Representative Volume Element (RVE) analysis using LS-DYNA

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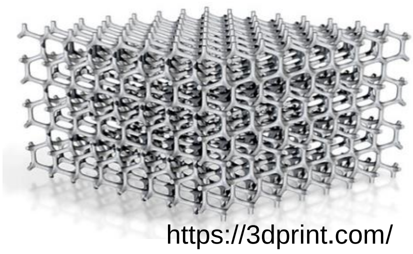
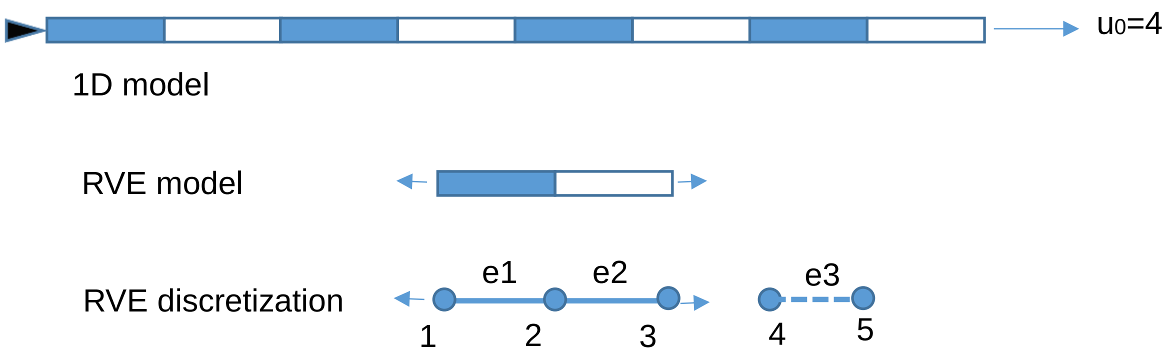
With the emerging of new materials and novel manufacturing techniques, periodic structures in different scales are increasingly important in the real application, for example, battery arrays in cars, sub-scale structures in 3D printing products and all kinds of microstructures in material design analyses shown in the following pictures.

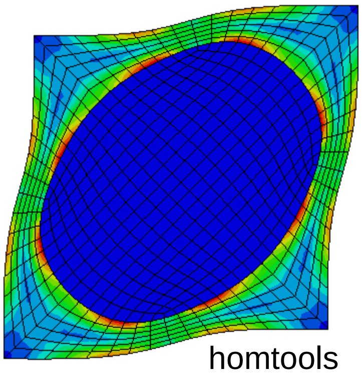


In the numerical simulation, it is very expensive to model the whole structure with a decent resolution for capturing fine details. For instance, when studying microstructure response under the macro level loading, the mesh size in the fine scale is orders of magnitude smaller than that of the macro structure. By introducing the assumption of periodicity, the large scale model can be simplified by RVE (Representative Volume Element) with periodic boundary conditions (PBC). In LS-DYNA, these PBC equations can be defined through *CONSTRAINED_MULTIPLE_GLOBAL. This short paper will focus on its use in RVE analysis and another keyword *INCLUDE_UNITCELL that simplifies the procedure of PBC definition。

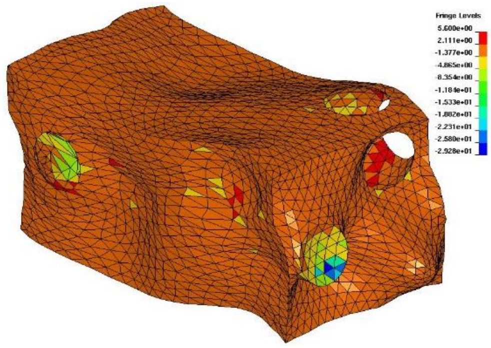
First, let’s talk about PBC equations using the following 1D model.



In this model, the left end is fixed and a prescribed displacement is imposed on the right end. By introducing periodic assumption and element discretization, we obtain the FEM model with 3 nodes and two elements. The corresponding PBC is u_3-u_1=u_4, where the node 4 is the control point. It is required by *CONSTRAINED_MULTIPLE_GLOBAL to define PBC by only nodal IDs and the coefficients. Since the node 4 is involved in PBC, we have to define a control element e3 with much higher stiffness and prescribe the displacement on the node 5 to indirectly impose the prescribed displacement boundary on RVE. You may have a question why not to define the conditions in a simple way like u_1=0， u_3=1. This works in 1D but generally not in 2D and 3D. In the following figures, we can see that the deformation along RVE boundaries is not homogeneous so that we have to define PBC equations to enforce periodicity along with prescribed loading conditions.



homtools



The PBC equation u_3-u_1-u_4=0 can be defined as follows:

*CONSTRAINED_MULTIPLE_GLOBAL

1	Group ID of PBC equations
3	The number of nodes in the current PBC equation
1 1 -1 3 1 1 4 1 -1	In every line, we need to list the nodal ID, the degree of freedom (DOF, 1:x; 2:y; 3:z), and the corresponding coefficient

Here are two remarks：

(1) Multiple PBC equations in the same degree of freedom should be defined under the same group ID. For example, all PBC equations in x direction are defined in the keyword *CONSTRAINED_MULTIPLE_GLOBAL using group ID 1.

(2) LS-DYNA supports user-define element type, where there can be more than 3 nodal DOFs. In this case, the DOF of RVE nodes in PBC definition should be -(i-3), where i is the global one. The control nodes are usually standard with only three DOFs in 3D. We

recommend to define unique control node for the PBC equation on every global DOF. For example, when using standard solid elements in RVE, we define three control nodes for PBC equations in x, y and z directions, respectively; when using user-defined element type with 7 nodal DOFs, we define 7 control nodes accordingly.

In practice, RVE often contains large number of elements and nodes for modeling the fine details of microstructure. For example, a RVE in material design analysis may have 100x100x100 elements where the number of PBC equations is more than 10 thousand. We developed the keyword *INCLUDE_UNITCELL to automatically define PBC equations in LS-DYNA:

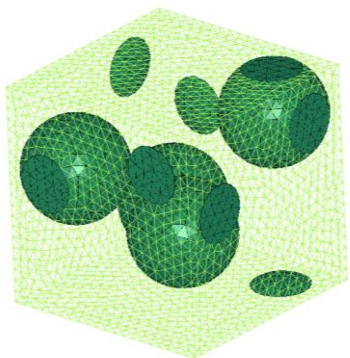
(1) Prepare the RVE mesh in a separated keyword file, e.g. mesh.k

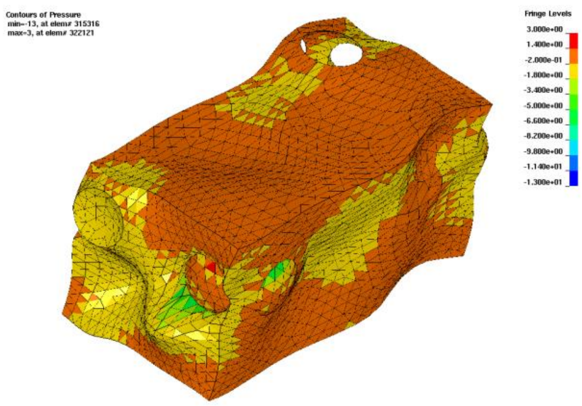
(2) Include mesh.k through *INCLUDE_UNITCELL in the main keyword file

(3) Define the control nodes starting from card 5 in *INCLUDE_UNITCELL

(4) Run LS-DYNA to generate a new include file, called uc_mesh.k, where all the PBC equations are automatically defined using *CONSTRAINED_MULTIPLE_GLOBAL

Here is an example of particle-reinforced rubber design analysis. The left figure below shows the demo model, where the matrix is rubber material and the spherical parts are the inclusions with much higher stiffness. By imposing PBC and prescribed displacement field, the rubber matrix deforms severely shown in the right figure below, where there is strong stress concentration near the interface between the matrix and inclusions. Based on the periodic assumption, the force-displacement result using RVE can well represent the material behavior and be applied to structure analysis in macro scale.





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