Multiscale Simulation of Short-Fiber-Reinforced Composites: From Computational Homogenization to Mechanistic Machine Learning in LS-DYNA

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1 Introduction

Injection-molded short-fiber-reinforced composites (SFRC) have been widely used for structural applications in automotive and electronics industries. Due to the heterogeneous microstructures across different length scales, the nonlinear anisotropic behaviors of SFRC are very challenging to model. Therefore, an effective multiscale approach that links the local microscopic properties (e.g., fiber orientation, fiber volume fraction) to the global behaviors is required. To this end, multiscale analysis functions are recently developed in the engineering simulation software LS-DYNA to enable high-fidelity micromechanical finite element analysis, mechanistic machine learning-based reduced-order modeling, and accelerated concurrent multiscale simulation of SFRC composite structures.

In this paper, we will firstly introduce the LS-DYNA RVE (Representative Volume Element) analysis module [1], which employs the FEM-based computational homogenization technique to predict high-fidelity microscopic stress/strain fields within the composite microstructures and averaged macroscopic constitutive responses. In addition, we will introduce a mechanistic machine learning technique referred to as Deep Material Network (DMN) [2,3,4]. Based on DMN, a highly accurate and efficient concurrent multiscale simulation framework is being developed in LS-DYNA to simulate injection-molded SFRC structures where microstructural distributions predicted by Moldex3D are imported into LS-DYNA through the LS-PrePost mapping function.

2 RVE-based Multiscale Virtual Testing of Materials

Constitutive models, especially those for nonlinear anisotropic materials, often involve many parameters, for which the parameter calibration requires a number of material data. Measuring these data from a series of physical experiments is quite time-consuming and expensive. These physical experiments, however, can be easily replaced by more cost-saving Representative Volume Element (RVE) analysis, which provides a rigorous numerical means to obtain homogenized macroscopic material properties at the upper length scale from the properties of the material constituents and structures at a lower length scale.

Recently, an RVE module (keyword: **`*RVE_ANALYSIS_FEM`**) is released in the multiphysics simulation software LS-DYNA to enable high-fidelity virtual testing of numerically re-constructed material samples at user-specified characteristic length scales. Given the material microstructural information (geometry and constitutive properties for base materials), this new feature enables LS-DYNA to perform high-fidelity RVE analysis in an efficient manner, and it includes the following functions:

1) Creation of periodic displacement boundary conditions (or linear displacement boundary conditions) automatically;
2) Nonlinear implicit finite element analysis of RVE under any loading conditions;
3) Calculation of the detailed distribution and evolution of microscopic stress/strain fields in the RVE;
4) Homogenization of the RVE's microscopic material responses to yield the macroscopic effective material responses.

2.1 Workflow for RVE Analysis

To prepare the input deck for RVE analysis in LS-DYNA R13, the following procedure and associated keywords can be considered:

Step 1. RVE Construction (**`*SECTION_xxx`**, **`*PART`**, **`*ELEMENT_xxx`**, **`*NODE`**):

a) define the microstructural geometry
b) generate finite element mesh

Step 2. Microscopic Material Model (**`*MAT_xxx`**):

a) define the constitutive model for each material constituent
b) provide the corresponding material constants

Step 3. Boundary Condition (**`*RVE_ANALYSIS_FEM`**, **`*DEFINE_CURVE`**, **`*CONTROL_TERMINATION`**):

a) choose the linear or periodic displacement boundary condition
b) define the loading history with a macroscopic displacement gradient

Step 4. Output Control (**`*DATABASE_RVE`**, **`*DATABASE_BINARY_D3PLOT`**):

a) define the output frequency for the d3plot file
b) define the output frequency for the rveout file

Step 5. Implicit Solver (**`*CONTROL_IMPLICIT_GENERAL`**, **`*CONTROL_IMPLICIT_AUTO`**, **`*CONTROL_IMPLICIT_SOLUTION`**, **`*CONTROL_IMPLICIT_SOLVER`**, *etc.*):

a) choose a direct or iterative solver
b) define the implicit solver parameters

After the input deck is prepared, the RVE analysis job can be submitted in the same way as other standard SMP/MPP LS-DYNA simulations. When the simulation is finished, 'd3plot' files will be generated, which contain the microscopic stress/deformation fields of the RVE, and these data can be visualized directly in the LS-PrePost software. Meanwhile, an 'rveout' file containing time histories of homogenized macroscopic stress/deformation fields is also created, and this file can be opened by any text editors.

2.2 Application of RVE Analysis

The RVE module is applicable to various types of materials, e.g., fiber/particle-reinforced polymers, metallic alloys, laminar composites, etc. In the following, let us consider a 3D RVE model for short-fiber-reinforced composites (SFRC).

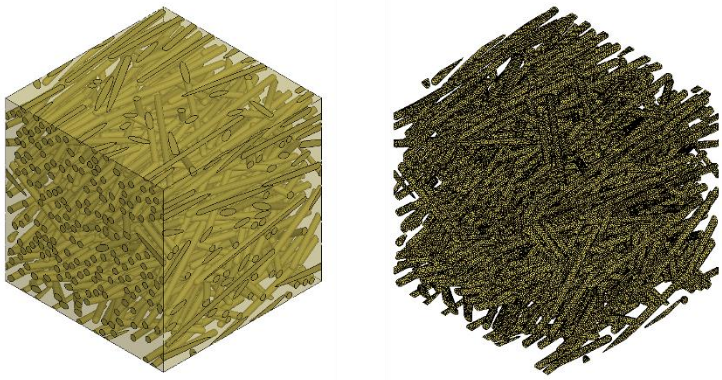


Fig.1: An RVE model for short-fiber-reinforced composites (SFRC). A finite element mesh for the matrix phase is also generated but not plotted here.

As shown in Figure 1, we can construct a 3D finite element model that represents the SFRC microstructure (i.e., fiber orientation, volume fraction, etc) of interest to our engineering applications. Next, we can simply follow the procedure listed in Section 2.1 to prepare the complete input deck. In this example, we choose to impose a periodic displacement boundary condition which represents a macroscopic uniaxial compression in the X-axis direction, and we assign elastic and elastoplastic constitutive laws to the fiber phase and matrix phase, respectively. The nonlinear 3D RVE model contains approx. 20 million displacement degrees-of-freedom (DOFs), so an iterative solver is chosen for its attractive efficiency in the implicit finite element computation.

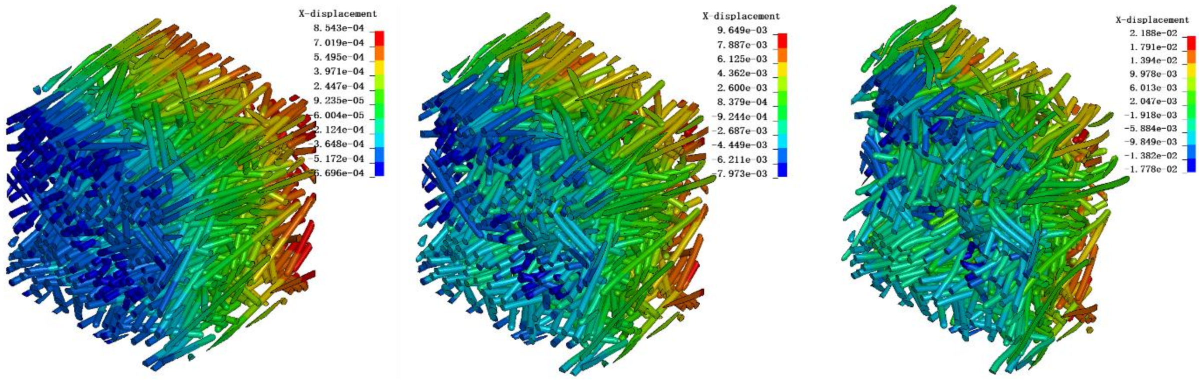


Fig.2: RVE simulation results for short-fiber-reinforced composites (SFRC). The fibers' x-direction displacement field is shown at different loading steps, where a displacement scale factor of 10 is used for plotting.

The double precision MPP R13 version LS-DYNA is adopted for the simulation, and after the finite element simulation is finished, we can open the d3plot file in LS-PrePost to check the microscopic stress and deformation. As expected, the overall RVE model experiences a uniaxial compressive deformation macroscopically (see Figure 2), while the microscopic deformation field is non-uniform within the RVE due to the heterogeneity of the short fiber distributions. Meanwhile, material nonlinearities are well captured in the RVE simulation, and the distributions of effective plastic strain and von Mises stress fields are plotted in Figure 3.

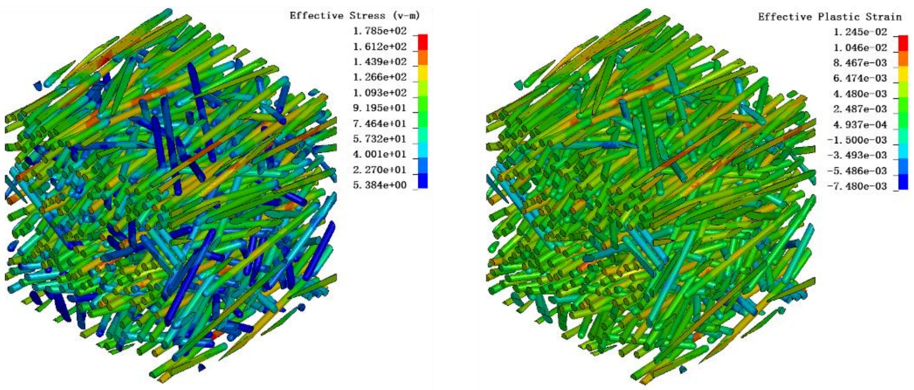


Fig.3: RVE simulation results for short-fiber-reinforced composites (SFRC). The fibers' von Mises stress and effective plastic strain fields are shown, where a displacement scale factor of 1 is used for plotting.

In addition, the homogenized macroscopic stress/strain results are available in the rveout file. By performing homogenization of properly designed material samples, RVE models can accurately predict the macro-scale material behaviors, which can then be adopted to identify the material parameters of the assumed constitutive model as illustrated in Figure 4.

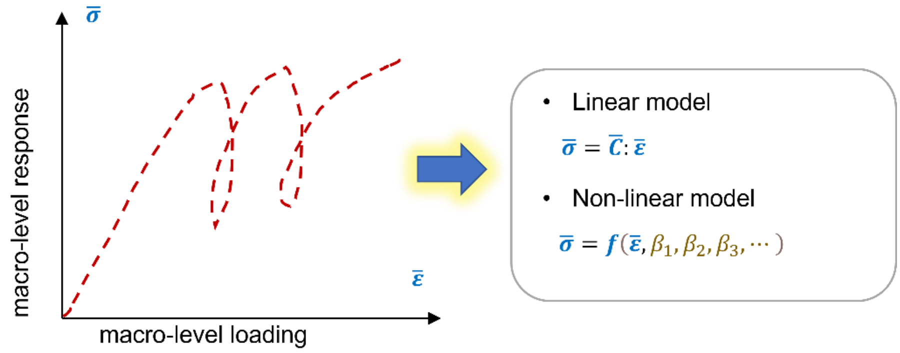


Fig.4: Constitutive model parameter calibration based on virtual material testing via RVE analysis.

3 DMN-based Concurrent Multiscale Simulation of SFRC Structures

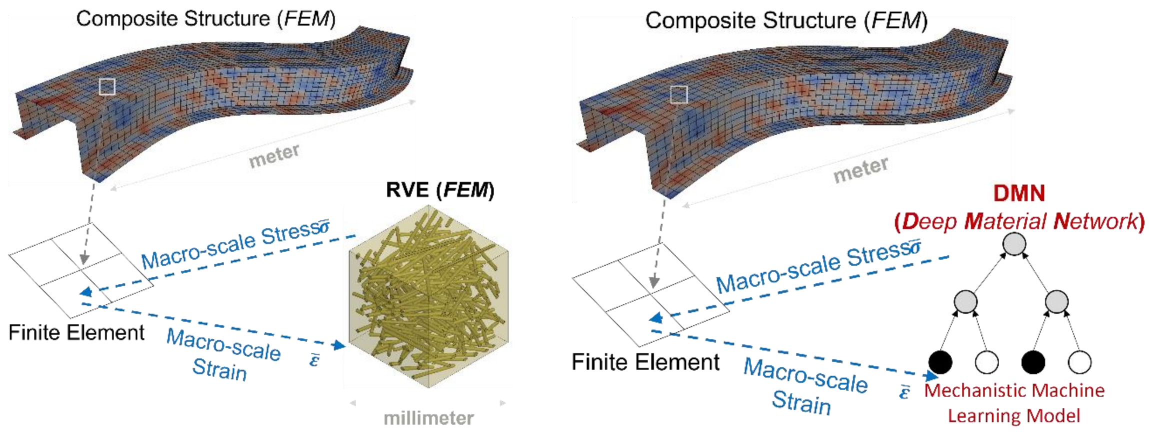
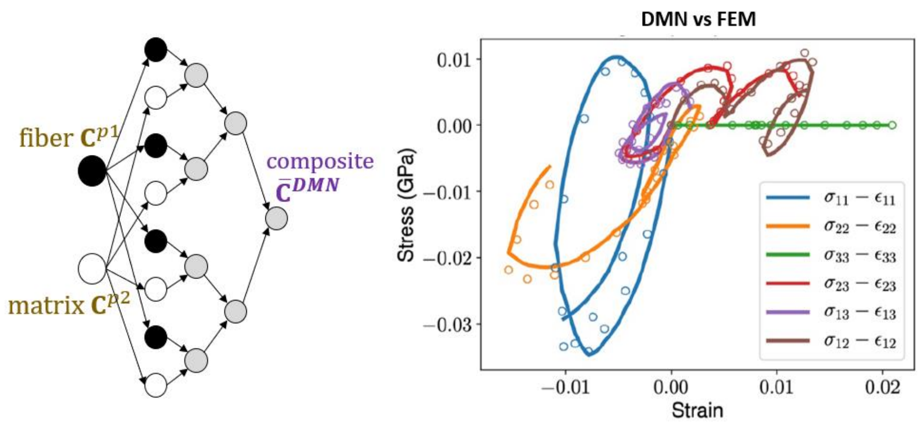


Fig.5: Concurrent multiscale simulation methods: the conventional FEM-based framework (left) vs. the DMN-based framework (right).

In a concurrent multiscale structural simulation, every material point (i.e., integration point) in a macroscale FE model is coupled with a microscopic RVE that corresponds to the local material microstructure. Instead of assuming any macroscopic constitutive law, the RVE model naturally provides the macroscopic stress response based on the local material microstructural information (geometry and constitutive properties for base materials), yielding a high-fidelity multiscale finite element model shown in Figure 5. For large-scale structures, however, such high-fidelity multiscale finite element models can consume extremely high CPU time and memory, which is not affordable for industrial applications, especially when material nonlinearities are considered.



Computational time

FEM	1100s on 8 CPUs
DMN	3s on 1 CPU

Fig.6: Comparisons of the stress-strain predictions by DMN and FEM for a short-fiber-reinforced composites (SFRC) RVE model [4]

To save computational costs, reduced-order models of RVEs can be created by employing a mechanistic machine learning technique called Deep Material Network (DMN) [2,3]. DMN can be trained in an offline stage to learn the microscopic material morphologies and physics hidden in linear composite material data (e.g., from linear elastic RVE numerical simulation), and afterwards the trained network is able to conduct online prediction of nonlinear multiscale constitutive behaviors at a computational speed orders-of-magnitude faster than high-fidelity FEM simulations, as shown in Figure 6. Note that the CPU time for FEM in Figure 6 comes from a finite element model containing approximately 1 million DOFs, while finite element models with more DOFs and higher CPU costs are often required for materials with more complicated microstructures. On the other hand, the computation by DMN is always fast for any material microstructures, which enables us to perform highly efficient concurrent multiscale simulations by coupling the trained DMN network to macroscale finite element models [4], as illustrated in Figure 5.

Recently, we have coupled trained DMN to finite element models in LS-DYNA to analyze short-fiber-reinforced composite (SFRC) structures, where microstructure distributions predicted by injection molding simulation (e.g., via Moldex3D) can be imported through the LS-PrePost mapping function. The proposed nonlinear concurrent multiscale simulation workflow is illustrated in Figure 7. This machine learning-based new feature is currently under development and will be released soon in LS-DYNA.

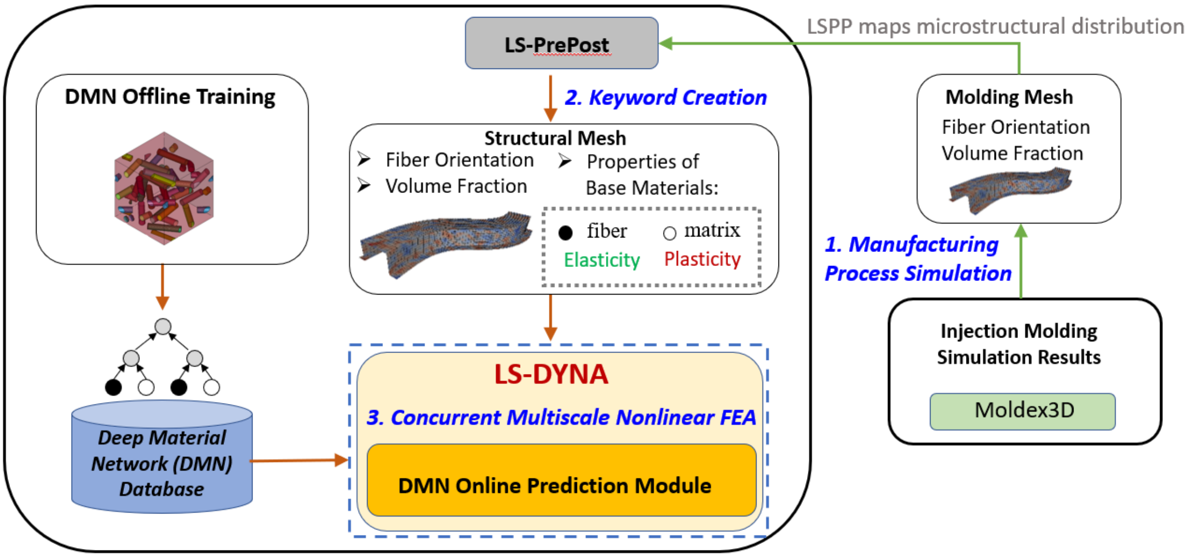


Fig.7: Workflow of the DMN-based nonlinear concurrent multiscale simulation for short-fiber-reinforced composite (SFRC) structures, where microstructural data predicted by Moldex3D are mapped by LS-PrePost onto LS-DYNA finite elements coupled with trained DMN.

4 Summary

In this article, we introduced two advanced techniques for multiscale modelling of short-fiber-reinforced composite (SFRC) materials and structures.

The RVE technique is available in LS-DYNA R13 to predict the macroscopic effective constitutive behaviors of composite materials. This function allows virtual testing of numerically re-constructed material samples, which is of great importance to design and analysis of advanced materials. More details on the RVE theory and input file preparation can be found in [1].

The DMN technique under development in LS-DYNA will be released soon. After the offline training, DMN can accurately predict the macroscopic material responses based on the microscopic material information, and the computation speed is much faster than the corresponding high-fidelity finite element models. Preliminary simulation results for SFRC structures based on this intelligent multiscale simulation technique can be found in [4]. Since this machine learning model is based on both physics and data, its simulation capability can be continuously enhanced as more high-quality training data are supplied.

It is noteworthy to mention that these multiscale methods are not only applicable to SFRC, but can also be adopted to model many other types of materials, such as particle-reinforced composites, laminar composites, polycrystalline metals, porous media, etc.

5 Acknowledgments

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6 Literature

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