

# **\*RVE**

The \*RVE keywords control a Representative Volume Element (RVE) analysis. This method can predict macroscopic material properties for various types of composites from their microstructural information. Using this method, you can conduct virtual testing of numerically re-constructed material samples at their characteristic length scales. The algorithms invoked with \*RVE keywords automatically create periodic or linear displacement boundary conditions, perform FEM-based computational homogenization, and predict the homogenized macroscopic constitutive responses as well as the detailed microscopic stress / strain fields.

The only available keyword is:

**\*RVE\_ANALYSIS\_FEM**

**\*RVE\_ANALYSIS\_FEM**

Purpose: Predict the macroscopic effective constitutive behaviors of composite materials under the micromechanics-based computational homogenization framework. Composite materials supported for this feature include but are not limited to fiber-reinforced composites, particulate composites, laminar composites, polycrystalline aggregates, and single-phase or multi-phase porous media.

We account for both the geometrical and material nonlinearities of the Representative Volume Element (RVE) with the nonlinear computational homogenization theory. Given the material microstructural information (geometry and constitutive properties for base materials), this keyword causes

1. Automatic creation of periodic displacement boundary conditions (or linear displacement boundary conditions) on the RVE finite element mesh;
2. A nonlinear quasi-static implicit finite element analysis of the RVE under user-defined loading conditions; and
3. The calculation of the macroscopic effective material responses through homogenization of the RVE's microscopic material responses as well as a detailed distribution and evolution of microscopic stress/strain fields within the RVE.

Double precision SMP/MPP LS-DYNA version R13 and newer versions support this RVE analysis function.

**Card Summary:**

**Card 1.** This card is required.

MESHFILE
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**Card 2.** This card is required.

INPT	OUPT	LCID	IDOF	BC	IMATCH	IMAGE	
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**Card 3.** This card is required.

H11	H22	H33	H12	H23	H13		
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**Card 4.** This card is required only if BC = 2.

PX	PY	PZ					
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**Data Card Definitions:**

Card 1	1	2	3	4	5	6	7	8
Variable				MESHFILE				
Type				C				
Default				none				

VARIABLE	DESCRIPTION							
MESHFILE	Name of an input file that contains the mesh information (nodal coordinates, element connectivity) of the RVE model. Note that this file should be in keyword format [basename].k. The finite element mesh given in this file is for the spatial discretization of the material microstructures. Do not include dummy nodes for specifying control points in boundary conditions. See <a href="#">Remark 1</a> .							

Card 2	1	2	3	4	5	6	7	8
Variable	INPT	OUPT	LCID	IDOF	BC	IMATCH	IMAGE	
Type	I	I	I	I	I	I	I	
Default	0	1	none	none	0	1	0	

VARIABLE	DESCRIPTION							
INPT	Type of input:  EQ.0: RVE boundary conditions are fully defined by two factors: (1) the parameter BC of this input card, and (2) the mesh information in the file specified in MESHFILE. When running an RVE simulation, LS-DYNA automatically creates a file named rve_[basename].k. This file contains all the necessary information (e.g., dummy nodes, displacement constraints, etc.) for boundary condition enforcement.  EQ.1: You provide a file named rve_[basename].k to specify the boundary condition keywords (e.g. *CONSTRAINED_MULTIPLE_GLOBAL, *BOUNDARY_SPC_NODE, etc.)							

<b>VARIABLE</b>	<b>DESCRIPTION</b>
	and dummy nodes for enforcing RVE boundary conditions. We do not recommend this option since it is usually nontrivial to manually define all the keywords for RVE boundary conditions. If the file <code>rve_[basename].k</code> is not found when running RVE simulations, then LS-DYNA creates <code>rve_[basename].k</code> based on the parameter BC and the mesh information in the file specified with MESHFILE.
OUPT	Type of output:  EQ.1: RVE homogenization results will be written out to a file named <code>rveout</code> . Please refer to the keyword *DATABASE_RVE.
LCID	Load curve ID for specifying loading history (see *DEFINE_CURVE) or flag to indicate that each component of the macroscopic deformation measure ( $H_{11}$ , $H_{22}$ , ..., $H_{13}$ on Card 3) is input as a load curve:  GT.0: Load curve ID. This curve gives a scale factor for the user-defined macroscopic deformation measure ( $H_{11}$ , $H_{22}$ , ..., $H_{13}$ input on Card 3) as a function of loading time. The scale factor is the ordinate (second column) while the loading time is the abscissa (first column).  LT.0: Flag to indicate that each component of the macroscopic displacement gradient, $H_{ij}$ , is input as a load curve on Card 3.
IDOF	Dimension of the RVE:  EQ.2: 2D geometry EQ.3: 3D geometry
BC	Type of the RVE boundary condition (see <a href="#">Remark 2</a> and <a href="#">Figure 44-1</a> ):  EQ.0: Periodic displacement boundary condition EQ.1: Linear displacement boundary condition EQ.2: Partially Periodic Displacement Boundary Condition (PDPC). Card 4 is required.
IMATCH	Type of the given RVE mesh (ignored unless BC = 0; see <a href="#">Remark 3</a> ):

<b>VARIABLE</b>	<b>DESCRIPTION</b>
	<p>EQ.0: The mesh is non-matching for periodic displacement boundary condition.</p> <p>EQ.1: The mesh is periodic displacement boundary condition matching.</p>
IMAGE	<p>Create image RVE in specified directions. This feature is only available for IMATCH = 1. See <a href="#">Remark 11</a> and <a href="#">Figure 44-2</a>.</p> <p>EQ.110: Create image RVE in <math>x</math> direction</p> <p>EQ.120: Create image RVE in <math>y</math> direction</p> <p>EQ.130: Create image RVE in <math>z</math> direction</p> <p>EQ.212: Create image RVE in both the <math>x</math> and <math>y</math> directions</p> <p>EQ.213: Create image RVE in both the <math>x</math> and <math>z</math> directions</p> <p>EQ.232: Create image RVE in both the <math>y</math> and <math>z</math> directions</p> <p>EQ.300: Create image RVE in the <math>x</math>, <math>y</math> and <math>z</math> directions</p>

Card 3	1	2	3	4	5	6	7	8
Variable	H11	H22	H33	H12	H23	H13		
Type	F	F	F	F	F	F		
Default	optional	optional	optional	optional	optional	optional		

<b>VARIABLE</b>	<b>DESCRIPTION</b>
H $ij$	Component $ij$ of the prescribed macroscopic displacement gradient, $\tilde{\mathbf{H}}$ . $\tilde{\mathbf{H}}$ is assumed to be symmetric (see <a href="#">Remark 4</a> ). To not impose the corresponding constraints on the RVE, leave the component H $ij$ empty (instead of setting it to be zero). If LCID < 0 on Card 2, the input value is assumed to be a load curve ID for a load curve giving the component as a function of time. Please refer to <a href="#">Remarks 2</a> and <a href="#">8</a> .

**PDBC Card.** This card is required for BC = 2.

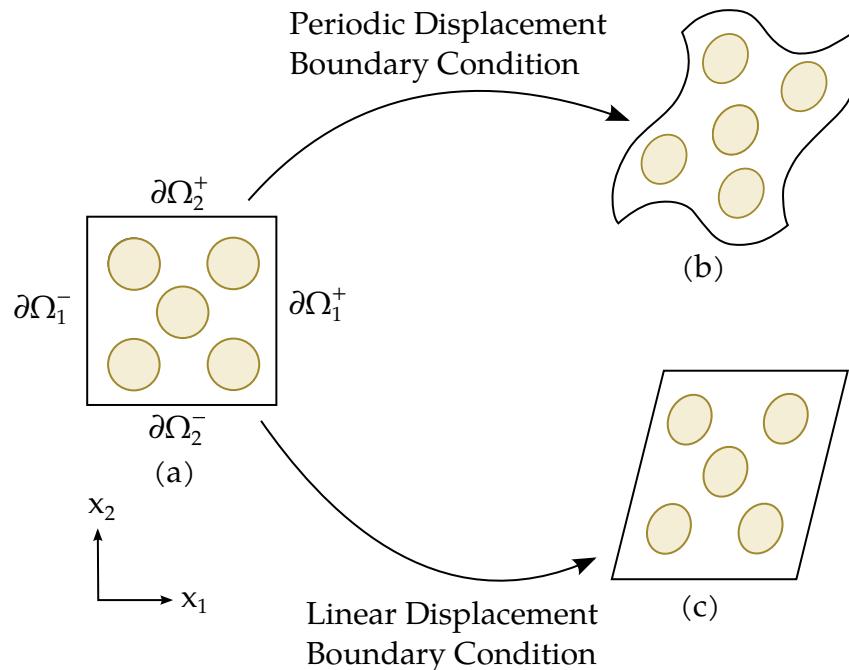
Card 4	1	2	3	4	5	6	7	8
Variable	PX	PY	PZ					
Type	I	I	I					
Default	0	0	0					

VARIABLE	DESCRIPTION
Pi	Flag to apply the periodic boundary condition in the $i^{\text{th}}$ direction ( $i = x, y, \text{ or } z$ ) for PDBC:
	EQ.0: Periodic boundary condition is not applied for this direction.
	EQ.1: Periodic boundary condition is applied for this direction.

### Remarks:

- RVE Mesh.** The RVE's mesh information (nodal coordinates, element connectivity) should be provided in a separate input file, of which the file name should be given in Card 1 of the keyword \*RVE\_ANALYSIS\_FEM. Usually, a 3D RVE model has a cuboid shape with its edges parallel to the X-, Y-, and Z-axes of the global coordinate system, respectively. A 2D RVE model is rectangular with its edges parallel to the X- and Y- axes of the global coordinate system, respectively. The size of the RVE should be large enough to include sufficient statistical microstructural information (fibers, particles, voids, grains, etc.) of the composite material. It should, however, remain small enough to be considered as a volume element of continuum mechanics. The 3D RVE should be meshed with solid elements (see \*ELEMENT\_SOLID) while the 2D RVE should be meshed with shell elements (see \*ELEMENT\_SHELL).
- Boundary Conditions.** LS-DYNA can automatically create boundary conditions on the external boundary  $\partial\Omega$  of the RVE. Two types of RVE boundary conditions can be created, depending on the input value of BC:
  - Periodic Displacement Boundary Condition (BC = 0).* When BC = 0, LS-DYNA imposes the following periodic displacement boundary condition:

$$\mathbf{w}_\alpha^+ - \mathbf{w}_\alpha^- = \tilde{\mathbf{H}}(\mathbf{X}_\alpha^+ - \mathbf{X}_\alpha^-) .$$



**Figure 44-1.** Schematic of the two types of displacement boundary conditions for RVE analysis. (a) The initial configuration of RVE occupying the domain  $\Omega$ , where  $\partial\Omega_\alpha^+$  and  $\partial\Omega_\alpha^-$  denote a pair of opposite external boundaries.  $\alpha = 1, 2$  for this 2D model. (b) The current configuration of RVE subjected to periodic displacement boundary conditions. (c) The current configuration of RVE subjected to linear displacement boundary conditions.

Here  $\mathbf{X}_\alpha^+ \in \partial\Omega_\alpha^+$  and  $\mathbf{X}_\alpha^- \in \partial\Omega_\alpha^-$  denote the microscale material points located on a pair of opposite external boundaries  $\partial\Omega_\alpha^+$  and  $\partial\Omega_\alpha^-$ , respectively, in the RVE's initial configuration (See Figure 44-1 for a 2D illustration).  $\mathbf{w}_\alpha^+$  and  $\mathbf{w}_\alpha^-$  are the microscale displacements of the material points  $\mathbf{X}_\alpha^+$  and  $\mathbf{X}_\alpha^-$ , respectively. The subscript  $\alpha = 1, 2, \dots, d$  where  $d = 2$  for 2D RVE models and  $d = 3$  for 3D RVE models. To impose the periodicity constraint, a control point-based method is implemented, which is similar to the keywords \*INCLUDE\_UNITCELL and \*CONSTRAINED\_MULTIPLE\_GLOBAL. Unlike these other keywords, \*RVE\_ANALYSIS\_FEM automatically creates these control points.

- b) *Linear Displacement Boundary Condition (BC = 1)*. When BC = 1, LS-DYNA imposes the following linear displacement boundary condition:

$$\mathbf{w}_\alpha = \widetilde{\mathbf{H}}\mathbf{X}_\alpha,$$

where  $\mathbf{X}_\alpha \in \partial\Omega_\alpha$  denotes any micro-scale material point located on the external boundaries  $\partial\Omega_\alpha = \partial\Omega_\alpha^+ \cup \partial\Omega_\alpha^-$  of the RVE. Note that the RVE's complete external boundary can be expressed as  $\partial\Omega = \bigcup_{\alpha=1}^d \partial\Omega_\alpha$ , in which  $d = 2$  for 2D RVE models and  $d = 3$  for 3D RVE models. It is noteworthy to mention that RVEs with linear displacement boundary conditions usually

appear to be stiffer than RVEs with periodic displacement boundary conditions. When the size of RVE is large enough, however, the influence of different types of boundary conditions on the homogenized material properties becomes negligibly small.

The assignment of a zero value to any component of the macroscopic displacement gradient  $\tilde{\mathbf{H}}$  indicates the imposition of the boundary constraint based on the above constraint equations. If you do not want to impose constraints in certain directions (i.e., allow the associated RVE boundaries to deform freely), then you should leave the corresponding component of  $\tilde{\mathbf{H}}$  empty in the input card. Please refer to [Remark 8](#) for an application scenario where most components of  $\tilde{\mathbf{H}}$  should be set empty.

3. **IMATCH for Periodic Displacement Boundary Conditions.** When the mesh is periodic displacement boundary condition matching, the nodal distributions on the RVE's opposite sides match well with each other. For instance, let us consider two opposite surfaces, surface A and surface B, that are both perpendicular to the X-axis. For any FEM node on surface A, if we draw a straight line that is parallel to the X-axis, then the intersection point of this line with surface B must also be an FEM node. For such periodic displacement boundary condition matching meshes, an efficient direct nearest neighbor search algorithm imposes the boundary condition. Thus, a matching mesh is preferred for imposing the periodic displacement boundary conditions. However, if complex material microstructures exist, it is not always straightforward to create matching meshes. In this case, set IMATCH to zero which calls a projection-based constraint imposition method.
4. **Prescribed Macroscopic Displacement Gradient.** The prescribed macroscopic displacement gradient is given as:

$$\tilde{\mathbf{H}} \equiv \nabla_{\tilde{\mathbf{x}}} \tilde{\mathbf{u}} = \tilde{\mathbf{F}} - \mathbf{I} ,$$

where  $\nabla_{\tilde{\mathbf{x}}}$  is the gradient operator with respect to the macroscale,  $\tilde{\mathbf{u}}$  is the macroscopic displacement field,  $\tilde{\mathbf{F}}$  is the macroscopic deformation gradient, and  $\mathbf{I}$  is the identity tensor. Generally,  $\tilde{\mathbf{F}}$  is not symmetric. Thus,  $\tilde{\mathbf{H}}$  is not usually symmetric. Through polar decomposition of the deformation gradient,  $\tilde{\mathbf{F}} = \tilde{\mathbf{R}}\tilde{\mathbf{U}}$ .  $\tilde{\mathbf{R}}$  represents the macroscopic rigid body rotation, and  $\tilde{\mathbf{U}}$  is a symmetric stretch tensor describing the pure material deformation. Since material constitutive behaviors are not affected by macroscopic rigid body rotations, we will assume  $\tilde{\mathbf{R}} = \mathbf{I}$  in the RVE analysis. Under this condition, both the macroscopic deformation gradient  $\tilde{\mathbf{F}}$  and macroscopic displacement gradient  $\tilde{\mathbf{H}}$  become symmetric.

Because  $\tilde{\mathbf{H}}$  is symmetric, only six components of  $\tilde{\mathbf{H}}$  are needed to prescribe boundary conditions for 3D RVE analysis. For 2D RVE problems, the inputs for H33, H23, and H13 are ignored, and only the inputs for H11, H22, and H12 are

adopted for enforcing the boundary condition. Note that you should leave the component  $H_{IJ}$  empty (instead of setting it to be zero) if you do not want to impose the corresponding constraints on the RVE. Please refer to [Remarks 2](#) and [8](#).

5. **Constitutive Models for Base Materials.** Depending on the actual morphology of material microstructures, an RVE finite element model can consist of many parts. Each part can be assigned a unique constitutive law to describe the behaviors of the corresponding base material (e.g., fiber, particle, matrix, grain, etc.). Any constitutive model (linear/nonlinear, isotropic/anisotropic, etc.) can be selected for the base materials as long as the model is supported for implicit analysis. The part and material information should be contained in the main input file, not in MESHFILE. See the [example](#) below.
6. **Accuracy Control for the Implicit Calculation.** To ensure high accuracy of the nonlinear implicit finite element simulation, we recommend using the 2<sup>nd</sup> order objective stress update scheme specified with OSU = 1 on \*CONTROL\_ACCURACY. We also suggest specifying other control parameters for the implicit solver in relevant keywords, such as \*CONTROL\_IMPLICIT\_GENERAL, \*CONTROL\_IMPLICIT SOLUTION, and \*CONTROL\_IMPLICIT\_SOLVER.
7. **Homogenization Results.** LS-DYNA writes out the homogenized material responses to a file named rveout. In this file, the macroscopic deformation gradient  $\tilde{\mathbf{F}}^t$ , Green strain  $\tilde{\mathbf{E}}^t$ , Cauchy stress  $\tilde{\mathbf{\tau}}^t$ , and the 1<sup>st</sup> Piola-Kirchhoff stress  $\tilde{\mathbf{P}}^t$ , are recorded at each output time  $t$ . Different measures for the macroscale stress and deformation can be obtained based on their relationships with the results in rveout. For instance, the 2<sup>nd</sup> Piola-Kirchhoff stress  $\tilde{\mathbf{S}}$  is defined as  $\tilde{\mathbf{S}} = \tilde{\mathbf{P}}\tilde{\mathbf{F}}^{-T}$ . It can be easily calculated since  $\tilde{\mathbf{P}}$  and  $\tilde{\mathbf{F}}$  are available in rveout.

Note that, as discussed in [Remark 4](#), the macroscale rigid body rotations are excluded from the macroscopic displacement gradient. Accordingly, the macroscopic deformation gradient  $\tilde{\mathbf{F}}^t$  and 1<sup>st</sup> Piola-Kirchoff stress  $\tilde{\mathbf{P}}^t$  obtained from RVE analysis are both symmetric, so only six components of each symmetric tensor are written to rveout.
8. **Degeneration to Small Strain Analysis.** Although a nonlinear computational homogenization formulation is implemented in LS-DYNA to capture the RVE's finite deformation effects, the homogenized quantities will be close to those calculated by small strain homogenization theories when the actual macroscopic deformation is small. In this situation, the macroscopic Green strain  $\tilde{\mathbf{E}}$  given in the rveout file will be approximately equal to the infinitesimal strain, and different stress measures ( $\tilde{\mathbf{P}}$ ,  $\tilde{\mathbf{S}}$ , and  $\tilde{\mathbf{\tau}}$ ) will have an identical magnitude.

For small strain linear analysis, if we conduct 3D RVE simulations with six orthogonal loading conditions (e.g., three uniaxial tensile loadings and three pure

shear loadings), respectively, then we will obtain the full macroscopic elasticity tensor for the composite material. Recall that the macroscale linear elastic constitutive relationship can be expressed as follows:

$$\tilde{\epsilon} = \tilde{C}\tilde{\sigma} .$$

$\tilde{C}$  is the  $6 \times 6$  macroscopic material compliance matrix:

$$\tilde{C} = \begin{bmatrix} \tilde{C}_{11} & \tilde{C}_{12} & \tilde{C}_{13} & \tilde{C}_{14} & \tilde{C}_{15} & \tilde{C}_{16} \\ \tilde{C}_{21} & \tilde{C}_{22} & \tilde{C}_{23} & \tilde{C}_{24} & \tilde{C}_{25} & \tilde{C}_{26} \\ \tilde{C}_{31} & \tilde{C}_{32} & \tilde{C}_{33} & \tilde{C}_{34} & \tilde{C}_{35} & \tilde{C}_{36} \\ \tilde{C}_{41} & \tilde{C}_{42} & \tilde{C}_{43} & \tilde{C}_{44} & \tilde{C}_{45} & \tilde{C}_{46} \\ \tilde{C}_{51} & \tilde{C}_{52} & \tilde{C}_{53} & \tilde{C}_{54} & \tilde{C}_{55} & \tilde{C}_{56} \\ \tilde{C}_{61} & \tilde{C}_{62} & \tilde{C}_{63} & \tilde{C}_{64} & \tilde{C}_{65} & \tilde{C}_{66} \end{bmatrix},$$

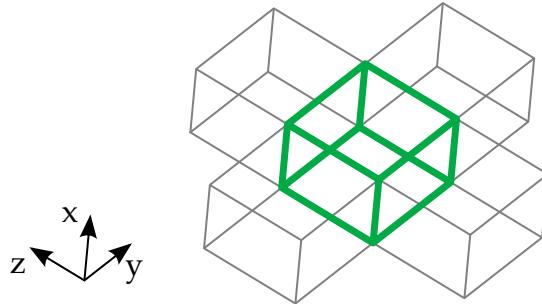
The vectors  $\tilde{\epsilon} = [\tilde{\epsilon}_{11} \quad \tilde{\epsilon}_{22} \quad \tilde{\epsilon}_{33} \quad \tilde{\epsilon}_{12} \quad \tilde{\epsilon}_{23} \quad \tilde{\epsilon}_{31}]^T$  and  $\tilde{\sigma} = [\tilde{\sigma}_{11} \quad \tilde{\sigma}_{22} \quad \tilde{\sigma}_{33} \quad \tilde{\sigma}_{12} \quad \tilde{\sigma}_{23} \quad \tilde{\sigma}_{31}]^T$  contain six macroscopic strain and stress components, respectively.

If we specify uniaxial tensile loading ( $H_{11} = \epsilon$ , where  $\epsilon$  is a non-zero small number, and all other components of the macroscopic displacement gradient are left empty) in Card 3, then the finite element simulation of RVE will yield a homogenized stress vector  $\tilde{\sigma} = [\tilde{\sigma}_1 \quad 0.0 \quad 0.0 \quad 0.0 \quad 0.0 \quad 0.0]^T$  and a homogenized strain vector  $\tilde{\epsilon} = [\tilde{\epsilon}_1 \quad \tilde{\epsilon}_2 \quad \tilde{\epsilon}_3 \quad \tilde{\epsilon}_4 \quad \tilde{\epsilon}_5 \quad \tilde{\epsilon}_6]^T$ . These results are available in rve-out. We can then calculate the first column of the macroscopic material compliance matrix as follows:

$$\begin{aligned} \tilde{C}_{11} &= \tilde{\epsilon}_1 / \tilde{\sigma}_1, & \tilde{C}_{21} &= \tilde{\epsilon}_2 / \tilde{\sigma}_1, & \tilde{C}_{31} &= \tilde{\epsilon}_3 / \tilde{\sigma}_1, \\ \tilde{C}_{41} &= \tilde{\epsilon}_4 / \tilde{\sigma}_1, & \tilde{C}_{51} &= \tilde{\epsilon}_5 / \tilde{\sigma}_1, & \tilde{C}_{61} &= \tilde{\epsilon}_6 / \tilde{\sigma}_1. \end{aligned}$$

Similarly, all the other macroscopic compliance coefficients can be computed by applying different uniaxial tensile and pure shear loading conditions. By inverting the compliance matrix  $\tilde{C}$ , we can obtain the macroscopic material stiffness matrix.

9. **Calibration of Macroscale Constitutive Laws.** If a functional form of the macroscopic constitutive equation is available, then a series of numerical material tests can be properly designed and conducted on the RVE model to identify the material parameters for the assumed constitutive model. In other words, by treating RVEs as virtual material samples, we can fit macroscale material model parameters while reducing the amount of expensive (or unfeasible) physical experiments for composite materials.
10. **De-homogenization/Localization analysis.** After performing a standard macroscale structural finite element analysis in LS-DYNA, we can obtain the macroscale deformation history at any element or integration point of the macrostructure. If we convert such information to the macroscopic displacement



**Figure 44-2.** Example of image RVEs in both the  $y$  and  $z$  directions. The green lines outline the real RVE while the grey lines outline the image RVEs.

gradient  $\tilde{\mathbf{H}} \equiv \nabla_{\mathbf{x}} \tilde{\mathbf{u}}$ , we can then apply this \*RVE\_ANALYSIS\_FEM keyword to perform the RVE localization analysis (also called de-homogenization analysis) to evaluate the actual micro-scale material responses, including the evolution and distribution of microscopic stress/strain fields within the heterogeneous RVE. These detailed microscale material responses are available in the standard LS-DYNA output files (e.g., d3plot). The multiscale simulation can provide useful guidance to both microscopic material design and macroscopic structural analysis.

11. **Image RVE.** The RVE feature in LS-DYNA generally imposes periodic boundary conditions on the RVE boundary but does not impose periodic contact constraints. For some special RVEs, such as textile RVEs, no matrix exists and the yarns in the RVE tend to untangle from other yarns during deformation. To resolve this issue, we developed the image RVE feature. When IMAGE is non-zero, image RVEs are generated automatically in the specified directions. The motion of the image RVE will follow the motion of the real RVE but with an offset distance (equal to the displacement of the control nodes in the specified direction). Specifically, the offset is defined as

$$u_J = u_R + \alpha u_c ,$$

where  $u_I$  is the displacement of the nodes in the image RVE,  $u_R$  is the displacement of the nodes in the real RVE,  $u_C$  is the displacement of the control nodes in a certain direction, and  $\alpha$  is the coefficient relating the position of the image RVE. The value of  $\alpha$  will be 1 or -1. The following figure gives an example of a real RVE (outlined with green lines) and image RVEs in both the  $y$  and  $z$  directions (outlined with grey lines).

## Example:

## Main RVE input.k:

## Mesh\_RVE.k:

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$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ * The finite element mesh represents the composite material micro-structures.
$ * For 3D models, this file should contain keywords *ELEMENT_SOLID & *NODE
$ * For 2D models, this file should contain keywords *ELEMENT_SHELL & *NODE
$ * Only a reduced input is given below
$  
*KEYWORD  
$  
*NODE  
...  
  
*ELEMENT_SOLID  
...  
  
$  
*END  
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
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