the material in response to an magnetisation field H . The iron sample treated with relaxation annealing exhibits the steepest curve and the strongest magnetic flux density. This leads to the assumption that the relaxation treatment is the best out of the three to temper the pure iron core to maximise the possible magnetic flux density it can relay from the electromagnet to the gap. With the tempered core, the setup was capable of producing electromagnetic fields with a field strength of up to 0.64 T, as measured with a magnetic field probe for a 5 mm gap size.

A.1.3 Failure Analysis

Several magnetisation experiments where performed using the described setup. It was observed that magnetisation in some directions resulted in the required permanent magnetic field strength. Other directions would show significantly decreased permanent magnetic properties. As such a strong anisotropy of the material was observed. Upon contacting the supplier this was confirmed. However, possible isotropic material was expected to show significantly lower magnetic field strength after magnetisation³. Therefore it was concluded that soft magnetic material could not be used to construct a programmable self-folding chain.

³McCallum, R.W., Kadin, A.M., Clemente, G.B. and Keem, J.E., 1987. High performance isotropic permanent magnet based on Nd-Fe-B. Journal of applied physics, 61(8), pp.3577-3579.

a)
Folding
mode 1



b)
Folding
mode 2

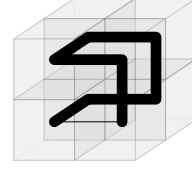


Figure A.4: Possible chain geometries to fold a cube.

A.2 Cube folding Simulation Results

Folding has been simulated for a chain of magnetic components with various sequences to fold into a $2 \times 2 \times 2$ cubical structure. Two primary modes to fold into such a cube have been defined as seen in Figure A.4. Each of these modes can be folded in sequence starting with the first or last component and is subject to one of four possible magnetic orientations.

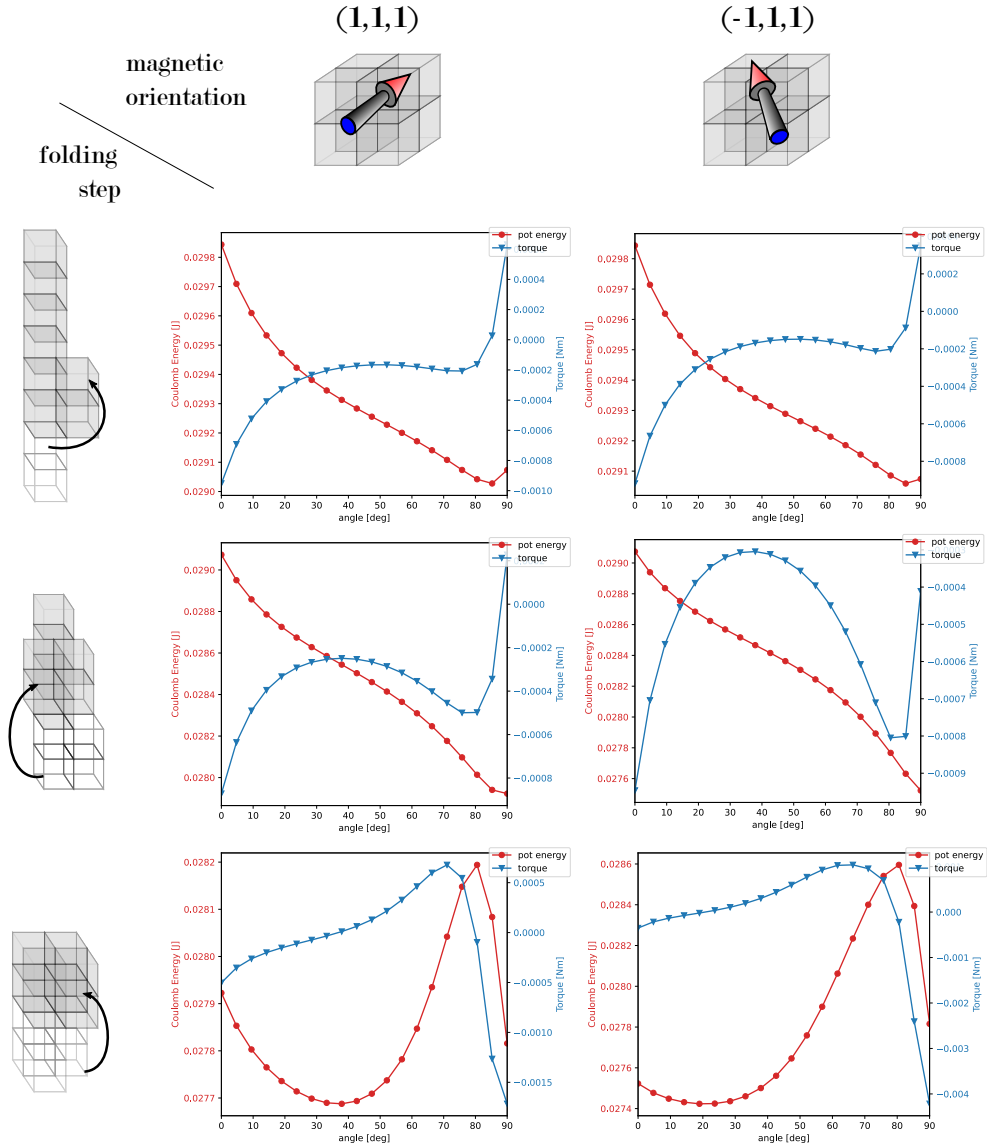


Figure A.5: Potential energy of sequential folding for cube mode 1, folding from component 1 to 6, for magnetic orientation $(1, 1, 1)$ and $(-1, 1, 1)$.

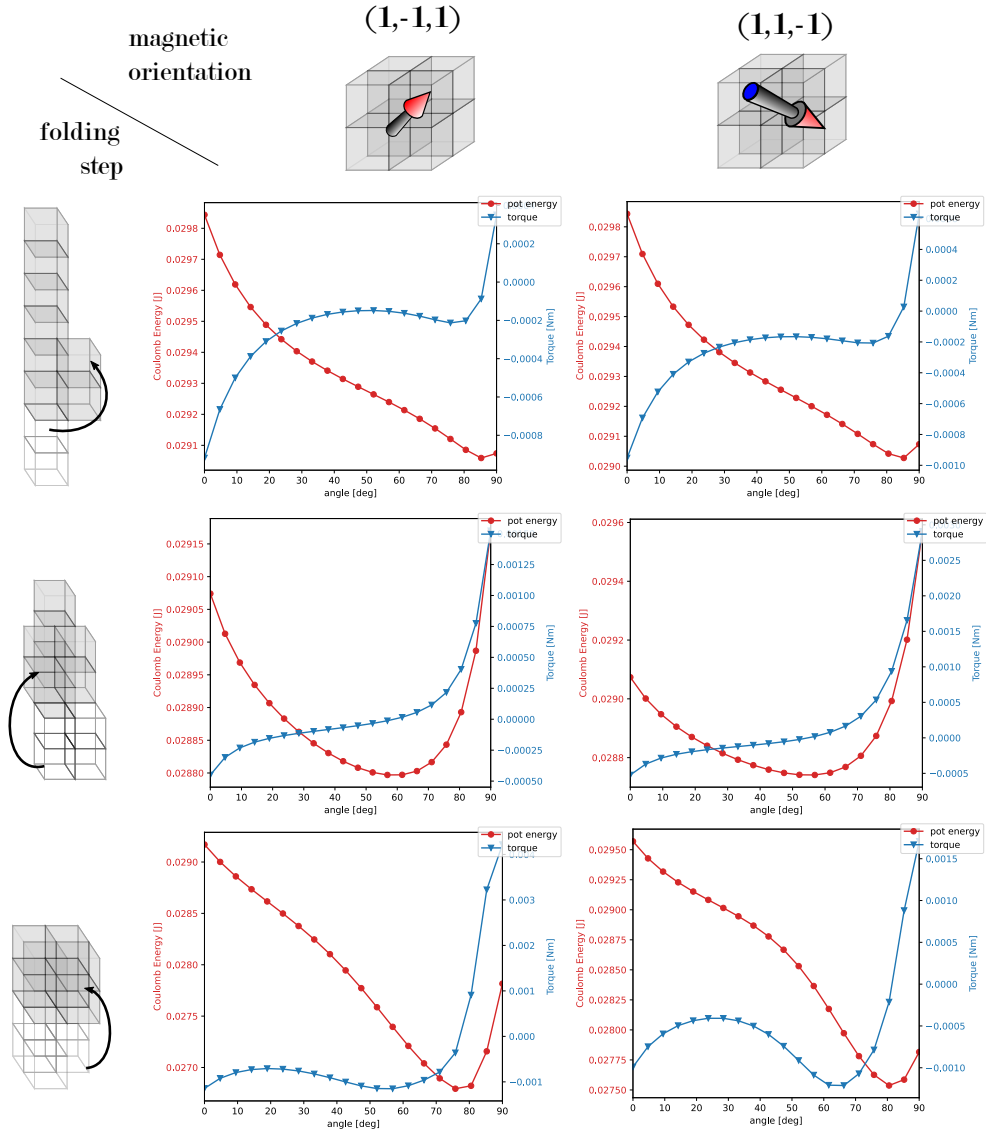


Figure A.6: Potential energy of sequential folding for cube mode 1, folding from component 1 to 6, for magnetic orientation $(1, -1, 1)$ and $(1, 1, -1)$.

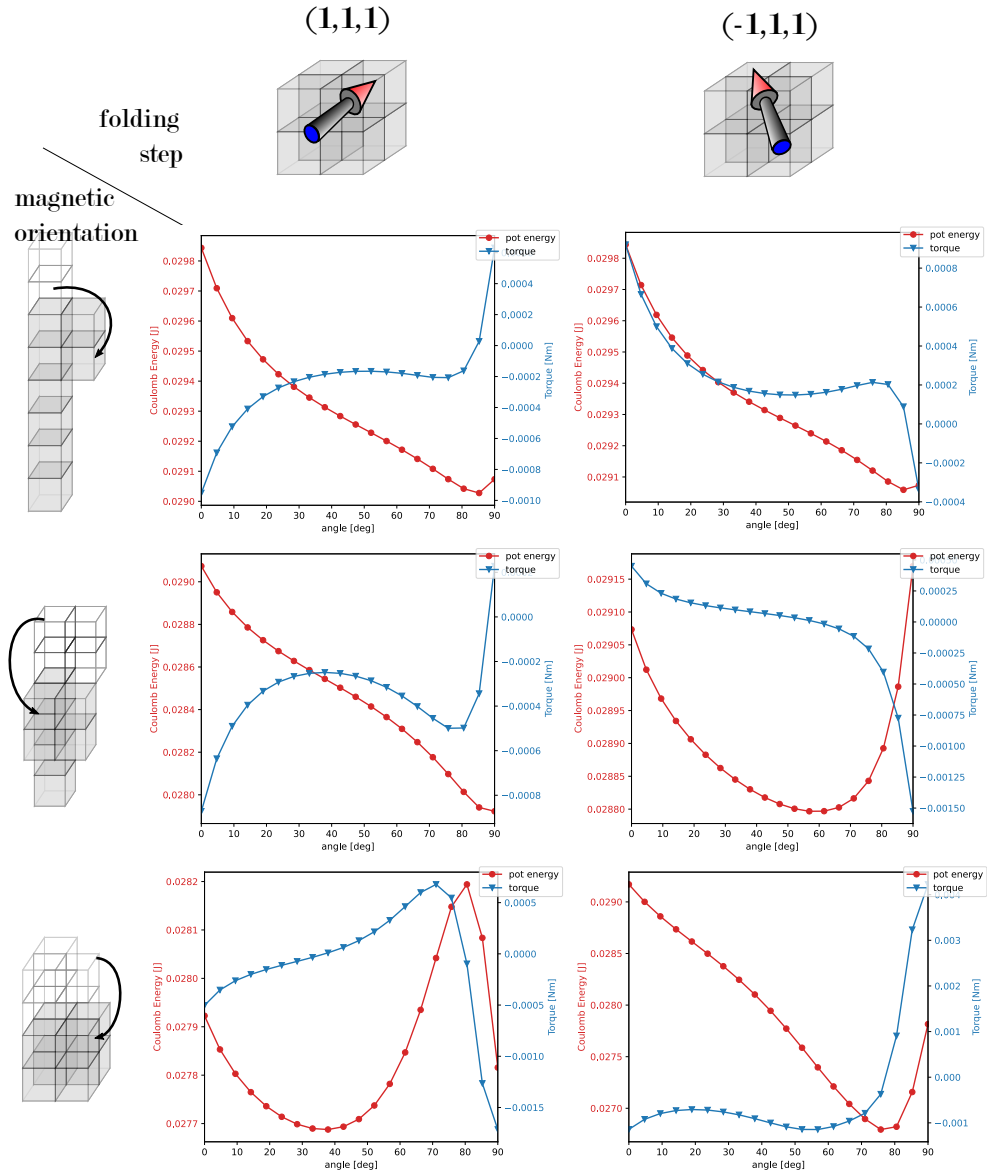


Figure A.7: Potential energy of sequential folding for cube mode 2, folding from component 6 to 1, for magnetic orientation $(1, 1, 1)$ and $(-1, 1, 1)$.

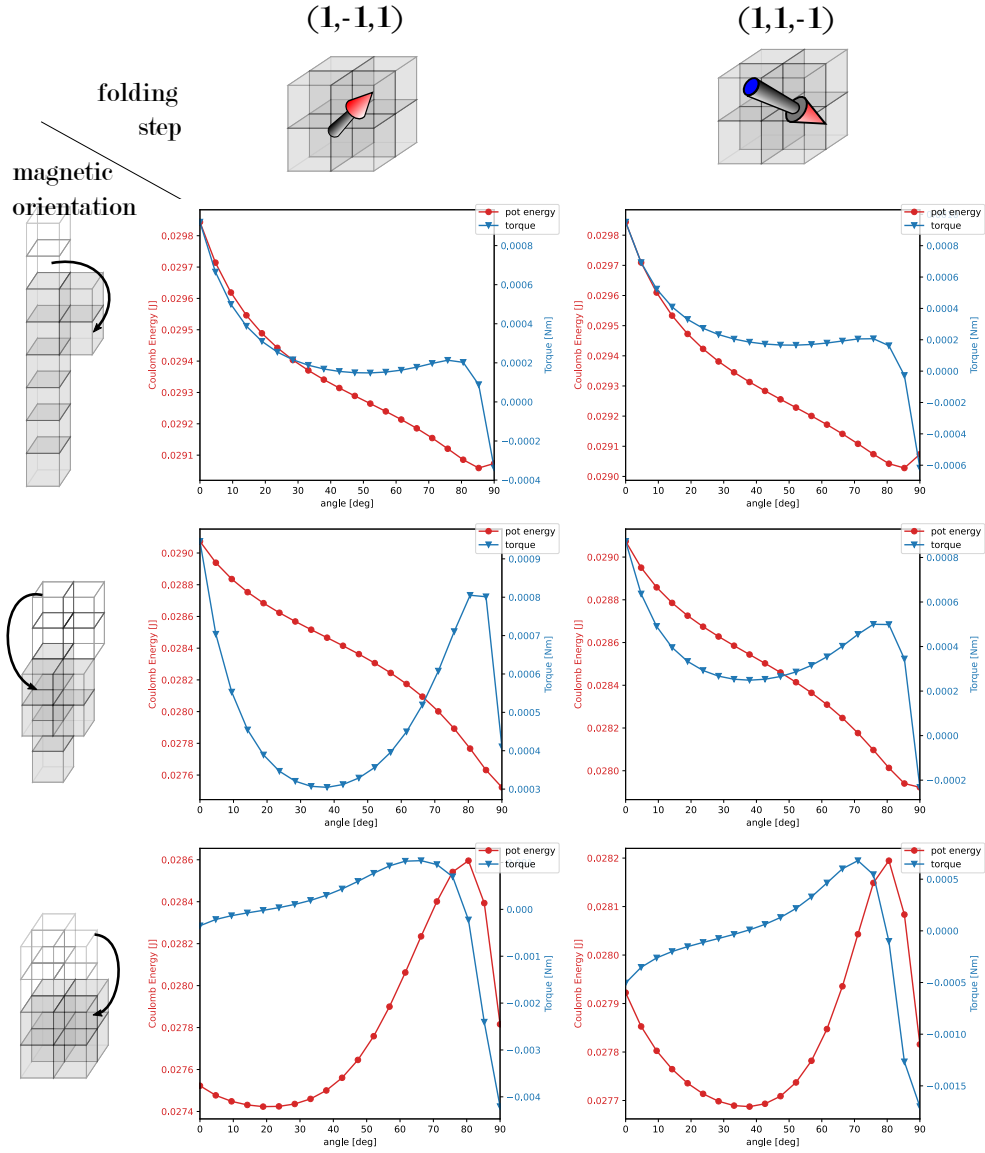


Figure A.8: Potential energy of sequential folding for cube mode 2, folding from component 6 to 1, for magnetic orientation $(1, -1, 1)$ and $(1, 1, -1)$.

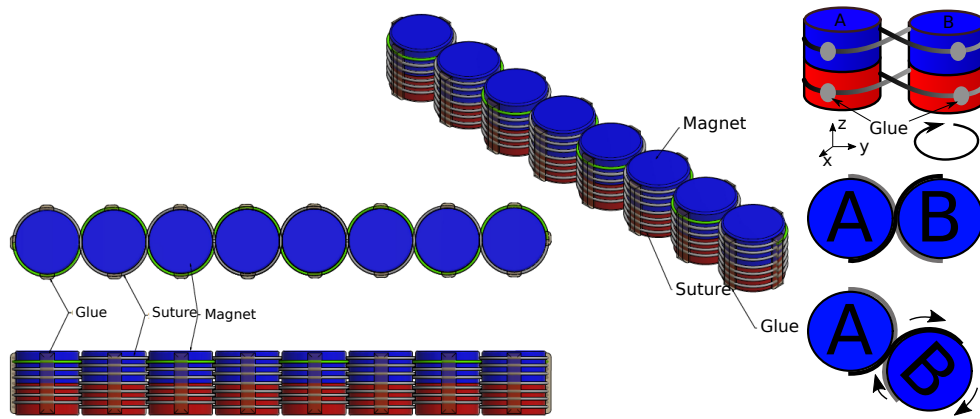


Figure A.9: Folding magnetic anastomosis device, schematics.

A.3 Folding Magnetic Anastomosis Device Operation and Production

This section specifies the manufacture and operation of the folding magnetic anastomosis device. The device schematics are given, followed by a detailed list of material and parts used. A step by step guide with pictures on how the device can be manufactured is documented, as well as a step by step guide on the usage and operation of the device.

A.3.1 Device Schematics

An even number of magnets is suspended by a string woven around cylindrical magnets as seen in Figure A.9. This weaving effectively acts as a core living hinge and allows for the components to roll on each other in a shared plane, while preventing any bending of the chain outside this plane. The magnetic polarisation of the magnets in the chain is parallel to ensure maximum magnetic interaction with other devices. Key components as seen in Figure A.10 are:

- A Magnet; Cylinder; height and diameter a
- B String; Nylon or silk; diameter b
- C Magnetic folding anastomosis device with n magnets
- D Nylon sheet with minimal thickness and broadness $< a$
- E Nylon wire with diameter d
- F Spacer: material polymer: Shape: thin Disk with diameter $< a$ and two holes with diameter b

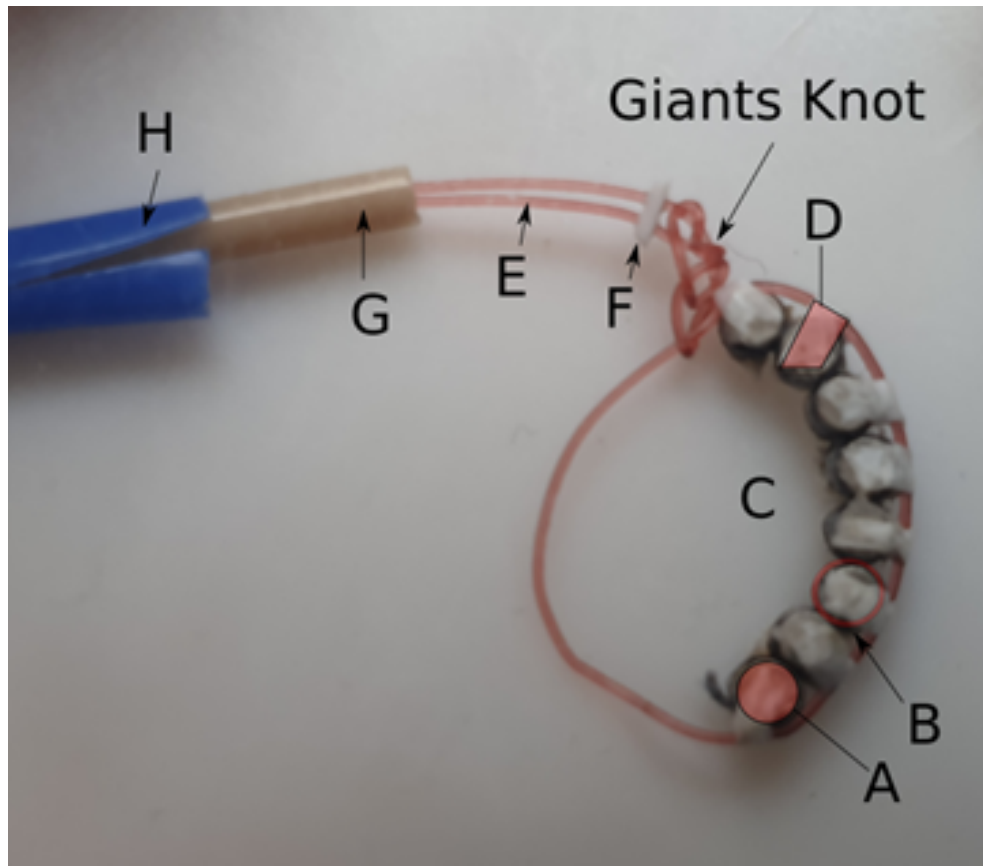


Figure A.10: Folding magnetic anastomosis device, closeup.

F Mantle; PTFE extrusion; diameter inner $ei \geq a$ outer eo ; length dl

G Pusher; PTFE extrusion; diameter inner $fi > 2d$ outer $fo < ei$; length $el = d + 5$

A.3.2 Hinge Design

The specific configuration of strings as seen in Figure A.11 allows a rolling of the magnets on each other but restricts all other movement including torsion. If we consider magnet A fixed in space, the strings restrict any movement of magnet B in x or y direction. The only possible movement is a rolling of magnet B along the surface of magnet A. This is implemented by weaving the magnets together as seen in Figure A.11 with one continuous string. To achieve this, an even number of magnets is required. The hinges are exposed to external forces as well as internal forces and torques. Strings, specifically sutures, are used in surgery due to their ability to withstand several Newtons of pulling force. The specific weaving is designed to absorb all forces in the Y-direction. However, due to the magnet configuration, internal torques force the magnets to rotate around the Y-axis. A small twist will result in

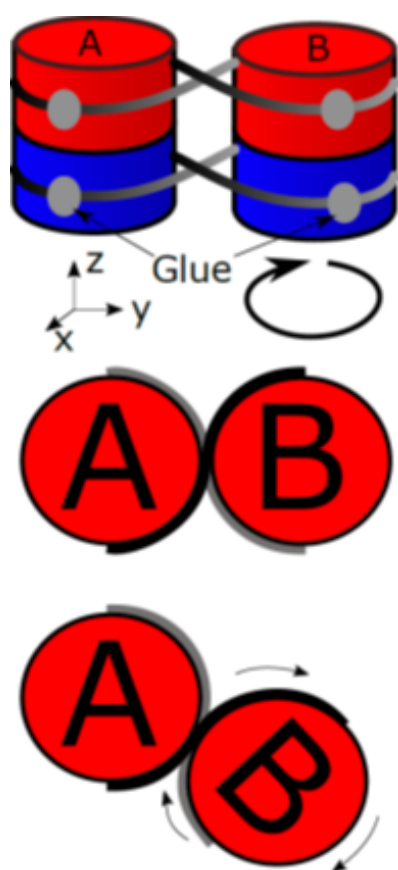


Figure A.11: Weaving acting as compliant CORE hinge design, with position of spot glue to fixture the weaving.

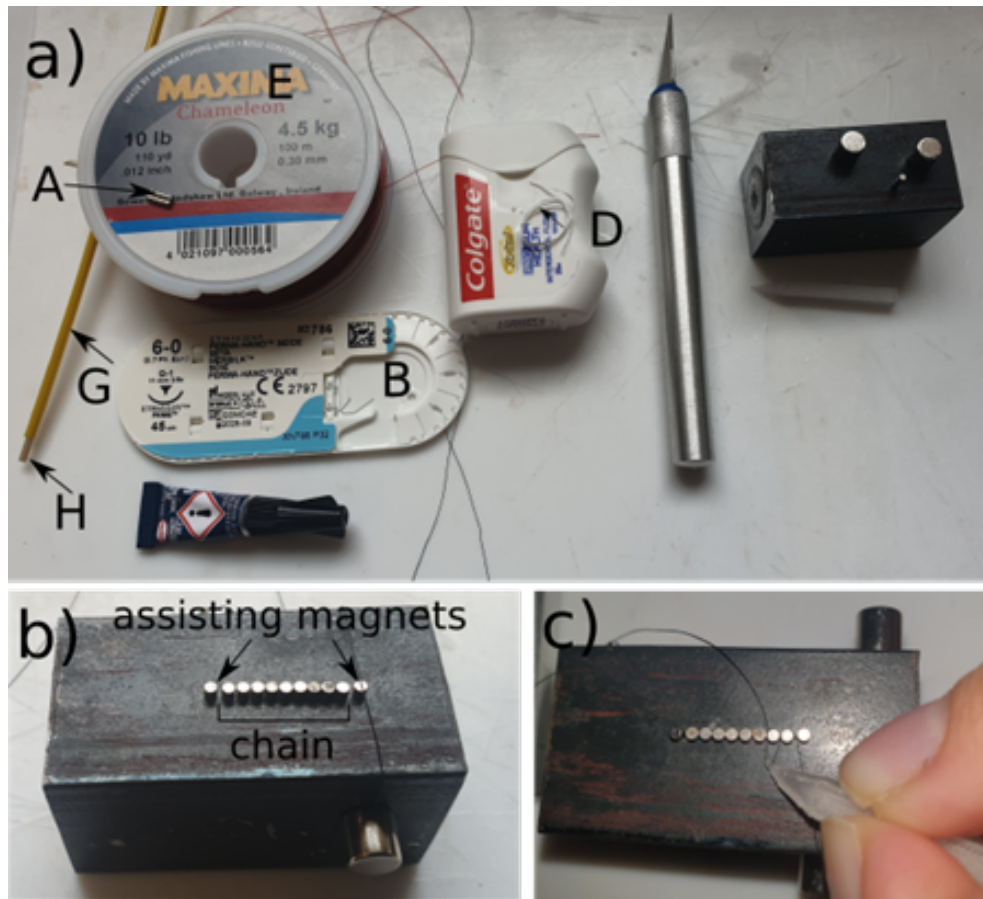


Figure A.12: Prototype production process with a) materials and tools used, b) initial setup for manufacture and c) weaving process.

the chain latching on itself upon folding and irreparably twisting the device. A tight weaving and a large number of weaving layers is required to minimise this effect. The thinner the suture, the more layers can be stacked and the smaller the distance between the magnets. As more layers also result in more layers of string resisting forces, thinner sutures are preferable to acquire a tighter more homogeneous weaving.

A.3.3 Production Process

The production process happens with the key step as documented in Figure A.12:

1. A nylon or silk string B is weaved around the magnets A;
2. The string B is fixed with glue at the shoulders of the magnet A;
3. Nylon D sheets are glued to one side of the magnets;
4. A nylon wire E of suitable length is placed close to the magnets A;

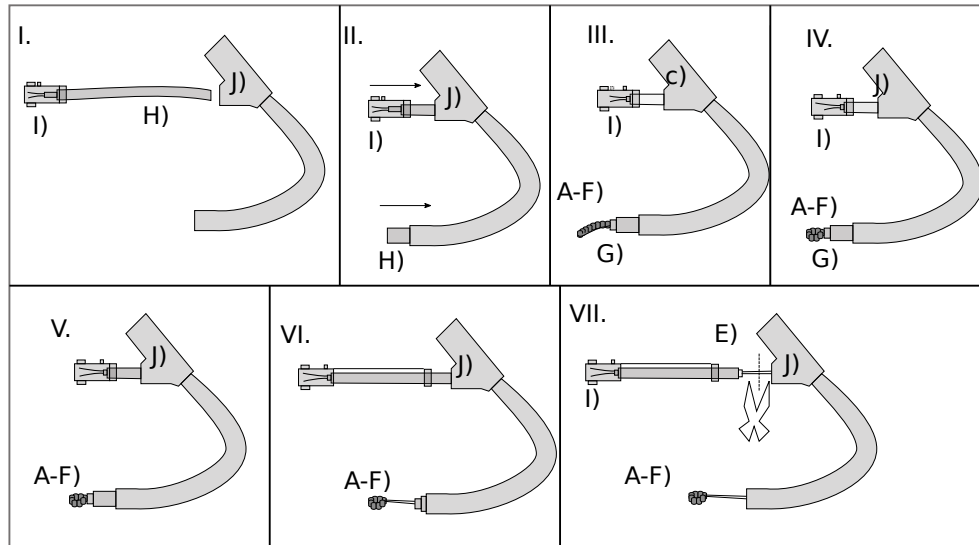


Figure A.13: Folding magnetic anatomises device, deployment process.

5. the Nylon sheet D is glued to the top of the magnets A to build a channel for the wire, forming device C;
6. The device C is placed at half length of the wire E and a Giants Knot [7] is formed, resulting in wire end Ec for closing the device and El for locking it;
7. The two ends of the wire H are fed through the polymer spacer F;
8. A cut with length $c+10$ is introduced to one end of mantle G;
9. Wire E is fed through the Pusher H;
10. Pusher H is fed through the mantle G;
11. Device B is fed into slid end of mantle G;

A.3.4 Deployment Process

The device is deployed as seen in Figure A.13 via a port that might be long and flexible, such as an endoscope, colonoscope or catheter. All control over the device is exerted via the handle, that operates the pusher, mantle and strings. The deployment happens in the following steps:

- I Once the device exits the port the device can be readied by pushing the pusher into the mantle by a distance $c+5$;
- II Wire end Ec is pulled by a distance c to close the device;
- III Wire end El is pulled by approximately 5% of el ;

- IV The device can be precisely placed aided by fluoroscopic guidance, X-ray or camera;
- V The Pusher H is carefully removed while feeding the wire ends Ec and El into the pusher;
- VI The wire ends Ec and El are cut to length as required;
- VII Mantle G and port might be removed.

A.3.5

A.3.6 Prototype

Several prototypes of the device have been produced with the outlined production method and have been tested in laboratory conditions as well as in a cadaveric pre-clinical study. This chapter details the specifications of the final prototypes.

Material requirements

All components need to fulfil highly specific functions that greatly rely on geometry and material properties. This section analyses the requirements for the component materials. As the central components allowing for magnetic coupling, the magnets, need to be of high grade and have a medically certified coating. Due to the high cost of a medically certified coating, this requirement was neglected in the early prototyping phase. The string B forming the living hinge needs to have a low elongation flexibility and a high bending flexibility. A silk weaving as used for sutures has proven best for this application. The Wire E needs to convey sufficient force to close and lock the magnet. Nylon is a material widely used in minimally-invasive surgery and proves to fulfil this purpose. The mantle and pusher need to be radially flexible to fit through possible curvature of a catheter or device channel while being axially rigid to allow the pusher H to move relative to the mantle G. The friction between pusher and wire E has to be minimal. The material of pusher and mantle has to be certified for use in medical procedures. Possible lubricant needs to be bio-compatible.

Dimensions & Material

The device specifications seen in Table A.1 have proven to be effective and allows an application in minimally-invasive surgery. The pusher and mantle

Table A.1: List of components of the folding magnetic anastomosis device with relative measurements and measurements of presented prototype iteration.

	Name	dimensions	material
A	Magnet	Height and diameter $a = 1/16$ inch = 1.5875 mm	N52
B	Suture	Diameter $b = 0.05$ mm	Silk
D	Support sheet, holds the guiding wire in place	thickness ≈ 0.1 mm and broadness = 1.5 mm	Nylon Floss
E	Guiding wire, folds the device	Diameter $e = 0.6$ mm	Nylon Floss
F	Spacer, allows for a reliable folding	Thin Disk with diameter $< a$ and two holes with diameter $b = 1.5$ mm	PP
G	Pusher, deploys devices out of mantle	Inner diameter $gi = 1.18$ mm outer $go = 1.77$ mm; length $gl = hl + c \approx 500$ mm	PEEK
H	Mantle, protects device and tissue	Inner diameter $hi = 2.8$ mm outer $ho = 3$ mm; length $hl \approx 1485$ mm	PTFE awg 11

are extrusions that have been provided by *Zeus Industrial Products*, USA. Suture was provided by Professor M.G. Ó Riordáin (Mercy University Hospital, Cork, Ireland). 8-0 Silk suture with a diameter of 0.05 mm from Ethicon, US was used. All other material originated from the internal resources of University College Cork, Power-electronics laboratory.

A.3.7 Device Testing

The prototype was deployed via a standard bronchoscope with a device channel diameter of 3.2mm. Seven out of eight deployments using three different prototypes were successful. One prototype failed due to low tension in the sutures and consequent twisting of the device, potentially induced by hand manufacturing. The other two prototypes proved to be highly reliable in their folding and could be reused three and four times without breaking. A full video documentation of the prototype folding can be seen online⁴.

The pre-clinical study was performed in Mater University Hospital Dublin by

⁴<https://media.heanet.ie/page/cd3d3629929e4f5c8f8a1cb6c3ed8f52>

the surgeon Ronan Cahill and his team. The mantle directly inserted into the abdomen, where the prototype was successfully deployed. A second prototype was deployed in a neighbouring part of the abdomen and a latching of both parts was observed.

A.3.8 Conclusion

The invention encompasses a specific configuration of a folding anastomosis ring that features a set of magnets linked by a specific weaving. This weaving acts as core hinge and allows for the manufacture at very small scales and potentially allows for fully or semi-automated production of folding anastomosis devices. Furthermore, the design uses a Giant's Knot to close the ring and secure it. This prevents issues with reopening and allows for a safe use of the device. Multiple prototypes have been produced and tested in a clinical setting, to provide a proof of concept. The prototypes have been produced manually in a research and development process but show a high reliability and efficiency in the folding. Compared to other existing designs, the design of a folding magnetic anastomosis ring presented in this thesis has proven to fold reliably at cm and mm scale as well as during clinical conditions and allows for a potential mass production.

A.4 Review of Medical Handle Constructed by External Company

The company (*Dolmen Design & Innovation*, Ireland) has been tasked with constructing a medical handle for the folding magnetic anatomises device presented in this thesis. As detailed in Appendix A.3, the device is deployed via a set of extrusions (pusher and mantle) and operated via two pull-wires that run inside these extrusions. After deployment and closing of the device, the extrusions are removed while the pull-wire stays in place. Due to the friction between the pull-wire and extrusions, the process is delicate and risks to misplace the already positioned device. Addressing this problem was the primary reason for employing an external company so as to utilise their experience and know-how to solve the issue. The request was to build a handle that would actively feed the pull-wires into the extrusion during retraction and therefore counteracting the friction. Parameters of this task have been:

- Creating CAD files for a medical handle to ease the use of the folding

magnetic anastomosis device;

- The handle has to be able to operate the device as outlined in Appendix A.3;
- The handle has to be usable by a surgeon and should fulfill ergonomic requirements;
- The handle should improve operation of the device by actively counteracting friction between pull wires and pusher during the final stages of device deployment.

The following analyses the product of this task. The handle prototype was communicated in a *SolidWorks* construction file. The required parts have been produced by *Materialise*, UK via laser sintering and assembled and tested in University College Cork. This section highlights the assembly as understood via the communicated data and lists arising issues with the existing construction in terms of its functionality.

A.4.1 Operation of Handle

This section details the steps to operate the handle as understood by the author. The handle has 4 points of interaction, as seen in Figure A.14:

- The crank A that moves mantle and pusher;
- The Switch B that switches between operating handle and pusher;
- The Switch B that switches between operating handle and pusher;
- The two levers C and D that pull the wires.

Operating the handle should happen in the following steps:

1. The switch B is set to operate the pusher. The crank A is turned by some degree counter clockwise to push the prototype out of the mantle;
- 2 The lever C is pulled to close the device;
- 3 The lever C is pulled to close the device;
- 4 The Crank is rotated clockwise until the Indicator shows a full retraction of the pusher;
- 5 The switch B is set to operate the Mantle and the Crank is turned Clockwise until the mantle exits the device channel.

A.4.2 Construction

The design as proposed has been assembled into the Prototype as seen in Figure A.14. In addition to the foremost mentioned parts A to D, it features:

- Pusher-wheel-gear E that drives the Pusher
- Pusher pressure carriage F that presses the Pusher against the pusher-wheel-gear E
- Mantle-wheel-gear G, that drives the Mantle
- Pusher pressure carriage H that presses the Pusher against the pusher-wheel-gear G
- Stopper I and J that stop the unused wheel-gear

Springs provide the force to the pressure carriages F and H to push the mantle and pusher against the wheel-gears to generate the friction necessary to move mantle and pusher. The wheel-gears E and G are positioned on a slider so that operating switch B will push one of them against the crank gear to be operated and the other against the respective stopper I and J to be stopped from rotating. When pusher and mantle are retracted, they are coiled up within the mantle.

A.4.3 Identified Issues

Unfortunately, the following issues have been identified while operating the prototype:

- I. The friction the wheel-gears E and G generate are barely sufficient to move the mantle and pusher.
- II. The pressure carriages F and H are physically prevented from exerting the necessary pressure to generate the required friction as they are blocked by implemented constraints.
- III. There is no force pressing the wheel-gears E and G against the crank gear. As a result the gears are pushed apart during operation and it is required to manually press the wheel-gears against the crank gear. This results in a very non-ergonomic operation of the device.
- IV. During step 5 when the mantle is moved, the switch B is set as to operate the mantle-wheel-gear G while the Pusher wheel gear E is pressed against the stopper and can not rotate. As such, the mantle

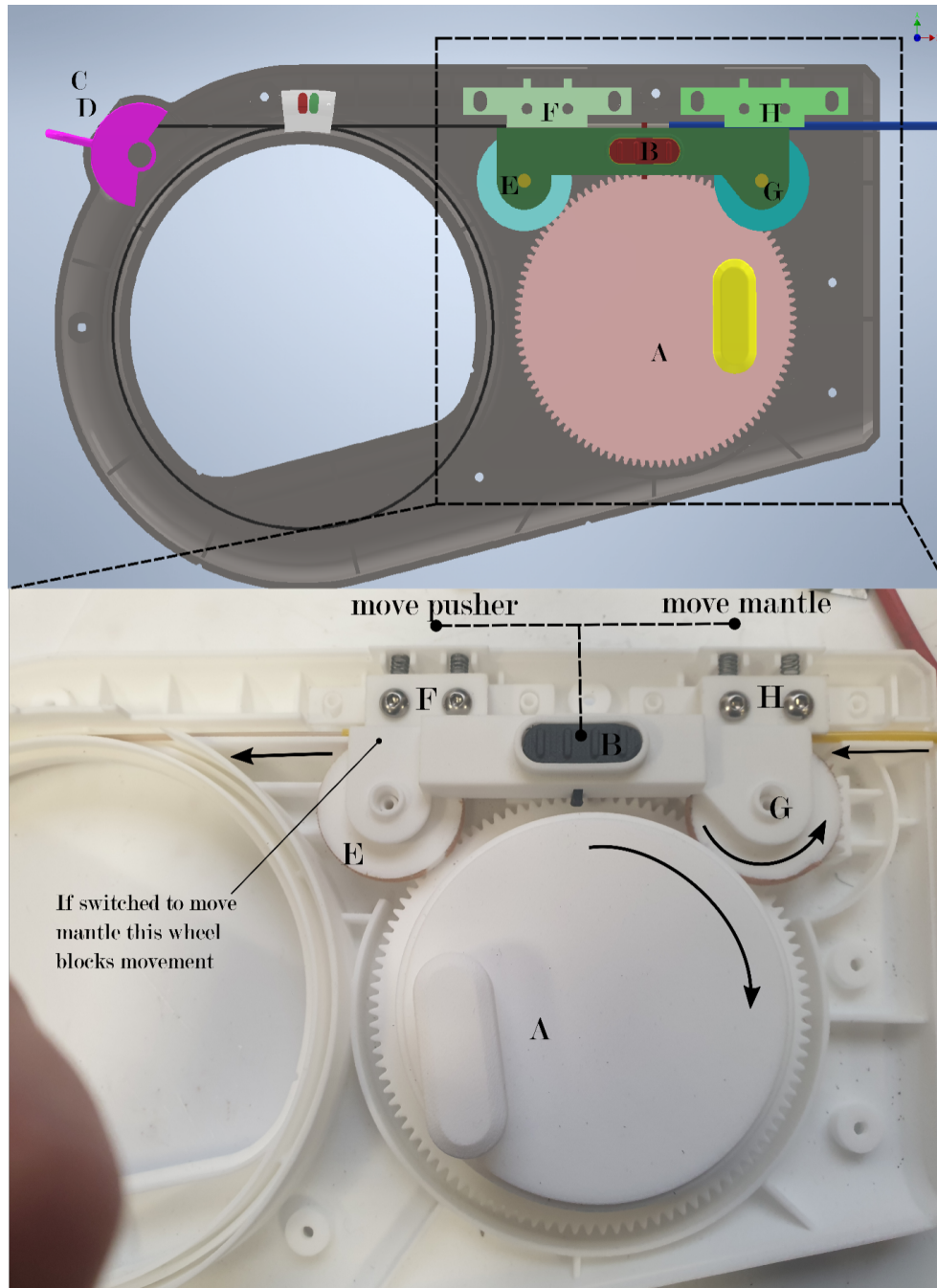


Figure A.14: Internal mechanism of folding magnetic anastomosis device handle, with Top: Construction; bottom: Assembled Handle.

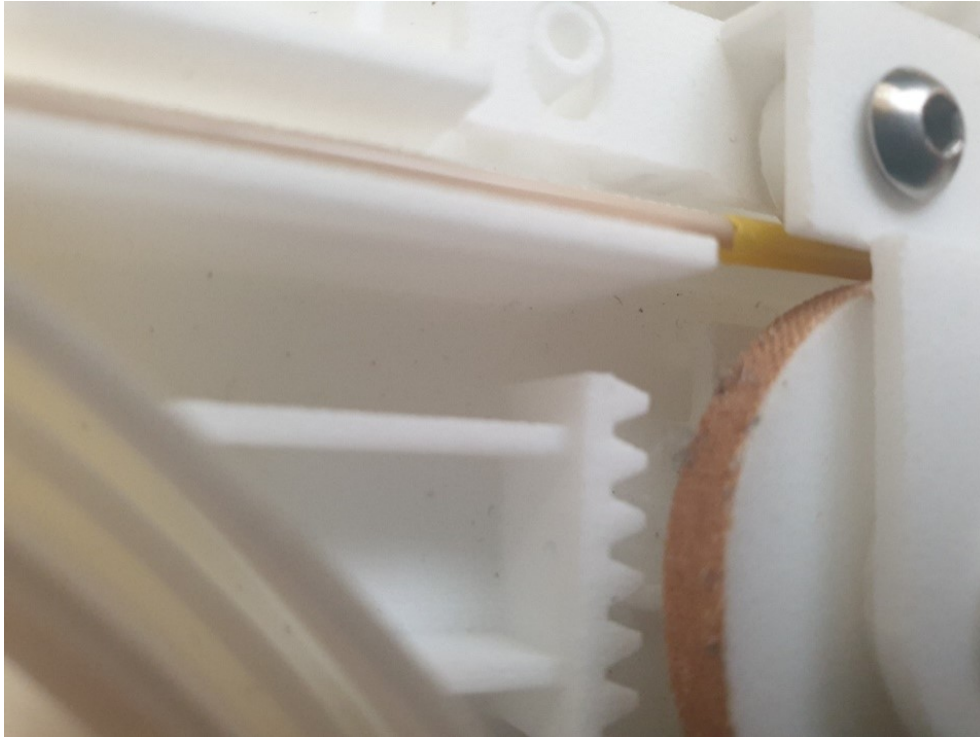


Figure A.15: Close-up of modified Pusher-wheel-gear.

has to be pushed past the stopped-wheel-gear E. This makes moving the mantle unnecessarily difficult.

- V. When mantle or Pusher are coiled up, it is virtually impossible to move them. The friction from coiling them up is significantly too high.

A.4.4 Conclusion

The central issue is the friction exerted by the wheel-gears required to move the mantle and pusher against the other and specifically while coiling up. As seen in Figure A.15, the wheel gears have been modified to increase their friction coefficient and increase their diameter to exert more force on the pusher and mantle. However, the mantle has to move past the pusher-wheel in step 5, as noted in Section A.4.1. The more the pressure and friction of the pusher-wheel-gear E increases, the more friction resists a successful retraction of the mantle. Finally, when the pusher and mantle begin to coil up, the resistance to move them increases drastically, up to the point that they can not be moved without damaging them. Considering that the wheel gears already have trouble moving them at all, it seems unlikely that friction within the handle can be managed to the point that it is operational. Increasing the size of the coil by increasing the bending radius to reduce friction in the coil would further increase the size of the handle. Considering

that the device already has a significant size we must conclude that the coiling approach is not suitable to implement this handle.

A.5 Software Documentation

A software package was developed that allows for the creation, manipulation and analysis of magnetic folding chains. The software was implemented in Python V3.8.0 and the full source code is available on *GitHub* ⁵. The software is dependent on the following openly available libraries:

- *numpy* V1.18.4
- *cupy* v10.1
- *trimesh* v3.9.29
- *scipy* v1.4.1
- *matplotlib* v3.2.1
- *tkinter* v3.8

The following libraries have been implemented

Chain_data_struct:

Contains the Chain object that builds the the data structure for magnetic folding chains. It depends on Component_data_struct, Function_lib and Coord_data_struct. Primary methods of the *CHain* object are:

- *calc_energy*: calculates internal energy for current state;
- *calc_force*: calculates internal forces for current state;
- *calc_torque*: calculates internal torques for current state;
- *set_mag*: sets the magnetic orientation of all components;
- *plot*: plots the chain using *matplotlib* library;
- *append*: appends a component to the chain;
- *remove*: removes a component from the chain;
- *from_types*: creates the chain from predefined archetypes;
- *simulate*: simulates the dynamics of the chain;
- *is_colliding*: calculates is components are colliding in the current state;
- *update_lists*: mandatory step to synchronise component positions;
- *get_centres*: returns absolute position of all components;

⁵GitHub, <https://github.com/THFass/Magnetic-Folding-Simulation-Tools.git>

- *get_angles*: returns relative angles between components;
- *get_state*: returns state of chain;
- *set_angles*: sets all joints in the chain to specific relative angles;
- *set_anglex*: sets the relative angle for a specific joint;
- *set_state*: sets the state of the chain.

Component_data_struct:

Contains the *Component* object, that handles all functionality for a singular component. Provides archetypes for the standardised cubic component defined in Section 4.1.1. It depends on *Magnet_data_struct*, *Coord_data_struct*, *Shape_data_struct* and *Function_lib*. Primary methods of the *Component* object are:

- *update_pos*: updates absolute position in chain;
- *plot* plots specific component;
- *make_next*: creates new component similar to this one;
- *get_Q*: return absolute rotation matrix of the component;
- *get_charge*: returns absolute position and magnitude of all point charges associated with the component;
- *get_centre*: returns absolute position of component;
- *set_mag*: sets magnetisation of the component;
- *set_angle*: sets joint corresponding to component.

Library provides basic magnet shape archetypes, that inherit from the *Component* object:

- *ACube*: Cube archetype "A" as defined in Section 4.1.1;
- *BCube*: Cube archetype "B" as defined in Section 4.1.1;
- *CCube*: Cube archetype "C" as defined in Section 4.1.1;
- *DCube*: Cube archetype "D" as defined in Section 4.1.1.

Magnet_data_struct:

This library contains the Magnet Object that provides functionality for magnet simulation. It depends on *Coord_data_struct* and *Shape_data_struct*.

Primary methods of the *Magnet* object are:

- `copy`: creates copy of the the object;
- `get_charge_abs`: returns absolute position and magnitude of all point charges associated with the magnet;
- `get_charge_rel`: returns relative position and magnitude of all point charges associated with the magnet.

Library provides basic magnet shape archetypes, that inherit from the *Magnet* object:

- *MCube*: Cube shaped magnet;
- *MSphere*: Sphere shaped magnet;
- *MCylinder*: Cylinder shaped magnet.

Coord_data_struct

The library contains the *RefFrame* Obejct that manages all coordinate transformations. Primary methods of the *Component* object are:

- `abs`: returns absolute position;
- `rel`: returns relative position;
- `rotate`: rotates by a specific transformation;
- `rotate_to`: rotates to an absolute transformation;
- `append`: returns *RefFrame* object with this reference frame as origin;
- `get_dcm`: returns absolute rotation matrix;
- `get_abs_axis`: returns axis in absolute transformation.

Shape_data_struct

This library includes the *Shapes* object that provides a framework for geometric shapes. Basic shapes such as sphere, cylinder and cube are currently implemented. support for generic shape via point cloud definition provided.

Function_lib

Is a collection of utility functions. Includes functions for vector algebra, block matrices and piloting.

GUI

Provides an alpha for a graphical user interface to create, manipulate and analyse magnetic chains and is dependent of Chain__data structure.

A.5.1 Primary Method Documentation

The primary functions for a user to interface with the software via text commands are listed together with their input and output in the following;

Chain.create

Inputs:

- *sequence*: is a list of component objects;
- *resolution*: is an arbitrary value corresponding to the number of point charges per magnetic surface. Absolute quantity depends on shape of magnet;
- *upper_boundary*: is a value for maximum angle between components. If not specified, set to 2π ;
- *lower_boundary*: is value for minimum angle between components. If not specified, set to 0;
- *fig*: can contain a handle for a figure to plot into. If not specified or 0 a new figure will be created for plotting. If not specified it is set to 2;
- *dtype*: defines the type of numerical values within the code. Can be used to increase computational speed at the cost of precision. If not specified, set to *numpy.float32*.

Output:

- *Chain*: object

Creates a chain object. Is the same as native *Chain.__init__* method.

Chain.append

Inputs:

- *comp_type*: is an input specifying the the type of component to append to the chain. Valid inputs are component objects or strings from {"A", "B", "C", "D"};

- *phi_0*: specifies the initial angle of the component. If not specified it is set to 0;
- *resolution*: is an arbitrary value corresponding to the number of point charges per magnetic surface. Absolute quantity depends on shape of magnet. If not specified it is set to 3;
- *dtype*: defines the type of numerical values within the code. Can be used to increase computational speed at the cost of precision. If not specified, set to *numpy.float32*.

Output: None

Appends a new object at the end of an exiting chain. Supports standard cube components as defined in Section 4.1.1.

Chain.set_state

Input:

- *state*: is a list of rotation matrices indicating the rotation of each component. Number of entries has to be at least number of components in the chain.

Output: None

Sets all components to a specific absolute rotation given in *state*. If given rotation can not be achieved a close approximation will be made.

Chain.set_state

Input: None

Output:

- *state*: is a list of rotation matrices indicating the rotation of each component. Number of entries equals number of components in the chain.

Returns a list filled with the absolute rotation matrix for each component.

Chain.set_angles

Input:

- *angles*: is a list of relative angles for the chain to be set to. Length of list has to be equal or shorter than number of components.

Output: None

Set all angles to a specific relative configuration.

Chain.set_angle

Input:

- *angle*: is a relative angle for the specific joint to take;
- *index*: specifies the joint that is supposed to be set.

Output: None

Set a specific angle to a specific relative configuration.

Chain.get_angles

Input: None

Output:

- *angles*: is a list of relative angles of the chain. Length of list is equal to number of components.

Returns the current configuration of the chain as a list of all relative angles.

Chain.set_mag

Input:

- *mag*: is a list, tuple or numpy-array with three entries specifying the direction of magnetisation. magnitude of the vector corresponds to maximum surface charge Br_{max} .

Output: None

Set the magnetic orientation of all components in accordance with their current orientation, resulting in all components being magnetised in direction of the input vector.

Chain.get_mag

Input: None

Output

- *mag*: list of numpy-arrays with three entries that indicate absolute orientation of the magnetic polarisation of all magnets in each component, for the current system state.

Output: None

Returns a list of numpy-arrays with three entries that indicate absolute orientation of the magnetic polarisation of all magnets in each component, for the current system state.

Chain.get_fen

Input: None

Output:

- *energy*: numerical value specifying the total potential energy in the system for the current system state in Joules;
- *force*: is a list of numpy-arrays, specifying the force that acts on each component's center of mass in [N];
- *torque*: is a list of numpy-arrays, specifying the torque that acts on each component's center of mass in [Nm].

Chain.plot

Input:

- *plt_hinges*: is a Boolean with true to plot hinges. If not specified it is set to True;
- *plt_charge*: is a Boolean with true to lot the point charges. If not specified it is set to False.

Output:

- *Figure*: returns the *matplotlib* library handler for the figure

GUIMain

Initiating this object will crate a rudimentary graphical user interface that allows for the creation, manipulation and analysis of magnetic chains.

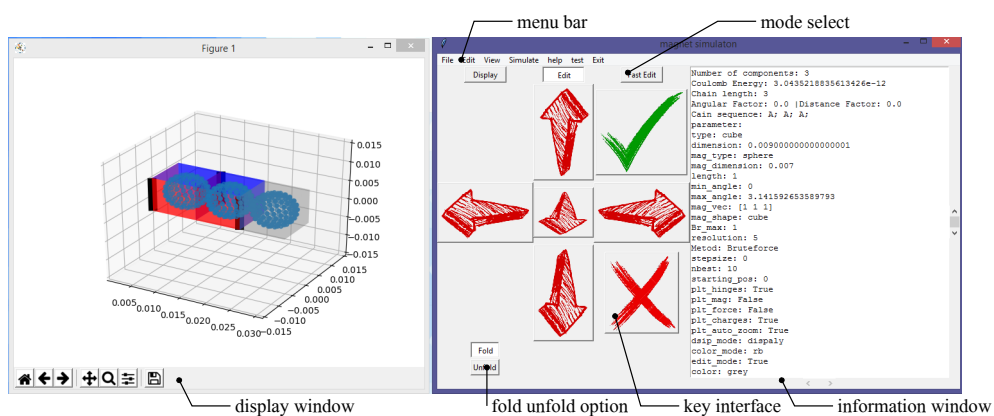


Figure A.16: Graphical User Interface to construct and test magnetic folding chains.