A parametric algorithm for computing scattering for distributions of spherical particles(Readme)

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1 Homogeneous spheres

This algorithm computes the scattering integral for homogeneous spheres given by:

$$I = \int_{x1}^{x2} \int_{m1}^{m2} p(m,x) C_{sca} dm dx$$

For an arbitrary probability density function $p(m,x)$. It uses Gaussian quadrature to reduce the number of evaluations of the integrand and then uses the periodicity of the scattering cross-section C_{sca} to compute by approximating it by a sinusoidal form. The descriptions of the functions and scripts used are given below.

1.1 sin_sq_alpha_along_mx_c_curves

This script approximates the periodicity of $\sin^2 \alpha_n$ and $\sin^2 \beta_n$ by calling the function calc_period for a c($c = mx$), the mode number n and the range of index m. The average periods of $\sin^2 \alpha_n$ and $\sin^2 \beta_n$ are found for different parameters c and is observed to be an oscillatory function with decreasing amplitude. For example the average period for $\sin^2 \alpha$ for $n = 1$ looks like:

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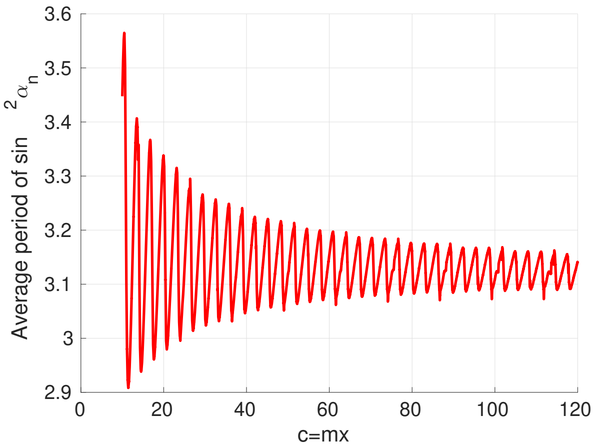

Figure 1: Average period T_α vs c

We can fit a function of c for the above, by doing a least square regression. We choose the basis functions of the form:

$$F_1(c) = p_1 \frac{1}{2c} + p_2 \frac{1}{2c^2} + p_3 \frac{sin(2c + (n-1)\pi)}{2c} + p_4 \frac{sin(2c + (n-1)\pi)}{2c^2} + \pi \quad (1)$$

$$F_2(c) = q_1 \frac{1}{2c} + q_2 \frac{1}{2c^2} + q_3 \frac{sin(2c + n\pi)}{2c} + q_4 \frac{sin(2c + n\pi)}{2c^2} + \pi \quad (2)$$

Where F_1 and F_2 are the basis functions for average period of $\sin^2 \alpha$ and $\sin^2 \beta$ respectively. The factor of $(n-1)\pi$ and $n\pi$ in F_1 and F_2 are due to the fact that it is observed that the oscillatory nature of the average periods changes phase by π for a change in the mode number by 1.

$$min(||T_\alpha(c) - f_\alpha(c)||_2) \implies \begin{bmatrix} \frac{1}{2c_1} & \frac{1}{2c_1^2} & \frac{\sin(2c_1)}{2c_1} & \frac{\sin(2c_1)}{2c_1^2} \\ \frac{1}{2c_2} & \frac{1}{2c_2^2} & \frac{\sin(2c_2)}{2c_2} & \frac{\sin(2c_2)}{2c_2^2} \\ . & . & . & . \\ . & . & . & . \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \\ p_3 \\ p_4 \end{bmatrix} = \begin{bmatrix} T_\alpha(c_1) \\ T_\alpha(c_2) \\ . \\ . \end{bmatrix}$$

$$min(||T_\beta(c) - f_\beta(c)||_2) \implies \begin{bmatrix} \frac{1}{2c_1} & \frac{1}{2c_1^2} & \frac{\sin(2c_1)}{2c_1} & \frac{\sin(2c_1)}{2c_1^2} \\ \frac{1}{2c_2} & \frac{1}{2c_2^2} & \frac{\sin(2c_2)}{2c_2} & \frac{\sin(2c_2)}{2c_2^2} \\ . & . & . & . \\ . & . & . & . \end{bmatrix} \begin{bmatrix} q_1 \\ q_2 \\ q_3 \\ q_4 \end{bmatrix} = \begin{bmatrix} T_\beta(c_1) \\ T_\beta(c_2) \\ . \\ . \end{bmatrix}$$

The coefficients p, q are found by using the inbuilt matlab solver. The coefficients p and q are stored in the variables Coeff_vec1, Coeff_vec2.
Alternatively, if one chooses to not mind a storage solution the average periods can be precomputed and stored.

1.2 calc_period

This function calculates the average periods of $\sin^2 \alpha_n$ and $\sin^2 \beta_n$. The function is called in the script sin_sq_alpha_along_mx_c_curves.m. Since $\sin^2 \alpha$ and $\sin^2 \beta$ are not *exactly* periodic but actually a weakly varying function of x, and to keep our model simple we calculate the average period by finding the points of minima/maxima of $\sin^2 \alpha_n$ and $\sin^2 \beta_n$ and finding the mean period by taking the mean of the difference between successive minima/maxima.

1.3 Scattering_eval

This script takes the inputs as the range of the limits of the integral I, the average periods and the nodes and weights for Gaussian quadrature(which are precomputed)-w_i, x_i and outputs the normalized scattering cross-section($k^2 \frac{C_{sca}}{2\pi}$) for the first three modes. The limits are assumed to be between $10 \leq x \leq 20$ for size parameter x and $1.2 \leq m \leq 1.8$ for index m. It calls the function gauss_quad_appx_algo which takes the ranges of m, x and the average periods of $\sin^2 \alpha$ and $\sin^2 \beta$ for the first 3 modes and gives the scattering cross-section as the output. Average periods for the first 3 modes for the given range have already been precomputed, stored and used in this script. Average periods for higher modes or for different ranges in m and x can be found by running the script sin_sq_alpha_along_mx_c_curves after making the appropriate changes.

1.4 gauss_quad_appx_algo

This function uses Gaussian quadrature in conjunction with trigonometric functions of form $\sin^2(T(x-c))$ to approximate the normalized scattering cross-section($k^2 \frac{C_{sca}}{2\pi}$). Where T is the average period of either $\sin^2 \alpha$ or $\sin^2 \beta$.

2 Layered spheres

The algorithm computes the scattering integral for layered spheres given by:

$$I = \int_{x1}^{x2} \int_{m1}^{m2} p(m,x) C_{sca} dm dx$$

For an arbitrary probability density function $p(m,x)$ over the 2D parametric space of the refractive index of the inner sphere m_1 and the size parameter of the inner sphere x. It uses Gaussian quadrature to reduce the number of evaluations of the integrand and then uses the periodicity of the scattering cross-section C_{sca} to compute by approximating it by using a nested trigonometric form.

2.1 sin_sq_alpha_along_mx_c_curves

This script approximates the periods and phase(ϕ) as a function of c, for $\sin^2 \alpha$ and $\sin^2 \beta$ by calling the function calc_period for a given c($c = m_1 x$), the range of the inner index m_1 and the mode number n.

2.2 calc_period

This function calculates the average periods of $\sin^2\alpha_n$ and $\sin^2\beta_n$. The function is called in the script sin_sq_alpha_along_mx_c_curves.m. Since $\sin^2\alpha$ and $\sin^2\beta$ are not *exactly* periodic but actually a weakly varying function of x, and to keep our model simple we calculate the average period by finding the points of minima/maxima of $\sin^2\alpha_n$ and $\sin^2\beta_n$ and finding the mean period by taking the mean of the difference between successive minima/maxima.
However unlike the homogeneous case $\sin^2\alpha_n$ and $\sin^2\beta_n$ cannot be fit with the approximation of $\sin^2(Tx+\phi)$ this is demonstrated for $\sin^2\alpha_1$:

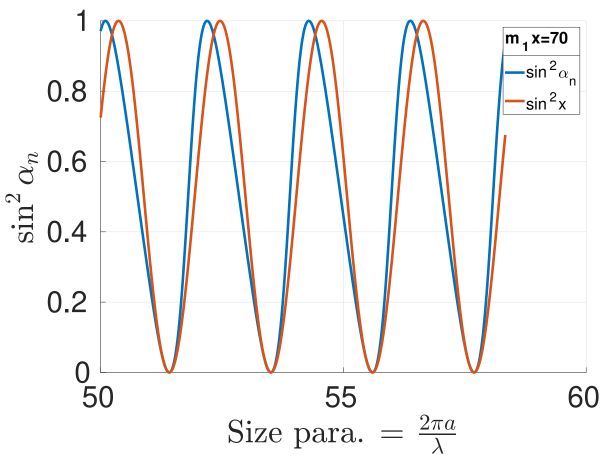

Figure 2: $\sin^2\alpha_n$ vs. inner size parameter x

Instead we use the nested trigonometric form for a given c:

$$f(x) = \frac{1}{t}\arctan\left(\frac{t\sin(Tx+\phi)}{1-t\cos(Tx+\phi)}\right)$$

Where T is the average period and ϕ is the phase which can be calculated for some initial value of $f(x)$. t is the degree of "slantness" and a value of 0.4 gives a reasonable accuracy. When $t=1$, $f(x)$ becomes

$$\arctan\left(\frac{\sin(Tx+\phi)}{1-\cos(Tx+\phi)}\right) = \arctan\left(\tan\left(\frac{x}{2}+\phi\right)\right)$$

Which is a sawtooth function. We can also see that when $t \to 0$,

$$\frac{1}{t}\arctan\left(\frac{t\sin(Tx+\phi)}{1-t\cos(Tx+\phi)}\right) \to \sin(Tx+\phi)$$

Which is a sinusoid. In order to scale the sinusoid to [0 1], we also need to perform a scaling of $f(x)$, so the fitting function becomes:

$$f_{fit}(x) = \frac{f(x)-min(f(x))}{max(f(x))-min(f(x))} \tag{3}$$

Where, f_{max}, f_{min} can be found by:

$$f_{max,min} = \pm\frac{1}{t}\arctan\left(\frac{t}{\sqrt{1-t^2}}\right) \tag{4}$$

Which for $t = 0.4$ becomes, $f_{max} = 1.0288$ and $f_min = -1.0288$. The phase ϕ can be found by substituting a minima $x = x_0$ in f_{fit} and noting that at the minima $f_{fit} = 0$. Thus solving the equation:

$$\frac{1}{t}\arctan\left(\frac{t\sin(Tx+\phi)}{1-t\cos(Tx+\phi)}\right) = -\frac{1}{t}\arctan\left(\frac{t}{\sqrt{1-t^2}}\right) \tag{5}$$

After some algebra we obtain:

$$\phi = -acos(t) - Tx_0 \tag{6}$$

We can then store the values of ϕ in an array.
The value of t, changes sign every alernate mode, and the values are always opposite in sign for the same mode for $\sin^2\alpha$ and $\sin^2\beta$. Thus $\sin^2\alpha_1\sin^2\beta_1 \leq 0$, $\sin^2\alpha_n\sin^2\alpha_{n+1} \leq 0$ and $\sin^2\beta_n\sin^2\beta_{n+1} \leq 0$

2.3 Scattering_eval

This script takes the inputs as the range of the limits of the integral I, the average periods, phase and the nodes and weights for Gaussian quadrature(which are precomputed)-w_i, x_i and outputs the normalized scattering cross-section($k^2\frac{C_{sca}}{2\pi}$) for the first three modes. The limits are assumed to be between $60 \leq x_1 \leq 100$ for inner size parameter x and $1.2 \leq m \leq 1.4$ for inner index m_1. The values of the outer index and size parameters are assumed to be constant and are equal to 1.51 and 150 respectively. Different values of outer indices and outer size parameters will change the average periods, phase ϕ and the parameter t, and they will have to be precomputed again my making the appropriate changes in the function calc_period.
The script calls the function gauss_quad_appx_algo which takes the ranges of m_1, x and the average periods and phase of $\sin^2\alpha$ and $\sin^2\beta$ for the first 3 modes and gives the scattering cross-section as the output. Average periods and phase for the first 3 modes for the given range have already been precomputed, stored and used in this script. Average periods for higher modes or for different ranges in m_1 and x can be found by running the script sin_sq_alpha_along_mx_c_curves after making the appropriate changes.

2.4 gauss_quad_appx_algo

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