Creating Representative Volume Element by LAMMPS for Finite Element Analysis

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Background

- To evaluate the properties of the Representative Volume Element (RVE), highly filled with fillers are often needed.
- However, creating such highly filled structure, e.g., filled around 50 vol.%, by modeling tools for FEM may not be easy.
- By using Molecular Dynamics, It is possible to create these models easily.

Purpose

- How high filling is possible ?
- How to create a target filling rate and target shapes ?

Types of Fiber

Create fiber models using 3 types of filler of different thickness and length.

Fiber Name	Length of Fiber	Radius of Fiber	Num. of Bead	Force Field Parameters for MD			
				LJ sigma	LJ epsilon	Bond (Harmonic)	Angle (Cosine)
A: L10R1.0	10	1.0	10	2.0	1.0	R0=1.0 K=200	Theta0=180 K=10,000
B: L10R0.5	10	0.5	20	1.0	1.0	R0=0.5 K=200	Theta0=180 K=10,000
C: L05R0.5	5	0.5	10	1.0	1.0	R0=0.5 K=200	Theta0=180 K=10,000

L10, R1.0

L10, R0.5

L05, R0.5

A

B

C
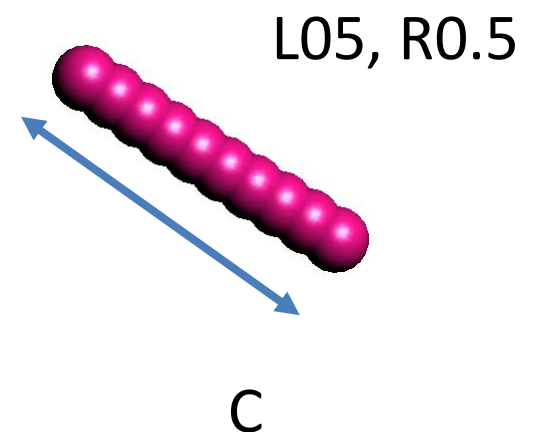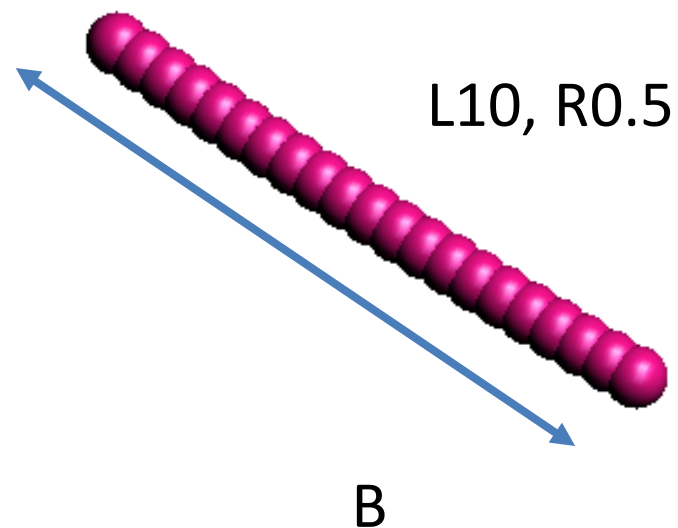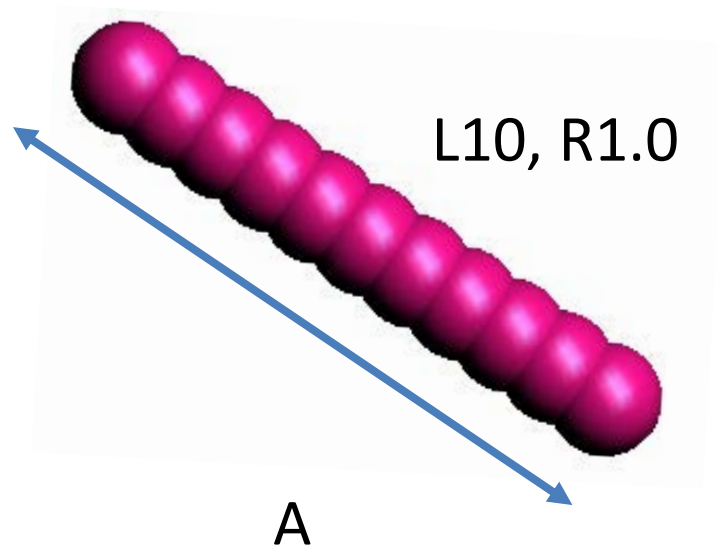
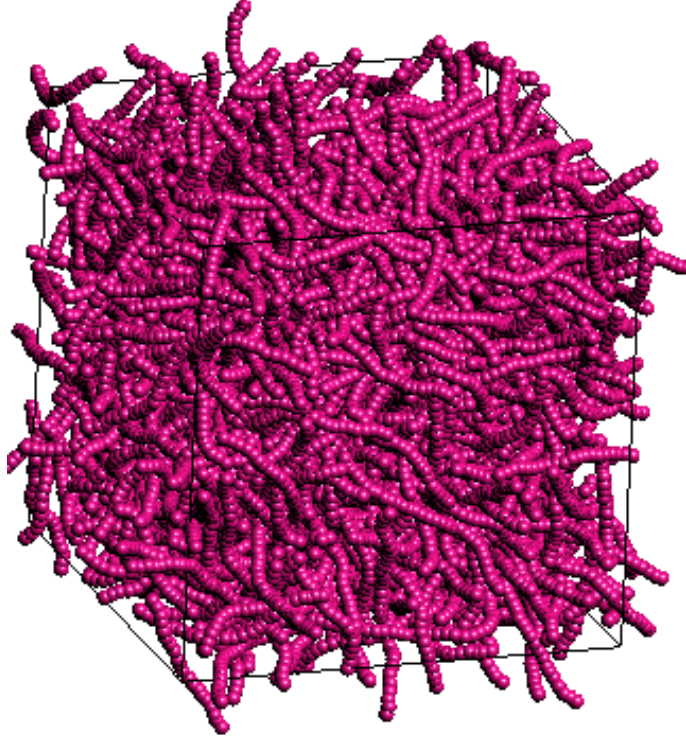# Process to Create RVE Model

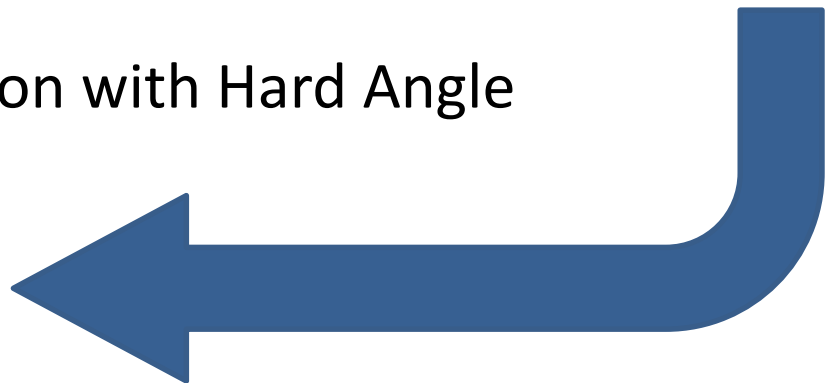**Particle Generation by COGNAC**
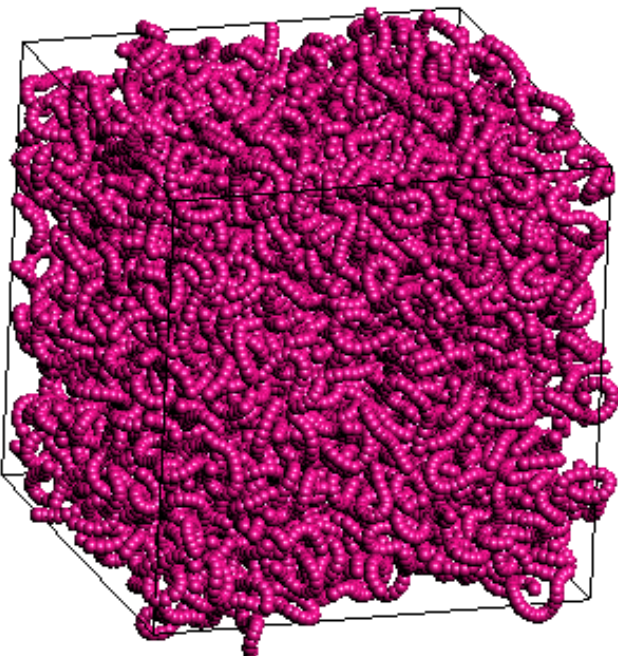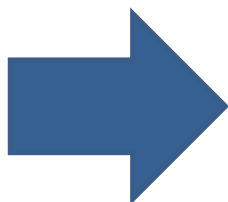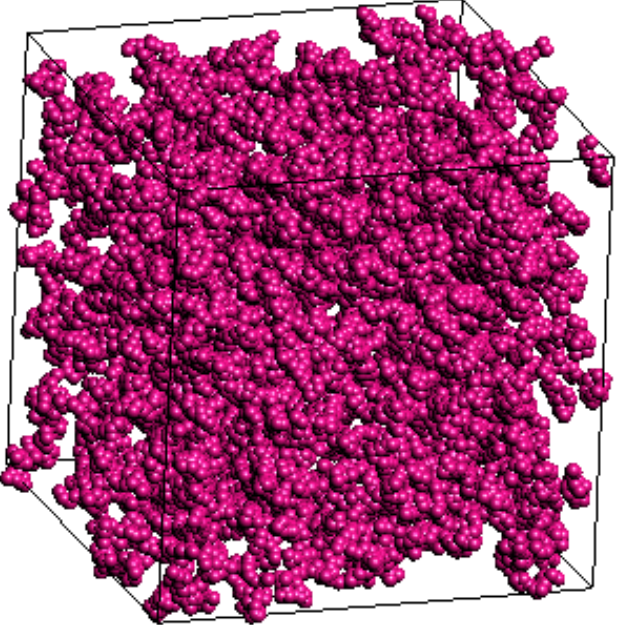
Short Relaxation with Soft Angle

Positioning by Random
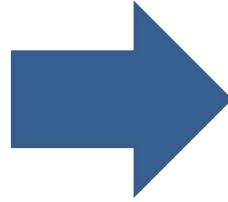
Molecular Dynamics by LAMMPS

Relaxation with Hard Angle
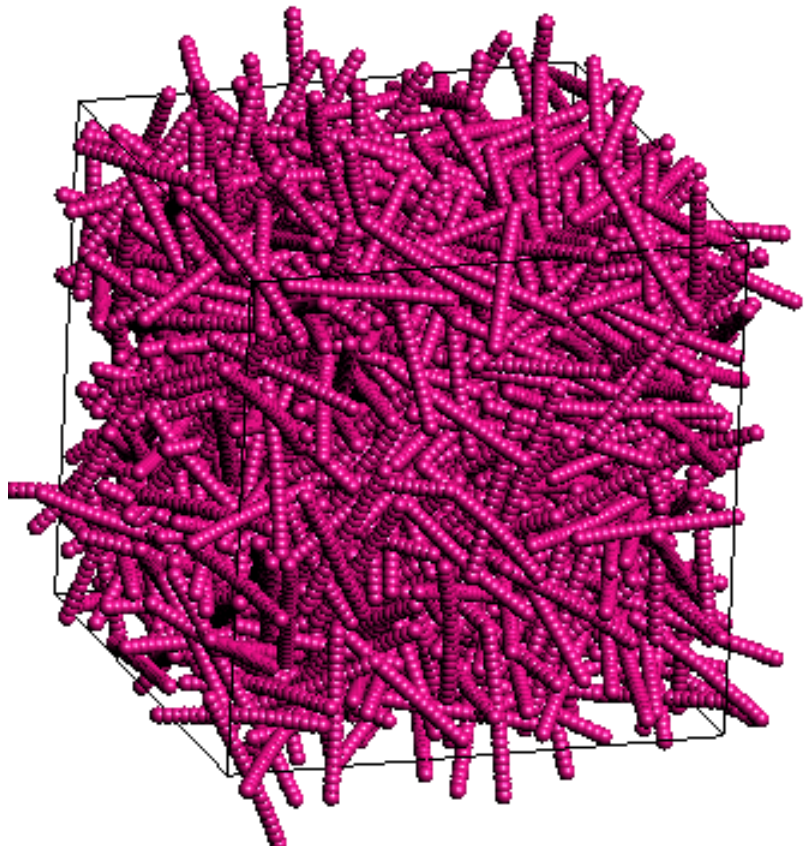
Parameters for MD Calculation

Particle Generation & Short Relaxation	Cognac (OCTA)
Delta Time	0.006
Total Step	10,000
Temperature	1.0
Angle Potential	K=500 (Soft)
Calculation Time	1 ~ 15 [min]

| Molecular Dynamics	LAMMPS
Delta Time	0.001
Total Step	500,000
Temperature	1.0e-3
Angle Potential	K=10000 (Hard)
Calculation Time	3 ~ 50 [min]

・Angle Potential
To keep a linear shape of fiber, it is necessary to set a large value as a spring constant of the angle potential.

・Temperature
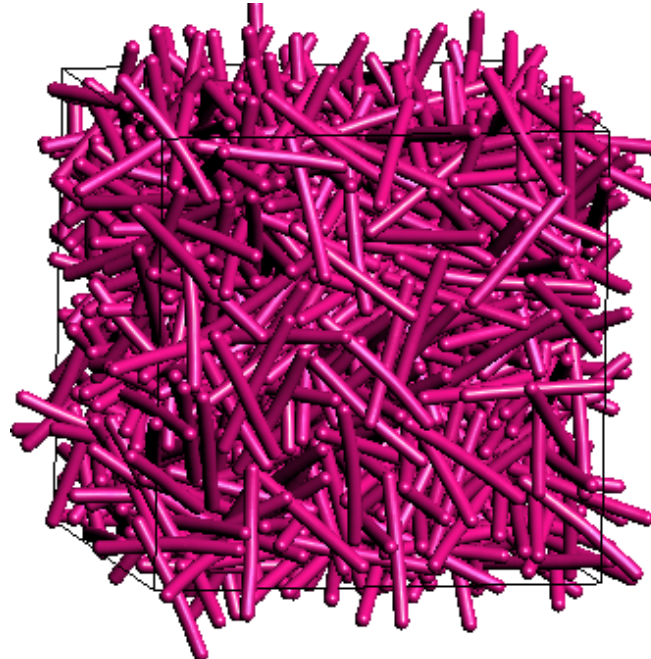To keep linear shape of fiber, temperature is also important. Sometimes it is effective to lower temperature.

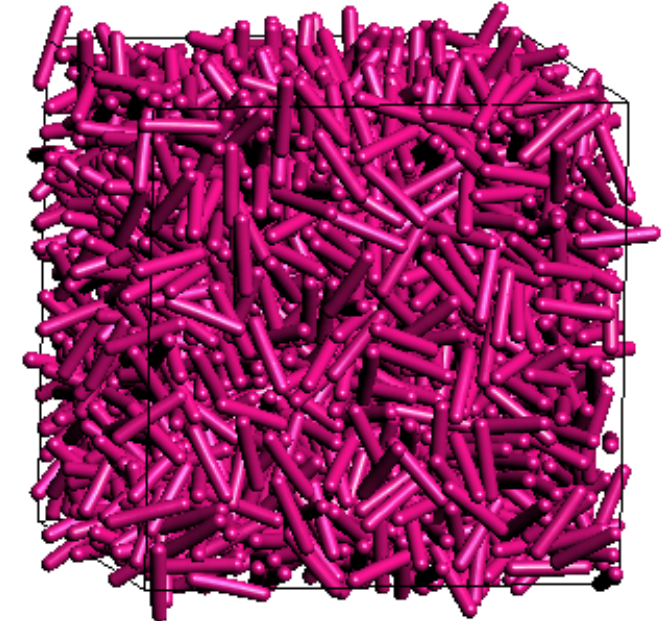# Fiber Shapes of MD Results

System Size	30 x 30 x 30
Volume	27,000

VF = 0.291
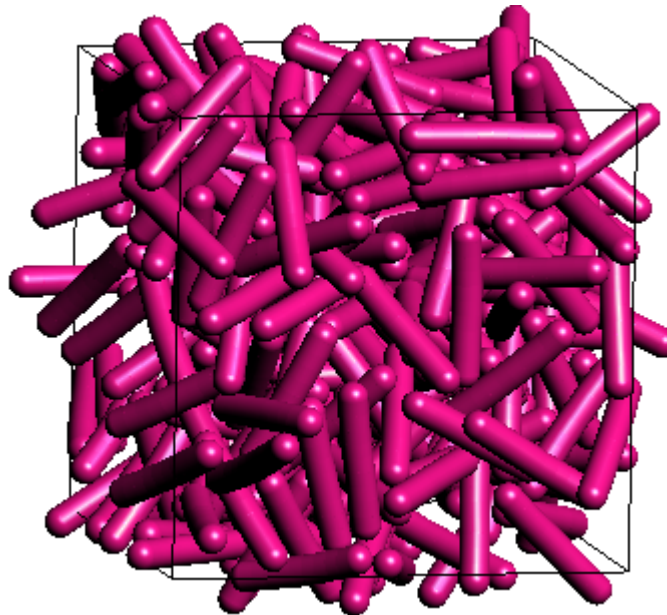
A: L10R1.0 x 250
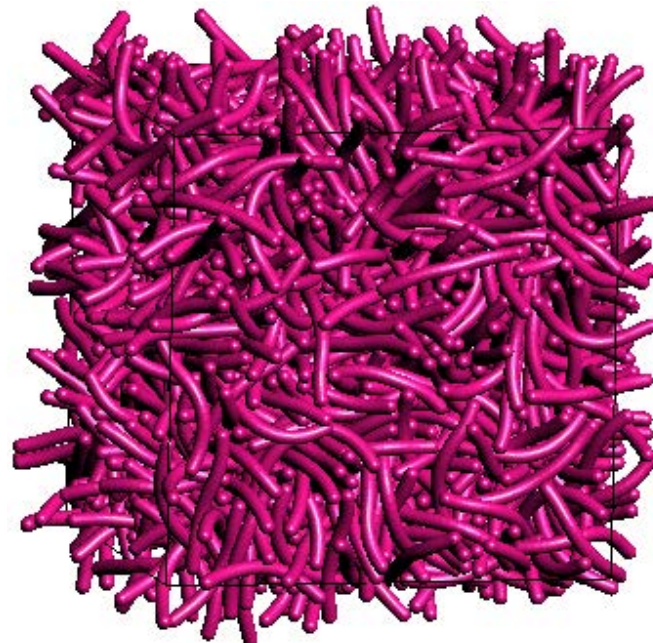
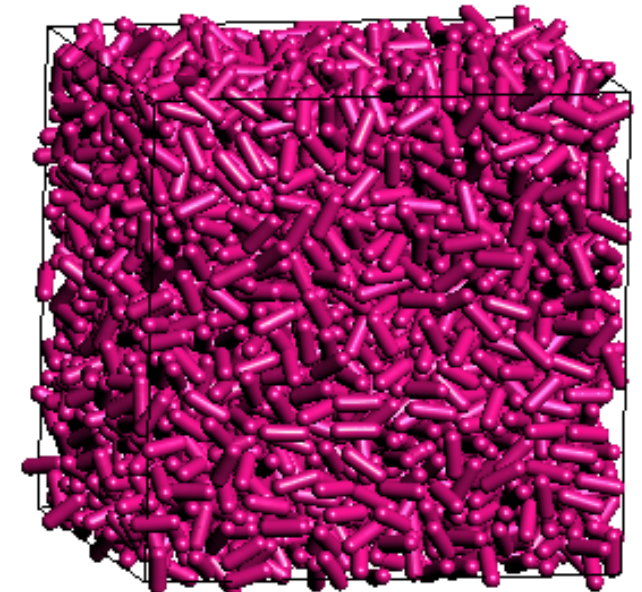**B: L10R0.5 x 1000**

C: L05R0.5 x 2000

VF = 0.523
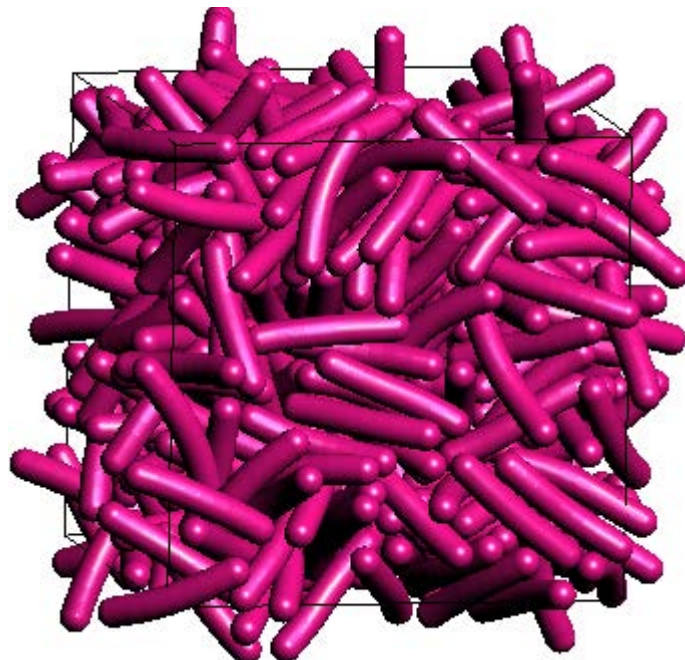
A: L10R1.0 x 450

B: L10R0.5 x 1800
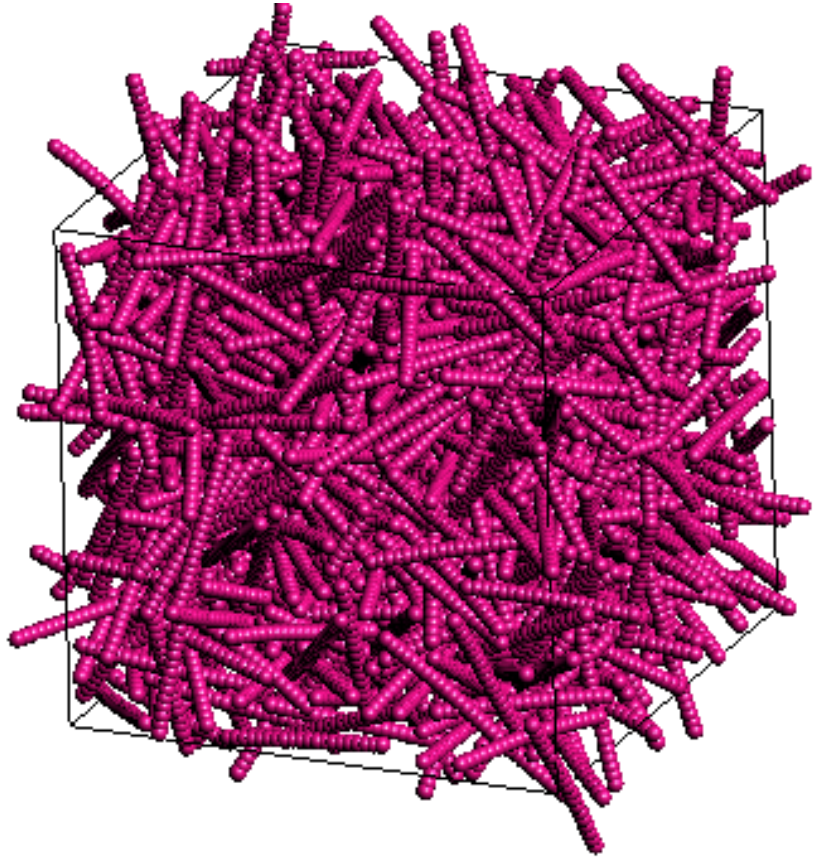
C: L05R0.5 x 3600

If lowly filled, the fiber shape is kept linear even if length=10.

If highly filled, it is difficult to keep fiber shape. If length=5, the shapes can be kept.
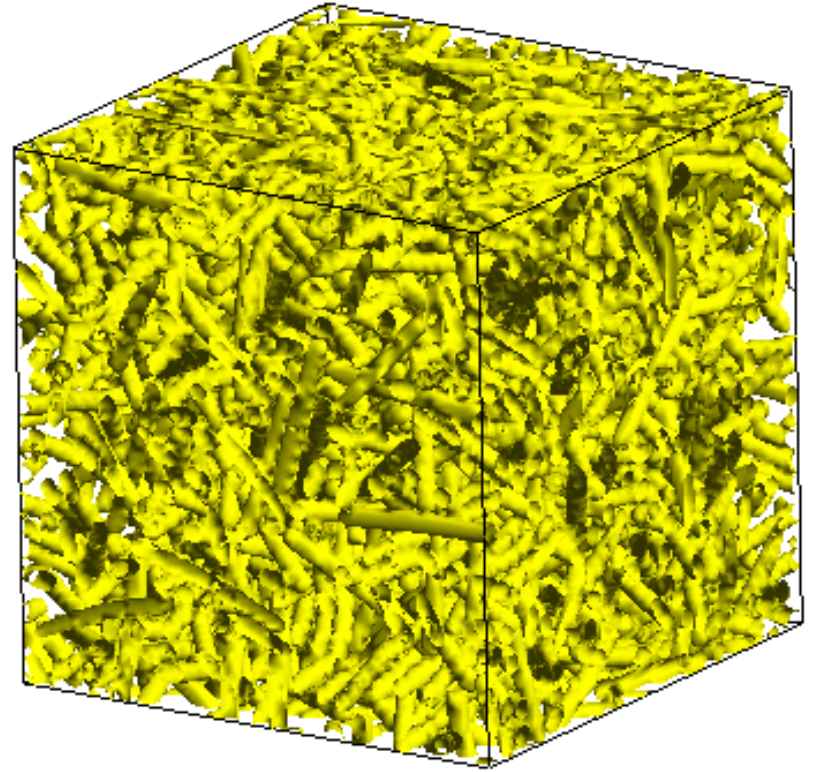
(In this model, even if highly filled and length=10, the shape can be kept by calculating for a longer time at higher temperature.)

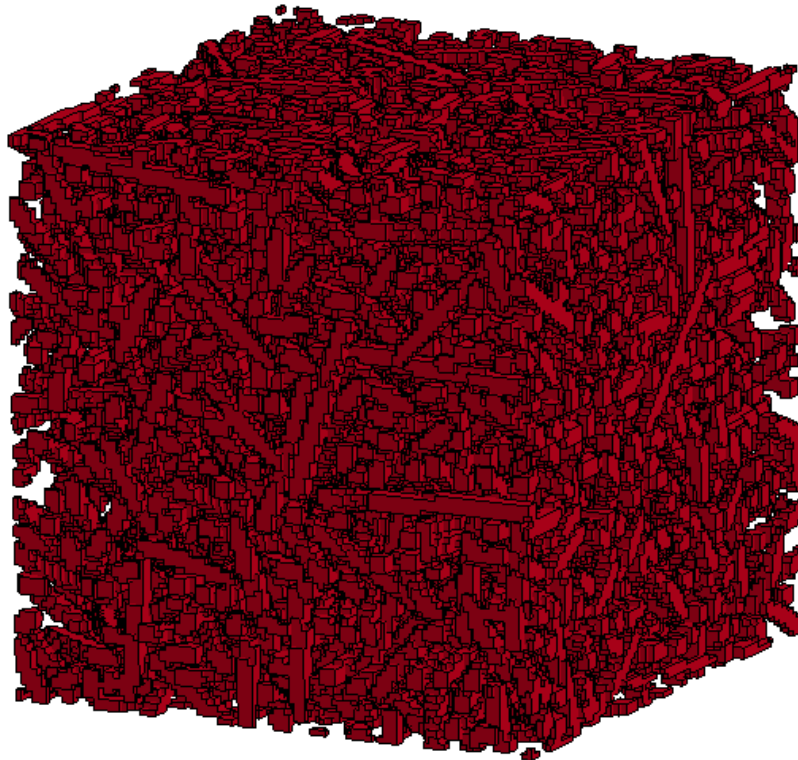Results of LAMMPS

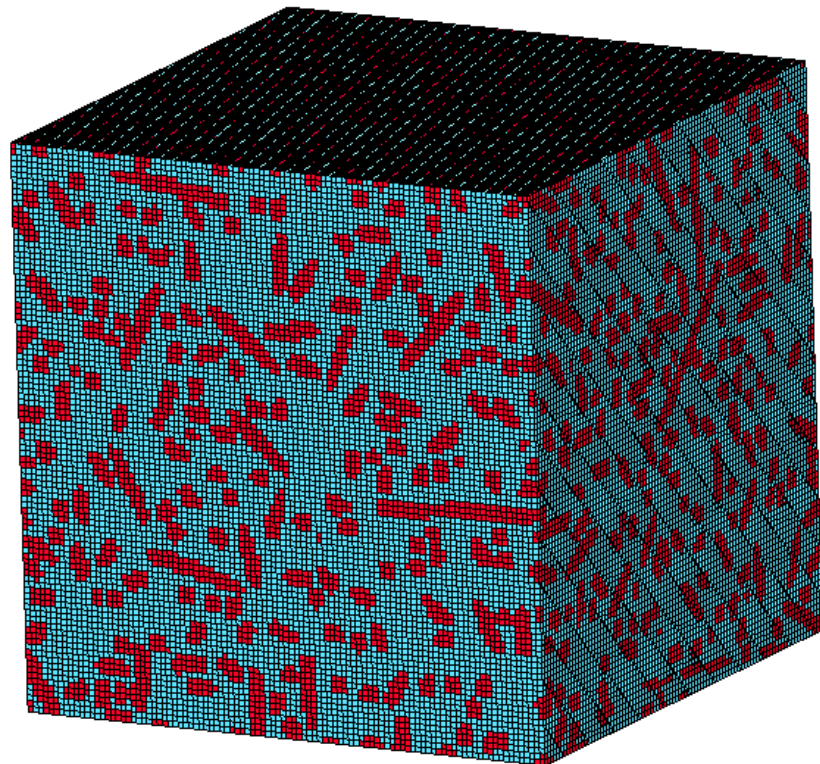Creating Mesh Model for FEM

Getting Densities by COGNAC

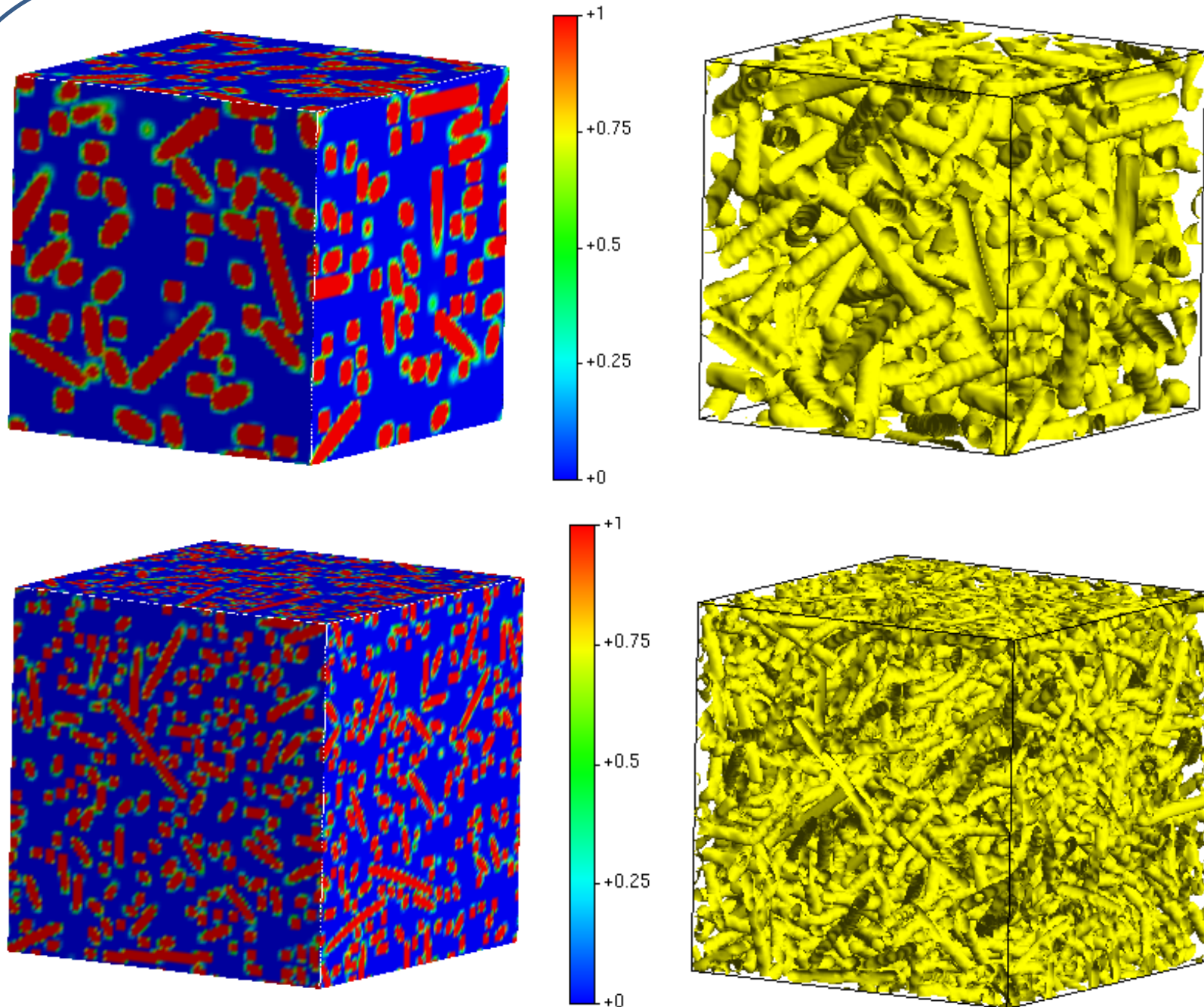Surface of Fiber

Voxel Meshing by J-OCTA

Voxel Mesh Model for FEM

Target Volume Fraction : 29 %
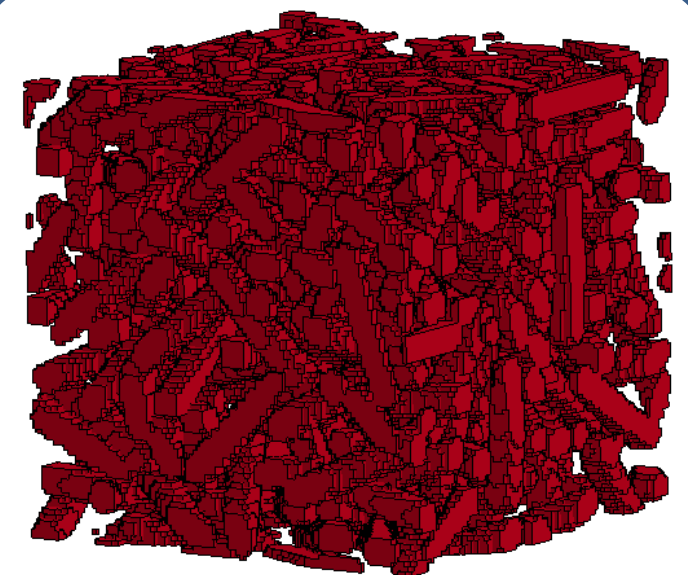
Density Field (Red: Fiber, Blue: Void)
& Surface of Filer (Isosurface value = 0.5)
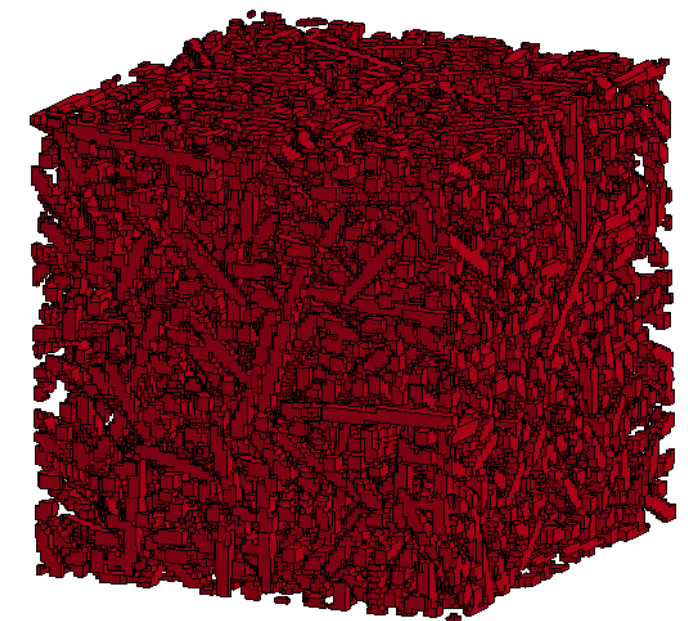Num. of Grid for getting density = 1,000,000

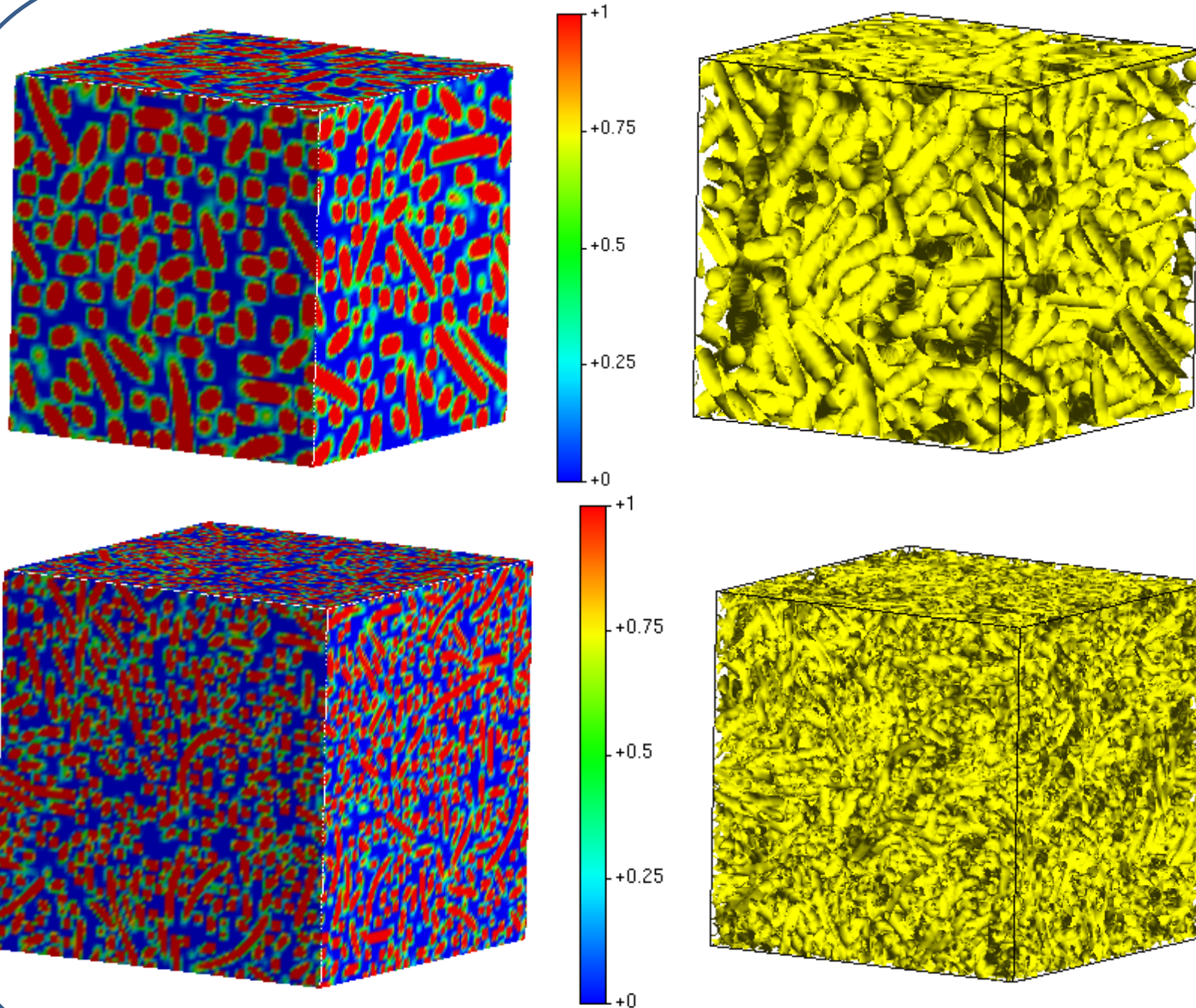Voxel Mesh for FEM
Num. of Mesh = 1,000,000

VF = 31.6%

VF = 30.9%

Target Volume Fraction : 52 %

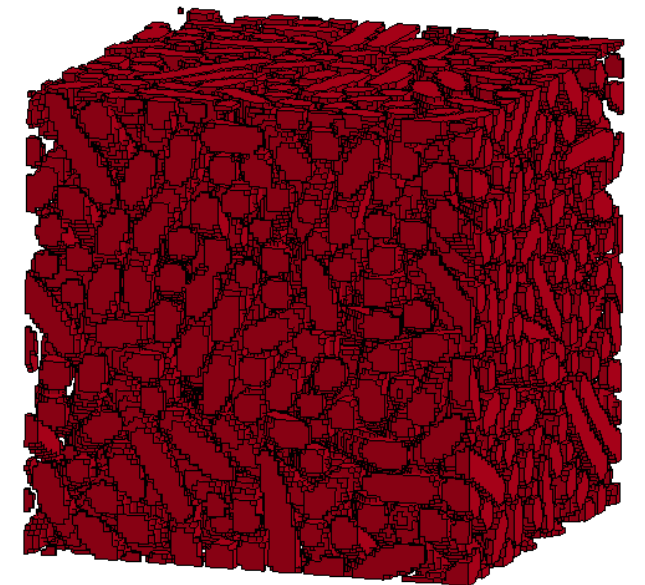Density Field (Red: Fiber, Blue: Void)
& Surface of Filer (Isosurface value = 0.5)
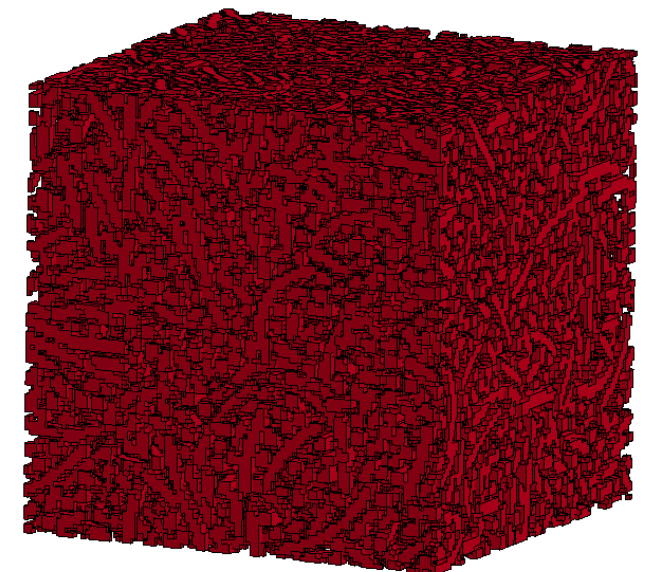Num. of Grid for getting density = 1,000,000

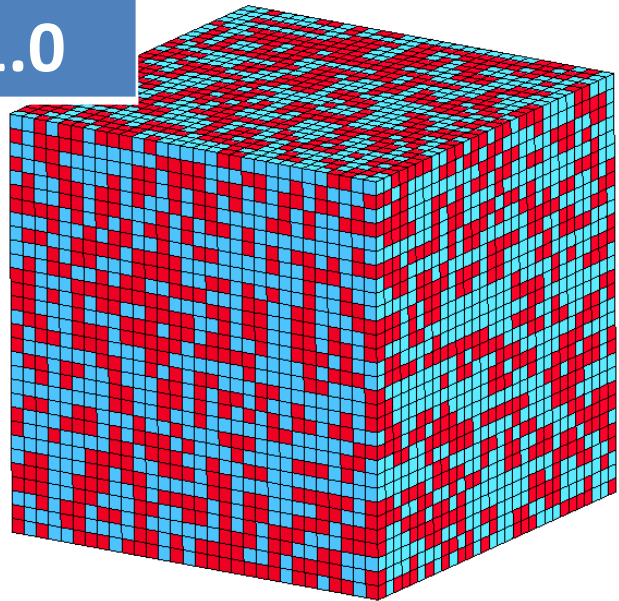Voxel Mesh for FEM
Num. of Mesh = 1,000,000

VF = 47.3%

VF = 46.2%

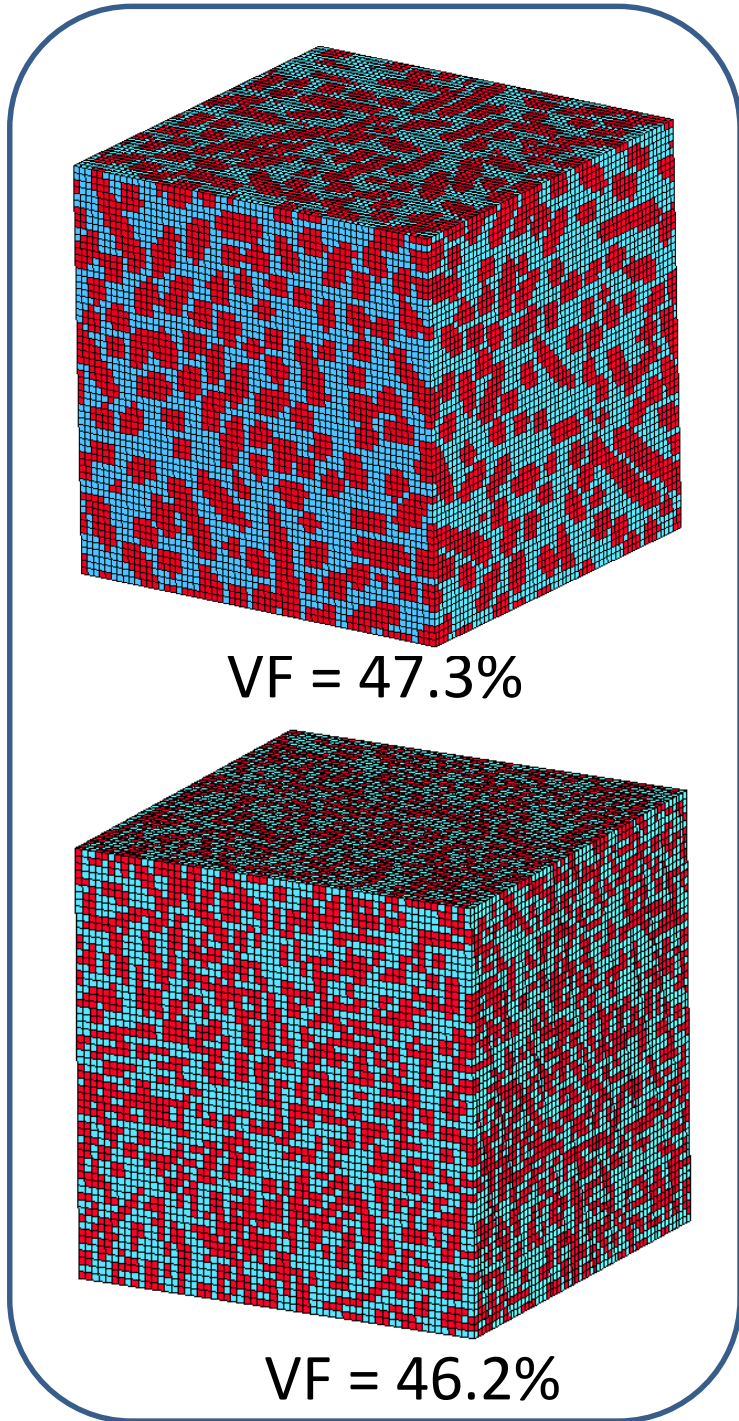# Effect of Number of Meshes (Target VF = 52.3%)

* Red: Fiber, Blue: void

	Num. of Mesh = 27,000 (30 x 30 x 30)	Num. of Mesh = 216,000 (60 x 60 x 60)	Num. of Mesh = 1,000,000 (100 x 100 x 100)

Rad = 1.0

VF = 47.5%   VF = 47.3%   VF = 47.3%

Rad = 0.5

NG

VF = 94.9%   VF = 46.2%   VF = 46.2%
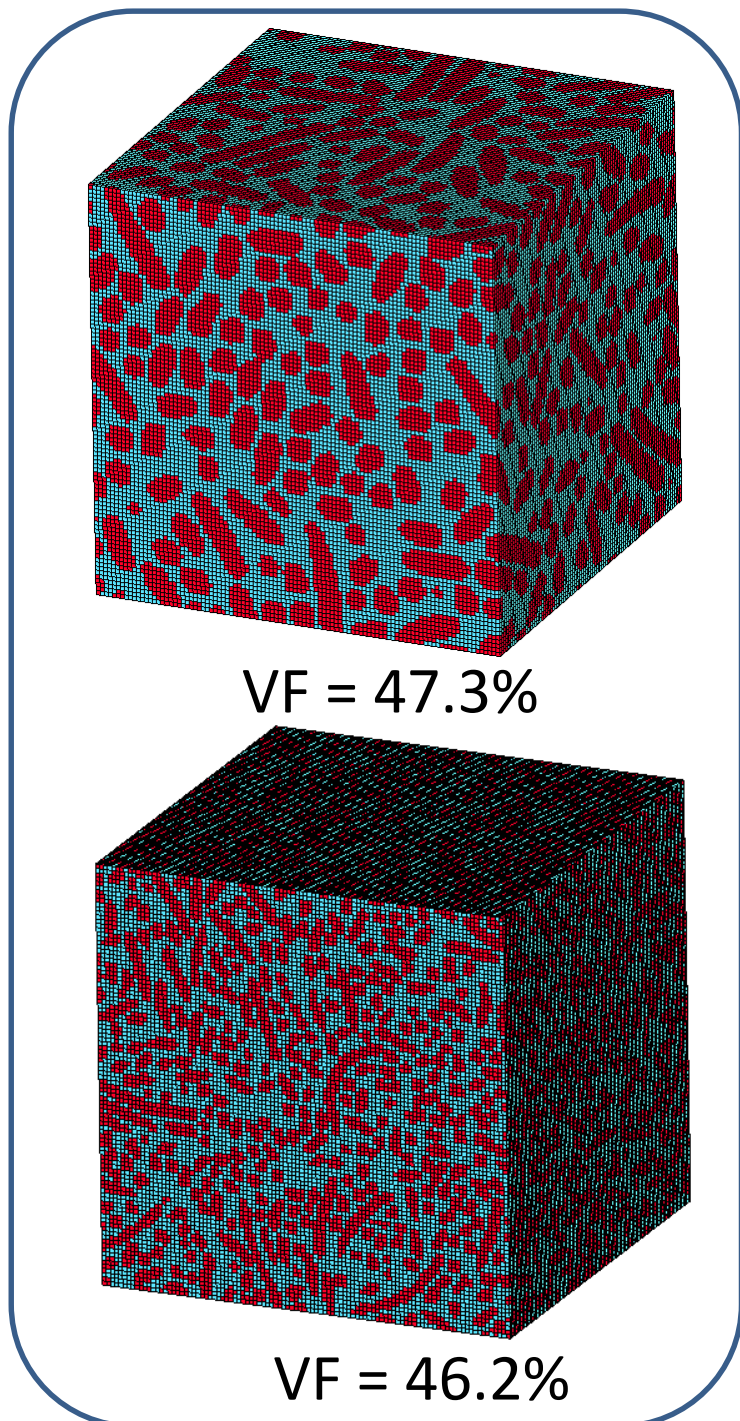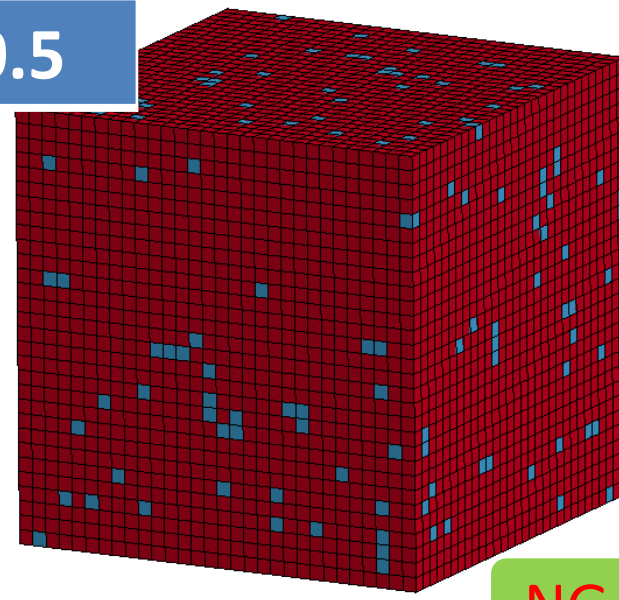
When the number of meshes is small, the fiber connection may not be expressed.
When Rad = 0.5, at least, mesh number of at least 60 (1 mesh size = 0.5) on a side is required.

Summary

1. By using molecular dynamics,
   the highly filled structure models could be created easily.

2. There are a few notes,
   - ✓ Key Parameters for MD
     - Potential Parameters of Angle
     - Temperature and Delta Time
   - ✓ Number of Meshes
     The number of meshes that can express the particle radius (fiber radius) is required.

3. Future work
   In case of highly filled, the accuracy of density distribution is important.
   The method for getting more accurate density distribution and grid size will be investigated.

Reference
[1] http://octa.jp
[2] http://www.j-octa.com