

Manual to Pyt-FFT-elas: The homogenization of elastic and visco-elastic materials

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1 Theory

In this section, we present the theory to FFT-based homogenization, analytical homogenization, and visco-elastic homogenization.

we use following **notation**: $a = a(\mathbf{x}) : \mathbb{R}^d \rightarrow \mathbb{R}$, $\mathbf{a} = (a_{\alpha\beta}(\mathbf{x}))_{\alpha,\beta=1}^d : \mathbb{R}^d \rightarrow \mathbb{R}^d$ and $\mathbf{A} = (A_{\alpha\beta\mu\nu}(\mathbf{x}))_{\alpha,\beta,\mu,\nu=1}^d : \mathbb{R}^d \rightarrow \mathbb{R}^{d \times d}$ denote scalar, second-order and fourth-order tensor quantities with Greek subscripts used when referring to the corresponding components, e.g. $A_{\alpha\beta}$. A multi-index notation is employed, in which $\mathbb{R}^{\mathbf{N}}$ with $\mathbf{N} = (N_1, \dots, N_d)$ represents $\mathbb{R}^{N_1 \times \dots \times N_d}$. The objects denoted with a capital letter in a serif font and bold style (e.g. $\mathbf{A} \in \mathbb{R}^{d \times d \times d \times d \times \mathbf{N} \times \mathbf{N}}$) are called matrices, further superscript and subscript indices are used to refer to components $A_{\alpha\beta\mu\nu}^{km}$, i.e. $\mathbf{A} = [A_{\alpha\beta\mu\nu}^{km}]_{\alpha,\beta,\mu,\nu=1,\dots,d}^{\mathbf{k},\mathbf{l} \in \mathbb{Z}_{\mathbf{N}}^d}$ with $\mathbb{Z}_{\mathbf{N}}^d$ defined as

$$\mathbb{Z}_{\mathbf{N}}^d = \left\{ \mathbf{k} \in \mathbb{Z}^d : -\frac{N_\alpha}{2} < k_\alpha \leq \frac{N_\alpha}{2}, \alpha = 1, \dots, d \right\}. \quad (1.1) \quad \{\text{eq: def } \mathbb{Z}_{\mathbf{N}}^d\}$$

Moreover, we denote by

$$\begin{aligned} \mathbf{A}_{\alpha\beta\mu\nu} &= [A_{\alpha\beta\mu\nu}^{km}]_{\mathbf{k},\mathbf{m} \in \mathbb{Z}_{\mathbf{N}}^d} \in \mathbb{R}^{\mathbf{N} \times \mathbf{N}}, & \text{for } \alpha, \beta, \mu, \nu = 1, \dots, d, \\ \mathbf{A}^{km} &= [A_{\alpha\beta\mu\nu}^{km}]_{\alpha,\beta=1,\dots,d} \in \mathbb{R}^{d \times d \times d \times d}, & \text{for } \mathbf{k}, \mathbf{m} \in \mathbb{Z}_{\mathbf{N}}^d, \end{aligned}$$

the submatrices of \mathbf{A} . With the same notation, the objects denoted with a small letter (e.g. $\mathbf{e} \in \mathbb{R}^{d \times d \times \mathbf{N}}$) are called vectors and the product of matrix by vector multiplication $\mathbf{A}\mathbf{e} \in \mathbb{R}^{d \times d \times \mathbf{N}}$ is defined as

$$\mathbf{A}\mathbf{e} = \left(\sum_{\mu,\nu=1}^d \sum_{\mathbf{m} \in \mathbb{Z}_{\mathbf{N}}^d} A_{\alpha\beta\mu\nu}^{km} e_{\mu\nu}^{\mathbf{m}} \right)_{\alpha,\beta=1,\dots,d}^{\mathbf{k} \in \mathbb{Z}_{\mathbf{N}}^d}. \quad (1.2) \quad \{\text{eq: MB multiplication}\}$$

The binary operator \odot denotes the elementwise multiplication, i.e. for $\mathbf{l}, \mathbf{N} \in \mathbb{R}^d$

$$\mathbf{l} \odot \mathbf{N} = (l_\alpha N_\alpha)_{\alpha=1}^d \in \mathbb{R}^d.$$

Since the second-order tensors $\boldsymbol{\varepsilon}$ and $\boldsymbol{\sigma}$ are symmetric, the engineering notation is used. We use a Mandel notation where in the two-dimensional case of plain strain, we can express strain and stress as

$$\tilde{\boldsymbol{\varepsilon}} = (\varepsilon_{11}, \varepsilon_{22}, \sqrt{2}\varepsilon_{12})^T \quad (1.3a) \quad \{\text{eq: stress strain Mandel}\}$$

$$\tilde{\boldsymbol{\sigma}} = (\sigma_{11}, \sigma_{22}, \sqrt{2}\sigma_{12})^T. \quad (1.3b)$$

Analogously, in order to express material law in Mandel notation as $\tilde{\boldsymbol{\sigma}} = \tilde{\mathbf{L}}\tilde{\boldsymbol{\varepsilon}}$, the stiffness matrix $\tilde{\mathbf{L}}$ can be expressed as

$$\tilde{\mathbf{L}} = \begin{pmatrix} L_{1111} & L_{1122} & \sqrt{2}L_{1112} \\ L_{2211} & L_{2222} & \sqrt{2}L_{2212} \\ \sqrt{2}L_{1211} & \sqrt{2}L_{1222} & 2L_{1212} \end{pmatrix} \quad (1.4) \quad \{\text{eq: stiffness Mandel}\}$$

1.1 Linear elasticity homogenization using FFT

A majority of computational homogenization techniques rely on the solution to the unit cell problem, which concerns the determination of local fields in a representative sample of a heterogeneous material under periodic boundary conditions. The behavior of any heterogeneous materials consisting of periodically repeating unit cell (occupying domain $\Omega = \prod_{\alpha=1}^d (-Y_\alpha, Y_\alpha) \subset \mathbb{R}^d$, where Y_α is the axial size and d denotes the space dimension) can be described with differential equations with periodic boundary conditions and prescribed macroscopic load $\boldsymbol{\varepsilon}^0$ as

$$\operatorname{div} \boldsymbol{\sigma}(\mathbf{x}) = \mathbf{0}, \quad \mathbf{x} \in \mathcal{Y} \quad (1.5a)$$

$$\boldsymbol{\sigma}(\mathbf{x}) = \mathbf{L}(\mathbf{x})\boldsymbol{\varepsilon}(\mathbf{x}), \quad \mathbf{x} \in \mathcal{Y} \quad (1.5b) \quad \{\text{eq:linear elastic material}\}$$

$$\langle \boldsymbol{\varepsilon} \rangle := \frac{1}{|\mathcal{Y}|_d} \int_{\mathcal{Y}} \boldsymbol{\varepsilon}(\mathbf{x}) \, d\mathbf{x} = \boldsymbol{\varepsilon}^0 \quad (1.5c)$$

where $\boldsymbol{\sigma}$ denotes second order stress tensor, $\boldsymbol{\varepsilon}$ second order strain tensor, \mathbf{L} the fourth order tensor of elastic stiffness, and $|\cdot|_d$ denotes d-dimentional Lebesgue measure. The effective (homogenized) material tensor \mathbf{L}_{eff} is such a tensor satisfying

$$\langle \boldsymbol{\sigma} \rangle = \mathbf{L}_{\text{eff}} : \langle \boldsymbol{\varepsilon} \rangle \quad (1.6) \quad \{\text{eq:hom stress strain rel}\}$$

for arbitrary macroscopic load $\boldsymbol{\varepsilon}^0 = \langle \boldsymbol{\varepsilon} \rangle$. In the two-dimensional case, it is calculated as a individual unit loads \mathbf{e}^0 are prescribed, i.e. step by step is described $\varepsilon_{11}^0 = 1$, $\varepsilon_{22}^0 = 1$ and $\varepsilon_{12}^0 = 1$. In fact, each unit load determines one column of the effective (homogenized) stiffness \mathbf{L}_{eff} meaning in the engineering notation, see Mandel notation at the end of the section.

Thus the problem of finding effective material tensor \mathbf{L}_{eff} is composed of finding corresponding strain field $\boldsymbol{\varepsilon}$ and associated stress field $\boldsymbol{\sigma}$ for known elastic properties \mathbf{L} and loading $\boldsymbol{\varepsilon}^0$ using differential equation Eq. (1.5).

We formulate the initial problem Eq. (1.5) as a weak formulation: Find $\bar{\boldsymbol{\varepsilon}} = \boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^0 \in V$ such that

$$(\mathbf{L}\bar{\boldsymbol{\varepsilon}}, \mathbf{v})_{L_{\mathcal{Y}}^2} = -(\mathbf{L}\boldsymbol{\varepsilon}^0, \mathbf{v})_{L_{\mathcal{Y}}^2} \quad (1.7)$$

where

$$V = \{\boldsymbol{\varepsilon} = (\varepsilon_{\alpha\beta})_{\alpha,\beta=1,\dots,d}; \varepsilon_{\alpha\beta} \in L_{\mathcal{Y}}^2 \text{ such that there exists vector field } u \in H_{\mathcal{Y}}^1 \text{ satisfying } \frac{\nabla u + (\nabla u)^T}{2} = \boldsymbol{\varepsilon}\},$$

$L_{\mathcal{Y}}^2$ denotes the measurable functions (vector valued), square integrable factorized with equivalence unifying two functions equaling one another almost everywhere.

The weak formulation is numerically solved using Galerkin approximation with numerical integration and trigonometric polynomials

$$\varphi_{\mathbf{N},\mathbf{m}}(\mathbf{x}) = \frac{1}{\prod_{\alpha=1}^d N_{\alpha}} \sum_{\mathbf{k} \in \mathbb{Z}_{\mathbf{N}}^d} \varphi_{\mathbf{k}}(\mathbf{x}) \omega_{\mathbf{N}}^{-\mathbf{m}\mathbf{k}} \quad (1.8) \quad \{\text{eq:basis Orig}\}$$

taken as a basis function where

$$\varphi_{\mathbf{k}}(\mathbf{x}) = \exp\left(\pi i \sum_{\alpha=1}^d \frac{k_{\alpha} x_{\alpha}}{Y_{\alpha}}\right), \quad \mathbf{m}, \mathbf{k} \in \mathbb{Z}_{\mathbf{N}}^d, \quad (1.9)$$

$$\omega_{\mathbf{N}}^{\mathbf{k}\mathbf{m}} = \exp\left(2\pi i \sum_{\alpha=1}^d \frac{k_{\alpha} m_{\alpha}}{N_{\alpha}}\right), \quad \mathbf{m}, \mathbf{k} \in \mathbb{Z}_{\mathbf{N}}^d, \quad (1.10)$$

$$\mathbb{Z}_{\mathbf{N}}^d = \left\{ \mathbf{k} \in \mathbb{Z}^d : -\frac{N_{\alpha}}{2} < k_{\alpha} \leq \frac{N_{\alpha}}{2}, \alpha = 1, \dots, d \right\}. \quad (1.11)$$

The basis functions $\varphi_{\mathbf{N},\mathbf{m}}(\mathbf{x})$ satisfy the dirac delta property, i.e. $\varphi_{\mathbf{N},\mathbf{m}}(\mathbf{x}^{\mathbf{k}}) = \delta_{\mathbf{m}\mathbf{k}}$, at nodal points

$$\mathbf{x}^{\mathbf{k}} := \sum_{\alpha=1}^d \frac{2Y_{\alpha} k_{\alpha}}{N_{\alpha}} \boldsymbol{\epsilon}_{\alpha} = \left(\frac{2Y_1 k_1}{N_1}, \frac{2Y_2 k_2}{N_2}, \dots, \frac{2Y_d k_d}{N_d} \right) \in \mathcal{Y} \subset R^d. \quad (1.12)$$

Since we store the nodal values of functions occurring in weak formulation

$$\mathbf{e} = \left(\varepsilon_{\alpha\beta}(\mathbf{x}^{\mathbf{k}}) \right)_{\alpha,\beta=1,\dots,d}^{\mathbf{k} \in \mathbb{Z}_N^d} \quad (1.13) \quad \{\text{eq:strain grid}\}$$

$$\mathbf{L} = \left(\delta_{\mathbf{k}\mathbf{m}} L_{\alpha\beta\mu\nu}(\mathbf{x}^{\mathbf{k}}) \right)_{\alpha,\beta,\mu,\nu=1,\dots,d}^{\mathbf{k},\mathbf{m} \in \mathbb{Z}_N^d} \quad (1.14)$$

$$\mathbf{e}^0 = \left(\varepsilon_{\alpha\beta}^0 \right)_{\alpha,\beta=1,\dots,d}^{\mathbf{k} \in \mathbb{Z}_N^d} \quad (1.15) \quad \{\text{eq:MBe}\}$$

the Galerkin approximation with numerical integration is then equivalent to solution of linear system

$$\mathbf{P}\mathbf{L}\bar{\mathbf{e}} = -\mathbf{P}\mathbf{L}\mathbf{e}^0 \quad (1.16) \quad \{\text{eq:linear system}\}$$

where \mathbf{P} is a projection on a discrete space corresponding to the space V of admissible strain fields, i.e. on the space

$$\mathcal{E} = \left\{ \mathbf{e} \in \mathbb{R}^{d \times d \times N}; \sum_{\mathbf{k} \in \mathbb{Z}_N^d} \mathbf{e}^{\mathbf{k}} \varphi_{N,\mathbf{k}} \in V \right\} \quad (1.17)$$

and the matrix \mathbf{P} can be explicitly expressed as

$$\mathbf{P} = \mathbf{F}^{-1} \hat{\mathbf{F}} \mathbf{F} \quad (1.18)$$

where matrices $\mathbf{F}^{-1}, \mathbf{F} \in \mathbb{C}^{d \times d \times d \times d \times N \times N}$ are composed of Discrete Fourier Transform, i.e.

$$\mathbf{F} = \frac{1}{\prod_{\alpha=1,\dots,d} \omega_N} \left(\delta_{\alpha\mu} \delta_{\beta\nu} \omega_N^{-\mathbf{k}\mathbf{m}} \right)_{\alpha,\beta,\mu,\nu=1,\dots,d}^{\mathbf{k},\mathbf{m} \in \mathbb{Z}_N^d} \quad \mathbf{F}^{-1} = \left(\delta_{\alpha\mu} \delta_{\beta\nu} \omega_N^{\mathbf{k}\mathbf{m}} \right)_{\alpha,\beta,\mu,\nu=1,\dots,d}^{\mathbf{k},\mathbf{m} \in \mathbb{Z}_N^d} \quad (1.19)$$

and matrix $\hat{\mathbf{F}}_{K_0, G_0}$ is derived from a green function expressed in a Fourier space, i.e.

$$\hat{\mathbf{F}}_{K_0, G_0} = \left[\delta_{\alpha\mu} \delta_{\beta\nu} \left(\frac{1}{2G_0} \cdot \frac{(\delta_{ik} \xi_j \xi_l + \delta_{il} \xi_j \xi_k + \delta_{jk} \xi_i \xi_l + \delta_{jl} \xi_i \xi_k)}{2\|\boldsymbol{\xi}\|_2^2} - \frac{3K_0 + G_0}{G_0(3K_0 + 4G_0)} \cdot \frac{\xi_i \xi_j \xi_k \xi_l}{\|\boldsymbol{\xi}\|_2^4} \right) \right]_{\alpha,\beta,\mu,\nu=1,\dots,d}^{\mathbf{k},\mathbf{m} \in \mathbb{Z}_N^d} \quad (1.20)$$

where $\boldsymbol{\xi} = (\xi_\alpha(\mathbf{k}))_{\alpha=1,\dots,d}$, $\xi_\alpha(\mathbf{k}) = \frac{k_\alpha}{Y_\alpha}$ for $\alpha = 1, \dots, d$ and $\mathbf{k} \in \mathbb{Z}_N^d$, and K_0, G_0 are bulk and shear modulus of reference stiffness, the parameter of the method.

The assumption occurring through the whole program is that the material is isotropic in each point. Next, the indentation provides the bulk and shear modulus $K(\mathbf{x}), G(\mathbf{x}) \in \mathbb{R}, \mathbf{x} \in \mathcal{Y}$ at nodal points $\mathbf{x}^{\mathbf{k}} \in \mathcal{Y}$ for $\mathbf{k} \in \mathbb{Z}_N^d$. It determines the matrix \mathbf{L} required for the solution of linear system (1.16) as

$$\mathbf{L}(\mathbf{x}^{\mathbf{k}}) = 3K(\mathbf{x}^{\mathbf{k}}) \boldsymbol{\Lambda}_V + 2G(\mathbf{x}^{\mathbf{k}}) \boldsymbol{\Lambda}_D, \quad \mathbf{k} \in \mathbb{Z}_N^d \quad (1.21) \quad \{\text{eq:isotropic material}\}$$

where $\boldsymbol{\Lambda}_V, \boldsymbol{\Lambda}_D \in \mathbb{R}^{d \times d \times d \times d}$ are volumetric and deviatoric projections, i.e.

$$\mathbf{I}_S := \left(\frac{\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}}{2} \right)_{i,j,k,l=1,\dots,d}, \quad (1.22)$$

$$\boldsymbol{\Lambda}_V := \left(\frac{1}{d} \delta_{ij} \delta_{kl} \right)_{i,j,k,l=1,\dots,d}, \quad (1.23)$$

$$\boldsymbol{\Lambda}_D := \mathbf{I}_S - \boldsymbol{\Lambda}_h. \quad (1.24)$$

We note that the indentation files contains Young's modulus E and Poisson's ration ν rather than bulk and shear modulus, however they are equivalent with the equations

$$K = \frac{E}{3(1-2\nu)} \quad (1.25) \quad \{\text{eq:relation KG'Emu}\}$$

$$G = \frac{E}{2(1+\nu)}. \quad (1.26)$$

Next, the parameters of reference stiffness $K_0, G_0 \in \mathbb{R}$ are chosen as a mean of K and G at the set of nodal points, i.e.

$$K_0 = \frac{1}{\text{card } \mathbb{Z}_N^d} \sum_{\mathbf{k} \in \mathbb{Z}_N^d} K(\mathbf{x}^{\mathbf{k}}), \quad (1.27)$$

$$G_0 = \frac{1}{\text{card } \mathbb{Z}_N^d} \sum_{\mathbf{k} \in \mathbb{Z}_N^d} G(\mathbf{x}^{\mathbf{k}}). \quad (1.28)$$

In the implementation, the nodal points, e.g. $K(\mathbf{x}^{\mathbf{k}})$ for $\mathbf{k} \in \mathbb{Z}_N^d$, are stored in a matrices $\mathbf{K} \in \mathbb{R}^N$ defined as

$$\mathbf{K} = (K(\mathbf{x}^{\mathbf{k}}))_{\mathbf{k} \in \mathbb{Z}_N^d}. \quad (1.29)$$

The linear elasticity is generally described in the three-dimensional case, $d = 3$, but some simplifications can be done if one variable is omitted leading to two-dimensional case. In our work we assume the problem of plain strain where $\varepsilon_{33} = \varepsilon_{23} = \varepsilon_{32} = \varepsilon_{13} = \varepsilon_{31} = 0$. Another simplification having the benefit in computation is Engineering notation, i.e. Mandel notation stated at the end of previous section, which employ the symmetry of undergoing tensors $\mathbf{L}, \boldsymbol{\varepsilon}$ and $\boldsymbol{\sigma}$. Hence linear system (1.16) can be alternatively rewritten as

$$\tilde{\mathbf{P}}\tilde{\mathbf{L}}\tilde{\mathbf{e}} = -\tilde{\mathbf{P}}\tilde{\mathbf{L}}\tilde{\mathbf{e}}^0 \quad (1.30) \quad \{\text{eq:linear system Mandel}\}$$

where $\tilde{\cdot}$ denotes Mandel notation and matrices $\tilde{\mathbf{P}}, \tilde{\mathbf{L}}$ are from the space $\mathbb{R}^{3 \times 3 \times N \times N}$ instead of $\mathbb{R}^{2 \times 2 \times 2 \times N \times N}$. Specifically, the matrix \mathbf{L} is block diagonal in the sense that submatrices are zero, $\mathbf{L}^{\mathbf{k}\mathbf{m}} = \mathbf{0}$, for $\mathbf{k} \neq \mathbf{m}$ and $\mathbf{k}, \mathbf{m} \in \mathbb{Z}_N^2$, and the diagonal can be expressed as

$$\tilde{\mathbf{L}}^{\mathbf{k}\mathbf{k}} = \begin{pmatrix} \mathbf{K}^{\mathbf{k}} + \frac{4}{3}\mathbf{G}^{\mathbf{k}} & \mathbf{K}^{\mathbf{k}} - \frac{2}{3}\mathbf{G}^{\mathbf{k}} & 0 \\ \mathbf{K}^{\mathbf{k}} - \frac{2}{3}\mathbf{G}^{\mathbf{k}} & \mathbf{K}^{\mathbf{k}} + \frac{4}{3}\mathbf{G}^{\mathbf{k}} & 0 \\ 0 & 0 & 2\mathbf{G}^{\mathbf{k}} \end{pmatrix}, \quad \mathbf{k} \in \mathbb{Z}_N^2. \quad (1.31) \quad \{\text{eq:stiffness}\}$$

The linear system is then solved using the conjugate gradient method as shown in [4]. Numerically, the algorithm is stopped when the number of iterations exceeds the user defined number or the required tolerance ε_{CG} for the 2-norm of residuum is reached, i.e.

$$\|\tilde{\mathbf{P}}\tilde{\mathbf{L}}\tilde{\mathbf{e}}^{(i)} + \tilde{\mathbf{P}}\tilde{\mathbf{L}}\tilde{\mathbf{e}}^0\| < \varepsilon_{\text{CG}} \quad (1.32) \quad \{\text{eq:tol}\}$$

where $\tilde{\mathbf{e}}^{(i)}$ denotes the i -th conjugate gradient approximation of the solution.

1.2 Visco-elasticity FFT-homogenization

In previous section, we deal with linear elasticity and isotropic material, see Eq. (1.5b) and (1.21). In this section, we describe homogenization of visco-elastic material. In the whole section, we assume that the material, that we are concerned with, is visco-elastic in the deviatoric part meaning that the bulk modulus $K(\mathbf{x})$ is time independent while shear modulus $G(\mathbf{x})$ obeys the viscoelastic properties.

In section 1.2.1, we describe the identification of parameters from the nanoindentation experiment. We assume that the material points are describable by Kelvin-Voigt-Maxwell model (KVM) with a scheme shown in Fig. 1. Since the viscoelastic parameters are identified, we describe in section 1.2.3 the homogenization of those parameters. Then we again assume that the behaviour at the macroscopic level again occurs only in deviatoric part and that it behaves like the KVM model.

1.2.1 Identification of parameters

In this section, we describe the identification of viscoelastic parameters that are very well cover in [2]. The idea is to link the indentation force vs. indentation depth to viscoelastic properties, in our case to parameters occurring in KVM model.

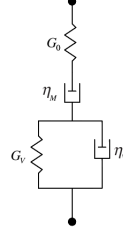


Figure 1: Kelvin-Voight-Maxwell model

The indentation experiment is prescribed with linear loading, constant holding and linear unloading indentation force. The example of such experiment for particular point is shown in Fig. 2 where the begin of loading phase t_1 , holding phase t_2 and unloading phase t_3 are identified. Then

$$t_L = t_2 - t_1 \quad (1.33)$$

$$t_H = t_3 - t_2 \quad (1.34)$$

refers to the duration of loading and holding phase resp.

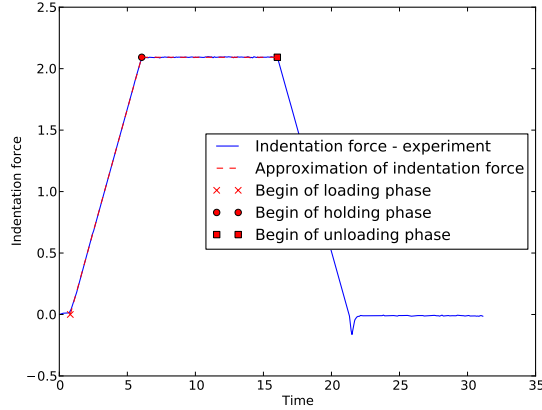


Figure 2: Example of indentation force diagram

Next to the indentation force, cf. Fig 2, the indentation depth is obtained as it is shown in Fig. 3(a). From the initial phase, the Young's modulus E and Poisson's ratio ν or bulk or shear moduli K, G_0 are identified, likewise in the case of obtaining parameters for linear elasticity.

Since the shear modulus G_0 from KVM model is identified, it is still necessary to obtain viscoelastic parameters η_M, η_V , and G_V . Vandamme and Ulm in [2] shown that the indentation depth in the holding phase can be expressed as

$$y_H = \frac{5 - 4\nu_0}{1 - \nu_0^2} + \frac{M}{G_V} - \frac{MT_2}{G_V t_L \exp\left(\frac{-t}{T_2}\right) \left(\exp\left(\frac{t_L}{T_2}\right) - 1\right)} + \frac{M}{\eta_M \left(t - \frac{t_L}{2}\right)} - \frac{(1 - 2\nu_0)^2}{t_L(1 - \nu_0^2) \left(\frac{1}{T_1} - \frac{1}{T_3}\right)} \left[\left(\frac{T_3}{T_2} - 1\right) \exp\left(\frac{-t}{T_3}\right) \left(\exp\left(\frac{t_L}{T_3}\right) - 1\right) + \left(1 - \frac{T_1}{T_2}\right) \exp\left(\frac{-t}{T_1}\right) \left(\frac{t_L}{T_1} - 1\right) \right] \quad (1.35)$$

where $M = M(E, \nu)$, $T_1 = T_1(\eta_M, G_V, \eta_V)$, $T_2 = T_2(\eta_M, G_V, \eta_V)$, and $T_3 = T_3(\eta_M, G_V, \eta_V)$ are defined

as

$$M = \frac{E}{1 - \nu^2}, \quad (1.36)$$

$$T_1 = \frac{6\eta_M\eta_V}{E_0(\eta_M + \eta_V) + 3\eta_M G_V + (E_0^2(\eta_M + \eta_V)^2 + 6E_0\eta_M G_V(\eta_M - \eta_V) + 9\eta_M^2 G_V^2)^{1/2}}, \quad (1.37)$$

$$T_2 = \frac{\eta_V}{G_V}, \quad (1.38)$$

$$T_3 = \frac{6\eta_M\eta_V}{E_0(\eta_M + \eta_V) + 3\eta_M G_V - (E_0^2(\eta_M + \eta_V)^2 + 6E_0\eta_M G_V(\eta_M - \eta_V) + 9\eta_M^2 G_V^2)^{1/2}}. \quad (1.39)$$

Thus, it is now possible to identify the searched parameters (η_M , η_V , and G_V) using least squares. The red line in Fig. 3(a) and in a more detail in Fig. 3(b) shows the indentation depth during the force holding phase while the green line corresponds to the best fit of KVM model with the least squares method.

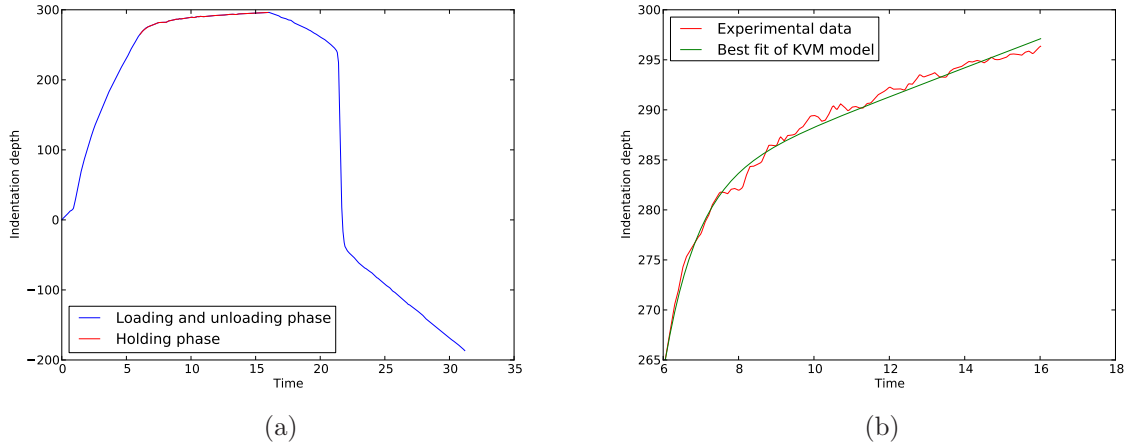


Figure 3: Example of indentation depth (ID); (a) Development of ID during the whole experiment (b) Approximation of experimental data with KVM model

1.2.2 Kelvin-Voight-Maxwell viscoelastic model at material point

In this section, we describe the Kelvin-Voight-Maxwell viscoelastic model shown in Fig. 1. We are interested in a stress $\sigma(t)$ vs. strain $\varepsilon(t)$ relation defined by this model dependent on four parameters, i.e. G_0 , η_M , G_V , and η_V , as it will be useful in the next sections. The Kelvin-Voight-Maxwell model can be described by the system of ordinary differential equations

$$\varepsilon(t) = \varepsilon_G(t) + \varepsilon_{\eta_M}(t) + \varepsilon_V(t) \quad (1.40a)$$

$$2G_0\varepsilon_G(t) = \sigma(t) \quad (1.40b)$$

$$2\eta_M\dot{\varepsilon}_{\eta_M}(t) = \sigma(t) \quad (1.40c) \quad \{\text{eq:strain } \mathcal{M}\}$$

$$2G_V\varepsilon_V(t) + 2\eta_V\dot{\varepsilon}_V(t) = \sigma(t) \quad (1.40d) \quad \{\text{eq:KV}\}$$

where $\dot{\varepsilon}$ denotes time derivative of ε , i.e. $\dot{\varepsilon}(t) = \frac{d\varepsilon}{dt}(t)$, $\varepsilon_G(t)$, $\varepsilon_{\eta_M}(t)$, and $\varepsilon_V(t)$ are strains of individual parts of the model.

First, we are interested in the strain response while loaded by stress with linear loading and constant

holding phase

$$\sigma(t) = \begin{cases} 0, & t \leq 0 \\ \frac{\sigma_{\max}}{t_L} t, & 0 < t \leq t_L \\ \sigma_{\max}, & t_L < t \end{cases} \quad (1.41) \quad \{\text{eq:stress load}\}$$

The analytical solution can be expressed with Volterra type of integral equation

$$\varepsilon(t) = \int_0^t J(t-\tau) \dot{\sigma}(\tau) d\tau \quad (1.42) \quad \{\text{eq:Volterra}\}$$

where $J := J(t)$ denotes the creep function, explicitly expressed as

$$2J(t) = \frac{t}{\eta_M} + \frac{1}{G_0} + \frac{1}{G_V} \left[1 - \exp - \frac{G_V t}{\eta_V} \right], \quad (1.43) \quad \{\text{eq:creep}\}$$

denoting a strain response exhibit by unit stress load. The well known Eq. 1.43 can be found among others in [2] and can be calculated using Laplace Transform, cf. MATLAB[®] routine published in [3]. Expressing the time derivative in Eq. (1.41) and substituting in Eq. (1.42) leads to the analytical solution in loading phase

$$\varepsilon_L(t) = \int_0^t J(t-\tau) \frac{\sigma_{\max}}{t_L} d\tau, \quad 0 \leq t \leq t_L \quad (1.44)$$

and explicitly in holding phase

$$\varepsilon_H(t) = \int_0^{t_L} J(t-\tau) \frac{\sigma_{\max}}{t_L} d\tau, \quad t_L < t \quad (1.45a)$$

$$= \frac{\sigma_{\max}}{2} \left\{ \frac{1}{G_0} + \frac{1}{G_V} + \frac{t}{\eta_M} - \frac{t_L}{2\eta_M} - \frac{\eta_V \left(\exp \frac{G_V t_L}{\eta_V} - 1 \right)}{G_V^2 t_L \exp \frac{G_V t}{\eta_V}} \right\}. \quad (1.45b)$$

Although the analytical solution (1.42) can always be used, the complicated stress load can lead to difficulties in expression of the integral, thus we are interested in numerical solution of KVM model. We solve numerically the differential equations (1.40), rather than the numerical expression of Volterra type of integral equation (1.42).

The numerical solution of system (1.40) is based on time discretization with time step $\Delta t > 0$, with time-levels

$$t_i = i\Delta t, \quad i \in \mathbb{Z}. \quad (1.46)$$

Next, ε^i will denote the calculated strain at time-level t_i and define $\sigma^i := \sigma(t_i)$. We express the searched strain in time-level t_i as a sum of individual contributions

$$\varepsilon^i = \varepsilon_G^i + \varepsilon_{\eta_M}^i + \varepsilon_V^i. \quad (1.47) \quad \{\text{eq:strain at time-level}\}$$

Simply, the first term can be expressed as

$$\varepsilon_G^i = \frac{\sigma^i}{2G_0}. \quad (1.48)$$

The second term is based on numerical integration of Eq. (1.40c)

$$\varepsilon_{\eta_M}(t) = \frac{1}{2\eta_M} \int_0^t \sigma(\bar{t}) d\bar{t} = \frac{1}{2\eta_M} \int_{t_{i-1}}^t \sigma(\bar{t}) d\bar{t} + \varepsilon_{\eta_M}(t_{i-1}), \quad (1.49)$$

hence

$$\varepsilon_{\eta_M}(t_i) = \frac{1}{2\eta_M} \int_{t_{i-1}}^{t_i} \sigma(\bar{t}) d\bar{t} + \varepsilon_{\eta_M}(t_{i-1}) \quad (1.50)$$

$$\varepsilon_{\eta_M}^i = \frac{\Delta t}{2\eta_M} \cdot \frac{\sigma^i + \sigma^{i-1}}{2} + \varepsilon_{\eta_M}^{i-1}. \quad (1.51) \quad \{\text{eq:strain'etaM}\}$$

The last term is based on solution of Eq. (1.40d) that is fully described e.g. in [1]. Since, we approximate the right-hand side of (1.40d) with constant $\frac{\sigma^i + \sigma^{i-1}}{2}$, it is possible to find a approximate solution $\bar{\varepsilon}_V$

$$\bar{\varepsilon}_V(t) = \frac{\sigma^i + \sigma^{i-1}}{4G_V} + C \exp\left(-\frac{G_V t}{\eta_V}\right) \quad (1.52)$$

where the constant C can be determined with a known initial value $\bar{\varepsilon}_V(t_{i-1}) = \varepsilon_V^{i-1}$. Hence

$$\bar{\varepsilon}_V(t) = \beta \varepsilon_V^{i-1} + (1 - \beta) \frac{\sigma^i + \sigma^{i-1}}{4G_V}, \quad (1.53)$$

$$\varepsilon_V^i = \beta \varepsilon_V^{i-1} + (1 - \beta) \frac{\sigma^i + \sigma^{i-1}}{4G_V}, \quad (1.54) \quad \{\text{eq:epV}\}$$

where $\beta = \exp\left(-\frac{G_V \Delta t}{\eta_V}\right)$.

Finally, substitution into Eq. (1.47) leads to affine relation between strain and stress at material point

$$\varepsilon^i = a\sigma^i + b^i \quad (1.55) \quad \{\text{eq:viscoelastic'law}\}$$

where

$$a = \frac{1}{2G} + \frac{\Delta t}{4\eta_M} + \frac{1 - \beta}{4G_V}, \quad (1.56)$$

is a constant independent on time levels while

$$b^i = \frac{\Delta t}{4\eta_M} \sigma^{i-1} + \varepsilon_{\eta_M}^{i-1} + \beta \varepsilon_V^{i-1} + \frac{1 - \beta}{4G_V} \sigma^{i-1}. \quad (1.57)$$

depends on previous time level t_{i-1} , particularly on stress σ^{i-1} and individual strain contributions $\varepsilon_{\eta_M}^{i-1}$ and ε_V^{i-1} that are necessary to calculate for the next time level according to Eq. (1.54) and (1.51).

1.2.3 Viscoelastic homogenization

The viscoelastic homogenization is based on finding the relation between the mean stress $\langle \boldsymbol{\sigma}(t) \rangle$ and mean strain $\langle \boldsymbol{\varepsilon}(t) \rangle$. In our case, assuming the viscoelastic properties occurring in the deviatoric part, we are mainly concerned with the relation of shear parts, i.e. $\langle \sigma_{12}(t) \rangle$ and $\langle \varepsilon_{12}(t) \rangle$, that is further approximated with KVM model. Analogically to the indentation experiment, where the indentation force is prescribed and indentation depth is measured, we prescribe the shear stress¹ and calculate strain².

In the section 1.1 about Linear elasticity we discuss the simplification into engineering Mandel's notation and we denoted the quantities with tilde operator, cf. Eq. (1.3a) and (1.4). In this section, we omit the tilde operator to simplify the notation.

¹The shear stress $\sigma_{12}(t)$ is prescribed as in Eq. (1.41) or as is shown in Fig. 4, i.e. with t_L and t_H being the duration of loading and holding phase, while the other stress components $\sigma_{11}(t), \sigma_{22}(t)$ are hold zeros.

²Although only $\sigma_{12}(t)$ is nonzero, all of calculated strain components are nonzero. Since we are interested in mean of both shear stress $\langle \sigma_{12}(t) \rangle$ and strain $\langle \varepsilon_{12}(t) \rangle$, the other strain components $\varepsilon_{11}(t)$ and $\varepsilon_{22}(t)$ are neglected.

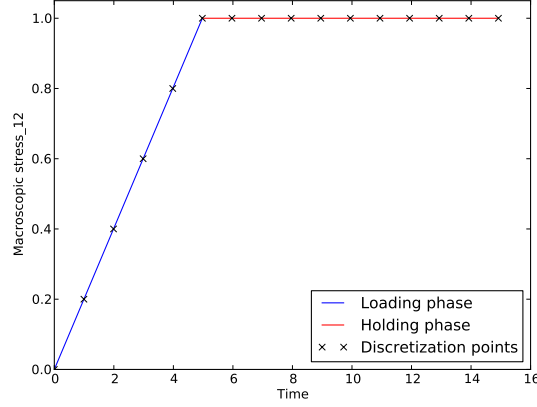


Figure 4: Example of loading test for obtaining homogenized parameters

First, we amend the viscoelastic material (1.55) to fit for the homogenization purposes. We rewrite it for particular nodal point \mathbf{x}^k as

$$\varepsilon_3^{k,i} = a^k \sigma_3^{k,i} + b^{k,i} \quad (1.58)$$

$$\sigma_3^{k,i} = \frac{1}{a^k} \varepsilon_3^{k,i} - \frac{b^{k,i}}{a^k} \quad (1.59)$$

$$= 2G_{ve}^k \varepsilon_3^{k,i} - (B_{ve}^i)_3^k \quad (1.60)$$

where $\varepsilon_3^{k,i}$ and $\sigma_3^{k,i}$ denotes shear strain and stress components at time level t_i and G_{ve}^k , $(B_{ve}^i)_3^k$ are components of matrices $\mathbf{G}_{ve} \in \mathbb{R}^N$, $\mathbf{B}_{ve}^i \in \mathbb{R}^{3 \times N}$, explicitly expressed as

$$\mathbf{G}_{ve} = (G_{ve}^k)_{k \in \mathbb{Z}_N^d} \quad G_{ve}^k = \frac{1}{2a^k}, k \in \mathbb{Z}_N^d \quad (1.61) \quad \{\text{eq:Gve}\}$$

$$\mathbf{B}_{ve}^i = ((B_{ve}^i)_\alpha^k)_{\substack{k \in \mathbb{Z}_N^d \\ \alpha=1,\dots,3}} \quad (B_{ve}^i)_3^k = \frac{b^{k,i}}{a^k}, k \in \mathbb{Z}_N^d \quad (B_{ve}^i)_\alpha^k = 0, k \in \mathbb{Z}_N^d, \alpha = 1, 2 \quad (1.62) \quad \{\text{eq:Bve}\}$$

Next, we define a matrix $\mathbf{L}_{K,G_{ve}}$ as a matrix $\tilde{\mathbf{L}}$ in Eq. (1.31) with bulk and shear moduli \mathbf{K} and \mathbf{G}_{ve} rather than with \mathbf{G} .

Then the material law, in engineering notation, can be expressed as

$$\mathbf{s}^i = \mathbf{L}_{K,G_{ve}}^i (\bar{\mathbf{e}}^i + (\mathbf{e}^0)^i) - \mathbf{B}_{ve}^i \quad (1.63)$$

where $\mathbf{e}^i = (\bar{\mathbf{e}}^i - (\mathbf{e}^0)^i)$ and \mathbf{s}^i denotes strain and stress resp. in Mandel's notation at nodal points for time-level t_i analogically to Eq. (1.13).

Substitution of material law into the linear system (1.30) leads to

$$\mathbf{P}\mathbf{L}_{K,G_{ve}} \bar{\mathbf{e}}^i = -\mathbf{P}\mathbf{L}_{K,G_{ve}} (\mathbf{e}^0)^i + \mathbf{P}\mathbf{B}_{ve}^i \quad (1.64) \quad \{\text{eq:linear system 'Mandel'}\}$$

where $(\mathbf{e}^0)^i \in \mathbb{R}^{3 \times N}$ depends only on macroscopic strain $(\boldsymbol{\varepsilon}^0)^i \in \mathbb{R}^3$ as in Eq. (1.15) thus later on we will often replace both quantities.

We repeat that we are interested in the mean stress $\boldsymbol{\sigma}^0(t) := \langle \boldsymbol{\sigma}(t) \rangle$ and mean strain $\boldsymbol{\varepsilon}^0(t) := \langle \boldsymbol{\varepsilon}(t) \rangle$ relation while the stress is prescribed as in Fig. 4. Unfortunately the linear system (1.64) is appropriate for the macroscopic strain prescription that we are interested in to calculate. Thus we split the linear system into two as we split the right-hand side

$$\mathbf{P}\mathbf{L}_{K,G_{ve}} \bar{\mathbf{e}}_{\mathbf{e}^0}^i = -\mathbf{P}\mathbf{L}_{K,G_{ve}} (\mathbf{e}^0)^i, \quad (1.65) \quad \{\text{eq:linear system 'A'}\}$$

$$\mathbf{P}\mathbf{L}_{K,G_{ve}} \bar{\mathbf{e}}_{\mathbf{B}_{ve}}^i = \mathbf{P}\mathbf{B}_{ve}^i, \quad (1.66) \quad \{\text{eq:linear system 'B'}\}$$

where the searched solution \mathbf{e}^i can be expressed as a sum of particular solutions $\bar{\mathbf{e}}_{\mathbf{e}^0}^i$ and $\bar{\mathbf{e}}_{\mathbf{B}_{ve}}^i$, i.e. $\mathbf{e}^i = \bar{\mathbf{e}}_{\mathbf{e}^0}^i + \bar{\mathbf{e}}_{\mathbf{B}_{ve}}^i$. Then, the stress \mathbf{s}^i can be split accordingly

$$\mathbf{s}^i = \mathbf{s}_{\mathbf{e}^0}^i + \mathbf{s}_{\mathbf{B}_{ve}}^i \quad (1.67)$$

where

$$\mathbf{s}_{\mathbf{e}^0}^i = \mathbf{L}_{\mathbf{K}, \mathbf{G}_{ve}} (\bar{\mathbf{e}}_{\mathbf{e}^0}^i + (\mathbf{e}^0)^i), \quad (1.68a)$$

$$\mathbf{s}_{\mathbf{B}_{ve}}^i = \mathbf{L}_{\mathbf{K}, \mathbf{G}_{ve}} (\bar{\mathbf{e}}_{\mathbf{B}_{ve}}^i - \mathbf{B}_{ve}^i). \quad (1.68b) \quad \{\text{eq:MBs'MBBve}\}$$

The quantities $\mathbf{s}_{\mathbf{B}_{ve}}^i$ and $\bar{\mathbf{e}}_{\mathbf{B}_{ve}}^i$ can be calculated from the linear system (1.66). Then we will calculate the macroscopic strain $(\mathbf{e}^0)^i$ in a way to satisfy the prescribed macroscopic stress $\boldsymbol{\sigma}^0(t_i)$. Since

$$\boldsymbol{\sigma}^0(t_i) = \langle \mathbf{s}^i \rangle := \frac{1}{N_1 N_2} \sum_{\mathbf{k} \in \mathbb{Z}_N^2} \mathbf{s}^{\mathbf{k}} \in \mathbb{R}^3, \quad (1.69)$$

we express at least the mean of searched quantity $\mathbf{s}_{\mathbf{e}^0}^i$

$$\langle \mathbf{s}_{\mathbf{e}^0}^i \rangle = \langle \mathbf{s}^i \rangle - \langle \mathbf{s}_{\mathbf{B}_{ve}}^i \rangle. \quad (1.70)$$

Since $(\mathbf{L}_{\mathbf{K}, \mathbf{G}_{ve}})_{\text{eff}}$ connects the mean stress and mean strain, cf. Eq. (1.6), we can express the mean of searched strain $\mathbf{e}_{\mathbf{e}^0}^i = \bar{\mathbf{e}}_{\mathbf{e}^0}^i + (\mathbf{e}^0)^i$

$$\langle \mathbf{e}_{\mathbf{e}^0}^i \rangle = (\mathbf{L}_{\mathbf{K}, \mathbf{G}_{ve}})_{\text{eff}}^{-1} \langle \mathbf{s}_{\mathbf{e}^0}^i \rangle \quad (1.71) \quad \{\text{eq:counting'MBe0}\}$$

Since $\langle \mathbf{e}_{\mathbf{e}^0}^i \rangle = \langle \mathbf{e}^0 \rangle$, we can calculate $\bar{\mathbf{e}}_{\mathbf{e}^0}^i$ using linear system (1.65) and consequently $\mathbf{s}_{\mathbf{e}^0}^i$. The calculated stress $\mathbf{s}^i = \mathbf{s}_{\mathbf{e}^0}^i + \mathbf{s}_{\mathbf{B}_{ve}}^i$ than satisfies the required stress loading $\langle \mathbf{s}^i \rangle = \boldsymbol{\sigma}^0(t_i)$.

However, the linear system (1.65) do not need to be calculated for each macroscopic strain $\langle \mathbf{e}^0 \rangle$ but the superposition of solutions can be used as the system is linear. Thus we calculate the solutions $\mathbf{e}_\alpha = \bar{\mathbf{e}}_\alpha + \mathbf{e}_\alpha^0$ of linear system

$$\mathbf{P} \mathbf{L}_{\mathbf{K}, \mathbf{G}_{ve}} \bar{\mathbf{e}}_{(\alpha)} = \mathbf{P} \mathbf{L}_{\mathbf{K}, \mathbf{G}_{ve}} \mathbf{e}_{(\alpha)}^0 \quad (1.72)$$

where $\mathbf{e}_{(\alpha)}^0$ depends on unit loads $\boldsymbol{\varepsilon}_{(\alpha)}^0 = (\delta_{\alpha\beta})_{\alpha=1, \dots, 3}$ for $\alpha = 1, \dots, 3$. Then since the arbitrary macroscopic strain is prescribed $\langle \mathbf{e}_{\mathbf{e}^0}^i \rangle$ we can express the solution as

$$\mathbf{e}_{\mathbf{e}^0}^i = \sum_{\alpha=1, \dots, d} \bar{\mathbf{e}}_{(\alpha)}^i (\mathbf{e}_{(\alpha)}^0)^i + \mathbf{e}^0. \quad (1.73) \quad \{\text{eq:MBs'MBe0'linear'com}\}$$

Finally, the effective parameters can be calculated. First the effective bulk and shear moduli K_{eff} , G_{eff} are calculated from the effective stiffness $(\mathbf{L}_{\mathbf{K}, \mathbf{G}})_{\text{eff}}$ obtained as in a linear elasticity and assuming that it is isotropic matrix, i.e.

$$G_{\text{eff}} = \frac{((\mathbf{L}_{\mathbf{K}, \mathbf{G}})_{\text{eff}})_{33}}{2} \quad (1.74a)$$

$$K_{\text{eff}} = \frac{((\mathbf{L}_{\mathbf{K}, \mathbf{G}})_{\text{eff}})_{11} + ((\mathbf{L}_{\mathbf{K}, \mathbf{G}})_{\text{eff}})_{22}}{2} - \frac{4}{3} G_{\text{eff}} \quad (1.74b)$$

where $((\mathbf{L}_{\mathbf{K}, \mathbf{G}})_{\text{eff}})_{\alpha\beta}$ is a component of $(\mathbf{L}_{\mathbf{K}, \mathbf{G}})_{\text{eff}}$ at position $\alpha\beta$, cf. Eq. (1.4) and (1.31). The mean stress and mean strain relation in the holding phase, i.e. prescribed $(\boldsymbol{\sigma}^0(t_i))_{t_L \leq t_i \leq t_H, i \in \mathbb{N}}$ and calculated $((\mathbf{e}^i))_{t_L \leq t_i \leq t_H, i \in \mathbb{N}}$, is used to find, using least square method, the effective viscoelastic parameters $(\eta_M)_{\text{eff}}$, $(G_V)_{\text{eff}}$, and $(\eta_V)_{\text{eff}}$, analogically to identification of parameters stated in Section 1.2.1. For this purpose, the analytical expression of shear strain in the holding phase (1.45) is used. Fig. 5(a) then shows macroscopic shear strain as the response to macroscopic shear stress load shown in Fig. 4 and Fig. 5(b) shows its part in the holding phase with a best fit of KVM model with effective (homogenized) viscoelastic parameters.

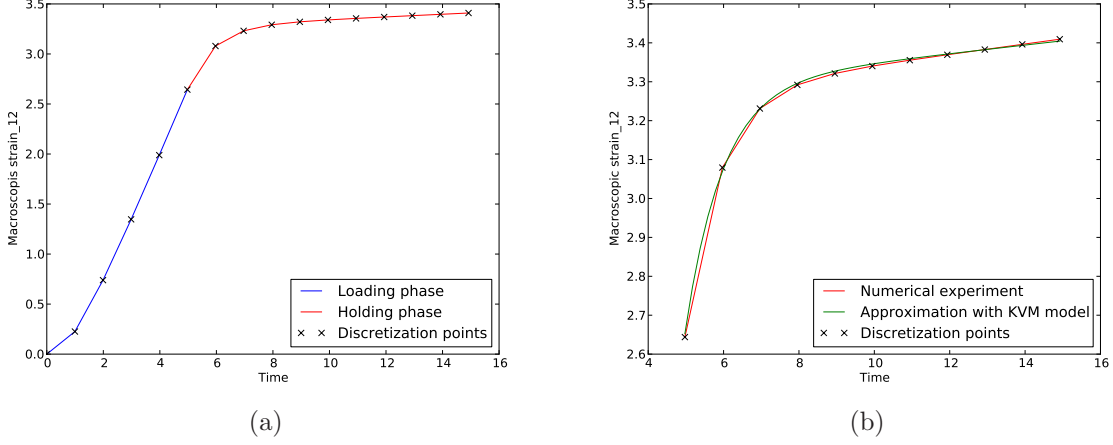


Figure 5: Numerical test obtained by loading as in Fig. 4; (a) Strain response during the whole experiment (b) Approximation of KVM model in the holding phase

Require: Material parameters $\mathbf{K}, \mathbf{G}, \eta_M, \mathbf{G}_V, \eta_V \in \mathbb{R}^N$; Time step Δt and number of time steps $n = n_L + n_H$ such that the loading phase $t_L = n_L \Delta t$ and holding phase $t_H = n_H \Delta t$; Macroscopic shear stress load $\boldsymbol{\sigma}^0(t) \in \mathbb{R}^3$ defined with t_L and t_H with the maximal value at holding phase equal to 1.

- 1: Calculate \mathbf{G}_{ve} as in Eq. (1.61), set stiffness matrix $\mathbf{L}_{\mathbf{K}, \mathbf{G}_{ve}}$ and projection matrix \mathbf{P}
- 2: Solve the linear system $\mathbf{P} \mathbf{L}_{\mathbf{K}, \mathbf{G}_{ve}} \bar{\mathbf{e}}_{(\alpha)} = -\mathbf{P} \mathbf{L}_{\mathbf{K}, \mathbf{G}_{ve}} \mathbf{e}_{(\alpha)}^0$ where $\mathbf{e}_{(\alpha)}^0$ corresponds to unit loads $(\delta_{\alpha\beta})_{\beta=1, \dots, 3}$ for $\alpha = 1, \dots, d$; obtain effective parameters $(\mathbf{L}_{\mathbf{K}, \mathbf{G}_{ve}})_{\text{eff}} \in \mathbb{R}^{3 \times 3}$ and vectors $\mathbf{e}_{(\alpha)} = \bar{\mathbf{e}}_{(\alpha)} + \mathbf{e}_{(\alpha)}^0 \in \mathbb{R}^{3 \times N}$
- 3: Calculate macroscopic strain $\langle \mathbf{e}_{e^0}^i \rangle = (\mathbf{L}_{\mathbf{K}, \mathbf{G}_{ve}})_{\text{eff}}^{-1} \boldsymbol{\sigma}^0(t_1) \in \mathbb{R}^3$, cf. Eq. (1.71).
- 4: Calculate strain at time level t_1 as $\mathbf{e}^1 = \sum_{\alpha=1, \dots, 3} \mathbf{e}_{(\alpha)} \langle \mathbf{e}_{e^0}^i \rangle_{\alpha}$ and stress as $\mathbf{s}^1 = \mathbf{L}_{\mathbf{K}, \mathbf{G}_{ve}} \mathbf{e}^1$
- 5: **for** $i = 2, \dots, n$ **do**
- 6: Calculate \mathbf{B}_{ve}^i as in Eq. (1.62)
- 7: Find strain $\mathbf{e}_{B_{ve}^i}^i = \bar{\mathbf{e}}_{B_{ve}^i}^i - \mathbf{B}_{ve}^i$ the solution of linear system $\mathbf{P} \mathbf{L}_{\mathbf{K}, \mathbf{G}_{ve}} \bar{\mathbf{e}}_{B_{ve}^i}^i = \mathbf{P} \mathbf{B}_{ve}^i$, cf. Eq. (1.66).
- 8: Calculate stress corresponding to $\mathbf{e}_{B_{ve}^i}^i$ as $\mathbf{s}_{B_{ve}^i}^i = \mathbf{L}_{\mathbf{K}, \mathbf{G}_{ve}} (\bar{\mathbf{e}}_{B_{ve}^i}^i - \mathbf{B}_{ve}^i)$, cf. Eq. (1.68b)
- 9: Calculate macroscopic strain for linear system (1.65) as $\langle \mathbf{e}_{e^0}^i \rangle = (\mathbf{L}_{\mathbf{K}, \mathbf{G}_{ve}})_{\text{eff}}^{-1} (\boldsymbol{\sigma}^0(t_i) - \langle \mathbf{s}_{B_{ve}^i}^i \rangle) \in \mathbb{R}^3$, cf. Eq. 1.71.
- 10: Find $\mathbf{e}_{e^0}^i = \bar{\mathbf{e}}_{e^0}^i + \mathbf{e}^0$, a solution of linear system (1.65), where $\mathbf{e}^0 = \langle \mathbf{e}_{e^0}^i \rangle$ as a linear combination $\bar{\mathbf{e}}_{e^0}^i = \sum_{\alpha=1, \dots, d} \bar{\mathbf{e}}_{(\alpha)}^i (\mathbf{e}_{(\alpha)}^0)^i + \mathbf{e}^0$, cf. Eq. (1.73).
- 11: Calculate strain $\mathbf{e}^i = \mathbf{e}_{e^0}^i + \mathbf{e}_{B_{ve}^i}^i$
- 12: Calculate stress $\mathbf{s}^i = \mathbf{L}_{\mathbf{K}, \mathbf{G}_{ve}} \mathbf{e}^i + \mathbf{B}_{ve}^i$
- 13: **end for**
- 14: Calculate $(\mathbf{L}_{\mathbf{K}, \mathbf{G}})_{\text{eff}}$ as in the case of linear elasticity
- 15: Calculate effective bulk and shear moduli K_{eff} and G_{eff} from $(\mathbf{L}_{\mathbf{K}, \mathbf{G}})_{\text{eff}}$ using Eq. 1.74.
- 16: Find effective viscoelastic properties $(\eta_M)_{\text{eff}}$, $(G_V)_{\text{eff}}$, and $(\eta_V)_{\text{eff}}$ as a best fit of KVM model to relation between calculated mean stress and strain, $(\boldsymbol{\sigma}^0(t_i))_{t_L \leq t_i \leq t_H, i \in \mathbb{N}}$ and $(\langle \mathbf{e}^i \rangle)_{t_L \leq t_i \leq t_H, i \in \mathbb{N}}$, using analytical expression (1.45)

Algorithm 1: Visco-elastic homogenization

2 Manual

2.1 Indentation

This section describes tab Indentation as is shown in Fig. 2. It primarily reads and adjust the data from files obtained from nanoindentation.

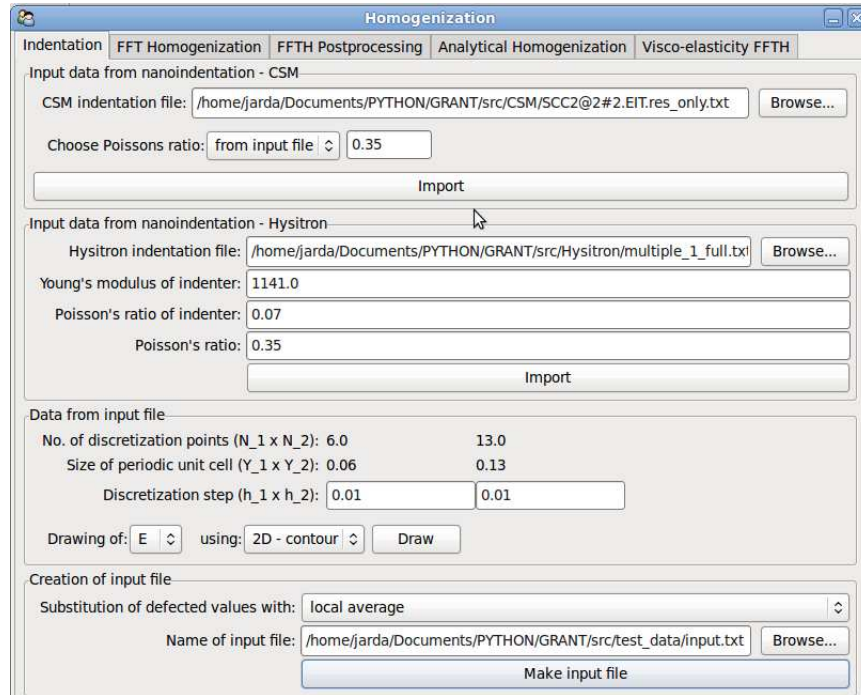


Figure 6: 'Indentation'

2.1.1 Input data from nanoindentation - CSM

This section is operated with a button 'Import' reading the data from the file stated as 'CSM indentation file'. It reads the Young's modulus E , Poisson's ratio ν and the position of each indenter in PUC that is used to identify the size of PUC (\mathbf{Y}) and the number of discretization points (\mathbf{N}) in each direction. In fact the Poisson's ratio can be obtained in two ways stated in option 'Choose Poisson's ratio':

- 'from input file' - it reads the values from 'CSM indentation file',
- 'as' - it sets the value of Poisson's ratio to value stated further for all indentation points.

2.1.2 Input data from nanoindentation - Hysitron

This section is operated with a button 'Import' reading the scaled Young's modulus³ $\bar{\mathbf{E}} = (\bar{E}^{\mathbf{k}})^{\mathbf{k} \in \mathbb{Z}_N^d} \in \mathbb{R}^N$ from the file stated as 'Hysitron indentation file'.

The scaled Young's modulus has to be recalculated into the real one $\mathbf{E} \in \mathbb{R}^N$ with the following formula

$$E^{\mathbf{k}} = \frac{1 - \nu^2}{\frac{1}{\bar{E}^{\mathbf{k}}} - \frac{1 - \nu_i^2}{E_i}}, \quad \mathbf{k} \in \mathbb{Z}_N^d \quad (2.1)$$

³The components of $\bar{\mathbf{E}}$ denotes the Young's modulus of individual indenter, i.e. $\bar{E}^{\mathbf{k}}$ represents its value in the point $\mathbf{x}^{\mathbf{k}}$ for $\mathbf{k} \in \mathbb{Z}_N^d$.

where ν is a Poisson's ratio of real material taken the same for all points, E_i and ν_i are Young's modulus and Poisson's ratio resp. for a material of indenter.

2.1.3 Data from input file

This section shows the number of discretization points N , size of periodic unit cell \mathbf{Y} and discretization step $\mathbf{h} := (\frac{Y_1}{N_1}, \frac{Y_2}{N_2})$ that can be adjusted leading to recalculation of the size of PUC, \mathbf{Y} . Moreover, the read values of \mathbf{E} can be plotted.

2.1.4 Creation of input file

This section is operated by button 'Make input file' producing an input file named 'Name of input file' that is used in the tab 'FFT homogenization'⁴.

The indentation process can produce some defected values of Young's modulus; since it is recognized by user, those Young's modulus are set up to some negative value. Hence, there are some possibilities to deal with those non-physical negative values stated in choose option 'Substitution of defected values with':

- 'none' - this option leaves the negative values and write it into the input file; this option is especially used when the user wants to recognized those defected values in input file,
- 'local average' - it substitutes the negative value with a value calculate as a mean of the closest adjacent values. When the negative value occurs at the margin the periodicity assumption is utilized.
- 'global average' - the negative values are substituted with the mean of all positive Young's modulus.

2.2 FFT homogenization

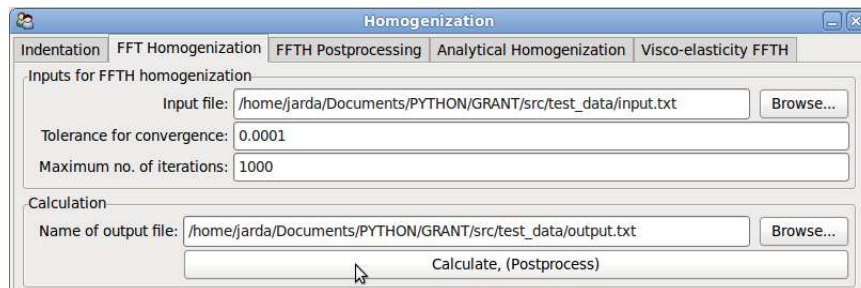


Figure 7: 'FFT Homogenization'

This section describes tab FFT homogenization as is shown in Fig. 7. The tab is operated with a button 'Calculate' proceeding a Linear elasticity homogenization using FFT as is described in Section 1.1.

First, it reads the input file named 'Input file' where the size of PUC \mathbf{Y} and material parameters $\mathbf{E}, \nu \in \mathbb{R}^N$ are stored. Then bulk and shear modulus $\mathbf{K}, \mathbf{G} \in \mathbb{R}^N$ are calculated from the components of \mathbf{E} and ν as

$$\mathbf{K}^k = \frac{\mathbf{E}^k}{3(1 - 2\nu^k)} \quad (2.2)$$

$$\mathbf{G}^k = \frac{\mathbf{E}^k}{2(1 + \nu^k)} \quad (2.3)$$

⁴The name of input file 'Input file' in the tab 'FFT homogenization' is filled up with the value 'Name of input file'.

for $\mathbf{k} \in \mathbb{Z}_N^d$.

Then the FFT-based homogenization is proceeded as it is described in Sec. 1.1. The linear system (1.30) is then solved with the maximal number of iterations stated in 'Maximal no. of iterations' and the required tolerance of convergence stated in 'Tolerance for convergence'.

The output files contains following variables

- L_{eff} - homogenized matrix in Mandel's notation
- resnorm - residual based norm calculated for unit loads, i.e. sequentially for $\varepsilon_0 = [1, 0, 0]$; $\varepsilon_0 = [0, 1, 0]$ and $\varepsilon_0 = [0, 0, 1]$
- kit - number of iteration of Conjugate gradients reached for unit loads
- maxit - maximal number of iteration for Conjugate gradients
- tol - required tolerance for residual based norm to reach a convergence of Conjugate gradients
- time - time in seconds to calculate Conjugate gradients for a particular unit load
- L - the object from $\mathbb{R}^{3 \times 3 \times N_1 \times N_2}$ storing the stiffness coefficients
- strain - the object from $\mathbb{R}^{3 \times 3 \times N_1 \times N_2}$ storing the stiffness coefficients

2.3 FFTH postprocessing

In this section, we describe the postprocessing of output file of FFT homogenization. It is operated with button 'update' that reads the file 'Name of output file' and primarily shows the effective stiffness in group 'Outputs'. Next, it shows the number of iterations necessary to reach the required tolerance of residual norm. Both quantities are in sum of three as the effective stiffness is calculated for three unit loads.

Finally, the section 'Drawing of local fields' enable to show the local strain and stress fields for arbitrary macroscopic strain.

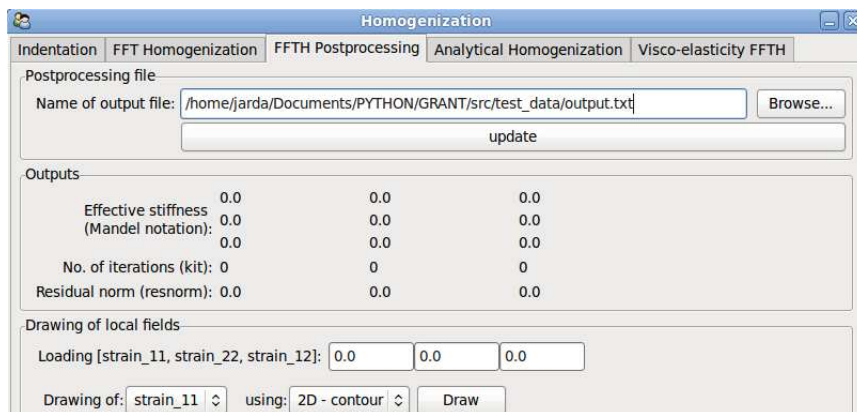


Figure 8: 'FFTH postprocessing'

2.4 Analytical homogenization

In this section, we describe the tab 'Analytical Homogenization' that homogenize the material in a fully different approach than FFT homogenization. It is based on a assumption that the material is composed of some finite phases each having the phase volume ratio and material parameters, in our case isotropic. After pushing the button 'Import and calculate' those quantities are read and various analytical

homogenization proceeded. The Voigt-Reuss homogenization makes the bounds for the real effective parameters that are improved by the Hashin-Shtrikman-Walpole method. Finally Self Consistent method and Mori-Tanaka calculate the estimates of effective parameters. The second method requires to identify the matrix phase, usually the phase with maximal phase ratio. It is provided by field 'No. of matrix phase'.

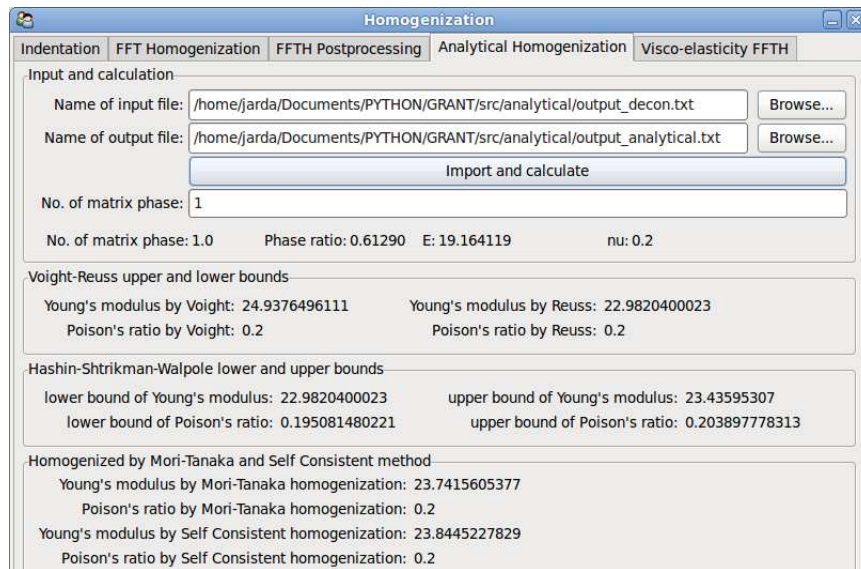


Figure 9: 'Analytical Homogenization'

2.5 Visco-elastic FFTH

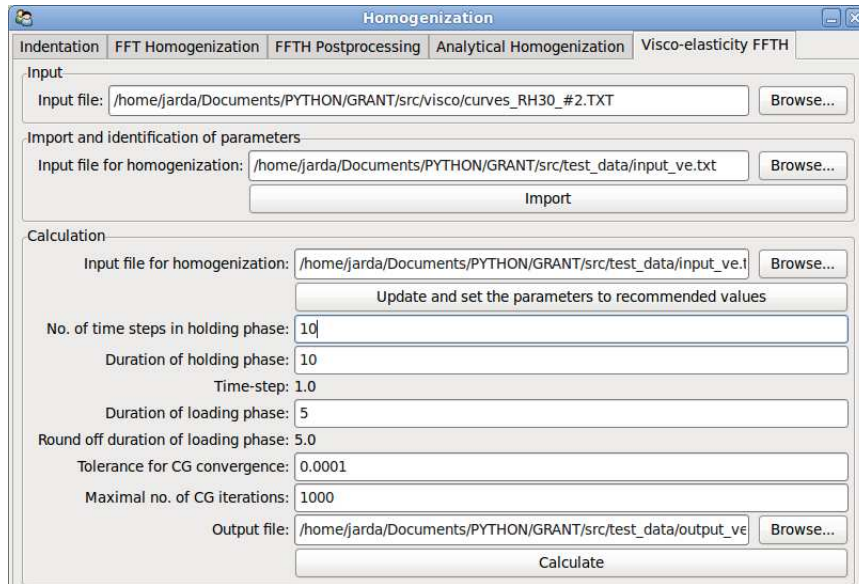


Figure 10: 'Visco-elasticity FFTH'

This section describes tab 'Visco-elasticity FFTH', see Fig. 7, dealing with homogenization of visco-elastic material.

2.5.1 Import and identification of parameters

This section is operated with button 'Import' that reads the data from 'Indentation file', identifies the visco-elastic parameters and write it into the file defined as 'Input file for homogenization'. Moreover, it directly set the recommended values for the section 'Calculation'.

The identification of visco-elastic parameters follows the description from Sec. 1.2.1. Briefly, for each indentation point from regular grid, the nanoindentation force is prescribed as in Fig. 2 and the indentation depth is measured as in Fig. 3. The part of indentation depth that corresponds to holding phase in indentation force is fitted with Kelvin-Voight-Maxwell model, cf. Fig. 1, emerging the visco-elastic parameters.

2.5.2 Calculation

This section is operated with two buttons 'Update and set the parameters to recommended values' and 'Calculate'. The first read the data from the file stated in 'Input file for homogenization' and set the parameters to recommended values. The number of time steps in holding phase n_H is predefined in the source code, however it can be adjusted and dependent quantities are recalculated. Next, the quantity 'Duration of holding phase', t_H , can also be set up and directly influence the quantity 'Time-step', Δt , as

$$\Delta t = \frac{t_H}{n_H}.$$

'Duration of loading phase', t_L^{init} , can be set up, however it is round-off in order to be multiplier of time-step Δt , i.e.

$$t_L = \Delta t \cdot \text{round} \left(\frac{t_L^{\text{init}}}{\Delta t} \right).$$

Finally, two quantities that control the solution of linear system by Conjugate gradients can be regulated. First, 'Tolerance for CG convergence', ε_{CG} , controls the 2-norm of residual as in Eq. (1.32). Next, 'Maximal no. of CG iterations' regulate CG iterations especially in case of not convergence.

Then, the homogenization itself follows the theory stated in Sec. 1.2.3. The duration loading and holding phase defines a macroscopic shear stress load with maximal value equal to one. Than the strain and especially macroscopic one is calculated using visco-elastic material law with parameters identified from nanoindentation for particular points from regular grid.

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