Implementation of periodic boundary conditions in the finite element program ABAQUS

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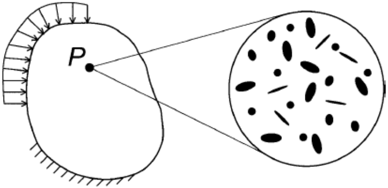
Representative volume element

- Representative volume element (RVE) is the statistical representation of properties of a material
- Contains all informations of microstructure
- Significantly smaller than the macroscopic structural dimensions
- Deformation gradient is known from Macro Model $\rightarrow$ should be applied to Micro Model



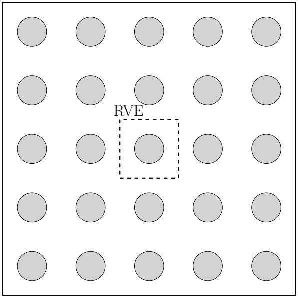
The same informations can be obtained using the RVE while significantly reducing the computational effort.

Representative volume element

Periodic features

1. Periodic repeating geometry
   - RVE represents whole microstructure

2. Periodic boundary conditions
   - Boundary conditions are whether **free** nor **fixed**
   - Opposite sides are deforming in the same manner (**periodic**) but allowing lateral shrinkage due to Poisson's ratio



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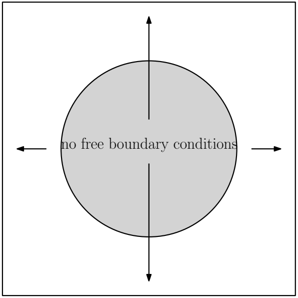

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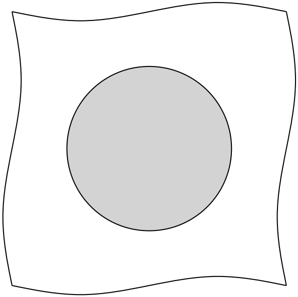
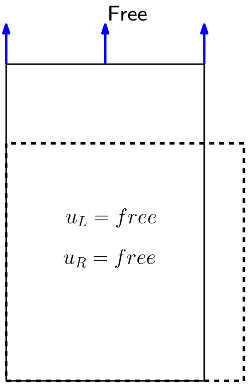
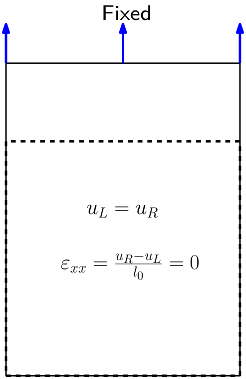


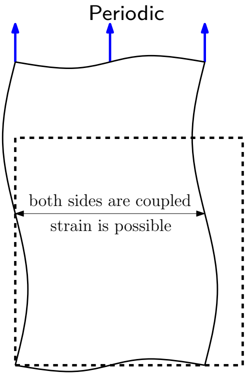
Boundary conditions



- To soft



- To stiff



- Presents periodicity

Periodic boundary conditions

- $u_i^{\text{Side}} - u_j^{\text{Opposite side}} = \Delta\varepsilon_{ij} \cdot l_i$

- $u_x^{\text{Right}} - u_x^{\text{Left}} = \Delta\varepsilon_{xx} \cdot l_x$
- $u_y^{\text{Top}} - u_y^{\text{Bottom}} = \Delta\varepsilon_{yy} \cdot l_y$
- $u_y^{\text{Right}} - u_y^{\text{Left}} = \Delta\varepsilon_{xy} \cdot l_x$
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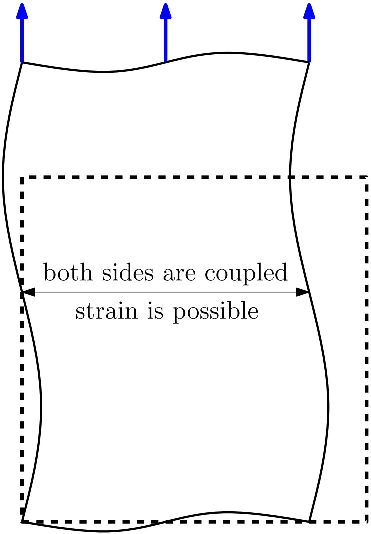

Key features

- Ability to apply displacement boundary conditions
- Correctly represent strains due to Poisson's ratio
- Avoid overconstrained model

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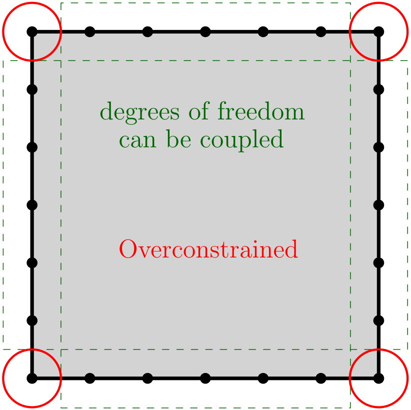


Periodic boundary conditions - Abaqus implementation 2D

Left to right

- $\mathbf{u}_i^R - \mathbf{u}_i^L = \mathbf{u}^{V_2} - \mathbf{u}^{V_1}$

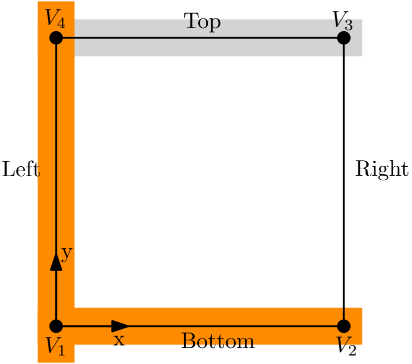
Bottom to top

- $\mathbf{u}_i^T - \mathbf{u}_i^B = \mathbf{u}^{V_4} - \mathbf{u}^{V_1}$

Dependent vertex

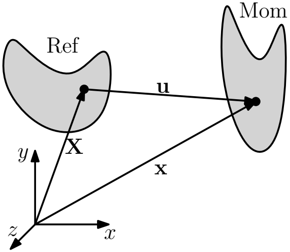
- $\mathbf{u}^{V_3} - \mathbf{u}^{V_4} = \mathbf{u}^{V_2} - \mathbf{u}^{V_1}$

$\mathbf{u}$:= Displacement vector



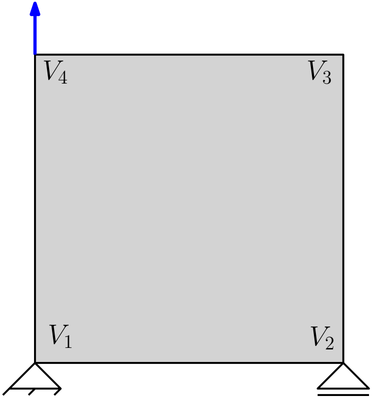
Application of deformation gradient

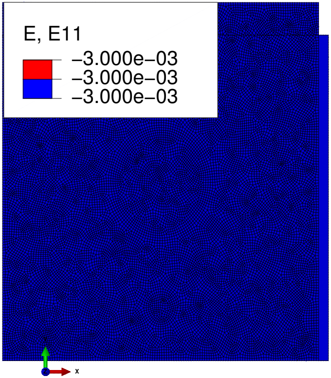
- $\mathbf{F} = \begin{pmatrix} \frac{\partial x_1}{\partial X_1} & \frac{\partial x_1}{\partial X_2} \\ \frac{\partial x_2}{\partial X_1} & \frac{\partial x_2}{\partial X_2} \end{pmatrix}$
- $\mathbf{x} = \mathbf{X} + \mathbf{u} \quad \rightarrow \mathbf{F} = \mathbf{I} + \begin{pmatrix} \frac{\partial u_1}{\partial X_1} & \frac{\partial u_1}{\partial X_2} \\ \frac{\partial u_2}{\partial X_1} & \frac{\partial u_2}{\partial X_2} \end{pmatrix}$
- Prescribing boundary conditions to vertices V_1, V_2, V_4 can present any arbitrary deformation gradient



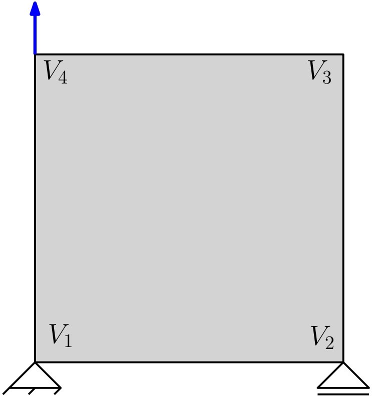
Simple tension test

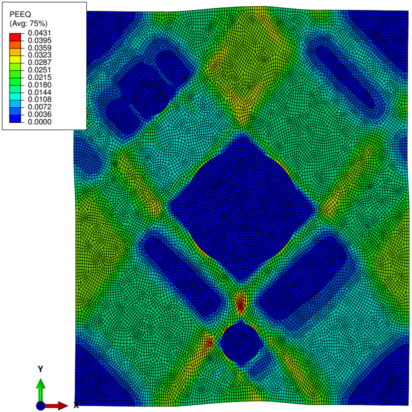
- Applied strain $\varepsilon_{yy} = 1\%$ due to displ. BC at V_4
- Due to Poisson's ratio $(\nu = 0.3) \rightarrow \varepsilon_{xx} = 0.3\%$ from analytics





Complex tension test (Y-Dir)





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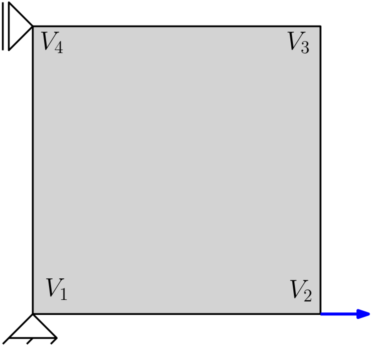
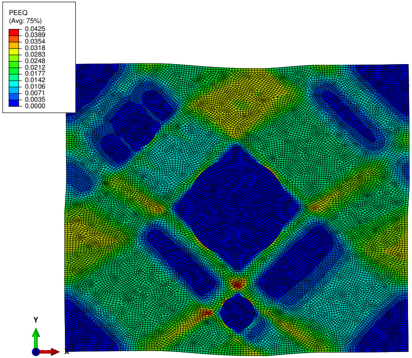
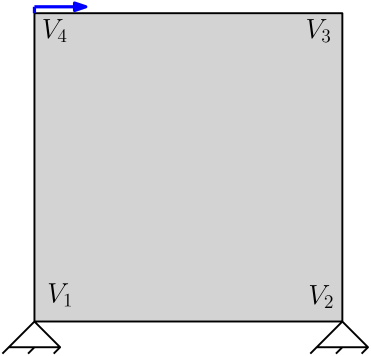
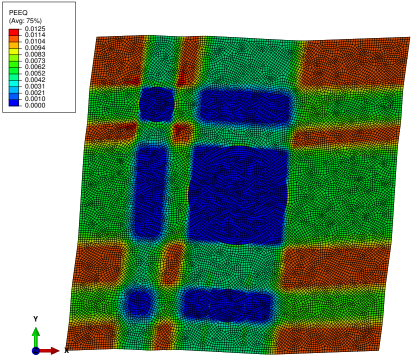




Shear test

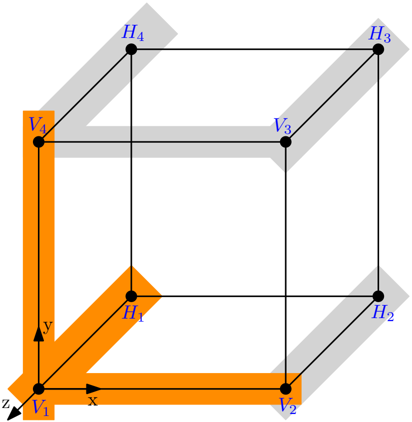

V_4
V_3
V_1
V_2


PEEQ
(Avg: 75%)
0.0125
0.0114
0.0104
0.0094
0.0083
0.0073
0.0062
0.0052
0.0042
0.0031
0.0021
0.0010
0.0000
Y
X

Periodic boundary conditions - Abaqus implementation 3D

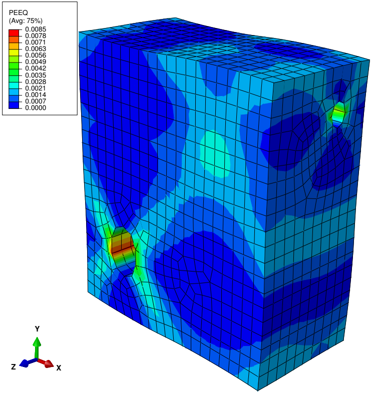
Procedure

- All surface nodes have to be coupled to opposite surface
- Special treatment for edge nodes and vertex nodes to avoid overconstraining
- Orange system is independent and deformation gradient can be prescribed
- Grey system is dependent and follows the applied deformation



3D Applications

Tension test



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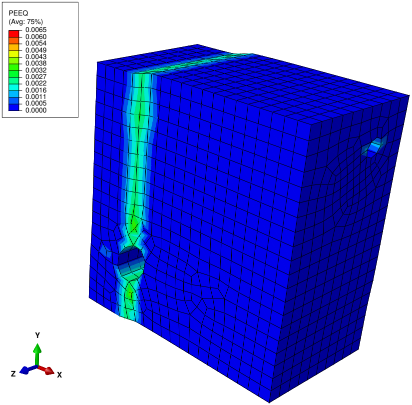
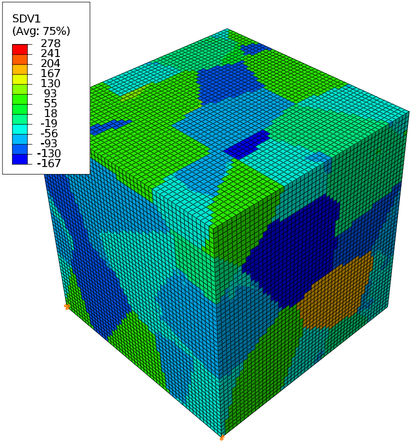
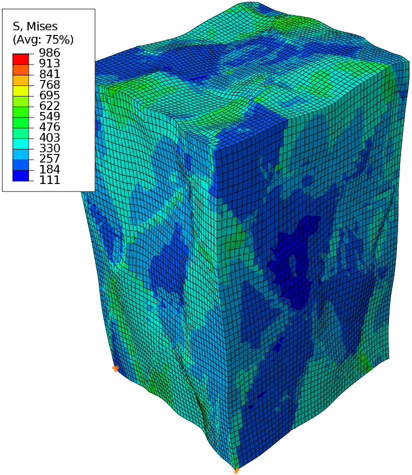


Periodic RVE

Initial grain orientation



Mises stress



Homogenisation approach

Averaged stress tensor

$$\bar{\boldsymbol{\sigma}}_{\mathsf{RVE}} = \frac{1}{V_{\mathsf{RVE}}} \int_{\mathbf{y} \in V_{\mathsf{RVE}}} \boldsymbol{\sigma}(\mathbf{y}) dV \tag{1}$$

$$\bar{\boldsymbol{\sigma}}_{\mathsf{RVE}} = \frac{1}{A} \mathsf{sym} \left[\left(\mathbf{u}^{V4} - \mathbf{u}^{V1} \right) \mathbf{f}^{V4} + \left(\mathbf{u}^{V2} - \mathbf{u}^{V1} \right) \mathbf{f}^{V2} \right] \tag{2}$$