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Percus–Yevick radial distribution function calculation for a water-saturated granular medium

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ABSTRACT

This paper presents a practical technique to evaluate the Percus–Yevick (PY) radial distribution function (RDF) for a water-saturated granular medium with a high volume fraction of grains. This is based on the weighted average of the PY RDF's recursive formula (Goodwin et al., 1992) and the PY integral equation's numerical solution using the filtered fast Fourier transform. In a highly dense medium, the combination of both models produces more accurate and stable results. The error analysis for the volume fraction of scatterers and the distance is given for validation. Finally, using the proposed PY RDF result, we solve an acoustic multiple-scattering equation with quasi-crystalline approximation (QCA) to obtain the effective bulk modulus and attenuation of the water-saturated granular medium, and confirm that our method provides a reasonable result.

1. Introduction

The radial distribution function (RDF) describes the particle distribution from a reference particle in a granular medium. In a classical fluid, an analytic expression of RDF can be obtained by solving the Ornstein–Zernike integral equation with the closure relation of Percus and Yevick (PY) (Wertheim, 1963). The PY RDF is an approximate result, which has successfully been applied in various fields from molecular physics to ocean sediment physics (Smith and Henderson, 1970; Henderson, 2009; Tsang and Kong, 1980; Caleap et al., 2012; Varadan et al., 1989).

The PY RDF evaluation can be performed by calculating the analytic formula for the inverse Laplace transform, where the high-order derivatives rise as the distance increases. Goodwin et al. (1992) derived a recursive formula to calculate high-order derivatives and evaluated the PY RDF up to $20d$ with a hard sphere diameter, d. Although their results were better than those in other similar studies, the repetitive arithmetic multiplication and division still leads to numerical instability in distances above $15d$ (Goodwin et al., 1992). Similar numerical errors occurred in the numerical solution based on the difference equation derived from the Baxter factorization method (Perram, 1975). Kahl and Pastore (1991) directly solved the inverse Laplace transform without kernel expansion at a short distance. At a long distance, they applied the asymptotic method to the calculation. A drawback of this method is that the complex roots of the kernel denominator are found numerically (Goodwin et al., 1992). A more efficient method would be to use the Fourier transform of the direct correlation function (DCF) (Mandel et al., 1970; Tsang et al., 2001). The PY RDF is obtained from the inverse transform of the relation of DCF and RDF in the Fourier domain. This method is fast, but still has numerical errors due to the Gibbs phenomenon (in particular at the first contact of the sphere (Tsang et al., 2001)) and aliasing.

In general, difficulties in the aforementioned numerical methods are not significant problems in a weakly dense medium with a volume fraction below 0.4. This is because the PY RDF in a diffused medium shows relatively regular behavior and rapidly converges to 1 at distances over $4d$ (Tsang et al., 1982). However, in highly dense packing such as sand, gravel, or artificial balls (Aste et al., 2005; Panaitescu and Kudrolli, 2010; Lee et al., 2009), the PY RDF goes up sharply at the beginning distance, and exhibits much slower convergence for distance. In this case, the aforementioned methods fail to yield a stable value for the PY RDF, which will be entered into a main acoustic solver.

The purpose of this study is to develop a more accurate and stable solver of PY RDF in highly dense packing. We suggest a hybrid technique using the analytic evaluation method for short distances and the filtered Fourier-transform method for long distances. This method is easy to implement with existing algorithms, and provides very good results up to $60d$ for the volume fraction of 0.6. Moreover, we confirm that the proposed method is sufficiently applicable to an acoustic multiple-scattering problem for a highly dense medium.

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This paper is categorized as follows: Section 2 provides the details of our approach with the description of the analytic evaluation method and the Fourier transform method. In particular, the use of a filter is considered to suppress the Gibbs phenomenon in the original Fourier-transform method (Gottlieb and Shu, 1997). The section also deals with the validation test and error analysis as a function of the volume fraction of scatterers and of the distance. Section 3 describes an application of the proposed technique to an acoustic multiple-scattering problem for highly dense spheres. The conclusion is presented in Section 4.

2. Hybrid approach

2.1. Analytic evaluation method

Following the Smith and Henderson (1970) expression, the PY RDF for uniform spheres is written as

$$g(x) = \sum_{n=1}^{\infty} H(x-n) g_n(x), \tag{1}$$

where $H(x)$ is the Heaviside step function with 0 for $x<0$ and 1 for $x>0$, x is the scaled distance of r/d with the distance r, and $g_n(x)$ is a piecewise continuous function defined as follows.

$$xg_n(x) = \frac{(-12\eta)^{n-1}}{(n-1)!} \sum_{i=0}^{2} \lim_{t \to t_i} \frac{d^{n-1}}{dt^{n-1}} \left[(t-t_i)^n t \left(\frac{L(t)}{S(t)} \right)^n \exp\,[t(x-n)] \right], \tag{2}$$

where

$$L(t) = (1+0.5\eta)t + 1 + 2\eta, \tag{3}$$

$$S(t) = (1-\eta)^2 t^3 + 6\eta(1-\eta)t^2 + 18\eta^2 t - 12\eta(1+2\eta), \tag{4}$$

and t_i is each root of the cubic polynomial $S(t)$. η is the volume fraction of spheres and relates to the number density ρ as $\eta = \pi\rho d^3/6$.

To simplify Eq. (2), Goodwin et al. factorized $S(t)$ into the monic polynomial $(1-\eta)^2(t-t_0)(t-t_1)(t-t_2)$ and substituted it into Eq. (2). The result is rearranged as

$$xg_n(x) = \frac{(-12\eta)^{n-1}}{(n-1)!} \sum_{i=0}^{2} \frac{1}{(1-\eta)^{2n}} \lim_{t \to t_i} \frac{d^{n-1}}{dt^{n-1}} \left[\frac{tL^n(t) \exp\,[t(x-n)]}{(t-a)^n (t-b)^n} \right], \tag{5}$$

where a and b are the other two roots of $S(t)$ excluding t_i.

The high-order derivatives of brackets in the above equation can be easily calculated by the recursive formula derived by Goodwin et al. (1992). Although Eq. (5) is an analytic form, it is noted that the arithmetic operations are numerically performed by a computer. As indicated in Ref. Goodwin et al. (1992), this method shows numerical instability above $15d$ for hard spheres of $\eta = 0.47$. We calculate Eq. (5) for the volume fraction of spheres and check similar tendencies, plotted in Fig. 1. The sphere diameter used in the calculation is set to 0.545 μm and identical for all following examples.

2.2. Fourier transform (FT) method

With spherical symmetry assumption, the DCF is written in the Fourier domain k as

$$c(k) = \frac{24\eta}{(2\pi)^3 \rho} \left[\frac{(\alpha+\beta+\delta)}{(kd)^2} \cos\,kd - \frac{(\alpha+2\beta+4\delta)}{(kd)^3} \sin\,kd - \frac{2(\beta+6\delta)}{(kd)^4} \cos\,kd + \frac{2\beta}{(kd)^4} + \frac{24\delta}{(kd)^6} (\cos\,kd - 1) \right], \tag{6}$$

where $\alpha = (1+2\eta)^2/(1-\eta)^4$, $\beta = -6\eta(1+\eta/2)^2/(1-\eta)^4$, and $\delta = \eta(1+2\eta)^2/2(1-\eta)^4$ (Tsang et al., 2001).

The relation between the DCF and the total correlation function $h(k)$ is obtained from the Ornstein–Zernike integral equation and given as $h(k) = c(k)/[1-(2\pi)^3 \rho c(k)]$.

Since $g(r) = h(r)+1$ in the physical domain r, the PY RDF is simply obtained by taking the inverse Fourier transform of $h(k)$. The final expression is arranged to

$$g(r) = 4\pi \int_0^{\infty} k^2 \left(\frac{\sin\,kr}{kr} \right) h(k) dk + 1. \tag{7}$$

Note that due to spherical symmetry, the 3D integral transform is reduced to 1D integral transform.

Due to the ‘no overlapping’ condition between particles, the PY RDF is inherently discontinuous at $r=d$. This discontinuity causes the Gibbs phenomenon in the numerical evaluation. This is the main reason that the high-order convergence of this method is degraded and the numerical accuracy of the solution is reduced.

To mitigate the Gibbs phenomenon, we apply the Lanczos filter (Gottlieb and Shu, 1997; Duchon, 1979; Vandeven, 1991) into

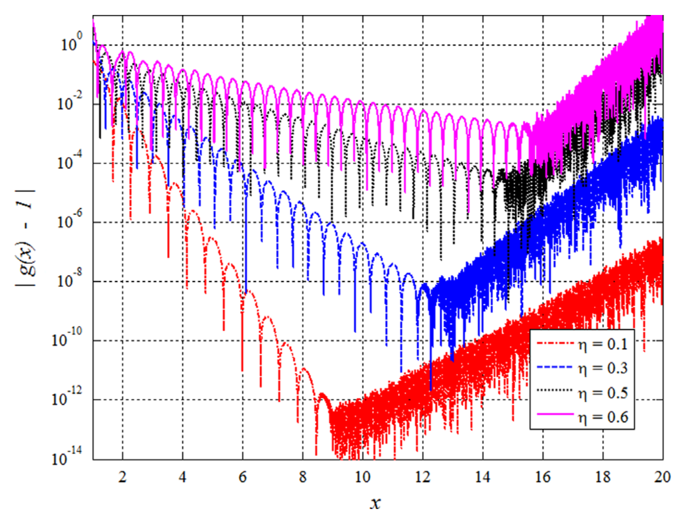

Fig. 1. Absolute value of PY RDF minus one versus the scaled distance for volume fractions of 0.1, 0.3, 0.5 and 0.6 calculated by Eq. (5).

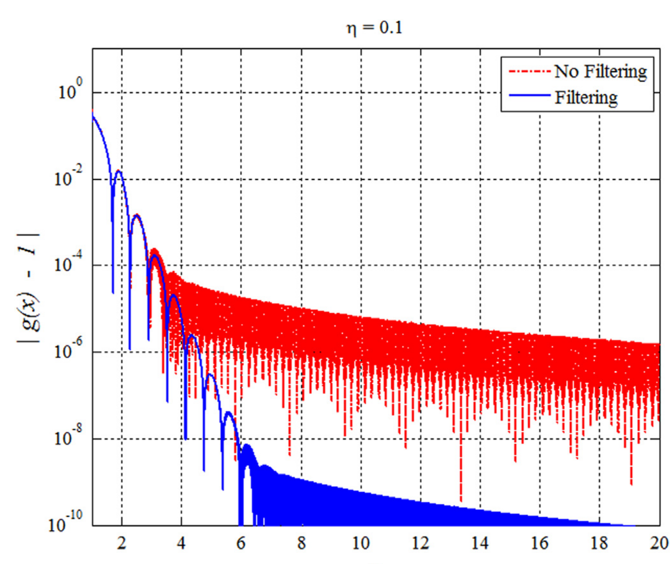

Fig. 2. Comparison of the original and filtered FT method as a function of the scaled distance for the volume fraction of 0.1.