Graph-Based View of an Equilibrium Model for Nonwoven Tensile Strength Simulations

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Abstract Focus of this work is the graph-based analytical treatment of the equilibrium model introduced in [4], which allows to determine the tensile behavior of nonwovens over the interaction of the individual fiber connections in the material. We use the representation of fiber structures as arbitrarily directed graphs to derive a compact nonlinear system of equations with characteristic divergence structure and to investigate its solvability and the uniqueness of solution. Further, we discuss the identification of subgraphs for which trivial solutions can be found.

1 Equilibrium Model

The microstructure of nonwovens consists of thousands of fibers bonded, for example, by thermal or chemical means. Their topology can be described by arbitrarily oriented graphs $\mathcal{G} = (\mathcal{N}, \mathcal{E})$, where the nodes $\mathcal{N}$ represent both adhesive joints and fiber ends, and the edges $\mathcal{E}$ represent the individual fiber connections between them (see Fig. 1). The spatial positions of the adhesive joints and fiber ends (nodes) are denoted by $\mathbf{x} \in \mathbb{R}^{3|\mathcal{N}|}$. To refer to the position of an individual node $\nu \in \mathcal{N}$ we write $\mathbf{x}_\nu \in \mathbb{R}^3$. Similarly, $\ell_\mu \in \mathbb{R}_+$ refers to the (positive) length of the fiber connection represented by edge $\mu \in \mathcal{E}$, yielding a global length vector $\ell \in \mathbb{R}_+^{|\mathcal{E}|}$.

To model the nonwoven tensile behavior, we consider the truss-based approach introduced in [4]. Thus, we distinguish further between boundary nodes $\mathcal{N}_B$ and interior nodes $\mathcal{N}_I$, such that $\mathcal{N} = \mathcal{N}_I \dot{\cup} \mathcal{N}_B$. Thereby, the positions of the boundary nodes are fixed, while the positions of the remaining interior nodes are determined

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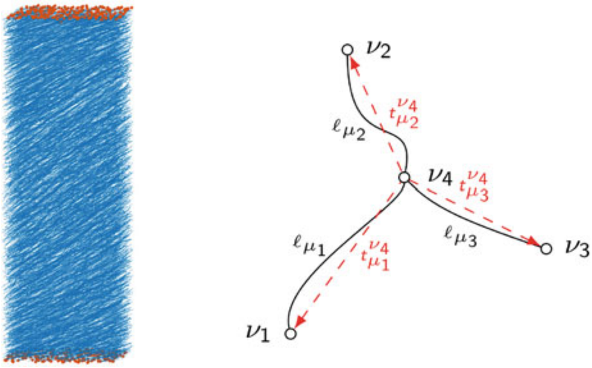

Fig. 1 Graph representation. Left: Topology of a virtually generated nonwoven material sample, cf. [4], with boundary nodes highlighted in red. Right: Simple fiber structure constellation, where the black lines mark fiber connections between the nodes and the dashed red lines indicate the corresponding edges representing the fiber connections

by a force equilibrium condition that accounts for the static material behavior. For the forces acting on the interior nodes, the model is restricted to the stresses caused by strain on incident fiber connections, which results in the following system:

$$\mathbf{x}_\nu = \mathbf{g}_\nu, \qquad \forall \nu \in \mathcal{N}_B, \tag{1}$$

$$\sum_{\mu \in \mathcal{E}(\nu)} \mathbf{f}_\mu^\nu(\mathbf{x}) = \mathbf{0}, \quad \mathbf{f}_\mu^\nu(\mathbf{x}) = \frac{\mathbf{t}_\mu^\nu(\mathbf{x})}{\|\mathbf{t}_\mu^\nu(\mathbf{x})\|_2} N(\epsilon(\|\mathbf{t}_\mu^\nu(\mathbf{x})\|_2, \ell_\mu)), \quad \forall \nu \in \mathcal{N}_I, \tag{2}$$

where $\mathbf{g}_\nu \in \mathbb{R}^3$ is the position specified for node $\nu \in \mathcal{N}_B$, the set $\mathcal{E}(\nu) \subset \mathcal{E}$ consists of all edges incident to node ν and $\mathbf{f}_\mu^\nu : \mathbb{R}^{3|\mathcal{N}|} \to \mathbb{R}^3$ expresses the force acting on node $\nu \in \mathcal{N}_I$ which is caused by stress on edge $\mu \in \mathcal{E}(\nu)$. According to (2), we have that $\mathbf{f}_\mu^\nu$ acts in the normalized direction $\mathbf{t}_\mu^\nu(\mathbf{x}) = \mathbf{x}_{\tilde{\nu}} - \mathbf{x}_\nu$ for $\mu = (\nu, \tilde{\nu})$, where the amplitude $N : [-1, \infty[\to \mathbb{R}_+$ depends on the relative strain of the fiber connection with respect to its length ℓ_μ, i.e., $\epsilon : \mathbb{R}^+ \times \mathbb{R}^+ \to [-1, \infty)$, $(l, \ell) \mapsto (l - \ell)/\ell$. Thereby, N denotes the fibers' material law for which we make the following assumption.

Assumption 1 *We have that $N \in C^2([-1, \infty), \mathbb{R}_+)$ and for some constant $c \geq -1$ the material law satisfies $N(\varepsilon) = 0$ for $\varepsilon \leq c$ and N is strictly increasing for $\varepsilon > c$.*

This expresses a solely elastic stress-strain behavior, as an increase in stress is associated with further elongation of the fibers. Thereby, c is the strain from which the fibers are under tension. For a material law using $c > 0$, thus, incorporating a zero phase in the stress-strain behavior we refer to [4]. For a strictly increasing choice, implying $c = -1$, we refer to [3] where crimp on the fibers is considered.

2 Graph Structure and Solvability

We consider the model (1)–(2) introduced in [4] and use the representation of the fiber structure as arbitrarily directed graph (e.g., obtained by imposing edge directions according to an underlying node enumeration) to embed it in a compact formulation with characteristic divergence structure. This allows to investigate the solvability and the uniqueness of a solution for the equilibrium model.

Subsequently, $\mathbf{A} \in \mathbb{R}^{|\mathcal{N}|\times|\mathcal{E}|}$ denotes the underlying graph's incidence matrix with

$$\mathbf{A}_{i,j} = \begin{cases} -1 & \text{, if } \ \nu_i = \operatorname{init}(\mu_j) \\ 1 & \text{, if } \ \nu_i = \operatorname{ter}(\mu_j) \\ 0 & \text{, else.} \end{cases} \tag{3}$$

Hereby, $\operatorname{init}(\mu_j)$ refers to the start node and $\operatorname{ter}(\mu_j)$ to the end node of edge μ_j. Given an arbitrary node constellation $\mathbf{x} \in \mathbb{R}^{3|\mathcal{N}|}$, the edge vectors can be collectively determined through

$$\mathbf{t}(\mathbf{x}) = \begin{pmatrix} \mathbf{t}_{\mu_1}(\mathbf{x}) \\ \vdots \\ \mathbf{t}_{\mu_{|\mathcal{E}|}}(\mathbf{x}) \end{pmatrix} = (\mathbf{A} \otimes \mathbf{I}_3)^T \mathbf{x} \tag{4}$$

where $\otimes$ denotes the Kronecker product, $\mathbf{t}_\mu(\mathbf{x})$ is the vector representing the directed edge μ and $\mathbf{I}_3 \in \mathbb{R}^{3\times 3}$ is the identity matrix.

In contrast to (2), let $\phi : \mathbb{R}^{3|\mathcal{E}|} \to \mathbb{R}^{3|\mathcal{N}|}$ denote the forces acting in normalized edge direction expressed in terms of the edge vectors collected in $\mathbf{t} \in \mathbb{R}^{3|\mathcal{E}|}$. That is

$$\phi(\mathbf{t}) = \begin{pmatrix} \phi_{\mu_1}(\mathbf{t}) \\ \vdots \\ \phi_{\mu_{|\mathcal{E}|}}(\mathbf{t}) \end{pmatrix}, \ \text{with } \phi_\mu(\mathbf{t}) = \frac{\mathbf{t}_\mu}{\|\mathbf{t}_\mu\|_2} N(\epsilon(\|\mathbf{t}_\mu\|_2, \ \ell_\mu)), \tag{5}$$

where ϕ_μ is continuously continuable in zero for each $\mu \in \mathcal{E}$. To accumulate the forces acting on an interior node $\nu \in \mathcal{N}_I$ according to (2), we add ϕ_μ if μ is an outgoing edge, i.e., $\nu = \operatorname{init}(\mu)$, and subtract it if μ is an incoming edge, i.e., $\nu = \operatorname{ter}(\mu)$. This is to account for the arbitrarily imposed edge directions which yields

$$\sum_{\mu\in\mathcal{E}(\nu)} \mathbf{f}_\mu^\nu(\mathbf{x}) = -\sum_{\mu\in\mathcal{E}} \mathbf{A}_{\nu,\mu}\phi_\mu(\mathbf{t}(\mathbf{x})) = -(\mathbf{A}_{\nu,\cdot} \otimes \mathbf{I}_3)\phi((\mathbf{A}\otimes\mathbf{I}_3)^T\mathbf{x}). \tag{6}$$

Due to (1), the fixation of the boundary nodes, the variables are the positions of the interior nodes only. Let $\mathbf{z} \in \mathbb{R}^{3|\mathcal{N}_I|}$ denote the interior node positions and $\mathbf{g} \in \mathbb{R}^{3|\mathcal{N}_B|}$ that of the boundary nodes. Thus, to express the node positions in terms of $\mathbf{z}$ we introduce

$$\mathbf{x}_\mathbf{g}(\mathbf{z}) = (\mathbf{P}_I \otimes \mathbf{I}_3)^T\mathbf{z} + (\mathbf{P}_B \otimes \mathbf{I}_3)^T\mathbf{g} \tag{7}$$

with orthogonal projections $\mathbf{P}_I \in \mathbb{R}^{|\mathcal{N}_I|\times|\mathcal{N}|}$ and $\mathbf{P}_B \in \mathbb{R}^{|\mathcal{N}_B|\times|\mathcal{N}|}$ onto the interior nodes and boundary nodes, respectively. Then (4) can be expressed in terms of $\mathbf{z}$ through

$$\mathbf{t}(\mathbf{x_g}(\mathbf{z})) = (\mathbf{A}\otimes\mathbf{I}_3)^T\mathbf{x_g}(\mathbf{z}) = (\mathbf{P}_I\mathbf{A}\otimes\mathbf{I}_3)^T\mathbf{z}+(\mathbf{P}_B\mathbf{A}\otimes\mathbf{I}_3)^T\mathbf{g} = \tilde{\mathbf{A}}_I^T\mathbf{z}+\tilde{\mathbf{A}}_B^T\mathbf{g}, \quad (8)$$

where $\tilde{\mathbf{A}}_I = \mathbf{P}_I\mathbf{A}\otimes\mathbf{I}_3$ and $\tilde{\mathbf{A}}_B = \mathbf{P}_B\mathbf{A}\otimes\mathbf{I}_3$ are defined for notational convenience. Apparently, $\tilde{\mathbf{A}}_I \in \mathbb{R}^{3|\mathcal{N}_I|\times 3|\mathcal{E}|}$ and $\tilde{\mathbf{A}}_B \in \mathbb{R}^{3|\mathcal{N}_B|\times 3|\mathcal{E}|}$ are the incidence matrices containing only the rows belonging to interior nodes and boundary nodes, respectively, that are blown up to three dimensions.

Equation (8), also, allows to express (6) in terms of $\mathbf{z}$. Hence, collecting the individual equations (6) for all interior nodes $\nu \in \mathcal{N}_I$ yields the nonlinear system

$$\mathbf{F_g}(\mathbf{z}) := -\tilde{\mathbf{A}}_I\phi(\tilde{\mathbf{A}}_I^T\mathbf{z}+\tilde{\mathbf{A}}_B^T\mathbf{g}) = \mathbf{0}, \quad (9)$$

with $\mathbf{F_g}\colon \mathbb{R}^{3|\mathcal{N}_I|} \to \mathbb{R}^{3|\mathcal{N}_I|}$, which is subsequently referred to as Network Equation System (NES). Each interior node constellation $\mathbf{z}$ satisfying $\mathbf{F_g}(\mathbf{z}) = \mathbf{0}$, for a given boundary node constellation $\mathbf{g}$, meets the conditions (1)–(2).

Particularly noteworthy is the divergence structure in (9), which is similarly found in the context of electrical circuit simulations [2], where the circuit topology determines the solvability of the associated differential-algebraic equations. For the NES, which can be embedded in a quasi-static framework to perform tensile strength simulations, we have the following result.

Theorem 1 *Let $\mathcal{G} = (\mathcal{N}, \mathcal{E})$ be connected and let N satisfy Assumption 1. Then, given a fixed boundary node constellation $\mathbf{g} \in \mathbb{R}^{3|\mathcal{N}_B|}$, we have that*

1. *There exists an interior node constellation $\hat{\mathbf{z}} \in \mathbb{R}^{3|\mathcal{N}_I|}$ with $\mathbf{F_g}(\hat{\mathbf{z}}) = \mathbf{0}$.*
2. *If N is strictly increasing on $[-1, \infty)$ then $\hat{\mathbf{z}} \in \mathbb{R}^{3|\mathcal{N}_I|}$ is an unique solution.*

Proof We show the existence of a potential $E_\mathbf{g}\colon \mathbb{R}^{3|\mathcal{N}_I|} \to \mathbb{R}$, which satisfies $\nabla E_\mathbf{g} = -\mathbf{F_g}$. Then the existence of a minimum to $E_\mathbf{g}$ implies that of a solution to the nonlinear system $\mathbf{F_g}(\mathbf{z}) = \mathbf{0}$ by first order optimality conditions.

For a given constellation of boundary nodes $\mathbf{g} \in \mathbb{R}^{3|\mathcal{N}_B|}$ we define the fiber structure's potential, depending on the interior node positions $\mathbf{z} \in \mathbb{R}^{3|\mathcal{N}_I|}$, through

$$E_\mathbf{g}(\mathbf{z}) = \sum_{\mu\in\mathcal{E}} \ell_\mu G(\varepsilon(\|\mathbf{t}_\mu(\mathbf{x_g}(\mathbf{z}))\|, \ell_\mu)), \quad \text{where} \quad G(\varepsilon) = \int_{-1}^{\varepsilon} N(s)\, ds.$$

That is the weighted sum of the potential energies of the individual fiber connections caused by stretching them. Straightforward application of the chain rule yields

$$
\begin{aligned}
\nabla_{\mathbf{z}} E_{\mathbf{g}}(\mathbf{z}) &= \sum_{\mu\in\mathcal{E}} \ell_\mu \frac{d}{d\varepsilon} G(\varepsilon(\|\mathbf{t}(\mathbf{x_g}(\mathbf{z}))\|, \ell_\mu))\nabla_{\mathbf{z}}\varepsilon(\|\mathbf{t}(\mathbf{x_g}(\mathbf{z}))\|, \ell_\mu)) \\
&= \sum_{\mu\in\mathcal{E}} \frac{\mathbf{t}_\mu(\mathbf{x_g}(\mathbf{z}))^T}{\|\mathbf{t}_\mu(\mathbf{x_g}(\mathbf{z}))\|} N(\varepsilon(\|\mathbf{t}(\mathbf{x_g}(\mathbf{z}))\|, \ell_\mu))(\mathbf{A}_{\cdot,\mu}\otimes \mathbf{I}_3)^T(\mathbf{P}_I\otimes \mathbf{I}_3)^T \\
&= \sum_{\mu\in\mathcal{E}} (\mathbf{P}_I\mathbf{A}_{\cdot,\mu}\otimes \mathbf{I}_3)\phi_\mu(\mathbf{t}(\mathbf{x_g}(\mathbf{z}))) \\
&= \tilde{\mathbf{A}}_I\phi(\tilde{\mathbf{A}}_I^T\mathbf{z}+\tilde{\mathbf{A}}_B^T\mathbf{g}),
\end{aligned}
$$

which shows that $\mathbf{F_g}$ is the negative gradient field of $E_{\mathbf{g}}$. To verify the existence of a global optimum we show that $E_{\mathbf{g}}$ is coercive, i.e., $E_{\mathbf{g}}(\mathbf{z}) \to \infty$ for $\|\mathbf{z}\| \to \infty$.

Apparently, $\|\mathbf{z}\| \to \infty$ implies $\|\mathbf{x}_\nu\| \to \infty$ for at least one interior node $\nu \in \mathcal{N}_I$. Due to the connectivity of $\mathcal{G}$, we have that any boundary node $\tilde{\nu} \in \mathcal{N}_B$ is connected to ν over a finite path $P = (\mathcal{N}_P, \mathcal{E}_P) \subseteq \mathcal{G}$, with nodes $\mathcal{N}_P = \{\nu_{p_0}, \dots, \nu_{p_q}\} \subseteq \mathcal{N}$, edges $\mathcal{E}_P = \{(\nu_{p_0}, \nu_{p_1}), \dots, (\nu_{p_{q-1}}, \nu_{p_q})\} \subseteq \mathcal{E}$ and $q \in \mathbb{N}$ such that $\nu_{p_0} = \nu$ and $\nu_{p_q} = \tilde{\nu}$. As the boundary node $\tilde{\nu} \in \mathcal{N}_B$ is fixed to a given position $\mathbf{g}_{\tilde{\nu}}$, we can conclude

$$
\|\mathbf{x}_\nu - \mathbf{g}_{\tilde{\nu}}\| \le \sum_{j=1}^{q} \|\mathbf{x}_{\nu_{p_j}} - \mathbf{x}_{\nu_{p_{j-1}}}\| \to \infty, \quad \text{for} \quad \|\mathbf{z}\| \to \infty. \tag{10}
$$

Hence, for at least one $k \in \{1, \dots, q\}$ it holds that $\|\mathbf{x}_{\nu_{p_k}} - \mathbf{x}_{\nu_{p_{k-1}}}\| \to \infty$, for $\|\mathbf{z}\| \to \infty$, as otherwise we would have a contradiction to (10). Let $\tilde{\mu} = (\nu_{p_k}, \nu_{p_{k-1}})$ denote the respective edge in $\mathcal{E}_P$, then

$$
E_{\mathbf{g}}(\mathbf{z}) \ge \ell_{\tilde{\mu}} G(\varepsilon(\|t_{\tilde{\mu}}(\mathbf{x_g}(\mathbf{z}))\|, \ell_{\tilde{\mu}})) \to \infty, \text{ for } \|\mathbf{z}\| \to \infty, \tag{11}
$$

since Assumption 1 implies $G \ge 0$ and $G(\varepsilon) \to \infty$ for $\varepsilon \to \infty$. Apparently, (11) corresponds to $E_{\mathbf{g}}$ being coercive. Thus, by the continuous differentiability of $E_{\mathbf{g}}$ we can conclude the existence of a global minimum, cf. [1].

Moreover, if N is strictly increasing on $[-1, \infty)$, then $E_{\mathbf{g}}$ is strictly convex, as

$$
\begin{aligned}
G(\varepsilon(\|t_\mu(\mathbf{x}(\lambda\mathbf{z} + (1-\lambda)\tilde{\mathbf{z}}))\|, \ell_\mu)) &= G(\varepsilon(\|\lambda t_\mu(\mathbf{x}(\mathbf{z})) + (1-\lambda)t_\mu(\mathbf{x}(\tilde{\mathbf{z}}))\|, \ell_\mu)) \\
&< \lambda G(\varepsilon(\|t_\mu(\mathbf{x}(\mathbf{z}))\|, \ell_\mu)) + (1-\lambda)G(\varepsilon(\|t_\mu(\mathbf{x}(\tilde{\mathbf{z}}))\|, \ell_\mu))
\end{aligned}
$$

for $\lambda \in (0, 1)$ and any pair $\mathbf{z}, \tilde{\mathbf{z}} \in \mathbb{R}^{3|\mathcal{N}_I|}$ with $\mathbf{z} \neq \tilde{\mathbf{z}}$. Here, the equality holds by linearity and the inequality is explained by the fact that ε is convex and that G is strictly increasing and convex. This implies a unique solution for the nonlinear system $\mathbf{F_g}(\hat{\mathbf{z}}) = \mathbf{0}$, cf. [6]. □

3 Structural Analysis

Except for $\mathcal{G}$ being connected, there are no topological restriction to Theorem 1, which is even applicable for multigraphs. This differs from typical requirements for electrical circuit simulation, where additional structural assumptions must be made, e.g., to avoid short circuits. However, we can exploit the topology of the fiber structure to identify subgraphs that have a trivial solution for which the associated equations of the NES are satisfied. This includes loose subgraphs and simple linking nodes, cf. [4], that are subject to following discussion.

Definition 1 A connected subgraph $\mathcal{L} \subset \mathcal{G}$ is refered to as loose if it is connected to the remainder $\mathcal{R} = \mathcal{G} \setminus \mathcal{L}$ over a cutvertex $\nu_c \in \mathcal{N}$ and if it does not contain a boundary node, i.e., $\mathcal{N}(\mathcal{L}) \cap \mathcal{N}_B = \emptyset$.

Loose subgraphs can be neglected, as their constellation is determined by the associated cutvertex. To convince ourselves of this statement, assume that $\mathcal{L}$ is a loose subgraph with associated cutvertex ν_c and remainder $\mathcal{R}$, and that the edges are arranged so that the edges of $\mathcal{R}$ come first. Then we have $\mathbf{A} = [\mathbf{A}_R, \mathbf{A}_L]$, which implies

$$\tilde{\mathbf{A}}_I = [\tilde{\mathbf{A}}_{IR}, \tilde{\mathbf{A}}_{IL}], \quad \mathbf{t} = \begin{pmatrix} \mathbf{t}_R \\ \mathbf{t}_L \end{pmatrix}, \quad \text{and} \quad \phi(\mathbf{t}) = \begin{pmatrix} \phi_R(\mathbf{t}_R) \\ \phi_L(\mathbf{t}_L) \end{pmatrix}, \tag{12}$$

where the indices R and L indicate the edges, edge vectors, and acting forces corresponding to the remainder $\mathcal{R}$ and the loose subgraph $\mathcal{L}$, respectively. The information regarding edges connecting the loose subgraphs to the cutvertex is thereby included in the terms indicated by L. Accordingly, $\tilde{\mathbf{A}} = [\tilde{\mathbf{A}}_R, \tilde{\mathbf{A}}_L]$ for $\tilde{\mathbf{A}} = \mathbf{A} \otimes \mathbf{I}_3$. Then, for node constellation $\mathbf{x} \in \mathbb{R}^{3|\mathcal{N}|}$, the NES can be split up, since

$$\tilde{\mathbf{A}}_I \phi(\tilde{\mathbf{A}}^T \mathbf{x}) = \tilde{\mathbf{A}}_{IR} \phi_R(\tilde{\mathbf{A}}_R^T \mathbf{x}) + \tilde{\mathbf{A}}_{IL} \phi_L(\tilde{\mathbf{A}}_L^T \mathbf{x}), \tag{13}$$

where the first term corresponds to the NES associated to the remainder $\mathcal{R}$ and the second term to that of the loose subgraph $\mathcal{L}$. Definition 1 implies that the positions of all nodes in $\mathcal{L}$ are variable and that they are either incident to ν_c or another node in $\mathcal{L}$. Hence, for any $\mathbf{x}$ satisfying $\mathbf{x}_\nu = \mathbf{x}_{\nu_c}$ for all $\nu \in \mathcal{L}$ we have $\mathbf{x} \in \ker(\tilde{\mathbf{A}}_L^T)$ which implies $\phi_L(\tilde{\mathbf{A}}_L^T \mathbf{x}) = \mathbf{0}$ with regard to (5). Hence, for this trivial constellation of loose subgraph nodes the second term in (13) vanishes. Thus, it suffice to determine a solution to the NES of the remainder $\mathcal{R}$, which exists according to Theorem 1.

Definition 2 A node $\nu \in \mathcal{N}_I$ is referred to as simple linking node, if it has degree 2.

Apparently, simple linking nodes link a pair of fiber connections, that can be treated equally as single fiber connection of cumulated length. This can be attributed to the force equilibrium condition (2) and Assumption 1.

For solving the NES, trivial parts of the solution can be neglected, e.g., by removing loose subgraphs and merging fiber connections linked by a simple linking node. Apart from such trivial parts of the solution, it may come to a lack of uniqueness to a solution of the NES when considering a material law that is not strictly increasing. In this case the Newton-Raphson Method may fail, for which a diagonal perturbation of the Jacobian of $\mathbf{F_g}$ can be considered. This corresponds to a Tikhonov Regularization for the minimization of $E_{\mathbf{g}}$, cf. [5]. In the context of nonwoven tensile strength simulations a friction-based regularization approach was introduced in [4] to cope with the ill-posedness of the associated quasi-static simulation approach.

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