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A MULTISCALE METHODOLOGY FOR SIMULATION OF MECHANICAL PROPERTIES OF PAPER

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Abstract. In this work a multiscale framework developed for simulation of mechanical properties of paper is presented. The framework consists of two major parts. In the first part the forming process of a paper machine is simulated using the fiber suspension model developed in [8]. Fluid dynamics together with an advanced contact calculation method enables detailed simulation of the lay down process. The resulting paper sheet is used as input to the second part of the framework. In the second part the fiber configuration attained from the unique forming simulations is transformed into a network representation, enabling simulation of mechanical properties. The paper mechanics is governed by a fiber network model. To study macroscale properties a novel numerical upscaling method for networks has been developed. In this paper the complete simulation methodology is outlined and discussed.

1 INTRODUCTION

Paper making is an old-established manufacturing process. Paper making machines all around the world produce each year hundred million tons of paper and cardboard. The genuinely complex process is not fully understood and there is still much room for improvement. The global trend of digitalization reduces the need of printing paper at the same time as the increased use of packaging leads to an industry in urgent need to improve production methods and product quality, as well as to develop new ways to use paper and fiber-based materials.

One crucial stage of paper making is the forming process taking place in the forming section of the paper machine. There a dilute suspension of cellulose fibers is leaving the head box, flowing down onto a forming fabric over which the suspension is drained and a paper structure forms. After the forming section the resulting paper is pressed, further affecting the configuration of fibers. Lastly the paper is dried and the resulting product is a material that can be seen as a fiber network held together by bonds.

The mechanical properties of the final paper product is important, and increasing the knowledge of how the different sections of the paper making machine affect the properties of the end product is utterly desirable. By developing simulation tools that are accurate, robust and fast, a product development iteration methodology could be applied to the paper making process that would be pioneering for the paper industry.

In this paper a framework for investigating the mechanical properties of paper through simulation is presented. The aim of the framework is to study how the forming process affects the mechanical properties of the resulting paper. By developing such a simulation tool plenty of different production parameters can be investigated and the resulting effect on the paper studied. Example of such parameters are the forming fabric structure, the flow conditions during lay down, the injection velocity and angle, the fiber composition and distribution, and the fiber type.

The simulation framework consists of two main parts, one part for simulation of the paper forming, and one part for simulation of the mechanical properties of the resulting paper. The paper forming simulation framework was presented in [8, 13, 23] and is built on a fiber suspension model consisting of four submodels: one for the fluid flow, one for the fibers, one for the fluid-fiber interaction, and one for the fiber-fiber interaction. The framework is reviewed in Section 2.2.

The new contribution of this work is the second part of the simulation framework, a methodology for simulating the mechanical properties of the resulting paper sheet. Properties which are closely linked to the paper forming simulation. By taking advantage of the realistic fiber sheet configuration attained from the forming simulations, the fiber sheet in its fiber suspension representation is transformed into a new representation, in the form of a fiber network. By representing the fiber sheet as a fiber network and adding bonds between close fibers a setup is attained which is more suitable for simulation of mechanical properties compared to the initial fiber suspension model which on the contrary is necessary to capture the fluid mechanical features during the forming process.

By utilizing cyclic boundary conditions during the forming simulations, sheets can be periodically replicated into a fiber network of macroscale size. Resolving mechanical properties of this large network will however not be computationally feasible. Therefore a numerical upscaling method has been developed suitable for materials represented by network models.

In this paper this simulation methodology is outlined. In Section 2 a brief background is presented together with a review of the forming simulation framework. In Section 3 a fiber network model is presented based on three types of force contributions. In Section 4 a numerical upscaling method is presented, which is directly applicable to the network model. In Section 5 the simulation framework as a whole is described and lastly, in Section 6, some concluding discussion is contained.

2 BACKGROUND

2.1 Previous work

To investigate macroscale properties of paper products with a simulation methodology as presented in this paper, based on a fiber network approach, three crucial steps in the modeling procedure have to be considered. Firstly, the configuration of fibers and bonds in the network has to correspond well to the real paper material. Secondly, the model for fibers and bonds in the network has to be sufficiently detailed to correctly transfer the mechanical properties to the macroscale. Thirdly, to be able to handle the scale separation of the macroscale and microscale, and to accurately resolve the macroscale properties from the microscale model, a robust numerical multiscale method has to be used.

Different methods have been used to create the network configuration. Kulachenko and Uesaka [9] use a deposition technique, where fibers are generated with Gaussian based random orientation and deposited one by one on a flat surface such that the fiber deforms from contact with previously deposited fibers. In other works [10, 5], fibers are randomly generated without intersection in the space between two plates and the plates are pressed against each other. For fibers modeled as one-dimensional lines, a simpler method is to randomly position them in the plane [18, 11]. At Fraunhofer-Chalmers Centre, a unique framework has been developed to attain the network configuration from simulation of the real process. A fiber suspension, governed by fluid dynamics, is flowing down onto a forming fabric and fibers start to build up the paper structure, similarly to the process in the forming section of a paper machine. In this way the flow conditions during lay down and the forming fabric structure, two important variables during the forming process, are included when creating the network configuration.

When modeling the fiber network a variety of different representations are used in the literature, ranging from simple representations, where fibers are modeled as chains of springs with bonds represented as common nodes, to networks where fibers are modeled as beams with bonds modeled by FEM-contact elements. Wilbrink et al. [27] use the spring approach, while others [9, 10, 5, 11] model fibers as beams, e.g. with 3-node Timoshenko beam elements. Mao et al. model their bonds using mutual nodes between beam elements prescribing the translational and rotational degrees, while Kulachenko and Uesaka use beam-to-beam contact elements.

There is a long research tradition in upscaling of partial differential equations (PDE) with heterogeneous data. In homogenization theory efficient material parameters are determined for periodic and random structures. Several numerical methods have also been proposed during the last twenty years; see e.g. [26]. A recent contribution in multiscale methods for elliptic problems was achieved in [15]. In that work an optimal generalized finite element space is constructed, using an orthogonal split of the full solution space, and a rigorous mathematical analysis for non-periodic data is derived. This technique is referred to as the localized orthogonal decomposition method (LOD).

Numerical upscaling of networks has not been as extensively studied as upscaling of PDE. On the numerical side there are results for porous media flow problems based on the heterogeneous multiscale method [2] and heat conductivities of fibrous materials such as glass and mineral wool [7], which has a similar structure as paper. Mechanical properties of network materials have been investigated using upscaling methods requiring a continuum representation of the material [22]. A method not requiring a continuum description is the quasicontinuum (QC) method [24, 1], which enables multiscale calculation of fracture propagation. QC is however restricted regarding the generality of the network structure. The numerical upscaling method for fiber networks presented in this work is based on the LOD method, enabling fiber networks of arbitrary structure and a rigorous error analysis.

2.2 Paper forming simulation framework

To attain a realistic fiber network configuration as input to the network model the first part of the simulation framework is developed to simulate the forming process of a paper making machine, where a fiber suspension flows down onto the forming fabric and the fibers lay down and build up the sheet structure. To enable such microstructure simulations, the involved fiber suspension flow has to be modeled. In this section the fiber suspension model developed in [8] is reviewed. That model, used to simulate the forming process, consists of the four sub-models: a fluid model, a fiber model, a fluid-fiber and fiber-fluid interaction model, and a fiber-fiber interaction model.

The fluid is governed by the Navier-Stokes equations, consisting of the momentum and the continuity equation

$$\begin{aligned} \rho\frac{\partial u}{\partial t} + \rho u \cdot \nabla u - \mu \nabla^2 u = -\nabla p + f, \\ \nabla \cdot u = 0, \end{aligned} \tag{1}$$

where u is the velocity, p is the pressure, t is the time, and ρ and μ are the density and viscosity of the fluid, respectively. The flow is solved using the incompressible finite-volume based fluid solver IBOFlow (immersed boundary octree flow solver).

The fibers are modeled as beams using a finite-strain rod model developed by Simo and Vu-Quoc [19, 20, 21]. Their model is a nonlinear rod model including finite bending, shearing and extension, permitting deformations which are arbitrarily large in regard to rotation and strain. The forming fabric used in the forming simulations is attained from a voxel representation of a real fabric. The voxel representation is meshed and the fabric is considered as a rigid static object.

The effect from the immersed fabric and fibers on the fluid is handled by the non-distributive, second-order accurate, immersed boundary method developed by Mark and co-workers [14, 12]. It is a hybrid mirroring immersed boundary method, which by an implicit boundary condition, constrains the fluid velocity at the immersed boundary to the velocity of the surface. The effect from the fluid on the fibers is calculated using an empirical drag force relation derived from experiments.

The fiber-fiber interaction model was developed in [8] and can resolve contact forces acting at small scales without requiring the time step of the discretized fiber motion to be reduced. It is based on so called contact points which are distributed over the fibers. Between these contact points contact forces are calculated. The force formulas are the DLVO [3, 25] forces together with a steric repulsion force, adapted to, in a numerically stable way, manage the repulsive forces acting on the smallest separation distances where overlaps occur. By solving the motion of the contact points locally during each fiber time step, average forces can be calculated which are added to the fibers.

The fiber suspension model described above is used to simulate the lay down of fibers during the forming process. In the lay down simulations an axis-aligned rectangular box is used as simulation domain. The forming fabric is positioned in the lower half of the domain and the domain is filled with water and a pressure drop across the fabric accelerates the flow and a steady state solution is found. Thereafter fibers are injected in the upper part of the domain and they flow down onto the fabric. When the fibers have laid down the fluid is reset to zero and a horizontal rigid plane is used to press the fiber sheet. The resulting fiber configuration is then used as input to the fiber network model.

3 FIBER NETWORK MODEL

In this section a two-dimensional elasticity network model is presented which is used to represent the fiber sheet as a fiber network. The structure is attained from the forming simulations described in Section 2.2. The basic building blocks of the network are nodes, edges and edge pairs. Fibers are modeled as chains of edges transformed from the FEM representation used in the fiber suspension model. The nodes represent the connection between each edge of fibers. Bonds between fibers can be represented either in the most simple way as nodes mutual to different fibers, or more advanced bonds can be build up using one or several edges connecting fibers.

The network model in this work is based on internal forces arising when nodes are displaced, acting to restore the displacements. These forces act at two types of elements, the edges or the edge pairs. There are three types of internal forces that are included in this model, one type is related to edges, and two types are related to edge pairs. The model in this paper is two dimensional, static and assumes small deformations.

When nodes of edges or edge pairs are displaced, the three internal force contributions give rise to forces acting on the nodes and by assembling force equilibrium equations at each node the governing equation of the network is attained. All force equilibrium equations can be assembled into a system of the form $-Ku + F = 0$, where K is called the elasticity matrix, u contains the node displacements, and F are the external forces. The three types of force contributions are related to stretching, bending and the Poisson effect. In the following sections the forces are described in more detail. First some nomenclature is introduced.

Let the network consist of n nodes. Let (i, j) denote the edge connecting node i to j and let $\mathcal{E}$ denote the set of all edges. Edge pairs are denoted by (i, j, l) where j is the center node. Denote by $\mathcal{P}$ the set of all edge pairs. Note that $(i, j) = (j, i)$ and $(i, j, l) = (l, j, i)$. Each node i has two degrees of freedom, the x-directed displacement u_i and the y-directed displacement v_i.

Let the length of edge (i, j) be denoted L_{ij} and assume that the edge has a width w_{ij}. All edges are assumed to have a uniform thickness z in the direction into the plane. The direction vector, d^a_{ij}, of an edge (i, j) with respect to node $a \in \{i, j\}$ is calculated as

$$d^a_{ij} = \frac{p_b - p_a}{|p_b - p_a|}, \quad b \in \{i, j\},\ b \neq a. \tag{2}$$

The length change of edge (i, j), denoted ΔL_{ij}, is given by $\Delta L_{ij} = (\delta_j - \delta_i) \cdot d^i_{ij}$.

3.1 Extension of edges

The first force contribution is a basic spring force used in lattice-spring models. It acts on edges, and when the nodes of the edge are displaced such that the projection of the node displacement onto the initial edge direction is nonzero, anti-parallel forces arise at the nodes of the edge to restore the length. The tendency of an edge to restore its length is described by the edge's elastic modulus k_{ij}.

Consider an edge (i, j). When the nodes are displaced the edge (i, j) will give rise to two forces $F^{\mathrm{I}}_a(i, j)$, $a \in \{i, j\}$, acting on node a according to

$$F^{\mathrm{I}}_a(i, j) = k_{ij} \frac{w_{ij} z}{L_{ij}} \Delta L_{ij} d^a_{ij}, \quad a \in \{i, j\}. \tag{3}$$

3.2 Angular deviations of edge pairs

The second force contribution introduces bending resistance of pair of edges and works similarly as angular springs used in lattice-spring models. When the nodes of an edge pair are displaced such that the angle between the edges is changed, two torques arise at the central node acting to restore the initial angle. By transforming these torques to force couples the effect can be converted into the force equilibrium equations.

Consider an edge pair (i, j, l). When the nodes are displaced an angular change $\Delta\theta_{ijl}$ occurs, giving rise to two torques

$$\begin{aligned} \tau_i &= \kappa_{ijl} V_{ijl} \Delta\theta_{ijl} \hat{z}, \\ \tau_l &= -\tau_i, \end{aligned} \tag{4}$$

acting on edge (i, j) and (j, l) respectively, at the position of node j. The parameter V_{ijl} is the joint volume at the connection between the two edges, and the parameter κ_{ijl} is the bending resistance. The angular change is a sum of two contributions according two

$$\Delta\theta_{ijl} = \delta\theta_{ji} + \delta\theta_{jl}. \tag{5}$$

Each term is the angle deviation of the respective edge from its initial orientation. By using the assumption $\alpha \approx \tan\alpha$ the angles $\delta\theta_{ja}, a \in \{i, l\}$ can be calculated according to

$$\delta\theta_{ja} \approx \tan\theta_{ja} = \frac{(\delta_a - \delta_j)\cdot n^j_{ja}}{L_{ja}}, \quad a \in \{i, l\}, \tag{6}$$

where the edge normals are calculated as

$$\begin{aligned} n^j_{ji} &= d^j_{ji} \times \hat{z}, \\ n^j_{jl} &= -d^j_{jl} \times \hat{z}. \end{aligned} \tag{7}$$

Transforming the torques to force couples gives the resulting three forces $F^{\mathrm{II}}_a(i, j, l), a \in \{i, j, l\}$ from edge pair (i, j, l), acting on node a, according to

$$\begin{aligned} F^{\mathrm{II}}_a(i, j, l) &= -\frac{\kappa_{ijl} V_{ijl} \Delta\theta_{ijl}}{L_{aj}} n^j_{ja}, \quad a \in \{i, l\}, \\ F^{\mathrm{II}}_j(i, j, l) &= -F^{\mathrm{II}}_i(i, j, l) - F^{\mathrm{II}}_l(i, j, l). \end{aligned} \tag{8}$$

3.3 Poisson effect of edge pairs

The third force contribution models the Poisson effect. It acts on edge pairs and when the nodes are displaced forces arise at all three nodes to counteract changes in the sum of the length of the two edges.

Consider an edge pair (i, j, l). The forces arising at the outer nodes $a \in \{i, l\}$ will be

$$F^{\mathrm{III}}_a(i, j, l) = -\eta_{ijl}\frac{w_{aj} z}{L_{aj}}\left(\Delta L_{aj} + \gamma_{ijl}\frac{w_{bj}}{2}\frac{\Delta L_{bj}}{L_{bj}}|n^j_{aj}\cdot d^j_{bj}|\right) d^j_{aj}, \quad a, b \in \{i, l\},\ b \neq a, \tag{9}$$

and at the central node

$$F^{\mathrm{III}}_j(i, j, l) = -F^{\mathrm{III}}_i(i, j, l) - F^{\mathrm{III}}_l(i, j, l). \tag{10}$$

The parameter γ_{ijl} is the Poisson's ratio, and η_{ijl} describes how much each edge in the edge pair is effected by the Poisson expansion of the other edge.

4 UPSCALING METHOD

In this section a brief description of the numerical upscaling method is presented. The method is based on the LOD [15], which was developed for multiscale solution of elliptic PDE:s and is based on FEM. The LOD method has been modified and extended to handle network models of the type described in this paper. The new method is fully decoupled from any governing PDE and the network structure can be of arbitrary geometry. All input that is required is the network structure and an equation system of the form $Ku = F$ governing the network mechanics.

Consider an arbitrary fiber network. Assembling the force equilibrium equations from the network model described in Section 3 gives a linear system

$$Ku = F, \tag{11}$$

where K is the elasticity matrix, u contains the displacements of the network nodes, and F are externally applied node forces. In the upscaling method a coarse grid is introduced representing the network at the macroscale. This coarse grid is a FEM grid with basis functions defined at each node as in standard FEM. Sought for are the displacements of the grid nodes. To include effects from the network scale, each basis function is modified by solving a system using information contained in the elasticity matrix K.

Denote by $\Lambda_i : \mathbb{R}^2 \to \mathbb{R}$ the FEM basis function at grid node i. Note here that a two-dimensional problem is assumed, however the upscaling method works also for three dimensions. Define network basis vectors by λ_i, being the interpolation of Λ_i onto the network nodes, i.e. $\lambda_i(j) = \Lambda_i(p_j)$, where p_j is the position of network node j. Each such basis vector is modified by solving a system

$$\begin{bmatrix} K & C^T \\ C & 0 \end{bmatrix} \begin{bmatrix} \phi_i \\ \eta_i \end{bmatrix} = \begin{bmatrix} K\lambda_i \\ 0 \end{bmatrix}, \tag{12}$$

attaining the vector ϕ_i and the modified basis function will be $\lambda_i - \phi_i$. The newly introduced matrix C, called the constraint matrix, is defined as

$$C(i,:) = \lambda_i^T, \quad i = 1, \ldots, M, \tag{13}$$

where M is the number of grid nodes. The kernel of the matrix C represents the fine network scales not included in the finite element space of the coarse grid. The new modified basis is orthogonal to these fine scales with respect to the scalar product attained from K. This orthogonal splitting of the fine and multiscale space is the main feature of LOD [15].

All modified basis functions are assembled in a matrix B_M according to

$$B_M = [\lambda_1 - \phi_1 \ldots \lambda_M - \phi_M]^T. \tag{14}$$

Finally, this matrix is used to calculate the node displacements of the coarse grid, denoted u_G, by solving the system

$$B_M K B_M^T u_G = B_M F. \tag{15}$$

5 SIMULATION METHODOLOGY

To simulate the mechanical properties of paper based on information from the microscale, a simulation framework is designed consisting of the different models outlined in the previous sections. In Figure 1 a schematic overview of the framework is shown.

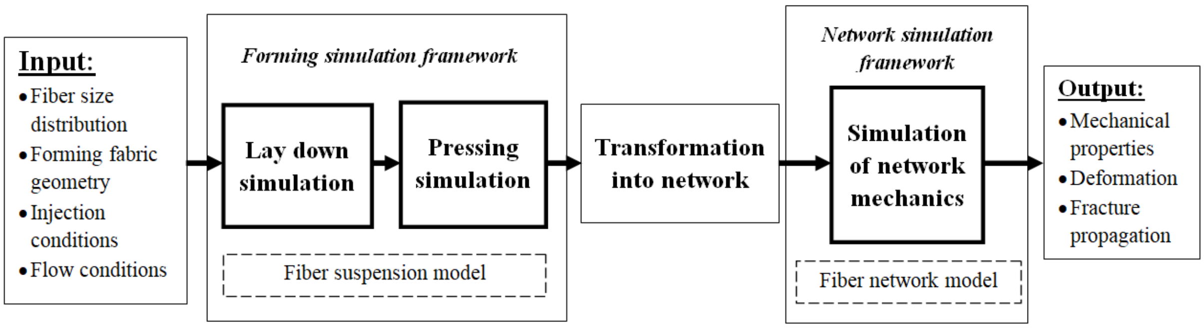


Figure 1: *A schematic overview of the different parts of the simulation framework.*

The two main elements are the simulation of the forming process using a fiber suspension model, and the simulation of mechanical properties using a fiber network model. To connect these two parts a link is required which transforms the sheet resulting from the forming simulation into the fiber network representation.

The input to the forming simulation framework is parameters such as the type of fibers and their distribution, the geometry of the fabric, different kind of injection conditions, flow conditions, etc. Variation of these parameters will affect the forming process and different sheet structures are attained. When transforming the fiber suspension into a fiber network, fibers have to be re-represented and appropriate bonds between fibers have to be created. Using the network representation simulations can be performed such as stretching or bending of the sheet, or fracture propagation investigations. These simulations will result in information regarding the mechanical properties of the sheet. To enable simulation of large paper sheets the multiscale method is used.

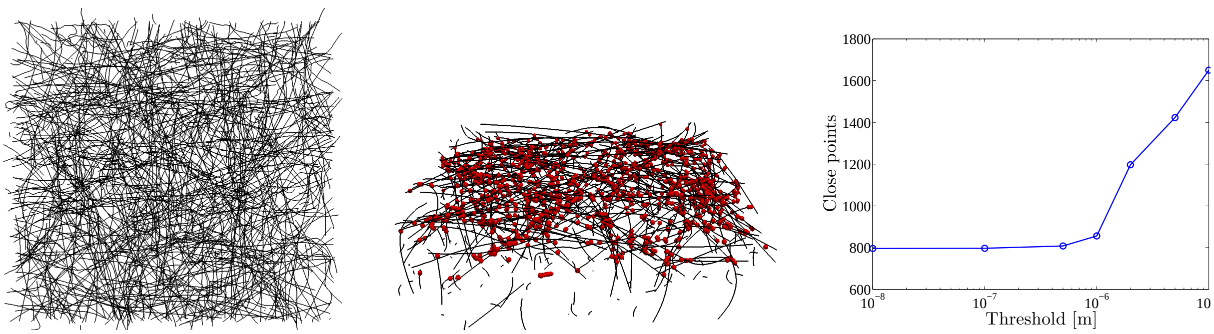
In Figure 2(a) a snapshot from a forming simulation is shown, where thousands of fibers with circular cross-section flow down onto a 3x3 mm real forming fabric structure, and a sheet structure starts to form. In Figures 2(b)-2(c) a resulting sheet structure is shown before and after pressing has been applied.

(a) Lay down simulation. (b) Unpressed simulated sheet. (c) Pressed simulated sheet.

Figure 2: *Three snapshot from the forming simulations framework: during lay down, after lay down, and after pressing.*

Studies of how variation of the input data affects the mechanical properties can increase the understanding of the process. Another type of investigation is to generate different regular network structures and plug them in to the network simulation framework. In this way desirable configurations with special mechanical properties can be found. With such structures in mind the forming simulation framework can be used to find ways to create such structures during the forming process by finding appropriate fiber injection, fabric geometry and flow conditions.

In Figure 3(a) a snapshot is shown of a fiber network, where the fibers from the forming simulations have been transformed into network edges. Close points between fibers are found using geometrical routines resulting in possible bond points as seen in Figure 3(b). Depending on the threshold distance for when two fiber surfaces are regarded as close enough for bonding, different numbers of close points are found. In Figure 3(c) the number of found contact points is plotted versus the threshold distance. Interesting to note is the plateau when the threshold is smaller than approximately 0.5 μm.



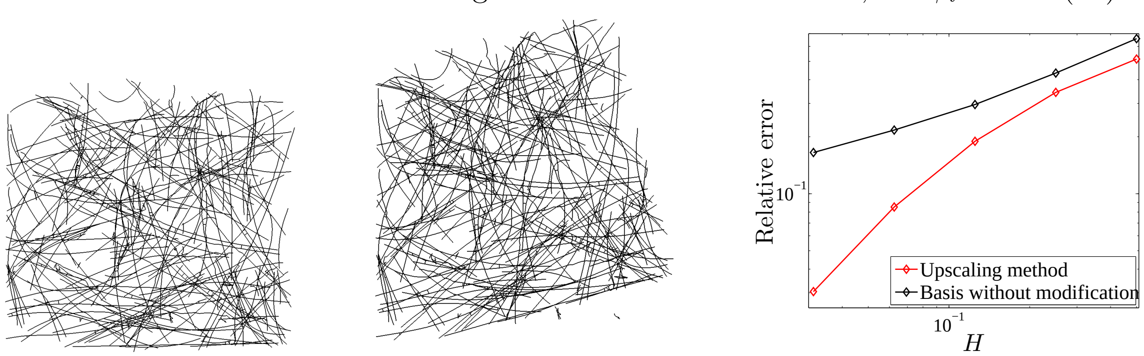
(a) Fiber network with configuration from simulation.

(b) Close points between fibers marked with red dots.

(c) Number of close points depending on threshold distance.

Figure 3: *Pictures related to the transformation from fibers suspension representation to fiber network.*

In Figures 4(a)-4(b) two networks are shown after network simulation. First all fibers not connected to any other fiber were removed. In the first case a horizontal force was applied on the right side of the network, and in the second case a vertical force was applied. In Figure 4(c) the convergence rate for the multiscale method is shown for a basic test case of a regular unit square network. The multiscale method is plotted versus the case when no modification of the grid basis functions are used, i.e. $\phi_i = 0$ in (14).



(a) Fiber network with horizontal force applied on right boundary.

(b) Fiber network with vertical force applied on right boundary.

(c) Error convergence of regular unit square network (relative error based on K).

Figure 4: *Pictures illustrating the fiber network simulation framework.*

6 CONCLUSIONS

In this paper a multiscale simulation methodology was presented with the aim to simulate the mechanical properties of paper. The framework is based on two different types of representations of the paper fibers. First the fibers are represented with a fiber suspension model enabling simulation of the forming process. By using this detailed model, realistic fiber sheet structures can be attained. Secondly the fiber suspension is transformed into a fiber network representation more suitable for simulation of mechanical properties. The fiber network approach is improved by adding a novel numerical upscaling method. By combining the realistic fiber configuration attained from the forming simulations with the upscaling method macroscale paper properties can be investigated.

The next step in the development of this framework is to further investigate the transformation from fiber suspension to fiber network studying how fiber bonds should be added. The upscaling approach has so far been tested on small networks of regular structure analyzing its accuracy, large samples remains to be investigated. With an improved transformation from suspension to network, and a parallel implementation of the upscaling method, interesting investigations of mechanical properties can be achieved, using the methodology presented in this work.

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