# Assembly and Solution of the High-Fidelity Generalized Method of Cells with Interface Damage

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The assembly of the system of equations and its solution are presented for the High-Fidelity Generalized Method of Cells (HFGMC) with interface damage. The direct stiffness assembly, which is used in the Finite Element Method with its unknown nodal displacements, is applied to the HGFMC. The nonlinear set of equations due to damage is solved with Newton's Method for the microscopic surface-averaged displacements, which are the unknowns in the efficient version of the HFGMC.

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## **1** Introduction

The HFGMC, see [1], with interface damage provides the basis for modeling brittle failure of unidirectional fiber-reinforced composites with the inter-element crack method. The fine scale point of view reduces the macroscopic matrix failure mode to two elementary processes: cohesive failure within the matrix phase and debonding of the fiber/matrix interface. In the numerical implementation, zero thickness interfaces are inserted for both failure types along the intercell boundaries of the discretized repeating unit cell (RUC), see Fig. 1. These interfaces serve as predefined sites for crack initiation and growth.

# 2 System of Equations on the Subcell Level

The system of equations (1) has been published in [2] for a linear-elastic solid subcell  $\Omega^{(\beta,\gamma)}$ , which is labeled by the superscripts  $\beta$  and  $\gamma$ , see Fig. 1. It is derived from a surface-averaging process, which is denoted by  $(\bar{.})$ , of the traction t and the microscopic displacement u' at the four boundaries  $\partial \Omega^{n\pm(\beta,\gamma)}$ , where  $n\pm$  stands for the right, left, upper, or lower face, see Fig. 1. Eq. (1) links the surface-averaged tractions  $\bar{t}^{n\pm(\beta,\gamma)}$  to their displacement counterparts  $\bar{u}'^{n\pm(\beta,\gamma)}$  and to the macroscopic strain  $\varepsilon^0$  by a stiffness matrix  $\mathbf{K}^{(\beta,\gamma)}$  and a matrix  $\mathbf{D}^{(\beta,\gamma)}$  containing elements of the elastic stiffness tensor. Both hypermatrices are written down briefly by means of the submatrices  $\mathbf{K}_{ij}^{(\beta,\gamma)} \in \mathbb{R}^{3\times3}$  and  $\mathbf{D}_{i1}^{(\beta,\gamma)} \in \mathbb{R}^{3\times6}$ , with i, j = 1, 2, 3, 4.

$$\begin{cases} \bar{\mathbf{t}}^{2+} \\ \bar{\mathbf{t}}^{2-} \\ \bar{\mathbf{t}}^{3+} \\ \bar{\mathbf{t}}^{3-} \end{cases}^{(\beta,\gamma)} = \begin{bmatrix} \mathbf{K}_{11} & \mathbf{K}_{12} & \mathbf{K}_{13} & \mathbf{K}_{14} \\ \mathbf{K}_{21} & \mathbf{K}_{22} & \mathbf{K}_{23} & \mathbf{K}_{24} \\ \mathbf{K}_{31} & \mathbf{K}_{32} & \mathbf{K}_{33} & \mathbf{K}_{34} \\ \mathbf{K}_{41} & \mathbf{K}_{42} & \mathbf{K}_{43} & \mathbf{K}_{44} \end{bmatrix}^{(\beta,\gamma)} \begin{cases} \bar{\mathbf{u}}^{\prime 2+} \\ \bar{\mathbf{u}}^{\prime 3+} \\ \bar{\mathbf{u}}^{\prime 3-} \end{cases}^{(\beta,\gamma)} + \begin{bmatrix} \mathbf{D}_{11} \\ \mathbf{D}_{21} \\ \mathbf{D}_{31} \\ \mathbf{D}_{41} \end{bmatrix}^{(\beta,\gamma)} \\ \{\boldsymbol{\varepsilon}^{0}\} \end{cases}$$
(1)

A similar system results for the *k*-th interface  $S^{(k)}$ , see Fig. 1, from treating it more like a separate subcell embedded between two solid subcells. This point of view differs from former ones proposed in [3] and [4]. The constitutive behavior of the interfaces is described by an elasto-damage model that is utilized in a surface-averaged sense, i. e.  $\bar{\mathbf{t}}^{(k)} = \mathbf{\Omega}^{(k)} (\bar{d}^{(k)}) \bar{\mathbf{\Delta}}^{'(k)}$ , and defined in a local coordinate system  $\mathbf{e}_n \cdot \mathbf{e}_t \cdot \mathbf{e}_b$ , see Fig. 1. Therein,  $\bar{\mathbf{t}}^{(k)}$  is the traction vector,  $\mathbf{\Omega}^{(k)}$  the interface stiffness matrix,  $\bar{d}^{(k)}$  the damage variable, and  $\bar{\mathbf{\Delta}}^{'(k)} = \bar{\mathbf{u}}^{'+(k)} - \bar{\mathbf{u}}^{'-(k)}$  the separation, which is the relative displacement between the displacement at the positive crack face  $\bar{\mathbf{u}}^{'+(k)}$  and the displacement at the negative one  $\bar{\mathbf{u}}^{'-(k)}$ , see Fig. 1. Eq. (2) is found by imposing the traction continuity  $\bar{\mathbf{t}}^{+(k)} + \bar{\mathbf{t}}^{-(k)} = \mathbf{0}$  and using the elasto-damage model. The surface-averaged tractions  $\bar{\mathbf{t}}^{\pm(k)}$ on both crack faces are linked to their displacement counterparts  $\bar{\mathbf{u}}^{'\pm(k)}$  by the matrix  $\mathbf{I}^{(k)}$  comprising the elements of  $\mathbf{\Omega}^{(k)}$ . Here, the mean damage variable  $\bar{d}^{(k)}$  is assumed to be driven by the surface-averaged separation, i. e.  $\bar{d}^{(k)} = \bar{d}^{(k)}(\bar{\mathbf{\Delta}}^{'(k)})$ .

$$\begin{cases} \frac{\tilde{t}_{n}^{+}}{\tilde{t}_{b}^{+}} \\ \frac{\tilde{t}_{b}^{+}}{\tilde{t}_{b}^{-}} \\ \frac{\tilde{t}_{b}^{-}}{\tilde{t}_{b}^{-}} \end{cases} = \begin{bmatrix} -\Omega_{nn}(\bar{d}) & 0 & 0 & \Omega_{nn}(\bar{d}) & 0 & 0 \\ 0 & -\Omega_{tt}(\bar{d}) & 0 & 0 & \Omega_{tt}(\bar{d}) & 0 \\ 0 & 0 & -\Omega_{bb}(\bar{d}) & 0 & 0 & \Omega_{bb}(\bar{d}) \\ \Omega_{nn}(\bar{d}) & 0 & 0 & -\Omega_{nn}(\bar{d}) & 0 & 0 \\ 0 & \Omega_{tt}(\bar{d}) & 0 & 0 & -\Omega_{tt}(\bar{d}) & 0 \\ 0 & 0 & \Omega_{bb}(\bar{d}) & 0 & 0 & -\Omega_{bb}(\bar{d}) \end{bmatrix}^{(k)} \begin{cases} \bar{u}_{n}^{+} \\ \bar{u}_{n}^{+} \\ \bar{u}_{b}^{+} \\ \bar{u}_{n}^{-} \\ \bar{u}_{t}^{-} \\ \bar{u}_{b}^{-} \end{cases} \\ \vdots \end{cases}$$

$$(2)$$

$$\bar{t}^{\pm(k)} = \mathbf{I}^{(k)} \qquad \mathbf{\bar{u}}^{\prime\pm(k)}$$

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#### System of Equations and Direct Stiffness Assembly 3

The overall system of equations to be solved is formally obtained by enforcing the traction conditions (3), either between solid and solid subcells or solid and interface subcells. In the latter case, the interface orientation must be taken into account.

solid-solid:  

$$\frac{\bar{\mathbf{t}}^{2+(\beta,\gamma)} + \bar{\mathbf{t}}^{2-(\beta+1,\gamma)} = \mathbf{0}}{\bar{\mathbf{t}}^{3+(\beta,\gamma)} + \bar{\mathbf{t}}^{3-(\beta,\gamma+1)} = \mathbf{0}}, \text{ solid-interface: } \bar{\mathbf{t}}^{-(k)} = \begin{cases} \bar{\mathbf{t}}^{2+(\beta,\gamma)}, \mathbf{e}_n = \mathbf{e}_2\\ \bar{\mathbf{t}}^{3+(\beta,\gamma)}, \mathbf{e}_n = \mathbf{e}_3 \end{cases}, \ \bar{\mathbf{t}}^{+(k)} = \begin{cases} \bar{\mathbf{t}}^{2-(\beta+1,\gamma)}, \mathbf{e}_n = \mathbf{e}_2\\ \bar{\mathbf{t}}^{3-(\beta,\gamma+1)}, \mathbf{e}_n = \mathbf{e}_3 \end{cases}.$$
(3)

Instead, the task of setting up the overall system is conducted by means of the direct stiffness assembly, see [5], which is wellknown from the Finite Element Method. This procedure needs a location vector for each solid subcell  $\mathbf{L}^{(\beta,\gamma)}$  and one for each interface subcell  $\mathbf{L}^{(k)}$ . They store the information about the assignment of the degrees of freedom (DOFs) of the RUC (global level), called  $\bar{\mathbf{r}}'$  here, to the corresponding DOFs of the subcells (local level). The DOFs are the surface-averaged microscopic displacements in the efficient form of the HFGMC and visualized in Fig. 1 from both perspectives. Based on [6], the assembly process is written symbolically with the assembly operators **A** and **B** for the solids and interfaces. These operators represent the assembly procedure, which is an assignment rule that uses the location vectors, as a mathematical expression:

$$\widehat{\mathbf{K}} = \overset{N_{\beta}, N_{\gamma}}{\underset{\beta=1, \gamma=1}{\overset{\mathbf{A}}{=}}} \left[ \mathbf{K}^{(\beta, \gamma)} \right], \qquad \widehat{\mathbf{I}}(\overline{\mathbf{r}}') = \overset{N_{\text{int}}}{\underset{k=1}{\overset{\mathbf{B}}{=}}} \left[ \mathbf{I}^{(k)} \left( \overline{d}^{(k)} \left( \overline{\mathbf{A}}^{\prime(k)} \left( \mathbf{B}^{-1}[\overline{\mathbf{r}}'] \right) \right) \right) \right], \qquad \widehat{\mathbf{D}} = \overset{N_{\beta}, N_{\gamma}}{\underset{\beta=1, \gamma=1}{\overset{\mathbf{A}}{=}}} \left[ \mathbf{D}^{(\beta, \gamma)} \right].$$
(4)

The local separation  $\bar{\Delta}'^{(k)}$  is related to the unknown local surface-averaged displacements  $\bar{\mathbf{u}}'^{\pm(k)}$ . The inverse assembly operator  $\mathbf{B}^{-\bar{1}}$  in Eq. (4)<sub>2</sub>, applied to  $\bar{\mathbf{r}}'$ , contains the assignment rule from the global DOFs  $\bar{\mathbf{r}}'$  to the local DOFs  $\bar{\mathbf{u}}'^{\pm(k)}$  for each interface by using the same location vectors as for the assembly process. The direct stiffness assembly leads to the set of equations (5), in which  $\hat{\mathbf{K}} - \hat{\mathbf{I}}(\mathbf{\bar{r}}')$  is the nonlinear stiffness matrix of the RUC and  $\mathbf{\bar{r}}'$  the vector of unknowns. The procedure presented provides another assembly technique compared to the other two: the connectivity matrix in the efficient version of the HFGMC, see [7], or a rigorous collecting of each unknown, see [8].



Fig. 1: Left: Spatially discretized single-fiber RUC in  $N_{\beta} \times N_{\gamma}$  solid subcells and  $N_{\rm int}$  interfaces as well as global coordinate system e<sub>1</sub>-e<sub>2</sub>-e<sub>3</sub>, Center: Depiction of the DOFs of the RUC (global level), Right: Subcell DOFs of a solid and interface subcell (local level)

#### **Iterative Solution with Newton's Method** 4

Eq. (5) is solved iteratively for an applied macroscopic strain  $\varepsilon^0$  by Newton's Method in each step *i*:

$$\widehat{\mathbf{J}}\left(\bar{\mathbf{r}}_{i}^{\prime}\right)\Delta\bar{\mathbf{r}}_{i+1}^{\prime} = -\mathbf{R}\left(\bar{\mathbf{r}}_{i}^{\prime}\right), \quad \text{with} \quad \mathbf{R}\left(\bar{\mathbf{r}}_{i}^{\prime}\right) = \left(\widehat{\mathbf{K}}-\widehat{\mathbf{I}}\left(\bar{\mathbf{r}}_{i}^{\prime}\right)\right)\bar{\mathbf{r}}_{i}^{\prime} - \widehat{\mathbf{t}}^{0}, \quad \widehat{\mathbf{J}}\left(\bar{\mathbf{r}}_{i}^{\prime}\right) = \widehat{\mathbf{K}}-\widehat{\mathbf{I}}\left(\bar{\mathbf{r}}_{i}^{\prime}\right) - \frac{\partial\mathbf{I}\left(\bar{\mathbf{r}}_{i}^{\prime}\right)}{\partial\bar{\mathbf{r}}_{i}^{\prime}}\bar{\mathbf{r}}_{i}^{\prime}. \tag{6}$$

The forming of the third summand of the Jacobian  $\widehat{\mathbf{J}}$  by linearization and matrix-vector multiplication is conducted on the local interface level. Afterwards, these contributions are added by means of the direct stiffness assembly to  $\hat{J}$ .

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