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Roadmap on metamaterial theory, modelling and design

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Roadmap

Roadmap on metamaterial theory, modelling and design

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Abstract

This Roadmap surveys the diversity of different approaches for characterising, modelling and designing metamaterials. It contains articles covering the wide range of physical settings in which metamaterials have been realised, from acoustics and electromagnetics to water waves and mechanical systems. In doing so, we highlight synergies between the many different physical domains and identify commonality between the main challenges. The articles also survey a variety of different strategies and philosophies, from analytic methods such as classical homogenisation to numerical optimisation and data-driven approaches. We highlight how the challenging and many-degree-of-freedom nature of metamaterial design problems call for techniques to be used in partnership, such that physical modelling and intuition can be combined with the computational might of modern optimisation and machine learning to facilitate future breakthroughs in the field.

Keywords: mechanical, electromagnetic, modelling, artificial intelligence, homogenisation, optimisation, acoustic

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Introduction

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The growth of metamaterial science has brought to the fore the power of micro-structuring materials to achieve previously unattainable properties. Metamaterial-based breakthroughs have had wide-ranging technological implications, including realising materials with effectively negative material parameters [1, 2], allowing for design freedoms such as the ability to finely tune highly anisotropic properties [3] or practical considerations such as being able to greatly reduce mass. However, the often complex and many-degree-of-freedom nature of the small-scale geometries that have facilitated these breakthroughs come with associated challenges. Traditional direct numerical simulations can incur significant computational costs (due to the need to use very fine meshes). This, combined with the high-dimensional associated parameter spaces, can render design problems computationally intractable. As a result, researchers have developed a variety of strategies to characterise metamaterials' properties, seeking approaches that greatly simplify problems while still capturing the material's key features.

The pre-eminent approach to succinctly characterising metamaterials is to use asymptotic homogenisation to capture their 'effective' properties. These techniques have a long history in mathematics [4, 5] and are based on the principle that very small-scale periodic structures (which are, for example, at least an order of magnitude smaller than the operating wavelength) can be averaged out. As a result, it is possible to derive a homogeneous material (possibly with some strongly anisotropic or dispersive properties) that displays the same properties as the metamaterial in question (up to some quantifiable errors). It was within this framework that the possibility to create materials with effectively negative permeability and permittivity were created, paving the way for negative refraction [6].

Homogenisation is still at the heart of many of the most important breakthroughs in metamaterial science. In this Roadmap, we will explore how homogenisation strategies have been developed to meet the various needs of the broad and scientifically diverse field of metamaterials. This has included materials with local resonances and strong local dispersion as well as strategies for describing effective properties at non-zero frequencies. Similarly, the contributors will highlight some of the remaining challenges in this domain.

Given the many degrees of freedom available when designing a metamaterial, such design problems are ideal candidates for treatment through numerical optimisation. This Roadmap will explore strategies for topology optimisation as well as recent applications of artificial intelligence (AI). Consistent with the rapid growth in the usability and accessibility of machine learning for problems across the physical sciences, the use of data-driven approaches for designing metamaterials has grown rapidly in recent years. This Roadmap will cover some of the highlights of these breakthroughs and focus on some of the key challenges, particularly related to assembling the quality and quantity of data needed to facilitate data-driven design.

Several of the main challenges and opportunities in the field of metamaterial modelling and design are related to resolving the differences in scientific approach and philosophy between physics-based modelling and data-driven methods. These two schools of thought can occasionally seem to be at odds with one another, but they have the potential to unlock and accelerate breakthroughs when combined effectively. For example, physics-based models (based on techniques such as homogenisation) have an important role to play in offering concise frameworks for numerical optimisation and machine learning. Conversely, the complexity and high dimensionality of metamaterial design problems mean they stand to benefit significantly from the unparalleled insight possible through modern computation and machine learning. Combining these two sometimes disconnected communities is a major opportunity for the field. The applied metamaterials and engineering communities are ideally placed to manage the synergy between generative AI and rigorous, physics-based techniques, offering intuition and efficiency while also ensuring adherence to the laws and safety regulations. In this way, the development of AI techniques is envisioned to support and augment human creativity, where AI-generated ideas can be fine-tuned, experimentally validated and assessed considering complex regulatory and ethical frameworks.

This Roadmap contains contributions from leading experts in the field which outline the cutting edge and highlight some possible avenues to overcoming the most important challenges. The 16 sections cover a diversity of physical regimes, including electromagnetism, acoustics, mechanical metamaterials and water waves. The contributions are grouped into four main sections. First, analytic approaches (such as homogenisation and other analytic methods) are covered, reflective of the field's roots in asymptotic homogenisation. Following this, numerical methods are considered, ranging from numerical topology optimisation strategies to data-driven machine learning approaches. In the third part, the contributors will cover some of the most exciting frontiers in metamaterials science and explore the new modelling and design challenges that have arisen as a result. This will include time-modulated metamaterials, quasicrystalline metamaterials, polaritonic metamaterials and active metamaterials. Finally, the Roadmap will end with two contributions exploring the theoretical challenges posed by designing metamaterials for industrial applications, such as for biomedical engineering, soft robotics and ocean wave energy harvesting.

The broad and multi-disciplinary nature of metamaterial science means that its grand challenges require breakthroughs in many different areas of science. In this article, we have focused on theoretical, modelling and design challenges. Other notable challenges are, for example, the need to develop scalable manufacturing techniques and to develop metamaterials for use in extreme environments (such as the extreme temperatures experienced in space).

1. Modelling in mechanical metamaterials

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Status

Progress in mechanical metamaterials research has attracted significant attention in the past decade, resulting in a plethora of designs with distinct complex geometries and mechanical characteristics [7]. Exploration into multifunctional metamaterials is also growing, with a focus on seamlessly integrating constitutive properties with additional functionalities such as thermal conductivity, acoustic insulation, and electromagnetic (EM) response. This has also led to an increasing shift towards nonlinear and tuneable metamaterials [8], emphasising the quest for dynamic control and adaptability in response to varying conditions. The interplay between the structural components of metamaterials and their responses to stimuli is evolving into a focal point of study, drawing inspiration from other complex systems such as active matter that exhibit emergent behaviours and dynamic transformations [9].

These increasing complexities and multiphysics requirements demand the development of sophisticated mathematical and computational tools to allow the accurate representation and analysis of these systems. Of these, Finite Element Analysis and Topology Optimisation are central, allowing precise customisation of mechanical properties by strategically distributing matter within structures. Principle to these modelling approaches is the underlying structural system of smaller constituents, the meta-atom (figure 1), from which large-scale properties emerge. However, often the microscopic representation of these structures is not efficient when applying these modelling tools due to the large number of degrees of freedom that need to be resolved, resulting in a computationally expensive design process. Modelling methods that reduce the computational cost, whilst capturing the relevant phenomenology, are therefore in high demand. Developing these tools will enable the efficient characterisation of highly complex metamaterials with multiphysics interactions, enabling the realisation of their purported industry application potential from within the research community.

Current and future challenges and opportunities

Homogenisation techniques, where at the long wavelength limit the micro-structured material behaves like a homogenous material [14], remain indispensable for predicting macroscopic properties. Recent advancements have highlighted their computational efficiency, particularly when dealing with the complexities of large-scale metamaterial systems [15]. Key to the successful application of these methods is correctly capturing the quasi-static phenomenology of meta-atoms—even though generalisations to a dynamic scenario are also relevant [9, 10].

To characterise the phenomenology of meta-atoms, there exist useful mathematical tools in the following fields: rigidity theory; topological mechanics; nonlinear mechanics and stability theory. These tools can capture the emergent behaviour from meta-atoms and are applied to design metamaterials. For instance, rigidity theory allows for the design of Origami inspired metamaterials, where the crease pattern of these structures prescribe their kinematics and can be designed so that the underpinning mechanism has a single degree of freedom, i.e. the Miura-ori crease pattern (figure 1(a)). Moreover, rigidity theory is applied to determine the behaviour that dominates the bulk properties: e.g. nodal connectivity of the octet truss (figure 1(b)) results in stretching dominated behaviour. Alternative meta-atoms may be dominated by bending or membrane forces (e.g. beams, plate or minimal surface-based topologies [7]), enabling the effective design of structures with a diverse set of properties.

In parallel, within topological mechanics, there is a pronounced focus on manipulating robust properties, such as soft edge modes, offering an additional layer of tuneability. This can be leveraged to control failure modes, such as the buckling location of a polarised kagome lattice [12] (figure 1(c)).

Additionally, non-linear mechanics stands out for its potential in deliberately engineering instabilities as a means of functionalization, thus enabling controlled responses like energy absorption or precisely orchestrated deformation under specified conditions [8]. Meta-atoms that exhibit snap-through instability are one such example (figure 1(d)).

While traditional homogenisation techniques are commonly applied to attempt to model these phenomena, such theories are often limiting us to systems that assume infinite repetition of meta-atoms and typically they do not manage to capture large deformations, complex loading paths, and evolving microstructures. These challenges manifest as the microstructural length scale approaches the size of the macrocomponent or the length scale associated with macroscopic spatial variability [16]. In such instances, the introduction of higher-order gradients or non-local continua becomes necessary to capture size effects and derive a higher-order constitutive response without requiring assumptions at the macroscopic level.

Advances in methods and techniques to meet challenges

Currently, one way in which these challenges are navigated is through a computational homogenisation approach, involving the utilisation of two interrelated boundary value problems for both macroscopic and microscopic evolving geometries [15, 17]. However, placing more emphasis on an analytical understanding of higher-order homogenisation techniques could be immensely beneficial in providing fundamental insights into challenging questions. These include forward homogenisation, focused on extracting effective material properties from a known microstructural architecture, and inverse homogenisation, which seeks to identify microstructures that exhibit a specified combination of target properties. Furthermore, an

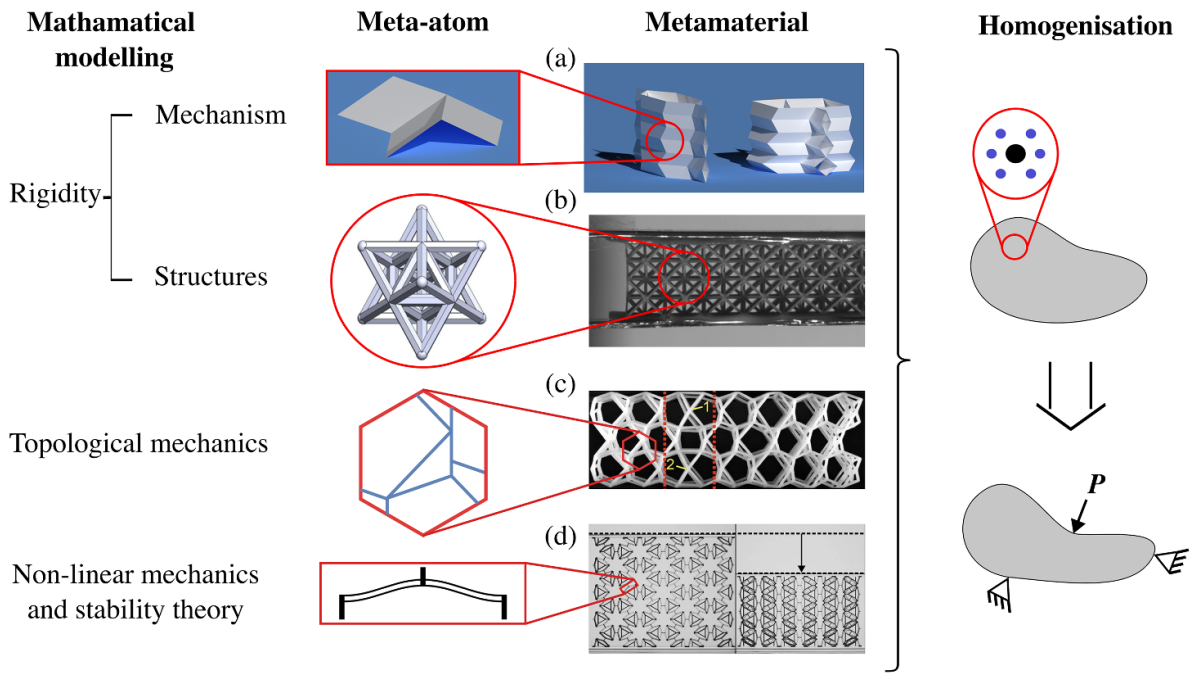

Figure 1. (a) Miura-ori pattern. Reprinted from [10], Copyright (2021), with permission from Elsevier. (b) Octet truss. Reproduced from [11]. CC BY 4.0. (c) Topological metamaterial. Reproduced with permission from [12]. (d) Phase transforming cellular material. Reproduced from [13]. CC BY 4.0.

analytical focus would yield additional advantages, such as eliminating the need for constitutive assumptions regarding overall material behaviour, accommodating large deformations and rotations at both scales, and being applicable to arbitrary material behaviours, including nonlinearities and time-dependency.

Yet, another challenge lies in current trends in nonlinear and tuneable metamaterials [8]. Homogenisation techniques that can capture nonlinear behaviour in metamaterials present a significant mathematical challenge, as bifurcations occurring at the meta-atom scale are closely linked to the loss of rank-one convexity observed at the macroscopic scale [18, 19]. Such energy functionals may, for instance, explain global properties driven by instabilities, phase transformation such as the formation of shear bands, and softening behaviour.

The predominant focus in the modelling of mechanical metamaterials has centred on the constitutive behaviour of meta-atoms. However, the multidisciplinary nature and broad applications of these structures necessitate a more comprehensive understanding of meta-atoms' interaction with other multiphysics phenomena such as thermal conductivity, acoustic damping and electromagnetism. The coupling and resolution of the multiphysics inherently increases the complexity of the models and requires theories that are thermodynamically consistent at the scale of the meta-atom. Addressing this need introduces a set of challenges in the homogenisation modelling of mechanical metamaterials. Firstly, achieving a seamless integration of physical phenomena into a unified model poses a significant hurdle. This requires accounting for couplings of these multiphysics interactions. Secondly, the variability in material properties at smaller scales, alongside the nonlinear behaviours exhibited by mechanical metamaterials, complicates the modelling process. Thirdly, the scale discrepancy across multiple length scales demands computationally intensive multiscale modelling techniques.

Concluding remarks

A mechanical metamaterial, a complex system of smaller constituent materials or meta-atoms, showcases transformative potential where collective characteristics surpass those of individual components. By leveraging this potential, many innovative metamaterials are being developed to improve the performance of structures in our built environment. These structures often have complex geometries and increasingly require the coupling of their mechanical properties with other multiphysics properties, resulting in significant computational cost when attempting to characterise their behaviour. Homogenisation methods show great potential in addressing this issue, by reducing the complexity and therefore computational cost. However, significant steps are needed to augment these methods to capture large deformations, complex loading paths, evolving microstructures and coupling with other multiphysics phenomena accurately.

Providing an accurate homogenised description of metamaterial simplifies their design process, opening up new possibilities for the creation of metamaterials that not only passively respond to external factors but actively adapt their mechanical properties, presenting a paradigm shift towards materials that can autonomously navigate and adjust in a dynamic and unpredictable environment. Discovering more advanced modelling techniques and principles will signal a new era in metamaterials, crafted not only for strength, but also for dynamic, responsive, and adaptive functionalities.

2. Analytical methods in metamaterial design

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Status

In 1967 Victor Veselago proved that negative-index materials and superlenses are possible by employing analytical methods. Thirty-three years later, when these material where obtained experimentally, this opened up a new subdiscipline of physics and engineering: metamaterials [20]. Likewise, many analytical methods which are now used to study and design metamaterials pre-date the field of metamaterials, for example, methods to analyse periodic materials. Metamaterials possess unusual properties due to the internal structuring of the material. In particular, if the parameters of the internal structure change, then the properties change. This means that in order to design metamaterials we should be able to tailor the parameters to achieve desired effects. The advantage of using analytical methods is that in an ideal situation the material properties are expressed in terms of the parameters. This offers a huge advantage over methods that simply provided properties for given parameters and then require numerous trial and error in order to find the right parameter sets.

In most realistic situations it is currently not possible to obtain desired properties of a material expressed in terms of the structural parameters. Nevertheless, analytical methods are useful in designing metamaterials when used in conjunction with other methods

1. Employing partially analytical methods can dramatically speed up computation. Some hybrid methods are frequency independent or allow to reuse part of the computed solution for large parameters spaces [21].
2. Analytical methods can help increase accuracy especially since many interesting behaviours can occur at 'singularity' or resonances [22].

In this section we will concentrate on analytical methods other than homogenisation, which has been covered in other sections.

Current and future challenges and opportunities

There is a huge variety of different metamaterial, in this section we will concentrate on phononics/photonic crystals which have been extensively studied using analytical methods [23]. In the simplest setting they are 2D and doubly periodic materials with a repeated unit cell. When the unit cell is simple there are exact analytical solutions. The challenge is to be able to extend these analytical results to more realistic settings by:

1. Changing the unit cell from the simplest point scatterer to consider much more complicated unit cells [23];
2. Extending to 3D were some of the analytical methods need significant modifications;
3. To allow for edges and corners in the periodic material [24];
4. To model variation in parameters from cell to cell (which can be a change is size or spacing), they are refereed as graded metamaterial or rainbow metamaterials;
5. To consider some local/non-local perturbations to the periodic structure which can lead to interesting effects such as localisation [25].

When addressing the challenges outlined above it might be possible to design hybrid analytical/ numerical methods that allow to capture the key behaviour analytically and use this within a numerical scheme to make it versatile and easy to use.

Advances in methods and techniques to meet challenges

A good example of the advantage of understanding the nature of the phenomena comes from the study of black-hole waves [22]. By studying the associated eigenvalue problem, it is shown that the local behaviour at the corner is analogous to the behaviour at infinity. This allows to pick the correct mesh at the corner for the finite element computation to capture the black-hole waves well. In fact, it is shown that there is a transformation which maps the corner behaviour to a region at infinity. The idea of picking a correct transformation is key in other areas of metamaterial design, for example cloaking [26]. Other applications which have been extensively studied mathematically are filtering and polarisation [23] as well as localisation [25].

One interesting feature of periodic structures is the possibility of resonance effects [23]. In the context of array scattering, it is frequently referred to as Wood's anomaly. Typically, around the resonant state, interesting phenomena can be observed such as, for example, abnormal transmission or reflection [27]. Also, some frequently used models for example Foldy's approximation can give non-unique solution at these frequencies [24]. This is different to the existence of Rayleigh–Bloch waves (modes that propagate along the grating and decay exponentially in orthogonal directions) which can also lead to non-uniqueness in certain circumstances [28].

The key in obtaining correct solution fast is to capture the correct behaviour. Matched asymptotic expansion is a popular analytical method which allows to capture the key singular behaviour in different regions and then match the solution together [29]. Also, there are a number of methods that allow to pose an ansatz made up of functions capturing the singular behaviour and then use numerical methods to find the coefficients of the ansatz numerically [21]. Sometimes the singular behaviour can be eliminated by looking at the integral in the complex plane and deforming the contour, this is for example used in the Wiener–Hopf technique or Cauchy's theorem to deal with removable singularity [24].

Concluding remarks

Modelling wave propagation through metamaterials frequently results in difficult to solve integral equations. Analytical methods played a central role in solving them prior to computers making numerical methods readily available. Now analytical methods are a valuable tool in designing hybrid numerical schemes which can offer the advantage of accuracy and speed over conventional numerical methods. Further developments are required to make the hybrid methods more flexible, versatile and user-friendly to increase their use in designing metamaterials. In the meantime, the analytical understanding of metastructures might be used to perform computations and solve equations instead of a computer [20].

3. Two-scale homogenisation of high-contrast subwavelength resonances

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Status

For a periodic array of high-contrast 'soft' inclusions within a 'stiff' matrix of comparable density (figure 2), waves of the same frequencies produce much shorter wavelengths in the inclusion material compared to the matrix. If the inclusion's wavelength is comparable with their size, the frequencies are comparable with the inclusions' natural frequencies while we are in a long wavelength regime relative to the matrix. This is reflected in a two-scale asymptotics of Bloch waves, which displays a frequency bandgap opening near the subwavelength inclusion resonances. This was probably first formally observed in [30] and then made mathematically rigorous in [31, 32]. Auriault and Bonnet [30] also provided interpretations in terms of frequency-dependent as well as sign-changing effective density and related time-nonlocality. In the context of electromagnetism, similar effects were rigorously interpreted in [33] in terms of artificial magnetism. Analogous effects are observed for highly anisotropic periodic fibres, see [34] where for a scalar static model the macroscopic equations are shown to be spatially non-local. This was advanced in [35], where more general 'inter-connected' partially degenerating elastic inclusions serve as generalised micro-resonances. Resulting two-scale formal asymptotics suggests behaviours with a Willis-type coupling in the macroscopic constitutive relations and related coupled directional and frequency gaps. Two-scale homogenisation and spectral convergence for another model with a partial degeneracy is studied in [36], for stiff in compression but soft in shear elastic inclusions. A general convergence theory for two-scale homogenization of partially degenerating systems with periodic coefficients was developed in [37]. The emergence of localised modes due to defects was established for high-contrast periodic media (accompanied by error bounds) in [38], and recently for some high-contrast stochastic media in [39]. In [40], bandgap opening in high-contrast periodic elastic beam lattices was shown. An exciting recent development is on constructing two-scale type operator approximations with error bounds, see [41] and numerous references therein. Such approximations were first constructed in [42] for a basic scalar high-contrast model, and then developed further in e.g. [43] which has also uncovered certain macroscopic dispersive properties at high contrasts. In [41], a general approach was developed constructing such approximations for a broad class of multi-scale problems in terms of associated two-scale limit problems and a 'connecting operator' J_ε. The latter provides a key link between the original oscillatory and the two-scale limit problems, and appears to be a composition of certain 'translation' operators and a 'two-scale interpolation operator' I_ε (as well their more abstract analogues). Operator

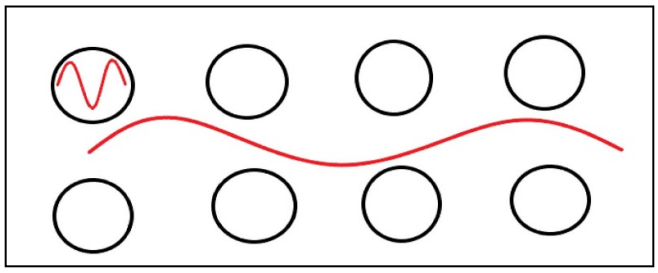

Figure 2. A basic configuration: inclusions of 'soft' material periodically distributed within a matrix occupied by a 'stiff' material. As a result, the wavelength in the inclusion material is much shorter than in the matrix material (both wavelengths are visualised in red). If the former is comparable to the inclusion size, one is in a micro-resonant regime. With the macroscale comparable with the matrix wavelength, the inclusions serve as subwavelength resonators.

I_ε was introduced, in an equivalent form, in [44] under the name of 'periodic two-scale transform', and appears to be a two-scale version of a classical Whittaker–Shannon interpolation from signal processing.

Current and future challenges and opportunities

The field of high-contrast homogenization, developed over the last 40+ years, is receiving a renewed interest from the point of view of metamaterial modelling thanks to the importance of locally resonant materials for realising metamaterials [3, 45–47]. Indeed, for the underlying mathematical models with a strong interaction between micro and macro-scales, related two-scale type approximations are often capable of displaying certain non-standard and unusual effects in an asymptotically explicit way. This often clarifies the nature and the microscopic mechanism of the observable macroscopic effects (such as the role of the micro-resonances in bandgap opening, frequency and directional dispersion and localisation, etc). A key general challenge here is to construct tractable but accurate approximations of two-scale type, with controllably small error. The mathematical approach is often capable of achieving this in a systematic and rigorous way, leading to tractable approximate models with tight error bounds. Works like [41] provide certain new mathematical tools for achieving this, both in part of constructing improved approximations and controlling the errors, for a broad class of multiscale scenarios. This is so far restricted however to although broad but still quite specific class of models, which generalises those infinitely periodic and obeying certain 'spectral gap' condition (the latter rules out, for example, models with highly anisotropic fibres and their further extensions like in [34, 35] with associated additional interesting effects). A challenge is therefore to tackle such models, as well as physically more realistic problems in bounded domains, higher-order, time-dependent, and non-periodic problems. The latter may range from locally-periodic models to fully random ones. Indeed, if one allows for certain randomness of the micro-resonances, the inclusions' eigenvalues vary and each inclusion tends to capture

the energy at frequencies close to its natural frequencies. As a wide range of such eigenfrequencies is represented, the inclusions may collectively try to prevent the wave from propagation. This may lead to some interesting phenomena like localisation due to the collective effect of random micro-resonances. A very challenging open problem is to analyse this rigorously, i.e. to control the macroscopic effect of all the interactions of the high-contrast micro-resonances with the macroscopic field and each other.

Advances in methods and techniques to meet challenges

To address the above as well as various other challenges, one may need to advance some recently developed methods in new and exciting ways. The approach developed in [41] is based on very few basic principles and looks promising for its further advance in diverse directions. Indeed, it allows to identify very few generic features of multiscale problems for which two-scale type approximations with error estimates can be constructed. In particular it allows to naturally arrive at such versatile tools as the above mentioned two-scale connecting operators, which bear all the desirable properties and can in principle be used on their own, i.e. even when the Floquet–Bloch transform (from which it was derived in the first place) may be not anymore directly applicable. This opens-up avenues for the approach's potential applicability to locally periodic problems, problems with boundaries, etc. For tackling the problems with locally periodic (two-scale) coefficients, an emerging exciting prospect is to develop a natural two-scale analogue of semiclassical pseudodifferential calculus. Moreover, the approach of [41] is based on analysis of a general family of asymptotically degenerating variational problems, i.e. not necessarily coming from the Floquet–Bloch transform, with one example of such other families—for 'concentrated perturbations'—already treated in [41]. This also makes the underlying ideas potentially applicable to other non-periodic problems, which could include quasi-periodic problems as well as some random ergodic ones. That may require advancing the approach of [41] e.g. in the direction of relaxing the spectral gap condition, or combining it with some other recently advanced techniques see e.g. [48], which could also allow tacking some of the other open problems mentioned above. Another possible exciting direction is towards development of new asymptotic-numerical hybrid approaches for multiscale problems, cf. precedents in asymptotic-numerical hybrid methods in high-frequency scattering [49] as well as in numerical analysis of some wave problems in high contrast heterogeneous media [50, 51]. Indeed, the approach of [41] approximates (with a controllable error) the highly oscillatory solutions of the original problem by non-oscillatory solutions of (higher-dimensional) two-scale limit problems, with the two linked by a two-scale connecting operator. The latter involves data sampling and interpolation, and it may be an exciting challenge to combine the asymptotic approaches with numerical ones for achieving controllably accurate computable approximations for a wide range of scale separation parameters.

Concluding remarks

High-contrast two-scale homogenization is a field with several decades of history. In the context of wave propagation, the critical scaling between the two small parameters of the spatial scale separation and contrast appears to be a micro-resonant scaling. Renewed interest to this area in the context of metamaterial modelling is due to the two-scale asymptotic models' ability to display often unusual macroscopic physical effects in an asymptotically explicit way, clarifying the nature and the microscopic mechanism of the observable effects due to the subwavelength resonances. Recent advances make substantial progress on constructing improved approximations of a two-scale type with a controllable error for a broad and growing set of models of physical interest. Most recent developments provide exciting opportunities for addressing current and future challenged in metamaterial modelling.

4. High-frequency homogenization for periodic media

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Status

Metamaterials are known for their unique properties arising from their internal structure. When this structure exhibits periodicity, effective properties describing these materials can be derived using asymptotic methods [14]. These methods offer numerous advantages:

- The effective properties mimic those of a homogeneous medium, providing analytical insights into wave behaviour more readily than within the microstructure itself.
- Eliminating the need to mesh the fine scale of the microstructure results in significant computational efficiencies.
- These models can serve as a solid foundation for topological optimization or inverse design strategies.

A classical setting for these methods is the low-frequency regime where the typical wavelength is much larger than the periodicity of the material. This results in an effective macroscopic equation for the fields and an approximation that is valid near the origin of the dispersion diagram, i.e. in the quasi-static regime.

However, intriguing phenomena specific to metamaterials emerge at higher frequencies, such as Bragg band gaps where propagation is inhibited, or Dirac points that form the basis for topological considerations. High-frequency homogenization techniques, introduced in [52], enable the extraction of effective properties for the media when the wavelength is comparable to the periodicity, facilitating a deeper understanding of these materials at different frequency ranges.

High-frequency homogenization relies on identifying a specific point on the dispersion diagram and its associated eigenfunction, see figure 3. The eigenfunction represents the rapid-scale variations, which are predominant phenomena at high frequencies, such as standing waves at the corners of the Brillouin zone. Through high-frequency homogenization, an effective equation for the long-scale function that modulates the eigenfunction around the identified point on the dispersion diagram is derived, along with an approximation of the dispersion relation. This process encapsulates all relevant information about the physics and geometry in the effective parameter (or tensor) present in the effective equation for long-scale modulation function.

The methodology has been applied successfully across a wide range of configurations, including discrete lattices, frame structures, optics, elastic plates, full vector wave systems, elastic composites, reticulated structures, imperfect interfaces, dispersive media. Furthermore, progress has also been achieved in considering source terms, closely located branches of the dispersion diagram [53], and time domain derivations.

Current and future challenges and opportunities

While significant progress has been made in adapting high-frequency homogenization to various scenarios, there are still several challenges that need to be addressed in dealing with more realistic or unconventional settings.

An intriguing scenario involves metasurfaces, where the periodic structure is confined to a single surface rather than the entire space. These metamaterial categories are compelling for size reduction and wavefront manipulation but necessitate specific asymptotic methods to model the boundary effects occurring at the transition between the structured surface and the homogeneous embedding medium.

Moreover, while many metamaterials are based on periodic structures, quasiperiodic materials showcase intriguing wave scattering and transmission properties, offering the potential to greatly broaden the design possibilities for metamaterials. However, transferring the well-established characteristics of wave phenomena from periodic media to quasiperiodic media presents a substantial challenge. Effective properties have been studied at low-frequency [54] and recent mathematical research has concentrated on extending Floquet–Bloch theory [55] and characterising super band gaps [56]. Developing a high-frequency effective model could bolster these efforts and address the scarcity of mathematical techniques, which has prevented the widespread utilization of quasiperiodic media thus far.

Another topical issue is the case of time-modulated media, where properties vary both in time and space. This emerging class of materials has garnered considerable attention due to its potential for wave manipulation, such as enabling non-reciprocal behaviour. Despite some efforts at low frequencies to propose effective models capturing this effect [57–59], addressing this issue remains an open question at higher frequencies. A deeper understanding of the unique dispersion diagrams that exhibit asymmetric band gaps in frequency or unusual gaps in wavenumber could be of significant interest and importance.

Advances in methods and techniques to meet challenges

At low-frequency, effective models are built for metasurfaces thanks to matched asymptotic expansions [60]. They allow to end up with effective jump conditions encapsulating the geometry and the physics of the microstructured surface. These effective jump conditions are able to take into account the boundary effect mentioned above and to provide valuable insights into scattering coefficients. There is a desire to expand these methodologies to address higher frequency scenarios. This could then be a basis for topological optimization

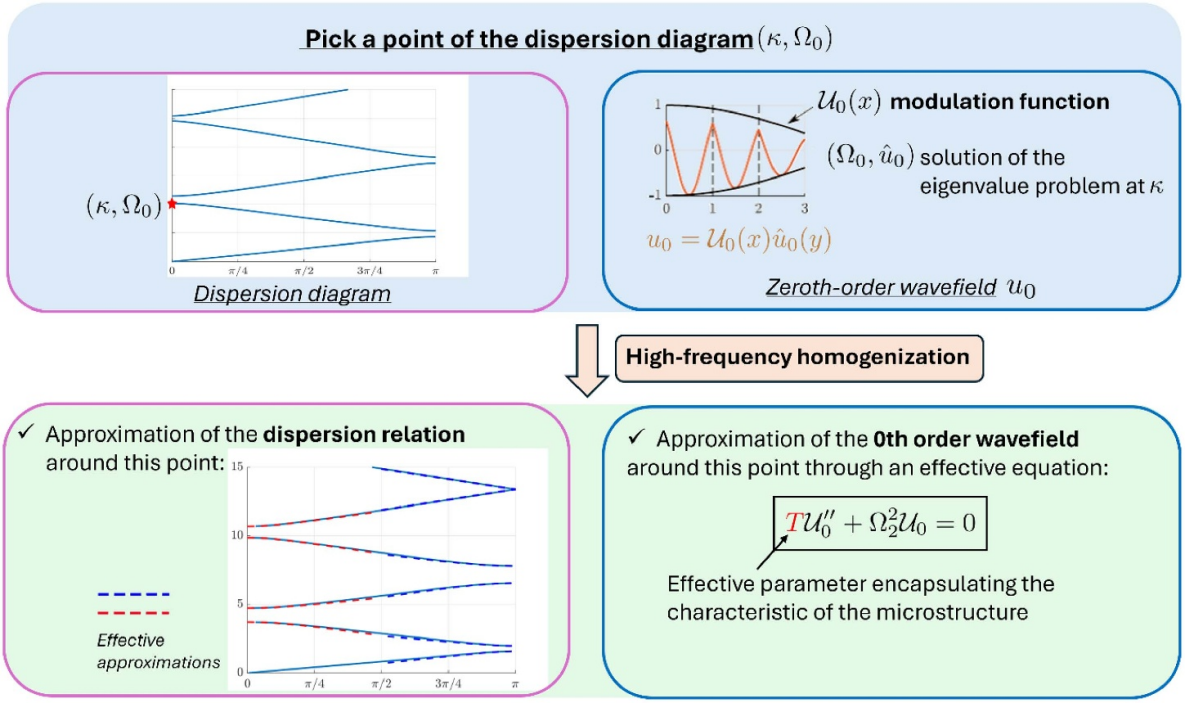

Figure 3. Schematic representation of high-frequency homogenization process in 1D.

techniques [61] of the microstructure in order to optimize the characteristics of the bandgaps or the dispersion.

Getting effective properties at low frequency for quasicrystals [54], or the extension of Floquet–Bloch theory to quasi-periodic structures [55], involves lifting the problem onto a higher-dimensional problem with periodic coefficients. In the higher-dimensional space, the equation obtained is degenerate and more intricate to solve. However, once this problem addressed, information about the physical quasi-periodic system can be obtained by projecting back the solutions into the real space. However, the adaptation of high-frequency homogenization to this scenario remains a complex challenge. While applying high-frequency homogenization to the periodic higher-dimensional space appears feasible, establishing a connection to an effective equation for the real space is not a straightforward step. Another strategy could be to consider periodic approximants of the material [56], with however similar questions regarding the connection with an effective equation for the physical quasi-periodic problem.

Regarding time-domain media, recent theoretical works have been conducted for a laminate whose properties are modulated in a wave-like fashion. This unique setup enables the consideration of a moving frame where properties are dependent on a single variable, facilitating the application of standard techniques like the Floquet–Bloch theorem. This framework could serve as a foundation for the advancement of high-frequency methods. However, one should be careful regarding the model precision equivalence in both frames. Additionally, addressing gaps in wavenumber is expected to require a special care beyond current high-frequency homogenization treatments. Extending this analysis to other space-time modulations remains an ongoing area of exploration.

Concluding remarks

High-frequency homogenization has proved to be numerically efficient, enabling a deeper understanding of wave behaviour across a wide range of frequencies. This technique has been successfully applied to various metamaterial configurations. Expanding the application of this method to new areas will require to address open questions but could play a crucial role in the modelling of the next generation of metamaterials. For example, metasurfaces, time-varying materials or quasi-periodic media, which are fast-developing research areas, would benefit from the development of high-frequency asymptotic techniques.

5. Adjoint based methods for the design of large-scale non-periodic electromagnetic materials

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Status

Electromagnetic scattering problems are typically cast in terms of a known material distribution and an incident, or source field. A variety of numerical and analytical methods can then be applied to solve Maxwell's equations for the full electromagnetic field. By contrast, *inverse design problems* are characterised by having the full solution, often only part of it, specified from the outset. One must then devise a way to find the material distribution that yields this field for a specific input wave. Solutions to such inverse problems are crucial for designing metamaterial-based devices that can address key challenges in energy, healthcare and defence.

Topology optimization via the adjoint method has recently emerged as a route to solve inverse design problems in electromagnetics [62]. The adjoint method simplifies the problem of finding the gradient of a figure of merit into two field calculations a 'forwards' field and an 'adjoint' field. As only two field evaluations are required to find how to change the structure at every single point in space, this technique is extremely numerically efficient and can be applied to a huge range of problems. For example, it has enabled the design of mode sorters [63], beam steering devices [64, 65], and even structures that can solve integral equations [66]. Nevertheless, while extremely powerful, in certain contexts the adjoint method can produce graded structures that are challenging to fabricate.

One way to alleviate both the problem of simulating aperiodic metamaterials, and the complex fabrication requirements of adjoint based designs is to concentrate on designs that use an aperiodic distribution of known resonators. Treating such an array as a collection of dipole (or higher order multipole) scatterers greatly simplifies the computational complexity (as depicted in figure 4). Recently, methods have been developed that begin from a particular distribution of scatterers and iteratively move them in order to increase some figure of merit, thus solving the inverse design problem [64, 67]. Treating all scatterers as dipoles enables the calculation of the gradients of figures of merit analytically, making this technique both much more numerically efficient than full wave simulations, and leads to designs that are straightforward to fabricate.

Current and future challenges and opportunities

Despite great progress over the last few decades in solving the inverse design problems, many open challenges remain. For several applications, such as next-generation communications, there is a desire for devices to operate over a wide frequency band, something which is often neglected in inverse problems. Typically, performance over a large band is achieved by stacking resonances [68], however this requires many independent designs. Instead, one might define a figure of merit in terms of the bandwidth of a system and seek to optimise this algorithmically. This would allow for precise control over the frequency response, allowing for peaks or nulls to be placed arbitrarily, while retaining the convenience of existing fabrication techniques.

There has also been a great deal of recent activity in designing materials that vary in time as well as space: here the inverse design problem is largely unexplored. This new class of material shows great promise for the manipulation of the frequency content of a wave, however the question of how to modulate a material to achieve a desired spectrum remains open. A formulation of the adjoint method in the time domain was recently proposed [69], although has yet to be fully exploited.

Finally, the ability perform inverse design in real time might benefit the application of reconfigurable intelligent surfaces (RISs) to communications challenges. The real-time reconfigurability of these surfaces is often electronic and it is desirable to adapt the EM environment as quickly as possible. If one had reliable physical model that could be quickly evaluated [70], or access to a feedback loop, one could update the structure to manipulate the EM field in real-time. This would allow, for example, a beam to track a moving target. While at lower frequencies, the elements of a RIS can reasonably assumed to be strongly subwavelength thereby scattering as dipoles, at higher frequencies they resonators may be larger with respect to the wavelength causing the dipole approximation to break down (something that could be mitigated through including higher order multipoles, although this comes at the expense of greater numerical demands).

Advances in methods and techniques to meet challenges

To address the challenges presented above, several potential advances to the adjoint method and dipole-based design techniques will be required. Manipulation of the bandwidth of materials using the adjoint method might require a way to algorithmically distribute different materials with different dispersion properties in space, to achieve the desired effect. Alternatively, a range of resonances could be employed for example mixtures of dipole, quadrupole, octupole etc. resonators could be distributed in space. While the theory of collections of interacting multipolar resonators is well developed, the application of this to design scattering systems has yet to be explored.

Applying the usual inverse design techniques to time-varying systems presents a more fundamental challenge. A key feature of the adjoint method is that reciprocity is exploited to convert a gradient evaluation into two field calculations. For time-varying materials, which are not reciprocal, how to formulate the adjoint field remains an open question, although some progress has been made in the context of non-reciprocal materials [71]. There will then be many challenges related

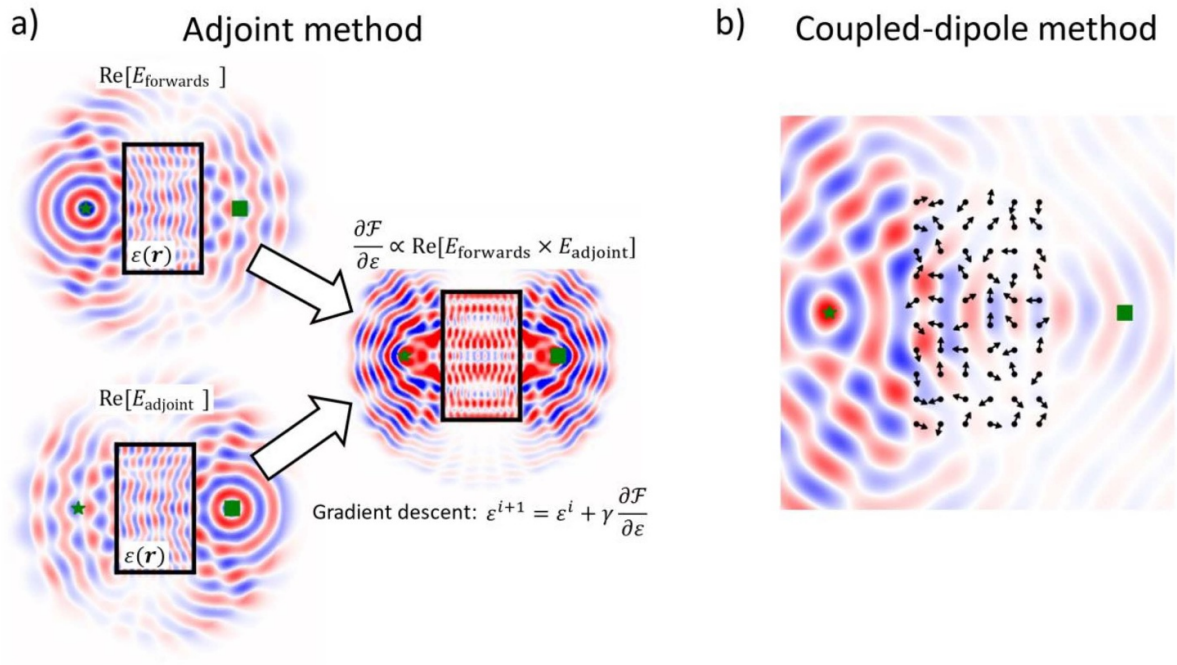

Figure 4. Schematic representations of using (a) the adjoint method and (b) the coupled dipole method to design a lens. We seek to design a structure that focuses radiation from a source at the location indicated by the green star to the location given by the green square. The design region is indicated by the black rectangle. For the adjoint method, only two field calculations a 'forwards' and an 'adjoint' are required to form the gradient of the figure of merit (field amplitude at the green square) with respect to the whole structure. This allows one to iteratively update the structure according to gradient descent to increase a figure of merit $\mathcal{F}$. Using the coupled dipole framework, the gradient of the figure of merit with respect to the scatterer locations can be found analytically, providing a map of how to move the scatterers.

to imposing fabrication constraints, as realising time-varying materials experimentally remains challenging.

Concluding remarks

Numerically efficient and conceptually simple, adjoint discrete dipole based inverse design techniques have already shown great promise for designing novel wave-shaping devices that can be a periodic and many wavelengths in size. Bringing these techniques to new areas of application, such as time-varying materials or real-time reconfiguration, will require many open questions to be addressed. The realisation of an 'adjoint' method in the time domain might enable the design of bespoke frequency shifters or amplifiers and real time inverse design might be important in the next generation of communication technologies.

6. Design optimisation of hierarchical structural metamaterials

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Status

The field of structural metamaterials has gained significant interest in recent years due to the increasingly widespread adoption of additive manufacturing (AM). AM has permitted the manufacture of complex structures including those which span a range of scales and hierarchies. This allows an architected internal structure to be designed and manufactured, with characteristics significantly different from the bulk material. This can lead to complex or even counter-intuitive structural responses from the designed component, for example auxetic behaviour [72], programmed nonlinear behaviour [73], including negative stiffness. The design of complex hierarchical structures now means that in addition to the design of the component's external boundary, the internal structural arrangement can be designed, providing additional exploitable properties. One of the major challenges presented by the new capability is how to design components with architected interiors and where the grading of an internal structure might lead to enhanced structural characteristics, but where the design itself is hard to visualise and therefore design without formal optimisation methods. This presents significant challenges, especially if emerging properties of graded structures are to be exploited rather than utilising a single repeated unit geometry to give uniform structural characteristics. To achieve these, computational methods are required which go far beyond CAD and visualisation tools.

Three approaches are often used to describe the small-scale, (i) the geometric parameters [74] or orientation and thickness of lattice members [75], (ii) the resulting properties of the small-scale geometry (essentially a subset of the elasticity terms in a multiscale problem) [76] and (iii) the small-scale geometry is spatially optimised using inverse homogenisation-based techniques [77]. In (i), sub-optimal small-scale geometries are often employed and (ii) has the equally significant problem that the mapping from graded material properties to small-scale geometries does not guarantee slowly varying geometries. This leads to a breakdown of the underlying assumption on which the heterogenous multiscale method is based and which is often used as a basis for multiscale structural analysis. Some significant progress has been made to address these deficiencies using the computationally expensive (iii) approach, but there is still work to be done in this area. There has been some excellent work going beyond classical homogenisation methods for multiscale approaches [78] and the potential for this to be extended to nonlinear complex problems is significant.

Current and future challenges and opportunities

The additional design flexibility afforded by the ability to tailor both the internal and external structure extends well beyond the linear elastic regime. Large deformations, nonlinear viscoelastic tailoring of materials, abrupt material changes resulting from internal contact or failure, and tailored multifunctionality could all be areas which could be better realised with the application of hierarchical structures [79]. Coupling these structural metamaterial-based opportunities arising from those of other disciplines such as electromagnetics adds further opportunities to the class of new materials. A further open challenge is how to optimise multiscale structures in a way which allows design flexibility across the scales. Approaches which rely on de-homogenisation of a large scale FGM structure via analytical means require a small-scale approximation to be known [80] or approximated using simulation [81]. The former is typically only available for simple, and usually 2D, geometries in the linear elastic regime and the latter is challenging in highly complex, nonlinear settings.

Some of the major challenges to the development and wider adoption of structural metamaterials are presented below, these do not include challenges which go beyond the computational design of the metamaterial structures, and therefore only touches on the geometric representation of the geometry using CAD, and manufacturing challenges related to computational design rather than the broader challenges. The development of implicit geometry [82] definition is an active are of research which overcomes some of the challenges associated with conventional geometry surface representations. It also focuses on the design optimisation or inverse design of structures, rather than more ad-hoc design methods based on trial-and-error or a human designer's intuition.

One area of significant potential is the development of hierarchical structures which are optimised for nonlinear responses. This includes the development of optimal structures which account for, (i) large displacements, (ii) internal contact, (iii) failure and post failure characteristics. Optimising metamaterials for these requirements pose significant challenges. Multi-level approaches, where small-scale characteristics are stored in a database and an optimisation algorithm relies on design sensitivities, frequently arrived at using a finite element and adjoint method, pose considerable computational processing and storage challenges. This is due to the high level of multidimensionality of the characteristic space (both the material properties in terms of the local displacement field and geometric definition). The underlying assumptions permitting homogenisation theory may also start to breakdown, for example small scale buckling of members potentially no longer being consistent with the assumption of a slowly changing and periodic displacement field. Developing model order reduction approaches which go beyond classical homogenisation approaches could provide a means of accessing complex, nonlinear material properties, allowing assembly of small-scale geometry to form components optimised across scales.

Loaded structures exhibiting contact, negative stiffness and failure all have the potential to dramatically change how we consider metamaterials if they become accessible to formal design optimisation methodologies. An example of this is that if we are able to optimise the progressive failure of a metamaterial. By considering internal contact and fracture, safer, impact resistant structures for a wide range of applications could be designed. The potential to go far beyond ad-hoc design and testing of structures will no doubt deliver not only improved performance, but also the ability to direct impact, as well as gain an understanding of the overall compromise between the impact resistance of a structure and its other functionality, such as stiffness.

Multifunctionality of structures, where components go beyond purely structural response, for example to include actuation, sensing or energy storage, require a multifunctional analysis of the problem and an understanding of the combined objective of the system. The optimisation of such systems is frequently made more complex by the significantly different approaches to parameterisation required for the different discipline [79]. The optimisation of the metamaterial will then not only provide an optimal design, but of equally importance also tell the designer something about the compromises required and how the discipline specific requirements interact.

Advances in methods and techniques to meet challenges

There are a number of exciting model order reduction methods being developed, as previously described, to analyse structural metamaterials efficiently. This leads to the potential to go beyond analysis and to optimise the system. The complexity of structural metamaterials means that a model order reduction technique is commonly required to make the analysis and optimisation of the problem accessible. Much of the model order reduction has thus far centred on the application of homogenisation or small-scale analytical approaches. However, homogenisation relies on the underlying assumption of a slowly spatially varying geometry, property field and solution field. There exist a range of approaches which do not rely on homogenisation methods which could potentially be exploited to design and optimise metamaterial structures rather than for analysis. Examples include hyper-reduction approaches [83] and the use of subspace methods [84]. The latter potentially facilitated by the use of machine learning as an efficient model order reduction tool to enable the design of metamaterials and going beyond the more well-established approaches of using machine learning for the efficient interpolation of databases of already designed structures. Developing such methods with efficient optimisation approaches, typically gradient-based methods, with similarities to classical SIMP-based topology optimisation, could deliver optimisation of complex hierarchical structures without requiring a separation of scales and all the associated challenges. Contact, failure or problem scales which are non-separable reduce the relevance of the approach and require other methods to be considered.

Concluding remarks

Much work on structural metamaterial design often focuses on the efficient graphical and geometric representation of a design. The authors believe that unlocking the potential of complex nonlinear, multifunctional metamaterials lies in the application of formal optimisation methods which go beyond CAD and instead consider the functional grading of a structure. The renewed interest in machine learning approached and other model order reduction approaches hold significant promise in dealing with the efficient coupling between scales required.

7. Artificial intelligence for electromagnetic metamaterial design

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Status

Artificial intelligence (AI) has gained widespread recognition in the mainstream consciousness in the last twelve months due to the immergence of significant large language models such as ChatGPT. However, AI has been developed for the design of electromagnetic (EM) structures for over 20 years [85]. Due to the recent increase in interest in this area there is a significant increase in the amount of hype in this area alongside excellent technical progress. Sorting the hype from the truly novel work will take time as the research community implements these developments.

Deep learning and neural networks have been used to predict the response of metamaterials with a wide variety of structures, examples include split ring resonators [86] and coded metasurfaces [87]. A summary of deep learning techniques for EM metamaterials is given by Khatib *et al* [88]. An alternative technique, sometimes making use of deep learning techniques, involves replacing the computational expensive steps with a simpler model by fitting to known data points, known as a surrogate model. This has been done in an adjacent field using finite element method modelling in determining the stress within a sample subject to a controlled increase in temperature [89]. This surrogate modelling technique has the potential to supplement full computational electromagnetic modelling (CEM) in producing training data for deep learning models.

AI has the potential to provide a benefit to the design of EM metamaterials due to the difficulty inherent in the inverse design problem for metamaterials. The inverse design problem for metamaterials is challenging as metamaterials are often a high dimensional optimisation problem which is solved using CEM techniques. These techniques, involving solving Maxwell's equations across the metamaterial structure, are time consuming for each individual iteration of the structure and determine the maximum number of simulations that are practical and therefore the number of iterations available to the optimiser. Were AI able to reduce the time for each iteration in the traditional optimisation process or improve the approximation of the design space, for example through surrogate modelling, this would provide a significant benefit to metamaterial optimisation.

Current and future challenges and opportunities

The biggest issue facing using AI for EM metamaterial design is actually a wider issue; the inverse design problem [90]. Inverse problems involve attempting to calculate cause from effect, see figure 5, which leads to a variety of challenges. Inverse problems, in particular the inverse EM metamaterial design problem, are almost always 'ill-posed problems'. Ill-posed problems violate at least one of the following principles of 'well-posed problems':

Criteria 1: Existence (a solution exists)
Criteria 2: Uniqueness (there is only one solution)
Criteria 3: Stability (the solution depends continuously on initial conditions)

In inverse EM metamaterial design we can reasonably expect to design problems that are; not physically realisable e.g. violate the laws of physics (violates Criteria 1), is physically realisable but the solution is not within the bounds of the design space (violates Criteria 1) or is physically realisable but with multiple solutions within the design space (violates Criteria 2).

Another major issue with using AI for EM metamaterial design is a wider issue in AI development which is the requirement for significant quantities of data required to train the model, in our case this data is often generated using time-consuming CEM. For instance, the training data required for a neural network is often between 1000 and 10 000 data points across the design space [88]. This requirement means that the main driver of the time taken for these models is the CEM time to generate the training and test dataset. If a single optimisation is required then it is often quicker to simply perform a traditional optimisation, where multiple solutions can be drawn from the same design space an AI method is significantly more beneficial.

The major open problem, related to a large range of AI problems, is mitigating the dependency of AI models on large amounts of training data. Reducing the training data burden for future models would enable an expansion of the use of AI models to design and optimise EM metamaterials.

Advances in methods and techniques to meet challenges

Given the difficulty of the inverse design problem the primary focus of future techniques will likely be on reducing the requirement for substantial amounts of training data. This has the advantage of being useful across a wide range of AI applications, not just EM metamaterials. Two promising avenues are active learning and transfer learning; active learning involves allowing the neural network to influence, or choose, the training data that it uses to build and model, whilst transfer learning involves leveraging trained models from adjacent problems to help reduce the training time.

Active learning has been studied extensively across the machine learning community and can be particularly helpful where an optimisation goal is known [91]. Another widely-used technique is to use 'uncertainty sampling' where the model adds further training data at points where the model solution has the greatest uncertainty. This is a very useful technique for EM metamaterial development since obtaining the training data involves time-consuming CEM simulations for a given point within the design space and therefore 'uncertainty sampling' can improve the AI model accuracy for the

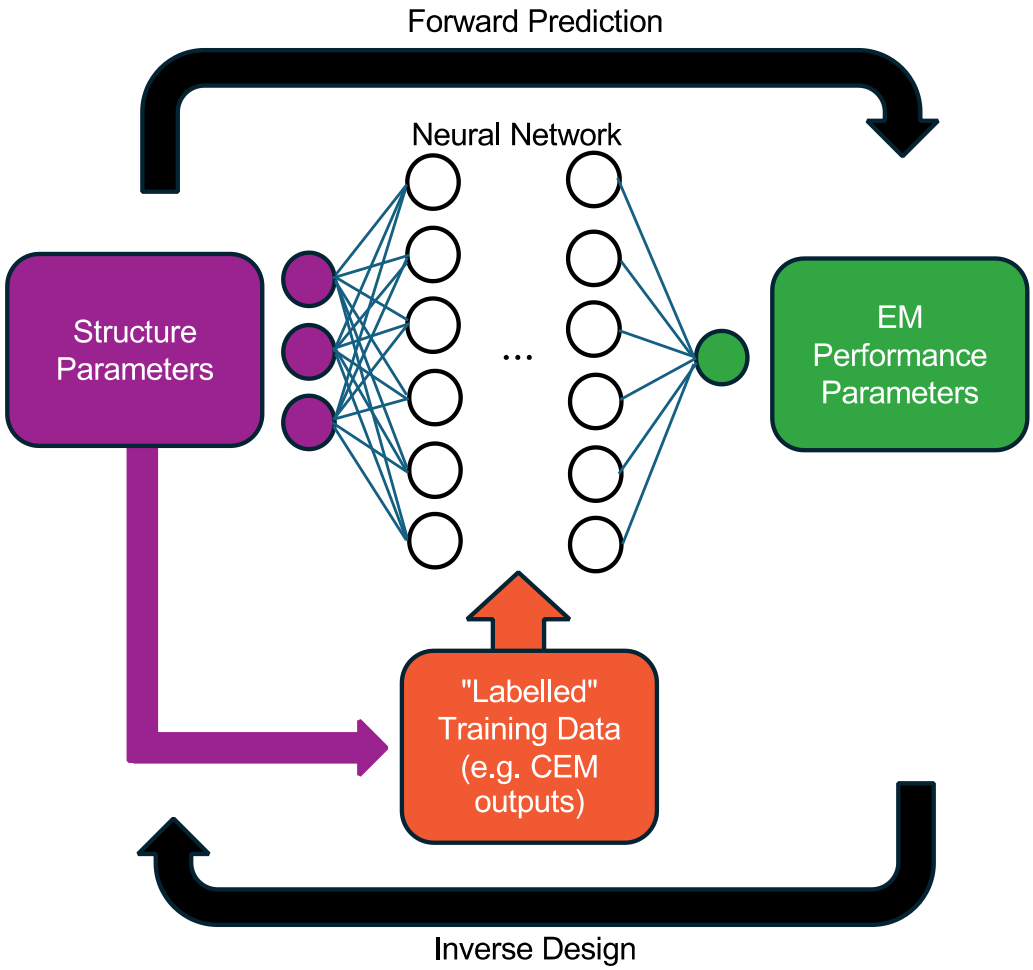

Figure 5. Schematic illustration of the use of a neural network to take the place of time consuming computational electromagnetic modelling. This also shows the difference between forward prediction and inverse design.

same amount of training data. Alternatively, Transfer learning, involves using training data from an adjacent problem to supplement the training data of the problem being studied. This can be done by pre-training a neural network on the adjacent problem before refining it on the training data for the real problem or by training the network on both problems simultaneously. Given that all EM metamaterial design tasks involve solving Maxwells equations transfer learning could provide a significant benefit in this area.

Another area that is currently being explored is physics informed neural networks (PINNs). PINNs introduce limitations on the neural network to enforce some of the underlying physics on the network result. Previous work has [92–94] enforced the neural network solution obeys partial differential equations and included the problem boundary conditions to limit the available solutions within the neural network. The combination of PINNs and transfer learning, for problems with the same or similar boundary conditions (e.g. infinite planar metasurfaces), could provide a step change in training neural networks.

Concluding remarks

AI has the potential to revolutionise the optimisation of EM metamaterials. However significant challenges remain, some of which are associated with the wider issue of the inverse design problem. In this context AI tools will be best deployed in a ‘train once, use many’ application where future iterations of a metamaterial can be rapidly generated once the AI tool has been trained sufficiently. If further progress can be made on reducing the training data required to develop the AI models, through some of the methods discussed above, then these AI tools have the potential to provide a route to efficient optimisation of EM metamaterials for industrial applications.

8. Strategies to overcome difficult data

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Status

Historians chronicle human civilizations development through the stone, bronze, and iron ages, underlining how materials discovery enables new technology. In each instance, right up to the present day, materials were discovered by a time-consuming and expensive process of experiment-driven trial-and-improvement. However, recently AI has emerged as a tool for materials discovery, offering significant time and cost savings. The first application of AI to materials was in 2003 to design a new steel [95]. Since then, there has been rapid development of AI for materials and chemicals design with a range of industrially proven examples [96], and early commercial adoption.

Artificial intelligence learns from historic data, and so the amount and quality of this historic data is key to success. We discuss two approaches to improve this fundamental underpinning of AI:

1. **Additional data:** sections 1–3 and 6 of this roadmap offer complementary analytical methods that offer additional information about a system. Therefore, we propose the development of AI that can exploit all possible knowledge about a system, combining the strengths of experimental data, first principles computer simulations, and physical rules of thumb.
2. **Explainability and reliability of data:** section 7 discusses physics and chemistry aware AI. Therefore, we propose improvements to the explainability of AI, which will not only provide critical insights to scientists and engineers, but moreover assess reliability of data to fulfil a common regulatory requirement for evidence of the underlying mechanisms.

Current and future challenges and opportunities

Artificial intelligence is a powerful tool that has found applications across materials and chemical systems, spanning both research and also industrial settings. In the face of inevitably challenging training data, researchers are pursuing approaches that exploit additional information to accelerate further applications in materials and chemicals:

There are several open problems in AI, pertaining to handling difficult data, that if solved, would open significant opportunities in the application of machine learning to metamaterials. We highlight just two opportunities below:

Exploit all available information: Data is often sparse, for example values are not all measured or individual companies curate private data silos but guard them jealously even when it may be mutually beneficial to share. Furthermore, there is much untapped knowledge beyond traditional experimental data, including first principles computer simulations and physical rules of thumb. The development of AI methods that can juxtapose these sources of knowledge would lead to a predictive tool more powerful than the sum of its parts.

Explainability and reliability of data: Experimental data often carries uncertainty. However, scientists and engineers often require more than accurate predictions and designs, they need to understand that a design will be reliable and why the design works. This not only provides the insights that drive future development, but moreover is often demanded by regulators for safety critical products. The development of an AI tool that can open the box, explore robustness, and explain the physical insights behind its predictions would be a gamechanger for the practical applications.

Sometimes the supplied training data could simply be insufficient to train a reliable model. There are then two possible ways forward that we discuss below:

Design of experiments: Sometimes there is not enough data available to build an AI model, or even for a human scientist to infer the underlying mechanisms. The solution is often to gather more data, which can often be gathered in a judicious pattern to efficiently cover design space. Standard methods do this without any knowledge of the behaviour of the end-goal properties, but methods are under development in AI can take advantage of existing knowledge and the end goal to more efficiently explore space, saving experimental time and cost.

Design of formulations: An even more powerful use of AI is to propose new formulations that fulfil a target specification. However, models can be uncertain owing to either lack or noise in data. Another area of active research, this requires not only the algorithmic development to enable more accurate predictions, but also a measure of their confidence, so that only the most robust proposals are taken forward.

Advances in methods and techniques to meet challenge of difficult data

In the materials and chemicals sectors experiments remain the key tool to understand the properties of materials, including metamaterials. However, experiments are expensive and time consuming, and moreover are not always performed to completion. Therefore, AI that can extract value from highly sparse and noisy data has emerged as a key opportunity in the materials and chemicals sectors. Three approaches have emerged to overcome sparse data:

Modelling technique ignores sparsity: Perhaps the clearest approach is to adopt a modelling technique that ignores the missing values. The straightforward approach is to simply discard entries where any single component is missing, however this can leave no data remaining. Alternatively, missing values can be simply ignored, or replaced by an average value, for example k-means clustering skips around missing input values by simply sampling those inputs present [97].

Multi-output neural network: The model is set up so the two linked properties share many hidden nodes, with the two properties distinguished only by the final hidden layer [98]. Therefore, the bulk of the physics is captured by the common hidden nodes, and so can be learnt from both properties, extracting more information from sparse data.

Self-consistent imputation: A third approach is to make guess at the missing values, thereby generating a complete dataset [96]. From this a standard AI algorithm can be applied to make predictions for all values, including those that were missing. These improved estimates for the missing values can be used as inputs in successive training and prediction cycles until the predictions reach self-consistency.

Experimental data is often noisy, stemming from inevitable experimental uncertainty. Artificial intelligence methods can not only average over this noise (rather than overfit), they can also estimate the uncertainty in their prediction owing to this noise. Additional contributions to the uncertainty arise when extrapolating beyond the range of the training data. By understanding this uncertainty, AI can focus on the most robust predictions that are most likely to fulfil the target specification [96].

Concluding remarks

We have demonstrated that there are many opportunities to ensure quality and availability of data to apply AI to metamaterials. The holistic exploitation of all sources of information and explainability to ensure reliability in face of difficult data are two especially important themes for further development.

9. Metamaterials genome: towards synergy between mathematical modelling and AI analysis

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Status

What is the best use of machine learning techniques in the context of computational mechanics and relatively scarce experimental data sets? One could attempt to gain a general understanding of the design possibilities by aggregating results from a large number of targeted engineering projects, i.e. tapping into the so-called 'data exhaust' of the broader research and engineering community. Understanding the limits of the design space is a key aspect in optimising complex hierarchical structures and is vital for exploring and designing novel Metamaterials.

The development of machine learning and AI technologies has been accelerated by abundant data (mostly text, images, geographical coordinates) aggregated by multinational corporations. Although increasingly conceptually advanced, the origins of machine learning can be traced back to traditional statistical methods and data-centric analysis. These techniques have been used in fields where establishing relationships and using differential equations or closed-form descriptions have been challenging due to the systems' complexity. However, well-established, and validated physics-based modelling tools offer direct solutions for various physical domains relevant to metamaterials.

Fundamentally, numerous research groups and companies repeatedly carry out physics-based calculations, all employing the same fundamental equations such as Maxwell, wave, or dynamic equations of motion. Therefore, one can recognise the potential for a large collection of results, which are currently scattered across various research groups and frequently guarded in private data silos. In many instances, the results are discarded at the completion of specific projects or placed in disparate archives for a limited time. As recognised by several US federal agencies [99–101], creating an open research commons and appropriate standards and infrastructure for sharing, reusing and recycling existing data (including computational tools) can accelerate the development of novel materials, reduce effort duplication, and facilitate creative, fast-paced knowledge generation.

Current and future challenges and opportunities

To create an open research commons that can integrate multiple physical domains like mechanical, optical, EM, etc it is necessary to establish common data standards [102]. This requires input and agreement from both academic and industrial groups. Moreover, these standards may change over time. Therefore, it is important to establish methods for migrating and adapting data.

Shared repositories of knowledge require the trust of all stakeholders [103], sustainable funding, and a transparent governance structure. To achieve satisfactory cyber security resilience, such a repository might require distributed storage across academic and industrial stakeholders and specialist cybersecurity support. Low barriers for adaptation and usage are also required to facilitate broader benefits and adaptation by the widest possible group of stakeholders.

Optimising the process of organising and utilising data that already exists can save time and resources for all stakeholders. Additionally, establishing a shared open research commons can lead to improved collaboration and knowledge mapping by linking research groups based on similarity and proximity metrics of the structures they produce. By enabling search engines for specific required properties, manufacturers and industrial stakeholders can quickly identify the key research groups and technology suppliers in the design space.

Shared data from 'adjacent' problems can be used to inform and suggest solutions for the problem being studied (also in different physical domains). Since Metamaterial problems solve a limited number of physical laws, transfer learning provides significant benefits in this area and suggests good starting points for developing Metamaterials with specific properties. This can be achieved by leveraging prior iterations and the experience of other academic groups and stakeholders. Transverse learning can be facilitated using approximate surrogate models trained on prior data. Such fast-running surrogate models are also vital for optimisation and can underpin AI generative design, which could suggest promising areas for novel material discoveries. However, performing final design checks can be reliable and accurately achieved using computational physics and mechanics, guaranteeing accurate results, ensuring adherence to known laws of physics and offering explainable results.

Another interesting application is the use of large language models to suggest suitable physical models, regulatory requirements, design equations, and modelling code snippets. In such instances, AI tools are focused on enhancing human productivity and easing access to knowledge. However, the validation and reliability of such co-generative tools remain an issue.

An example of an unsolved problem in the field is the development of a compact topology parameterisation compatible with machine learning tools. Such encoding should be able to generate any suitable Metamaterial topologies

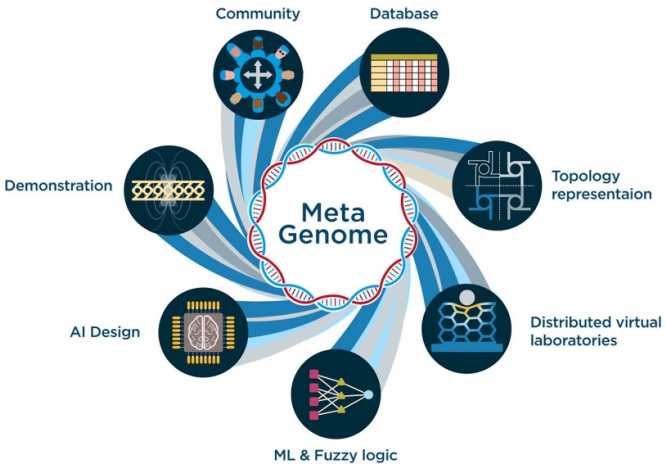

Figure 6. Synergy between physics-based modelling tools, the scientific community, AI toolboxes, manufacturers, and end-users is essential for a successful development ecosystem.

without being restricted to a specific subclass of structures. Another challenge is incorporating manufacturability, cost, and sustainability aspects into the optimisation process, as well as the generative capabilities of the shared open research commons. What is the best pathway to standardise such data to enable interoperability and facilitate data sharing?

Advances in methods and techniques to meet challenges

The National Institute of Standards and Technologies (NIST) has developed an open-source platform called the configurable data curation system (CDCS) [104] that can curate complex data structures. This platform is designed with cybersecurity in mind and is continuously updated and supported by NIST. We have used this platform to create a prototype of a shared database of metamaterials, which is accessible online [105] and outlined in figure 6. The database can handle complex hierarchical XML data structures, including topology information in discrete voxel formats and more parametric, vector-like descriptions such as step formats. The open-source code can also be cloned, and independent repositories can be created while leveraging shared data standards and programmatic developments in toolkits for working and processing large datasets. This database is particularly relevant in the context of recent developments in the computer science community, where tools like VQGAN [106] are being used to describe topologies. These tools hold promise in establishing critical links between physical information in the Metamaterials community and rapidly developing AI toolboxes with generative capabilities demonstrated for other material domains [107]. Recent developments of AI-generated mechanical metamaterials [108–110] further underscore the benefits of shared data repositories for the overall progress of the discipline.

Concluding remarks

Through the establishment of a shared open research commons, collaboration and knowledge mapping can be improved by utilising property-based norms and metrics. This will enable the community to quickly identify key research groups, manufacturers, and industrial stakeholders in the design space by searching for specific required properties. Secondly, it will enable researchers to focus on the most interesting and high-value activities, minimising duplication of effort and leveraging prior material discoveries. Thirdly, a standardised shared data platform lays the foundation for experimentation with and developing generative AI toolkits to augment and guide future meta-material discoveries. Establishing a thriving ecosystem where all skill bases are complementary is fundamental for ensuring benefits for all stakeholders.

10. Electromagnetics of time-modulated metamaterials

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Status

The interaction of light with structured media is now commonplace: photonic crystals are widely deployed to control light, and metamaterials appear in many. Structure should be on the same scale as, or less than the wavelength of radiation. Initially this was technically demanding but technology has advanced to the point where photonic crystals and metamaterials are commonplace. The obvious extension is to structuring in time, and once more the length scale for effectiveness is dictated by the radiation concerned: is should be on the same scale or shorter than the radiation's temporal period. The time challenge is a much more demanding experimentally than the spatial one and has held up development of the field until recently when technology has opened new horizons for us.

Just as the static Bragg grating is the starting point for diffraction theory, so a grating in space and time,

$$\varepsilon(x,t) = \varepsilon_1 [1 + 2\alpha \cos(gx - \Omega t)]$$

has been the workhorse of theory for time modulated materials [111]. In almost all studies it is assumed that the material itself does not move but is locally modulated, rather as a water wave spreads over the ocean without carrying the water with it. This ensures that the velocity of the structure, $c_g = \Omega/g$, is not limited by the speed of light. It also avoids complications that arise from performance of mechanical work when materials physically move.

Early theoretical work showed that the model is PT symmetric and gives rise to real dispersion relations, $\omega(k)$. The exception is the so called trans-luminal regime defined by the grating travelling at a speed comparable to the velocity of light such that there is a point in the grating where light travels at the same speed as the grating [112]. This is a trapping point where radiation is compressed and amplified: the PT symmetric model breaks down and $\omega(k)$ can no longer be defined. Figure 7 shows the dramatic consequences. A recent review gives more [113].

Current and future challenges and opportunities

The most obvious opportunity is the breaking of time reversal symmetry [114]. This means systems can dispense with the need for magnetic fields to produce isolators and replace them with more compact devices. As space-time structure becomes more elaborate, systems show true topological protection of the flow of light, rather than relying on spin conservation. For example, helical structures have been studied where polarizability rotates in time giving a spin dependence to its response. The surface states of these structures have rich potential for topological properties.

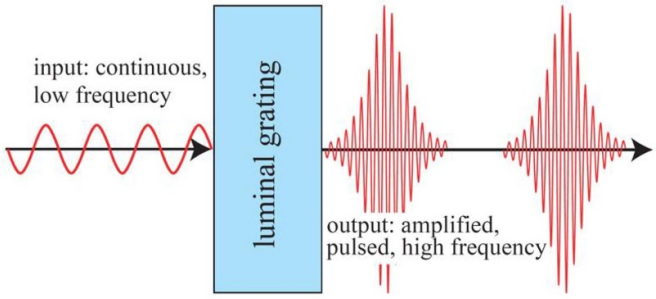

Figure 7. Schematic transmission through a luminal grating. Incident radiation grows exponentially in intensity undergoing compression into a series of pulses separated by the time period of the grating.

Most fascinating is the transluminal regime. Theory has identified the mechanism by which light is amplified and compressed in this regime: lines of force are conserved and energy added by compressing them as in compression of a magnet's quasistatic field as it approaches a superconductor [115]. In quantum terms amplification takes place by photons climbing a ladder of frequencies in units of Ω.

The quantum nature of light is very much emphasised by time dependent structures [116]. A simple periodic modulation in time of frequency Ω will give rise to a band gap at $\omega = \Omega/2$ by hybridising states at $\pm\Omega/2$, i.e. by mixing positive and negative frequencies giving rise to parametric amplification with amplitude growing exponentially in time. In quantum terms this amounts to creation of qubits—highly correlated pairs of photons. This process is well known but there is another mechanism for pair creation which has only recently been identified. In the transluminal regime light is amplified irrespective of the frequency, trapped at the accumulation points referred to in the previous section. For upward movement of frequency photons are conserved. In contrast downward movement of frequency meets an impasse when attempting to cross from positive to negative frequencies and can only do so by creating a qubit with one of the components having a negative frequency. This mechanism is analogous to Hawking radiation which although in a totally different context also involves a singularity in the propagation of light at the Schwarzschild radius and the creation of negative frequency photons.

The quantum domain is ripe for future studies with many questions waiting to be answered.

Advances in methods and techniques to meet challenges

For theory to be taken seriously it must connect to experiment. There are now several experiments showing extremely fast modulation of materials properties. An early example is the so called 'push broom' effect [117]: a sufficiently intense pump pulse of light travels in an optical fibre changing the refractive index at the leading edge. A probe pulse travels at a different frequency at a lower velocity and is overtaken by the pump which then captures the probe into the transluminal region created by the pump and compresses

it, even though the modulations in refractive index may be tiny.

More substantial modulation has been achieved in recent experiments. The Sapienza group exploited the 'epsilon near zero' property of indium tin oxide (ITO) combined with plasmonic enhancement of an incident pump pulse to turn the ITO into a reflecting surface [118]. Modulation of the reflectivity of 230 GHz radiation in this experiment was substantial—of the order of 50%. The problem they faced was that the onset of reflectivity was so sudden that neither the pump not the probe could resolve it, both being of the order of 800fs wide. This issue was resolved by creating two windows of reflectivity to make a time domain analogy of a Young's slits experiment. In the original experiment slits separated in real space disperse radiation over a range of angles and fringes arise from interference. The decay of fringe intensity with angle is dictated by how narrow the slits are. In the Sapienza experiment the 'slits' now appear in the time domain, and the interference fringes in the frequency shift of the probe. The decay of fringe visibility with frequency shift is a measure of how narrow the time-slits are remarkably the experiment revealed that the rise time of the reflectivity was at least as rapid as the 5fs period of the radiation. Work is underway to combine this very rapid time variation with spatial modulation.

Experiments at Technion-Israel Institute of Technology, and Purdue University had a different approach [119]. They were able to compress the pump pulse to 6fs and under the assumption that the material responds more or less instantaneously, produced a very sharp rise time of refractive index which was measured by observing the colour shift of a probe as the refractive index is modulated.

Concluding remarks

Time modulated metamaterials are a rapidly expanding field with encouraging experimental progress. In my opinion the chief challenges lie in the further development of experiments. Theory makes a vital contribution and is well prepared for their interpretation and will press on to exploit opportunities in the quantum domain.

11. Irrational metamaterials and their development

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Status

Quasicrystals, which were experimentally observed 40 years ago by the team of the Nobel Prize winner Dan Shechtman [120], are arrangements of particles or elements in such a fashion that they do not present translational symmetries, but they show long-range order. They can be modelled from a cut and projection of a periodic structure in a higher dimensional space onto a hyperplane as in [121–123]. Other kinds of structures [124–126], incommensurately modulated crystals, also present non-periodic features. They derive from Harper's equation, which can be understood by Bellissard's K-theory of C*-algebras [127], linking their properties to the bulk-boundary theorem and topology. Alternatively, they can be engineered with diffraction orders disallowed by the crystallographic restriction theorem [128].

Effective properties of quasicrystals can be rigorously derived from elliptically degenerate differential operators depending upon some irrational coefficients [54]. There are oddities in their effective properties in the infinite conducting case [127]. When rational approximants are considered, periodic structures with increasingly large unit cells are generated [121] whose effective properties approximate those of corresponding quasiperiodic structures. In [121], the nearly isotropic effective speed of sound is approached in chiral crystalline mechanical metamaterials (see figure 8, panels (a)–(c)).

In the Bragg regime, some phenomena akin to stop bands occur [55, 122, 129]. Applications are for instance, transmission problems between periodic half-spaces with incommensurate periods along the interface. Such systems are analogous to edge waves in quasiperiodic arrays of scatterers studied in [124, 126]. Figure 8 panels (d) and (e) taken from [123] show that when the slope of the hyperplane is spatially graded, some fractal rainbow effect revealing features of the Cantor spectrum of quasicrystals can be observed.

The spectrum of quasiperiodic crystals can be explored in the phase space in conjunction with the Hofstadter butterfly, which reveals the existence of topological edge states like those in periodic structures [124, 125]. The quantum Hall effect can then be generalized to quasiperiodic structures such as Moiré lattices [130]. Localization is related to topology [126, 131], and the edge states in quasiperiodic structures possess unique properties, making them suitable for wave-control devices. In figure 9, two examples of edge states are shown, in mechanics and optics, in both one and two dimensions, proving the versatility of these structures.

Current and future challenges and opportunities

The transposition of the well-known features of wave phenomena in periodic media (effective properties, stop bands, topological effects, etc) to quasiperiodic media is challenging, as we have discussed. Exploration of irrational acoustic, EM, and mechanical metamaterials requires some mathematical background (with some knowledge of functional analysis, spectral theory, number theory), computational skills (numerical exploration of their properties guides the theoretical conjectures before they can eventually be proven), and physical interpretation (one should be careful to not jump at a conclusion based on what is known for periodic structures).

Several challenges are still open in the field of quasiperiodic structures; understanding the propagation of waves in quasicrystals might bridge the gap between ordered media (studied with the Floquet–Bloch theory) and disordered media (commonly analysed in Anderson's localization framework). An alternative classification for long-range ordered systems is hyperuniformity [132]. Hyperuniform materials include perfect crystals, perfect quasicrystals, and some amorphous states of matter. In this sense, quasicrystal properties might also be formulated under the hyperuniform framework.

Moreover, not only propagation is relevant, but as we have stated before, localization of waves is essential for novel modern wave devices. Certain quasicrystal structures present Cantor spectra, which allows us to theoretically define band stops in every frequency range, even at extremely low frequencies [121, 126], and this makes possible to create structures exhibiting forbidden bands, i.e. perfect reflection at extremely large wavelengths, in complete contradiction with periodic structures [133]. This property makes them appealing for the realization of deep-subwavelength wave devices, but it remains a challenge to implement them effectively. Not only the lower part of the spectrum presents its challenges, but also at higher frequencies the spectrum becomes complex and difficult to decipher.

Advances in science and technology to meet challenges

From the theoretical point of view, although massive efforts were devoted to understanding quasicrystals and their properties during the '90s, ongoing research lines still produced compelling advances in the last years. In [55], Floquet–Bloch theory is generalized to quasiperiodic structures by treating two wave propagation problems first in the periodic high dimensional space and then projecting the solutions into the real space by adequately solving the elliptically degenerate differential operators. In [56], a theorem is established for the

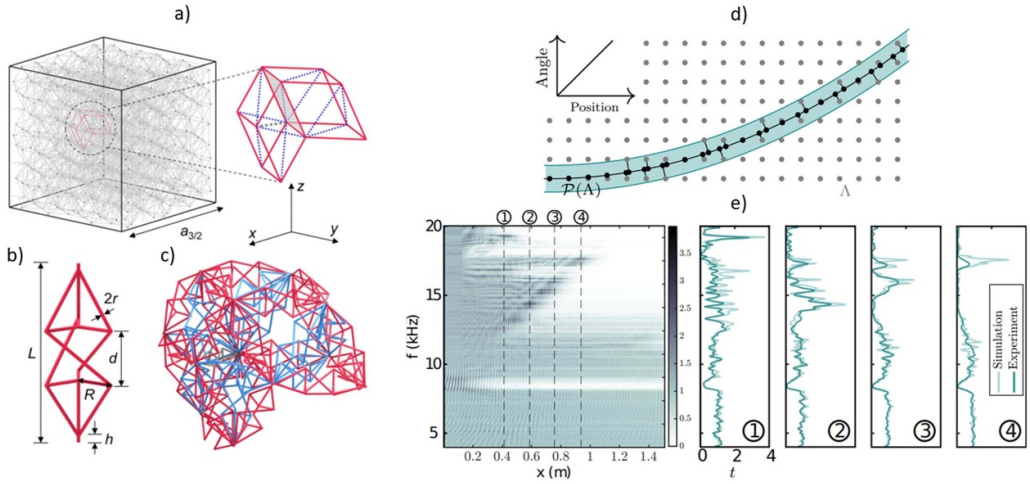

Figure 8. Two examples of quasicrystalline structures generated with the cut-and-project method. The first example, reproduced from [121], is generated from a high dimensional space of order 6 to a 3D icosahedral quasicrystalline metamaterial (a). After replacing each rod with either an achiral homogeneous cylindrical rod or with a homogeneous uniaxial chiral rod, an achiral or a chiral 3D structure is approached. (b) The homogeneous uniaxial chiral rod is approximated by the metarod depicted in (b), resulting in the structure shown in (c). (a)–(c) Reprinted (figure) with permission from [121], Copyright (2020) by the American Physical Society. The second example, reproduced from [123], shows a quasicrystalline structure obtained by grading the slope of the cut-and-project technique from dimension 2 into dimension 1 (d). (e) Demonstration of the fractal rainbow effect by smoothly grading the slope of the hyperplane. The frequency spectra are shown as a function of position. The numbered lines show the measurement positions, with a comparison between experiments and simulation shown in the numbered plots. (d), (e) Reproduced from [123]. CC BY 4.0.

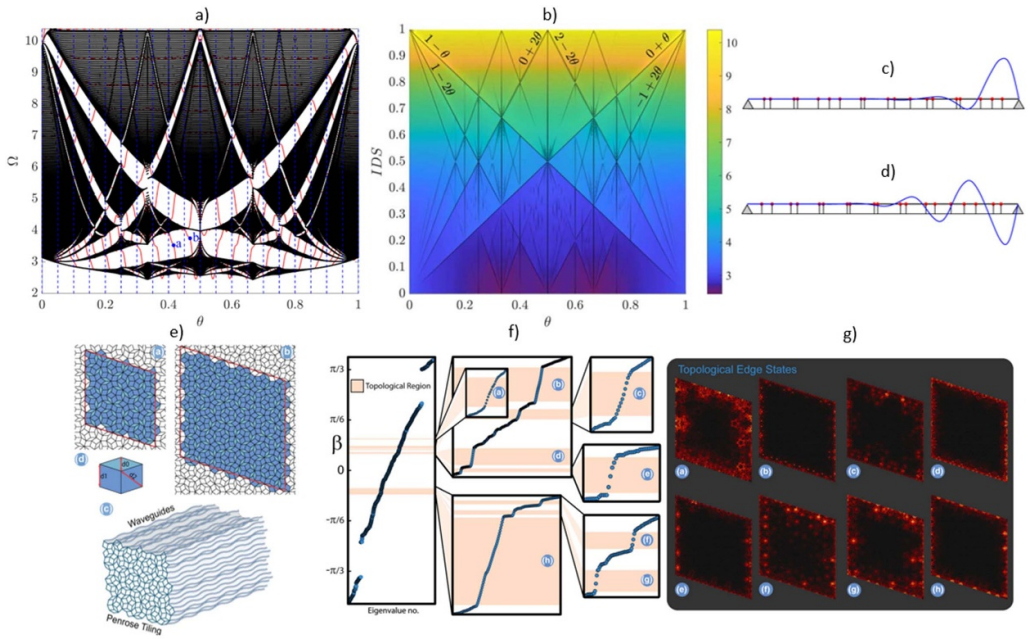

Figure 9. Two examples of topological edge states in quasicrystals. The first one, reproduced from [126], is a one-dimensional finite mechanical beam with mass-spring resonators attached at some positions along the beam. (a) The spectrum of a finite system with $S_f = 20$ scatterers attached to it (red) superimposed by the bulk spectrum (black) as a function of θ (the modulation parameter). Red curves spanning the bulk gaps are topological edge modes localized at the right boundary of the finite beam. (b) The integrated density of states (IDS) with θ exhibiting sharp jumps at the bandgaps. The colormap indicates frequency Ω. (c), (d) mode shapes corresponding to the eigenfrequencies marked by blue dots with labels (a) and (b), respectively, in panel (a). (a)–(d) Reproduced from [126]. © IOP Publishing Ltd. CC BY 3.0. The second example, reproduced from [131], is photonic fibre modulated as a Penrose quasicrystal. (e) Periodic Penrose approximants of Penrose quasicrystals and a sketch of the photonic Floquet quasicrystal. (f) Topological features at different levels of the energy spectrum. (g) Topological edge states associated with the fractal spectrum of a finite topological quasicrystal. (e)–(g) Reproduced from [131]. CC BY 3.0.

apparition of super band gaps in periodic approximants of generalized Fibonacci sequence, which might be especially useful for practically implementing quasicrystals in photonic and phononic systems.

The advances in AI can help design quasiperiodic structures with complex features, as in figure 8. It is difficult to visualize periodic structures in dimension higher than 3 for a human being, but computers can explore periodic structures in high dimensions provided they have been trained in cases that can be visualized by human beings. Furthermore, optimization algorithms and neural networks might help solve inverse problems when design quasiperiodic structures for a given purpose. Generally, these problems are ill-posed and require an iterative process that is computationally expensive and time consuming.

Advances in nanomanufacturing allow for the creation of nanostructures that can perform the most sophisticated and efficient tasks on the smallest scale. The exhaustive control in the manufacturing process has reduced tolerances and errors, which paves the way for implementing structures that are not so robust against disorder. This technology has opened the field of nanomaterials and beyond, and the reachable wavelengths and frequencies have led to the control of wave packets at their lowest level. Noticing that quasiperiodic arrangements of layered media allow for a larger photonic state density than that of their periodic counterparts makes possible polarization insensitive broadband optical absorbers [134].

Concluding remarks

Irrational metamaterials is a fast-developing research area. Quasicrystals have proved to be suitable for a wide range of wave applications, from tailoring effective properties of the material to trapping energy efficiently in space. Advancements in computational techniques and nanomanufacturing allow us to envisage solving inverse problems to design 3D quasicrystal metamaterials with optimized properties and at useful wavelengths for desired applications. Some questions remain unsolved for the lower part of the spectrum, which is the one that gives access to their effective properties, such as the appearance of stop bands at extremely low frequencies [121, 126]. Furthermore, moving to higher frequencies, the spectrum becomes so complex that its mathematical properties are still elusive, even in the one-dimensional case [55, 124, 132]. There is much that remains to be done with one-dimensional quasicrystals in terms of localization and topological states, but it seems timely to start exploring their two-dimensional and three-dimensional counterparts.

12. Polaritonics and metamaterials

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Status

The field of metamaterials has been evolving over time, encompassing a wide range of wave phenomena, frequencies and functionalities. An important role in this progress has been played by the material platforms used to build these engineered materials. *Plasmonics* [135] has been at the basis of the first generation of metamaterials, due to the strong field confinement and enhanced light-matter interactions emerging at the interface between metals and dielectrics, driven by the coupling of light with electrons that supports *plasmon polaritons*. However, the challenges posed by these materials, mostly in the context of losses and poor compatibility with integrated and silicon-based platforms, has driven a quest to explore low-loss plasmonic alternatives and heterostructures [136].

In the last few years an interest in a broader range of material phenomena supporting strong light-matter interactions has emerged, in the context of *polaritonics* [137, 138]. Polaritons are quasi-particles, half-light half-matter, emerging when light is so tightly coupled with the material response that the optical and material response cannot be separated. While plasmons are arguably the most widely explored form of polaritons, new opportunities have emerged in the context of alternative polariton species, based on light coupled to phonons, excitons, magnons, or other material excitations. In turn, these responses have been opening a wide range of opportunities for metamaterials, with new functionalities and new frequency regimes. Of particular interest is the recent surge of interest around phonon polaritons, which enable low-loss and highly directional excitations in the mid-infrared frequency range [139]. This platform can naturally support hyperbolic bulk waves and surface waves, with broadband highly-confined and low-loss light-phonon transport. Coupling phononic materials with meta-structures, as in figure 10(a) for the case of boron nitride, enables to transfer exotic optical features to polaritons [140], which may be directly observed in the far-field response. Other materials, such as molybdenum trioxide (figure 10(b)) or calcite (figure 10(c)), naturally offer even more exotic polaritonic modes at their interfaces with air, which may be further controlled using metamaterial principles by rotations and twists [141, 142]. Other exciting opportunities for metamaterials have emerged leveraging exciton polaritons, supported by 2D materials and transition-metal dichalcogenides [143], or magnon polaritons in chromium sulfide bromide [144].

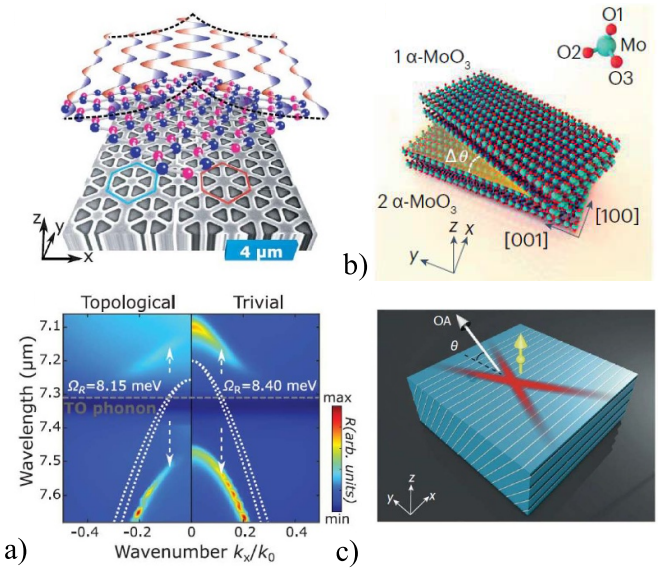

Figure 10. Polaritonic metamaterials: (a) A topological metasurface strongly coupled to a thin layer of boron nitride enables exotic topological phase transfer from light to phonon polaritons [140]. From [140]. Reprinted with permission from AAAS; (b) twisted bilayers of molybdenum trioxide can drastically modify the nature of the supported surface modes as a function of the twist angle [141]. Reproduced from [141], with permission from Springer Nature; (c) the angle between the calcite crystal axis and its interface with air drastically controls the confinement and directionality of surface polariton modes [142]. Reproduced from [142], with permission from Springer Nature.

Current and future challenges and opportunities

These recently emerged classes of polaritonic materials offer unique opportunities for wave control when combined with metamaterial concepts. Yet, they also pose unique challenges in the context of modelling and simulations. First, these exotic wave-matter interactions are inherently dispersive, both in time—leading to strong resonances and large variations with frequency—and in space—leading to nonlocality phenomena that impact light localization and transport. Special efforts must be made to properly capture these features in analytical and numerical models, and suitably characterize the underlying material constituents. In this framework, density functional theory and other *ab-initio* techniques to model the underlying materials and polaritonic phenomena become necessary to properly model the EM problem. In this context, it is also crucial to make sure that causality relations are considered in modelling the frequency and momentum dispersion of the underlying materials and polaritonic metamaterials.

Dispersion is also associated with material losses, which poses a challenge not only in terms of the functionality of the resulting devices, but also in the modelling aspects. Carefully capturing the associated retardation phenomena and dissipation is crucial to model polaritonic metamaterials. Similarly, active materials, nonlinearities and lasing phenomena naturally emerge in polaritonic systems, leading to even more complex modelling requirements that need to carefully analyse stability and causality.

Polaritons are commonly associated with extreme light confinement, with wavelengths shortened by up to two orders of magnitude compared to free space. This leads to challenging multi-scale modelling problems, in which largely different spatial scales need to be considered in the modelling and simulations. Similarly, the recent interest in

exploring time modulation and Floquet phenomena in polaritonic metamaterials implies analogous challenges in the temporal domain, in which the scale of modulation is largely different from the relevant polariton dynamics. A related challenge is associated with the inherent multi-physics nature of polaritons: the fact that light is so tightly coupled with material responses implies that optical modelling alone is not sufficient to capture the phenomena at stake. Multi-physics modelling, both analytical and numerical, and co-simulations emerge as important in this context, with finite-element and semi-analytical methods playing a prominent role in this context.

Clearly, the described challenges are closely tied to exciting opportunities that emerge in polaritonic metamaterials. These new needs for modelling and simulations are tightly linked to the new physics emerging in these structures and the strong opportunities associated with them, both from the fundamental standpoint and in the context of emerging technologies.

Advances in methods and techniques to meet challenges

The challenges and opportunities mentioned in the previous section open interesting directions for the future of modelling techniques aimed at the analysis and design of polaritonic metamaterials. Analytical methods offer a powerful way to capture the fundamental aspects of the problem. Coupled-mode theories, properly augmented to consider the multi-physics aspects at play, offer an elegant platform to describe in compact ways the polaritonic response. Efforts to expand the multi-physics nature of these theories is important, as well as to capture in efficient ways the nonlocalities, both in space and time, stemming from polaritonic responses.

Sophisticated numerical tools that involve multi-scale meshing, both in space and time are necessary tools to efficiently study polaritonic metamaterials. In this context, new numerical approaches and new expansion basis functions need to be devised, keeping in mind also the trade-offs between general purpose models and ad-hoc complexity. For time-varying structures, finite-difference time-domain techniques appear to be the only general modelling solution, but given the widely different time scales involved it also implies excruciatingly long and intense simulations. In the case of periodic modulations, augmented frequency-domain techniques or mixed time-domain/frequency-domain approaches can offer large speed-ups. These approaches can be also extended to spatial modulations to study space-time gratings made of polaritonic materials.

Opportunities to link these efforts to other fields of theoretical physics also emerge. For instance, the field of Floquet matter has been making progress in modelling driven systems composed of resonant particles, very relevant to polaritonic metamaterials. Also the excitement around chiral phonons has relevance in the context of phonon-polariton metamaterials, in which chiroptical responses can be transferred to phonon polaritons. More generally, the field of polaritonic metamaterials inherently leads to a highly inter-disciplinary effort, bringing together different communities that can feed and guide the modelling efforts discussed in this section. Close work with experimentalists and with *ab-initio* theorists is likely to lead to new breakthroughs on the modelling side, paving the way to exciting prospects to capture the polaritonic metamaterial response, and apply them in larger systems for new technologies, from quantum to classical waves.

Concluding remarks

The field of polaritonic metamaterials has been blossoming in recent years, pushing forward a new paradigm of material responses for light, matter and wave control. The opportunities that stem from coupling structured light in metamaterials with phonons, excitons, magnons and electronic responses in materials open exciting directions for science and technology. Yet, they need to be properly supported by new modelling tools—analytical and numerical—that allow to capture the underlying multi-physics phenomena, and enable analysis, design and optimization of the resulting devices. In turn, these efforts are likely to expand and enrich the theoretical physics and engineering communities, with new mathematical tools and numerical techniques uniquely suited to address these challenging problems. A bright future for polaritonic metamaterials is ahead, both from the modelling and from the experimental perspective.

13. Active chirality in mechanical metamaterials using gyroscopes

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Status

Since the inception of metamaterials as a field of study, there have been several challenges in the physical realisation of their designs. For example, metamaterials must be manufactured on length scales comparable to the wavelengths of the fields with which they should interact, which can be a significant issue for optical metamaterials [145]. However, recent developments in manufacturing techniques have allowed for the implementation of many designs that were previously impossible [146]. In contrast to photonic metamaterials, the science of elastic metamaterials has attracted less attention, but represents a rapidly expanding area of study due to the growing interest in the applications to solid mechanics and mechanical systems [147]. For example, elastic lattices of beams—combined with various supports, such as pillars and Winkler foundations—have been used to model real-world systems, such as bridges, with particular emphasis on improving their resilience against earthquakes [148]. Despite the requisite length scales being typically larger for mechanical metamaterials compared with optical metamaterials, the physical realisation of many elastic metamaterials now faces similar challenges to those that have long affected the manufacturing of photonic metamaterials.

Although there is significant scope for the translation of ideas between elasticity and electromagnetism, it must be emphasised that the underlying frameworks are very different for the two classes of metamaterials—indeed, even the physical laws governing individual classes of mechanical metamaterials (elastic, flexural, gyroscopic, etc) have significant differences. Achieving negative refraction was pivotal to the development of EM metamaterials, and while the mechanism is very different, concepts have been proposed for inducing the negative refraction of elastic waves on lattices of beams at rotational inertia interfaces [149]. However, currently, there is no formal analogue of a negative index of refraction in photonic media for elastic media. Furthermore, elastic 'invisibility cloaks' have been proposed, with experimental results showing significant success at cloaking voids in plates [147].

Another parallel between elastic and photonic metamaterials arises in relation to the growing interest in chiral lattices. Photonic metamaterials are usually associated with passive chirality, that is, molecules that are chiral because of their geometry [150]. However, recently methods have been devised to induce chirality on elastic arrays through the incorporation of gyroscopic resonators. Gyroscopes are described as 'actively' chiral, which differs from passive (geometric) chirality in that two identical gyroscopes become chiral only when they are spinning in different directions, in which case they are mirror images, but cannot be super-imposed [151], as demonstrated in figure 11.

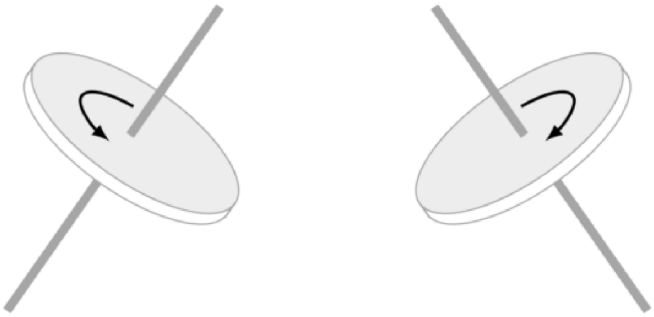

Figure 11. Two geometrically identical tilted gyroscopes that are spinning in opposite directions, demonstrating their active chirality.

Current and future challenges and opportunities

Several studies have demonstrated remarkable effects with systems of gyroscopes and flexural elements. In the papers [152, 153] strongly localised uni-directional waves were produced at chiral interfaces by setting gyroscopes on either side of the interface spinning in different directions. This was achieved in [152] for flexural plates with arrays of upright beams topped by gyroscopes; whereas [153] used a 2D triangular lattice of beams that was supported by a network of tilted gyroscopes at the beam junctions. In [152, 153] the localisation was so strong that waves were successfully bent around corners with minimal backscattering. The acronym Dynamic Amplification by Spinners in Elastic Reticulated systems was coined in [153] to describe the phenomena of interfacial waves travelling in closed loops, amplifying the original signal.

While the results of [152, 153] are indeed impressive, such structures requiring hundreds (if not thousands) of gyroscopes that are all perfectly synchronised would be exceedingly difficult to build and control. Although there are many physical systems that have inherent gyroscopic motion—wind turbines, boat propellers, and motorcycles to name a few—gyroscopes are often considered difficult to model analytically. Even simulating gyroscopes numerically is a computationally challenging multi-body dynamics problem. Moreover, there are several accepted conventions which are often employed for analytically modelling flexural systems that would need to be considered when building physical models. For example, it is commonplace to neglect the effects of gravity on systems, and the coupling of flexural and torsional rotations between elastic elements. Although there are some works that have studied these effects in elastic systems [149, 154] wherein it was demonstrated that the effects of gravity and the coupling of rotations can be significant.

Advances in methods and techniques to meet challenges

In the papers [151, 155] 'chiral boundary conditions' were developed, which provide a set of forces and moments that account for the presence of a gyroscope without needing to

solve the full equations of motion for the spinner. While deriving analytical solutions for any system would rarely be described as simple, using these boundary conditions provides significant simplifications when considering the equations of motion of chiral systems. Additionally, the chiral boundary conditions can be employed in finite element simulations, eliminating the need to model the full gyroscopic system, which in turn greatly reduces the computation time. The chiral boundary conditions contain a quantity called the *gyricity* which is defined as the sum of the rate of spin and rate of precession of the spinner (although, it is noted that the term 'gyricity' has had different definitions in other works, such as in [156]). With this, the ability to change the direction of spin of the gyroscope resides solely in changing the sign of the gyricity constant. The papers [152, 154] both employed these chiral boundary conditions to produce large scale models of chiral resonators.

There has also been progress in forming parallels between gyroscopic spinners and existing experiments. For example, the work reported in [154] has not only included the effects of gravity in studying gyropendulums (hanging rods with gyroscopes at the tips) but also showed the same ray tracing as Foucault's pendulum—whereby a swinging pendulum precesses due to the rotation of the earth. Furthermore, there have been studies that have drawn parallels between systems of beams and gyroscopes and gyrobeams—that is, beams with continuously distributed rotational inertia. In [155], a chain of beams with gyrohinges at the junctions was shown to be a good discrete approximation of a gyrobeam. Gyrobeams have been proposed in the designs of earthquake protection systems [157] and even for use in the propulsion of spacecraft [156]. Similar to [155], in [154] a chain of gyropendulums was shown to be a discrete approximation of a chiral rope.

Concluding remarks

The field of metamaterials is still considered a young area of research, with technology often significantly lagging the theoretical developments. The first concept of negative refractive indices [1] put forward by Veselago in the 1960's was in danger of fading into obscurity. It took another 30 years for the significance of the results to be recognised and another decade for optical metamaterials to be implemented [145]. In the same way that recent advances in manufacturing have made the realisation of photonic metamaterials for optical wavelengths possible, advances in manufacturing technology could well make many of the designs discussed in this review achievable in the near future.

Studies of periodic arrays of gyroscopic resonators could provide insights into the behaviour of large-scale systems of spinning rotors, such as wind farms formed of arrays of spinning turbines. With the hopes that, this research could determine method for reducing the vibrations of offshore wind farms, which are known to affect marine ecosystems [158].

14. The challenges of underwater acoustics

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Status

In the broad field of acoustics, ultrasound undoubtedly occupies the top position in terms of maturity, broad applications, and R&D outputs. Air-borne sound has received a rejuvenation through the advent of acoustic metamaterials. Underwater acoustics, covering the frequency range of few hundred to few thousand Hertz, is however up to now firmly in the third position both in terms of published research outputs as well as commercialized applications. This is due to the longer wavelength involved, as well as the much smaller contrast in its impedance with solids, as compared to that of air. These differences can translate into larger required sizes for wave manipulating devices, thereby hindering their applications and relevant experiments. It is a valid question on whether acoustic metamaterials can alter this situation for underwater acoustics. Some works have already been done along this direction, but still far short of the range and depth attained in the airborne acoustics (see, e.g. the review article [159]).

Current and future challenges and opportunities

In terms of underwater acoustic wave attenuation, one can have either absorption or blocking (reflection). Whereas the former is limited by the causality constraint in terms of the sample thickness necessary to attain the target absorption performance, the latter is governed by the mass density law. These constraints are especially stringent for low frequency applications.

We propose to re-examine the use frequency gap for low frequency acoustic blocking. The well-known phononic crystal bandgaps would imply very large lattice constants for low frequency bandgaps, as the phononic crystals' bandgaps are based on the Bragg scattering mechanism. So, in this context a frequency gap that starts at just above zero frequency and has an upper gap frequency ω_0, denoted here as the zero frequency gap, would be impractical for phononic crystals owing to the periodicity required. The question here is: Are there other avenue (s) to realize a zero-frequency gap? In this regard an earlier publication [160] has pointed out that for a solid plate with periodically perforated holes, a zero-frequency gap can be realized provided the zero-displacement condition is applied to the edges of the holes. The zero-displacement condition implies that practical realization requires the whole plate to be fixed to the ground, or some infinite mass; i.e. without the rigid overall translation degrees of freedom. Can the zero-frequency gap be realized with only the centre of mass be fixed, so that there is no rigid translational motion of the whole sample, i.e. immobilize the $k = 0$ mode in the frequency ω versus wave vector k dispersion relation for a solid plate? Below we will use the term 'zero frequency gap' to denote a frequency gap that excludes the rigid translational motion of the whole sample.

Advances in methods and techniques to meet challenges

Offshore structures usually require underwater support that extends to the seabed. Such structures can often generate very significant underwater low frequency noise. Shielding such noise would be beneficial to marine creatures and the relevant ecology. Here we propose the use of geometric design that is inherent to the central theme of acoustic metamaterials, to enhance the magnitude of the bending modulus for a structured solid plate, in order to realize something that is second best to the zero-frequency gap, i.e. a zero-frequency gap beyond a minimum wavevector k. In a sense this is exactly the finite size effect: The fact that a finite-sized plate (which has a natural minimum cutoff k corresponding roughly to the size of the plate $1/k$) would have a gap in its frequency of excitations. If the centre of mass of the plate is fixed, e.g. by fixing its edges, then the minimum excitation frequency ω_0 would be related to its size and to its bending modulus. However, what we hope to do is not to have a small square sample which would be of little practical use, but something that is meter (s) off in size so that it can exhibit a significant difference with a uniform plate of similar size, thickness, and mass density.

The consideration of solid plate does not mean to exclude other potentially possible avenues for attaining the same goal of shielding low frequency noise, e.g. absorption by bubbles. However, in this article we focus only on solid plates owing to their ease of application if realized, and lack of any pressure effects that can be a serious consideration in underwater acoustics.

The fact that a zero-frequency gap is directly linked to the bending modulus can be easily seen from the eigenfunctions expansion of the Green's function (1), here defined as the local displacement ξ of the solid plate in response to the pressure modulation p:

$$G(x,x'=x,\omega)=\frac{\xi}{p}=\sum_{n=1}^{N}\frac{\phi_n^*(x)\,\phi_n(x'=x)}{m_n\left(\omega_n^2-\omega^2-\mathrm{i}\beta\omega\right)}=\sum_{n=1}^{N}\frac{\left|\phi_n(x)\right|^2}{m_n\left(\omega_n^2-\omega^2-\mathrm{i}\beta\omega\right)},\tag{1}$$

where x is the lateral coordinate of the plate, ϕ_n is the nth eigenfunction in unit of displacement, $\omega_n=2\pi f_n$ is the associated eigenfrequency of the solid, $\omega=2\pi f$ is the frequency of the acoustic wave, β is the solid's dissipation coefficient, and m_n is the averaged mass of the sample weighted locally by the eigenfunction magnitude. Hence, the displacement at x can be expressed as equation (2) below:

$$\xi(x)=p\sum_{n=1}^{N}\frac{\left|\phi_n(x)\right|^2}{m_n\left(\omega_n^2-\omega^2-\mathrm{i}\beta\omega\right)}.\tag{2}$$

For fixed p, the magnitude of displacement ξ is inversely related to the response modulus. Smaller displacement implies

a larger modulus. In the case of a zero-frequency gap, with no excitations below the frequency $\omega_0 \gg \omega$, then in the low-frequency range above the zero frequency, we have an approximate expression (3):

$$\xi(x) \cong \frac{|\phi_0(x)|^2}{m_0\omega_0^2} p. \tag{3}$$

That displacement can be very small, implying a very large effective modulus.

The above discussion can also be made plausible through the simple qualitative description. Consider the dispersion of the two plate modes, S_0 and A_0, the symmetric and antisymmetric modes, in the limit where the relevant wavelength is much larger than the plate thickness. Whereas the dispersion relation of S_0 is linear, that of A_0 is quadratic. They are both governed by the biharmonic equation of motion with the bending modulus as the only physical parameter. If the bending modulus is large, then both the slope of the linear dispersion and the curvature of the quadratic dispersion will increase accordingly. If we have a fixed ω_0 on the vertical frequency axis, then we can imagine that both dispersion relations will intersect the horizontal line, located at the height of ω_0, in two values of k. The larger value of the two can be denoted the minimum wavevector beyond which there is a zero-frequency gap. Larger the bending modulus, smaller would be the minimum wavevector. That in turn implies the realization of the zero-frequency bandgap can be realized in a large, though finite, sample.

There are existing structures that are light and have a high bending modulus, e.g. the honeycomb lattice made of aluminium sheets is one such example. To be used for acoustic attenuation, two skin layers need to be attached to the honeycomb lattice to form a sandwich structure. These have already been commercialized for acoustic applications [161]. However, it is not always easy to attach the skin layers to the honeycomb lattice, and the bending modulus does depend on the height of the honeycomb structure. Larger the height, larger the bending modulus. However, that would mean a thick structure if the target bending modulus is large. The acoustic result as reported (in the website) shows that it does not display the ideal zero frequency gap behaviour for acoustic attenuation. Hence the search for such a metamaterial structure remains an open topic.

Concluding remarks

There can be multiple applications to underwater acoustics for a metamaterial with a zero-frequency gap, provided a suitable structure can be found. A material/structure that can display static rigidity significantly beyond that of water can effectively attenuate the underwater acoustic wave transmission, beyond the limitation imposed by the mass density law at low frequencies. Work in this direction is presently underway.

15. Metamaterials for ocean wave control, manipulation and harvesting

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Status

Strong winds over the open ocean generate surface gravity water waves, in the form of vertical fluctuations at the air–water interface that travel along the ocean surface. The wave fields are random and dispersive, consisting of a spectrum of frequencies and directions, with characteristic periods on the order of seconds to tens of seconds and amplitudes order metres. They carry huge stores of energy over great distances across the ocean—with power comparable to the capacity of a power plant—before breaking at the coastline.

Ocean waves are a potentially fatal hazard for offshore and coastal structures and dictate their design. This is an area of topical interest as humans increasingly encroach into the ocean, to extract natural resources (e.g. seabed mining), to capture renewable energy (e.g. using offshore wind farms), and to utilise the space offered on the ocean surface (e.g. using very large floating structures). Moreover, ocean waves play an important role in coastal morphology, which is also a subject of topical interest as climate change enhances coastal erosion.

Metamaterial-inspired ideas to control ocean waves are gaining traction in three broad application areas. Methods are being explored to *cloak objects* from ocean waves, based on the transformation media and metamaterials approach developed in optics, and in the context of reducing or eliminating hydrodynamic loads on the cloaked objects. There have only been a few experimental realisations of water-wave cloaking theories, using an array of vertical cylinders [162] and corrugations in the bathymetry [163]. Further, a water-wave cloak in a channel has been realised using bathymetric variations, with potential applications for controlling wave impacts in ports and wharfs [164]. There is also a so-called direct method for water-wave cloaking, in which the geometry (i.e. the bathymetry) or a structure surrounding the cloaked object is optimised to minimise wave scattering and, hence, the drift force on the cloaked object [165].

Metamaterial concepts have revitalised concepts for *harvesting ocean wave energy* for human use. There has been major progress over recent decades to the point of small-scale deployments. Most of the devices used to capture ocean wave energy (so-called wave energy converters; WECs) are designed to resonate at a chosen frequency, but, in general, they are narrow-banded and display poor performance in real (random) seastates, as the prevailing wave field at the WEC array may not carry significant energy at the resonant frequency. Metamaterial-esque structures have been proposed to focus wave energy into a target region, where it can be efficiently harvested by a WEC or WECs (an idea that dates back to the late 1970s). Designs have also been proposed in which the WECs themselves are the unit elements of the array, analogous to locally resonant metamaterials in optics and acoustics. These WEC-arrays aim to focus energy within the array, such that the WECs forming the array can absorb the energy. Arrays of offshore structures have an alternative application for *coastal protection* [166]. In contrast to standard breakwaters that block all water flow, offshore structures have been designed with band-structures that reflect [167–169] or redirect [170] wave energy over the damaging frequency bands (e.g. causing coastal erosion), whilst allowing transmission of bands associated to beneficial coastal processes (see figure 12).

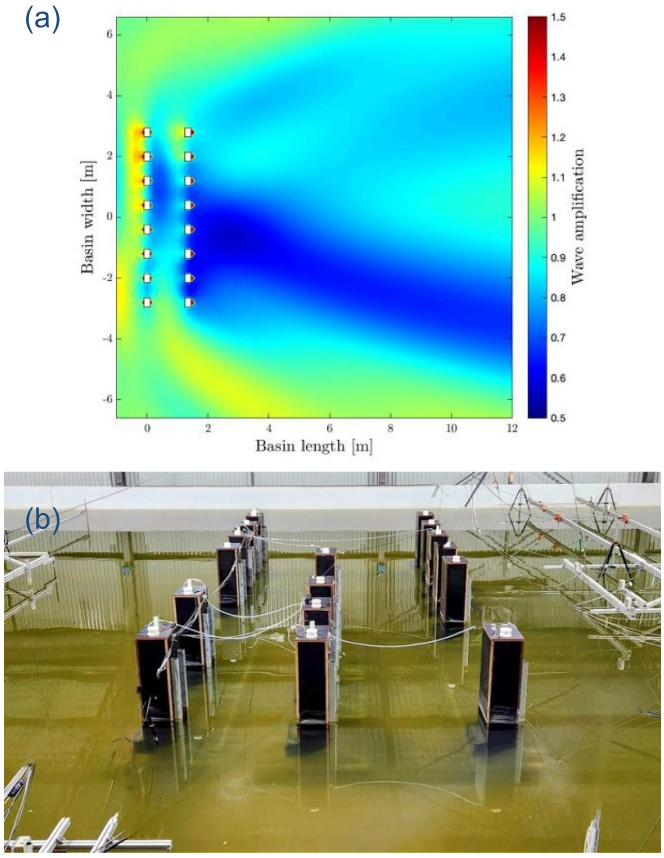

Figure 12. Potential combined wave energy harvesting and coastal protection by refraction created by a graded array of oscillating water column-type WECs. (a) Numerical prediction of wave amplification by a 8 × 2 array of WECs (graded in increasing natural period from 1.4 s on top row to 1.7 s on bottom row), for a regular incident wave of period 1.6 s that propagates from left to right. (b) Experimental set-up of a similar array, with an optimised configuration proposed by [166].

There are other examples of metamaterial-type structures for controlling water waves that do not fit into the three main application areas of cloaking, energy harvesting or coastal protection. These include negative refraction, reflectionless bends in channels, interface states, hydroelastic scattering cancellation, and spoof surface water wave polaritons along structured breakwaters.

Current and future challenges and opportunities

Cloaking offshore structures: Transformation media and metamaterial approaches to designing water wave cloaks have only been applied for simplified models, such as shallow water, for which the governing equations are equivalent to those of acoustics and optics. Extending the approach to the full linear water wave equations is an open challenge. The direct method allows greater freedom, such as finite water depths, and has been applied to finite depth water with cloaks formed from the bathymetry [165, 171] or an annular thin floating elastic plate [172]. However, the direct method has only been used to cloak at isolated frequencies, leaving the design of broadband cloaks an open challenge. Moreover, the direct method includes wave scattering by the cloaked objects, and, hence, the relationships to transformation media and metamaterials are unclear.

Wave energy converters: WEC-arrays require broadband absorption from an economical design to become a competitive renewable energy source. Over the past five years, there has been a move towards graded structures [173], inspired by rainbow trapping in optics and its translation into seismology and acoustics. The structures are broadband, with water wave energy amplified at locations chosen according to frequency, using standard vertical cylinders [174, 175], resonant C-shaped cylinders [176] and submerged cylinders [177], and where the grading is in terms of the cylinder spacing or the cylinder dimensions. Theories have been developed in 2D (one horizontal dimension plus depth) in which WECs are embedded in a graded structure to form quasi-perfect broadband wave energy capture [178]. The effect has also been achieved for structures formed from the WECs [179]. The design of 3D versions of the graded WEC-array for absorption over a broad range of frequencies and directions is an open challenge.

Coastal protection: To date, proposed designs are based on periodic arrays with wide, low-frequency bandgaps to block selected frequency ranges. The bandgaps are generated by local resonances of C-shaped cylinders [167] and fast wave speeds in stationary disk arrays at the water surface [168, 170]. Questions remain about how to control and optimise the bandgap properties. However, the most pressing challenge is to design practical and (relatively) cost-efficient arrays. The arrays should occupy as little surface area and/or contain as few unit elements as possible. Ideally, the unit elements themselves would be easy to deploy, not requiring bottom mounting or a separate structure to hold the elements in place.

Advances in methods and techniques to meet challenges

The challenges outlined above should be considered in the context of the high cost of installing and maintaining structures and devices in the ocean. This overarching challenge is a defining feature of metamaterials for ocean waves. It will direct modelling and design towards dual use structures to increase their cost effectiveness. WEC-arrays for combined energy harvesting and coastal protection have already been proposed, although, thus far, without fully utilising existing metamaterial concepts. Similarly, WECs have been proposed to stabilise larger offshore structures, such as floating wind turbines. This appears to be an area that will benefit from metamaterial techniques for energy harvesting and cloaking.

It is advantageous for costs and other practical considerations that metamaterials for ocean waves consist of relatively few units. Thus, there is a need to move beyond the band-structure paradigm for metamaterial design and develop analysis techniques for metamaterials of finite dimensions. Further, modelling and design tools must be suitable for lossy metamaterials, as energy absorbing WECs are likely to be their standard units.

Current modelling and design of metamaterials for ocean waves is almost exclusively based on linear water wave theory (or its degenerate shallow water variant), which assumes the water is incompressible, inviscid and irrotational, in addition to small wave amplitudes. Software that can be used to test metamaterial designs when operational considerations in the ocean, such as nonlinear energy transfers, wave breaking, currents, realistic bathymetries and coastlines, and more, will accelerate progress of the research field.

Concluding remarks

There have been significant advances in the modelling and design of water-wave metamaterials in recent years, backed by small-scale experiments. Although key research challenges remain, large scale testing of the metamaterial concepts is the next major frontier in the move towards ocean applications. The tests will help to refine the modelling and design challenges, among other benefits. Closer interactions between the metamaterials research community and those with expertise in ocean structures will drive the next major steps for the field.

16. Designing mechanical metamaterials for biomedical engineering and (soft) robotics

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Status

The research into mechanical metamaterials started with the rational design of micro-architected materials with unusual mechanical properties. These include negative stiffness or negative thermal expansion coefficients, extreme anisotropy, and ultra-high stiffness coupled with ultra-light weight, etc [3]. Over the last decade, the focus has gradually shifted from unusual properties to functionalities that are otherwise challenging or impossible to realize, such as shape morphing, adaptive mechanical behaviour, mechanical logic, and (re-)programmable actuators [180].

Recent advancement in mechanical metamaterials have transcended their exceptional mechanics into the realm of multifunctional and application-oriented designs [181, 182]. Multifunctional metamaterials demonstrate a range of advanced mechanical properties simultaneously, such as shape morphing, targeted elasticity, along with tunable or extreme or double-negative elastic moduli [3]. Alternatively, multifunctionality can be attained by integrating unique mechanical features with unusual dynamic, acoustic, thermal, biomedical, and other properties. Notable examples include high-static combined with zero-dynamic stiffness, shape morphing with adaptable mechanical properties for regulating biomechanical behaviour [183], and metamaterials combining targeted mechanical responses with sound- or energy-absorbing functionalities.

Two rapidly developing application areas for metamaterials are biomedical engineering and (soft) robotics. In biomedical engineering, engineered materials with unique combination of mechanical, biophysical and biological properties are defined as meta-biomaterials [184]. These two examples of mechanical metamaterials require the integration of three pillars: design, fabrication, and functionality (figure 13). For instance, the design space of meta-biomaterials can be tuned to combine auxetic (i.e. negative Poisson's ratio) and non-auxetic behaviour, creating hybrid meta-implants designed to improve implant longevity through enhanced primary and secondary fixations. This is achieved by rationally integrating both types of metamaterial unit cells to enhance bone-implant contact [184]. In the field of robotics, metamaterials significantly expand the range of geometric parameters and deformation degrees of freedom, thereby offering exciting prospect to equip robots with sensing, actuating, and interactive functionalities that are otherwise inaccessible [185].

As far as manufacturing is concerned, 3D printing techniques have already been widely used in biomedical engineering and robotics. Depending on the application, meta-biomaterials cover a wider range of materials from metals to polymers, while in robotics, the focus is on polymers and particularly smart polymers (e.g. shape memory polymers). The primary concern from the material viewpoint for biomedical applications is their biocompatibility and adaptability within the human body.

Current and future challenges and opportunities

Periodic architectures, which are common in all metamaterials, often limit the functionalities of mechanical metamaterials. Therefore, a key design challenge is to identify non-periodic combinations of architectural elements that cannot only deliver the desired mechanical properties but also can ensure structural integrity and manufacturability (figure 14). Non-periodic architectures are particularly crucial for applications such as shape morphing, deployability, and programmability. These can be obtained by various design strategies, which are currently limited to relatively simple deformations and randomness [3, 180, 183, 184].

Another challenge is achieving multifunctionality, specifically in terms of integrating electrical, magnetic, optical, or thermal properties with mechanical characteristics within a single construct. This integration is not straightforward, or sometimes even impossible, for microarchitectures composed of linear-elastic elements. Additionally, the use of functional materials possessing nonlinear, time-varying, or evolving material properties is still in the early stages of development. This area represents a significant research gap that requires further exploration and has the potential to unlock novel features in mechanical metamaterials, including strain-rate dependent functionalities [181].

The challenges associated with meta-biomaterials are closely linked to patient-specific designs, which, despite their benefits, remain labour-intensive and costly. Additionally, there are often contradictory requirements regarding their mechanical behaviour. This is illustrated by the need to enhance the strength of porous meta-biomaterials, which, intuitively, could be addressed by increasing their density. This approach, however, leads to reduced porosity and lower permeability, which are undesirable for biological functionalities. Other challenges include ensuring compatibility of the developed meta-biomaterials with existing manufacturing techniques and the stringent requirements of clinical applications. This complexity complicates the realization of design objectives, such as bone-mimicking mechanical properties or osteogenic behaviour, in clinically approved materials. It also affects the ability to achieve a desired pores size or customized surface (nano)pattern [184].

In robotics, the large number of design parameters becomes burdensome for many optimization methods, complicating the analysis of non-trivial deformations. The design complexity is

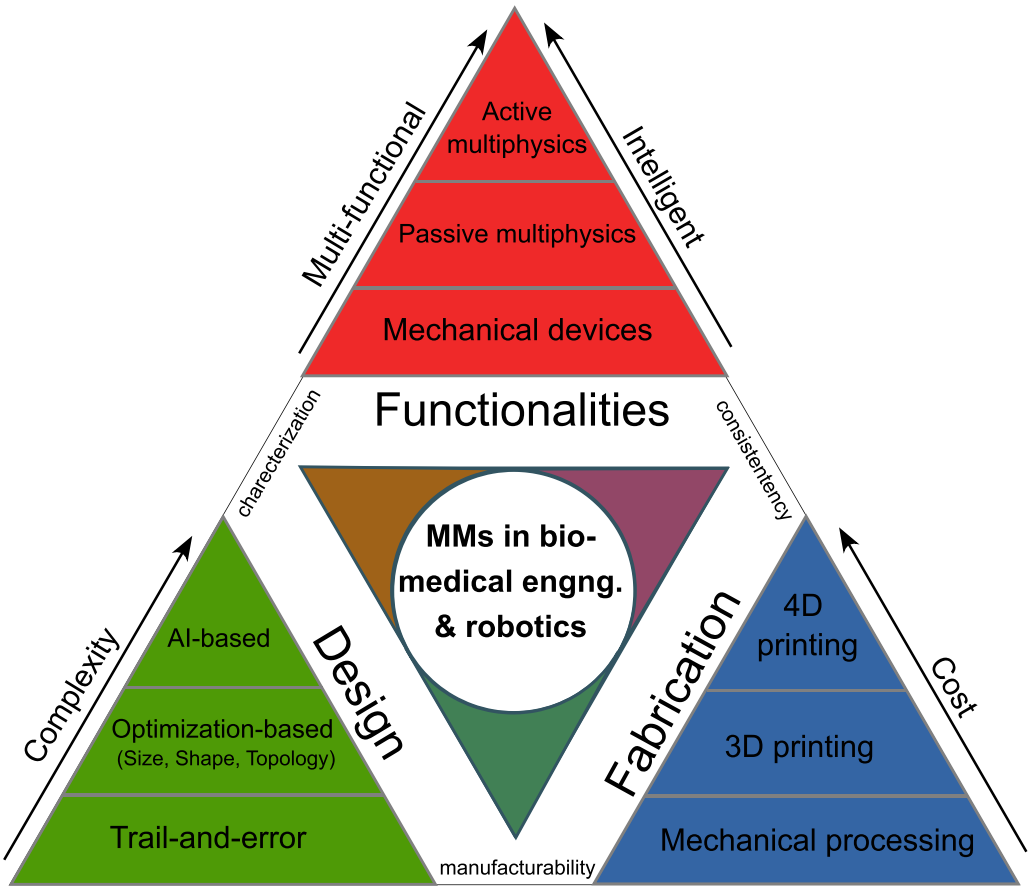

Figure 13. Three pillars for biomedical and robotic mechanical metamaterials.

further increased in compliant metamaterials due to the nonlinear behaviour of their hyperelastic or viscoelastic constituents [180]. Implementation challenges arise from the limitations of cost-efficient additive-manufacturing techniques, which hinder the resolution of a microarchitecture and the minimization of residual stresses and post-processing effects. Robotic applications demand excellent motion controllability, reversibility, stability, and robustness, which are difficult to simultaneously integrate into a design approach that also considers fabrication constraints.

Advances in methods and techniques to meet challenges

Multifunctional metamaterials hold significant potential in thermal control, energy storage, condition monitoring, power absorption, and energy harvesting. Their responsiveness to electric, magnetic, light, or thermal stimuli can be harnessed to enable adaptivity, shape-locking, or tunability activated by external stimuli or environmental conditions. The design of such metamaterials can be advanced by data-driven and AI-based techniques surpassing the limitations of gradient-based, topology, and evolutionary optimization. These tools have demonstrated potential in exploring design possibilities, optimizing performance control, addressing computational complexity, and overcoming technical challenges to guarantee fabrication feasibility and accurate response prediction [181]. They appear to be the most suitable approaches for utilizing randomness as a design tool, thereby expanding the design space of mechanical metamaterials to achieve even more exotic properties [180]. Accelerated inverse design of metamaterials based on AI shows great promise in tackling challenges from meta-implants to soft robotics [109]. For instance, video diffusion generative models can predict and tune nonlinear deformations and stresses in large-strain regimes, including buckling and contact, and can be extended to estimate deformation paths and full-field internal stress distribution.

Practical implementation of such solutions requires materials with non-trivial constitutive behaviour, including, e.g. flexible, nonlinear, photo- or magneto-sensitive materials. The careful selection of constituent materials is especially crucial for meta-biomaterials, as the right material can add another level of functionality, such as high corrosion or fatigue resistance, improved biocompatibility, or superelasticity. For instance, ceramic-reinforced metals form meta-biomaterials that combine the mechanical properties of metal with the biological functionalities of ceramic [184].

The emergence of multi-material and advanced additive manufacturing is promising for producing high-quality final meta-structures. Significance progress has been made by 3D grey-tone two-photon lithography in manufacturing thermoelastic metamaterials [189]. Inkjet and extrusion-based

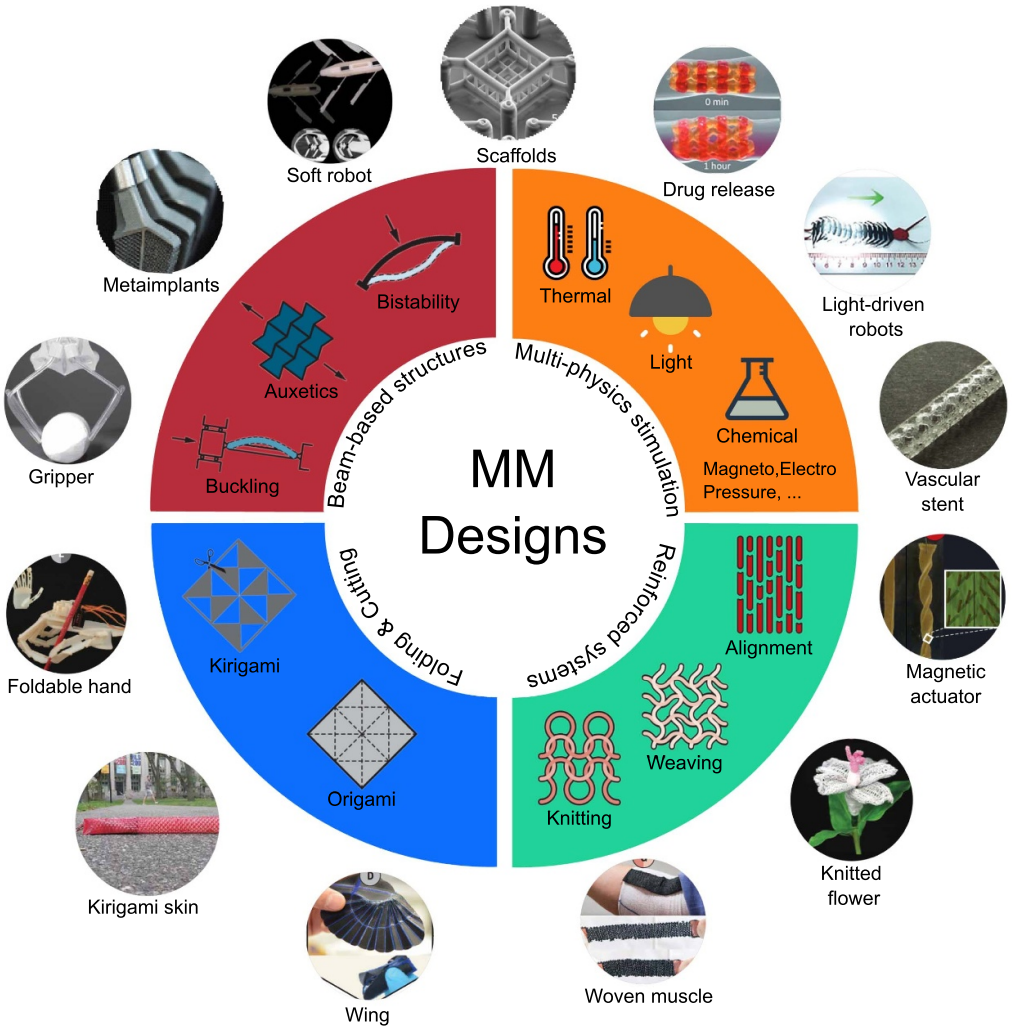

Figure 14. Mechanical metamaterial designs and examples of applications. Reproduced icons: beam-based structures, folding & cutting, reinforced systems, soft robot, gripper, foldable hand, kirigami skin, wing, woven muscle, knitted flower, magnetic actuator: from [185]. Reprinted with permission from AAAS. Multi-physics stimulation, drug release, light-driven robots, vascular stent: Reproduced from Qi *et al* [186]. CC BY 4.0. Metaimplants: Reproduced with permission from Kolken *et al* [187]. CC BY-NC 3.0. Scaffolds: Greiner *et al* [188] John Wiley & Sons. [Copyright © 2012 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim].

printing have been used to expand the range of materials, e.g. to metals with biodegradable properties [184]. Optimizing ink formulations for printability and adjusting bio-ceramic powder particles can facilitate the creation of multifunctional meta-biomaterials with modulated scaffold biodegradation rates. An emerging area is the application of 4D printing techniques to produce shape-morphing meta-implants [184]. The consistency between an initial design and the fabricated structure can be improved by topology optimization considering fabrication uncertainty or robustness theories at the design stage.

Robotic metamaterials with integrated soft logic modules can potentially simplify control systems while maintaining unrestricted mobility [109]. This approach, combined with scalable manufacturing, could facilitate the development of autonomous robotic systems that can perform complex motions.

Concluding remarks

Mechanical metamaterials, when combined with advanced manufacturing techniques, not only expand the range of realizable mechanical and multi-physical properties and functionalities but also demonstrate strong potential for a paradigm shift in mechanics and several other disciplines. In biomedical engineering, meta-biomaterials may enable treatment of skeletal diseases by encapsulating improved physical and biological performance, stability, longer service life, and shape customization within unique metamaterial (micro)architectures. This opens a new perspective for truly personalized medical treatments, moving beyond the current ‘one-size-fits-all’ approach [184]. In robotics, metamaterials have transformed design approaches and perceptions by proposing adaptable systems that can undergo complex motion and perform different tasks, thanks to

their programmable architecture [184]. Nevertheless, most metamaterials have only been developed up to proof-of-concept stage. This highlights the need for further research into fatigue, long-term local buckling, damage, and future design optimization, which are highly relevant for practical applications [190].

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Luke G Bennetts

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16. Designing mechanical metamaterials for biomedical engineering and (soft) robotics

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Data availability statement

No new data were created or analysed in this study.

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