DEFINITION OF PERIODIC BOUNDARY CONDITIONS IN EXPLICIT DYNAMIC SIMULATIONS OF MICRO- OR MESO-SCALE UNIT CELLS WITH CONFORMAL AND NON-CONFORMAL MESHES

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Abstract
Although Periodic Boundary Conditions (PBCs) have been extensively used in finite elements to analyze unit cell models of composites, there are few reported investigations using explicit dynamic simulations. While different formulations and implementations of PBCs do not affect the results of quasi-static simulations solved by an implicit solver, they have an impact on the results of dynamic simulations solved by an explicit solver. A simple benchmark with a cubic unit cell of an isotropic linear elastic material is used to compare the results of different scenarios, which have different formulations and implementation of PBCs. The stress-strain curves under simple uniaxial tension shows that, in some scenarios, the explicit analyses do not follow the expected linear elastic behavior. These unexpected results are remarkable when the characteristic length of the model is in the range of few microns. This work encapsulates the relevant features of the different formulations and implementations of PBCs, and indicates in which scenarios the PBCs must be carefully applied.

1. Introduction

Periodic boundary conditions (PBCs) are a set of equations applied to a small domain in a way that the domain can be replicated through the different dimensions of the model. Using PBCs, the small domain called unit cell represents an infinite large system.

PBCs have been extensively used in finite element models to analyze composites with periodic geometries. They have been applied in simulations of micro and meso-scale unit cells to obtain homogenized properties [1–4]. The implementation of the equations in the finite element solvers have been done with different formulations and implementations[5–7].

In a quasi-static model solved by an implicit analysis, the kinematic constraints defined by the PBCs reduce the model degrees of freedom. Therefore, different formulations and implementations of PBCs are mathematically equivalent and their results are in good agreement. In a dynamic simulation solved by explicit analysis, however, the kinematic constraints (PBCs) and constitutive equations of the model are solved simultaneously. In this way, there is no reduction of the degrees of freedom. Consequently,

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different solutions can be obtained for mathematically equivalent formulations or implementations of PBCs applied at the micro- or meso-scale.

There are few reported investigations using finite element explicit analysis with PBC [8]. To our knowledge, there is no mention about possible differences with respect to the equivalent analysis performed with an implicit solver.

This study focuses on how to correctly apply PBCs in dynamic simulations using an explicit finite element solver. First, the different formulations and implementations of PBCs in a finite element model are presented. Then, results of explicit analysis with PBCs are compared with the equivalent implicit analysis. Finally, some conclusions about the implementation of PBCs in explicit analysis are reported.

2. Formulations and implementations of the PBCs

Formulations and implementations of the PBCs have been developed in 3D. For the sake of simplicity, they are described for a 2D parallelepiped unit cell (Fig. 1). The following sets of equations (Eq. 1, 2) describe the correlation between each node on one edge and its counterpart on the opposite edge,

$$u_j^{BC} - u_j^{AD} = \bar{\epsilon}_{xj}\Delta x = u_j^{RPX}. \tag{1}$$

$$u_j^{DC} - u_j^{AB} = \bar{\epsilon}_{yj}\Delta y = u_j^{RPY}. \tag{2}$$

u_j is the displacement of the node where $j = x, y$, $\bar{\epsilon}_{xj}$ and $\bar{\epsilon}_{yj}$ are the components of the average strain, Δx and Δy are the horizontal and vertical length of the parallelepiped. For each set of equations, the components of the average strain multiplied by the corresponding length are the perturbations that can be described with the displacements of each dummy node, u_j^{RPX} and u_j^{RPY} respectively. Using the displacements of the dummy nodes, the formulation can be easy implemented in whatever finite element solver. The load conditions are introduced through the displacement of the dummy nodes.

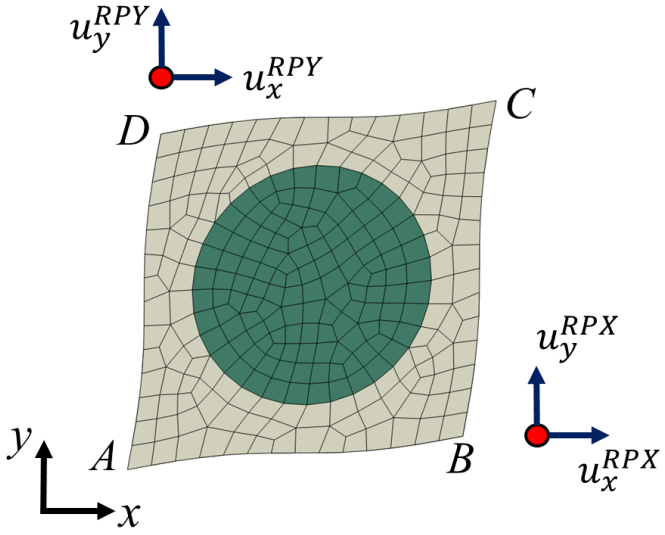

Figure 1. Unit cell with PBCs in 2D.

2.1. Relative and absolute formulation

When the sets of equations (Eq. 1, 2) are applied to the 2D unit cell, there are two equations to describe the displacement of C. To avoid duplicity of equations, only one of them or a combination must be used.

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Therefore, different formulations can be distinguished from this point on.

If the displacement of C is described by the equation $u_j^C - u_j^B = u_j^{RPY}$ from (Eq. 2), a *relative* formulation is obtained because the displacement of B is calculated by $u_j^B - u_j^A = u_j^{RPX}$ from (Eq. 1).

Another formulation can be written calculating the displacement of all vertices from one of them, which is called origin. Choosing A as origin, the displacement of B and D are calculated from (Eq. 1, 2) and the displacement of C can be formulated by $u_j^C - u_j^A = u_j^{RPX} + u_j^{RPY}$. Then, the formulation is *absolute*.

2.2. Node-to-node or surface-coupling implementation

Regardless of using relative or absolute formulation, the kinematic equations (Eq. 1, 2) are written node-to-node. This implementation of the PBCs so called node-to-node coupling requires a conformal mesh, where each node on an edge has its counterpart on the opposite edge.

When the mesh is non-conformal, a different implementation of the PBCs is necessary. There are some approaches that overcome this problem [5, 9]. The solution described by Al Kassem [5] is easy to implement in a finite element solver. The nodes from the original edge (AD) are copied to the opposite edge (BC) as reference points (Fig. 2). Then, the equations of PBCs can be applied between the original nodes on edge (AD) and the copied ones on opposite edge (BC). Finally, the copied nodes are coupled with the nodes of the mesh located on the edge (BC). The same procedure is done in the other direction between the edges (AB) and (DC). We call this implementation of the PBCs surface-coupling because the copied nodes are tied to the corresponding edge. This implementation can be used with conformal and non-conformal meshes.

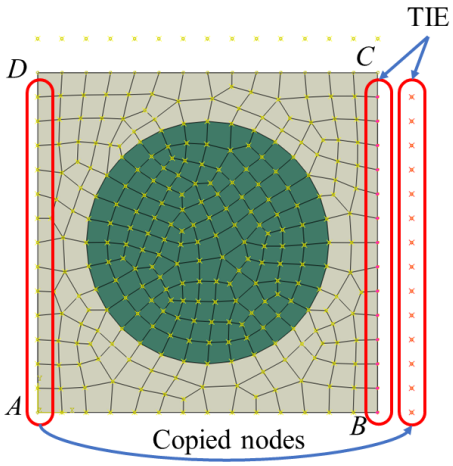

Figure 2. Unit cell with surface-coupling PBCs in 2D.

3. Benchmark using PBCs with an explicit solver

The benchmark has been performed using a cubic unit cell (Fig. 3). The PBCs have been applied with a 3D formulation using three dummy nodes. Four different scenarios with different implementations of the PBCs have been created (Table 1). There are two scenarios assuming node-to-node coupling with relative and absolute formulation. And two more scenarios assuming surface-coupling (although the

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mesh is conformal) with relative and absolute formulation.

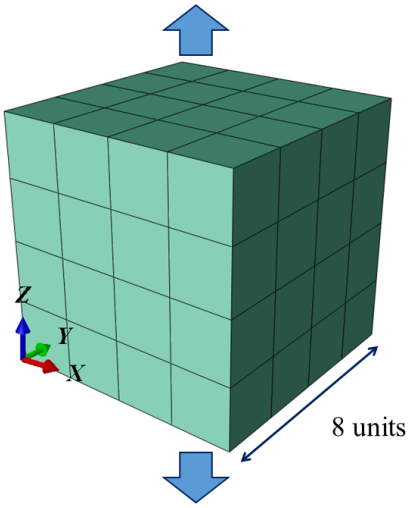

Figure 3. Mesh of the cubic unit cell with the applied load.

Table 1. Scenarios for different implementation of PBCs.

Scenario	Coupling	Formulation
N2N-REL	Node-to-node	relative
N2N-ABS	Node-to-node	absolute
STIE-REL	Surface-coupling	relative
STIE-ABS	Surface-coupling	absolute

The cubic unit cell has an edge length of 8 units. The mesh is regular with 64 linear hexagonal elements (Fig. 3). The material is isotropic linear elastic with density = 1174.3 Kg/m^3, Young modulus = 2600 MPa, and Poisons ratio = 0.4. The selected units for the model are: length in microns (μm), pressure in MPa, time in seconds (s), density in Kg/μm^3. Working with microns, the results show notable differences between the different implementation of the PBCs. Simulations in the length of millimeters also show different results but less noteworthy.

The load condition is a simple uniaxial tension in Z direction, where $u_z^{RPZ} = 0.02$ while the other components are zero. The strain rate is fixed in 10/s. The dependency with strain rate has been studied but not included in this paper. When the strain rate decreases, the results show bigger differences between the scenarios. The used finite element software is ABAQUS which has implicit and explicit solver.

The results are presented in Fig. 4 with stress-strain curves. The expected linear behavior is correctly calculated using the implicit solver for all the scenarios, see *std* curve with dots (Fig. 4). When the scenarios are solved with the explicit solver, different results from the linear behavior are shown. The scenario with node-to-node coupling and relative formulation (xpl N2N_REL) has a stress-strain behavior far away from the expected linear behavior. In this scenario, the final solution does not respect the boundary conditions imposed in the transverse direction where the average strain must be zero. In addition, the simulation introduces two unexpected results: an average shear strain, and a local expansion of the elements on the corners. Conversely, the scenario with node-to-node coupling and absolute formula-

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tion (xpl N2N_ABS) matches perfectly with the linear elastic behavior. As conclusion, the formulation of PBCs is very important in dynamic simulations. Relative kinematic equations can accumulate errors using the explicit solver.

In the case of surface-coupling, the stress-strain behavior using relative (xpl STIE_REL) or absolute equations (xpl STIE_ABS) are quite similar (Fig. 4). In both cases the curves are below the linear elastic behavior. Again, the same unexpected results than in the scenario (xpl N2N_REL) are found but less pronounced. Although (xpl STIE_ABS) use an absolute formulation between the nodes in one surface and the copied nodes on the counterpart, the surface-coupling introduces relative equations in the model. It is important to mention that every copied node has mass which is usually the mean average mass of the nodes. Therefore, they add mass to the model. Comparing the surface-coupling (xpl STIE_REL) with node-to-node coupling (xpl N2N_REL), it seems that the results improve when the mass of the model increases. This later hypothesis has been confirmed increasing numerically the density of the material.

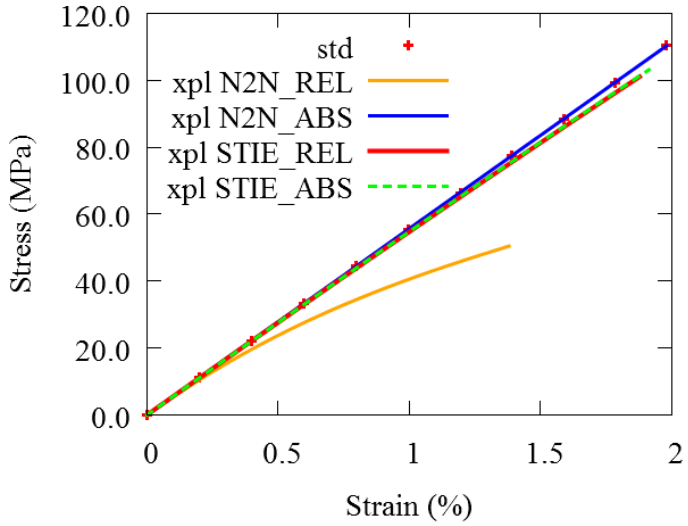

Figure 4. Stress-strain behavior for the different scenarios of PBCs under simple uniaxial load.

4. Conclusion

A systematic study of different formulations and implementations of PBCs in a finite element model has been done using an explicit solver. The PBCs implemented with node-to-node coupling and absolute formulation show results in good agreement with the theoretical ones. When a node-to-node coupling with relative formulation is used, the results move away from the theoretical ones. The discrepancy is more pronounced in micro-scale finite element models. On the other hand, the surface-coupling approach with both relative and absolute formulation gives results close to the theoretical ones with small differences. The advantage of the surface-coupling is that conformal and non-conformal meshes can be used, which is useful to model complex or random periodic units cells. As conclusion, none of the approaches analyzed is consistently better. However, these analysis results in useful advice to increase the reliability of the dynamic simulations and avoid unexpected results.

We are currently applying the PBCs to models at the micro- and meso-scale solved by an explicit finite element solver. The PBCs have been successfully implemented in different composite micro-scale models: under impact load [10], and in a damping study [11]. At the meso-scale, we are studying what is the best formulation and implementation in an accurate representative unit cell for textile composite [12].

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