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A COMPARATIVE STUDY OF FFT ALGORITHMS FOR CONVOLUTION CALCULATION IN NON-PERIODIC ELASTIC CONTACTS

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Abstract: The interaction of machine elements in direct mechanical contact generates responses of the elastic bodies best described in the frame of computational contact mechanics by finding numerical solutions for the contact area, the contact tractions, deformations and stresses. In most cases, the mathematical model for the discrete contact problem involves convolutions whose calculation yields the body response to a surface load. The main idea of the FFT-based methods is to execute the convolution calculation in the frequency domain, where the convolution operation reduces to an element-wise product between the convolution members. This paper analyses and compares two methods for assessment of the elastic half-space response to arbitrary, yet known, surface loads. The starting point is the analytical solutions to fundamental problems of elasticity, concerned with the response to unit loads, also referred to as the impulse responses in digital signal processing theory. These solutions exist in the space domain and/or in the frequency domain, and different algorithms and manipulations are required in each case. The main issue when computing the convolution in the frequency domain is to deal with the implicit problem periodization, which induces an error when applied to intrinsically non-periodic problems. The displacement induced by a Hertz pressure distribution is chosen as a case study and relative errors are computed for each algorithm. The influence of parameters that must be chosen based on numerical experimentations is discussed. The paper is expected to provide additional insight to a very important topic in computational contact mechanics and to guide the application of FFT based algorithms to convolution calculations.

Key words: elastic contact, convolution, fast Fourier transform, frequency domain.

1. INTRODUCTION

A contact algorithm first seeks information on the contacting interface, such as the contact area and the pressure distribution, followed by a boundary-value problem assessing the stresses in each contacting body. Convolution products arise in both stages of the contact solution as displacement calculation is a prerequisite for finding the contact area. The classic evaluation of two-dimensional convolutions by direct multi-summation is very computationally intensive, which limits dramatically the number of discrete elements in the numerical contact model. Many research efforts in computational contact mechanics were therefore concerned with acceleration of calculation of convolution products. Algorithms based on the fast Fourier transform (FFT) have emerged [1-7] in response to this challenge, and various methods were developed based on the convolution theorem.

The solution of a contact mechanics problem involves at least two sets of convolutions [5,8-10]: one for the contribution of contact tractions to the surface displacements, and a second one to compute the stresses developing in the contacting bodies in response to the calculated surface tractions. Each type of contribution is based on the solution to a fundamental problem for the elastic half-space, which is usually expressed in closed form, e.g., for the first set of convolutions, the Boussinesq and Cerruti displacements induced by a unit point force acting on the boundary of an elastic half-space. The latter solutions are also referred to as the Green's functions, when they are computed in the space domain, or as the frequency response functions (FRFs), when expressed in the frequency domain. By making an analogy with the digital signal processing theory, the Green's functions or the FRFs are the so-called unit impulse responses, whose convolution with the input signal yields the output signal.

More complicated problems [11-19] can also be formulated with the aid of convolutions. The displacements and stresses arising in a material containing inclusions or inhomogeneities can also be assessed based on the eigenstrain theory and the

associated Green's functions. These frameworks led to the solution of essentially non-linear contact problems, such as the elastic-plastic, the viscoelastic, or the contact between inhomogeneous materials.

Given the large variety of contact problems and contact scenarios that can benefit from efficient calculation of convolution products assisted by the FFT, many algorithms, reviewed in [20,21], have been developed in the last two decades. This paper attempts a comparative study of the two most important methods for convolution calculation, applied to the computation of displacement in elastic contacts. This type of convolution appears in the first stage of a contact process solution, and its efficient and precise estimation is of paramount importance for the contact solution. The choice is based on the existence of a closed-form solution [22] for the elastic displacement arising in a Hertz contact problem, and allows assessing the influence of different algorithm parameters that are usually chosen by numerical experimentation, on the solution precision.

2. MODEL OVERVIEW

The computation of the convolution due to the relationship between contact tractions and the surface displacement allows the formulation of an iterative strategy for finding simultaneously the contact area and the pressure distribution, which are both a priori unknown. An analytical solution to the contact problem was only achieved under strong limiting assumptions, under the Hertz contact framework. Once the contact geometry is not as prescribed by the latter model, or when the contacting bodies are not homogeneous, the analytical treatment fails and numerical analysis steps in, with its iterative approach. A guess contact area and pressure distribution are adopted and subsequently adjusted, until all model equations are checked to an imposed precision. Usually, the static force equilibrium is employed as a convergence criterion, as the corresponding equation is not comprised in the linear system to be solved. During the iterative process, the displacement field must be computed for each trial pressure, therefore an efficient algorithm is needed to assure the algorithm robustness.

In order to use the Green's functions, the contacting bodies must be approximated with semi-infinite mediums, i.e., half-spaces, which is reasonable in the frame of small deformations for concentrated contacts, with contact areas evolving from a point or a line to surface regions of small dimensions compared to the radii of curvature of the contacting bodies.

The analytical correlation between a pressure distribution $p(x,y)$ acting on a surface region A_C and the resulting normal displacement $u(x,y)$ can be expressed based on the Boussinesq and Flamant equations [22]:

$$u(x,y)=\frac{1-\nu^2}{\pi E}\iint_{A_C}\frac{p(\xi,\eta)}{\sqrt{(x-\xi)^2+(y-\eta)^2}}d\xi d\eta\ , \quad (1)$$

which is in fact a convolution product between pressure and the Green's function $G(x,y)$ (or the unit impulse response) for the pressure - normal displacement correlation:

$$G(x,y)=(1-\nu^2)\Big/(\pi E\sqrt{x^2+y^2})\ . \quad (2)$$

Here, E and ν are the Young modulus and the Poisson's ratio for the half-space material. Equation (2) stands for the normal displacement induced by a unit point force acting normally on the half-space boundary. In the solution process for a general contact problem, the integration (1) must be performed repeatedly for various pressure distributions and integrations domains, as resulting during the iterative search progression; therefore, only a numerical technique may be applicable.

Discretization of the contact problem involves the meshing of the contact surface using rectangular elements of uniform size (on each direction), indexed by integers, on which all problem parameters are piece-wise constant. The discrete counterpart of (1) can be expressed as:

$$u(i,j)=\sum_{(k,\ell)\in A_P}K(i-k,j-\ell)\,p(k,\ell)=\sum_{k=1}^{N_1}\sum_{\ell=1}^{N_2}K(i-k,j-\ell)\,p(k,\ell)\ , \quad (3)$$

where A_P is a domain comprising $N_1\times N_2$ rectangular elements, with $A_C\subset A_P$, and $K(i-k,j-\ell)$ the so-called influence coefficient, expressing the displacement contribution of a uniform unit pressure acting in the (k,ℓ) grid element to the displacement observed in the (i,j) element. For increased accuracy, the influence coefficients should be calculated from analytical solutions, in this case from the solution [23] for uniformly distributed pressure on a rectangular half-space boundary element:

$$K(i-k,j-\ell)=\int_{y(\ell)-\Delta_y/2}^{y(\ell)+\Delta_y/2}\int_{x(k)-\Delta_x/2}^{x(k)+\Delta_x/2}G(x_1(i)-x_1',x_2(j)-x_2')\,dx_1'dx_2'\ , \quad (4)$$

where $x(k)$ and $y(\ell)$ are the coordinates of the control point for the (k,ℓ) grid element, and Δ_x and Δ_y the side lengths of the rectangular grid element.

The closed-form expression for the pressure-displacement influence coefficient is:

$$K(i,j)=\frac{1-\nu^2}{\pi E}\left(\begin{array}{l} f(x(i)+\Delta_x/2,y(j)+\Delta_y/2)+f(x(i)-\Delta_x/2,y(j)-\Delta_y/2)... \\ -f(x(i)+\Delta_x/2,y(j)-\Delta_y/2)-f(x(i)-\Delta_x/2,y(j)+\Delta_y/2) \end{array}\right), \quad \text{with} \quad (5)$$
$$f(x,y)=x\ln\left(y+\sqrt{x^2+y^2}\right)+y\ln\left(x+\sqrt{x^2+y^2}\right).$$

The calculation of the convolution product in (3) by direct multi-summation is an operation with an order of complexity of $O(N^2), N=N_1N_2$, which strains the method application to rough contact problems, where finer grid resolutions with $N>10^6$ are needed to accurately capture in a deterministic manner the specifics of the microtopography. The solution adopted in the last two decades is to transfer the convolution calculation in the frequency domain, where an improved order $O(N\log N)$ is achieved due to the convolution theorem. The latter states that a $O(N^2)$ convolution product in the space domain can be substituted by an $O(N)$ element-wise product in the frequency domain. Considering that the discrete Fourier transform can be efficiently computed in $O(N\log N)$ using the FFT, an efficient way to speed up the multi-summation (3) can be derived, however not without difficulties, as described in the following section.

3. THE DCFFT TECHNIQUE

Equation (3) is a convolution that can be computed efficiently in the frequency domain, where the convolution series are transferred via discrete Fourier transform, followed by inverse Fourier transform. In this section, the model equations will be written in one dimension only for brevity. Different types of convolution may be calculated [21], and the choice for the appropriate one should take into consideration the periodicity of the investigated problem. When the discrete Fourier transform of a finite series is computed, one tacitly assumes that the series comes from a periodic distribution having the considered window as a period. Moreover, this periodization affects the convolution result. From a physical point of view, the calculated displacement is due to an infinite series of pressure distributions, each similar to the considered period. This error was identified in the early implementations of the method, and resulted in an overestimation of displacement at the edges of the computational domain, due to the contribution of the false neighboring pressure periods. An early solution [1-3] was to move away the pressure periods by considering the discretization of a domain much larger than the one expected to encompass the contact area. This idea proved its efficiency, but the choice for the domain extension ratio remained a topic of numerical experimentation. This method weakness was circumvented by Liu and Wang [7], who studied in detail the different types of convolution and the sources of errors when a continuous infinite convolution is evaluated and substituted by a discrete convolution.

For non-periodic contact problems such as the concentrated contact, in which the initial contact area is a point that grows into a finite contact region, the type of convolution with no periodicity implied is the one referred to as a cyclic circular convolution [21]. If K_i and p_i, $i=1\ldots N$, are discrete series of finite length N, obtained from calculation of relation (5) for all involved indexes, and from discretization of pressure, respectively, the element-by-element product between their discrete Fourier transforms $\hat{K}(m)$ and $\hat{p}(m)$, with m the frequency variable, produces the spectral analogue of the needed elastic displacement:

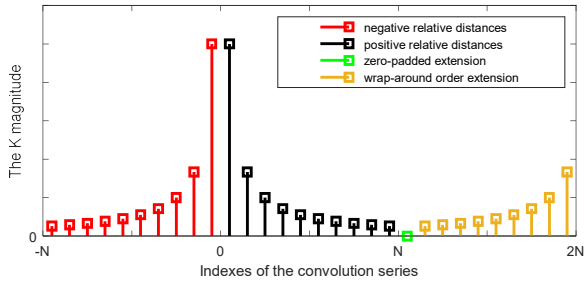
$$\hat{u}_i=\hat{K}_i\cdot\hat{p}_i. \quad (6)$$

For the latter product to be free of any periodicity artefacts, the product (6) should be performed between series of $i=1\ldots 2N$ terms with a special arrangement, as first suggested by the Discrete Convolution Fast Fourier Transform (DCFFT) technique [6]. It should be noted that the domain for which the displacement is calculated is $i=1\ldots N$, but the convolution series are calculated for a domain twice (in each direction) the original one. The influence coefficient series $K_i=K(k-\ell)$, $i=1\ldots 2N$, $k,\ell=1\ldots N$, is computed so that the first N terms are for negative relative distances, i.e., $k<\ell$, whereas the remaining ones are for positive relative distances, i.e., $k>\ell$. If $i=k-\ell$, the index of the series would vary between $-N$ and N, thus $2N$ terms. An additional simplification can be made by considering the symmetry of the influence coefficients: for the dependence of displacement on pressure, $K(k-\ell)=K(\ell-k)$, but other dependencies may be anti-symmetric. After computation, the terms of the K series are rearranged as depicted in Figure 1(a): the terms for the negative indices, i.e., the first N terms, are shifted after the positive ones. This wrap around order defines the circular nature of the resulting series. As suggested in [6], an additional treatment involves a one term zero padding of the terms with positive relative distances, i.e., $K_{N+1}=0$.

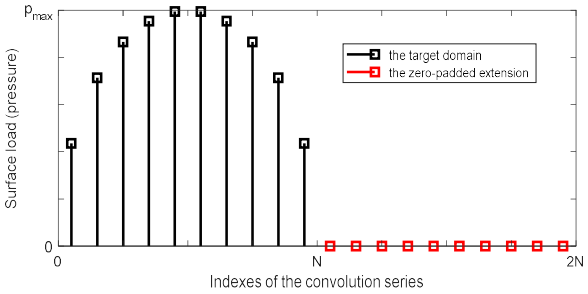
The second convolution member, i.e., pressure, is simply digitized in the target domain $i=1\ldots N$ and zero-padded in the extended window $i=N+1\ldots 2N$. With this treatment suggested in Figure 1(b), performed in the space domain, the transfer to and from the frequency domain can be performed via

FFT. The DCFFT steps are restated for clarity and brevity:

1. Choose the target computational domain and perform its digitization with N grids.
2. Compute the influence coefficients $K_i, i=1\ldots 2N$ from (5).
3. Rearrange the K series in wrap around order with zero padding, as suggested in Figure 1(a).
4. Transfer the latter series into the frequency domain via FFT, thus obtaining $\hat{K}$ with $2N$ terms.
5. Digitize and expand by zero-padding the pressure series, Figure 1(b).
6. Transfer p to the frequency domain via FFT, to get a complex $\hat{p}$ with $2N$ terms.
7. Compute convolution result as element-wise product in the frequency domain, according to (6).
8. Use inverse FFT (IFFT) to obtain the convolution result in the space domain, as a $2N$ series.
9. Discard the terms in the zero-padded region of pressure.



(a)



(b)

Fig. 1. The schematic of DCFFT: a) zero-padding and wrap-around of K; b) zero-padding of pressure

4. FRF-BASED COMPUTATIONS AND ALGORITHMS

The Fourier transform of the Green's function (2) can be obtained by Fourier analysis:

$$\tilde{u}(m,n)=\frac{2(1-\nu^2)}{E\sqrt{m^2+n^2}}, \qquad (7)$$

where m and n are the coordinates in the frequency domain corresponding to the space directions x and y, respectively. It is tantalizing to develop algorithms that use the frequency response function (7) instead of the Green's function (2) because in many contact scenarios, such as the contact of layered materials, only the FRFs can be expressed in closed-form. The DCFFT cannot thus be directly applied to contacts involving coatings unless a method for derivation of the influence coefficients is found, other than the one based on the integration of the Green's functions.

An alternative approach is to compute the convolution product directly in the frequency domain, by using a discrete counterpart of the FRF and the Fourier transform of the pressure. The discretization performed directly in the frequency domain adds unwanted artefacts such as aliasing and the Gibbs phenomenon [7], which together with the periodicity error can compromise the method accuracy. These drawbacks can be addressed by extending the physical domain on which the convolution product is performed, which conversely translates to an increase in resolution in the frequency domain that reduces the unwanted artefacts mentioned above. A method for displacement computation that uses the FRFs $\tilde{g}(m)$ instead of the Green's function was advanced by this author [24] and can be summarized in the steps described below:

1. Choose the target computational domain (in the space domain), of size L, and the domain extension ratio χ ($\chi=2\ldots 12$).
2. Compute a series of discrete frequencies that digitizes a frequency domain associated to the extended space domain.

$$m_i=2\pi(i-\chi N/2)/(\chi L), \quad i=1\ldots\chi N \qquad (8)$$

3. Digitize the FRF to obtain a new series $\hat{g}_i=\tilde{g}(m_i), i=1\ldots\chi N$. The value at the origin of the frequency domain, i.e., $\tilde{g}(0)$, should be computed by quadrature, as suggested in [3].
4. Rearrange the terms in the latter series in wrap-around order, as depicted in Figure 1(a).
5. Perform digitization with χN grids, thus obtaining the pressure series $p_i, i=1\ldots\chi N$. The original pressure is kept in the $i=1\ldots N$ span, whereas the rest of the series is zero-padded.
6. Compute the FFT of this series $\hat{p}=\mathrm{FFT}(p)$.
7. Compute the element-wise product $\hat{u}_i=\hat{g}_i\hat{p}_i, i=1\ldots\chi N$.
8. Transfer the resulting series in the space domain: $u=\mathrm{IFFT}(\hat{u})$.
9. Retain the middle N terms as algorithm output.

An alternative method is to derive the influence coefficients $K_i, i=1\ldots 2N$ needed in the DCFFT algorithm, from the discrete spectral series $\hat{g}_i, i=1\ldots \chi N$ calculated in step 3 of the abovementioned algorithm. A new algorithm variant can be formulated, with the first four steps, involving digitization of the FRF in the frequency domain, identical to the previous version. The remaining algorithm steps are detailed below:

1. Compute the inverse FFT of the $\hat{g}_i, i=1\ldots \chi N$ series to get a new series in the space domain, $g_i, i=1\ldots \chi N$.
2. From the latter series, retain the middle $2N$ terms as the influence coefficients $K_i, i=1\ldots 2N$
3. Rearrange the $K_i, i=1\ldots 2N$ series in wrap-around order and perform zero-padding as suggested in Figure 1(a).
4. Perform the rest of the DCFFT process (i.e., steps 5-9) to obtain the needed displacements.

These methods provide an efficient way to tackle contact problems for which the Green's functions have not been derived, e.g., the contact of layered bodies. The need for a numerical evaluation of the FRF in the origin of the frequency domain (step 3 of the algorithm) introduces a potential instability in the algorithm, considering that the numerical integration may fail when too strong convergence criteria are imposed, or its precision may not be reliable for very permissive convergence standards. It should be noted, however, that an error in the evaluation of $\tilde{g}(0)$ induces an error in the convolution calculation that is uniform over the whole computational domain, as detailed in [24]. Consequently, the displacement is known except for a constant, or, in other words, only the relative displacements are known on the computational domain. A contact solver however only needs relative displacements to derive iteratively the contact area and the pressure distribution. Therefore, the precise calculation of $\tilde{g}(0)$ may not be needed, unless the rigid-body approach between the contacting bodies is the required algorithm output. In the latter case, an accurate evaluation of $\tilde{g}(0)$ becomes of critical importance.

5. RESULTS AND DISCUSSIONS

The computer programs implementing the presented algorithms are benchmarked against the closed form expression [22] for the displacement in a point Hertz contact of central pressure p_H and contact area a_H, expressed in radial coordinates:

$$u^{(analytical)}(r)=\begin{cases}\pi\eta p_H(2a_H^2-r^2)/(2a_H), & |r|<a_H;\\ \eta p_H\left[(2a_H^2-r^2)\sin^{-1}(a_H/r)+ra_H\sqrt{1-(a_H/r)^2}\right]/a_H, & |r|\geq a_H.\end{cases} \quad (9)$$

Figure 2 shows the distribution of the dimensionless relative error $\varepsilon=(u^{(numerical)}-u^{(analytical)})/\delta$, normalized by the rigid body approach $\delta=u^{(analytical)}(0)$. The iso-contours depicted in Figure 2(a) prove that the most important errors in DCFFT displacement computation appear at the edges of the contact area (at $x/a_H=\pm 1$ and $y/a_H=\pm 1$), and are probably related to the inability of a reunion of rectangular elements to approximate a circular boundary (i.e., a discretization error). Figure 2(b) proves that the relative error decreases with the mesh density, thus the process converges to the required solution. Even with a coarse mesh of 32×32, the error is kept under 1.5%.

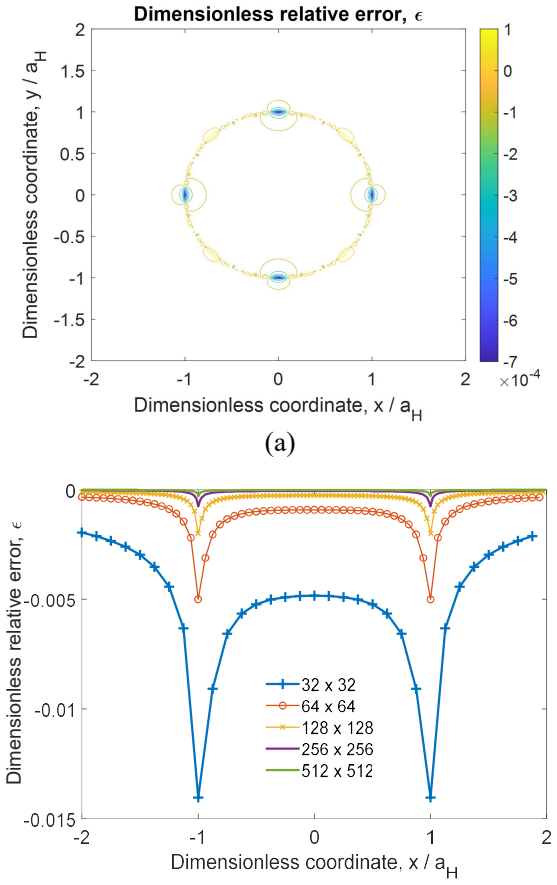


Fig. 2. Relative error in Hertz displacement calculation by DCFFT: a) iso-contours; b) influence of grid density

The influence of the numerical parameters affecting the relative error resulting from FRF calculations is shown in Figure 3. Figure 3(a) proves that a domain extension with a ratio $\chi=2$ results in an overestimation of displacement of up to 5% at the edges of the computational domain. The latter error may be attributed to the contribution of the spurious neighboring periods assumed implicitly by the FFT. The latter error is reduced with increasing χ,

suggesting a convergent process. Figure 3(b) suggests that solution accuracy can be increased by using smaller tolerances in the numerical quadrature employed to evaluate $\tilde{g}(0)$, i.e., by imposing stronger tolerances in the "quad2d" Matlab function, but with sometimes prohibitive added computational effort. Moreover, the added precision acts as a scalar not affecting the relative displacements, in accord with the theory developed in [24].

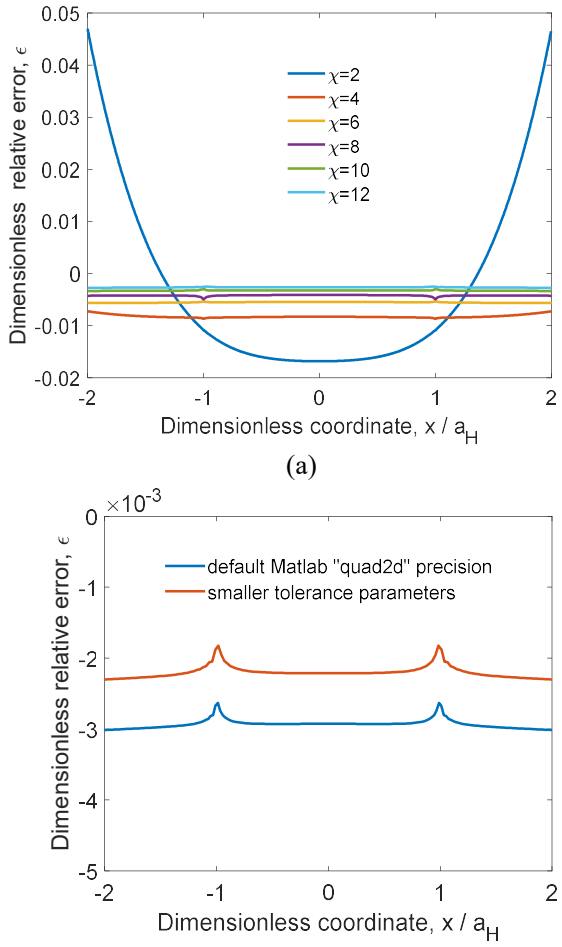


Fig. 3. Relative error in Hertz displacement calculation by FRF conversion: a) influence of χ ratio; b) influence of $\tilde{g}(0)$ calculation

6. CONCLUSIONS

The solution of contact problems encountered in engineering applications requires very efficient numerical techniques for the calculation of displacement induced by arbitrary, yet known, surface tractions. The computational methods that involve the convolution computations in the frequency domain show dramatic speed advantages over multi-summation in the space domain. This paper attempts a comparative study of the spectral methods for non-periodic contact problems and studies the influence of different parameters on the precision that can be achieved with each algorithm variant.

The artefacts related to the implicit periodicity assumed by transfer to the frequency domain via FFT can be eliminated by zero-padding and wrap around order. When the Green's functions exist in closed-form, the convolution calculation by the DCFFT technique introduces no additional error other than the discretization error, with an extension of the target domain with a ratio of two in each direction.

When the Green's functions cannot be obtained in analytical form, but their Fourier transform counterpart, i.e., the frequency response functions, is available, two algorithm variants can be employed: (1) digitization of the FRFs followed by element-wise product in the frequency domain, or (2) conversion of the influence coefficients from the FRFs followed by DCFFT. The methods have comparable precision and efficiency, but shear the same weakness: the evaluation of the FRF at zero frequency, where the FRF is singular, but numerically integrable over a vicinity containing the origin. However, this may not an issue when the contact solver only needs relative displacements to assess the contact area and the contact tractions.

The spectral methods for the convolution calculation not only provide important computational advantages over the classic multi-summation in the space domain, but also provide ways to approach models lacking analytical solutions in the space domain, such as the contact of layered materials.

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