Dynamic Homogenization Technique

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For single scale dynamic problem, the equilibrium equation takes the following form:

 $\frac{d}{dt}\Phi - \nabla_0 \cdot P = 0 \tag{1}$

where $\Phi = \rho_0 \dot{u}$, P is the 1st PK stress, the subindex 0 of ∇ is represent the gradient with respect to material coordinate.

For multiscale problem, the material properties and also the equilibrium equation at the microscale is known, *the goal* is to homogenize the microscale information to get a homogeneous macroscale medium. Specifically saying, the equilibrium equation at microscale is,

$$\frac{d}{dt}\Phi_m - \nabla_{0m} \cdot P_m = 0 \tag{2}$$

where $\Phi_m = \rho_{0m}\dot{u}_m$. The homogenized macroscale medium should also satisfy the equilibrium equation with the form of

$$\frac{d}{dt}\Phi_M - \nabla_{0M} \cdot P_M = 0 \tag{3}$$

where $\Phi_M = \rho_{0M} \dot{u}_M$. The problem is how to extract the microscale information in order to properly define the macroscopic quantities Φ_M and P_M . Indeed, equation 3 needs to be complemented by the effective constitutive behavior that links the macroscopic kinematic quantities (\dot{u}_M, F^M) (velocity and deformation) to their dual quantities (Φ_M, P_M) (macroscopic linear momentum and stress)¹.

Of course, one natural idea is to average every microscopic physical quantity, for instance, 1st PK stress P, deformation gradient F and strain energy density W, over the RVE domain. For example,

$$P_M = \langle P_m \rangle = \frac{1}{|\Omega_{0m}|} \int_{\Omega_{0m}} P_m d\Omega_{0m} \tag{4}$$

As we already known, equation (4) is verified to be a good assumption for quasistatic problem. However, this average technique is not always appropriate for every physical quantity in dynamic problem. In other words, the rule of mixture is not always appropriate for multiscale modeling of dynamic problem.

1 Rule of mixture

Let me take the linear momentum Φ as an example. The macroscopic momentum $\Phi_M = \rho_M \dot{u}_M$. One would say that just use the rule of mixture for the density, namely, for a two-phase material shown in Fig. 1 the macroscopic density is defined as,

$$\rho_M = \rho_1 \chi_1 + \rho_2 \chi_2 \tag{5}$$

where volumetric fraction $\chi_1 = \frac{|\Omega_1|}{|\Omega|}$, $\chi_2 = \frac{|\Omega_2|}{|\Omega|}$, $\chi_1 + \chi_2 = 1$. This is true for law frequency (long wave length). The reasoning process is shown below,

¹The tensor and vector in this document is not made bold explicitly, it should be self-explanatory.

The displacement field is

$$u_m = u_M + (F_M - I) \cdot (X - X_M) + w \tag{6}$$

Therefore the velocity field is:

$$\dot{u}_m = \dot{u}_M + \dot{F}_M \cdot (X - X_M) + \dot{w} \tag{7}$$

The averaged momentum is calculated as,

$$\Phi_{M} = \frac{1}{V_{0}} \int_{V_{0}} \rho \dot{u} dV_{0}$$

$$= (\rho_{1}\chi_{1} + \rho_{2}\chi_{2})\dot{u}_{M} + \frac{1}{V_{0}}\dot{F}_{M} \cdot \int_{V_{0}} \rho(X - X_{M}) dV_{0} + \frac{1}{V_{0}} \int_{V_{0}} \rho \dot{w} dV_{0}$$

$$\approx (\rho_{1}\chi_{1} + \rho_{2}\chi_{2})\dot{u}_{M} + \frac{1}{V_{0}} \int_{V_{0}} \rho \dot{w} dV_{0}$$

$$\approx (\rho_{1}\chi_{1} + \rho_{2}\chi_{2})\dot{u}_{M} + (\frac{1}{V_{0}} \int_{V_{0}} \rho dV_{0}) \cdot (\frac{1}{V_{0}} \int_{V_{0}} \dot{w} dV_{0})$$

$$= \langle \rho \rangle (\dot{u}_{M} + \langle \dot{w} \rangle)$$

$$= \langle \rho \rangle \langle \dot{u} \rangle$$
(8)

In the above derivation, the following conditions are used: $\dot{F}_M \approx 0$, $\langle \rho \dot{w} \rangle \approx \langle \rho \rangle \langle \dot{w} \rangle$. Therefore, it can be observed that the macroscopic velocity is related to the momentum by the averaged density $\langle \rho \rangle$. In other words, the rule of mixture is still valid at this scenario.

However, as long as the long wave assumption is not valid, the rule of mixture is no longer valid. This means that for dynamic problem, the macroscopic momentum is not always equal to the multiply of averaged density and averaged velocity. For multiscale problem, averaging is not always working.

2 Kinematic assumptions

The kinematic assumptions employed are:

$$u_m = u_M + (F_M - I) \cdot (X - X_M) + w \tag{9}$$

To satisfy the condition of $F^M = \langle F^m \rangle$, the fluctuation term w has to be periodic.

Remark. In this document, the separation of scales is assumed. Specifically saying, if we call l_k the typical size of the k-th microstructural constituent in the RVE e.g. the characteristic size of the cavities, grains. The separation of scale says that

$$l_k < \lambda_k \tag{10}$$

where λ_k is the shortest characteristic wavelength in the k-th constituents of the RVE. This is a relaxation of long wave length assumption, i.e. $l_k \ll \lambda_k$, in which the micro-inertia effect is generally not present.

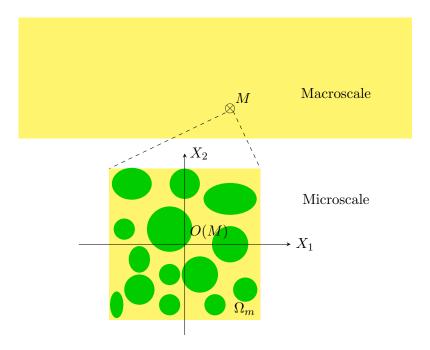


Figure 1: Two scales

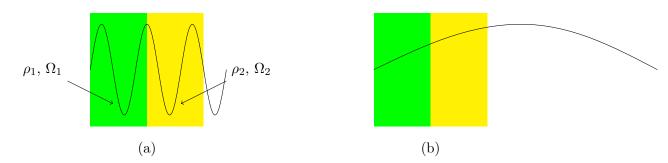


Figure 2: Real material constituents(phase 1 and 2) of RVE. (a) short wave length; (b) long wave length.

3 Definition of macroscopic stress

There are several ways to derive the definition of macroscopic stress, including asymptotic homogenization (Fish et al., 2012), generalized Hill-Mandel condition (Pham et al., 2013) and variational principle (Liu and Reina, 2017). These methods, however, arrives at similar definition (although some uses Cauchy stress for infinitesimal deformation others may use 1st PK stress for finite deformation). The effect of micro-inertia is introducing a inertia force at the macroscale, so the macroscopic equilibrium is enriched with a micro-inertia term. This is seen from,

1. Asymptotic homogenization leads to an equilibrium equation at macroscopic scale like,

$$\frac{\partial}{\partial x_j^M} \left(\sigma_{ij}^M + \zeta^2 D_{ijkl} \ddot{\varepsilon}_{kl}^M \right) = \rho^M \ddot{u}_i^M \tag{11}$$

The second term at the LHS represents the inertia force, in which D_{ijkl} is called dispersion tensor.

2. Generalized Hill-Mandel condition of the following form,

$$P: \delta F - f \cdot \delta u = \frac{1}{|\Omega_{\mu}|} \int_{\Omega_{\mu}} (P_{\mu}: \delta F_{\mu} + \rho_{\mu} \ddot{u}_{\mu} \cdot \delta u_{\mu}) d\Omega_{\mu}$$
 (12)

derives a macroscopic 1st PK stress,

$$P^{M} = \frac{1}{|\Omega_{m}^{0}|} \int_{\Omega_{m}^{0}} P^{m} d\Omega_{m}^{0} + \frac{1}{|\Omega_{m}^{0}|} \frac{d}{dt} \left(\int_{\Omega_{m}^{0}} p^{m} \otimes (X^{m} - X^{M}) d\Omega_{m}^{0} \right)$$
(13)

where microscopic momentum $p^m = \rho^m \dot{u}^m$. The first term at RHS of equation (4) is defined as the macroscopic stress for static problem. The second term at RHS of equation (4) represents the contribution of microinertia.

3. Variational technique based on the stationary potential energy starts with the following variational form,

min
$$\Pi(\varphi^M) = \int_{\Omega_0} W^M(\varphi^M, \nabla^M \varphi^M) dV^M - \int_{\partial \Omega_\sigma} \overline{T}^M \cdot \varphi^M dS^M$$
 (14)

This will give the strong form of the macroscopic problem:

$$\frac{\partial W^M}{\partial \varphi^M} - \nabla^M \cdot \frac{\partial W^M}{\partial F^M} = 0, \quad in \ \Omega$$
 (15)

$$\frac{\partial W^M}{\partial F^M} \cdot N^M - \overline{T}^M = 0, \quad @ \partial \Omega_{\sigma}$$
 (16)

Therefore the definition of macroscopic stress becomes,

$$P^{M} = \frac{\partial W^{M}}{\partial F^{M}} = \frac{\partial \langle W^{m} \rangle}{\partial \langle F^{m} \rangle} = \langle P^{m} + \rho_{0} \ddot{\varphi}^{m} \otimes X^{m} \rangle \tag{17}$$

where the energetic consistency condition $W^M = \langle W^m \rangle$ and kinematic assumption $F^M = \langle F^m \rangle$ are used in the above equation. The last equality comes from elaborate mathematical manipulations so it is not mentioned here

From the equation (8), it is also seen that the micro-inertia acts a inertia force in the macroscopic scale, this form is the same as the second method and is comparable to the first method.

4 Consistent tangent

For the FE² approach, the macroscopic consistent tangent is needed to perform global Newton-Raphson scheme at macroscopic scale. For static problem without body force, the static condensation technique is used to achieve this goal.

• Direct enforcement (elimination of dependent DOFs);

$${}^{4}C^{M} = \frac{1}{V_{0}} \sum_{i=1,2,4} \sum_{j=1,2,4} \left(X_{(i)} K_{M}^{\star(ij)} X_{(j)} \right)^{LC}$$
(18)

where the superscript LC denotes left conjugation, which for a fourth-order tensor ${}^{4}T$ is defined as $T_{ijkl}^{LC} = T_{jikl}$.

- Penalty approach (Temizer and Wriggers, 2008);
- Lagrangian Multiplier (Miehe and Bayreuther, 2007);

Now, the problem is how to define a proper consistent tangent for dynamic problem. I proceed with the first method (Direct enforcement) while the other two methods are **not** considered in this document.

4.1 Consistent tangent for quasi-statics

The direct enforcement method eliminates the dependent DOFs from the system equation and the extraction consistent tangent only needs the information of prescribed nodes $\{1,2,4\}$.

4.1.1 Elimination of dependent DOFs

Let me take a RVE consisted of 4 elements and 9 nodes as an example (Fig. 3). In this case, the nodes {9, 8, 3} are dependent nodes and nodes {1, 2, 4, 6, 5, 7} are independent nodes. When the periodic boundary condition is applied, namely,

$$u_T = u_B + u_4 - u_1 \tag{19}$$

$$u_R = u_L + u_2 - u_1 \tag{20}$$

Expanding the equations 19 and 20, we can get

$$u_{9x} = u_{5x} + u_{4x} - u_{1x} (21)$$

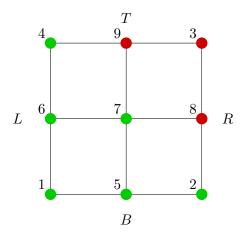


Figure 3: RVE mesh discretization (red circle—dependent nodes; green circle—independent nodes)

$$u_{9y} = u_{5y} + u_{4y} - u_{1y} (22)$$

$$u_{8x} = u_{6x} + u_{2x} - u_{1x} (23)$$

$$u_{8y} = u_{6y} + u_{2y} - u_{1y} (24)$$

$$u_{3x} = u_{4x} + u_{2x} - u_{1x} (25)$$

$$u_{3y} = u_{4y} + u_{2y} - u_{1y} (26)$$

The constraints equation can be further rewritten into matrix format,

$$\begin{bmatrix} C_i & C_d \end{bmatrix} \begin{bmatrix} u_i \\ u_d \end{bmatrix} = 0 \tag{27}$$

where the matrix C_i and C_d containing the constraint coefficients are defined as:

$$C_d = \begin{bmatrix} 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \end{bmatrix}_{6\times6}$$

$$(29)$$

and the independent DOFs u_i and dependent DOFs u_d are defined as,

$$u_{i} = [u_{1x}, u_{1y}, u_{2x}, u_{2y}, u_{4x}, u_{4y}, u_{5x}, u_{5y}, u_{6x}, u_{6y}, u_{7x}, u_{7y}]_{12 \times 1}^{T}$$
(30)

$$u_d = [u_{3x}, u_{3y}, u_{8x}, u_{8y}, u_{9x}, u_{9y}]_{6 \times 1}^T$$
(31)

Solve for the dependent displacements yields,

$$u_d = C_{di}u_i \quad \text{with} \quad C_{di} = -C_d^{-1}C_i \tag{32}$$

Using equation 32, the nodal displacement can be further rewritten as

$$u = \begin{bmatrix} u_i \\ u_d \end{bmatrix} = \begin{bmatrix} u_i \\ C_{di}u_i \end{bmatrix} = \begin{bmatrix} I \\ C_{di} \end{bmatrix} u_i = Tu_i, \text{ with } T = \begin{bmatrix} I \\ C_{di} \end{bmatrix}$$
 (33)

The system equation $K\delta u = \delta r$ is expanded as²,

$$\begin{bmatrix} (K_{ii})_{12\times12} & (K_{id})_{12\times6} \\ (K_{di})_{6\times12} & (K_{dd})_{6\times6} \end{bmatrix} \begin{bmatrix} \delta u_i \\ \delta u_d \end{bmatrix} = \begin{bmatrix} \delta f_i \\ \delta f_d \end{bmatrix}$$
(34)

Substitution of equation 33 into equation 34 and solve for the independent DOFs lead to the following reduced system equation,

$$K^{\star}\delta u_i = \delta f^{\star} \tag{35}$$

with,

$$K^{\star} = K_{ii} + K_{id}C_{di} + C_{di}^{T}K_{di} + C_{di}^{T}K_{dd}C_{di}$$
(36)

$$\delta f^{\star} = \delta f_i + C_{di}^T \delta f_d \tag{37}$$

4.1.2 Extraction only prescribed nodes

Independent dofs δu_i can be further split into prescribed δu_p and remaining free δu_f dofs. In this case, $\{1,2,4\}$ are prescribed nodes and $\{5,6,7\}$ are remaining free nodes³.

$$\begin{bmatrix} (K_{pp}^{\star})_{6\times6} & (K_{pf}^{\star})_{6\times6} \\ (K_{fp}^{\star})_{6\times6} & (K_{ff}^{\star})_{6\times6} \end{bmatrix} \begin{bmatrix} (\delta u_p)_{6\times1} \\ (\delta u_f)_{6\times1} \end{bmatrix} = \begin{bmatrix} (\delta f_p^{\star})_{6\times1} \\ (0)_{6\times1} \end{bmatrix}$$
(38)

The microscopic reduced stiffness matrix K_M^{\star}

$$(K_M^{\star})_{6\times 6}(\delta u_p)_{6\times 1} = (\delta f_p^{\star})_{6\times 1}, \text{ with } K_M^{\star} = K_{pp}^{\star} - K_{pf}^{\star}(K_{ff}^{\star})^{-1}K_{fp}^{\star}$$
 (39)

Divide the K_M^{\star} into submatrixs,

$$K_{M}^{\star} = \begin{bmatrix} \begin{bmatrix} K_{11}^{(11)} & K_{12}^{(11)} \\ K_{21}^{(11)} & K_{22}^{(11)} \end{bmatrix} & \begin{bmatrix} K_{11}^{(12)} & K_{12}^{(12)} \\ K_{21}^{(12)} & K_{22}^{(12)} \end{bmatrix} & \begin{bmatrix} K_{11}^{(14)} & K_{12}^{(14)} \\ K_{21}^{(14)} & K_{22}^{(14)} \end{bmatrix} \\ \begin{bmatrix} K_{11}^{(21)} & K_{12}^{(21)} \\ K_{21}^{(21)} & K_{22}^{(21)} \end{bmatrix} & \begin{bmatrix} K_{12}^{(22)} & K_{12}^{(22)} \\ K_{21}^{(22)} & K_{22}^{(22)} \end{bmatrix} & \begin{bmatrix} K_{11}^{(24)} & K_{12}^{(24)} \\ K_{21}^{(24)} & K_{22}^{(24)} \end{bmatrix} \\ \begin{bmatrix} K_{11}^{(41)} & K_{12}^{(41)} \\ K_{21}^{(41)} & K_{22}^{(41)} \end{bmatrix} & \begin{bmatrix} K_{11}^{(42)} & K_{12}^{(42)} \\ K_{21}^{(42)} & K_{22}^{(42)} \end{bmatrix} & \begin{bmatrix} K_{11}^{(44)} & K_{12}^{(44)} \\ K_{21}^{(44)} & K_{22}^{(44)} \end{bmatrix} \end{bmatrix}_{6 \times 6}$$

²The derivation in this document are based on the assumption that the material is elastic. Extension to inelastic material maybe straightforward.

³The components corresponding to the remaining free nodes $\{5,6,7\}$ in the nodal force vector δf^* is zero. The reason for that is explained in the "Remark" of this section.

Rewrite equation 39 as,

$$\sum_{j=1,2,4} K_M^{\star(ij)} \cdot \delta u_{(j)} = \delta f_{(i)}, \quad i = 1, 2, 4$$
(41)

where the sub-matrix $K_M^{\star(ij)}$ is

$$K_M^{\star(ij)} = \begin{bmatrix} K_{11}^{(ij)} & K_{12}^{(ij)} \\ K_{21}^{(ij)} & K_{22}^{(ij)} \end{bmatrix}, \quad \text{with} \quad i, j = 1, 2, 4$$
 (42)

$$\delta u_{(j)} = \begin{bmatrix} \delta u_{jx} \\ \delta u_{jy} \end{bmatrix}, \text{ with } j = 1, 2, 4$$
 (43)

Remark. Notice that the nodal force components of δf^* corresponding to the nodes $\{5,6,7\}$ is zero. This can be understood by looking at the same RVE shown in Fig. 4.

The periodicity condition Equation 19 and 20 is applied for the outer surface. For FEM discretization, this can be realized by applying the periodic boundary condition at the nodes of mesh, namely,

$$u_9 = u_5 + u_4 - u_1 \tag{44}$$

$$u_8 = u_6 + u_2 - u_1 \tag{45}$$

$$u_3 = u_4 + u_2 - u_1 \tag{46}$$

This fact can be derived by using FEM shape function. For a point located between point 4 and point 9 on the upper edge, the displacement is

$$u_T(x) = L_1(x)u_4 + L_2(x)u_9 (47)$$

The displcement of the corresponding point on the lower edge is,

$$u_B(x) = L_1(x)u_1 + L_2(x)u_5 \tag{48}$$

Therefore, using equation 47, 48 and 44 we can get,

$$u_{T}(x) - u_{B}(x) = L_{1}(x)(u_{4} - u_{1}) + L_{2}(x)(u_{9} - u_{5})$$

$$= L_{1}(x)(u_{4} - u_{1}) + L_{2}(x)(u_{4} - u_{1})$$

$$= (u_{4} - u_{1})(L_{1}(x) + L_{2}(x))$$

$$= (u_{4} - u_{1})$$

$$(49)$$

where the $L_1(x)$ and $L_2(x)$ are the 1st order Lagrangian interpolation function. The periodicity condition Equation 19 is recovered. Similarly, the periodicity condition Equation 20 can also be recovered.

For simplicity reason, it is assumed that the nodal force at y-direction is zero. This does not influence the conclusion. As it is shown in Fig. 4, the nodal force

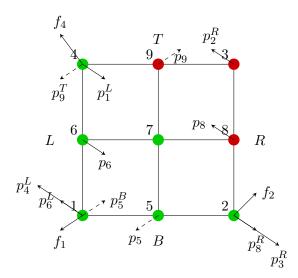


Figure 4: RVE mesh discretization (red circle—dependent nodes; green circle—independent nodes)

is (see Equation 34),

$$\delta f_{i} = \begin{bmatrix} p_{4}^{L} + p_{6}^{L} + f_{1} + p_{5}^{B} \\ 0 \\ p_{8}^{R} + p_{3}^{R} + f_{2} \\ 0 \\ f_{4} + p_{1}^{L} + p_{9}^{T} \\ 0 \\ p_{5} \\ 0 \\ p_{6} \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$(50)$$

$$\delta f_d = \begin{bmatrix} p_2^R + p_4^T \\ 0 \\ p_8 \\ 0 \\ p_9 \\ 0 \end{bmatrix}$$
 (51)

The dependent matrix C_{di} is calculated as (Equation 32),

According to the condition that the virtual work of the constraint force is zero. The following relations are valid,

$$p_6^L = -p_6 = p_8 = -p_8^R (53)$$

$$p_4^L = -p_1^L = p_2^R = -p_3^R (54)$$

$$p_5^B = -p_5 = p_9 = -p_9^T (55)$$

Use equations 53, 54, 55, 52 and 37,

$$\delta f^{\star} = \begin{bmatrix} \delta f_{1} - \delta p_{8} - \delta p_{9} + + \delta p_{5}^{B} + \delta p_{4}^{L} + \delta p_{6}^{L} - \delta p_{2}^{R} \\ 0 \\ \delta f_{2} + \delta p_{8} + \delta p_{2}^{R} + \delta p_{3}^{R} + \delta p_{8}^{R} \\ 0 \\ \delta f_{4} + \delta p_{9} + \delta p_{1}^{L} + \delta p_{2}^{R} + \delta p_{9}^{T} \\ 0 \\ \delta p_{5} + \delta p_{9} \\ 0 \\ \delta p_{6} + \delta p_{8} \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} \delta f_{1} \\ 0 \\ \delta f_{2} \\ 0 \\ \delta f_{4} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$= \begin{bmatrix} (\delta f_{p})_{6 \times 6} \\ (0)_{6 \times 6} \end{bmatrix}$$

$$\delta f_{4} + \delta p_{9} + \delta p_{1}^{L} + \delta p_{2}^{R} + \delta p_{3}^{R} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$= \begin{bmatrix} (\delta f_{p})_{6 \times 6} \\ (0)_{6 \times 6} \end{bmatrix}$$

$$\delta f_{4} + \delta p_{9} + \delta p_{1} + \delta p_{2} + \delta p_{3} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$= \begin{bmatrix} (\delta f_{p})_{6 \times 6} \\ (\delta f_{p})_{6 \times 6} \\ (\delta f_{p})_{6 \times 6} \end{bmatrix}$$

$$\delta f_{4} + \delta p_{9} + \delta p_{1} + \delta p_{2} + \delta p_{3} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$(56)$$

4.1.3 Definition of consistent tangent

Variation of displacements of the prescribed nodes $\{1,2,4\}$ according to the macroscopic deformation gradient F_M^4 ,

$$\delta u_{(j)} = \delta F_M \cdot X_{(j)}, \quad \text{with} \quad j = 1, 2, 4 \tag{57}$$

The variation of macroscopic stress tensor is calculated as⁵:

$$\delta P_M = \frac{1}{V_0} \sum_{p=1,2,4} \delta f_p X_p \tag{58}$$

Substitutions equations 41 and 57 into equation 58,

$$\delta P_{M} = \frac{1}{V_{0}} \sum_{i=1,2,4} \sum_{j=1,2,4} (K_{M}^{\star(ij)} \cdot \delta u_{(j)}) X_{(i)}
= \frac{1}{V_{0}} \sum_{i=1,2,4} \sum_{j=1,2,4} (K_{M}^{\star(ij)} \cdot \delta F_{M} \cdot X_{(j)}) X_{(i)}$$
(59)

Therefore, the constitutive tangent is identified as:

$${}^{4}C^{M} = \frac{1}{V_{0}} \sum_{i=1,2,4} \sum_{j=1,2,4} \left(X_{(i)} K_{M}^{\star(ij)} X_{(j)} \right)^{LC}$$

$$(60)$$

where the superscript LC denotes left conjugation, which for a fourth-order tensor 4T is defined as $T_{ijkl}^{LC} = T_{jikl}$.

⁴At prescribed nodes, the fluctuation term w in Equ. 9 is zero.

⁵The equation 58 will be justified in the next section

4.1.4 Constraint force

The application of periodic displacement boundary condition introduces constraint forces at the boundary of the RVE. There are three kinds of constrain forces introduced. The first one is the externally applied force to impose the prescribed boundary condition at points $\{1,2,4\}$. The second one is tying force introduced to impose the periodic boundary condition between the left (L) edge and right (R) edge of the RVE. The third one is tying forces between the top (T) edge and bottom (B) edge⁶.

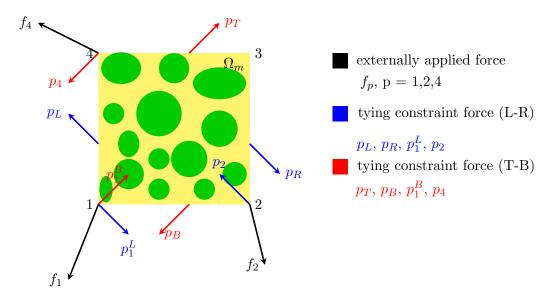


Figure 5: constraint forces

The constraints are:

$$u_T = u_B + u_4 - u_1 (61)$$

$$u_R = u_L + u_2 - u_1 \tag{62}$$

The constraint force should do zero virtual work.

$$p_T \delta u_T + p_B \delta u_B + p_4 \delta u_4 + p_1^B \delta u_1 = 0$$
 (63)

Remark. The fact that the constraint force should do zero virtual work is the property of constraint force. It can be understood by looking at a simple pendulum problem as shown in Fig. 6. The constraint forces f_1 applied to the ball is always perpendicular to the virtual displacement direction so the virtual work will always be zero. While the constraint force f_2 applied to the fixed base of course does zero virtual work. Namely, $\delta W_{cons} = f_1 \cdot \delta u_1 + f_2 \cdot \delta u_2 \equiv 0$.

⁶Herein, we apply the constraint force for every point in the surface. However, at the end of this section, another way of looking at this problem based on FEM discretization is presented at the "Remark".

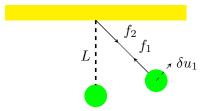


Figure 6: Pendulum problem

Substitution equations 61 into equation 63,

$$0 = p_T(\delta u_B + \delta u_4 - \delta u_1) + p_B \delta u_B + p_4 \delta u_4 + p_1^B \delta u_1 = (p_T + p_B) \delta u_B + (p_T + p_4) \delta u_4 + (p_1^B - p_T) \delta u_1$$
(64)

Considering the arbitrary of the virtual displacement δu_B , δu_4 and δu_1 , the following relation should be valid,

$$p_B = -p_T = -p_1^B = p_4 (65)$$

Likewise, the constrain force tying the left and right edge should also do zero virtual work. It means,

$$p_L \delta u_L + p_R \delta u_R + p_2 \delta u_2 + p_1^L \delta u_1 = 0 \tag{66}$$

Substitution of equation 62 into equation 66 will lead to

$$p_L = -p_R = -p_1^L = p_2 (67)$$

The definition of macroscopic stress tensor is

$$P_M = \frac{1}{V_0} \int_{S_0} p \otimes X dS_0 \tag{68}$$

where p is the surface traction show in Fig. 5.

Use equations 65, 67 and the following periodicity conditions on the RVE geometry,

$$X_T - X_B = X_4 - X_1 (69)$$

$$X_R - X_L = X_2 - X_1 (70)$$

The macroscopic stress can be simplified by (dyadic product \otimes is omitted for

clarity)

$$\begin{split} P_{M} &= \frac{1}{V_{0}} \bigg(\int_{S_{T}} p_{T} X_{T} dS + \int_{S_{T}} p_{4} X_{4} dS + \int_{S_{B}} p_{B} X_{B} dS + \int_{S_{B}} p_{1}^{B} X_{1} dS \\ &+ \int_{S_{R}} p_{R} X_{R} dS + \int_{S_{L}} p_{L} X_{L} dS + \int_{S_{R}} p_{2} X_{2} dS + \int_{S_{T}} p_{1}^{L} X_{1} dS \\ &+ f_{1} X_{1} + f_{2} X_{2} + f_{4} X_{4} \bigg) \\ &= \frac{1}{V_{0}} \bigg(\int_{S_{T}} p_{T} X_{T} dS + \int_{S_{T}} p_{4} X_{4} dS + \int_{S_{B}} -p_{T} X_{B} dS + \int_{S_{B}} p_{1}^{B} X_{1} dS \\ &+ \int_{S_{R}} p_{R} X_{R} dS + \int_{S_{L}} -p_{R} X_{L} dS + \int_{S_{R}} p_{2} X_{2} dS + \int_{S_{T}} p_{1}^{L} X_{1} dS \bigg) \\ &+ \frac{1}{V_{0}} \sum_{p=1,2,4} f_{p} X_{p} \\ &= \frac{1}{V_{0}} \bigg(\int_{S_{T}} p_{T} (X_{T} - X_{B}) dS + \int_{S_{R}} p_{4} X_{4} dS + \int_{S_{R}} -p_{4} X_{1} dS \\ &+ \int_{S_{R}} p_{R} (X_{R} - X_{L}) dS + \int_{S_{R}} p_{2} X_{2} dS + \int_{S_{T}} -p_{2} X_{1} dS \bigg) \\ &+ \frac{1}{V_{0}} \sum_{p=1,2,4} f_{p} X_{p} \\ &= \frac{1}{V_{0}} \bigg(\int_{S_{T}} p_{T} (X_{T} - X_{B}) dS + \int_{S_{T}} p_{4} (X_{4} - X_{1}) dS \\ &+ \int_{S_{R}} p_{R} (X_{R} - X_{L}) dS + \int_{S_{R}} p_{2} (X_{2} - X_{1}) dS \bigg) + \frac{1}{V_{0}} \sum_{p=1,2,4} f_{p} X_{p} \\ &= \frac{1}{V_{0}} \sum_{p=1,2,4} f_{p} X_{p} \end{split}$$

Remark. The same conclusion can be derived by using FEM discretization. For a RVE shown in Fig. 4, the constraint forces are only applied at nodes on the

surface. The calculation of macroscopic stress P_M becomes,

$$P_{M} = \frac{1}{V_{0}} \int_{S_{0}} p \otimes X dS_{0}$$

$$= \frac{1}{V_{0}} \left((f_{1} + p_{4}^{L} + p_{6}^{L} + p_{5}^{B}) X_{1} + (p_{8}^{R} + p_{3}^{R} + f_{2}) X_{2} + p_{2}^{R} X_{3} + (p_{9}^{T} + p_{1}^{L} + f_{4}) X_{4} + p_{5} X_{5} + p_{6} X_{6} + p_{8} X_{8} + p_{9} X_{9}) \right)$$

$$= \frac{1}{V_{0}} \sum_{p=1,2,4} f_{p} X_{p} + \frac{1}{V_{0}} \left((-p_{1}^{L} + p_{8} + p_{9}) X_{1} + (-p_{8} + p_{1}^{L}) X_{2} - p_{1}^{L} X_{3} + (-p_{9} + p_{1}^{L}) X_{4} - p_{9} X_{5} - p_{8} X_{6} + p_{8} X_{8} + p_{9} X_{9} \right)$$

$$= \frac{1}{V_{0}} \sum_{p=1,2,4} f_{p} X_{p} + \frac{1}{V_{0}} \left(p_{1}^{L} (-X_{1} + X_{2} - X_{3} + X_{4}) + p_{8} (X_{1} - X_{2} - X_{6} + X_{8}) + p_{9} (X_{1} - X_{4} - X_{5} + X_{9}) \right)$$

$$= \frac{1}{V_{0}} \sum_{p=1,2,4} f_{p} X_{p}$$

In the above derivation, equations 53, 54, 55, 69 and 70 are used.

4.2 Consistent tangent for dynamics

For dynamic problem, the following scale transition rule is true,

$$\Phi_M = \frac{1}{V_0} \int_{V_0} \Phi_m dV_0 \tag{71}$$

$$P_{M} = \frac{1}{V_{0}} \int_{V_{0}} P_{m} dV_{0} + \frac{1}{V_{0}} \frac{d}{dt} \left(\int_{V_{0}} \Phi_{m} \otimes (X - X_{M}) dV_{0} \right)$$

$$= \frac{1}{V_{0}} \int_{S_{0}} (P_{m} \cdot N_{m}) \otimes (X - X_{M}) dS_{0}$$

$$(72)$$

The goal is to find the consistent tangent matrix,

$$\delta P_M = {}^{4}C_M^{(1)} : \delta F_M + {}^{3}C_M^{(2)} \cdot \delta u_M \tag{73}$$

$$\delta\Phi_M = {}^{3}C_M^{(3)} : \delta F_M + {}^{2}C_M^{(4)} \cdot \delta u_M \tag{74}$$

4.2.1 Kinematic assumption

The kinematic assumption of the form shown below is introduced⁷,

$$u_m = u_M + (F_M - I) \cdot X + w \tag{75}$$

In order to satisfy the condition that $F_M = \langle F_m \rangle$, the fluctuation term w should be periodic.

To remove the rigid body motion, the following two conditions are introduced,

$$w_{n_1} = w_{n_2} = w_{n_4} = 0 (76)$$

 $^{^{7}}X_{M}=0$

$$u_M = \frac{1}{V_0} \int_{V_0} u_m dV_0 \tag{77}$$

The first condition says that the fluctutation term at nodes $\{1,2,4\}$ is zero. The second condition says that the averaged displacement in RVE is equal to the macroscopic displacement u_M .

The expansion of Equation 77 is,

$$u_{M} = \frac{1}{V_{0}} \int_{V_{0}} (u_{M} + (F_{M} - I) \cdot X + w) dV_{0}$$

$$= u_{M} + \frac{1}{V_{0}} \int_{V_{0}} w dV_{0}$$
(78)

This means that,

$$\frac{1}{V_0} \int_{V_0} w dV_0 = 0 \tag{79}$$

Remark. For FEM implementation of the equ. 77, it means that one more dependent DOF is introduced. This is because,

$$\frac{1}{V_0} \int_{V_0} \sum_{k=1,2,\dots,n_{total}} N_m^k u_m^k dV_0 = u_M$$
 (80)

$$\sum_{k=1,2,\dots,n_{total}} \left(\frac{1}{V_0} \int_{V_0} N_m^k dV_0 \right) u_m^k = u_M$$
 (81)

If we define $c^k := \frac{1}{V_0} \int_{V_0} N_m^k dV_0$, then

$$\sum_{k=1,2,\dots,n_{total}} c^k u_m^k = u_M \tag{82}$$

The variation of the above equation gives,

$$\sum_{k=1,2,\dots,n_{total}} c^k \delta u_m^k = 0 \tag{83}$$

This means that the constraints applied is a holonomic constraint. As we know that a holonomic constraint reduces the number of degrees of freedom. The constraint force for each node is therefore identified as c^k .

4.2.2 dynamic condensation

Let me take a RVE consisted of 4 elements and 9 nodes as an example (Fig. 9). In this case, the nodes {9, 8, 3} are dependent nodes and nodes {1, 2, 4, 6, 5, 7} are independent nodes. When the periodic boundary condition is applied, namely,

$$u_T = u_B + u_4 - u_1 (84)$$

$$u_R = u_L + u_2 - u_1 \tag{85}$$

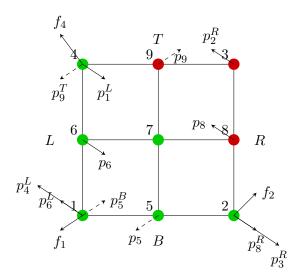


Figure 7: RVE mesh discretization (red circle—dependent nodes; green circle—independent nodes)

Expanding the equations 84 and 85, we can get

$$u_{9x} = u_{5x} + u_{4x} - u_{1x} (86)$$

$$u_{9y} = u_{5y} + u_{4y} - u_{1y} (87)$$

$$u_{8x} = u_{6x} + u_{2x} - u_{1x} (88)$$

$$u_{8y} = u_{6y} + u_{2y} - u_{1y} (89)$$

$$u_{3x} = u_{4x} + u_{2x} - u_{1x} (90)$$

$$u_{3y} = u_{4y} + u_{2y} - u_{1y} (91)$$

Following the same condensation process presented at Section 4.1.1, the nodal displacement can be further rewritten as

$$u = \begin{bmatrix} u_i \\ u_d \end{bmatrix} = \begin{bmatrix} u_i \\ C_{di}u_i \end{bmatrix} = \begin{bmatrix} I \\ C_{di} \end{bmatrix} u_i = Tu_i, \text{ with } T = \begin{bmatrix} I \\ C_{di} \end{bmatrix}$$
 (92)

Remark. The system equation for dynamic problem is normally expressed as,

$$f_{\rm in}^t(\Delta u) + M\ddot{u}^t = f_{\rm ext}^t \tag{93}$$

Take the variance of both sides of equ. 93, it yields,

$$\delta f_{\text{ext}}^t = \delta f_{\text{in}}^t (\Delta u) + M \delta \ddot{u}^t
= K \delta u + M \delta \ddot{u}^t$$
(94)

This also applies for nonlinear materiality.

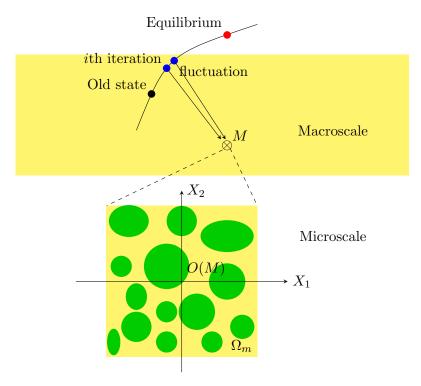


Figure 8: Two scales

The system equation 94 is further expanded as,

$$\begin{bmatrix} (K_{ii})_{12\times12} & (K_{id})_{12\times6} \\ (K_{di})_{6\times12} & (K_{dd})_{6\times6} \end{bmatrix} \begin{bmatrix} \delta u_i \\ \delta u_d \end{bmatrix} + \begin{bmatrix} (M_{ii})_{12\times12} & (M_{id})_{12\times6} \\ (M_{di})_{6\times12} & (M_{dd})_{6\times6} \end{bmatrix} \begin{bmatrix} \delta \ddot{u}_i \\ \delta \ddot{u}_d \end{bmatrix} = \begin{bmatrix} \delta f_i \\ \delta f_d \end{bmatrix}$$
(95)

Substitution of equation 92 into equation 95 and solve for the independent DOFs lead to the following reduced system equation,

$$K^{\star}\delta u_i + M^{\star}\delta \ddot{u}_i = \delta f^{\star} \tag{96}$$

with,

$$K^* = K_{ii} + K_{id}C_{di} + C_{di}^T K_{di} + C_{di}^T K_{dd}C_{di}$$
(97)

$$M^* = M_{ii} + M_{id}C_{di} + C_{di}^T M_{di} + C_{di}^T M_{dd}C_{di}$$
(98)

$$\delta f^{\star} = \delta f_i + C_{di}^T \delta f_d \tag{99}$$

Introducing the Newmark time discretization into equation 96 and consider it at time step n + 1,

$$\delta f^{\star,n+1} = K^{\star} \delta u_i^{n+1} + M^{\star} \delta \ddot{u}_i^{n+1}
= K^{\star} \delta u_i^{n+1} + M^{\star} (c_0 \delta u_i^{n+1})
= (K^{\star} + c_0 M^{\star}) \delta u_i^{n+1}
= \overline{K} \delta u_i^{n+1}$$
(100)

where a new stiffness matrix $\overline{K} := K^* + c_0 M^*$ and c_0 is a coefficient related to Newmark- β time integration scheme.

Remark. According to the Newmark- β time integration scheme, the acceleration and velocity at time step n + 1 are,

$$\ddot{u}^{n+1} = c_0(u^{n+1} - u^n) - c_1\dot{u}^n - c_2\ddot{u}^n \tag{101}$$

$$\dot{u}^{n+1} = \dot{u}^n + c_3 \ddot{u}^n + c_4 \ddot{u}^{n+1} \tag{102}$$

where $c_0 = \frac{1}{\beta \Delta t}$, $c_1 = \frac{1}{\beta \Delta t}$, $c_2 = \frac{1}{2\beta} - 1$, $c_3 = (1 - \gamma)\Delta t$, $c_4 = \gamma \Delta t$, Δt is the time step size. Normally, the so-called "average acceleration method" with $\beta = 0.25$, $\gamma = 0.5$ is adopted as it is unconditional stable.

Independent dofs δu_i can be further split into prescribed δu_p and remaining free δu_f dofs. In this case, $\{1,2,4\}$ are prescribed nodes and $\{5,6,7\}$ are remaining free nodes.

$$\begin{bmatrix}
(\overline{K}_{pp})_{6\times6} & (\overline{K}_{pf})_{6\times6} \\
(\overline{K}_{fp})_{6\times6} & (\overline{K}_{ff})_{6\times6}
\end{bmatrix}
\begin{bmatrix}
(\delta u_p)_{6\times1} \\
(\delta u_f)_{6\times1}
\end{bmatrix} = \begin{bmatrix}
(\delta f_p^{\star})_{6\times1} \\
(0)_{6\times1}
\end{bmatrix}$$
(103)

The microscopic reduced stiffness matrix K_M^{\star} ,

$$(\overline{K}_M)_{6\times 6}(\delta u_p)_{6\times 1} = (\delta f_p^{\star})_{6\times 1}, \text{ with } \overline{K}_M = \overline{K}_{pp} - \overline{K}_{pf}(\overline{K}_{ff})^{-1}\overline{K}_{fp}$$
 (104)

Divide the \overline{K}_M into submatrixs,

$$\overline{K}_{M} = \begin{bmatrix} \begin{bmatrix} \overline{K}_{11}^{(11)} & \overline{K}_{12}^{(11)} \\ \overline{K}_{21}^{(11)} & \overline{K}_{22}^{(11)} \end{bmatrix} & \begin{bmatrix} \overline{K}_{11}^{(12)} & \overline{K}_{12}^{(12)} \\ \overline{K}_{21}^{(12)} & \overline{K}_{22}^{(12)} \end{bmatrix} & \begin{bmatrix} \overline{K}_{11}^{(14)} & \overline{K}_{12}^{(14)} \\ \overline{K}_{21}^{(14)} & \overline{K}_{22}^{(14)} \end{bmatrix} \\ \begin{bmatrix} \overline{K}_{11}^{(21)} & \overline{K}_{12}^{(21)} \\ \overline{K}_{21}^{(21)} & \overline{K}_{22}^{(21)} \end{bmatrix} & \begin{bmatrix} \overline{K}_{11}^{(22)} & \overline{K}_{12}^{(22)} \\ \overline{K}_{21}^{(22)} & \overline{K}_{22}^{(22)} \end{bmatrix} & \begin{bmatrix} \overline{K}_{11}^{(24)} & \overline{K}_{12}^{(24)} \\ \overline{K}_{21}^{(24)} & \overline{K}_{22}^{(24)} \end{bmatrix} \\ \begin{bmatrix} \overline{K}_{11}^{(41)} & \overline{K}_{12}^{(41)} \\ \overline{K}_{21}^{(41)} & \overline{K}_{22}^{(41)} \end{bmatrix} & \begin{bmatrix} \overline{K}_{11}^{(42)} & \overline{K}_{12}^{(42)} \\ \overline{K}_{21}^{(42)} & \overline{K}_{22}^{(42)} \end{bmatrix} & \begin{bmatrix} \overline{K}_{11}^{(44)} & \overline{K}_{12}^{(44)} \\ \overline{K}_{21}^{(44)} & \overline{K}_{22}^{(44)} \end{bmatrix} \end{bmatrix}_{6 \times 6}$$

$$(105)$$

Rewrite equation 104 as,

$$\sum_{j=1,2,4} \overline{K}_{M}^{(ij)} \cdot \delta u_{(j)} = \delta f_{(i)}, \quad i = 1, 2, 4$$
(106)

where the sub-matrix $\overline{K}_{M}^{(ij)}$ is

$$\overline{K}_{M}^{(ij)} = \begin{bmatrix} \overline{K}_{11}^{(ij)} & \overline{K}_{12}^{(ij)} \\ \overline{K}_{21}^{(ij)} & \overline{K}_{22}^{(ij)} \end{bmatrix}, \text{ with } i, j = 1, 2, 4$$
 (107)

$$\delta u_{(j)} = \begin{bmatrix} \delta u_{jx} \\ \delta u_{jy} \end{bmatrix}, \text{ with } j = 1, 2, 4$$
 (108)

Variation of displacements of the prescribed nodes $\{1,2,4\}$ according to the macroscopic deformation gradient $F_M^{\ 8}$,

$$\delta u_{(j)} = \delta u_M + \delta F_M \cdot X_{(j)}, \quad \text{with} \quad j = 1, 2, 4 \tag{109}$$

The variation of macroscopic stress tensor is calculated as⁹:

$$\delta P_M = \frac{1}{V_0} \sum_{p=1,2,4} \delta f_p X_p \tag{110}$$

Substitutions equations 106 and 109 into equation 110,

$$\delta P_{M} = \frac{1}{V_{0}} \sum_{i=1,2,4} \sum_{j=1,2,4} (\overline{K}_{M}^{(ij)} \cdot \delta u_{(j)}) X_{(i)}$$

$$= \frac{1}{V_{0}} \sum_{i=1,2,4} \sum_{j=1,2,4} (\overline{K}_{M}^{(ij)} \cdot \delta F_{M} \cdot X_{(j)} + \overline{K}_{M}^{(ij)} \delta u_{M}) X_{(i)}$$

$$= \frac{1}{V_{0}} \sum_{i=1,2,4} \sum_{j=1,2,4} (\overline{K}_{M}^{(ij)} \cdot \delta F_{M} \cdot X_{(j)}) X_{(i)} + \frac{1}{V_{0}} \sum_{i=1,2,4} \sum_{j=1,2,4} (\overline{K}_{M}^{(ij)} \delta u_{M}) X_{(i)}$$
(111)

Therefore, the constitutive tangents are identified as:

$${}^{4}C_{M}^{(1)} = \frac{1}{V_{0}} \sum_{i=1,2,4} \sum_{j=1,2,4} \left(X_{(i)} \overline{K}_{M}^{(ij)} X_{(j)} \right)^{LC}$$
(112)

$${}^{3}C_{M}^{(2)} = \frac{1}{V_{0}} \sum_{i=1,2,4} \sum_{j=1,2,4} \left(\overline{K}_{M}^{(ij)} X_{(i)} \right)^{RC}$$
(113)

where the superscript LC denotes an operation, which for a fourth-order tensor ${}^{4}T$ is defined as $T_{ijkl}^{LC} = T_{jikl}$ and the superscript RC denotes an peration, which for a third-order tensor ${}^{3}L$ is defined as $L_{ijk}^{RC} = L_{ikj}$.

The variation of macroscopic linear momentum according to Equation 71 is,

$$\delta\Phi_{M} = \frac{1}{V_{0}} \int_{V_{0}} \delta\Phi_{m} dV_{0}
= \frac{1}{V_{0}} \int_{V_{0}} \rho_{0} \delta\dot{u}_{m} dV_{0}
= \frac{1}{V_{0}} \int_{V_{0}} \rho_{0} c_{4} c_{0} \delta u_{m} dV_{0} \quad \text{(Equ. 101 and 102)}
= \frac{1}{V_{0}} \int_{V_{0}} \rho_{0} c_{4} c_{0} (\delta u_{M} + \delta F_{M} \cdot X + \delta w) dV_{0} \quad \text{(Equ. 75)}
= \frac{1}{V_{0}} \int_{V_{0}} \rho_{0} c_{4} c_{0} (\delta u_{M} + \delta F_{M} \cdot X) dV_{0}
= {}^{3}C_{M}^{(3)} : \delta F_{M} + {}^{2}C_{M}^{(4)} \cdot \delta u_{M}$$

Therefore, the constitutive tangent is identified as,

$${}^{3}C_{M}^{(3)} = I \otimes \left(\frac{1}{V_{0}} \int_{V_{0}} \rho_{0} c_{4} c_{0} X dV_{0}\right)$$
(115)

⁸At prescribed nodes $\{1,2,4\}$, the fluctuation term w in Equ. 75 is zero

⁹The equ. 110 is justified in section 4.1.4.

$${}^{2}C_{M}^{(4)} = \rho_{0}c_{4}c_{0}I \tag{116}$$

where I is the second-order identity tensor.

Remark. In the above derivation, the condition that,

$$\frac{1}{V_0} \int_{V_0} w dV_0 = 0 \tag{117}$$

is used. This means that the following condition is true,

$$\frac{1}{V_0} \int_{V_0} \delta w dV_0 = 0 \tag{118}$$

5 Questions

The remaining questions can be summarized as,

- How to eliminate the rigid body motion (translation and rotation) for quasi-static and dynamic scenario?
- How to introduce the kinematic assumptions generally?
- The application of $u_M = \int_{\Omega} u_M dV$ introduces what kind of constraint force?

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A FEM discretization

The introduction of FEM discretization does not introduce extra external force. The displacement at any node p in one element is,

$$u_p(x) = \sum_{i=1,2,3,4} N_i u_i \tag{119}$$

Since the constrain force should do zero virtual work, the following condition is true.

$$f_p \delta u_p + f_1 \delta u_1 + f_2 \delta u_2 + f_3 \delta u_3 + f_4 \delta u_4 = 0$$
 (120)

Substitution of equ. 119 yields,

$$f_p(N_1\delta u_1 + N_2\delta u_2 + N_3\delta u_3 + N_4\delta u_4) + f_1\delta u_1 + f_2\delta u_2 + f_3\delta u_3 + f_4\delta u_4 = 0$$
(121)

Considering the arbitrary of the δu_1 , δu_2 , δu_3 and δu_4 ,

$$f_1 = -N_1 f_p \tag{122}$$

$$f_2 = -N_2 f_p \tag{123}$$

$$f_3 = -N_3 f_p \tag{124}$$

$$f_4 = -N_4 f_p \tag{125}$$

The external force vector, when the dependent node p is eliminated, can be calculated as,

$$f^{\star} = f_i + C_{di}^T f_d \tag{126}$$

where the vector,

$$f_i = \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \end{bmatrix} \tag{127}$$

The dependent matrix,

$$C_{di} = -C_d^{-1}C_i = [N_1, N_2, N_3, N_4]; (128)$$

Therefore,

$$f^{\star} = \begin{bmatrix} f_1 + N_1 f_p \\ f_2 + N_2 f_p \\ f_3 + N_3 f_p \\ f_4 + N_4 f_p \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$
 (129)

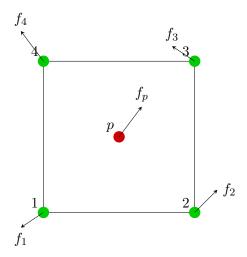


Figure 9: RVE mesh discretization (red circle—dependent nodes; green circle—independent nodes)

B Additional constraint force

The constraint condition is,

$$\sum_{i=1,2,\dots,9} c^k u^k = u_M \tag{130}$$

If we define $c^k := \frac{1}{V_0} \int_{V_0} N_m^k dV_0$

$$u_9 = u_5 + u_4 - u_1 \tag{131}$$

$$u_8 = u_6 + u_2 - u_1 \tag{132}$$

$$u_3 = u_4 + u_2 - u_1 \tag{133}$$

$$u_7 = \frac{1}{c^7} (u_M - \sum_{k=1,2,\dots,6} c^k u^k - c^8 u^8 - c^9 u^9)$$
 (134)

The dependent matrix C is,

General FEM equation

$$u(x,t) = \sum_{i}^{N} q_i(t)\phi_i(x)$$
(135)

Use Hamilton principle to derive the system equation, and then use the condensation technique.

$$0 = \sum_{k=1}^{N} \sum_{i=1}^{3} (m_k \ddot{u}_{ik} - X_{ik}) \delta u_{ik}$$

$$= \sum_{k=1}^{N} \sum_{i=1}^{3} \left(m_k \frac{d}{dt} (\dot{u}_{ik} \delta u_{ik}) - m_k \dot{u}_{ik} \delta \dot{u}_{ik} - X_{ik} \delta u_{ik} \right)$$
(136)

Therefore,

$$\sum_{k=1}^{N} \sum_{i=1}^{3} m_{k} \frac{d}{dt} (\dot{u}_{ik} \delta u_{ik}) = \sum_{k=1}^{N} \sum_{i=1}^{3} (m_{k} \dot{u}_{ik} \delta \dot{u}_{ik} + X_{ik} \delta u_{ik})$$

$$= \sum_{k=1}^{N} \delta T_{k} + \sum_{k=1}^{N} \delta W_{k}$$

$$= \delta T + \delta W$$
(137)

The integration of the above equation gives,

$$\int_{t_{1}}^{t_{2}} (\delta T + \delta W) dt = \int_{t_{1}}^{t_{2}} \sum_{k=1}^{N} \sum_{i=1}^{3} m_{k} \frac{d}{dt} (\dot{u}_{ik} \delta u_{ik}) dt$$

$$= \sum_{k=1}^{N} \sum_{i=1}^{3} m_{k} (\dot{u}_{ik} \delta u_{ik}) \Big|_{t_{1}}^{t_{2}}$$

$$= 0$$
(138)

When split the external force into conservative force and non-conservative force, the Hamilton principle can be rewritten as,

$$0 = \int_{t_1}^{t_2} (\delta T + \delta W^{\text{cons}} + \delta W^{\text{ncons}}) dt$$
$$= \int_{t_1}^{t_2} (\delta T - \delta V + \delta W^{\text{ncons}}) dt$$
(139)

Here the functional takes the form of $\delta T = \delta T(u_{ik}(t))$ and therefore $\delta u_{ik}(t_1) = \delta u_{ik}(t_2) = 0$. Normally, the potential energy is the strain energy in continuum system.

Continuum medium. The Hamilton principle says that,

$$\delta T = \int_{\Omega} m(x)\dot{u}(x,t)\delta \dot{u} \,dV = \sum_{i=1}^{N} m_i \dot{u}_i(x,t)\delta \dot{u}_i \tag{140}$$

$$\delta V = \int_{\Omega} \sigma \delta \varepsilon \, dV = \int_{\Omega} \nabla (\sigma \delta u) - \nabla \sigma \delta u \, dV$$

$$= \int_{\Gamma} \bar{t} \delta u \, dS - \int_{\Omega} \nabla \sigma \delta u \, dV \qquad (141)$$

$$= \sum_{k=1}^{N_s} t_k \delta u_k - \sum_{i=1}^{N} \nabla \sigma_i \delta u_i \Delta V_i$$

$$\delta W^{\text{ncons}} = \int_{\Omega} p \delta u \, dV + \int_{\Gamma} \bar{t} dS = \sum_{i=1}^{N} f_i(x, t) \delta u_i + \sum_{k=1}^{N_s} t_k \delta u_k dt$$
 (142)

$$0 = \int_{t_{1}}^{t_{2}} \sum_{i=1}^{N} \left(m_{i} \dot{u}_{i}(x, t) \delta \dot{u}_{i} + \nabla \sigma_{i} \delta u_{i} \Delta V_{i} + f_{i}(x, t) \delta u_{i} \right) dt$$

$$= \sum_{i=1}^{N} m_{i} \dot{u}_{i} \delta u_{i} \Big|_{t_{1}}^{t_{2}} - \int_{t_{1}}^{t_{2}} \sum_{i=1}^{N} m_{i} \ddot{u}_{i} \delta u_{i} dt + \int_{t_{1}}^{t_{2}} \sum_{i=1}^{N} \left(\nabla \sigma_{i} \delta u_{i} \Delta V_{i} + f_{i}(x, t) \delta u_{i} \right) dt$$

$$= \int_{t_{1}}^{t_{2}} \sum_{i=1}^{N} \left(\nabla \sigma_{i} \delta u_{i} \Delta V_{i} + f_{i}(x, t) \delta u_{i} - m_{i} \ddot{u}_{i} \delta u_{i} \right) dt$$

$$(143)$$

Considering that the constraint forces are not included into the δW . **Beam in bending.** The kinetic energy of the system,

$$T = \int_0^L \frac{1}{2} m(x) [\dot{w}(x,t)]^2 dx \tag{144}$$

The conversative energy of the system,

$$V = \int_0^L \frac{1}{2} EI(x) \left[\frac{\partial^2 w(x,t)}{\partial x^2} \right]^2 dx \tag{145}$$

The non-conversative energy of the system,

$$W^{\text{ncons}} = \int_0^L p(x,t)w(x,t)dx \tag{146}$$

Application of Hamilton principle yields,

$$\delta T = \int_0^L m(x)\dot{w}(x,t)\frac{d}{dt}(\delta w) dx \tag{147}$$

$$\delta V = \int_0^L EI(x) \left[\frac{\partial^2 w(x,t)}{\partial x^2} \right] (\delta w)'' dx \tag{148}$$

$$\delta W^{\text{ncons}} = \int_0^L p(x, t) \delta w(x, t) dx \tag{149}$$

$$\begin{aligned} 0 &= & \int_{t_{1}}^{t_{2}} \left(\int_{0}^{L} m(x) \dot{w}(x,t) \frac{d}{dt} (\delta w) \, dx - \int_{0}^{L} EI(x) \left[\frac{\partial^{2} w(x,t)}{\partial x^{2}} \right] (\delta w)'' \, dx + \int_{0}^{L} p(x,t) \delta w(x,t) dx \right) dt \\ &= & \int_{0}^{L} \int_{t_{1}}^{t_{2}} m(x) \dot{w}(x,t) \frac{d}{dt} (\delta w) \, dt \, dx - \int_{t_{1}}^{t_{2}} \int_{0}^{L} EI(x) \left[\frac{\partial^{2} w(x,t)}{\partial x^{2}} \right] (\delta w)'' \, dx \, dt \\ &+ \int_{t_{1}}^{t_{2}} \int_{0}^{L} p(x,t) \delta w(x,t) dx \, dt \\ &= & \int_{0}^{L} m(x) \dot{w}(x,t) (\delta w) \Big|_{t_{1}}^{t_{2}} dx - \int_{0}^{L} \int_{t_{1}}^{t_{2}} m(x) \ddot{w}(x,t) \delta w dt dx \\ &- \int_{t_{1}}^{t_{2}} EI(x) \left[\frac{\partial^{2} w(x,t)}{\partial x^{2}} \right] (\delta w)' \Big|_{0}^{L} dt + \int_{t_{1}}^{t_{2}} \int_{0}^{L} (EI(x) w''(x,t))' (\delta w)' dx \, dt \\ &+ \int_{t_{1}}^{t_{2}} \int_{0}^{L} p(x,t) \delta w(x,t) dx \, dt \\ &= & - \int_{0}^{L} \int_{t_{1}}^{t_{2}} m(x) \dot{w}(x,t) \delta w dt dx - \int_{t_{1}}^{t_{2}} EI(x) \left[\frac{\partial^{2} w(x,t)}{\partial x^{2}} \right] (\delta w)' \Big|_{0}^{L} dt + \int_{t_{1}}^{t_{2}} (EI(x) w''(x,t))' \delta w \Big|_{0}^{L} dt \\ &- \int_{t_{1}}^{t_{2}} \int_{0}^{L} (EI(x) w''(x,t))'' \delta w dx \, dt + \int_{t_{1}}^{t_{2}} \int_{0}^{L} p(x,t) \delta w(x,t) dx \, dt \\ &= & \int_{t_{1}}^{t_{2}} \int_{0}^{L} \left(p(x,t) - (EI(x) w''(x,t))'' - m(x) \ddot{w}(x,t) \right) \delta w dx \, dt \\ &- \int_{t_{1}}^{t_{2}} EI(x) \left[\frac{\partial^{2} w(x,t)}{\partial x^{2}} \right] \delta w' \Big|_{0}^{L} dt + \int_{t_{1}}^{t_{2}} (EI(x) w''(x,t))' \delta w \Big|_{0}^{L} dt \end{aligned}$$

where the conditions $\delta w(x, t_1) = \delta w(x, t_2) = 0$ are used.

The equation of motion is identified as,

$$p(x,t) - (EI(x)w''(x,t))'' - m(x)\ddot{w}(x,t) = 0$$
(150)

and boundary conditions are,

$$EI(x)w''(x,t) = 0$$
 or $\delta w' = 0$, at $x = 0, L$ (151)

and

$$(EI(x)w''(x,t))' = 0$$
 or $\delta w = 0$, at $x = 0, L$ (152)