# Homework Set #8

assigned: Friday, January 20th, 2017
due: Friday, February 10th, 2016, 3 pm
drop boxes outside 374 Firestone

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**Review: Periodic Boundary Conditions**

Periodic BCs enforce the condition (written for finite kinematics)

$$\boldsymbol{f}_c(\boldsymbol{U}^h) = \boldsymbol{u}^+ - \boldsymbol{u}^- - (\boldsymbol{F}^* - \boldsymbol{I})(\boldsymbol{X}^+ - \boldsymbol{X}^-).$$

for each pair of boundary nodes. Moreover, for a 2D RVE we showed that the above turns into

$$\begin{aligned}
\boldsymbol{f}_1(\boldsymbol{U}^h) &= \boldsymbol{u}^1, \\
\boldsymbol{f}_3(\boldsymbol{U}^h) &= \boldsymbol{u}^3 - \boldsymbol{u}^2 - \boldsymbol{u}^4, \\
\boldsymbol{f}_{\mathsf{lr}}(\boldsymbol{U}^h) &= \boldsymbol{u}^+ - \boldsymbol{u}^- - \boldsymbol{u}^2 \qquad \text{for each left/right pair,} \\
\boldsymbol{f}_{\mathsf{tb}}(\boldsymbol{U}^h) &= \boldsymbol{u}^+ - \boldsymbol{u}^- - \boldsymbol{u}^4 \qquad \text{for each top/bottom pair}
\end{aligned}$$

along with essential BCs at the corner nodes,

$$\begin{aligned}
\boldsymbol{u}^2 &= (\boldsymbol{F}^* - \boldsymbol{I})\boldsymbol{L}_{21}, \\
\boldsymbol{u}^4 &= (\boldsymbol{F}^* - \boldsymbol{I})\boldsymbol{L}_{41}
\end{aligned}$$

for *strain-controlled loading* with average deformation gradient $\boldsymbol{F}^*$ and/or

$$I[\boldsymbol{\varphi}] = \int_\Omega W(\boldsymbol{F})\,\mathrm{d}V - \boldsymbol{u}^4 \cdot \hat{\boldsymbol{F}}^4 - \boldsymbol{u}^2 \cdot \hat{\boldsymbol{F}}^2 \qquad \text{with} \qquad \hat{\boldsymbol{F}}^2 = \boldsymbol{P}^* \int_{\partial\Omega_r} \boldsymbol{N}_r \,\mathrm{d}S, \quad \hat{\boldsymbol{F}}^4 = \boldsymbol{P}^* \int_{\partial\Omega_t} \boldsymbol{N}_t \,\mathrm{d}S$$

for *stress-controlled loading* with average stress tensor $\boldsymbol{P}^*$.

**Problem 1: code development (25 points).**

Let us develop a concept for the implementation of the above periodic boundary conditions in 2D. To this end, conceive a viable and efficient implementation of the following components:

(i) Modify/replace the `EssentialBoundaryCondition` object to allow for general linear constraints

$$f_c(\boldsymbol{U}^h) = \sum_{a=1}^{n} \sum_{i=1}^{d} \alpha_i^a u_i^a - \delta = 0.$$

(ii) Modify the Newton-Raphson solver to correctly impose the your new `EssentialBoundaryCondition`.

(iii) Create a method that identifies all node pairs and corners for a given periodic rectangular mesh.

(iv) Develop a `Main` file or (ideally) modular code structure to conveniently impose components of $\boldsymbol{F}^*$ and $\boldsymbol{P}^*$ via the above periodic BCs (you can use the existing `ConstantForce` class).

Write pseudo-code for each component and propose interfaces for each class/method.

*Hint*: `EssentialBoundaryCondition` is defined in `core/Definitions.h`.

**Problem 2: periodic BCs (50 points).**

Implement the above new code structure in our finite element code and test it for a homogeneous RVE (using, e.g., CST elements and a Neo-Hookean material model in 2D – you will have to modify the existing 3D Neo-Hookean model for this purpose). Use the tools from set #7 to compute $\langle \boldsymbol{P} \rangle$.

Note that, when applying $\boldsymbol{F}^*$ to a homogeneous RVE, you can expect a uniform solution so that $\langle \boldsymbol{P} \rangle = \boldsymbol{P}(\boldsymbol{F}^*)$, which can be used to verify the accuracy of the scheme.

**Problem 3: homogenization (20 points).**

Use your new code structure to compute the response of the random microstructure of problem set #1 (using the Neo-Hookean model here). Compute the stress-strain response under uniaxial straining using periodic boundary conditions (i.e., apply a stretch $\lambda$ in the loading direction, while the RVE is stress-free in the transverse directions).

**Problem 4: project (5 points).**

Decide on a topic for your final project, which should involve the theory discussed and/or tools developed during this class. For example, use the homogenization techniques developed above in order to determine the effective response of a particular material with microstructure and investigate the influence of choice of boundary conditions.

*total: 100 points*

**Note**: You are welcome to solve this problem set in a *team of 1–3 students* – choose wisely so that the team can stay together for the final project as well (you are, of course, welcome to choose a different team for the final project but it may help to use the same team since the code developed here may be used).