An Efficient Multiscale Virtual Testing Platform for Composites Via Component-wise Models

IBRAHIM KALEEL, MANISH NAGARAJ, MARCO PETROLO, ERASMO CARRERA and ANTHONY M. WAAS

ABSTRACT

The aim of the current work is to develop a multiscale framework based on higher-order 1D finite elements developed using the Carrera Unified Formulation (CUF). The multiscale framework consists of a macroscale model to describe the global structure, and a CUF micromechanical model described using the Component-Wise approach. Such an approach allows for the explicit modelling of the fiber and matrix at the microscale, resulting in a high-fidelity finite element model at both scales. The use of refined CUF elements result in a computationally efficient analysis, due to a reduction in the degrees of freedom at both scales, as well as the reduction in total computational time when compared to standard 3D finite element analysis. The parallel implementation of the multiscale framework results in additional savings in computational time.

INTRODUCTION

The accurate description of the global behavior of composite structures often necessitates a detailed investigation of the material behaviour at lower scales, due to the physical processes which occur at the microstructural level [1]. Material models used to describe nonlinear behavior such as damage and plasticity are defined for individual constituents of the composite material, and a multi-scale analysis is thus well suited for such material systems, where the analysis at the macroscale assumes the material to be homogenous, and the inherent material heterogeneity at the microscale is explicitly defined via a Representative Volume Element (RVE). In such a procedure, each integration point at the macroscale is interfaced to a micromechanical boundary value problem (BVP), where the solution of the RVE and subsequent homogenisation of the material properties results in the macroscale property of the material system, at the given integration point [2]. Such two-scale procedures, when analysed using the finite element method, are often referred to as FE^2 techniques [3]. A non-incremental iterative scheme for multiscale modelling based on LATIN methods was developed by Ladavèze et al. [4]. FE^2 techniques have been used for the nonlinear analysis of composite structures [5], and to solve multiphysics problems such as thermo-mechanical analysis of heterogenous solids [6] and micro-diffusive damage modelling [7].

The most important issue which precludes the wide-spread adoption of multiscale procedures is the immense computational effort involved, stemming from the need to solve a micromechanical BVP for each integration point of the global structure at the macroscale. Considering nonlinear behavior adds on to the issue of computational cost since incremental iterative schemes are often employed to solve problems of nonlinearity. These factors result in a prohibitive computational cost, and correspondingly long solution time for the multiscale analysis of heterogenous materials systems. The most common solution to the reduction of the time required for the computation is by the application of parallel computing [3,8].

For instance, a parallel GPU-based implementation of a computational homogenisation method for visco-plastic materials was developed by Fritzen et al. using the CUDA framework, resulting in a net speedup in the order of 10^4 [9]. Another approach to improve computational time is via the use of computationally inexpensive analytical and semi-analytical methods for the micro-scale analysis, since the effort required to solve the microscale problem directly influences the overall computational cost [10, 11]. An example of such an approach is that of Lagoudas et al., where the Mori-Tanaka scheme was used to perform elasto-plastic analysis of binary composites [12]. Another numerical framework for multiscale analysis is the High-Fidelity Generalized Method of Cells (HFGMC), which is an extension of the Generalized Method of Cells (GMC) [2]. The HFGMC framework has been used to model damage and failure of composite structures at their constituent level [11, 13, 14]. A novel multiscale framework to determine nonlinear response of composites was developed by Zhang et al. by combining a macroscale FE model with analytical formulations for the micromechanical analysis [15]. The framework was then extended for the case of failure analysis of hybrid 3D textile composites [16]. Other approaches for multiscale analysis are based on reduced order methods and proper orthogonal decomposition techniques which are used to solve the micromechanical problem, thus improving the overall computational efficiency of the multiscale analysis [5, 17, 18].

The objective of the current work is to develop a novel multiscale procedure within the framework of the Carrera Unified Formulation (CUF), where expansion functions are used to enrich the cross-section kinematics of 1D finite elements [19, 20]. The use of advanced structural theories in CUF leads to a class of refined 1D elements which reduces the computational cost associated with the analysis of a structural problem. CUF has been used to solve various types of problems such as micromechanical progressive failure analysis of composite structures, rotordynamics, hygrothermal analysis and incompressible flow analysis [21, 22, 23, 24]. In the current work, refined beam models developed using CUF are used to model both the RVE at the microscale, as well as the global structure at the macroscale. The combination of higher-order theories derived using CUF and the parallel implementation leads to the development of a multiscale framework which is efficient in terms of both computational cost and solution time.

1-D CARRERA UNIFIED FORMULATION

Considering an arbitrary beam element aligned in the CUF Cartesian coordinate system, as shown in Fig. 1, the generalized displacement field can be expressed as:

$$u(x,y,z) = F_\tau(x,z)u_\tau(y), \tau = 1,2,\dots,M \quad (1)$$

Where $F_\tau(x,z)$ is an expansion function described across the cross-section, u_τ is the generalized displacement vector, and M is the number of terms in $F_u(x,z)$.

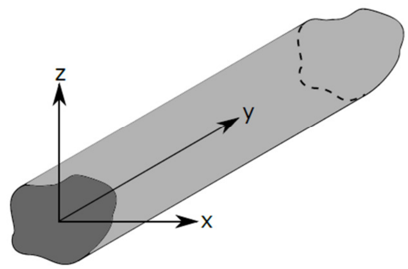


Figure 1. An arbitrary beam aligned in the CUF Cartesian reference system.

The expansion function and the number of terms M can be arbitrarily chosen and is a user input. The current work uses the Component-Wise (CW) approach, where Lagrange polynomials are used to enhance the cross-section kinematic field of the 1D finite elements. Such a formulation results in purely displacement degrees of freedom at each node. The displacement field obtained using a bi-quadratic Lagrange polynomial is given below:

$$u_x = \sum_{i=1}^{9} F_i(x,z)u_x(y) \quad (2)$$

where *x* denotes the displacement component of a node, and *i* is the node number.

Finite Element Formulation

The stress and strain fields can be denoted in vector notation as:

$$\boldsymbol{\sigma} = \{\sigma_{xx}\ \sigma_{yy}\ \sigma_{zz}\ \sigma_{xy}\ \sigma_{xz}\ \sigma_{yz}\} \quad (3)$$

$$\boldsymbol{\epsilon} = \{\epsilon_{xx}\ \epsilon_{yy}\ \epsilon_{zz}\ \epsilon_{xy}\ \epsilon_{xz}\ \epsilon_{yz}\} \quad (4)$$

Considering infinitesimal strains, the linear strain-displacement relation is given by:

$$\boldsymbol{\epsilon} = \mathbf{Du} \quad (5)$$

where **D** is the linear differentiation operator. The constitutive relation is given in a general manner as:

$$\boldsymbol{\sigma} = \mathbf{C}^{tan}\boldsymbol{\epsilon} \tag{6}$$

where $\mathbf{C}^{tan}$ is the material tangent matrix obtained from the material model considered in the analysis. In the current work, material nonlinearity has been considered for the matrix phase of the composite material system. Discretizing the beam axis using standard finite element shape functions $N_i(y)$, the displacement field can be written as:

$$\mathbf{u}(x, y, z) = F_\tau N_i(y)\mathbf{u}_{\tau i} \tag{7}$$

According to the Principle of Virtual Displacement,

$$\delta W_{int} = \delta W_{ext} \tag{8}$$

where W_{int} is the internal work, W_{ext} is external work due to the applied forces, and δ denotes the virtual variation. The virtual variation of the internal work is given by

$$\delta W_{int} = \int_l \int_\Omega \delta\boldsymbol{\epsilon}^T \boldsymbol{\sigma}\, d\Omega dl \tag{9}$$

where *l* represents the beam length and *Ω* is the beam cross-section. The use of Eqs. (5-8) leads to the development of the fundamental nucleus, which is a 3x3 matrix, as given below:

$$\mathbf{k}_{ij\tau s}^{tan} = \int_l \int_\Omega \mathbf{D}^T\big(N_i(y)F_\tau(x, z)\big)\mathbf{C}^{tan}\mathbf{D}\big(N_i(y)F_\tau(x, z)\big)d\Omega dl \tag{10}$$

The indices *i* and *j* refer to the finite element shape functions along the beam axis i.e. $N_i(y)$ and $N_j(y)$, while the indices τ and *s* refer to the expansion functions F_τ and F_s, described across the cross-section. Looping through the four indices results in the element stiffness matrix, which is assembled to obtain the global stiffness matrix of the structure.

MULTISCALE FRAMEWORK

In the current multiscale framework, the microstructure is explicitly modeled using a representative volume element (RVE), and a micromechanical analysis of the RVE is performed at each integration point of the macroscale structural model. The multiscale analysis procedure in CUF is illustrated in Fig. 2. The macroscale strain at each integration point is applied on the microscale RVE using periodic boundary conditions. The two scales are linked via homogenization, where volume averaging of the microscale quantities is done to obtain the effective values at the structural level.

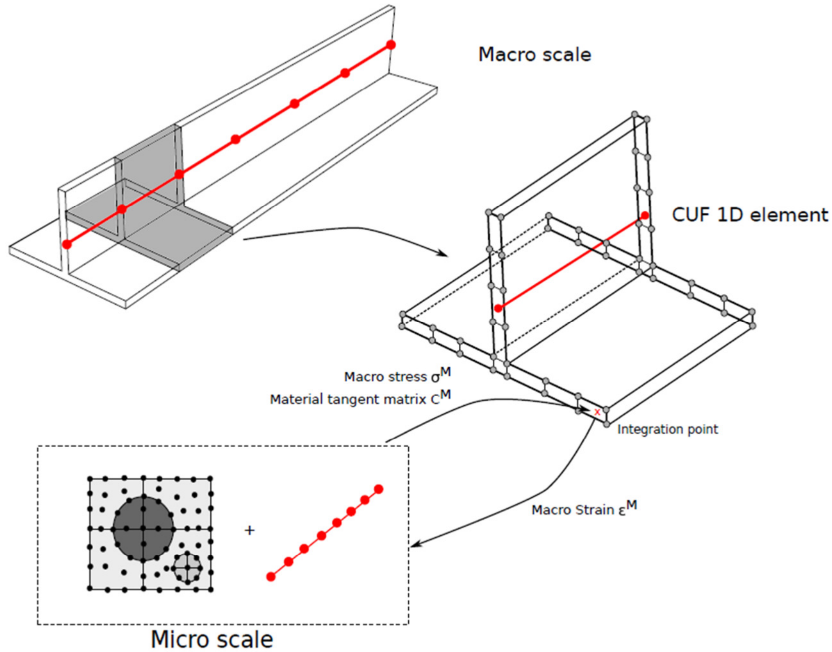


Figure 2. The multiscale analysis procedure in CUF.

The volume averaging of the microscale stress and strain fields is given below:

$$\bar{\epsilon}_{ij} = \frac{1}{V}\int_V \epsilon_{ij}\,dV \tag{11}$$

$$\bar{\sigma}_{ij} = \frac{1}{V}\int_V \sigma_{ij}\,dV \tag{12}$$

The material matrix of the homogenized RVE can then be obtained from:

$$\bar{\sigma}_{ij} = \bar{\mathbf{C}}_{ijkl}\bar{\epsilon}_{kl} \tag{13}$$

Further details of the micromechanical analysis within CUF can be found in [25].

Parallel Implementation

Since a micromechanical analysis is to be performed at each integration point of the macroscale, the computational effort can quickly become very prohibitive. In addition, the computation of stiffness matrices can be intensive [26]. In view of these points, the current work focuses on the parallelization of (a) assembly of the global stiffness matrices, (b) solving the system of linear equations, and (c) state variable update of the macroscale integration points. Standard MPI commands are used for the parallel implementation [27], with the equal distribution of the finite elements among the various processors.

NUMERICAL RESULTS

A single-ply notched laminate has been considered as a numerical example in the current work to showcase the capabilities of the proposed multi-scale framework. The geometry of the notched laminate is based on [28], and a schematic representation of the structure has been shown in Fig. 3. The material considered in the current example is a unidirectional glass fibre-epoxy composite, whose properties are listed in Table 1. The nonlinear characteristics of the epoxy matrix has been obtained from the experimental works of Fiedler et al. [29] and is plotted in Fig. 4. The structure has a thickness of 0.38 mm.

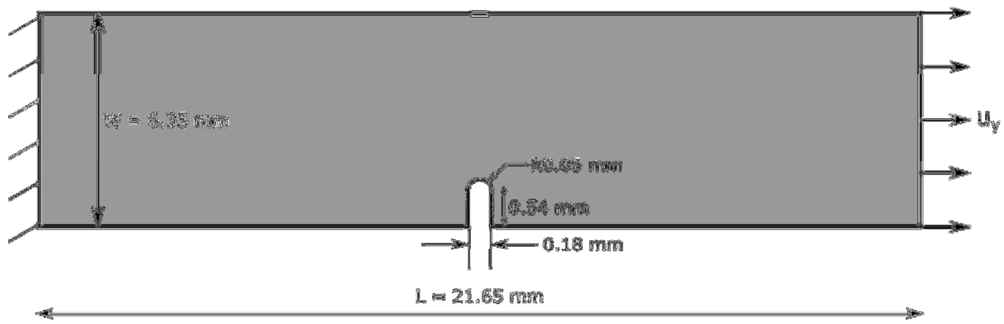


Figure 3. A schematic representation of the notched laminate.

TABLE 1. MATERIAL PROPERTIES.

Property	Glass Fiber	Epoxy Matrix
Young's Modulus E [Gpa]	74.0	3.9
Poisson's ratio ν [-]	0.20	0.39
Yield Stress σ_y [MPa]	-	29.0

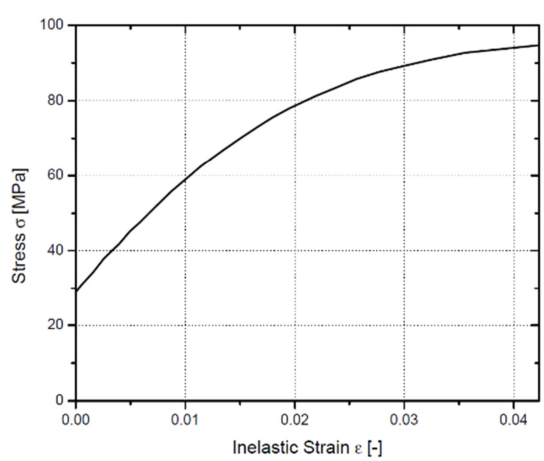


Figure 4. Nonlinear material behavior of the epoxy matrix [29].

The above structure is analysed using the nonlinear multiscale framework described in the previous section. A square-packed RVE has been considered for the micromechanical analysis. Two classes of finite element models have been generated in the current example. In the first type, the analysis has been performed using refined beams models at both the macro- and microscale and is hence termed 1D-1D. The 1D mesh for the RVE is shown in Fig. 5, where 2 cubic beam elements (B4) are used to model the RVE along the y-axis, while 20 biquadratic Lagrange elements (L9) are used to define the cross-section, thereby explicitly modeling the fiber and the matrix. In the second type of the mesh, the structure is modeled at the macroscale using classical 3D 8-node elements, with refined 1D elements at the microscale. The second finite element model is thus termed 3D-1D. The contour plots of the von Mises stress near the notch have been given in Fig. 6, while that of the inelastic strains have been shown in Fig. 7. Model information related to the mesh used, as well as memory requirements and computation time is listed in Table 2 for both the 1D-1D and 3D-1D cases.

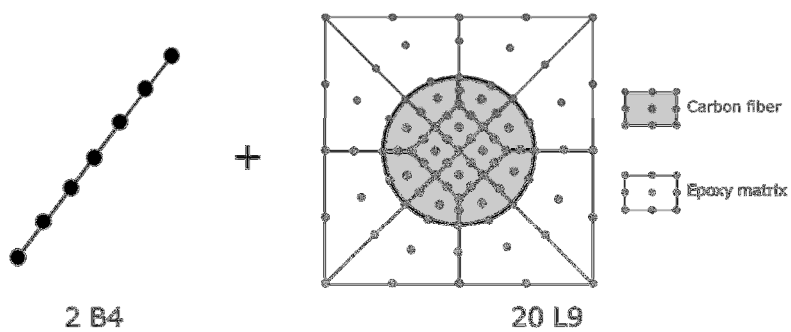
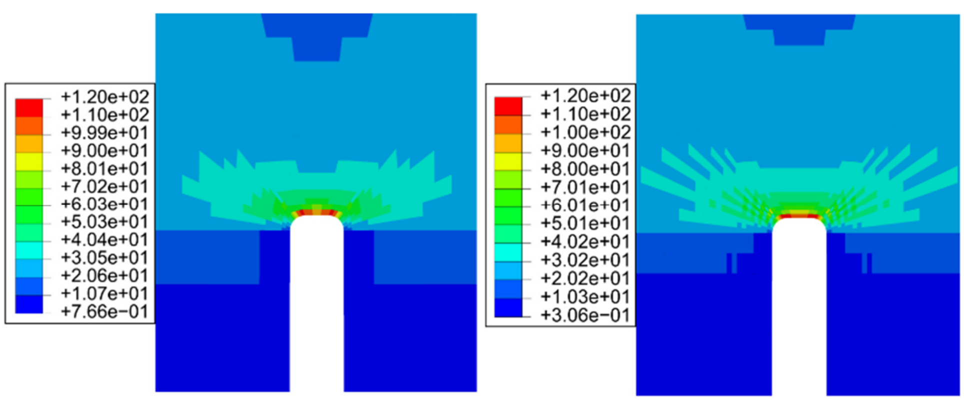


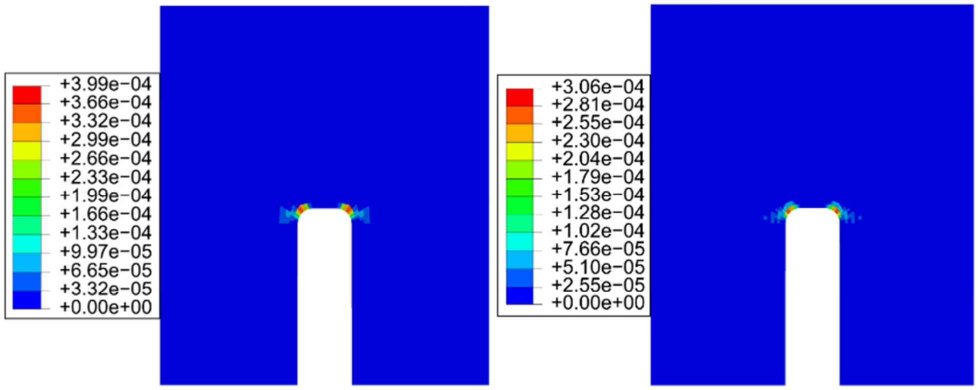
Figure 5. 1D discretization of the representative volume element.



(a) CUF 1D-1D

(b) 3D-1D

Figure 6. von Mises stress near the notch. (a) CUF 1D-1D, (b) 3D-1D.



(a) CUF 1D-1D (b) 3D-1D

Figure 7. Inelastic strains near the notch. (a) CUF 1D-1D, (b) 3D-1D.

TABLE 2. MACRO MODEL DATA ON MESH AND COMPUTATIONAL TIME.

Model	Mesh	DOF	No. of Gauss Points	Total CPU Time (hh:mm:ss)	Memory Required (GB)
CUF 1D-1D	8L9-1B4 for end sections, 124L9-1B3 for central notched region.	5849	3924	00:49:02	1.224
3D-1D	2408 linear 8-node 3D solid element	15552	19264	05:22:48	5.1

The following comments can be made:

1. The stress results obtained from the 1D-1D analysis are in excellent agreement with those obtained by the 3D-1D case, as can be seen in Fig. 6.
2. The inelastic strain fields obtained by both the analyses are in good qualitative agreement with each other, as can be seen from Fig. 7.
3. The proposed multiscale framework is efficient both in terms of computation time as well as memory required. This is shown in Table 2, where the use of refined 1D models at both scales results in a ~6.5x reduction in wall time and a ~3.9x reduction in the amount of memory required, when compared to the 3D-1D case.

CONCLUSIONS

An efficient framework has been developed for the nonlinear multiscale finite element analysis of composite structures, using refined beam elements obtained using the Carrera Unified Formulation (CUF). The microstructure of the composite material is explicitly modelled using a Representative Volume Element (RVE), and the micromechanical analysis is performed at each integration point of the macroscale model via the application of macro strains as periodic boundary conditions on the

RVE. The RVE analysis results in homogenized material properties at the macroscale, and volume averaging of the micro stress and strain fields results in the corresponding macro fields. The use of refined beam elements within CUF, along with the implementation of a parallel framework for the multiscale analysis, results in a very computationally efficient method both in terms of computational time and memory required.

REFERENCES

1. Liu, X., Furrer, D., Kosters, J., & Holmes, J. (2018). Vision 2040: A Roadmap for Integrated, Multiscale Modeling and Simulation of Materials and Systems.
2. Aboudi, J., Arnold, S. M., & Bednarcyk, B. A. (2013). *Micromechanics of composite materials: a generalized multiscale analysis approach*. Butterworth-Heinemann.
3. Feyel, F. and J. L. Chaboche, J. L. (2000). “Fe2 multiscale approach for modelling the elastoviscoplastic behaviour of long fibre SiC/Ti composite materials. Computer Methods in Applied Mechanics and Engineering”, 183(3):309 - 330.
4. Ladevèze, P., Loiseau, O., & Dureisseix, D. (2001). “A micro–macro and parallel computational strategy for highly heterogeneous structures”. *International Journal for Numerical Methods in Engineering*, *52*(1□2), 121-138.
5. Radermacher, A., Bednarcyk, B. A., Stier, B., Simon, J., Zhou, L., & Reese, S. (2016). “Displacement-based multiscale modeling of fiber-reinforced composites by means of proper orthogonal decomposition”. *Advanced Modeling and Simulation in Engineering Sciences*, *3*(1), 29.
6. Özdemir, I., Brekelmans, W. A. M., & Geers, M. G. (2008). “FE2 computational homogenization for the thermo-mechanical analysis of heterogeneous solids”. *Computer Methods in Applied Mechanics and Engineering*, *198*(3-4), 602-613.
7. Nguyen, V. P., Lloberas-Valls, O., Stroeven, M., & Sluys, L. J. (2011). Homogenization-based multiscale crack modelling: from micro-diffusive damage to macro-cracks. *Computer Methods in Applied Mechanics and Engineering*, *200*(9-12), 1220-1236.
8. Tikarrouchine, E., Chatzigeorgiou, G., Praud, F., Piotrowski, B., Chemisky, Y., & Meraghni, F. (2018). Three-dimensional FE2 method for the simulation of non-linear, rate-dependent response of composite structures. *Composite Structures*, *193*, 165-179.
9. Fritzen, F., Hodapp, M., & Leuschner, M. (2014). GPU accelerated computational homogenization based on a variational approach in a reduced basis framework. *Computer Methods in Applied Mechanics and Engineering*, *278*, 186-217.
10. Aboudi, J. (1982). A continuum theory for fiber-reinforced elastic-viscoplastic composites. *International Journal of Engineering Science*, *20*(5), 605-621.
11. Haj-Ali, R., & Aboudi, J. (2009). Nonlinear micromechanical formulation of the high fidelity generalized method of cells. *International Journal of Solids and Structures*, *46*(13), 2577-2592.
12. Lagoudas, D. C., Gavazzi, A. C., & Nigam, H. (1991). Elastoplastic behavior of metal matrix composites based on incremental plasticity and the Mori-Tanaka averaging scheme. *Computational Mechanics*, *8*(3), 193-203.
13. Bednarcyk, B. A., Aboudi, J., & Arnold, S. M. (2010). Micromechanics modeling of composites subjected to multiaxial progressive damage in the constituents. *AIAA journal*, *48*(7), 1367-1378.
14. Naghipour, P., Arnold, S. M., Pineda, E. J., Stier, B., Hansen, L., Bednarcyk, B. A., & Waas, A. M. (2017). Multiscale static analysis of notched and unnotched laminates using the generalized method of cells. *Journal of Composite Materials*, *51*(10), 1433-1454.
15. Zhang, D., Patel, D. K., & Waas, A. M. (2015). A novel two-scale progressive failure analysis method for laminated fiber-reinforced composites. In *56th AIAA/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference* (p. 0969).
16. Zhang, D., Waas, A. M., & Yen, C. F. (2015). Progressive damage and failure response of hybrid 3D textile composites subjected to flexural loading, part II: mechanics based multiscale computational modeling of progressive damage and failure. *International Journal of Solids and Structures*, *75*, 321-335.

17. Ladevèze, P., Passieux, J. C., & Néron, D. (2010). The latin multiscale computational method and the proper generalized decomposition. *Computer Methods in Applied Mechanics and Engineering*, *199*(21-22), 1287-1296.
18. Ricks, T. M., Lacy Jr, T. E., Pineda, E. J., Bednarcyk, B. A., & Arnold, S. M. (2016). Computationally efficient High-Fidelity Generalized Method of Cells micromechanics via order-reduction techniques. *Composite Structures*, *156*, 2-9.
19. Carrera, E., Cinefra, M., Petrolo, M., & Zappino, E. (2014). *Finite element analysis of structures through unified formulation*. John Wiley & Sons.
20. Zappino, E. & Carrera, E. 2018. Multidimensional model for the stress analysis of reinforced shell structures. *Computer Methods in Applied Mechanics and Engineering, 56(4), 1647-1661*.
21. Kaleel, I., Petrolo, M., Waas, A. M., & Carrera, E. (2018). Micromechanical progressive failure analysis of fiber-reinforced composite using refined beam models. *Journal of Applied Mechanics*, *85*(2), 021004.
22. Carrera, E., & Filippi, M. (2016). A refined one-dimensional rotordynamics model with three-dimensional capabilities. *Journal of Sound and Vibration*, *366*, 343-356.
23. Cinefra, M., Petrolo, M., Li, G., & Carrera, E. (2017). Variable kinematic shell elements for composite laminates accounting for hygrothermal effects. *Journal of Thermal Stresses*, *40*(12), 1523-1544.
24. Varello, A., Pagani, A., Guarnera, D., & Carrera, E. (2018). Analysis of Stokes flows by Carrera unified formulation. *Advances in Aircraft and Spacecraft Science*, *5*(3), 363-383.
25. Kaleel, I., Petrolo, M., Waas, A. M., & Carrera, E. (2017). Computationally efficient, high-fidelity micromechanics framework using refined 1D models. *Composite Structures*, *181*, 358-367.
26. Chiang, K. N., & Fulton, R. E. (1990). Concepts and implementation of parallel finite element analysis. *Computers & Structures*, *36*(6), 1039-1046.
27. Dagum, L., & Menon, R. (1998). OpenMP: an industry standard API for shared-memory programming. *IEEE computational science and engineering*, *5*(1), 46-55.
28. Meyer, P., & Waas, A. M. (2015). Mesh-objective two-scale finite element analysis of damage and failure in ceramic matrix composites. *Integrating Materials and Manufacturing Innovation*, 1-18.
29. Fiedler, B., Hojo, M., Ochiai, S., Schulte, K., & Ando, M. (2001). Failure behavior of an epoxy matrix under different kinds of static loading. *Composites Science and Technology*, *61*(11), 1615-1624.