Periodic Boundary Conditions for 3D Representative Volume Element Models: Theory and Implementation in WARP3D

Robert H. Dodds, Jr., PhD, NAE

University of Illinois at Urbana-Champaign

cee.illinois.edu/directory/profile/rdodds

rhdodds@gmail.com

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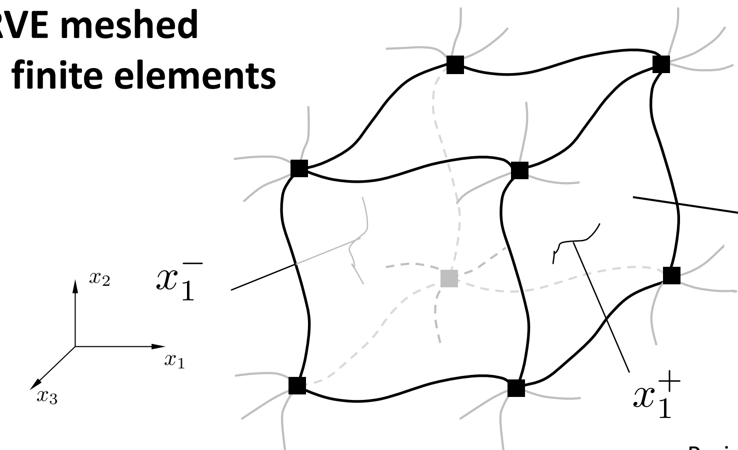
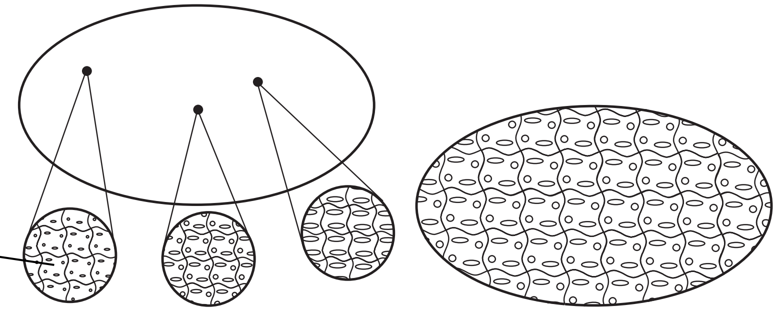
WARP3D input files available upon request

RVEs and PBCs

3D RVE meshed with finite elements





(a) (b)

$\bar{\varepsilon}_{ik}$ **Strain tensor computed for example at integration points of the macroscale finite element model**

u_i^* **Periodic part of the total displacement field. Must be identical at matching points (node pairs) on (+,-) surfaces, *e.g.*, (+,-) x faces as marked**

$$u_i\left(x_1,x_2,x_3\right)=\bar{\varepsilon}_{ik}\,x_k+\underbrace{u_i^*\left(x_1,x_2,x_3\right)}_{\text{Periodic part}},\quad i,k=1,2,3$$

$$u_i^{j+}=\bar{\varepsilon}_{ik}\,x_k^{j+}+u_i^*$$
$$u_i^{j-}=\bar{\varepsilon}_{ik}\,x_k^{j-}+u_i^*$$

$$u_i^{j+}-u_i^{j-}=\bar{\varepsilon}_{ik}\left(x_k^{j+}-x_k^{j-}\right)=\bar{\varepsilon}_{ik}\Delta x_k^j$$

$$\text{A}\quad\begin{cases}u_1^{j+}-u_1^{j-}=\bar{\varepsilon}_{11}\,\Delta x_1^j+\bar{\varepsilon}_{12}\,\Delta x_2^j+\bar{\varepsilon}_{13}\,\Delta x_3^j,\\ u_2^{j+}-u_2^{j-}=\bar{\varepsilon}_{21}\,\Delta x_1^j+\bar{\varepsilon}_{22}\,\Delta x_2^j+\bar{\varepsilon}_{23}\,\Delta x_3^j,\\ u_3^{j+}-u_3^{j-}=\bar{\varepsilon}_{31}\,\Delta x_1^j+\bar{\varepsilon}_{32}\,\Delta x_2^j+\bar{\varepsilon}_{33}\,\Delta x_3^j\ .\end{cases}$$

<u>One of first to employ this notation</u>: P.M. Suquet. Elements of homogenization for inelastic solid mechanics. In Homogenization Techniques for Composite Media. Edited by Sanchez-Palencia and A. Zaoui). Lecture Notes in Physics, 272, 1987.

Other References

Check for updates

M. M. Shahzamanian
Department of Mechanical Engineering,
The University of Mississippi,
University, MS 38677

T. Tadepalli
Department of Mechanical Engineering,
The University of Mississippi,
University, MS 38677
e-mail: tadepali@olemiss.edu

A. M. Rajendran
Department of Mechanical Engineering,
The University of Mississippi,
University, MS 38677

W. D. Hodo[1]
U.S. Army Engineer Research
and Development Center,
Vicksburg, MS 39180

R. Mohan
Joint School of Nano Science
and Nano Engineering,
North Carolina A&T State University,
Greensboro, NC 27411

R. Valisetty
U.S. Army Research Laboratory,
Aberdeen Proving Ground, MD

P. W. Chung
U.S. Army Research Laboratory,
Aberdeen Proving Ground, MD

J. J. Ramsey
U.S. Army Research Laboratory,
Aberdeen Proving Ground, MD

Representative Volume Element Based Modeling of Cementitious Materials

The current work focuses on evaluation of the effective elastic properties of cementitious materials through a voxel based finite element analysis (FEA) approach. Voxels are generated for a heterogeneous cementitious material (type-I cement) consisting of typical volume fractions of various constituent phases from digital microstructures. The microstructure is modeled as a microscale representative volume element (RVE) in ABAQUS® *to generate cubes several tens of microns in dimension and subjected to various prescribed deformation modes to generate the effective elastic tensor of the material. The RVE-calculated elastic properties such as moduli and Poisson's ratio are validated through an asymptotic expansion homogenization (AEH) and compared with rule of mixtures. Both periodic (PBC) and kinematic boundary conditions (KBC) are investigated to determine if the elastic properties are invariant due to boundary conditions. In addition, the method of "Windowing" was used to assess the randomness of the constituents and to validate how the isotropic elastic properties were determined. The average elastic properties obtained from the displacement based FEA of various locally anisotropic microsize cubes extracted from an RVE of size 100 × 100 × 100 μm showed that the overall RVE response was fully isotropic. The effects of domain size, degree of hydration (DOH), kinematic and periodic boundary conditions, domain sampling techniques, local anisotropy, particle size distribution (PSD), and random microstructure on elastic properties are studied.* [DOI: 10.1115/1.4025916]

Keywords: multiscale modeling, cement, RVE, FEA, calcium silicate hydrate, AEH

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A 3D RVE model with periodic boundary conditions to estimate mechanical properties of composites

Fathollah Taheri-Behrooz* and Emad Pourahmadi[a]

School of Mechanical Engineering, Iran University of Science and Technology, P.O.B. 1684613114 Tehran, Iran

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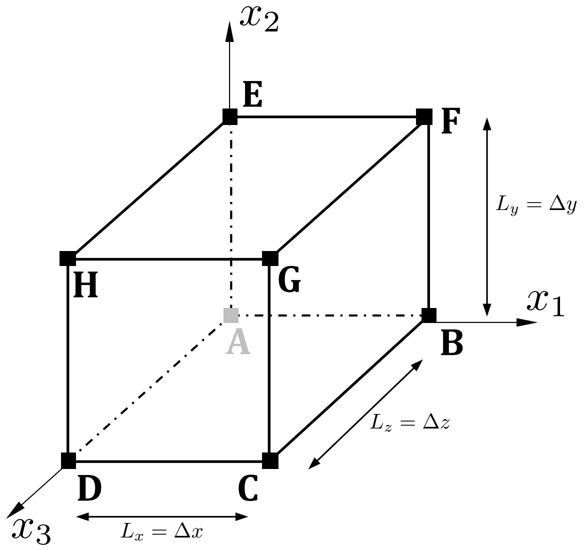
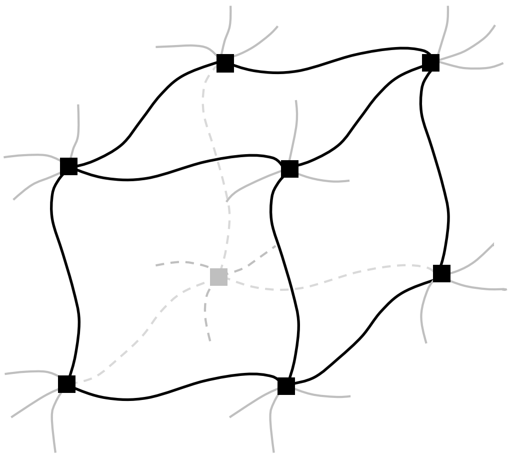
Abstract. Micromechanics is a technique for the analysis of composites or heterogeneous materials which focuses on the components of the intended structure. Each one of the components can exhibit isotropic behavior, but the microstructure characteristics of the heterogeneous material result in the anisotropic behavior of the structure. In this research, the general mechanical properties of a 3D anisotropic and heterogeneous Representative Volume Element (RVE), have been determined by applying periodic boundary conditions (PBCs), using the Asymptotic Homogenization Theory (AHT) and strain energy. In order to use the homogenization theory and apply the periodic boundary conditions, the ABAQUS scripting interface (ASI) has been used along with the Python programming language. The results have been compared with those of the Homogeneous Boundary Conditions method, which leads to an overestimation of the effective mechanical properties. According to the results, applying homogenous boundary conditions results in a 33% and 13% increase in the shear moduli G_{23} and G_{12}, respectively. In polymeric composites, the fibers have linear and brittle behavior, while the resin exhibits a non-linear behavior. Therefore, the nonlinear effects of resin on the mechanical properties of the composite material is studied using a user-defined subroutine in Fortran (USDFLD). The non-linear shear stress-strain behavior of unidirectional composite laminates has been obtained. Results indicate that at arbitrary constant stress as 80 MPa in-plane shear modulus, G_{12}, experienced a 47%, 41% and 31% reduction at the fiber volume fraction of 30%, 50% and 70%, compared to the linear assumption. The results of this study are in good agreement with the analytical and experimental results available in the literature

Keywords: Periodic boundary conditions; Asymptotic homogenization theory; Three-dimensional RVE; Mechanical properties; Python scripting; Non-linear resin behavior; USDFLD subroutine

Common Case: Rectangular Prisms





Node sets:

Vertex nodes: A B C D E F G H

Edge nodes: along the 12 edges excluding the vertex nodes

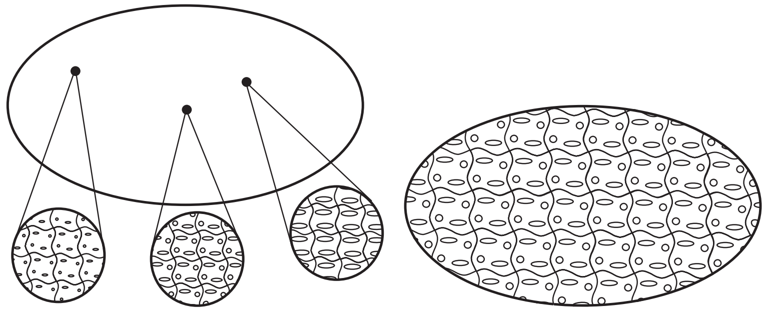
Face nodes: incident on faces, excluding vertex and edge nodes

Internal nodes: all other mesh nodes

RVE meshed with "pair nodes" to support application of periodic boundary conditions.

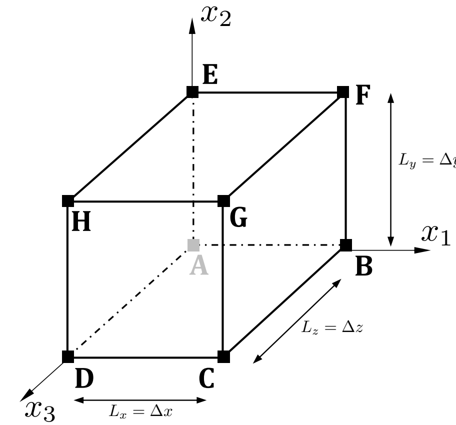
Pairs of nodes located on opposite faces of the RVE whose in-plane coordinates are identical. They represent the same physical point in the periodic material and are coupled by the periodic displacement constraints. GMSH and NEPER, for example, can generate RVE meshes with the required pair nodes.

Macroscale Strain to Load RVE



$$\bar{\varepsilon}_{ij} = \frac{1}{2}\left(\partial u_i/\partial x_j + \partial u_j/\partial x_i\right)$$

Known macroscale strain tensor to load the RVE

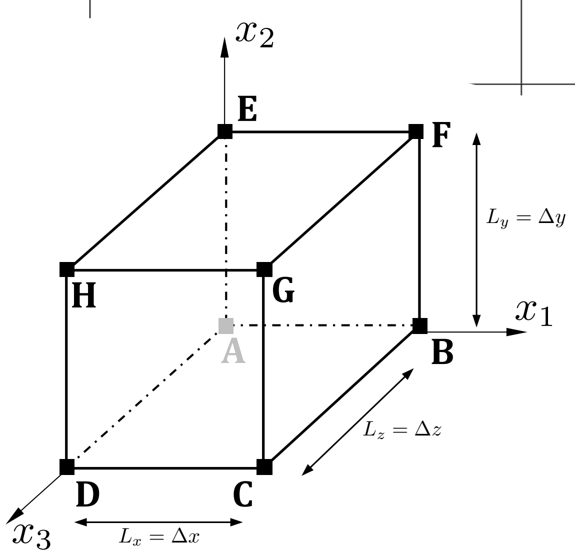


Developments here for multi-point constraint (MPC) equations to enforce the PBCs assume, but do not require, a symmetric strain tensor in the above equation.

For a simple RVE loaded only by $\bar{\varepsilon}_{12} = a$ and $\bar{\varepsilon}_{21} = b$, WARP3D computes/outputs $\gamma_{xy} = a + b$, even when $a \neq b$. The values a, b cannot $= 0$ but one can be made very small to approximate zero if needed.

3D PBCs (see A on pg. 2)

Face Nodes	Vertex Nodes	Edge Nodes
$u_i^{\mathrm{FGCB}} - u_i^{\mathrm{EHDA}} - L_x\,\bar{\varepsilon}_{i1} = 0$	$u_i^{\mathrm{G}} - u_i^{\mathrm{A}} - L_x\,\bar{\varepsilon}_{i1} - L_y\,\bar{\varepsilon}_{i2} - L_z\,\bar{\varepsilon}_{i3} = 0$	FG $\leftrightarrow$ AD: $u_i^{\mathrm{FG}} - u_i^{\mathrm{AD}} - L_x\,\bar{\varepsilon}_{i1} - L_y\,\bar{\varepsilon}_{i2} = 0$
$u_i^{\mathrm{FEHG}} - u_i^{\mathrm{BADC}} - L_y\,\bar{\varepsilon}_{i2} = 0$	$u_i^{\mathrm{F}} - u_i^{\mathrm{D}} - L_x\,\bar{\varepsilon}_{i1} - L_y\,\bar{\varepsilon}_{i2} + L_z\,\bar{\varepsilon}_{i3} = 0$	HG $\leftrightarrow$ AB: $u_i^{\mathrm{HG}} - u_i^{\mathrm{AB}} - L_y\,\bar{\varepsilon}_{i2} - L_z\,\bar{\varepsilon}_{i3} = 0$
$u_i^{\mathrm{GHDC}} - u_i^{\mathrm{FEAB}} - L_z\,\bar{\varepsilon}_{i3} = 0$	$u_i^{\mathrm{H}} - u_i^{\mathrm{B}} + L_x\,\bar{\varepsilon}_{i1} - L_y\,\bar{\varepsilon}_{i2} - L_z\,\bar{\varepsilon}_{i3} = 0$	GC $\leftrightarrow$ EA: $u_i^{\mathrm{GC}} - u_i^{\mathrm{EA}} - L_x\,\bar{\varepsilon}_{i1} - L_z\,\bar{\varepsilon}_{i3} = 0$
	$u_i^{\mathrm{C}} - u_i^{\mathrm{E}} - L_x\,\bar{\varepsilon}_{i1} + L_y\,\bar{\varepsilon}_{i2} - L_z\,\bar{\varepsilon}_{i3} = 0$	BC $\leftrightarrow$ EH: $u_i^{\mathrm{BC}} - u_i^{\mathrm{EH}} - L_x\,\bar{\varepsilon}_{i1} + L_y\,\bar{\varepsilon}_{i2} = 0$
		FE $\leftrightarrow$ CD: $u_i^{\mathrm{FE}} - u_i^{\mathrm{CD}} - L_y\,\bar{\varepsilon}_{i2} + L_z\,\bar{\varepsilon}_{i3} = 0$
		FB $\leftrightarrow$ HD: $u_i^{\mathrm{FB}} - u_i^{\mathrm{HD}} - L_x\,\bar{\varepsilon}_{i1} + L_z\,\bar{\varepsilon}_{i3} = 0$



Reduction to the 2D case is straightforward (vertexes H-G-D-C deleted)

$$L_z = 0;\ \ i = 1, 2;\ \ \bar{\varepsilon}_{i3} = 0$$

The RVE does not need to be located in the 1st quadrant with node A at (0,0,0)

Multi-Point Constraint Equations

- The PBCs are multi-point constraint (MPC) equations.
- When the known, (loading) strain terms in an equation are zero, the MPC is homogeneous.
- When one or more of the known (loading) strain terms is not zero, the MPC is inhomogeneous.
- Some finite element codes, including WARP3D, support only homogeneous MPC equations.
- The dummy node – rigid link technique is often used to overcome this limitation.

WARP3D input format

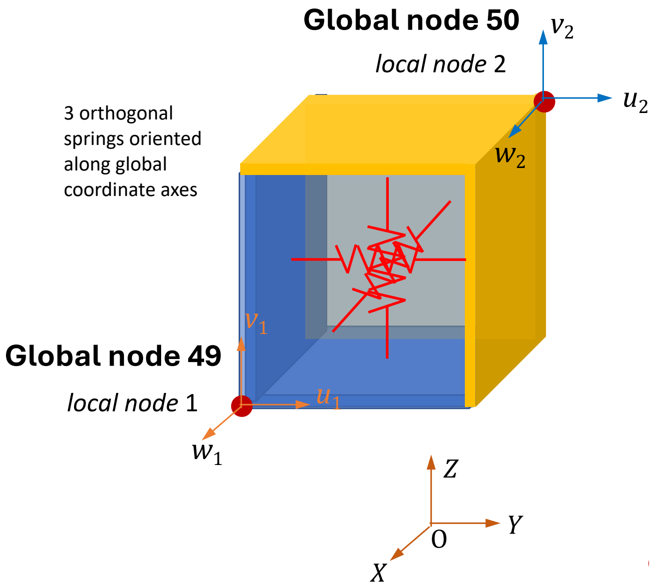
```
constraints
   14 u = 0 v = 0
   642 u = 0.1   w = -0.3
    …
    …

  multipoint
   23 1.0 v  - 5 1.0 v = 0.
   23 1.0 w  - 5 1.0 w = 0.
   18 1.0 u  - 10 1.0 u  - 28 1.0 u = 0.
   18 1.0 v  - 10 1.0 v = 0.
   18 1.0 w  - 10 1.0 w = 0.
   12 1.0 u  - 16 1.0 u  - 28 1.0 u = 0.
   12 1.0 v  - 16 1.0 v = 0.
      …
      …
```

1. The “absolute” constraint must come first.
2. The keyword “multipoint” ends the absolute constraints and starts the MPCs.
3. No absolute constraints can be mixed with the multipoint constraints.
4. Every MPC equation must be homogeneous.
5. No coefficient in an MPC equation may = 0.
6. Coefficients can be other than 1.0.
7. If the ”constraints” command appears again in the input, *all* existing constraint definition are deleted.

Dummy Node – Link Element Technique

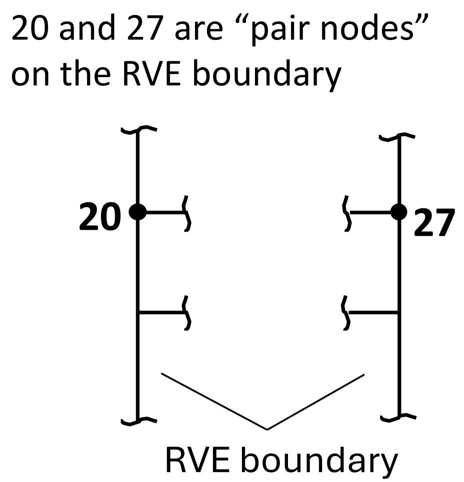
- Link element has 2 nodes, most often with identical coordinates – coordinates play no role in the element stiffness matrix (only connectivity and stiffness values matter).
- Placed away from RVE mesh for clarity but location has no effect on solution.
- Nodes connected by stiff, linear springs oriented along global X-Y-Z axes
- Connected to nodes 49, 50 in figure.
- In this example, displacements are applied to node 50 with node 49 appearing in the MPC equations.
- With sufficiently large spring stiffnesses, node 49 displacements are identical to those imposed at node 50.
- <u>But</u>, the MPC equations written using node 49 satisfy the requirement to be homogeneous.
- Node 49 is often termed the “dummy” node

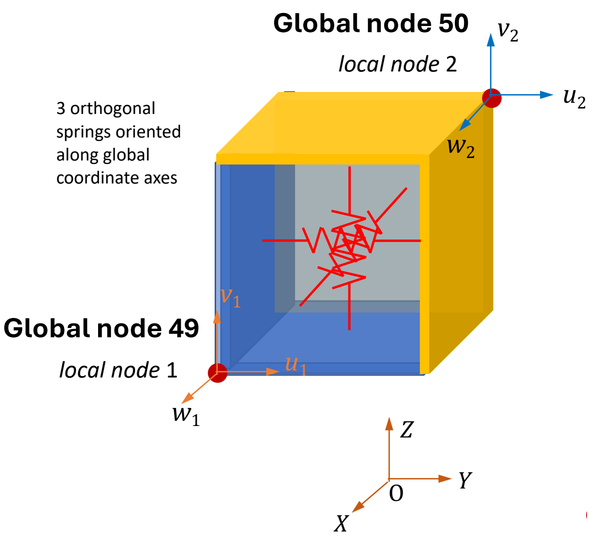


link2 element in WARP3D

<u>Remember:</u> in WARP3D the nodes must be numbered sequentially and the elements must be numbered sequentially. The dummy nodes and link elements are generally added after model nodes/elements.

Example: Dummy Node – Link Element





Example MPC equation using the dummy node 49 (WARP3D format):

$$27\ 1.0\ w\ -\ 20\ 1.0\ w\ -49\ 1.0\ w = 0$$

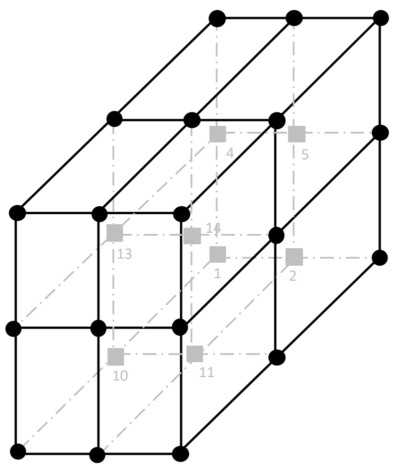
Where absolute constraints are imposed on node 50 (WARP3D format):

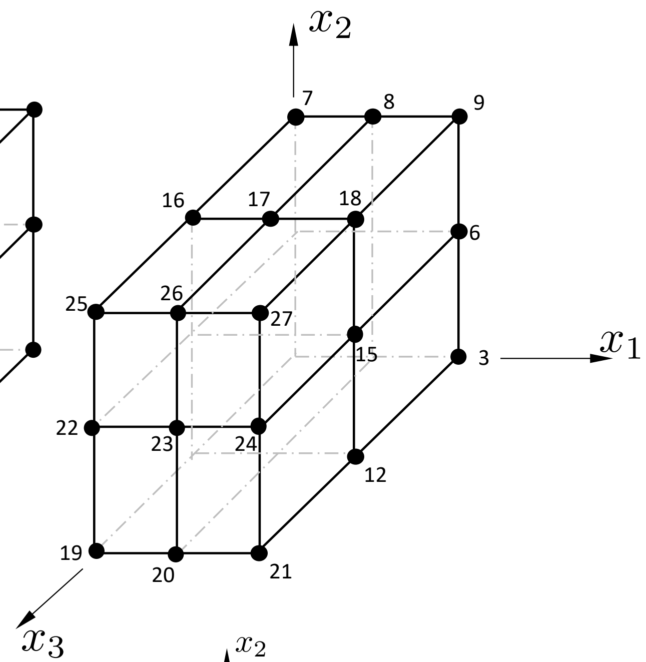
$$50\quad u\ = 0\quad v = 0\quad w = 0.0025$$

The u = v = 0 displacements on node 50 have no effect on the solution unless they appear in other MPC equations having node 49. For WARP3D, do not include terms in MPCs with a zero multiplier, *e.g.* $49\ 0.0\ w$

Verification Example

- Rectangular prism RVE
- 8, 8-node elements (l3disop)
- 4 link2 elements
- 27 nodes for prism
- 4 dummy-node pairs (8 total nodes)
- $L_x = 1$, $L_y = 2$, $L_z = 4$
- Linear-elastic material
- Confirm correct MPCs w/dummy nodes to enforce PBCs





Node Sets

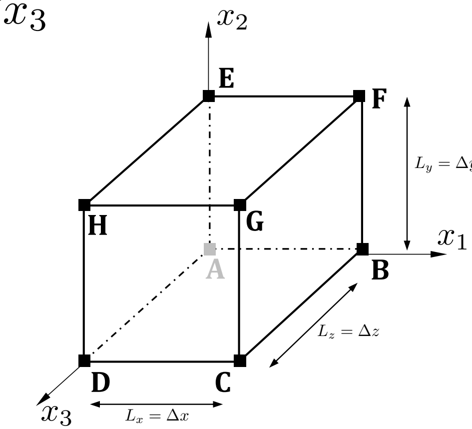
(A node can appear only once)

Vertex		Edge		Face	
A	1	FG	18	EHDA	13
B	3	AD	10	FGCB	15
C	21	HG	26	BADC	11
D	19	AB	2	FEHG	17
E	7	GC	24	FEAB	15
F	9	EA	14	GHDC	23
G	27	BC	12		
H	25	EH	16		
		FE	8		
		CD	20		
		FB	6		
		HD	22		

Internal

14

In more refined meshes, there will be many nodes on each edge, each face and internal to the RVE



Mesh Data

Coordinates

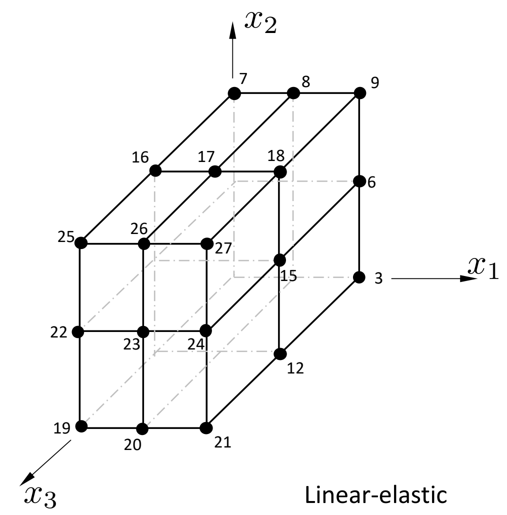
1	0.0	0.0	0.0
2	0.5	0.0	0.0
3	1.0	0.0	0.0
4	0.0	1.0	0.0
5	0.5	1.0	0.0
6	1.0	1.0	0.0
7	0.0	2.0	0.0
8	0.5	2.0	0.0
9	1.0	2.0	0.0
10	0.0	0.0	2.0
11	0.5	0.0	2.0
12	1.0	0.0	2.0
13	0.0	1.0	2.0
14	0.5	1.0	2.0
15	1.0	1.0	2.0
16	0.0	2.0	2.0
17	0.5	2.0	2.0
18	1.0	2.0	2.0
19	0.0	0.0	4.0
20	0.5	0.0	4.0
21	1.0	0.0	4.0
22	0.0	1.0	4.0
23	0.5	1.0	4.0
24	1.0	1.0	4.0
25	0.0	2.0	4.0
26	0.5	2.0	4.0
27	1.0	2.0	4.0
28	10	10	10
29	10	10	10
30	10	10	10
31	10	10	10
32	10	10	10
33	10	10	10
34	10	10	10
35	10	10	10

Dummy nodes

Incidences

1	1	2	5	4	10	11	14	13
2	2	3	6	5	11	12	15	14
3	4	5	8	7	13	14	17	16
4	5	6	9	8	14	15	18	17
5	10	11	14	13	19	20	23	22
6	11	12	15	14	20	21	24	23
7	13	14	17	16	22	23	26	25
8	14	15	18	17	23	24	27	26
9	28	29						
10	30	31						
11	32	33						
12	34	35						

Link2 elements



Linear-elastic

```
material steel
   properties mises e 30000  nu 0.3 n_power 10 yld_pt 60.e10
!
material rve_link
    properties link stiff_link 1.0e10 mass_link 0.0
!
elements
  1-8 type l3disop linear material steel order 2x2x2 bbar,
                        center_output short
 9-12 type link2 material rve_link
!
```

Put coordinates and incidences into file name: coords_incid.inp

Loadings, Dummy-Nodes

$$\boldsymbol{\varepsilon} = \varepsilon_{ij} = \begin{bmatrix} \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\ \varepsilon_{21} & \varepsilon_{22} & \varepsilon_{23} \\ \varepsilon_{31} & \varepsilon_{32} & \varepsilon_{33} \end{bmatrix}$$

$$\left.\begin{aligned} \varepsilon_{11} &= 0.1 \\ \varepsilon_{12} = \varepsilon_{21} &= 0.2 \\ \varepsilon_{13} = \varepsilon_{31} &= 0.5 \\ \varepsilon_{32} = \varepsilon_{23} &= 0.3 \\ \varepsilon_{22} = \varepsilon_{33} &= 0.0 \end{aligned}\right\}$$

Numerical values specified for easy verification that computed results in all mesh elements are identical to these strains.

- **4 dummy-node pairs and 4 corresponding stiff link2 elements are defined to impose displacements on the RVE that correspond to these macroscale strains.**
- **The RVE dimensions (1 x 2 x 4) are chosen to make clear the different displacement values required to impose specific macroscale strains**
- **One dummy-node pair and link2 element for each strain component (here the macroscale shear strains are symmetric)**
- **The (2,2) and (3,3) strain values could also be specified with non-zero values. Add 2 more dummy-node pairs and 2 link2 elements**
- **Coordinates for nodes 28-35 are set at 10.0 10.0 10.0 . The values are immaterial and do not affect the solution.**
- **link2 stiffnesses are set at 10^{10} – check that this value is sufficiently large to approximate a rigid-link**

Dummy-Node Pairs	Link2 element
28, 29	9
30, 31	10
32, 33	11
34, 35	12

Simple loading: Only $\varepsilon_{11} \neq 0$

- **All dummy-node pairs and link2 elements remain in model for convenience.**
- **Absolute displacements imposed:**
- **u = 0.1 at node 29 makes u at node 28 = 0.1**
- **The u = 0.1 makes macroscale strain ε_{11} = 0.1 since L_x = 1.0: $\varepsilon_{11} = u_{29} = u_{28}/1.0$**
- **<u>Recommended steps</u>:**
  - **Decide upon absolute constraints to prevent 3 rigid body translations and 3 rotations (rigid-body constraints).**
  - **Start with all equations on slide 6. Eliminate all the terms that become zero from the zero imposed ε_{ij} values.**
  - **Eliminate the terms that become zero from the rigid-body constraints.**
  - **Some of the MPCs to enforce the periodic boundary conditions will now have only 1 term remaining.**
  - **The MPC has become an absolute constraint and must be included with them.**

<u>Remove rigid-body motions</u>:

Node 1: $u = v = w = 0$

Node 3: $v = w = 0$

Node 7: $w = 0$

(other combinations will work as well)

<u>Impose dummy-node loading:</u>

Node 29 : $u = 0.1,\ v = w = 0$

<u>Periodic MPCs that become absolute constraints</u>:

Node 21 : $w = 0$

Node 25 : $v = 0\ w = 0$

Node 27 : $v = 0\ w = 0$

<u>What about dummy nodes 30-35</u>?

No constraints needed but can be set = 0 if desired. Nodes 29-35 do not appear in any MPCs for this simple loading with only ε_{11} non-zero. The stiff springs of the link elements 10, 11, 12 effectively attach them to ground - and they have no applied loads so zero displacements are computed.

<u>Solution</u>: all elements for this uniformly meshed RVE must have ε_{11} = 0.1 and other strains = 0

MPCs to Enforce Periodic Boundary

Multipoint

```
15 1.0 u  - 13 1.0 u  - 28 1.0 u = 0.
15 1.0 v  - 13 1.0 v = 0.
15 1.0 w  - 13 1.0 w = 0.
17 1.0 u  - 11 1.0 u = 0.
17 1.0 v  - 11 1.0 v = 0.
17 1.0 w  - 11 1.0 w = 0.
23 1.0 u  - 5 1.0 u = 0.
23 1.0 v  - 5 1.0 v = 0.
23 1.0 w  - 5 1.0 w = 0.
18 1.0 u  - 10 1.0 u  - 28 1.0 u = 0.
18 1.0 v  - 10 1.0 v = 0.
18 1.0 w  - 10 1.0 w = 0.
12 1.0 u  - 16 1.0 u  - 28 1.0 u = 0.
12 1.0 v  - 16 1.0 v = 0.
12 1.0 w  - 16 1.0 w = 0.
24 1.0 u  - 4 1.0 u  - 28 1.0 u = 0.
24 1.0 v  - 4 1.0 v = 0.
24 1.0 w  - 4 1.0 w = 0.
6 1.0 u  - 22 1.0 u  - 28 1.0 u = 0.
6 1.0 v  - 22 1.0 v = 0.
6 1.0 w  - 22 1.0 w = 0.
26 1.0 u  - 2 1.0 u = 0.
26 1.0 v  - 2 1.0 v = 0.
26 1.0 w  - 2 1.0 w = 0.
8 1.0 u  - 20 1.0 u = 0.
8 1.0 v  - 20 1.0 v = 0.
8 1.0 w  - 20 1.0 w = 0.
27 1.0 u  - 28 1.0 u = 0.
9 1.0 u  - 19 1.0 u  - 28 1.0 u = 0.
9 1.0 v  - 19 1.0 v = 0.
9 1.0 w  - 19 1.0 w = 0.
25 1.0 u  - 3 1.0 u  + 28 1.0 u = 0.
21 1.0 u  - 7 1.0 u  - 28 1.0 u = 0.
21 1.0 v  - 7 1.0 v = 0.
```

$\varepsilon_{11} = 0.1$, **all other macroscale strains = 0**

Put multipoint constraints into file name: mpc_eps_11_loading.inp

Complete Input File (1)

```
!
!     3D rectangular prism RVE. Lx = 1, Ly = 2, Lz = 4
!
!     Periodic boundary conditions (PBCs) applied to enforce the
!     RVE macroscale strain tensor:
!
!        0.1 0.0 0.0  #   eps_xx,  eps_xy,  eps_xz  alternate notation: eps_11,  eps_12,  eps_13
!        0.0 0.0 0.0  #   eps_xy,  eps_yy,  eps_yz
!        0.0 0.0 0.0  #   eps_xz,  eps_yz,  eps_zz
!
!
 material steel
    properties mises e 30000  nu 0.3 n_power 10 yld_pt 60.e10  $ linear-elastic
!
 material rve_link
     properties link stiff_link 1.0e10 mass_link 0.0
!
 structure prism
!
 number of nodes 35 elements 12
!
 elements
    1-8 type l3disop linear material steel order 2x2x2 bbar,
                          center_output short
    9 10 11 12 type link2 material rve_link
!
*echo off
 *input from file "coords_incid.inp"
*echo on
!
```

Complete Input File (2)

```
 blocking automatic
!
 constraints
!
  1 u 0.0 v 0.0 w 0.0   $ on nodes 1,3, 7 to prevent rigid motions
  3 v 0.0 w 0.0
  7 w 0.0
  21 w 0.0  $ on 21, 25, 27 as a result on MPCs becoming absolutes
  25 v 0.0 w 0.0
  27 v 0.0 w 0.0
  29 u 0.1  $  eps_11 strain
!
*input from file "mpc_eps_11_loading.inp"
!
 loading test
  nonlinear
    step 1 constraints 1.0
!
 nonlinear analysis parameters $ only those really needed here
   solution technique sparse direct
   time step 1.0e06
   maximum iterations 5 $ global Newton iterations
   minimum iterations 1
   convergence test norm res tol 0.001
   batch messages off
   trace solution on
!
 output model flat patran convention text file "model"
!
 compute displacements for loading test step  1
 output wide strains 1-8
 output wide stresses 1-12
 output wide displacements 1-35
 output flat text displacements     $ for ParaView visualization
 output flat text element stresses  $ for ParaView visualization
!
stop
```

For use by ParaView

More Complete Loading

- All dummy-node pairs and link2 elements in the model.
- Absolute displacements imposed on dummy nodes = macroscale strains.
- <u>Recommended steps</u>:
  - Decide upon absolute constraints to prevent 3 rigid body translations and 3 rotations (rigid-body constraints).
  - Start with all equations on slide 6. Eliminate all the terms that become zero from the zero imposed ε_{ij} values.
  - Eliminate the terms that become zero from the rigid-body constraints.
  - Some of the MPCs to enforce the periodic boundary conditions will now have only 1 term remaining.
  - The MPC has become an absolute constraint and must be included with them.

<u>Remove rigid-body motions</u>:**

Node 1: $u = v = w = 0$

<u>Impose dummy-node loading</u>:

Node 29 : $u = 0.1,\ v = w = 0$ $\leftarrow \boldsymbol{\varepsilon_{11}}$

Node 31 : $u = 0.2,\ v = 0.2,\ w = 0$ $\leftarrow \boldsymbol{\varepsilon_{12} = \varepsilon_{21}}$

Node 33 : $u = 0.5,\ v = 0.0,\ w = 0.5$ $\leftarrow \boldsymbol{\varepsilon_{13} = \varepsilon_{31}}$

Node 35 : $u = 0.0,\ v = 0.3,\ w = 0.3$ $\leftarrow \boldsymbol{\varepsilon_{23} = \varepsilon_{32}}$

$$\left.\begin{array}{l} \varepsilon_{11} = 0.1 \\ \varepsilon_{12} = \varepsilon_{21} = 0.2 \\ \varepsilon_{13} = \varepsilon_{31} = 0.5 \\ \varepsilon_{32} = \varepsilon_{23} = 0.3 \\ \varepsilon_{22} = \varepsilon_{33} = 0.0 \end{array}\right\} \text{Macroscale tensor}$$

<u>Periodic MPCs that become absolute constraints</u>:

*** none ***

** For this loading, there are sufficient non-zero imposed displacements (from the macroscale strain tensor) to suppress rigid-body rotations

<u>Solution</u>: all elements for this uniformly meshed RVE must have the imposed macroscale strain tensor

MPCs to Enforce Periodic Boundary

Multipoint

```
15 1.0 u  - 13 1.0 u  - 28 1.0 u = 0.
15 1.0 v  - 13 1.0 v  - 30 1.0 v = 0.
15 1.0 w  - 13 1.0 w  - 32 1.0 w = 0.
17 1.0 u  - 11 1.0 u  - 30 2.0 u = 0.
17 1.0 v  - 11 1.0 v = 0.
17 1.0 w  - 11 1.0 w  - 34 2.0 w = 0.
23 1.0 u  - 5 1.0 u  - 32 4.0 u = 0.
23 1.0 v  - 5 1.0 v  - 34 4.0 v = 0.
23 1.0 w  - 5 1.0 w = 0.
18 1.0 u  - 10 1.0 u  - 28 1.0 u  - 30 2.0 u = 0.
18 1.0 v  - 10 1.0 v  - 30 1.0 v = 0.
18 1.0 w  - 10 1.0 w  - 32 1.0 w  - 34 2.0 w = 0.
12 1.0 u  - 16 1.0 u  - 28 1.0 u  + 30 2.0 u = 0.
12 1.0 v  - 16 1.0 v  - 30 1.0 v = 0.
12 1.0 w  - 16 1.0 w  - 32 1.0 w  + 34 2.0 w = 0.
24 1.0 u  - 4 1.0 u  - 28 1.0 u  - 32 4.0 u = 0.
24 1.0 v  - 4 1.0 v  - 30 1.0 v  - 34 4.0 v = 0.
24 1.0 w  - 4 1.0 w  - 32 1.0 w = 0.
6 1.0 u  - 22 1.0 u  - 28 1.0 u  + 32 4.0 u = 0.
6 1.0 v  - 22 1.0 v  - 30 1.0 v  + 34 4.0 v = 0.
6 1.0 w  - 22 1.0 w  - 32 1.0 w = 0.
26 1.0 u  - 2 1.0 u  - 30 2.0 u  - 32 4.0 u = 0.
26 1.0 v  - 2 1.0 v  - 34 4.0 v = 0.
26 1.0 w  - 2 1.0 w  - 34 2.0 w = 0.
8 1.0 u  - 20 1.0 u  - 30 2.0 u  + 32 4.0 u = 0.
8 1.0 v  - 20 1.0 v  + 34 4.0 v = 0.
8 1.0 w  - 20 1.0 w  - 34 2.0 w = 0.
27 1.0 u  - 28 1.0 u  - 30 2.0 u  - 32 4.0 u = 0.
27 1.0 v  - 30 1.0 v  - 34 4.0 v = 0.
27 1.0 w  - 32 1.0 w  - 34 2.0 w = 0.
9 1.0 u  - 19 1.0 u  - 28 1.0 u  - 30 2.0 u  + 32 4.0 u = 0.
9 1.0 v  - 19 1.0 v  - 30 1.0 v  + 34 4.0 v = 0.
9 1.0 w  - 19 1.0 w  - 32 1.0 w  - 34 2.0 w = 0.
25 1.0 u  - 3 1.0 u  + 28 1.0 u  - 30 2.0 u  - 32 4.0 u = 0.
25 1.0 v  - 3 1.0 v  + 30 1.0 v  - 34 4.0 v = 0.
25 1.0 w  - 3 1.0 w  + 32 1.0 w  - 34 2.0 w = 0.
21 1.0 u  - 7 1.0 u  - 28 1.0 u  + 30 2.0 u  - 32 4.0 u = 0.
21 1.0 v  - 7 1.0 v  - 30 1.0 v  - 34 4.0 v = 0.
21 1.0 w  - 7 1.0 w  - 32 1.0 w  + 34 2.0 w = 0.
```

The L_x, L_y, L_z values apparent here

$$\boldsymbol{\varepsilon} = \varepsilon_{ij} = \begin{bmatrix} \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\ \varepsilon_{21} & \varepsilon_{22} & \varepsilon_{23} \\ \varepsilon_{31} & \varepsilon_{32} & \varepsilon_{33} \end{bmatrix}$$

$$\left.\begin{array}{l} \varepsilon_{11} = 0.1 \\ \varepsilon_{12} = \varepsilon_{21} = 0.2 \\ \varepsilon_{13} = \varepsilon_{31} = 0.5 \\ \varepsilon_{32} = \varepsilon_{23} = 0.3 \\ \varepsilon_{22} = \varepsilon_{33} = 0.0 \end{array}\right\}$$

Put multipoint constraints into file name: mpc_eps_all_loading.inp

Complete Input File (1)

```
!
!     3D rectangular prism RVE. Lx = 1, Ly = 2, Lz = 4
!
!     Periodic boundary conditions (PBCs) applied to enforce the
!     RVE macroscale strain tensor:
!
!        0.1 0.2 0.5  #   eps_xx,  eps_xy,  eps_xz  alternate notation: eps_11,  eps_12,  eps_13
!        0.2 0.0 0.3  #   eps_xy,  eps_yy,  eps_yz
!        0.5 0.3 0.0
!
!    *****    Note    *****
!
!         WARP3D outputs the engineering definition of shear strains, i.e.,
!         gamma_xy, gamma_yz, gamma_xz
!         The printed results should thus be gamma_xy = 0.4,
!         gamma_yz = 0.6 and gamma_xz = 1.0
!
 material steel
    properties mises e 30000  nu 0.3 n_power 10 yld_pt 60.e10  $ linear-elastic
!
 material rve_link
     properties link stiff_link 1.0e10 mass_link 0.0
!
 structure prism
!
 number of nodes 35 elements 12
!
 elements
    1-8 type l3disop linear material steel order 2x2x2 bbar,
                      center_output short
    9 10 11 12 type link2 material rve_link
!
*echo off
 *input from file "coords_incid.inp"
*echo on
!
```

Complete Input File (2)

```
 blocking automatic
!
 constraints
!
  1 u 0.0  v 0.0  w 0.0 $ non-zero displacements on dummy nodes are
!                       $ sufficient to prevent rigid rotations
!
! set node 29 u = eps_11 value
! set node 31 u, v = eps_12 value
! set node 33 u, w = eps_13 value
! set node 35 u, w = eps_23 value
!
   29   u 0.1  v  0.0  w 0.0
   31   u 0.2  v  0.2  w 0.0
   33   u 0.5  v  0.0  w 0.5
   35   u 0.0  v  0.3  w 0.3
!
   multipoint
!
    *input from "mpc_eps_all_loading.inp"

!
 loading test
  nonlinear
    step 1 constraints 1.0

     <<<< remainder of file same as eps_11 only loading >>>>
```

Program to Make MPCs

- **The simple example here makes clear that many thousands of MPC equations are needed to enforce the PBCs for RVEs with many elements**
- **A Python program, `rve_mpc_generator.py`, is available in the `RVE_support` directory of the WAR3D distribution**
- **Uses a small text input file of commands and the RVE nodal coordinates to generate a file of ready-to-use constraint data in WARP3D format**
- **The short manual for the program is named `manual.pdf` in the `RVE_support` directory.**