The Fretting Contact of Coated Bodies. Part II – The Stress State

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Abstract. The service life of contacting coated machine elements is ultimately determined by the distribution of stresses in the coating and in the substrate. By assuming the elastic bodies as elastic half-spaces, the contact stress computation entails the calculation of convolutions expressing the superposition of effects of unit point loads acting on the boundary. The fundamental solutions of stresses and displacements in multilayered materials have only been calculated in the frequency domain, and are known as the frequency response functions. An additional difficulty arises in the stress calculation, related to frequency response function valuation in the origin of the frequency domain, where a singularity is usually encountered. This case of undetermination is circumvented in this paper by substituting the required value with the mean value of the frequency response function over a vicinity centered in origin. The latter approach is endorsed by the fact that the frequency response function is singular, but numerically integrable in the aforementioned vicinity. The latter technique is validated by comparison with results obtained for the sliding contact, and then applied to derive the elastic stresses arising during a fretting loop in the coating and in the substrate. The stresses due to shear tractions are superimposed to those induced by contact pressure. The calculation is performed in layers of constant depth, and the algorithmic complexity is optimized by using state-of-the-art techniques for discrete convolution computation. The equivalent stress is discontinuous across interface between the two layers, and the location and intensity of the maximum von Mises stress is determined by the frictional coefficient and by the mismatch between the Young moduli of the coating and the substrate. The results obtained with the newly proposed numerical technique may extend the understanding of the fretting contact of coated materials and assist the design of improved coating configurations.

1. Introduction
The contact mechanics modelling of functionally graded materials and coatings, whose elastic properties vary in the depth direction, involves multi-layered systems consisting in perfectly bonded layers of different elastic constants, allowing for the half-space assumption valid for small contact region compared to the bulk body dimensions. The study of these materials pioneered with the stress and displacements analytical solutions given by Burminster [1] for a single layered material and axisymmetric normal loading. Chen [2], and Chen and Engel [3], extended these solutions to arbitrary
normal loadings. The case of multilayered transversely isotropic half-spaces was addressed by Kuo and Keer [4] using the boundary integral method together with the Hankel transform. The frequency response functions (FRFs) of bilayered materials, relating in the Fourier transform domain unit surface tractions to displacements and stresses, were derived by O’Sullivan and King [5] with the aid of the Papkovitch–Neuber potentials and the double Fourier transform. Their procedure was further employed to analyse various dry [6-12] or lubricated [13] contact scenarios, in which the elastic response of the layered material is assessed based on the FRFs.

From a computational point of view, an important breakthrough in the calculation of stresses arising in multi-layered systems due to general loadings, has been achieved with the development of the spectral techniques for the calculation of convolution products in the Fourier transform domain. Nogi and Kato [6] first employed the aforementioned FRFs in the derivation of the solution for the coated contact of rough surfaces with the aid of the fast Fourier transform (FFT). The source of the periodicity error linked to the application of the FFT to non-periodic problems such as the concentrated contact was discussed [14-16], and different correcting procedures were advanced. The extension of the physical computational domain coupled with the zero-padding of the excitation are now generally applied in evaluation of the discrete cyclic convolutions expressing stresses and displacements in contact problems.

Considering the complexity of the arising mathematical models, the derivation of the FRFs is an important prerequisite in stress calculation. Liu and Wang [16] obtained the FRFs for both normal and shear tractions in a closed-form that is well adapted to numerical implementations. In the same manner, the FRFs of tri-layer materials were derived [10], as well as the recurrence relation for the FRFs of multilayered materials [17].

In this paper, the stress fields in the fretting contact are obtained following the general procedure for stress calculation established in the literature of layered materials. The numerical implementation uses the FRFs derived by Liu and Wang [16], whereas the aliasing in the frequency domain is controlled by an extension of the computational target domain. The computer program is validated by comparison with results obtained for the sliding spherical contact of bilayered materials.

2. Elastic response of coated bodies

The half-space approximation employed in the framework of contact mechanics, together with the Linear Elasticity fundamental solutions, also referred to as the Green's functions, allow for the calculation of the response of an elastic half-space to arbitrary, yet known, loadings. In particular, displacements and stresses induced by surface general loadings result as integrals superimposing the individual contributions of concentrated forces applied on the boundary. Mathematically, the latter integrals are convolution products of the relevant Green’s function with the contact tractions. The Fourier transform of a Green’s function is also known as the frequency response function (FRF). Explicit expressions were derived in the literature for both the Green’s functions and the related FRFs of homogenous semi-infinities, but in case of layered materials, the Green’s functions still lack explicit expressions. The derivation of the FRFs suggests the numerical calculation of the layered half-space response in the frequency domain, assisted by the discrete convolution theorem, which brings additional advantages regarding the algorithmic efficiency: the convolution product of series with \(N\) terms is reduced in the frequency domain to an improved \(O(N \log N)\) order of operations, which is a substantial saving from the \(O(N^2)\) specific to the time/space domain. This decrease stems from the conversion of the convolution product in an element-wise product in the Fourier transform domain.

The main disadvantage of model digitization in the frequency domain is the problem periodization: the discrete Fourier transform of a discrete series, calculated with the fast Fourier transform (FFT), tacitly assumes the series as periodical. The physical meaning of the periodization is that a bogus periodical surface load is assumed instead of the actual one. The fake neighbouring periods of contact tractions are likely to perturb the half-space response to the non-periodical load. Important research efforts aimed to reduce or control this periodicity error. Nogi and Kato [6] protected the displacement solution of both homogenous and bilayered bodies by a grid refinement with a factor of two along
each direction, whereas Liu et al. [15] addressed the issue of the conversion of a linear convolution into its discrete cyclic counterpart, concluding in the Discrete Convolution FFT method (DCFFT) that allegedly brings no additional error beside the discretisation error in convolution computation. The aliasing and the Gibbs phenomena were identified [16] as the main sources of perturbation when the half-space response is calculated based on the FRFs directly in the Fourier transform domain. Based on their findings, the algorithm accuracy is assured in this paper by extending the target computational domain, resulting in a refinement of the mesh in the spectral domain that reduces aliasing, and by the zero-padding of the excitation (i.e., the contact tractions, pressure or shear), aiming to move away from the target domain the spurious neighbouring periods, thus limiting their contribution.

An algorithm for a more general problem is thus advanced, allowing the convolution computation when the convolution members are arbitrary, yet known functions, and one of the convolution members is only known in the frequency domain. In particular, the latter algorithm can be applied to derive numerically the elastic response (i.e., displacement and stresses) of a coated half-space to a general surface excitation in the form of pressure or shear tractions. It should be noted that, although the method implies digitization of the excitation, the employed fundamental solution (i.e., the FRF), is derived in closed-form. Therefore, similar methods are known in the literature of contact mechanics as semi-analytical [18].

For clarity and simplicity, but without losing generality, the method presentation is restricted to the line contact of infinitely long cylinders (i.e., the two-dimensional problem). Extension to the three-dimensional case is achieved by adding a new dimension, matching the second tangential direction from the contact 3D problem. The algorithm needs the following input: (a) the target domain \( L \), (b) the digitised surface loading \( p_i \), \( i = 1 \ldots N \), (c) the FRF closed-form for the needed response, \( \tilde{f} \), and (d) the extended domain \( \chi L \), defined with the aid of an extension ratio \( \chi \). It should be noted that the algorithm output should only be considered for the target domain \( L \), whereas results at the edge of the extended domain may be of a questionable precision. For the Fourier transform domain, the tilde (\( \sim \)) symbol is employed to denote continuous functions, as opposed to the hat (\( \hat{\cdot} \)) mark for discrete series. The extension of the target domain \( L \) into \( \chi L \) aims at the refinement of the mesh in the Fourier transform domain. This can only be achieved by preserving the original sampling interval in the spatial domain, \( \Delta = L/N \), and leads to a decrease of the sampling interval in the frequency domain from \( 2\pi/L \) to \( 2\pi/(\chi L) \). Thus, the number of samples in the spatial domain needs also to be increased from \( N \) to \( \chi N \). The value of the extension ratio \( \chi \) thus has a negative impact on the needed computational resources, and should be chosen as a compromise. Values between 2 and 8 make good candidates.

The spectral coordinates \( \zeta_i \) of the refined spectral mesh result as:

\[
\zeta_i = 2\pi (i - \chi N/2)/(\chi L), \quad i = 1 \ldots \chi N ,
\]

and represent discrete frequencies at which the FRF \( \tilde{f} \) is evaluated. A discrete spectral series \( \tilde{f}_i \), characterising the spectral response to a unit impulse response is achieved:

\[
\tilde{f}_i = \tilde{f}(\zeta_i), \quad i = 1 \ldots \chi N .
\]

One additional difficulty arise, as the stresses and displacements FRFs for both homogenous and layered materials are singular at \( \zeta = 0 \), i.e. the origin of the frequency domain. This shortcoming can be overcome depending on whether the calculated elastic response is needed in absolute or in relative terms. It was stated in the companion paper that, due to a particularity of the contact solver in both normal and tangential direction, only relative displacements are needed to achieve the contact solution. Therefore, if \( \tilde{f} \) is a displacement FRF, \( \tilde{f}(0) \) is not needed, as shown below, as it only introduces a constant to the calculated response field, and any value can be considered instead, e.g. \( \tilde{f}(0) = 0 \). The situation is similar to the 2D contact problem, in which the displacement field is known except for a
constant, but the contact pressure can be assessed in absolute terms. Relative calculation is not satisfactory in stresses computation, when absolute values are required to assess the propensity of plastic yielding via an equivalent stress tensor intensity such as the von Mises criterion. In the latter case, by taking advantage of the fact that the FRF is numerically integrable on a vicinity centred in origin, a mean value of the FRF can be considered as the best available indicator of the local function behaviour:

\[
\tilde{f}(0) \approx \frac{\chi L}{2\pi} \int_{-\pi/\chi L}^{\pi/\chi L} \tilde{f}(\tau) d\tau .
\]  

(3)

Following the requirements of the discrete cyclic convolution theorem [15], the series \( \tilde{f}_i \) is subsequently rearranged in wrap-around order, with the terms corresponding to negative frequencies shifted at the end of the series. Consequently, the first position in the series \( \tilde{f}_i \) will be occupied by the term calculated in eq. (3). Symmetrical zero-padding of the excitation in the extended domain is also required [15], resulting in a series of vanishing terms, apart from:

\[
p_{i+(\chi-1)N} \leftarrow p_i, \quad i = 1 \cdots N ,
\]  

(4)

series which is subsequently transferred to the frequency domain, \( \hat{p} = \text{FFT}(p) \). The convolution result \( \sigma_j \) is first calculated as element-wise product in the frequency domain, then transferred to the space domain via inverse FFT, as shown in eq. (10). The middle \( N \) terms match the target domain and are retained as output.

\[
\tilde{\sigma}_i = \hat{f}_i \cdot \hat{p}_i, \quad i = 1 \cdots 2N , \quad \sigma = \text{IFFT}(\tilde{\sigma}) .
\]  

(5)

One can verify that, when the first term of a series is perturbed with an arbitrary constant, all the terms in the FFT or the IFFT of the series are perturbed with a constant. Considering the way the convolution result is achieved in eq. (5), it can be seen that miscalculating the FRF in the origin of the frequency domain results in a constant added to the computed stress or displacement field.

The proposed algorithm not only circumvents the computation of the Green’s functions for the coated half-space, but also reduces the computational complexity due to the convolution calculation in the frequency domain in \( O(N) \) operations, as opposed to \( O(N^2) \) in the space domain. Considering that both FFT and IFFT are of order \( O(N \log N) \), the latter is the overall order of operations for displacement or stress calculation in layers of constant depth. The decrease is of paramount importance as the displacement field needs to be calculated many times during the iterative search of the contact area and the stick region. More so, the stress tensor components evaluation implies six convolutions for each traction component and each considered depth. The gap between \( O(N^2) \) and \( O(N \log N) \) becomes significant for \( N > 10^6 \), which is considered as a minimum threshold for the treatment of rough contact problems. Practically, a three-dimensional contact simulation with a surface grid of \( N = 128^2 \) points, multiplied 64 times in depth for stress calculation, and with a domain extension ratio \( \chi = 4 \), is performed on a quad-core 3.2 GHz CPU in less than 30 minutes.

The FRFs required in eq. (2) are given in the literature [5-7,16]. The closed-form expressions were obtained by taking the double Fourier transform of the Papkovich-Neuber potentials expressing the stress and displacement fields in layered materials, and by imposing the boundary conditions and the continuity conditions at the layers interface. From a computational point of view, the formulas obtained by Liu and Wang [16] are more convenient to use in a numerical implementation, as certain derivatives are not involved. The proposed algorithm can equally handle multilayered materials provided the required FRFs are made available, such as in [17].
3. Results and discussions
The validation of the sequence for the computation of stresses is attained by benchmarking the distributions of the calculated $J_2$ stress tensor second invariant with the data obtained by O’Sullivan and King [5] with a different approach. In this simpler case, the contact is in a full sliding, and the tangential tractions are simply proportional to the contact pressure via the frictional coefficient $\mu$. Two typical cases are presented in figure 1, but it should be noted that all results presented in [5] were closely reproduced with the newly advanced computer program. The Hertz parameters $a_H$ and $p_H$, calculated for the indentation of a homogenous half-space having the same elastic modulus as the substrate, by a rigid sphere, are used as normalizers. The coating thickness is denoted by $h_c$. The location of the maximum value in each distribution is depicted with an X mark, and its dimensionless magnitude is indicated on each plot. The comparison gives confidence in the sequence for the stress field computation in bilayered materials. The discontinuity in the equivalent stress at the interface $z = h_c = a_H$, suggests that, although the $\sigma_{xx}$, $\sigma_{xy}$ and $\sigma_{zz}$ stress tensor components are continuous across the interface, the remaining ones are not.

![Figure 1](attachment:image1.png)

**Figure 1.** $J_2/p_H$ contour plots in the plane $y = 0$, obtained for the sliding contact of coated bodies: (a) $E_1/E_2 = 2$, $\mu = 0.25$; (b) $E_1/E_2 = 1/2$, $\mu = 0.5$.

![Figure 2](attachment:image2.png)

**Figure 2.** $J_2/p_H$ contour plots in the plane $y = 0$, obtained for the fretting contact of coated bodies: (a) $E_1/E_2 = 1/2$; (b) $E_1/E_2 = 2$. 
The stress state in the fretting contact is then evaluated with the newly advanced computer program, corresponding to the contact tractions presented in the companion paper. The simulation parameters are: frictional coefficient $\mu = 0.1$, the coating thickness $h_c = \alpha_H$, the tangential force $T_\tau = 0.75 \mu W$, corresponding to the second pas of the increasing tangential force through zero (or the third zero value). Iso-contours of the dimensionless $J_2$ are depicted in figure 2, for different elastic moduli ratios between the coating and the substrate.

The computational process can take advantage of the fact the values of the FRF for the $q_2$ shear stress are permutations of those calculated for $q_1$. The numerical integration of the FRF in the vicinity of origin in the frequency domain was performed with the Matlab function “quad2d” with the default absolute and relative precisions, and no convergence issues were encountered.

4. Conclusions
The Green’s functions for the layered half-space are difficult to derive in closed-form expression, and therefore the method of influence coefficients cannot be directly applied as in the case of homogenous mediums. The stress and displacement elastic response of coated bodies is computed in this paper in the frequency domain, based on closed-form solutions for displacement and stresses induced in a coated half-space by unit point force, also known as the frequency response function. The evaluation of the latter leads to a series that is multiplied in the frequency domain with the transform of the excitation, thus substituting the convolution in the space domain. The rearrangement in wrap-around order and the zero-padding of the excitation are well-known techniques applied in discrete cyclic convolutions computations. The singularity in the origin is circumvented by replacing the missing sample with a mean value calculated around the vicinity of the singularity.

The program validation is achieved against classic results for the sliding contact of coated bodies. The simulations show the location and intensity of the maximum stress tensor second invariant, which is an indicator of the plastic flow susceptibility in the elastic body according to the von Mises criterion. The strong point of the proposed method consists in its computational efficiency, allowing for increased resolution in stress calculation. A map of the possible yield positions in the coated system subjected to fretting.

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