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Hybrid of monolithic and staggered solution techniques for the computational analysis of fracture, assessed on fibrous network mechanics

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Abstract

The computational analysis of fiber network fracture is an emerging field with application to paper, rubber-like materials, hydrogels, soft biological tissue, and composites. Fiber networks are often described as probabilistic structures of interacting one-dimensional elements, such as truss-bars and beams. Failure may then be modeled as strong discontinuities in the displacement field that are directly embedded within the structural finite elements. As for other strain-softening materials, the tangent stiffness matrix can be non-positive definite, which diminishes the robustness of the solution of the coupled (monolithic) two-field problem. Its uncoupling, and thus the use of a staggered solution method where the field variables are solved alternatingly, avoids such difficulties and results in a stable, but sub-optimally converging solution method. In the present work, we evaluate the staggered against the monolithic solution approach and assess their computational performance in the analysis of fiber network failure. We then propose a hybrid solution technique that optimizes the performance and robustness of the computational analysis. It represents a matrix regularization technique that retains a positive definite element stiffness matrix while approaching the tangent stiffness matrix of the monolithic problem. Given the problems investigated in this work, the hybrid solution approach is up to 30 times faster than the staggered approach, where its superiority is most pronounced at large loading increments. The approach is general and may also accelerate the computational analysis of other failure problems.

Keywords Damage · Fracture · Robustness · Convergence · Staggered · Monolithic · Coupled multi-field problem · Fiber network

1 Introduction

Fiber network structures define the mechanics of a wide range of materials with applications towards paper, packaging materials, rubber-like materials, hydrogels, soft biological tissues, and composites [1–8]. In addition to the elastic properties of such materials, their failure properties determine industrial applicability. The mechanics of fiber network structures may be described through the interaction of one-dimensional elements, such as truss-bars and beams [2, 9–15], where especially the numerical description of material failure is challenging.

The theory of strong discontinuities (e.g., see [16–30]) has made a significant impact on the computational analysis of fracture and extended the functionality of many commercial finite element method (FEM) packages. Strong discontinuities enrich the displacement solution space with jumps across the fracture surfaces. The embedded discontinuity finite element method (ED-FEM or E-FEM) and the extended finite element method (X-FEM) have gained the most popularity (e.g., see [31, 32] for comparative studies). The E-FEM and the X-FEM represent strong discontinuities via elemental and nodal enrichments of the displacement solution space, respectively. It allows the approximation of fracture problems using coarse FEM meshes and requires no re-meshing. Most importantly, it avoids pathological mesh-dependency as known from the solution of strain softening materials within the classical non-polar continuum. Whilst the
description of strain softening in non-polar continua results in an infinitesimally small (vanishing) localization volume [33–35], the failure in the discontinuity-based description is represented by an area;—the cross-section of the structural element in our applications. Since such an area remains finite, pathological mesh-dependency is not an issue in the discontinuity-based description, and it converges towards mesh-independent results. However, said approaches often require a crack-tracking algorithm (except for recent work [36] on E-FEM without crack tracking) and exhibit difficulties capturing crack branching and coalescence of multiple cracks, difficulties that are avoided with the newly emerged phase-field fracture method (e.g., see [37, 38]). Unlike discrete crack approaches, it is a smeared crack approach like damage mechanics [39–42] and therefore requires a localization limiter or a characteristic length scale parameter. Such measure is difficult to determine in practice [43] and can be difficult to implement upon unstructured meshes [44]. In addition, a sufficiently refined mesh is necessary to adequately describe the mechanics of the localization zone, leading to the high computational cost of smeared crack approaches. Thus, it prevents from an efficient analysis of failure in fiber networks where the fracture process zone is to be resolved in the individual fibers.

The tangent stiffness matrix of the two-field fracture problem can be indefinite or negative definite [45–48]. The energy potential to be minimized is therefore non-convex. Uncoupling the problem and using a staggered solution approach that solves for the displacement and the respective state of damage alternatingly, overcomes this issue and results in a convex alternating minimization problem. It is the preferred approach in phase-field modeling of fracture [49] and available in commercial software [50–52]. It results in a positive definite tangent stiffness matrix, but does not represent the linearized residuum, and the solution then converges much slower as compared to Newton–Raphson iterations. The efficiency of the consistently linearized coupled (monolithic) problem is therefore sacrificed towards the robustness of the staggered solution technique [53].

The E-FEM has received significant attention in the description of failure in truss-bars, beams, and structures thereof [54–68]. No crack-tracking algorithm is then needed [69]. The E-FEM framework allows static condensation of the additional DOF associated with the fracture kinematics [55] directly at the element level, resulting in an operator-splitting method [56] for the evaluation of these DOF. The implementation is based on the Hu-Washizu two-field variational principle, and given the discontinuity is positioned in the middle of the structural element, the orthogonality condition is a priori enforced [70, 71]. As with the phase-field method, a staggered solution method may be used, and the continuous and discontinuous fields are minimized alternatingly [61]. In the present work, we expand these ideas and propose a hybrid method to optimize the performance and robustness of the E-FEM models in the analysis of fiber network failure [61, 72, 73]. The hybrid solution approach is general and may also be applied to other fracture mechanics problems.

2 Enhanced finite element formulation

We consider a local Cartesian coordinate system \( \{e_x, e_y, e_z\} \) in the description of a 3D Timoshenko beam of the length \( L \) and the cross-section \( A \). The beam’s neutral axis \( x \in [0, L] \) is aligned with the \( x \)-coordinate along which distributed \( f \) as well as concentrated \( F \) loads are applied. The displacements \( u(x) \) and the rotations \( \theta(x) \) are collectively represented by the generalized displacement vector \( \overline{u} = [u_x \ u_y \ u_z \ \theta_x \ \theta_y \ \theta_z]^T \) with the subscripts \( x, y, \) and \( z \) denoting the respective displacement and rotation components. The generalized strain measures of the 3D Timoshenko beam then read

\[
\varepsilon = \frac{du}{dx} \ ; \ \gamma_y = \frac{du}{dx} + \theta_z; \ \gamma_z = \frac{du}{dx} + \theta_y; \\
\kappa_x = \frac{d\theta_y}{dx}; \ \kappa_y = \frac{d\theta_z}{dx}; \ \kappa_z = \frac{d\theta_x}{dx},
\]

where \( \varepsilon \) is the axial strain, \( \gamma_y, \gamma_z \) denote the shear strains along the \( y \) and \( z \) directions, \( \kappa_x \) is the change in the angle of twist \( \theta_x \) around the beam’s neutral axis and \( \kappa_y, \kappa_z \) represent bending curvatures. The stress resultants \( \sigma = \begin{bmatrix} N \ Q_y \ Q_z; M_x \ M_y \ M_z \end{bmatrix}^T \) are conjugate to the generalized strain measures \( \tau = \begin{bmatrix} \varepsilon \ \gamma_y \ \gamma_z \ \kappa_x \ \kappa_y \ \kappa_z \end{bmatrix}^T \). Here, the axial force \( N \), the shear forces \( Q_y, Q_z \) along the \( y \) and \( z \) directions, the torsional moment \( M_x \), and the bending moments \( M_y, M_z \) along the \( y \) and \( z \) directions have been introduced.

The strong form of the local equilibrium equations [74] reads

\[
\frac{dN}{dx} + q_x = 0; \ \frac{dQ_y}{dx} + q_x = 0; \ \frac{dQ_z}{dx} + q_z = 0; \\
\frac{dM_x}{dx} + m_x = 0; \ \frac{dM_y}{dx} - Q_z + m_y = 0; \ \frac{dM_z}{dx} - Q_y + m_z = 0,
\]

where \( q_x, q_y, q_z \) and \( m_x, m_y, m_z \) denote the components of the distributed forces and moments per unit length, respectively.

For simplicity, we consider a two-node beam element of the length \( l_e \) with the linear shape functions \( N_1 = 1 - x/l_e \) and \( N_2 = x/l_e \), and a single Gauss point in the center is used to integrate the FEM equations. The interpolated generalized displacement field then takes the form

\[
\overline{u} = \sum_{a=1}^{2} N_a \overline{u}_a = N_1 \overline{u}_1 + N_2 \overline{u}_2,
\]
where \( \mathbf{u}_1 \) and \( \mathbf{u}_2 \) are the six-dimensional generalized nodal displacement vectors. In addition, a softening hinge allows for the formation of localized failure in the center of the Timoshenko beam. We therefore enrich (3) with a discrete displacement/rotation jump \( \mathbf{\xi} = [\xi_{u_x}, \xi_{u_y}, \xi_{u_z}, \xi_{\theta_x}, \xi_{\theta_y}, \xi_{\theta_z}]^T \) situated in the center \( x_c \) of the element. Thus, \( \mathbf{u} = N_1 \mathbf{u}_1 + N_2 \mathbf{u}_2 + H_{x_c} \mathbf{\xi} \) represents the total displacements, where

\[
H_{x_c}(x) = \begin{cases} 1 & \text{at } x > x_c \\ 0 & \text{at } x \leq x_c \end{cases}
\]

represents the standard 6 \times 12 strain–displacement interpolation matrix, where \( B_1 = dN_1/dx = -1/l_e \) and \( B_2 = dN_2/dx = 1/l_e \).

Given the admissible variation \( \delta \mathbf{d} \) of the element nodal displacements, \( \delta \mathbf{u} \) of the displacement field and \( \delta \mathbf{\xi} \) of the corresponding jump, the internal and respective external virtual work of the beam formulation reads

\[
\delta w_{\text{int}} = \int_{l_e} \delta \mathbf{d}^T \mathbf{\sigma} \, dx = \int_{l_e} \mathbf{\delta d}^T (\mathbf{f} \mathbf{B}^T \mathbf{\sigma} \, dx + \mathbf{\delta \xi}^T (\int_{l_e} \mathbf{G} \mathbf{\sigma} \, dx + \int_{l_e} \delta \mathbf{\xi} \, dx)) ;
\]

\[
\delta w_{\text{ext}} = \int_{x_F} \delta \mathbf{u}^T \mathbf{F} + \int_{l_e} \delta \mathbf{u}^T \mathbf{f} \, dx = \int_{l_e} \mathbf{\delta d}^T \bigg( \mathbf{N}^T (x_F) \mathbf{F} + \int_{l_e} \mathbf{N}^T \mathbf{f} \, dx \bigg) + \int_{l_e} \delta \mathbf{\xi}^T (H_{x_c} - N_2(x_F)) \mathbf{F} ;
\]

where \( \mathbf{f} = [q_x q_y q_z m_x m_y m_z]^T \) represents a distributed load along the beam and \( \mathbf{F} \) a concentrated load applied at the position \( x_F \) along the beam. In the derivation of (11), we used the identity \( \int_{l_e} (H_{x_c} - N_2) \, dx = 0 \), a consequence of having the discontinuity in the middle of the beam, \( x_c = l_e/2 \). In addition, the second term of (11) vanishes if \( x_F = 0 \) or \( x_F = l_e \), which we apply here.

From the principle of virtual work, \( \delta w_{\text{int}} - \delta w_{\text{ext}} = 0 \), and the independence of the admissible variations \( \delta \mathbf{d}, \delta \mathbf{\xi} \), we obtain the two variational statements [55, 56, 75]

\[
\delta \mathbf{d}^T \bigg( \int_{l_e} \mathbf{B}^T \mathbf{\sigma} \, dx - \mathbf{N}^T (x_F) \mathbf{F} + \int_{l_e} \mathbf{N}^T \mathbf{f} \, dx \bigg) = 0 ;
\]

\[
\delta \mathbf{\xi}^T \bigg( \int_{l_e} \mathbf{G} \mathbf{\sigma} \, dx + \int_{l_e} \mathbf{t} \bigg) = 0 ,
\]

where the condition \( \mathbf{t} = \int_{l_e} \delta \mathbf{\sigma} \, dx \) has been used. The condition (12)_2 represents the local residual at the discontinuity, \( x = x_c \), and ensures the equilibrium between the vector of stress resultants \( \mathbf{t} \) at the discontinuity and the stress resultant \( \mathbf{\sigma} \) in the bulk material, \( -\mathbf{\sigma} + \mathbf{t} = \mathbf{0} \). To obtain the equilibrium condition \( \mathbf{\sigma} = \mathbf{t} \), we utilized the jump interpolation operator \( \mathbf{G} \) (9) and the fundamental property of the Dirac delta function \( \int_{-\infty}^{\infty} f(x) \delta(x - x_c) \, dx = f(x_c) \).
The implementation of (12) results in the set

\[ r_d^e = f^{\text{int}} - f^{\text{ext}} = 0; \quad r_{\xi}^e = \int_{l_e} G \sigma \, dx + t = 0 \]  

for \( e = 1, \ldots, 6 \).

of non-linear equations at the element level, where \( f^{\text{int}} = \int_{l_e} B^T \sigma \, dx \) and \( f^{\text{ext}} = \int_{l_e} N^T f \, dx + N^T (x_F) F \) are the internal and external element nodal force vectors, respectively.

Incremental formulations are used to express the constitutive relations of the bulk material and the fracture process zone, expressions that close the set of Eq. (13). We use the change in the stress resultant \( \Delta \sigma = C \Delta \epsilon_{\text{bulk}}; \Delta t = H \Delta \xi \) to describe the development of the stress resultants \( \sigma \) and \( t \), where \( C \) and \( H \) denote the respective tangent constitutive tensors.

\[
C = \begin{bmatrix}
EA & 0 & 0 & 0 & 0 & 0 \\
0 & k\mu A & 0 & 0 & 0 & 0 \\
0 & 0 & k\mu A & 0 & 0 & 0 \\
0 & 0 & 0 & \mu J & 0 & 0 \\
0 & 0 & 0 & 0 & EI_{11} & 0 \\
0 & 0 & 0 & 0 & 0 & EI_{22}
\end{bmatrix}
\]

(15)

determines the stress \( \sigma \), where \( k \) is the shear correction factor, \( J \) is the polar moment of inertia, whilst \( I_{11} \) and \( I_{22} \) denote the area moments of inertia. Note that (15) is the simplest set of uncoupled linear elastic constitutive equations and is based on the assumption that the beam’s cross-section possesses appropriate symmetries [76].

With the strain \( \epsilon_{\text{bulk}} \) in the bulk material (8), the increment of the stress resultant

\[
\Delta \sigma = C (B \Delta d + G \Delta \xi),
\]

and incremental local equilibrium across the discontinuity \( -\Delta \sigma + \Delta t = 0 \) are to be enforced.

The linearization of the residual force equations (13) with respect to the unknown displacement \( \Delta d \) and the discontinuous displacement \( \Delta \xi \) yields the system

\[
\begin{bmatrix}
K_{dd}^e & K_{d\xi}^e \\
K_{\xi d}^e & K_{\xi \xi}^e
\end{bmatrix}
\begin{bmatrix}
\Delta d \\
\Delta \xi
\end{bmatrix} = \begin{bmatrix}
f^{\text{int}} \\
0
\end{bmatrix}
\]

(17)

with the sub-matrices

\[
K_{dd}^e = \int_{l_e} B^T C B \, dx; \quad K_{d\xi}^e = \int_{l_e} B^T C G \, dx; \\
K_{\xi d}^e = \int_{l_e} G CB \, dx + C^* B; \quad K_{\xi \xi}^e = \int_{l_e} G^T C G \, dx + H.
\]

(18)

The term \( C^* B \) is explained in Sect. 4.

In the implementation of these equations, we distinguish between elastic and failure loading. We follow the framework of inelasticity [45, 77] and the decision is based on the introduction of a failure surface \( \Phi \), see Sect. 3. Given an elastic loading, or unloading, the increment \( \Delta \xi = 0 \) and the system reduces to the standard Timoshenko beam FEM model \( K_{dd} \Delta d = f^{\text{int}} - f^{\text{ext}} \). Different implementations concerning damage loading are discussed in the forthcoming sections.

3 Monolithic, staggered and hybrid FEM implementation

The monolithic implementation considers the consistently derived finite element stiffness as shown in (17), where off-diagonal terms couple the increment of the displacement \( \Delta d \) and the increment of the jump \( \Delta \xi \). As with other embedded approaches, our model allows for the static condensation of \( \Delta \xi \) directly at the element level, which then results in a displacement-based FEM implementation. The second equation in (17), the internal equilibrium, is then used to substitute \( \Delta \xi \) through

\[
\Delta \xi = -\left(K_{\xi \xi}^e\right)^{-1}K_{\xi d}^e \Delta d.
\]

(19)

In the limit \( l_e \to 0, G \to \infty \) and \( K_{\xi \xi}^e \) (18) therefore remains positive definite and invertible [21, 55]. In general, however, the condition (19) poses a limit on the size \( l_e \) of the finite element in the analysis of strain-softening materials. The substitution of \( \Delta \xi \) by (19) in (17) results in the system of equations

\[
K_{\text{mono}}^e \Delta d = f^{\text{int}} - f^{\text{ext}}
\]

at the element level, where

\[
K_{\text{mono}}^e = K_{dd}^e - K_{d\xi}^e \left(K_{\xi \xi}^e \right)^{-1} K_{\xi d}^e
\]

(21)

denotes the element stiffness. We emerged at a displacement-based model that may now be implemented through the standard user element interface of FEM packages. Whilst the aforementioned solution uses the consistent linearization of the residual forces, it results in a non-positive definite finite
Table 1  Predictor–corrector implementation of beam rupture

1. **Compute elastic trial force and test for failure loading**
   \[ N^{\text{trial}} = EA(\varepsilon + G\xi_n) \]
   \[ \Phi^{\text{trial}} = N^{\text{trial}} - (N_y + H\alpha_n) \]
   IF \( \Phi^{\text{trial}} \leq 0 \) THEN
   \[ N = N^{\text{trial}} ; \quad \xi = \xi_n ; \quad \alpha = \alpha_n \]
   END IF

2. **Return mapping**
   DO WHILE \( \Phi^{\text{trial}} > \text{THRESHOLD} \)
   \[ \Delta y = \frac{\Phi^{\text{trial}}}{H - EAG \text{sign}(N)} \]
   \[ N = N^{\text{trial}} + EAG\Delta y \text{sign}(N^{\text{trial}}) \]
   \[ \xi = \xi_n + \Delta y \text{sign}(N^{\text{trial}}) \]
   \[ \alpha = \alpha_n + \Delta y \]
   END DO

3. **Element stiffness** \( K_{\text{mono}}^e \), which then materializes through poor robustness of the monolithic implementation.

Towards reinforcing the robustness of the model, we may uncouple \( d, \xi \) and solve the problem in a staggered way. The internal equilibrium equation (13) is then solved at the nodal displacement \( d_n \) from the previous solution. It explicitly reads

\[ r^e_{\xi} = \int_{\xi} G_{\sigma}(d_n)dx + t = 0, \quad (22) \]

and the embedded formulation again allows to solve it directly at the element level. The system

\[ K_{\text{stag}}^e d = f^{\text{int}} - f^{\text{ext}} \quad (23) \]

of FEM equations may then be assembled, and the solution of the global system yields the nodal displacements. Here,

\[ K_{\text{stag}}^e = K_{dd}^e \quad (24) \]

determines the corresponding finite element stiffness, and given it represents an inconsistently linearized residuum, it results in poor convergence of the staggered approach.
Towards optimizing performance and robustness of the finite element model, we propose the hybrid definition

\[ K_{hyb}^c = \beta K_{mono}^c + (1 - \beta) K_{stagg}^c \]  

(25)

of the finite element stiffness, where \( \beta \) is a numerical parameter, chosen to ensure a positive definite finite element stiffness matrix \( K_{hyb}^c \). It is set according to

\[ 0 \leq \beta < \beta_{critical} \text{ such that } \det K_{hyb}^c > 0, \]  

(26)

where the condition for \( \beta_{critical} \) is derived as follows. Excluding the six rigid body motion-related DOFs from the system, the effective stiffness matrices are of the dimension 6 \( \times \) 6. The only physical root of \( \det K_{hyb}^c = 0 \) results in an expression for \( \beta_{critical} \), and (26) then guarantees a positive definite finite element stiffness matrix. Although our stiffness matrices are sparsely populated, the direct solution of \( \det K_{hyb}^c = 0 \) requires the eigenvalue analysis of one 12 \( \times \) 12 matrix at every Gauss point for each solution step; a faster and tailored implementation for beam rupture is discussed in Sect. 5.

4 Predictor–corrector implementation of beam rupture

Aiming at modeling the failure of soft fibers, we limit ourselves to the description of failure under tension. Therefore, only the component \( \xi_{u_t} = \xi \) of the jump \( \xi \) is allowed to evolve, whilst \( \xi_{u_s} = \xi_{u_c} = \xi_{\theta_s} = \xi_{\theta_c} = \xi_{\theta_t} = 0 \). The development of the stress resultant according to (14) is then determined by the tangent constitutive tensor component \( H_{11} = H < 0 \), whilst all the other components of \( H \) are 0. As a result, \( C^* \) (18) takes the form

\[ C^* = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & k\mu A & 0 & 0 & 0 & 0 \\ 0 & 0 & k\mu A & 0 & 0 & 0 \\ 0 & 0 & 0 & \mu J & 0 & 0 \\ 0 & 0 & 0 & 0 & EI_{11} & 0 \\ 0 & 0 & 0 & 0 & 0 & EI_{22} \end{bmatrix} \]  

(27)

because we only allow failure in tension. In (16), \( C^* B \) is the tangent when \( \Delta \xi_{u_t} = \Delta \xi_{\theta_t} = \Delta \xi_{u_c} = \Delta \xi_{\theta_c} = 0 \).

The failure criterion [56]

\[ \Phi = N - (N_y + H\alpha) \leq 0 \]  

(28)

in the stress resultant space, determines the beam’s loading condition. Here, \( N_y \) is the elastic limit resultant (force), whilst \( H < 0 \) and \( \alpha > 0 \) denote the softening modulus and an internal softening variable, respectively. Elastic deformation of the beam is then characterized by \( \Phi < 0 \), and a loading state that reaches the failure surface, \( \Phi = 0 \), results in the accumulation of failure. At complete rupture, \( N = 0 \), the linear softening law (28) yields \( \alpha_{max} = N_y/|H| \) and determines the fracture energy of \( G_f = \alpha_{max}|H|\alpha_{max}/2 = N_y^2/(2|H|) \).

Towards closing the failure description, the evolution of the internal softening variable is to be linked to the evolution of the jump displacement, and

\[ \Delta \alpha = 0 \text{ at } \phi < 0; \]  

\[ \Delta \alpha = |\Delta \xi| \text{ at } \phi = 0 \]  

(29)

specifies said correspondence at the cases of elastic and failure loading, respectively.

With (16), the internal equilibrium \( -\sigma + t = 0 \) for the only non-trivial loading mode reads \( -\alpha + t = 0 \), resulting in

\[ N = N_y + H\xi = EA(\varepsilon + G\xi). \]  

(30)

Here, \( \varepsilon_{bulk} = \varepsilon + G\xi \) denotes the strain in the bulk material, and \( \xi \) is the jump displacement with the initial condition \( \xi = 0 \) at \( N = N_y \). Given \( \xi_n \) and \( \alpha_n \) from the previous time point, we can iteratively derive \( \xi \) and \( \alpha \) at the current time point. We therefore expand (30) towards

\[ N = EA(\varepsilon + G\xi) = N_{trial} + N_{corr}/\xi_n. \]  

(31)

where \( N_{corr} \) eventually corrects the trial stress resultant \( N_{trial} = EA(\varepsilon + G\xi_n) \). The implementation follows the classical concept of computational inelasticity [77], and once \( \Delta \gamma \), the consistency parameter that ensures (28), is given, \( \xi = \xi_n + \Delta \gamma \text{sign}(N) \) updates the solution.

Alternatively, Eq. (31) may be expressed as \( (|N| - EAG\Delta \gamma) \text{sign}(N) = |N_{trial}| \text{sign}(N_{trial}) \), and with \( \Delta \gamma > 0 \), \( G < 0 \) and \( EA > 0 \), the term in the bracket to the left is always positive. Therefore, \( \text{sign}(N) = \text{sign}(N_{trial}) \) and \( |N| = |N_{trial}| + EAG\Delta \gamma \) follows.

With (31), the failure surface (28) then reads

\[ \Phi = N - (N_y + H\alpha) = \Phi_{trial} + (EAG\text{sign}(N) - H)\Delta \gamma, \]  

(32)

where \( \Phi_{trial} = N_{trial} - (N_y + H\alpha_n) \) describes the failure surface assuming an elastic load increment. At failure loading, \( \Phi = 0 \), the algorithmic consistency parameter therefore reads

\[ \Delta \gamma = \frac{\Phi_{trial}}{H - EAG\text{sign}(N)} > 0 \]  

(33)
Table 2 Implementation of monolithic, staggered and hybrid solution techniques for the computational analysis of fracture through the user-element interface of the software package ANSYS

| Step | Description |
|------|-------------|
| 1.   | Load $\alpha_n, \xi_n$ |
| 2.   | Global-to-local transformation $d = Td'$ |
| 3.   | Compute $\epsilon = Bd$ |
| 4.   | Compute $Q_y, Q_x, M_y, M_x$ as $\sigma = Ce$ |
| 5.   | Element degrees of freedom (DOF) deletion |
|      | IF ($\alpha_n > \alpha_{max}$) THEN |
|      | $K_{ij}^e = K_{ij}^e = K_{jj}^e = K_{jj}^e = 0$ ; $j = 1, ..., 12$ ; $N = 0$ |
|      | GOTO 8 |
|      | ENDIF |
| 6.   | Identify $\alpha, \xi, N$ according to Table 1 |
|      | IF ($\alpha_n > \alpha_{max}$) THEN |
|      | $K_{ij}^e = K_{ij}^e = K_{jj}^e = K_{jj}^e = 0$ ; $j = 1, ..., 12$ ; $N = 0$ |
|      | GOTO 8 |
|      | ENDIF |
| 7.   | IF (Monolithic) THEN $\beta = 1$ |
|      | ELSEIF (Staggered) THEN $\beta = 0$ |
|      | ELSE (Hybrid) THEN $K_{min} = \frac{h_{col} B A}{i_e}$ ; $\beta = \frac{K_{min} - K_{stag}^{e}}{K_{mon}^{e} - K_{stag}^{e}}$ |
|      | ENDIF |
| 8.   | Compute element stiffness $K^e = \beta K_{mon}^e + (1 - \beta) K_{stag}^e$ |
| 9.   | Compute nodal force vector $f^{e \text{ int}} = \int_{i_e} B^T \sigma \, dx$ |
| 10.  | Transform to global coordinates $K^e \rightarrow T^T K^e T$ and $f^{e \text{ int}} \rightarrow T^T f^{e \text{ int}}$ |
| 11.  | Return $\alpha, \xi, K^e, f^{e \text{ int}}$ |

and allows us to update the solution. The algorithmic consistency parameter $\Delta \gamma$ must be positive, a standard stability condition to be enforced to avoid snap-back behavior. Table 1 summarizes the predictor–corrector implementation.

5 Implementation

The description of beam rupture through failure under tension and the uncoupled constitutive model (15) result in an uncoupling of the condition (25). Consequently, the identification
Table 3 Fiber properties estimated from [79]

| Fiber properties               |       |
|-------------------------------|-------|
| Young’s modulus $E$           | 6500 MPa |
| Shear modulus $\mu$           | 3250 MPa |
| Shear correction factor $k$   | 0.84   |
| Length $\times$ Width $\times$ Height | $2.5 \times \sqrt{0.00028 \times \sqrt{0.00028}} \text{ mm}^3$ |
| Breaking force $N_y$          | 0.2352 N |
| Fracture energy $G_f$         | 0.1 Nmm or 0.2 Nmm |
| Fiber density $\rho_f$        | 1500 kg/m$^3$ |

of the stability parameter (26) yields the single scalar equation

$$\beta = \begin{cases} 
1 & \text{if } K_{\text{mono}11}^e > K_{\text{min}}; \\
\frac{K_{\text{mono}11}^e - K_{\text{stagg}11}^e}{K_{\text{stagg}11}^e} & \text{if } K_{\text{mono}11}^e < K_{\text{min}},
\end{cases} \quad (34)$$

and avoids then the eigenvalue analysis of the stiffness matrices $K_{\text{mono}}^e$ and $K_{\text{stagg}}^e$. Here, $K_{\text{min}} = h_{\text{tol}}E/A/l_e > 0$ determines a minimum stiffness, where the numerical tolerance level $h_{\text{tol}}$ is determined by the precision level of the hardware/software realization, whilst $l_e$ is the element length. To avoid ill-conditioning towards the development of complete fiber rupture, the corresponding elements in the global stiffness matrix are limited to be larger than the minimum stiffness $K_{\text{min}}$, where again said stiffness threshold has been used.

Given the finite element stiffness matrix (25) for the cases of a monolithic ($\beta = 1$), staggered ($\beta = 0$), or hybrid ($0 < \beta < 1$) implementation, we may now rotate the DOF vector $d$, the nodal force vectors $f_{\text{int}}^e$, and the stiffens $K^e$ into the global Cartesian coordinate system $\{e'_x, e'_y, e'_z\}$ [78]

$$d = T d'; \quad f_{\text{int}}^e = T^T f_{\text{int}}^e; \quad K^e = T^T K^e T. \quad (35)$$

Here,

$$T = \begin{bmatrix} 
A & 0 & 0 & 0 \\
0 & A & 0 & 0 \\
0 & 0 & A & 0 \\
0 & 0 & 0 & A 
\end{bmatrix}$$

(36)

denotes the corresponding transformation matrix, where $\Lambda_{ij} = e_i^T e'_j$; $i, j = x, y, z$ are the directional cosines between the global $\{e'_x, e'_y, e'_z\}$ and the local $\{e_x, e_y, e_z\}$ systems, respectively. Table 2 summarizes the implementation.

6 Benchmark exercises

6.1 Mesh independence

To illustrate the behavior of the finite element, we consider a 0.1 mm long cantilever beam that is loaded in tension. Young’s modulus $E = 1.0$ MPa, the cross-section area $A = 1.0$ mm$^2$, and the ultimate tensile force $N_y = 1.0$ N further describe the problem. The cantilever beam is discretized with one and ten evenly spaced finite elements, where the ultimate tensile force is lowered by 1% in the most left element. Otherwise, the homogenous stress field of the problem would have resulted in an ambiguous failure pattern, see Sect. 3 elsewhere [61]. Figure 1 presents the force–displacement response of our structural problem for three different fracture energies $G_f$, a property also expressed as the area under the curve (see Fig. 1). As expected from the fracture model, the force–displacement response is independent of the finite element discretization; it is identical between the one-element and ten-element discretization, respectively.

Fig. 2 Force-displacement response of fiber networks with the density of 300 kg/m$^3$ (yellow), 500 kg/m$^3$ (blue) and 1000 kg/m$^3$ (green). Dotted lines represent results achieved with the staggered solution method. The fibers within the network are modeled as Timoshenko beams with the properties listed in Table 3 and the fracture energy $G_f = 0.1$ Nmm (left column) and $G_f = 0.2$ Nmm (right column)
Fig. 3 Illustration of the development of failure in the fibrous network of the density 1000 kg/m³ (a–c) and 300 kg/m³ (d–f). The fibers within the network are modeled as Timoshenko beams with the properties listed in Table 3 and the fracture energy $G_f = 0.1$ Nmm (a–c) and $G_f = 0.2$ Nmm (d–f). The jump \( \xi \) [mm] in the displacement field is shown at points a, b, and c (left column) and d, e, and f (right column), highlighted in Fig. 2. At complete rupture, the jump $\xi_{\text{max}} = 0.85$ mm (a–c) and $\xi_{\text{max}} = 1.70$ mm (d–f). Any $\xi > \xi_{\text{max}}$ indicates the fiber has failed.
Fig. 4 Numerical stability with respect to the size of the displacement increment in the failure analysis of the 1000 kg/m³ dense fibrous network. The fibers within the network are modeled as Timoshenko beams with the properties listed in Table 3 and the facture energy $G_f = 0.2$ Nmm. Monolithic (solid line) and staggered (dotted line) solutions are explored, where a prescribed displacement was applied through 500, 2000, 4000, and 8000 steps, respectively. Crosses denote the point of termination of the (monolithic) computation.

6.2 Tensile test of a fibrous tissue specimen

A planar and random network of interconnected 3D beams describes the mechanics of a fiber network of the densities $\rho_s = \{300; 500; 1000\}$ kg/m³ and with the fiber properties listed in Table 3. In-plane it covers the area $18 \times 6$ mm² and the displacement $\delta_0 = 9.0$ mm is prescribed along one edge, while all six DOFs at the opposite edge are fixed. Out-of-plane displacements and rotations are prevented, and all information on how the mesh has been generated is reported elsewhere [12] together with the ANSYS input file [61]. A quasi-static failure analysis was computed through the incremental application of the prescribed displacement $\delta_0$.

Figure 2 shows the force-displacement response of the fiber networks. Computational results refer to the staggered solutions. As expected, we observe a more dissipative response of the fiber networks with the higher fracture energy of the fibers. As an example, Fig. 3 shows the evolution of the jump $\xi$ for the densest network of fibers with the fracture energy $G_f = 0.1$ Nmm. The fiber network configurations refer to the points A, B and C in Fig. 2. Given said fracture energy, the linear softening law (28) provides the jump $\xi_{\text{max}} = 0.85$ mm at the state of complete rupture.

6.2.1 Numerical stability

The numerical stability of the 1000 kg/m³ dense fibrous network made of fibers with the fracture energy of 0.2 Nmm was investigated with respect to the size of the displacement increment. The prescribed displacement was applied through 500, 2000, 4000, and 8000 steps. In each sub-step a maximum of 500 equilibrium iterations were allowed (NEQIT = 500 in ANSYS), before the next step was processed. Whilst the staggered solution converged for all step sizes, the monolithic failed for some step sizes. Figure 4 reports the results from the stability analysis and indicates the points of failure of the monolithic solution. Failure is most likely linked to the inability to minimize the related non-convex problem, and a further investigation of ANSYS’ internal algorithm was not feasible. Given the monolithic method did not fail, the monolithic and staggered approaches solve the same equilibrium equations (13) and therefore result in the same force-displacement response of the fibrous network.

6.3 Tensile test of a notched fibrous tissue specimen

The afore explored specimen geometry (see Sect. 6.2) is modified, and a sharp notch with an opening angle of 20° is introduced in the center of the tensile specimen. A 1000 kg/m³ dense fibrous network with the fiber properties listed in Table 3 is considered. Figure 5 shows the force-displacement response of the notched tensile specimen. See Fig. 6 for the visualization of the jump $\xi$ at the points G–K. Aligned with the previous problem, the monolithic approach is numerically unstable, given the prescribed displacement was applied through 2000 and 10,000 steps, respectively.


7 Performance and stability of the hybrid solution technique

Among all our simulations, the densest fibrous tissue specimens ($\rho_s = 1000 \text{ kg/m}^3$) were computationally most demanding. These cases will therefore be considered to explore the performance of the proposed hybrid solution technique (25) and benchmarking it against the monolithic and staggered schemes. Towards the optimization of the computation time of large fiber networks with many DOFs, we limit the maximum number of steps to 500 in our benchmarking exercise. Table 4 lists the cumulative iterations, the number of all iterations needed to compute the solution until the prescribed displacement $\delta_0$ is reached. It corresponds to the displacement at the endpoints in Figs. 2 and 5, and the number of cumulative iterations represents a measure that...
Table 4 Cumulative iterations (ANSYS variable CUM ITER) to analyze the failure of the fibrous tissue specimen formed by beams with the fracture energy $G_f$

| No. of displacement increments | Staggered | Monolithic $h_{tol} = 0.1$ | Hybrid $h_{tol} = 0.01$ |
|-------------------------------|-----------|---------------------------|------------------------|
|                               |           |                           |                        |
| (1) Notched fiber network: $G_f = 0.1$ Nmm, $\delta_0 = 1.08$ mm |           |                           |                        |
| 20                            | nc (2169) | nc                        | 296                    |
| 100                           | 1980      | nc                        | 354                    |
| 200                           | 1667      | nc                        | 463                    |
| 500                           | 1388      | nc                        | 936                    |
|                               |           |                           |                        |
| (2) Notched fiber network: $G_f = 0.2$ Nmm, $\delta_0 = 2.7$ mm |           |                           |                        |
| 20                            | 1669      | nc                        | 275                    |
| 100                           | 1663      | nc                        | 320                    |
| 200                           | 1383      | nc                        | 493                    |
| 500                           | 1230      | nc                        | 926                    |
|                               |           |                           |                        |
| (3) Fiber network: $G_f = 0.1$ Nmm, $\delta_0 = 2.57$ mm |           |                           |                        |
| 20                            | 1181      | nc                        | 155                    |
| 100                           | 1686      | nc                        | 322                    |
| 200                           | 1413      | nc                        | 422                    |
| 500                           | 1207      | 1171                      | 1000                   |
|                               |           |                           | 1035                   |
|                               |           |                           |                        |
| (4) Fiber network: $G_f = 0.2$ Nmm, $\delta_0 = 3.41$ mm |           |                           |                        |
| 20                            | 2514      | nc                        | 279                    |
| 100                           | 1788      | nc                        | 342                    |
| 200                           | 1568      | nc                        | 461                    |
| 500                           | 1267      | nc                        | 811                    |
|                               |           |                           | 1286                   |

The tissues have the density $\rho_s = 1000$ kg/m$^3$, $\delta_0$ denotes the prescribed displacement, and simulations that stopped without converging are indicated by ‘nc’.

Fig. 7 Comparison between staggered and hybrid solution approaches as a function of the number of prescribed displacement increments. Dots represent the outcome of individual simulations as reported in Table 4, and the curves denote second-order polynomial fits to such data. The numerical tolerance level of the hybrid method is denoted by $h_{tol}$.

is sensitive to the computational effort to solve the problem. The data reported in Table 4 is also shown in Fig. 7, where in addition a second-order polynomial fit visualizes the dependence of the cumulative iterations on the number of displacement increments. Whilst at large displacement increments the hybrid solution technique is clearly superior to the staggered approach, no such advantage is seen for small displacement increments. Searching for the solution in close vicinity of the previous solution, even a non-consistent linearization of the residuum, and thus the staggered solution approach, can find the solution within a low number (2–4) of iterations. We use the incremental constitutive implementation discussed in Sect. 4, and the result is therefore influenced by the size of the prescribed displacement increment. Figure 8 shows the resulting force-displacement curves for the hybrid solution technique as a function of the displacement increment and the numerical tolerance $h_{tol}$. Even the largest step size leads to results of practical use.
Fig. 8 Force-displacement response of fiber networks with the density of 1000 kg/m$^3$ and fibers modeled as Timoshenko beams with the properties listed in Table 3. The curves present results from the hybrid solution technique, where $h_{tol}$ denotes the related numerical tolerance. The numbering (1), (2), (3) and (4) refers to the performed benchmark exercises described in Table 4. The curves present results through the application of 20, 100, 200 and 500 displacement increments, denoted by a light-to-dark color transition, respectively.
8 Summary and conclusion

We studied the computational analysis of failure in fibrous materials, where the individual fibers are modeled as Timoshenko beams with embedded strong discontinuities. Representative benchmark examples have been used, where the recently proposed staggered solution method [61] has been tested against the monolithic solution strategy. Whilst the staggered approach is numerically robust, it does not use the consistent linearization of the nodal forces and therefore suffers from a poor convergence rate. This is especially the case for large displacement increments. The monolithic approach, in contrary, follows from the consistent linearization but can result in a non-positive definite element stiffness matrix, that then requires the solution of unstable equilibria. It is therefore practically not applicable to solve the benchmark problems studied in this work; it erratically fails, and step-size refinement is not always successful. We therefore proposed a novel hybrid solution method that forms the element stiffness through an adaptive ‘mixing’ of the stiffness of the monolithic and staggered approaches. It may also be seen as a matrix regularization technique to retain a positive definite element stiffness matrix while approaching the tangent stiffness matrix of the monolithic problem. The hybrid method results in a robust and computational efficient solution technique with an up to 30-fold performance gain in the exploration of failure in fibrous materials. The approach is general and may also accelerate the computational analysis of other failure problems.

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