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DOCTORATE IN MATERIALS SCIENCE AND ENGINEERING

REPORT

**DEFINITION OF A REFERENCE VOLUME
ELEMENT (RVE) MODEL FOR THE NUMERICAL
ANALYSIS OF THIN PLY MECHANICS**

Doctoral Candidate: Luca DI STASIO

Thesis Supervisors: Prof. Zoubir AYADI
Université de Lorraine
Nancy, France

Prof. Janis VARNA
Luleå University of Technology
Luleå, Sweden

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Acronyms

CAE Computer Aided Engineering

CF Carbon Fiber

CZM Cohesive Zone Model

EP Glass Fiber

FEM Finite Element Method

GF Glass Fiber

LEFM Linear Elastic Fracture Mechanics

RVE Reference Volume Element

UD Uni-Directional

VCCT Virtual Crack Closure Technique

Symbols

Symbol	SI units	Description
\bar{i}	$[-]$	Unit vector in the x-direction.
\bar{j}	$[-]$	Unit vector in the y-direction.
Ω_f	$[-]$	Fiber domain.
Ω_m	$[-]$	Matrix domain.
$\Omega_{[0^\circ]}^b$	$[-]$	Bottom Uni-Directional (UD) domain.
$\Omega_{[0^\circ]}^u$	$[-]$	Upper UD domain.
Γ_1	$[-]$	Fiber/matrix interface outside the crack region.
Γ_2	$[-]$	Fiber/crack interface.
Γ_3	$[-]$	Matrix/crack interface.
R_f	$[m]$	Fiber radius.
l	$[m]$	Square Reference Volume Element (RVE) half-length.
t_{ratio}	$[m]$	Ply thickness ratio.
$\bar{\varepsilon}_x$	$\left[\frac{m}{m}\right]$	Applied strain.
\bar{u}_x	$[m]$	Applied displacement.
θ	$[rad]$	Crack angular position.
$\Delta\theta$	$[rad]$	Crack angular semi-aperture.
a	$[m]$	Crack radial aperture.
V_f	$[-]$	Fiber volume fraction.
E_1	$[GPa]$	Young's modulus in longitudinal direction.
E_2	$[GPa]$	Young's modulus in transversal direction.
G_{12}	$[GPa]$	In-plane tangential modulus.
G_{23}	$[GPa]$	Out-of-plane tangential modulus.
ν_{12}	$[-]$	In-plane Poisson's ratio.
ν_{23}	$[-]$	Out-of-plane Poisson's ratio.
a_1	$\left[\frac{m}{mK}\right]$	Thermal expansion coefficient in longitudinal direction.
a_2	$\left[\frac{m}{mK}\right]$	Thermal expansion coefficient in transversal direction.

Abstract

In order to start probing the mechanics of thin ply composites from a numerical standpoint, a Reference Volume Element (RVE) model is developed for subsequent numerical simulations with the Finite Element Method (FEM).

The RVE is 2-dimensional and it is supposed to be taken from a $[90^\circ]$ ply inside a cross-ply laminate. The element lies inside the $[90^\circ]$ ply on a plane parallel to the $[0^\circ]$ direction of the laminate (global x-direction) and to the across-the-thickness direction of the laminate itself (global z-direction). Three different specifications of the RVE are developed: a simple single element made up by a fiber inside a square matrix domain; the latter element bounded by $[0^\circ]$ plies on the upper and bottom side; a periodic pattern constituted by the single RVE tiled in a 3×3 2D array.

The discretization of the geometry and the consequent mesh generation is performed by means of a custom-developed application written in C++. Such choice has been motivated by the need of generating a structured grid of quadrilateral elements capable of adapting to the curved geometry of the problem. Furthermore, as mesh geometry and size could affect significantly the final result of simulations, full control on the discretization process is fundamental for reliable numerical results. Hence the choice of developing a custom algorithm for the discretization step instead of using the ABAQUS FEA CAE interface. The main reason is the fact that numerical simulations of fracture mechanics are strongly dependent on mesh size and characteristics; thus it is better to have direct knowledge and control of the mesh generation process instead of leaving it to ABAQUS algorithms, which are kind of "black boxes" and thus not so easily customizable. Furthermore, based on author's experience, building a custom parametric mesh using ABAQUS FEA input file syntax is certainly possible but quite cumbersome and rigid. Hence the choice of C++, as it allows for flexibility and, if needed, custom-made features.

The main output of the C++ code is an ABAQUS FEA input file; using a Python script, the all process can be streamlined and automatized allowing parametric studies to be performed. In order to accommodate a grid of quadrilateral elements in a curvilinear geometry, the RVE geometry is split into different regions and a few parameters are introduced in order to control the outcome of the discretization process. The creation of multiple regions is important to control the localization of irregularities and elements' deformation. These can be in fact greatly reduced and smoothed out but not completely removed. Thus, transition zones are created in order to prevent irregularities to appear close to the fiber/matrix interface, where the fracture process takes place. The geometry is topologically transformed and discretized using transfinite interpolation and elliptic smoothing.

As the problem is 2-dimensional and in plane-strain, ABAQUS FEA elements CPEG4 (2D bi-linear plane strain elements) and CPEG8 (2D bi-quadratic plane strain elements) are chosen. CPEG8 are considered in addition to CPEG4 because only quadratic elements can capture curvature effects, as they might be present at a circular interface. Comparison of results from the same set-up with the two different elements

could show the presence (or absence) of curvature effects on the fracture process. Furthermore, the choice of CPEG4 and CPEG8 allows for a direct comparison with the work presented in [1].

Numerical simulations are then conducted with the Finite Element Method (FEM) using the commercial CAE software ABAQUS FEA. Two different analyses are conducted: a Linear Elastic Fracture Mechanics (LEFM) study and Cohesive Zone Model (CZM) approach. The details of the solving procedure and the corresponding ABAQUS FEA commands are described.

1 Geometries, loads and boundary conditions

Table 1: Model geometries summary.

Name	Description	Number of phases	Geometry of each phase	Boundary conditions	con- di- tional	Imposed conditions
single-RVE	Circular fiber inside a square matrix domain.	2	Fiber: circular; matrix: square with circular inclusion at its center.	Constant strain at $z = \pm l$; in order to have constant strain, the displacement has a linear functional form, i.e. $u_x _{z=\pm l} = \bar{u}_x \frac{x}{l}$.		Constant displacement $u_x _{z=\pm l} = \bar{u}_x = \bar{\epsilon}_x \cdot l$ at $x = \pm l$.
bounded-RVE	Circular fiber inside a square matrix domain, bounded by two UD rectangular domains on the upper and lower side.	3	Fiber: circular; matrix: square with circular inclusion at its center; UD: rectangular.	Free surface at $z = \pm l$.		Constant displacement $u_x _{z=\pm l} = \bar{u}_x = \bar{\epsilon}_x \cdot l$ at $x = \pm l$.
periodic-RVE	Periodically repeated unit cell, constituted by a circular fiber inside a square matrix domain.	2	Fiber: circular; matrix: square with circular inclusion at its center.	Periodic boundary conditions on all sides.		Constant displacement $u_x _{z=\pm l} = \bar{u}_x = \bar{\epsilon}_x \cdot l$ at $x = \pm l$.

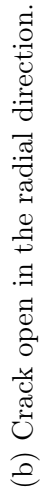


Figure 1: Single RVE model.

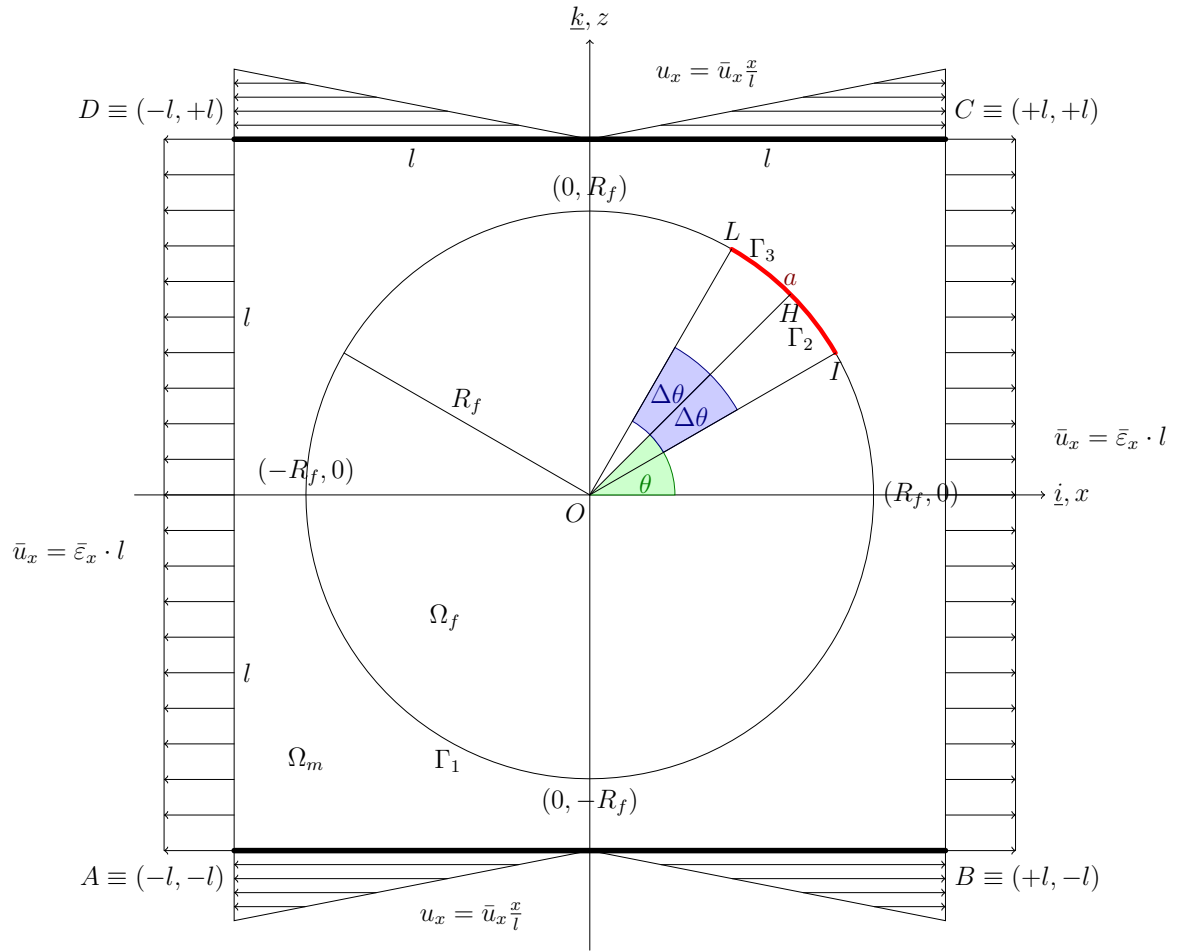


Figure 2: Initial state of single RVE model: crack closed in the radial direction.

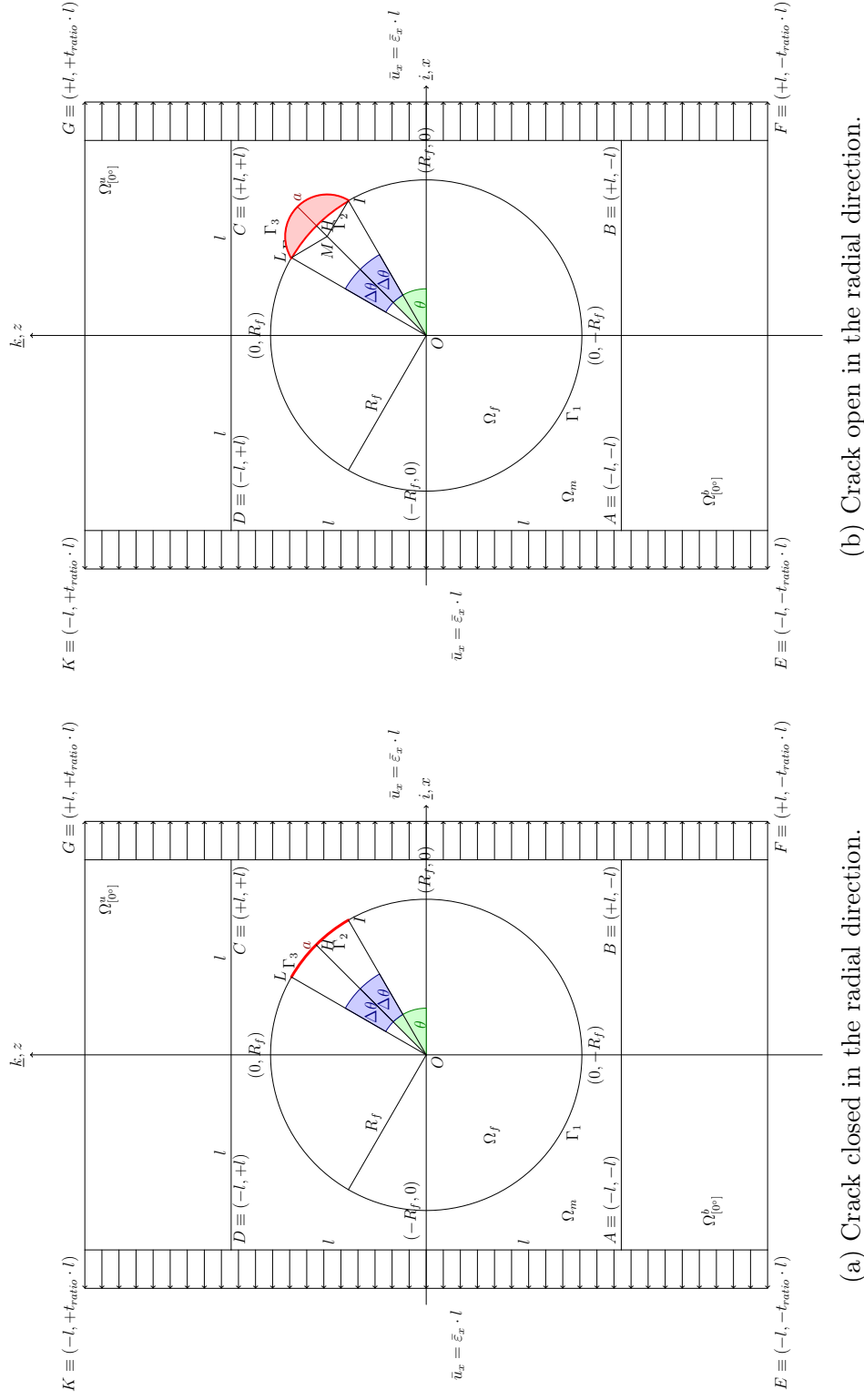


Figure 3: Bounded RVE model.

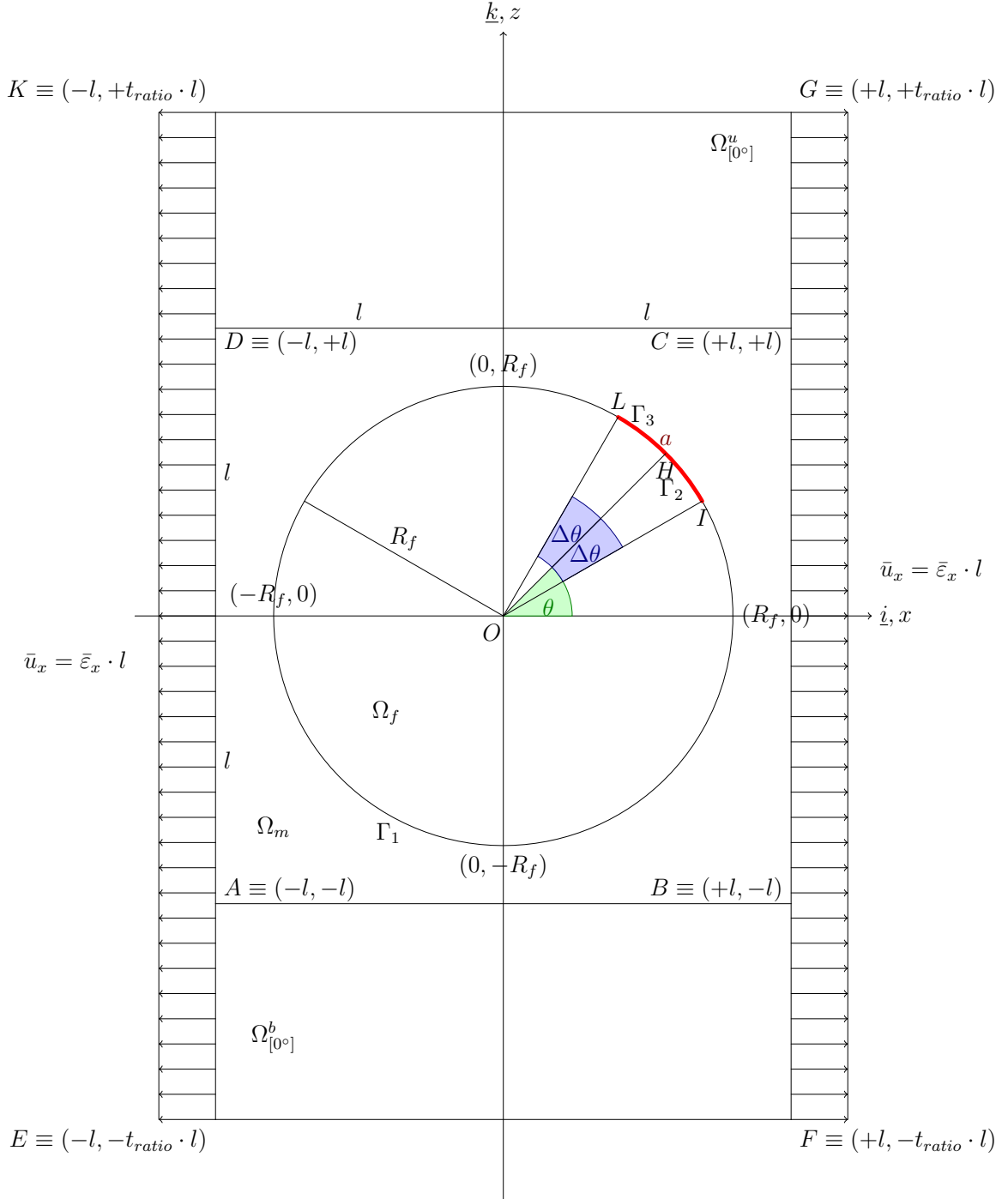
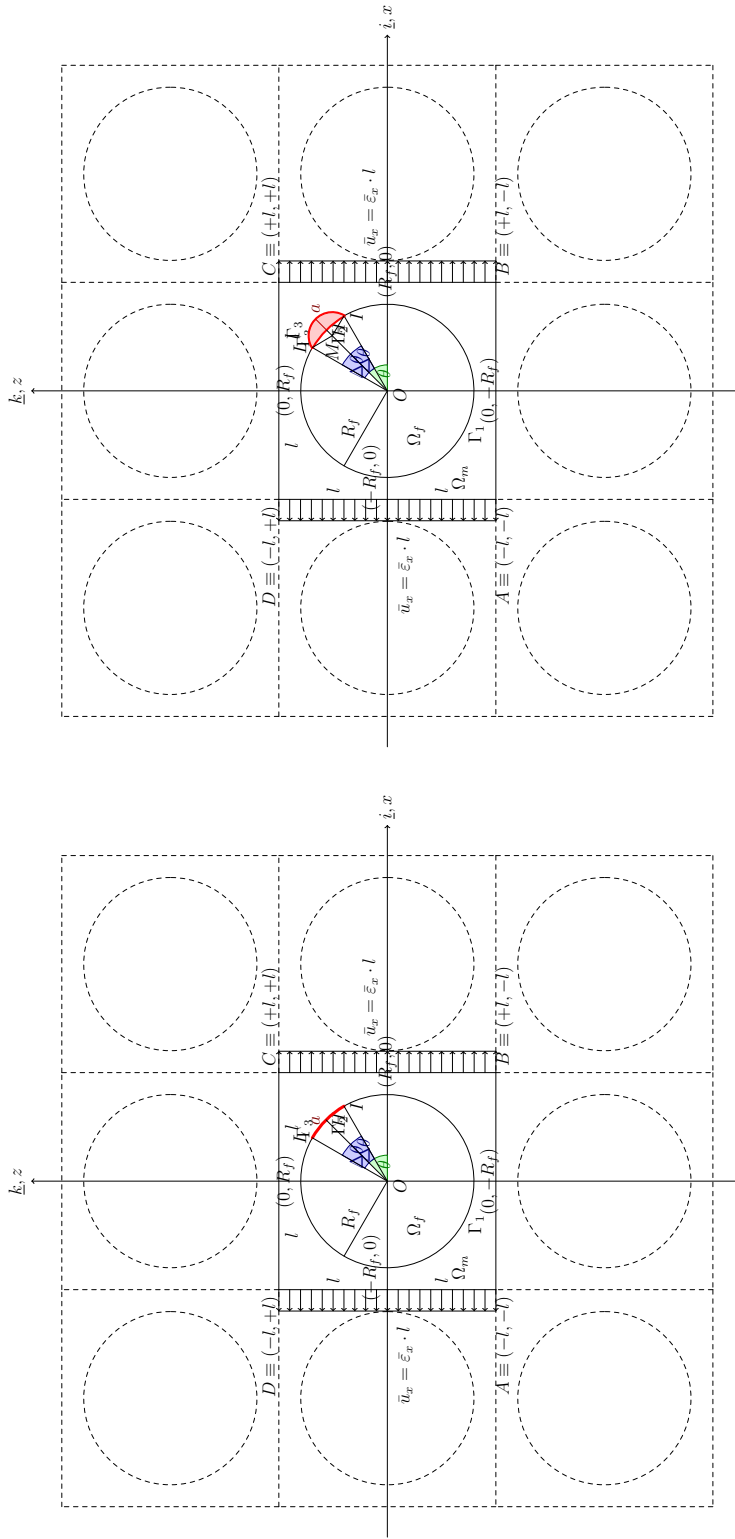


Figure 4: Initial state of bounded RVE model: crack closed in the radial direction.



(a) Crack closed in the radial direction.

Figure 5: Periodic RVE model.

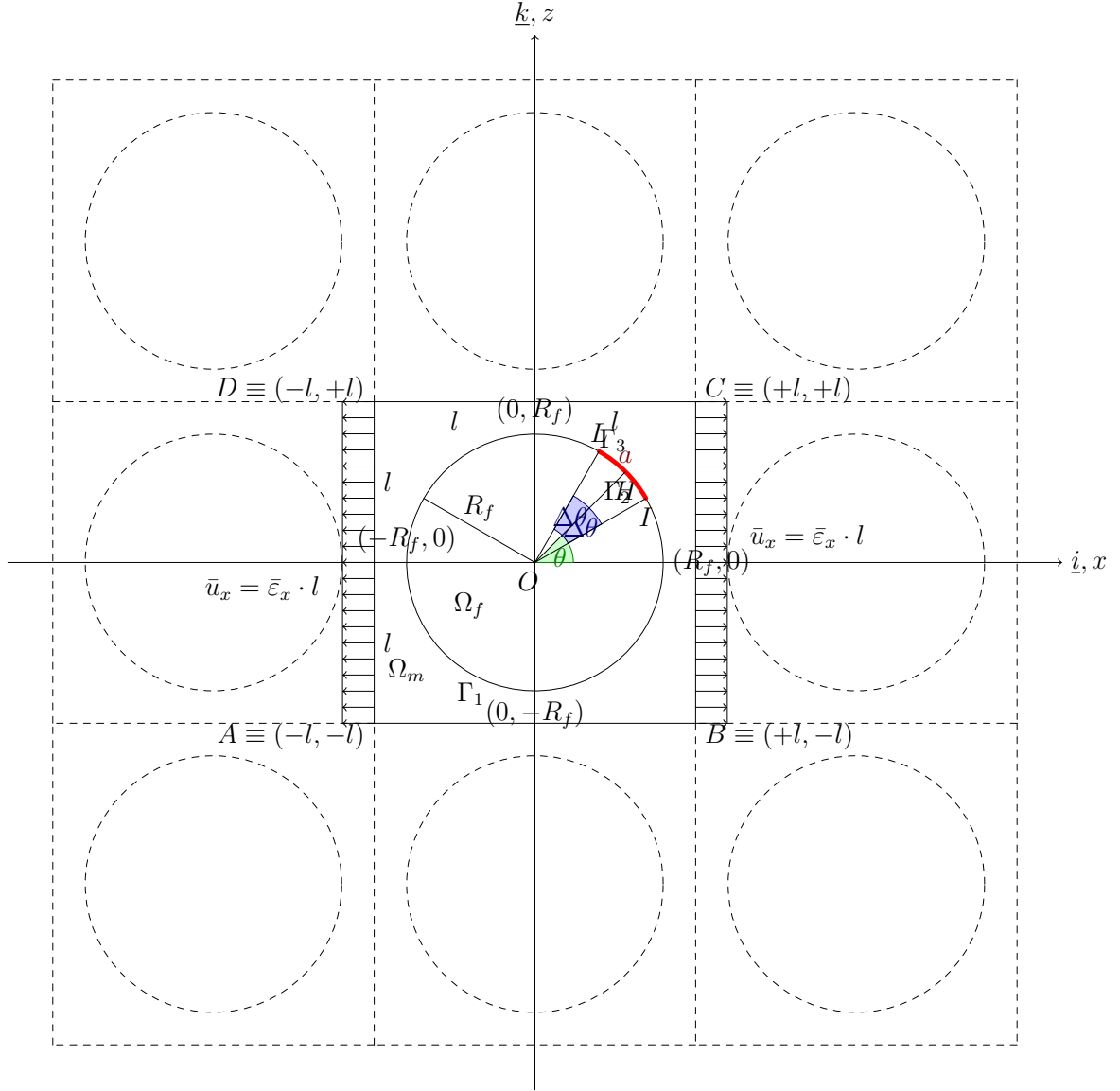


Figure 6: Initial state of periodic RVE model: crack closed in the radial direction.

2 Material properties

Table 2: Single phase properties summary.

Material	E_1 [GPa]	E_2 [GPa]	G_{12} [GPa]	ν_{12} [—]	ν_{23} [—]	a_1 [$10^{-6} \frac{m}{mK}$]	a_2 [$10^{-6} \frac{m}{mK}$]
CF	500,0	30,0	20,0	0,2	0,5	-1,0	7,8
GF	70,0	70,0	29,2	0,2	0,2	4,7	4,7
EP	3,5	3,5	1,3	0,4	0,4	60,0	60,0

Table 3: UD ply properties summary.

Material	V_f [—]	E_1 [GPa]	E_2 [GPa]	G_{12} [GPa]	G_{23} [GPa]	ν_{12} [—]	ν_{23} [—]
CF/EP	0,6	301,4422	11,0389	4,0625	3,5767	0,2734	0,5432
CF/EP	0,4	202,1433	7,5694	2,6136	2,3803	0,3133	0,5899
GF/EP	0,6	43,4425	13,7145	4,3140	4,6808	0,2726	0,4650

3 Mesh characteristics

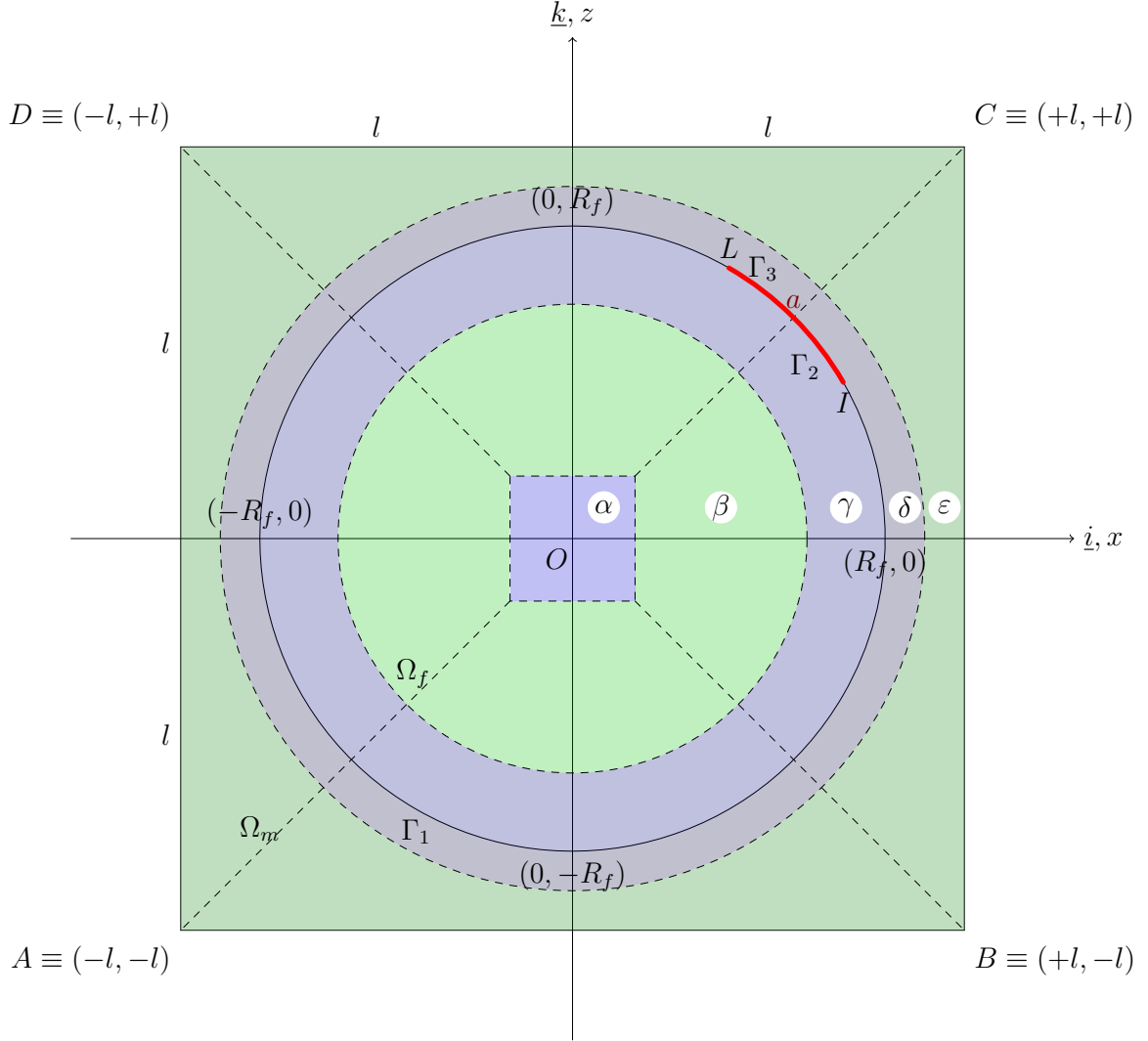
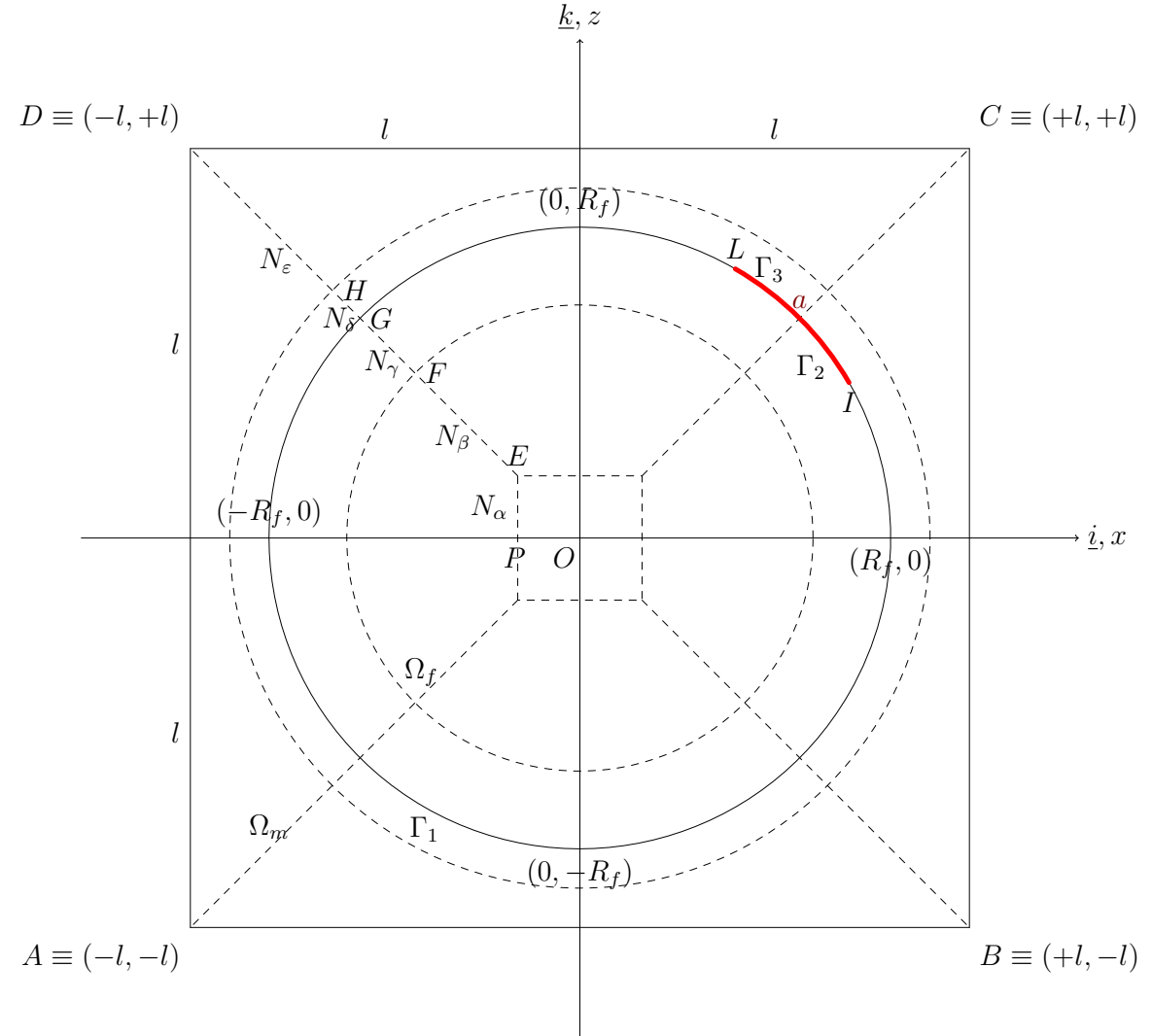


Figure 7: Block regions of the RVE geometry.

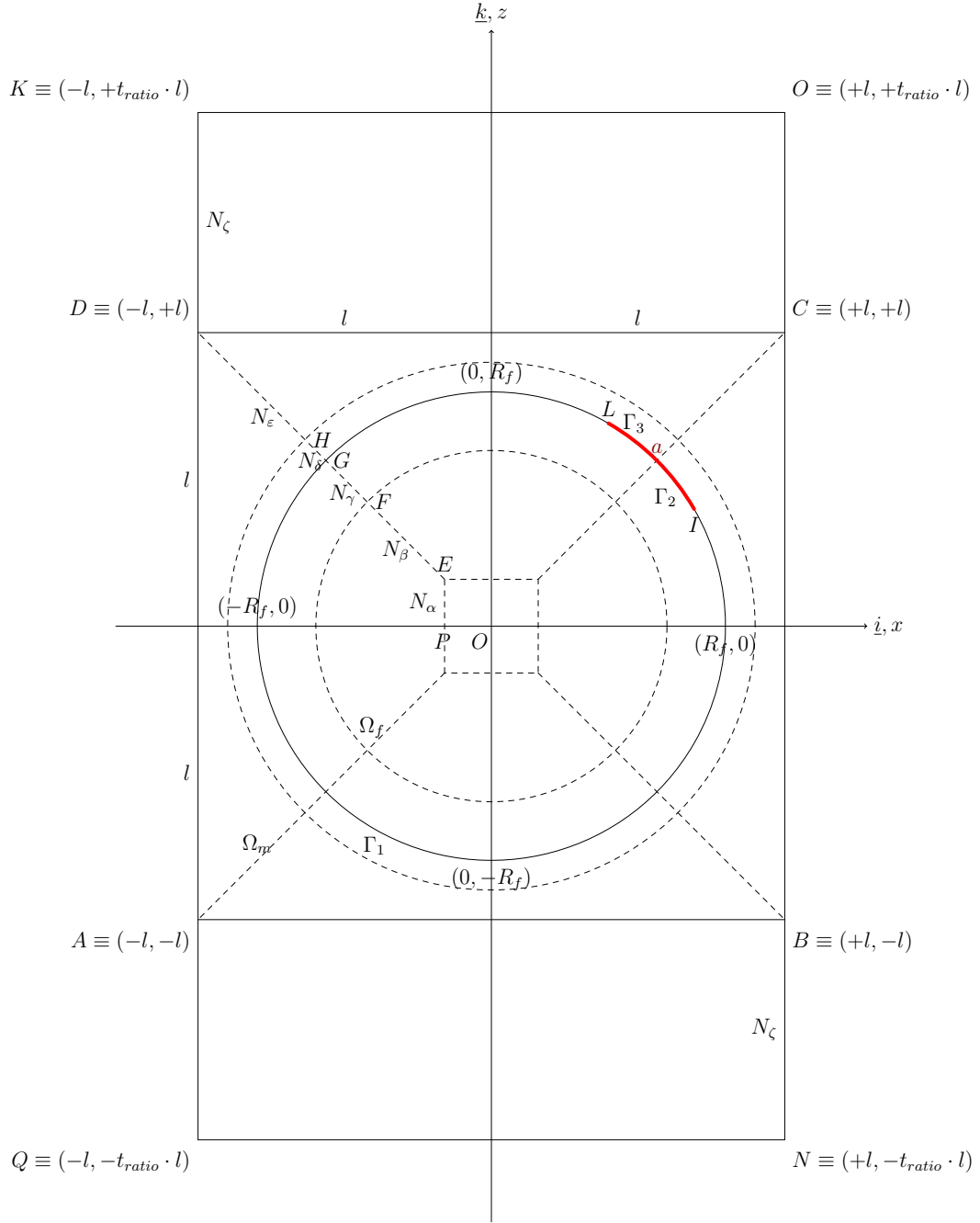


$$E \equiv (-f_1 \cdot R_f, +f_1 \cdot R_f) \quad F \equiv f_2 R_f (-\cos 45^\circ, \sin 45^\circ)$$

$$G \equiv R_f (-\cos 45^\circ, \sin 45^\circ)$$

$$H \equiv (R_f + f_3(l - R_f))(-\cos 45^\circ, \sin 45^\circ)$$

Figure 8: Parameters for mesh generation for the single and periodic RVE.



$$E \equiv (-f_1 \cdot R_f, +f_1 \cdot R_f) \quad F \equiv f_2 R_f (-\cos 45^\circ, \sin 45^\circ)$$

$$G \equiv R_f (-\cos 45^\circ, \sin 45^\circ)$$

$$H \equiv (R_f + f_3 (l - R_f)) (-\cos 45^\circ, \sin 45^\circ)$$

Figure 9: Parameters for mesh generation for the bounded RVE.

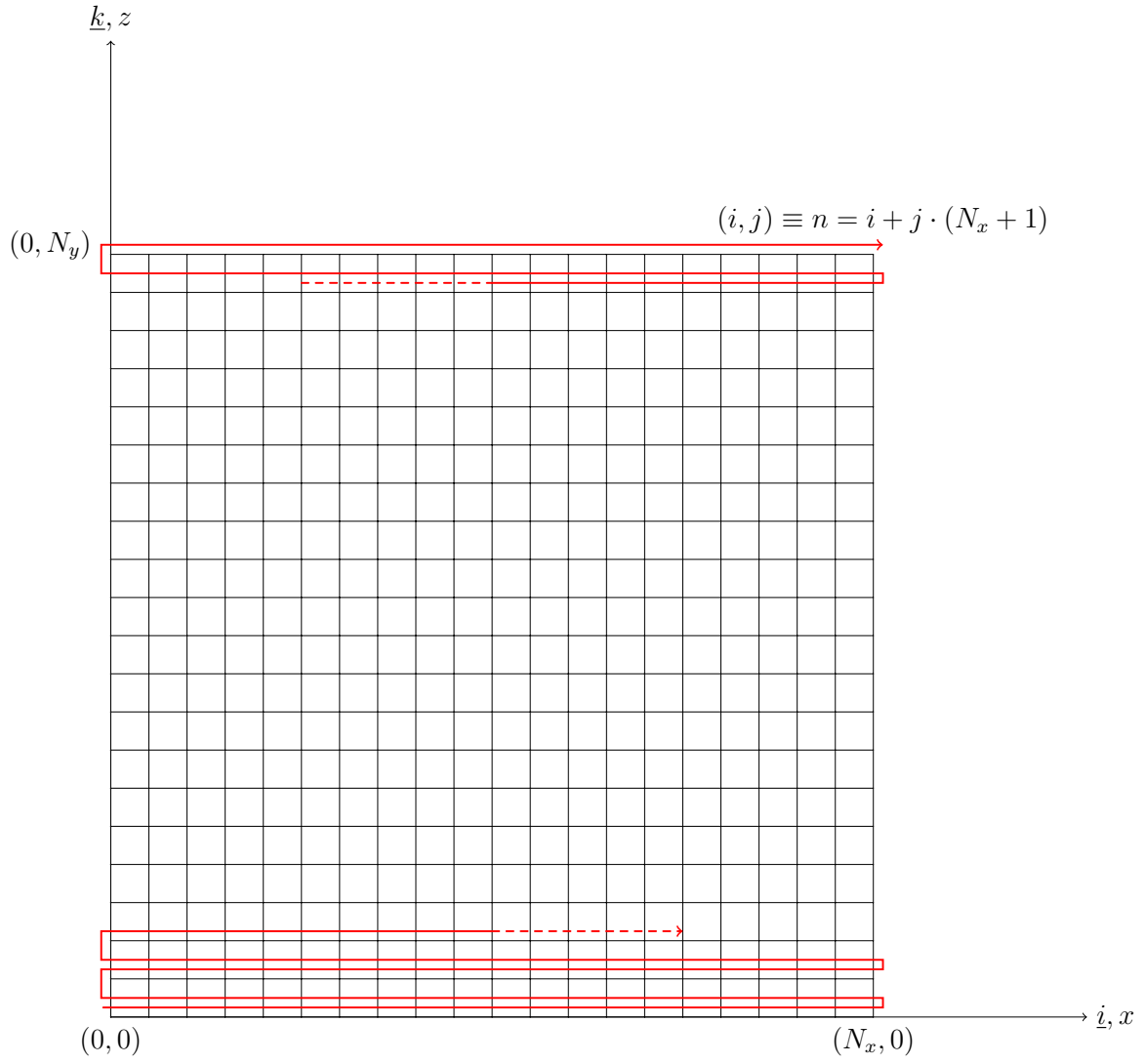
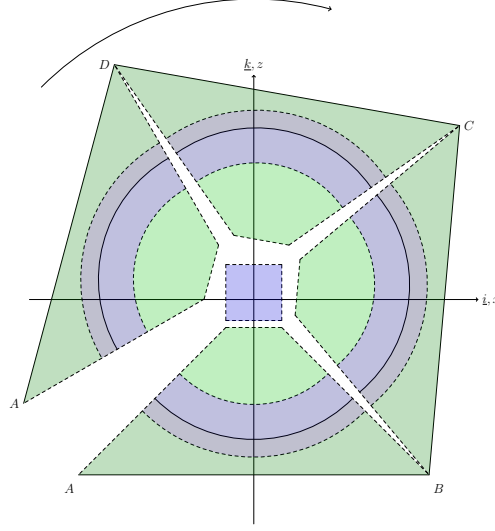
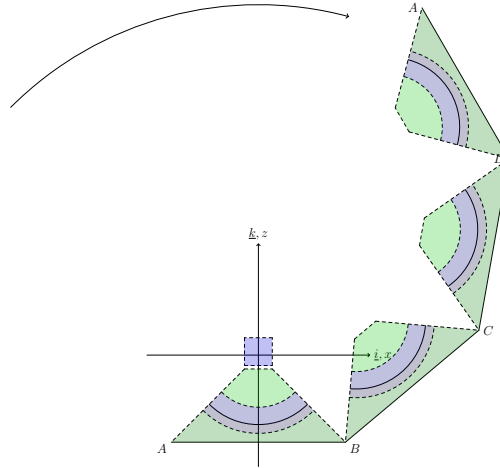


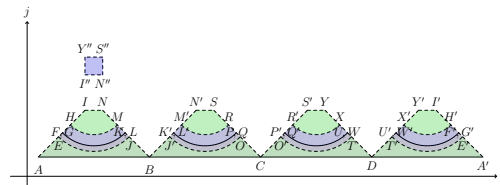
Figure 10: Representation of the helical numbering method.



(a) Initial state.



(b) Intermediate step of the transformation.



(c) Final state.

Figure 11: Main steps of the topological transformation for mesh generation.

Figure 12: Topological transformation for mesh generation.

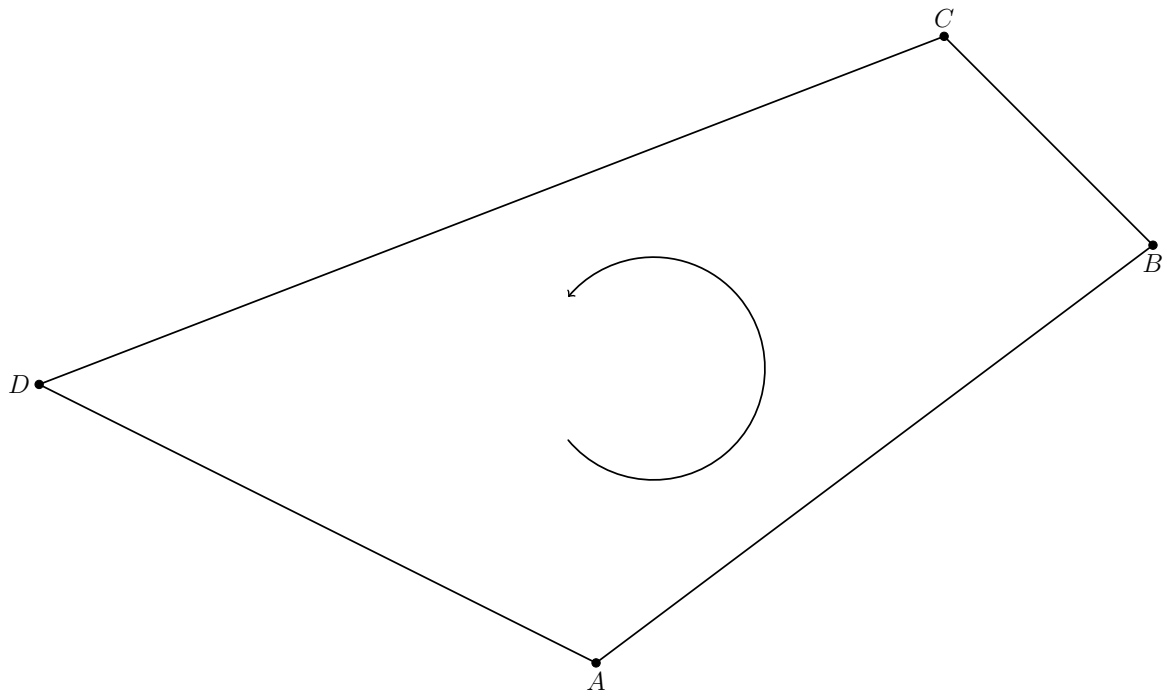


Figure 13: ABAQUS FEA CPEG4 first-order 4-node plane strain element (for details see [2]).

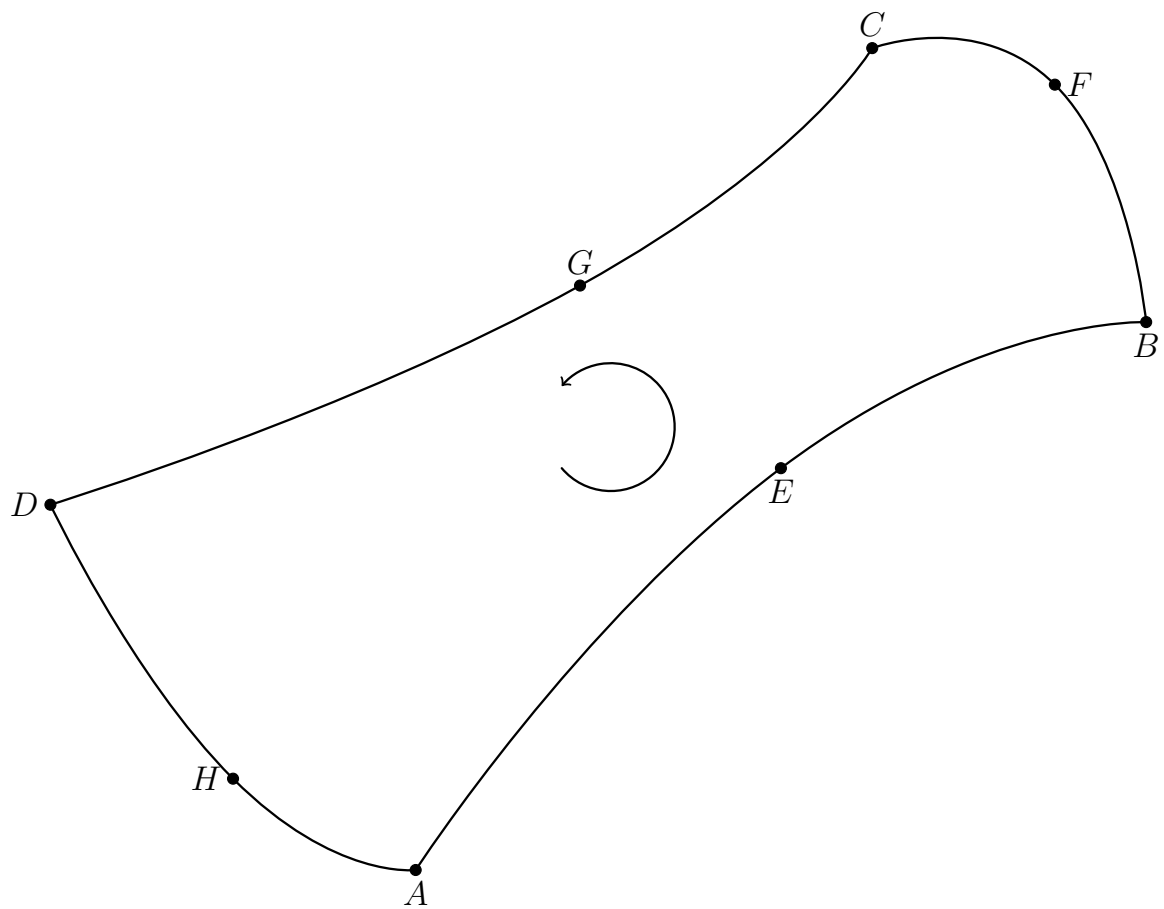


Figure 14: ABAQUS FEA CPEG8 second-order 8-node plane strain element (for details see [2]).

4 Types of analysis

Table 4: Analysis methods summary.

Method	Type	Elements	Interface	Input variables	Control ables	vari- ables	Output ables	vari-
ABAQUS FEA/STANDARD	The analysis is static, i.e. static analysis with the use of the VCCCT and the J-integral method.	CPEG4/CPEG8	Tied surface constraint on the fiber/matrix interface except inside the crack. In the crack region, the two surfaces are disjoint; contact mechanics is applied to avoid inter-penetration and resolve eventual friction between sliding crack surfaces.	Fiber radius, volume fraction, material properties.	Crack position, angular aperture, strain.	angular crack semi-aperture, applied stress factors, release rates, mean radial crack aperture.	Stress crack tip stress, stress intensity factors, energy rates, mean radial crack aperture.	field, stress, intensity
ABAQUS FEA/STANDARD	The analysis is static, i.e. static analysis with the use of the cohesive element method.	CPEG4/CPEG8 and COH2D4	The whole interface is discretized with cohesive elements.	Fiber radius, volume fraction, material properties.	Interface proper- ties, maximum stresses for crack onset, energy release rates, applied strain.	Crack position, angular crack aperture, mean radial crack boundary stresses.	Crack position, angular crack aperture, mean radial crack boundary stresses.	angu- lar position, angular

Table 5: ABAQUS FEA/STANDARD commands summary.

Method	ABAQUS FEA command
static analysis	*STATIC
VCCT	*FRACTURE CRITERION, TYPE=VCCT
J-integral method	*CONTOUR INTEGRAL
cohesive element method	*COHESIVE SECTION
tied surface constraint	*TIE
contact mechanics	*CONTACT
stress intensity factors	*CONTOUR INTEGRAL, TYPE=K FACTORS

Glossary

ABAQUS FEA (formerly ABAQUS) is a software suite for finite element analysis and computer-aided engineering, originally released in 1978.

ABAQUS FEA/STANDARD is part of ABAQUS FEA suite and tailored for the static or quasi-static analysis of problems in solid and structural mechanics.

C++ is a general-purpose programming language. It has imperative, object-oriented and generic programming features, while also providing facilities for low-level memory manipulation.

COH2D4 4-node two-dimensional cohesive element, from ABAQUS FEA special-purpose elements library.

CPEG4 4-node bilinear plane strain iso-parametric element, from ABAQUS FEA two-dimensional solid elements library.

CPEG8 8-node biquadratic plane strain iso-parametric element, from ABAQUS FEA two-dimensional solid elements library.

Python is a widely used general-purpose, high-level programming language.

References

- [1] Miguel Herráez et al. “Transverse cracking of cross-ply laminates: A computational micromechanics perspective”. In: *Composites Science and Technology* 110 (2015), pp. 196–204. ISSN: 0266-3538. DOI: 10.1016/j.compscitech.2015.02.008. URL: <http://www.sciencedirect.com/science/article/pii/S0266353815000792>.
- [2] Hibbit, Karlsson, and Sorensen. *ABAQUS Analysis User’s Manual*. USA: Hibbit, Karlsson, Sorensen Inc., 2013.