Development of simulation tools for bending and fracture of fiber-based materials

Final report, Åforsk’s young researcher grant ref.nr 22-166

January 2024

Utveckling av simuleringsverktyg för fiberbaserade materials böjning och sprickbildning

Ph.D. Gustav Kettil, Fraunhofer-Chalmers research centre for industrial mathematics, Chalmers Science Park Gothenburg

Summary of outcomes

This research project explores the potential of linear fiber network models for simulating key mechanical properties of paper relevant to product development, including tensile strength, z-strength, and bending resistance. The key findings from this investigation are as follows:

- Linear fiber network models prove effective in accurately simulating the behaviour of fiber-based materials in terms of fracture propagation and bending.
- To capture bending behaviour using fiber network models, it seems that a 3-dof Euler-Bernoulli beams is not enough, while a classic 6-dof Timoshenko model is adequate.
- Linear network models can successfully simulate paper strength tests by iteratively removing overloaded edges.
- Fiber network models effectively incorporate the essential characteristics of individual fibers and the bonds between them.
- The orientation, placement, and number of bond elements play a crucial role in determining the sheet's mechanical properties, especially the distribution of bonds and fibers in the thickness direction.
- The individual strength parameters of fibers and bonds directly influence the overall strength properties of the paperboard.
- The linear network approach facilitates the simulation of fundamental paper properties and product development tests using available computer resources within reasonable time frames.
- Using multiscale methods, even larger paper boards can be simulated.

These findings underscore the efficacy of linear fiber network models in understanding and predicting the mechanical properties of paper, offering valuable insights for product development in a computationally efficient manner.

Background

In Kettil's Ph.D. research (Kettil, 2019), the exploration of multiscale methods for simulating the papermaking process took center stage. The primary objective was to devise simulation techniques for paper formation, employing a fluid-structure interaction paradigm where fibers interacted with fluid, contributing to the formation of the paper sheet to replicate the lay-down step in a paper machine (Mark, o.a., 2011).

In the concluding phase of the Ph.D. work, a mathematical multiscale method initially designed for continuum partial differential equations (Målqvist & Peterseim, 2014) was extended to address discrete network problems, specifically applied to fiber networks. Proving effective with accurate convergence results (Kettil, o.a., 2019), this method was initially confined to simpler 2D network structures. The subsequent inquiry following the dissertation was whether linear fiber network models could enhance product development in the paper production process. The aim was to enable the simulation of four pivotal paper properties: tensile stiffness, tensile strength, bending resistance, and z-strength.

One notable strength of network models lies in their incorporation of individual fibers and the bonds between them, constituting the fundamental components of fiber-based materials (Sirviö, 2008). The mechanical properties of individual fibers, combined with their spatial distribution in the sheet, alongside bond quantities, locations, and mechanical properties, offer a comprehensive representation of a fiber-based material. However, this detailed representation introduces computational complexity.

While these models were explored years ago (Räisänen, Alava, Nieminen, & Niskanen, 1996), only in recent times has computational power become sufficient for handling such intricate problems. A central research question emerges regarding the requisite complexity of individual components in the model. Can linear beam models suffice, producing relevant results, or is the adoption of more complex, non-linear models necessary? The drawback of the latter lies in their limitation to small sheets, due to computational complexity, hence often impractical for real-world product development applications. In contrast to the network approach, continuum models (Borgqvist, Wallin, Ristinmaa, & Tryding, 2015) and stochastic approaches (Mansour, Kulachenko, Chen, & Olsson, 2019) have also been explored in previous research.

This pilot research study aims to assess the feasibility of using fiber network models, based on simpler linear beam models, to simulate fundamental paper properties typically tested in paper product development labs.

Project procedure

The project, funded by Åforsk's young researcher grant and performed by Gustav Kettil, entailed close collaboration with partners detailed in the Collaborations section. The work embraced both theoretical exploration and investigative simulation pursuits, with a primary goal of assessing the suitability of a network representation approach based on linear beam models for modelling and simulating paper product development. The focus revolved around four fundamental properties: tensile stiffness, bending resistance, tensile strength, and z-strength. The tensile stiffness and parts of tensile strength was proved possible in earlier work by the author and co-workers (Görtz, o.a., 2022).

The investigation was based on a network simulation framework initiated during Kettil's doctoral work (Kettil, 2019) and developed within the in-house structural solver at the Fraunhofer Chalmers Research Centre. To gauge the performance and validity of the fiber network model based on linear beam elements which the simulation framework was built on, results were systematically compared with experimental data. The data was obtained during a previous industry project, ISOP (Innovative Simulation of Paper), conducted at the Fraunhofer-Chalmers Research Centre in collaboration with partners from Stora Enso, Albany International, Akzo Nobel, and Tetra-Pack from 2009 and forward.

The investigative process for each paper property involved distinct experimental setups, necessitating the establishment of a robust simulation configuration for each test. Subsequent simulations were conducted, and the results were meticulously compared with the experimental data. Discrepancies between simulation and experimentation prompted in-depth examinations of model shortcomings. Some disparities were attributed to incorrect test procedure setups in the simulation, requiring rectification. In other instances, errors were identified in the implementation of network physics or the bonding procedure, prompting necessary corrections. Furthermore, in some cases, the chosen model seemed not adequate and other choices were investigated, for example as in the case of bending of paper sheets, where Timoshenko beams replaced the previous Euler Bernoulli beams.

Key findings of the project underscored the imperative to enhance the bonding algorithm and incorporate the cross-sectional directions of network edges to accurately reflect the features of the underlying beam model. Specifically, for fracture simulations, an adaptive iterative algorithm had to be developed in an efficient manner to ensure accurate representation and reliable results.

Summary of theory

A fiber network model characterizes paper-based materials by incorporating individual fibers and the bonds between them in the form of edges and nodes. In this study, fibers were modelled as chains of edges, and bonds between fibers were represented by placing edges where fibers intersect. The fiber geometry was derived from experimental pulp fiber data, including length, width, cross-sectional information, and shape. For a given sheet, defined by its size and grammage (surface weight), the generated fibers were randomly placed and oriented. Considering edges as volumes based on cross-sectional data, spatially proximate edges were evaluated for intersection, and bond edges were placed if sufficiently close, resulting in a connected network system.

The physical behaviour of the network was incorporated by modelling the edges as beams. Two beam models were explored: a simple Euler-Bernoulli beam model, encompassing only three translational degrees of freedom in each node (Kettil, o.a., 2019), and a standard Timoshenko model (Kulachenko & Uesaka, 2012), including both translational and rotational degrees of freedom. Assembling the element matrices for each edge produced a linear matrix equation. After applying boundary conditions according to the mechanical test considered, a solvable system was achieved and solved using a direct matrix solver.

The developed bonding algorithm extends the method used in (Görtz, o.a., 2022) where the closest points between edges were found and the edge volumes extracted from the cross-section definitions were used to check for intersections. Edges were considered pairwise and if intersecting, bond edges were placed with fixed distance until the edges ended. This gives uneven bond covering over edge connections. In the new method, instead of considering edges pairwise, whole fibers were instead considered, and a spreading procedure was used based on a local minimum criterion. For each pair of fibers close enough for bonding, all local minimum between the fibers were found. The local minimums are referred to points where the distance between fiber centrelines is locally at a minimum. When these points have been found, bonds can be spread by stepping along the fibers as long as the axis separation distance is increasing.

To simulate fracture propagation in fiber networks, crucial for determining the tensile strength and z-strength of paper sheets, an iterative approach with edge removals was employed. This involved applying strain to the paper sheet through boundary conditions, solving resulting deformations, and calculating individual edge strains and stresses. If edge stresses exceeded a predefined yield strength, the edge was considered broken and removed. The process was iteratively applied until the desired stretch of the whole sheet was achieved.

The iterative fracture algorithm's dependency on strain increments was addressed with an adaptive algorithm, adjusting the increment size based on the number of broken edges. Observing that the limits of broken edges could be categorized into fiber edges and bond edges, the limits could be kept higher, reducing the required number of iterations.

The multiscale method for partial differential equations extended to discrete network models (Kettil, o.a., 2019) during the Ph.D. work of Kettil was further elaborated in this project. The principle of the method is to consider a coarse scale representation of the network using a finite element basis space. This coarse solution space is not able to capture the microscale feature of the fiber network along, but a modification of the basis functions is necessary. That is performed by solving local sub problems incorporating fine scale features into new modified basis functions. These modified basis functions span a coarse scale space with improved representation properties and solving a coarse scale system using these modifications results in accurate coarse scale solutions.

Recap of important results

The research project yielded two pivotal outcomes, by demonstrating the feasibility of achieving realistic simulation results for the bending resistance and z-strength of paper sheets through a fiber network approach based on linear beam models. Notably, prior works in the literature have not achieved this, according to the author's knowledge.

In assessing bending resistance, simulations were conducted on three-ply, high-grammage paperboard. The results were compared to laminate material theory, revealing commendable agreement. Figure 1a illustrates the results of a study of 200-grammage boards with kraft pulp on the two outer layers and CTMP pulp in the central layer, with the weight fraction defined as the mass fraction of surface layers over the center layer. The simulated bending test was performed with both two-point and four-point methods. A key takeaway from the investigation was that the Euler-Bernoulli three-degree-of-freedom beam model proved insufficient to achieve realistic bending results. Instead, it became evident that a Timoshenko beam model was imperative for accurate representation.

Another significant finding for the bending resistance underscores the necessity of simulating large paper sheet sizes. This requirement arises from the fact that the bending resistance test, being particularly susceptible to shear bending effects with too short levers, demands substantial sample sizes. The requirement for large sheet sizes to obtain accurate bending results not only highlights the utility of the multiscale method investigated in this project but also emphasizes the practical aspect of its application. However, the paper boards examined in this project remained sufficiently compact to be accommodated on a standard working station computer.

For the z-strength investigation, Figure 1b presents results comparing simulations with experimental data for 60-grammage sheets with varying pulp compositions. Four sheet types were examined, including softwood and hardwood pulp, as well as two combinations (60-40% and 40-60%). The simulation input data for the pulps exhibited variations in terms of length, width, and cross-sectional geometry, while maintained uniformity in all other physical properties between the two pulp types. Concerning the bonds, identical properties were maintained, whether they occurred between the same fiber types or between different types, with the sole exception of the bond area, which was determined by the fiber widths.

Despite differences in pulp characteristics, the agreement between simulation and experiment was notable. The study's key finding emphasized the critical role of bonding extent in the thickness direction for proper behaviour. Randomly generated sheets, which was used in this project, results in a z-direction fiber distribution with unrealistic fiber overlap and voids, necessitating an increased padding distance to identify fiber bonds. Future analyses should delve deeper into this aspect, exploring networks generated through laydown methods for further comparison and understanding.

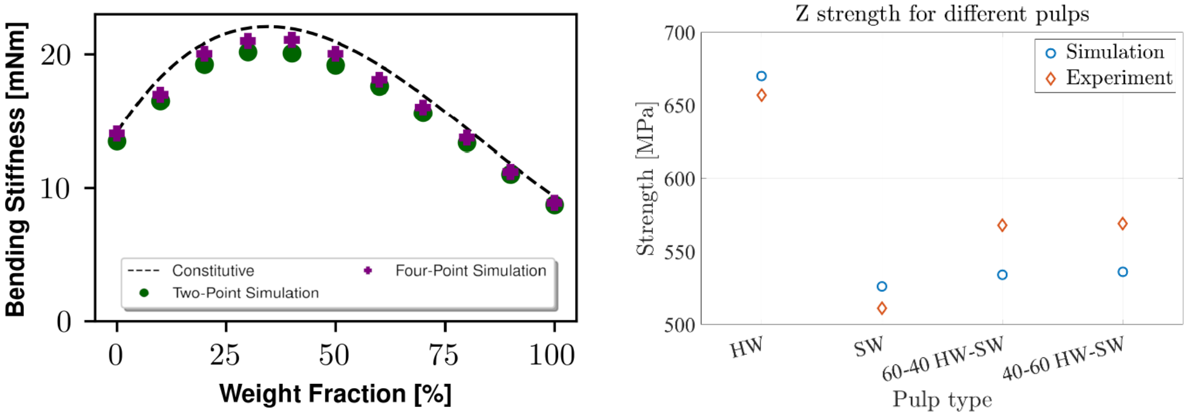

Figure 1. a) *Bending stiffness comparison between simulated paper board and laminate bending theory ("constitutive"). The paper board consisted of three plies and the grammage was 200 gsm.* ***b)*** *Z-strength comparison between simulation and experiments of 60 gsm sheets with four different pulp combinations.*

Collaborations

Gustav Kettil who performed this research projects worked closely with Morgan Görtz at Fraunhofer Chalmers Research Centre and Axel Målqvist at Chalmers University of Technology and Gothenburg University. Consultation and support were attained from Fredrik Edelvik at Fraunhofer Chalmers Research Centre. From industry partners, advice was seeked and supported from Mats Fredlund at Stora Enso and Kenneth Wester at Albany international.

Resulting publications

The research conducted in this project has so far resulted in two articles:

A. Numerical homogenization of spatial network models, Fredrik Edelvik, Morgan Görtz, Fredrik Hellman, Gustav Kettil, Axel Målqvist, Computer Methods in Applied Mechanics and Engineering, Vol 418, Part B, 2024, 11659
B. Iterative method for large-scale Timoshenko beam models, assessed on commercial-grade paperboard, Morgan Görtz, Gustav Kettil, Axel Målqvist, Mats Fredlund, Fredrik Edelvik, submitted December 2023

Article A presents theoretical aspects of the localized orthogonal decomposition method and highlights its capacity to solve complex networks such as fiber networks. Article B was submitted in December 2023 and covers bending of high grammage paperboards using a network model with Timoshenko beams. It also contains an iterative decomposition method implemented by Morgan Görtz. A third publication is currently in progress, with a primary emphasis on presenting findings related to the simulation of tensile strength and z-strength in paperboards. This upcoming publication will specifically showcase the iterative method, detailing its application and validation against experimental results for sheets with mid and high grammages.

Future considerations

The direct next step of this work is the compilation and submission of the article dedicated to the validation of strength simulations, particularly focusing on z-strength, presenting the preliminary results showed in Figure 1b.

To enhance the understanding of the fiber distribution in the z-direction and its impact on the properties of paper materials, a comprehensive investigation is warranted. Comparing various network generation methods is crucial to discern their effects on fiber and bond distribution in the z-direction of a virtual paper sheet. The random positioning method employed in this study, while remarkably speedy, results in unrealistic overlaps of fibers. It is worthwhile to invest efforts in refining this method to mitigate these overlaps. One approach could involve post-modification, reordering of fibers based on the degree of overlap. Alternatively, a statistical investigation might reveal a suitable padding distance for bond detection that ensures equivalent or nearly equivalent bonding coverage in the z-direction, even in the presence of unrealistic fiber overlaps.

The real physical process, where fibers are sequentially laid down and the sheet is pressed to tightly compact fibers in the thickness direction, was closely emulated by the method used in Kettil's Ph.D. work (Kettil, 2019). However, it is acknowledged that this method is slower due to increased simulation time. Despite this drawback, it remains invaluable for comparison purposes, as it accurately captures fiber interactions during forming, thereby avoiding unrealistic fiber overlaps. Achieving a correct fiber distribution and bond coverage in the z-direction holds significance not only for z-strength but also for other paper properties, such as shearing. Consequently, refining simulation methods to accurately represent these aspects is vital for advancing the understanding of paper properties.

As demonstrated in this study, the detailed fiber network representation of paper based on linear beam models proves robust by encompassing individual fibers and the interconnecting bonds. However, for specific applications or exceedingly large paper samples, relying solely on a direct solution approach may prove insufficient. In such scenarios, a multiscale approach becomes particularly pertinent. The method worked on in this research exhibits versatility, enabling the simulation of extensive samples, and demonstrating heightened efficiency when employing a periodic representation derived from a smaller domain.

In the pursuit of advancing multiscale approaches, the upcoming phase entails a meticulous focus on computational performance. The objective is to push the boundaries of paperboard size that can be effectively analysed through simulation utilizing the fiber network approach. This strategic emphasis on computational efficiency aims to enhance the applicability and scalability of the developed method in addressing the challenges posed by larger and more complex paper sheet configurations.

While initially planned but not addressed in this work, a captivating avenue for future investigation involves extending the fiber network model to incorporate time dependency. Although this will introduce additional computational complexity, delving into this aspect holds the promise of providing valuable insights. From the findings of this project, it appears that including time dependency is not necessary for certain paper properties like tensile strength, z-direction strength, and bending resistance. However, for more intricate paper tests, such as creasing, the inclusion of time dependency is likely to be essential.

Furthermore, integrating plasticity into the model can be achieved by introducing thresholds for which the stiffness of edges is altered, like the way edges currently break when specific stresses are reached. Similar plasticity approaches have been successfully tested in other breakage models (Tojaga, Kulachenko, Östlund, & Gasser, 2021).

Building on the insights gleaned from this project, which underscore the efficacy of the network fiber representation for simulating fundamental paper properties, the subsequent goal is to integrate this simulation framework into the development teams of industrial paper products. However, based on past experiences, this transition is not without its challenges. The process of digitization can be intricate, and embracing a simulation mindset may present hurdles. It is crucial to present the obtained results in an accessible manner, elucidating how the simulation framework can be utilized for parameter studies. This involves varying fiber and bond properties to comprehensively understand the impact on the resulting mechanical properties of paper material. Furthermore, an iterative collaboration with paper product developers is deemed appropriate to tailor the development of simulation tools according to their specific needs.

As evidenced by the ongoing discourse surrounding Swedish forestry, process changes are likely imperative to enhance biodiversity and mitigate the effects of climate change. Introducing new tree species and altering the composition of the current wood stock are potential measures. This, in turn, yields pulp types with distinct properties compared to the prevalent Scots pine, Norway spruce, or silver birch. The simulation tool developed in this work serves as an ideal instrument to assess the ramifications of new pulp properties on resulting paper properties. By doing so, it facilitates informed decision-making in the ever-evolving landscape of paper product development.

Acknowledgements

The author’s work was made possible due to the funding from Åforsk “Young researcher” grant. Simulations was performed by resources provided by Chalmers e-Commons at Chalmers.

References

Borgqvist, E., Wallin, M., Ristinmaa, M., & Tryding, J. (2015). An anisotropic in-plane and out-of-plane elasto-plastic continuum model for paperboard. *Composite Structures*, 184-195.

Görtz, M., Kettil, G., Målqvist, A., Fredlund, M., Wester, K., & Edelvik, F. (2022). Network models for predicting structural properties of paper. *Nordic Pulp & Paper Research Journal*, 712-724.

Kettil, G. (2019). *Multiscale methods for simulation of paper making.* Gothenburg, Sweden: Chalmers university of technology.

Kettil, G., Målqvist, A., Mark, A., Fredlund, M., Wester, K., & Edelvik, F. (2019). Numerical upscaling of discrete network models. *BIT Numerical Mathematics* , 67-92.

Kulachenko, A., & Uesaka, T. (2012). Direct simulations of fiber network deformation and failure. *Mechanics of Materials*, 1-14.

Mansour, R., Kulachenko, A., Chen, W., & Olsson, M. (2019). Stochastic Constitutive Model of Isotropic Thin Fiber Networks Based on Stochastic Volume Elements. *Materials*, 538.

Mark, A., Svenning, E., Rundqvist, R., Edelvik, F., Glatt, E., Rief, S., . . . Nyman, U. (2011). Microstructure Simulation of Early Paper Forming Using Immersed Boundary Methods. *TAPPI Journal*, *10*(11), 23-30.

Målqvist, A., & Peterseim, D. (2014). Localization of elliptic multiscale problems. *Mathematics of Computation*, 2583-2603.

Räisänen, V., Alava, M. J., Nieminen, R. M., & Niskanen, K. (1996). Elastic-plastic behaviour in fibre networks. *Nordic Pulp & Paper Research Journal*, 243-248.

Sirviö, J. (2008). FIbres and bonds. In K. Niskanen, *Paper Physics* (pp. 59-92). Helsinki: Finnish Paper Engineers' Association.

Tojaga, V., Kulachenko, A., Östlund, S., & Gasser, T. C. (2021). Modeling multi-fracturing fibers in fiber networks using elastoplastic Timoshenko beam finite elements with embedded strong discontinuities — Formulation and staggered algorithm. *Computer Methods in Applied Mechanics and Engineering*.