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Gaussian random ellipsoid geometry-based morphometric recovery of irregular particles using light scattering spectroscopy

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Abstract

The purpose of this study is to extend the capabilities of multispectral optical imaging techniques for morphological characterization of irregular particles, encountered in several applications. We have utilized the Gaussian random ellipsoid model to quantize the shape elongation and deviation in complex-shaped particles. Compared with the Gaussian random sphere model, it is more realistic and is applicable to wider range of irregular particles with minimum possible of free parameters. By processing the reduced light scattering spectra, the proposed inverse technique can simultaneously recover the size, volume fraction, elongation, and shape deformation of particles that are randomly oriented within a colloidal suspension. The discrete dipole approximation is employed in forward light scattering calculations and input synthetic data generation. To investigate the robustness of our algorithm in coping with real scenarios, we have added different levels of noise to the observed scattering spectra. The results demonstrate the potential of our technique to non-invasively recover the morphology parameters of irregular particles.

1. Introduction

Optical imaging techniques are proven to be efficient tools for non-invasive particle characterization [1–3]. Particle size, shape and the composition are all important characteristics that are crucial to many applications. Such applications include, but not limited to, industrial processes, standardization, smoke and aerosol detection and biomedical applications [4–8]. The objective is to extract the particle size and shape distribution parameters by processing the scattered light spectroscopy measured from a cluster of particles. Despite the simplicity of the idea involved, the problem is challenging because of inherent characteristics of inverse scattering problems [9].

The inverse light scattering problems have been considered by several researchers in the past. However the current techniques suffer from limitations in dealing with irregular particles, encountered in many applications. To avoid the complex calculations, particles were mostly modeled as independent spherical or spheroidal scatterers with homogenous dielectric properties [1–8]. However these simplified models are insufficient or inaccurate for applications in which the particle morphology parameters needed to be retrieved.

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The scattering response from a system of spherical particles, sufficiently far enough from each other, can be fully described with these parameters only: a size distribution function and the refractive indices of particles and the ambient medium. However, for irregular particles in real applications, additional parameters such as shape, orientation, and composition become necessary.

The Gaussian random spheres and ellipsoids are among the non-spherical models which can describe the shape of irregular particles with minimum possible free parameters. They have been applied in numerous forward light scattering calculations using the discrete dipole approximation [10–12]. In the discrete dipole approximation, the shape of an irregular particle is represented by a system of dipoles. After solving a system of equations, which express the interactions between the incident light wave and the dipoles and the interactions between the dipoles themselves, the scattering response from the particulate system can be calculated straightforwardly [13–14]. This technique is suitable to compute light scattering from complex-shaped and/or heterogeneous particles.

The previous model was able to recover the size, concentration and the shape deformation of particles using the data collected at multiples wavelengths. However, the Gaussian random sphere model is not adequate when irregular particles exhibit some preferential elongation or flattening [12].

Using experimental data, we already extracted the aspect ratio (e) in spheroidal particles, with a T-matrix based inverse algorithm [2]. The aspect ratio (e) is the ratio of the equatorial radius to the polar radius of the base spheroid. We also developed a technique for inverting the particle irregularity by utilizing the Gaussian random sphere model [15]. For some applications, it is important to recover the particle irregularity and the aspect ratio, simultaneously. The method, suggested in this work, integrates the capabilities of these techniques and it is expected to produce more accurate results for characterization of natural particles. There are several types of elongated irregular particles to which our technique can be applied. For example, feldspar and goethite particles show prolate deformation under microscope [16–17]. More importantly, the light scattering from cells and some biological particles can be better calculated using the Gaussian ellipsoid model. From the microscopic images of the breast slices, we observed that irregular nuclei show prolate deformation ($e < 1$) [18]. Red blood cells are another example, appearing as distorted particles with oblate shapes ($e > 1$) [19].

The Gaussian random ellipsoid is an extension of the Gaussian random sphere since it degenerates to Gaussian sphere when the base elongation and flattening vanishes. The shape of a Gaussian random ellipsoid can be fully described by standard deviation of the radial distance, the power law index of the covariance function, and the particle effective size with its elongation/flattening.

To generate the Gaussian random ellipsoids, we have multiplied the Gaussian random sphere geometry by ellipsoidal shapes. The irregular particles are assumed to have been randomly dispersed within a suspension. They are illuminated by light beams and the resultant reduced scattering spectra are related to the parameters of interest using an integral expression.

We have used the reduced scattering coefficient since it is a prevalent light scattering parameter in biomedical applications, and is suitable for characterization of particles deeply located inside tissues with considering the effect of multiple photon scatterings [9]. Furthermore, measurements of the reduced scattering coefficient are compatible with our ten-wavelength diffuse optical tomography system [9, 20].

The multispectral diffuse optical tomography (MS-DOT) system measures the values of the photon density along the boundary of a phantom containing the scattering particles. Afterwards, a finite element based DOT inverse algorithm retrieves the reduced scattering spectra using the photon diffusion equation [9]. The reduced scattering spectra are then used to extract the morphological parameters of particles. Therefore, as well as experimental uncertainties, the numerical errors in both inverse techniques (DOT and the particle characterization algorithms) can influence the final results. Several types of experimental uncertainties are associated with the MS-DOT system, including the positioning of the source/detector sites, calibration errors and the noise caused by optical fibers. There are also some errors in the DOT algorithm such as cross-talk between the absorption and scattering coefficients. However, our DOT algorithm has demonstrated acceptable performance for retrieving the reduced scattering spectra in biomedical applications. For more details regarding the experimental uncertainties in the MS-DOT system, please see Ref. [9]

The synthetic data are first generated using the discrete dipole approximation technique. Afterward, we have developed and implemented an inverse technique, based on a regularized version of the Newton update scheme, to simultaneously retrieve the parameters of interest in the target inclusion(s) and the background region. We have assumed that the refractive indices of particles and the surrounding medium are *a priori* known parameters. It is still possible to extend the algorithm for cases in which the refractive indices of scattering particles are unknown, but such calculations become much more demanding.

2. Methodology

2.1 The Gaussian random ellipsoid model

In this work, the nodes in Gaussian random spheres are scaled according to the required aspect ratio (particle elongation) in order to generate the surface boundary of Gaussian random ellipsoids. This approach is slightly different from the one followed in Ref. [12]. Furthermore, we have assumed that the base ellipsoid has two axes of equal length, making it a surface of revolution (alternatively 3referred as spheroid). In Gaussian random sphere model, the irregular particle is described with the mean radius, standard deviation of the radial distance, and the power-law index of the covariance function [10]. In spherical coordinates, the radius of a Gaussian random sphere, $r(\theta, \varphi)$, is defined as:

$$r(\theta, \varphi) = \frac{r}{\sqrt{1+\sigma^2}} \exp \left(\sum_{l=0}^{\infty} \sum_{m=-l}^l s_{lm} Y_{lm}(\theta, \varphi) \right) \quad (1)$$

$s(\theta, \varphi)$ is the logarithmic radial distance, r and σ are the mean radius and standard deviation for the radial distance respectively, $Y_{lm}(\theta, \varphi)$ s represent orthonormal spherical harmonics and s_{lm} s are Gaussian random variables with zero means. In this work, the power-law index of the covariance function is fixed and chosen to be $\nu=4$, which corresponds to non-fractal shapes without sharp features in the particle geometry [10]. The parameter σ is a measure of particle irregularity and it is referred as particle shape deviation in this work.

The $\nu=4$ is a reasonable choice for Gaussian random ellipsoids. The reason is that Gaussian random ellipsoids, considered in this work, are produced by multiplying the geometry of a regular-shape spheroid with that of a Gaussian random sphere. Therefore, sharp features will not appear in the particle structure provided that they are not available in the corresponding random sphere geometry.

In Fig. 1, the geometries of a Gaussian random ellipsoid with different power-law indices of the covariance function are shown. The selection of a small power law index ($\nu=2$) causes

sharp features in the particle geometry while the selection of a large power law index ($\nu=6$) results in a more regular structure and cancels the effect of the shape deviation factor(σ).

Suppose that a cluster of irregular particles, modeled as Gaussian random ellipsoids, are randomly oriented and dispersed within a suspension, as shown in Fig. 2. Light sources, placed sufficiently far away from the suspension, illuminate the particles in the infrared range. The presence of particles perturbs the propagation of light waves and the scattering responses are recorded by the light detectors. The averaged reduced scattering coefficient, measured by the light detectors, is related to the particle morphology parameters through the following expression:

$$\mu'_s(\lambda) = \varphi \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} f(r, \varepsilon, \sigma) \left(\pi r^2 Q_{sca}(\sigma, r, \varepsilon, m, \lambda) (1 - g(\sigma, r, \varepsilon, \lambda)) \right) dr d\varepsilon d\sigma \quad (2)$$

Where $\mu'_s(\lambda)$ is the reduced scattering coefficient of the bulk suspension at a wavelength of λ . The concentration of particles is represented by the symbol φ . The particle effective radius (mean radial distance in Eq. 1) is represented by the symbol r . The aspect ratio is represented by the symbol ε . σ is the shape deviation factor (the standard deviation of the radial distance in Eq. 1). $Q_{sca}(\cdot)$ is the scattering efficiency and $g(\cdot)$ is the asymmetry parameter [21]. m is the relative refractive index of the scattering particles, with respect to that of the ambient medium.

$f(r, \varepsilon, \sigma)$ is a distribution function which statistically describes the random perturbations in the shape parameters of irregular particles. In this work, we have utilized a tri-variate normal distribution function with zero correlation between the three variables, which is expressed by the following equation.

$$f(r, \varepsilon, \sigma) = \frac{1}{(2\pi)^{3/2} s(r)s(\varepsilon)s(\sigma)} \exp \left(-\frac{1}{2} \left(\frac{(r-r_m)^2}{s(r)^2} + \frac{(\varepsilon-\varepsilon_m)^2}{s(\varepsilon)^2} + \frac{(\sigma-\sigma_m)^2}{s(\sigma)^2} \right) \right) \quad (3)$$

Where r_m , ε_m and σ_m are the mean values of the variables r , ε and σ , respectively. The corresponding standard deviations are represented by the symbols $s(r)$, $s(\varepsilon)$ and $s(\sigma)$, respectively.

In Eq. 2, the multiple light scatterings between the irregular particles are not taken into consideration and the relationship between φ and the scattering coefficient is linear. This assumption is good for dilute to moderately concentrated suspension. As the concentration of particles within the suspension increases, the particle-particle interactions become significant and the scattering response is no longer a linear function of particle concentration (φ). In such scenario, some modifications to Eq. 2 become necessary. In this work, the particle concentration is expressed by the volume fraction of scattering particles within a unit volume of the suspension.

The volume fraction is the percentage of one milliliter of suspension taken up by particles and it is related to the particle concentration (φ) through the following expression:

$$VF(\%) \approx 0.1 \varphi (\text{in million per cubic millimeter}) \times \frac{4\pi}{3} r_m (\text{in } \mu m)^3 \quad (4)$$

The parameters of interest which are to be extracted from the light scattering measurements include: particle concentration (φ), particle mean radius (r_m), particle mean aspect ratio (ε_m),

the particle mean shape deviation (σ_m), as well as the three standard deviations $s(r)$, $s(\varepsilon)$ and $s(\sigma)$. In this work we assumed that the initial values standard deviations equal to 10% of their corresponding mean values. In Fig. 3, samples of Gaussian random ellipsoids with different combinations of the shape deviation factor (σ) and the aspect ratio (ε) are shown.

2.2 Calculation of the scattering efficiency and the anisotropy parameter

The proposed inverse algorithm, which shortly will be described in more details, requires the values of the $Q_{sca}(\cdot)$ and $g(\cdot)$ at different combinations of particle mean radius (r_m), particle mean aspect ratio (ε_m) and the particle mean shape deviation σ_m at multiple wavelengths. In the database, the particle effective radius is in the range $r \in [r_{\min} \ r_{\max}]$. The aspect ratio varies in the range $\varepsilon \in [\varepsilon_{\min} \ \varepsilon_{\max}]$ and the shape deviation factor $\sigma \in [\sigma_{\min} \ \sigma_{\max}]$. The bounds of these intervals are indicated according to the required application.

The values of $Q_{sca}(\cdot)$ and $g(\cdot)$ are calculated using the discrete dipole code (DDSCAT) and are averaged over several particle orientations [13–14, 22]. As the values of the particle shape deviation (σ) or the aspect ratio increase, the number of dipoles needed to accurately represent the irregular particle increases proportionally. This implies higher computational costs, which is to be expected.

In our discrete dipole database, the particle mean radius varies in the range of 0.1 μm –1 μm with the step of 0.1 μm and the shape deviation (σ) changes from 0.0 to 0.5 with the step of 0.05. The aspect ratio (ε) changes in the range of 0.5–1 with steps of 0.1. The discrete dipole database consists of 660 data per wavelength, which are averaged over 196 particle orientations.

The method chosen for solving the linear system in discrete dipole computations is called “BiConjugate Gradient with Stabilization”. More details about this technique are given in Ref. [23]. The maximum allowed tolerance is 10^{-5} . Maximum number of iterations is 300. However the solution converges fast in our calculations.

In Fig. 4, for different aspect ratios, the numbers of dipoles, required for discrete dipole calculations, are shown as functions of the shape deviation factor (σ). The plots show slight increasing trends, as the particles become more irregular.

The input data consists of reduced scattering spectra generated at eight wavelengths in the infrared range: 638 nm, 673 nm, 690 nm, 733 nm, 755 nm, 808 nm, 840 nm and 915 nm. The irregular particles are, assumedly, made of polystyrene with the refractive index of ~ 1.59 . The refractive index of polystyrene slightly varies over the wavelengths. The refractive index of the ambient medium, in which the particles are suspended, is 1.33 (e.g water). In this work, we assumed that the scattering particles are prolate-like, with an aspect ratio of smaller than 1.0 and they are randomly oriented within the ambient medium.

2.3 The Inverse algorithm

Our inverse algorithm is newton-based optimization approach, accompanied with the regularization schemes, which minimizes the discrepancy between the observed reduced spectra $\mu'_s(\lambda_j)^o$ and the calculated ones $\mu'_s(\lambda_j)^c$ using Eq. 2. Where $\lambda_j, j=1, 2 \dots$ are the measurement wavelengths.

$$\text{Find } \varphi, s(r), r_m, s(\sigma), \sigma_m, s(\varepsilon) \text{ and } \varepsilon_m \text{ .st. } \chi^2 = \sum_{\lambda_j} (\mu'_s(\lambda_j)^o - \mu'_s(\lambda_j)^c)^2 \text{ is minimum.} \quad (5)$$

If the vector $\Delta\chi$ represents the error between the observed and calculated reduced scattering coefficients and $\Delta\zeta$ is the vector updating the parameters of interest, as follows:

$$\Delta\chi = [\mu'_s(\lambda_1)^o - \mu'_s(\lambda_1)^c, \dots] \quad (6)$$

$$\Delta\zeta = \begin{bmatrix} \Delta\varphi & \Delta s(r) & \Delta r_m & \Delta s(\sigma) & \Delta\sigma_m & \Delta s(\varepsilon) & \Delta\varepsilon_m \end{bmatrix} \quad (7)$$

Then according to Newton's method, $\Delta\zeta$ is calculated by solving the following matrix equation:

$$J^T \Delta\chi^T = J^T J \Delta\zeta^T \quad (8)$$

where J is the Jacobian matrix. The elements of the Jacobian matrix are computed by direct derivation of Eq. (2) with respect to the model parameters (φ , $s(r)$, r_m , $s(\sigma)$, σ_m , $s(\varepsilon)$ and ε_m). For example, the element in the first row, second column of the Jacobian matrix is calculated as follows:

$$J_{12} = \frac{\partial \mu'_s(\lambda_1)}{\partial s(r)} = \varphi \int_{r_{\min}}^{r_{\max}} \int_{\sigma_{\min}}^{\sigma_{\max}} \int_{\varepsilon_{\min}}^{\varepsilon_{\max}} \left(\frac{\partial f(r, \varepsilon, \sigma)}{\partial s(r)} \right) (\pi r^2 Q_{sca}(\sigma, r, \varepsilon, m, \lambda) (1 - g(\sigma, r, m, \varepsilon, \lambda))) dr d\varepsilon d\sigma \quad (9.a)$$

$$\frac{\partial f(r, \varepsilon, \sigma)}{\partial s(r)} = \frac{(r - r_m)^2 - s(r)^2}{(2\pi)^{3/2} s(r)^4 s(\varepsilon) s(\sigma)} \exp \left(-\frac{1}{2} \left(\frac{(r - r_m)^2}{s(r)^2} + \frac{(\varepsilon - \varepsilon_m)^2}{s(\varepsilon)^2} + \frac{(\sigma - \sigma_m)^2}{s(\sigma)^2} \right) \right) \quad (9.b)$$

To combat the ill-conditioned Jacobian matrix in Eq. (8), we employed a scheme known as Tikhonov-Marquardt regularization [24]:

$$(J^T J + \alpha I) \Delta\zeta^T = J^T \Delta\chi^T \quad (10)$$

where α is an appropriately chosen regularization parameter and I is the identity matrix. After solving (10) for $\Delta\zeta$, the parameters of interests are subsequently updated. Newton-type optimization algorithms, including ours, are sensitive to initial guesses chosen for unknown parameters. Therefore, the reconstruction algorithm is preceded by pre-processing algorithm, which finds the appropriate values for the initial parameters such that the error between the observed and the calculated scattering spectra becomes minimum in a range of possible values for the four parameters of interest [2, 9, and 15].

The inverse algorithm recovers the particle size, volume fraction, shape deviation (σ) and the aspect ratio (ε) at all computational nodes belonging to either the target inclusion or the background region.

Most of the computational time is consumed for the generation of the discrete dipole database (several days). However, it is a one-time calculation for certain refractive indices chosen for the particles and the ambient medium. The total time for the initial parameter search and the reconstruction algorithms is about 5 minutes for 100 iterations.

3. Results and Discussion

In this section, we present some results obtained from our particle characterization algorithm, recovering the morphology parameters of irregular particles, based on the

Gaussian random ellipsoid geometry. There are two regions of interest in which the unknown parameters are to be extracted: The target inclusions with cylindrical boundary embedded off-center in the background with cuboidal shape. The irregular particles are present in both the inclusions and its surrounding medium. However, the particles in the cylindrical inclusion(s) exhibit more irregularity relative to the ones suspended in the background region.

3.1 Example one: single target inclusion embedded within a cuboidal background

The first example considers the reconstruction of particle morphology parameters inside a cylindrical inclusion embedded in a cuboidal background. The input data are synthetic and they are generated using Eq. 2 for the both regions with different parameters. In Table 1, the parameters chosen for the target inclusion and the background region are given. The particle size, volume fraction and the shape deviation have larger values in the target inclusion compared with those in the background region. On the other hand, the irregular particles suspended in the target inclusion demonstrate a more elongation which corresponds to a smaller aspect ratio.

We added different levels of the Gaussian noise to $\mu'_s(\lambda_j)$, generated by Eq. 2, and then the scattering data are fed into the reconstruction algorithm, elaborated in section 2.

The Gaussian noises are added to the values of reduced scattering coefficients at all computational nodes. In Fig. 5, the maps of reduced scattering coefficients at the shortest and the longest wavelengths are shown.

It is evident that as the wavelength of illuminating light wave increases, the resultant reduced scattering coefficient becomes smaller. In Fig. 6, the four reconstructed parameters using 10 % noise corrupted data are shown.

According to the obtained results, the recovered parameters are in relatively good agreement with the exact ones, presented in Table 1. There are some artifacts on the background region, due to the noise. However the target inclusion and its perimeter are clearly distinguishable from the background region. The reconstruction error which is defined by the following equation drops to 1.9% after 100 iterations.

$$\text{Error function(normalized)} = \sqrt{\sum_{\lambda_j} (\mu'_s(\lambda_j)^o - \mu'_s(\lambda_j)^e)^2} / \sqrt{\sum_{\lambda_j} (\mu'_s(\lambda_j)^o)^2} \quad (11)$$

We have also conducted other tests with 20% and 50% noise in the input scattering data. The final reconstruction errors for these cases drop to 3.7% and 9.7%, respectively. In Fig. 7, the quantitative plots of the four recovered parameters along line $y=0$ which passes through the target center are shown. As the level of noise in input data increases, the particle morphology parameters are reconstructed with larger discrepancies relative to the exact ones. However, even with 50% noise in the input data, the target location and the relative contrasts in the parameters are of interest are recovered reasonably well.

3.2 Example 2: two target inclusions embedded within a rectangular background

This example considers a more complex situation in which two targets with different particle morphology parameters are embedded in the background region. The parameters chosen to generate the synthetic scattering data are presented in table 2. The particles suspended in target one, centered at (15 mm, 0), scatter the light waves more strongly than those in target two, centered at (-15 mm,0) and the background region. This fact is observable from the

larger values of the reduced scattering coefficient at the target one position. In Fig. 8, the images of reduced scattering coefficients, with 10% added noise, at the first and last wavelengths are shown.

In Fig. 9, the two-dimensional maps of the four reconstructed parameters using 10% noise corrupted data in the XY plane are shown. Compared with the previous example, more artifacts and distortions appear in the reconstructed images. In Fig. 10, the reconstructed parameters along the line $y=0$, which passes through the targets centers, are presented. Results using 10% -noise and 20%-noise are similar and they are slightly better than those using 50% noise in input data. The final reconstruction errors for these cases are 1.8%, 3.9% and 10%, respectively (Eq. 11).

It is worth noting that the search and reconstruction algorithms are exactly the same for all the cases presented in this work.

As observed from Figures 10c and 10d, the effect of adding different levels of noise is not clear from the reconstructed aspect ratio (e). However, the reconstruction of other parameters show improvement as the noise level in the input data decreases. This could be due to the fact that we have chosen a relatively larger step for the aspect ratio ($\Delta e=0.1$), compared with the step chosen for the shape deviation ($\Delta \sigma=0.05$), in order to avoid excessive computational burden. As the number of unknown parameters increases, Newton-based optimization techniques could become more sensitive to the noise in the input data.

3.3 Error analysis

In this section, the errors in the reconstructed parameters, for all the examined cases, are presented. It should be noted that, the maximum error in the iterative optimization algorithm, defined by Eq. 11, is 10% even when the noise in the input data is as high as 50%. This implies that the inverse algorithm reasonably finds the optimum parameters. However, the errors in the reconstructed parameters (particle size, volume fraction, aspect ratio and the shape deviation) are generally larger. In Table 3, the mean percentage errors in the recovered parameters are presented at the target locations. The mean percentage error is defined as:

$$MPE\% = \frac{100}{n} \sum_{i=1}^n \frac{|P_{exact}(i) - P_{rec}(i)|}{P_{exact}(i)} \quad (12)$$

where n is the number of data points, P_{exact} is the exact parameter (see Tables 1 and 2) and P_{rec} is the recovered parameter.

According to Table 3, the particle sizes are recovered more accurately compared with the other parameters. The errors in the recovered volume fractions are relatively higher when two target inclusions with different parameters are embedded in the background medium. The errors in the shape deviation and the aspect ratio are also acceptable, particularly for the configuration with one target inclusion.

In the presented technique, the refractive indices of particles and the ambient medium have to be *a priori* estimated. This is a requirement for generating the scattering database needed for the inverse technique. Our group has already developed a technique to retrieve the refractive indices from optical measurements [9].

The refractive indices can have variations over wavelengths. But, all particles are assumed to be homogenous with identical refractive indices, at a specific wavelength. However, particles may have different refractive indices in a realistic setting.

It should be noted that, the effect of refractive index perturbations will appear in the reduced scattering coefficient. We tested our algorithm with up to 50% noise in the reduced scattering spectra. Therefore, it is reasonable to expect a tolerable performance from the algorithm in dealing with particles with small perturbations in their refractive indices.

In an alternative approach, one could generate the scattering database with a range of refractive index variations. In this case, the parameter optimization has to be done for several combinations of the particle size, aspect ratio, volume fraction, shape deviation and refractive index. Therefore, the computational time and burden will increase proportionally.

The inverse algorithm can be modified for other distribution functions, simply by replacing $f(\cdot)$ in Eq. 3, by other shape distribution functions such as log-normal or power-law distributions. This information is usually available depending on the application.

The proposed technique is good for dilute to moderately concentrated suspension, up to 16% VF [19]. For dense suspensions, highly multiple light scattering effects have to be taken into account in the particle scattering model. In that case, the reduced scattering coefficient is no longer a linear function of the particle concentration (ϕ) in Eq. 2. One way to work around this issue is by using static and angle-integrated structure factors [25].

4. Conclusions

In this work, we have developed and implemented an inverse technique for evaluating the morphological parameters of irregular and complex-shaped particles. Based on the Gaussian random ellipsoid geometry and the reduced scattering spectra, our technique can simultaneously and non-invasively recover the particle concentration and the three morphological parameters.

The proposed method has several limitations in dealing with particles in real applications. First, the scattering particles and the ambient medium are assumed to have constant refractive indices. Second, the effects of multiple scattering and sharp features in particle geometry are not considered. Finally, a database, containing the light scattering from Gaussian random ellipsoids with different combinations of the particle size, aspect ratio and the shape deviation, has to be *a priori* calculated and stored for the inverse technique.

Since the discrete dipole approximation is a volume-based light scattering technique, it is applicable to particles with heterogeneous dielectric properties. In addition, the algorithm can be extended for characterization of particles with more complex geometries, in the expense of considerably higher computational demand.

It should be noted that the morphological characterization of irregular particles is a challenging task. Different particle models, light scattering techniques and inverse schemes need to be integrated for this purpose. However, compared with our previously developed T-matrix based algorithm, the proposed technique can quantitatively recover the particle irregularity. This capability benefits many biomedical applications.

We plan to test our method against experimental data (e.g. for breast cancer detection) and to extend its capabilities for more generalized cases in the near future.

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Research Highlights

- Gaussian ellipsoid geometry is used to describe the shape of irregular particles.
- Discrete dipole method is utilized in forward scattering calculations.
- Four morphological parameters are simultaneously recovered using light measurement.
- The algorithm is compatible with diffuse optical tomography measurements.
- Our technique has relatively robust performance against noisy data.

Fig. 1.
The geometry of a Gaussian random ellipsoid with different power law indices of the covariance function

Fig. 2.
Irregular particles within a suspension are illuminated by light beams

Fig. 3. Gaussian random ellipsoids with different combinations of the aspect ratio and the shape deviation factor.

Fig. 4.
The number of dipoles representing the Gaussian random ellipsoid as a function of shape deviation for different aspect ratios

Fig. 5.

Reduced scattering coefficients at the shortest and longest wavelengths (a) μ'_s (mm⁻¹) at 638 nm (b) μ'_s (mm⁻¹) at 915 nm.

Fig. 6. two-dimensional maps of the reconstructed parameters using 10% noisy data (a) mean particle mean ($2 r_m$) (b) Volume fraction (%) (c) Shape deviation (σ_m) (d) Aspect ratio (ϵ_m)

Fig. 7. Quantitative plots of the reconstructed parameters along line $y=0$ passing through the target center, (a) particle size (b) volume fraction (c) shape deviation (d) aspect ratio

Fig. 8. Reduced scattering coefficients at the shortest and longest wavelengths for two target inclusions (a) μ'_s (mm⁻¹) at 638 nm (b) μ'_s (mm⁻¹) at 915 nm.

Fig. 9. two-dimensional maps the reconstructed parameters using 10% noisy data (a) mean particle mean ($2 r_m$) (b) Volume fraction (%) (c) Shape deviation (σ_m) (d) Aspect ratio (ϵ_m)

Fig. 10. Quantitative plots of the reconstructed parameters along line $y=0$ passing through the two target centers, (a) particle size (b) volume fraction (c) shape deviation (d) aspect ratio

Table 1

The exact parameters chosen for the cylindrical target inclusion and the cuboidal background

Region/Parameter	Particle size ($2r_m$)	Volume fraction	Shape deviation (σ_m)	Aspect ratio (e_m)
Target inclusion centered at (15 mm,0)	1.6 μm	1.0 %	0.3	0.5
Background	0.8 μm	0.05 %	0.05	1.0

Table 2

The exact parameters chosen for two cylindrical targets and the cuboidal background

Region/Parameter	Particle size ($2r_m$)	Volume fraction (%)	Shape deviation (σ_m)	Aspect ratio (e_m)
Inclusion#1 Centered at (15 mm,0)	1.6 μm	1.0	0.2	0.5
Inclusion#1 Centered at (-15 mm,0)	1.2 μm	0.5	0.3	0.7
Background	0.8 μm	0.05	0.05	1.0

Table 3

Mean Percentage Errors (MPE %) in the recovered parameters at the target locations

Configuration/ Parameter	Particle size ($2r_m$)	Volume fraction (VF%)	Shape deviation (σ_m)	Aspect ratio (e_m)
10% noise, one target	8.1%	19%	8%	20%
20% noise, one target	11.8%	36%	23%	27%
50% noise, one target	6.1%	18.8%	17.7%	26%
10% noise, two targets	6.7%	10.3%	40%	15%
20% noise, two targets	14.5%	37%	47%	19%
50% noise, two targets	22.1%	69%	45%	10%