Research report

1 Background

Many materials with high importance in engineering and biology are composed of random networks built from elastic rods. Such random networks constitute the structural component of various consumer products, i.e., rubber, paper, felt, textiles, baby diapers, various types of filters, heat or sound insulation, among others. Similar networks have an important role in biology as well, for example, connective tissue is formed by collagen and elastin fibers, cytoskeleton is formed by F-actin, microtubules and intermediate filaments. Rapid recent advance in the field of biological tissues, motivated by the hope to manufacture materials with superior properties, has given impetus to the research of the mechanical properties of these materials.

An important recent research direction is concerned with the behaviour of random fiber networks modelling the cytoskeleton, the component of eucaryotic cells providing internal support to maintain cell shape and to give the cell resistance against external mechanical loads. Similarly, collagen, the main structural protein in the extracellular space, the most abundant protein in mammals, exhibits peculiar mechanical behaviour. Investigating the mechanics of random network of rods can contribute to the understanding of the behaviour of the cytoskeleton and connective tissues containing collagen.

From a mechanical point of view, the cytoskeleton and similar biological networks can be viewed as a random network of elastic polymers. If the thermal fluctuations do not affect the mechanical properties of these (semiflexible) polymers, these random networks can be considered to consist of stiff elastic rods. The initial goal during this project was to investigate random networks of semiflexible polymers under athermal conditions, that is, neglecting thermal fluctuations. Quite surprisingly, such athermal, purely mechanical elastic random network models of biological materials can explain many experimental findings.

A remarkable property of biological networks like cytoskeleton and collageneous tissues is that they exhibit an extreme stiffening under applied mechanical loads. In some cases, this stiffening is on the order of a 100, that is, the shear modulus of the material, under shear strain, increases by two orders of magnitude before failure. Another interesting property of random elastic networks is that there is a sharp crossover between bending or stretching dominated regimes, depending on the density of rods in the network. This means that most of the elastic energy is stored as bending of the rods for low network density, and as stretching for large network density, respectively. Probably the simplest model to show this behaviour is the *mikado model*, where deformable rods of given length are dropped randomly on a square domain, and they are attached by hinges to each other wherever they intersect. It is found that there is a sharp transition between three distinct regimes depending on the network density. For very small density, the system is floppy, it cannot carry mechanical load. At larger densities, above the rigidity percolation, bending dominates: in this regime, there are sufficiently long free rod segments between cross-links that allows bending. At even higher network densities, the free segments become too short and the deformations are dominated by normal strains in the rods.

In order to perform its many important tasks, cytoskeleton or other biological networks need to be able to adapt to the external or internal signals, that is, they must be able to change their mechanical properties in a wide range. It has been observed that these almost floppy structures, under strain, show a very strong stiffening. This means that, depending on external stimulus, these structures are highly adaptable. The physical background of such adaptability is that they are working close to the transition between regimes of very different properties, that is, these highly complex systems can be highly tuned to their multiple tasks. Understanding the details of this highly adaptable mechanical behaviour can lead us to construct new adaptable materials with superior properties.

Most previous studies investigated random networks in which rods are connected either by hinges or by rigid connections that do not allow displacement or rotation. However, there are many types of cross-linking molecules e.g., in the cytoskeleton, that can connect the semiflexible polymers to each other. For example, α-actinin, fascin or filamin A can all cross-link actin filaments, but in different ways: α-actinin seems to provide hinged cross-links, while cross-linking with filamin A results in a preferential angle of 90° with a rotational spring included at the connection. Based on this observation, we proposed to investigate the inclusion of rotational springs in the mikado model: this way, the rods attached to each other can only rotate with respect to each other at an energy cost related to the spring modulus. In essence, the inclusion of these springs serves as a model of local shear stiffness, that is, stiffness against local angle changes. We asked the question of how the proportion of elastic energy associated to local bending, stretching or shearing varies with the parameters, and whether we find any transition between regimes of different mechanical properties.

Most models and simulations, with few exceptions, considered only one type of polymer to construct the random network, and dealt with only two-dimensional networks. Real networks often consist of different polymers, e.g., the cytoskeleton contains actin (providing initial stiffness under load), intermediate filaments (working under large load) and microtubules (supporting the other two). We intended to investigate the mechanical interplay of different types of rods in our random network.

The full description of the random network is inherently non-linear, and we initially aimed at using a non-linear investigation to find parasitic solutions, and also to include the effects of pre-stress.

The extension of the network modelling to include 3D effects was another goal we aimed for in the original proposal. This branch of our project took a slightly different direction by applying our results on filamentary network to the behaviour of bamboo, a natural, green material. From its 3D microscale ortotropic material properties up to 3D civil engineering structural levels, we reached important new results both computationally and experimentally in applying bamboo as a green building material or structural component.

We also intended to investigate the failure of filamentary networks and related engineering systems.

During the project, we addressed some additional problems not foreseen at the submission of the proposal. One of these problems is related to the averaged, mean-field-like description of the complexity of the network. We also opened a research direction related to the possiblecum string anisotropy of the network, which also lead to new results on the ortotropy of a new green building material, bamboo, which has a highly anisotropic internal microstructure.

2 Results

In order to study the behaviour of random elastic networks, we built a computational model, based on the mikado model used previously in the literature. The model has been implemented in a computer code in C for efficiency. Using this model, we were able to reproduce previous results concerning the transition between stretching dominated (affine) and bending dominated (non-affine) regimes. To overcome prohibitingly large (even several months) run times of the code, we implemented preconditioning and sparse matrices in our solver applying the conjugate gradient method.

We developed our model using two different boundary conditions. One uses a bounded load cell with pseudo periodic boundary conditions (rods hanging out of the load cell enter on the opposite edge, both segments fixed to the edge of the load cell). The other uses true periodic boundary conditions (rods hanging out of the investigated area enter along the opposite edge displaced according to the applied displacement load). Note that the first model, with the fixed load cell at the edges, can be considered as an initial pre-stress after loading, a more precise pre-stress model was not developed because of the large simulation times even without pre-stress. If the investigated network is large enough, the boundary conditions have negligible effect.

We also compared the results of our model with those obtained from a 2D, parametric finite element model developed and validated in Ansys Mechanical APDL environment. The model uses the pseudo periodic boundary conditions discussed above. At the intersection points of the rods either rigid connections, hinged connections or torsional and longitudinal springs with fixed stiffness can be placed connecting the intersecting rods. The results obtained from this model were close to the results of the model from our own code. The difference can be attributed to the different approximations used in the models.

Effect of local shear stiffness. During the investigation of the random elastic network, we applied our own C code with true periodic boundary conditions. We extended our implementation of the mikado model by applying rotational springs at the intersections to model moment bearing cross-links. This way we model the effect of local shear (angle change) in the network by computing the energy stored in the rotational springs as a function of the applied load or other network parameters (density, stiffness of rods, for example). The strain energy is proportional to the elastic modulus of the network, hence the energy stored in the various components is directly related to the contribution of the elements to the total network stiffness. We investigated the transition between the domains where stretching, bending or shear dominates the elastic energy and hence the stiffness. We found [24] that for small or large stiffness of the rotational springs, the total network stiffness is insensitive to the exact value of the local shear stiffness, and the energy stored in the rotational springs and hence the contribution of the shear springs to the network stiffness is zero. There is, however, a range of the local shear stiffness where the total network stiffness steadily increases; in this parameter range the energy in the rotational springs has a marked maximum. We explain this finding by observing that for small spring stiffness the rods are free to rotate at no energy cost, for large stiffness the rods cannot rotate and hence no strain energy is associated with the rotational springs. We can hence state that the rotational springs and hence local shear stiffness contribute directly to the total network stiffness in a well defined range of the parameters. In this regime, however, we find that there is an order of magnitude increase in the total network shear stiffness [24]. In essence, as the local shear stiffness increases, it makes it more difficult to bend the rods, leading to a more stiff network. At the same time, the role of the stretch component in the total network stiffness is enhanced, which can shift the network from its bending dominated non-affine regime to a stretch-dominated affine regime.

Mean-field approximation. We started to develop a mean-field approach to study the properties of the random network of rods. In general, the mean-field models in the literature apply some symmetric arrangement of the fibers and approximate the displacement field accordingly. As a first attempt, we implemented a Fourier-collocation-type method based on the Bernoulli-Euler rod model to realize that it becomes highly inefficient and inaccurate as the number of the randomly placed rods is increased. As the internal shear along the rods is discontinuous at crossings with other rods, we turned to establish a collocation method that accommodates functions with reduced regularity. Wavelet collocation is suggested to be a better method.

The stretch, shear and bending deformations of our network model are inherently coupled. To separate the effects of this coupling from the random nature of the network topology, we applied a similar methodology on a three dimensional regular unit cell of an open foam model, where it was possible to distinguish between the role of normal, bending and torsional stiffness. Numerical results allowed the derivation of a simple, mean-field like spring model and an analytical function for the calculation of a normal and a shear modulus. In essence, our method replaced the discrete model with a continuum model to achieve the computations [25].

Anisotropy. We also investigated the network with various levels of anisotropy. To this end, the network was generated by restricting the random rod directions to intervals around the horizontal and vertical angles. We found [24] that the more anisotropic the network is, the more important the local shear stiffness becomes in the overall stiffness of the network. In other words, the shear component of the total network stiffness shows a maximum for intermediate local shear stiffness, and this maximum increases with the anisotropy of the network. It was also found that anisotropy can suppress the transition to the affine regime with the increase of the local shear stiffness, although the increase in the stretch component is still observed.

We also investigated the mobility and stiffness of infinite planar networks, consisting of rods with hinged connections, exhibiting rotational symmetry, as a function of the choice of the unit cell. We found that interpreting the network as a material with microstructure leads to a 2D material law with -1 as the Poisson coefficient [15].

The mechanical behavior of random networks is interesting not just at the scale of cells: spider webs are highly optimized structures to carry an impact without failure. In an undergraduate research project, we studied the optimality of different possible arrangements of the net, including a random topology. We found, that the well-known radial-spiral arrangement is superior to the other topologies. This explains the way of spider web construction: in the beginning it resembles to a random network, but gradually the spider establishes the radial-spiral arrangement [1]. We also address a similar problem: the investigation of the mechanical performance of bone, in particular, the relation between random networks and the so called trabecuale palced at the end of mammal bones [2]. These topics were presented as undergraduate projects (TDK) winning prestigious prizes.

Different rod types. Our network model has also been extended to include three different types of rods mimicking the three different filaments found in cytoskeleton. The interplay of these rod types in the overall stiffness of the network typically leads to a layout in which one type is dominant in the overall network stiffness. However, for some parameter ranges, we find that the optimal, most stiff network is found to be the one with all three rod types simultaneously present [4,17].

Non-linear computations, parasites. When originally studying the mikado model, the equilibrium configuration was found by minimizing the elastic energy approximated up to second order in the displacements. This approximation simplifies the search for the equilibrium, however, it also might introduce errors. In order to extend the mikado model with a precise calculation of the energy functional, we derived the exact energy functionals for stretch, bending and local shear. An approximate implementation was used in the finite element model mentioned above. We also developed a computer code in C++ which is able to simulate the behaviour of a three-dimensional network of Euler-Bernoulli rods. In this latter model, the strains are assumed to be small, but the displacements can be large. The geometric discretisation of the rods is made by C1 continuous spline curves. This model allows for the modelling of local buckling of the rods of the 3D network. Unfortunately, the simulations with this model turned out to be prohibitively long on the computational resources we have access to (cluster at the Institute of Nuclear Techniques of BME). We therefore could not find any parasitic solutions.

Instead of full non-linearity of the random network model, the dynamics of a piecewise linear elastic structure (continuously suspended beam) was investigated with its status depending on the original or a reduced stiffness of buckled bar elements. The frequency and bifurcation diagrams were constructed [13]. A new algorithm was developed for the calculation of a steady-state response of the vibration problem with a single back-and-forth switching between the states during a period of the harmonic forcing. As opposed to the established classical methods, where the system is simplified to a reduced order model, our method uses only three parameters independent of the actual number of degrees of freedom, but finds all solutions in the search domain [16].

We also extended our studies towards the general behavior of complex, chaotic systems with parameter drift. We found that the concept of snapshot attractors, applied in studies related to climate change, can also be applied in mechanical systems [3]. Our results, based on an ensemble approach, can identify the level of complexity at different time instants [6]. These observations have far reaching consequences in other disciplines as well, where extreme events can be found using an ensemble approach. It was found that the method of sub-ensembles (initially close samples) can be useful in such cases [22].

Three-dimensional effects. We extended the model to include 3D effects by allowing the originally 2D model to displace out of plane. We found wrinkled solutions under load, however, the results depend too strongly on the actual details and scatter too much to draw meaningful conclusions. Instead, we looked for 3D effects in case of a green material investigated recently for its advantageous properties, that of bamboo as a constructional material. We constructed a representative volume element for constructional bamboo material based on the observed filamentary microstructure of natural bamboo. This simple model can explain the discrepancy between measured bamboo properties and theoretical predictions based on the differing material properties in 3 directions and on the spatially and directionally variable distribution of filamentary components [10,11]. The results obtained from the computational model (L.S. Al-Rukaibawi, S. Omirey, Gy. Károlyi: Multiscale simulation of bio-based composite materials, in preparation for submission to Construction and Building Materials, 2023) were confirmed in laboratory experiments [18], where the variation of bamboo strength in the radial direction was also investigated [19]. The properties of prefabricated structural elements made of bamboo lumber were also compared with the new standard of bamboo as a building material [21]. On an even larger scale, our findings were applied to application of bamboo in composite structural elements, like bamboo-steel hybrid composite beams [20], semi-rigid connection of laminated bamboo-steel hybrid composites I-section beam to steel column (L.S. Al-Rukaibawi, S.S. Weli, Gy. Károlyi: Evaluating the mechanical behaviour of a new semi-rigid connection of bamboo-steel hybrid composite I-shaped beam to steel column, in preparation for submission to Structures, 2023), laminated bamboo encased in Lipped channel cold-formed steel (L.S. Al-Rukaibawi, P. Hegyi, M. Kachichian, Gy. Károlyi: Mechanical behaviour of laminated bamboo encased in Lipped channel cold-formed steel columns under compression, in preparation for submission to Constructional Steel Research, 2023), and bamboo-expanded polystyrene composite sandwich block (L.S. Al-Rukaibawi, M. Kachichian, Gy. Károlyi: Design and mechanical test of bamboo-expanded polystyrene composite sandwich block for wall application, Construction and Building Materials, 2023). We also investigated the thermal properties of bamboo composites and their effect on overheating in housing applications [12], (L.S. Al-Rukaibawi, B. Nagy, Gy. Károlyi: Thermal conductivity measurements of cross-ply bamboo panels, in preparation for submission to Case Studies in Thermal Engineering, 2023).

Failure. In relation to the failure of networks, we followed experimentally the crack development in brittle hemispherical domes [14]. We developed a stochastic model to describe the fragment size distribution and proved that the new cracks appear either near previous cracks or in midpoints of the largest segments. In order to reveal the origin of quasi-equidistant spacing of cracks, commonly observable on hemispherical domes, we introduced a planar, pressurized, brittle ring model supported by a continuous elastic support [23]. This deterministic model, based on the Griffith theory of fracture and direct energy minimization demonstrates that the final cracking pattern obeys a quasi-equidistant spacing between the cracks as long as the variation in the support stiffness is moderate. It was also found that the emergence of the quasi-equidistant spacing is robust, i.e., the details of the mechanical model applied for the fragment hardly affects the close sizes of the fragments, The bending stiffness of the ring has some non-negligible effect on the order and position of the emerging cracks, while the bifurcation diagrams obtained as the critical points of the energy function determine the crack evolution, and the emerging cracks establish a discrete evolution along the global minima.

As a spin off, we also investigated dynamic, impact effects of rods on robust structures leading to potential failure. Using finite element simulations, we found that a single dimensionless parameter, which we named damage potential, can efficiently characterize the outcome of the impact [7]. We also found that this behaviour is valid even if the impacting rod is elasto-plastic, however, elastic waves travelling along the rod can enhance the impact load acting on the target structure [5]. We also carried out experiments at a military firing range to investigate the effect of impacts on the failure of reinforced concrete panels to verify our results. The raw experimental results have been reported already [8,9]. After the field tests, we evaluated the fractured concrete specimens by 3D scanning and by cutting them. We are in the middle of the evaluation of the results.

We published our results in 16 research paper, from which 11 is in highly ranked international journals with impact factors. There are three more papers that has been submitted in journals with impact factor, and there are 5 more in preparation.

Besides these research papers, a PhD has been submitted by one of the participants of the project (L.S. Al-Rukaibawi), an MSc thesis has been defended (supervised by Gy. Károlyi), and 3 student projects (TDK), supervised by the participants, won prizes.

The [references in square brackets] refer to the list of publication. The (references in round brackets) refer to manuscripts in preparation.