Modelling and validating average waves in random particulate materials

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Abstract

When you measure the scattered field from a material filled with randomly placed particles, you will have to perform the measurement many times, and then take the average, to get a repeatable result. How then do you relate this average measurement to the particles? Here we show how to mathematical model this average scattering, and present results on validating these models against heavier Monte Carlo simulations. The recent breakthrough that has enabled us to achieve a broadband numerical validation of the theory is that we now have rigorous models for scattering from a sphere filled with particles. A sphere, in contrast to a plate or halfspace, filled with particles can be easily simulated with a Monte Carlo approach.

Keywords: multiple scattering, random media, particulate. pair correlation

1 Introduction

Detailed derivations are given in [1]. Below we give a brief overview. To define the average scattered wave from a random particulate, we first need to define the scattered wave from just one configuration of particles. Figure 1 illustrates a scattered wave from one configuration, and the average over all particle configurations.

For a point $\boldsymbol{r}$, outside of all particles, we can write the total field $u(\boldsymbol{r})$ as a sum of the incident wave $u_{\text{in}}(\boldsymbol{r})$ and all scattered waves:

$$u(\boldsymbol{r}) = u_{\text{in}}(\boldsymbol{r}) + u_{\text{sc}}(\boldsymbol{r}), \tag{1}$$

$$u_{\text{sc}}(\boldsymbol{r}) = \sum_{i=1}^{J} \sum_{n} f_n^i \mathrm{u}_n(k\boldsymbol{r} - k\boldsymbol{r}_i), \tag{2}$$

where $\boldsymbol{r}_i$ is a vector pointing to the centre of the i-th particle, we assumed $|\boldsymbol{r} - \boldsymbol{r}_i| > a$ for $i = 1, 2, \ldots J$, with a being the particle radius, the u_n are the basis of outgoing spherical waves, and the coefficients f_n^i can be determined by applying the boundary conditions on all particles

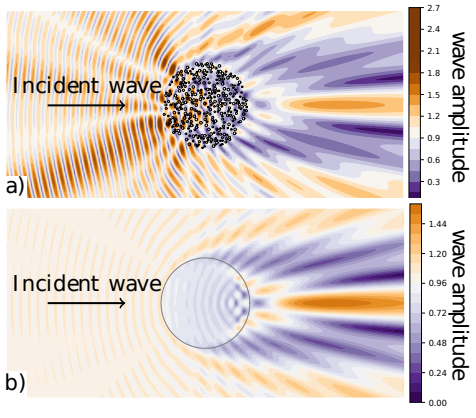

Figure 1: Scattering of an incident plane-wave from a) a sample of $J = 330$ particles, and b) the ensemble average of the scattered field over all possible particle positions. Taken with permission from [1].

(not shown). The field $\sum_n f_n^i \mathrm{u}_n(k\boldsymbol{r} - k\boldsymbol{r}_i)$ is the wave scattered from the i-th particle.

By taking an ensemble average of the above, and assuming all particles are the same, we reach

$$\langle u_{\text{sc}}(\boldsymbol{r})\rangle = J \sum_n \int_{\mathcal{R}} \langle f_n\rangle(\boldsymbol{r}_1) \mathrm{u}_n(k\boldsymbol{r} - k\boldsymbol{r}_1) p(\boldsymbol{r}_1) \mathrm{d}\boldsymbol{r}_1,$$

where $\mathcal{R}$ is the region where the particle centres are contained, $p(\boldsymbol{r}_1)$ is the probability of finding a particle centred at $\boldsymbol{r}_1$, when the position of all other particles is not known. The $\langle f_n\rangle(\boldsymbol{r}_1)$ are determined by ensemble averaging the boundary conditions (not shown above), which results in

$$\langle f_n\rangle(\boldsymbol{r}_1) = T_n G_n(\boldsymbol{r}_1) + \tag{3}$$
$$T_n \int_{\mathcal{R}} \mathcal{U}_{n'n}(k\boldsymbol{r}_1 - k\boldsymbol{r}_2) \langle f_{n'}\rangle(\boldsymbol{r}_2, \boldsymbol{r}_1) g(\boldsymbol{r}_1, \boldsymbol{r}_2) \mathrm{d}\boldsymbol{r}_2,$$

where $\mathcal{U}_{n'n}(k\boldsymbol{r}_1)$ is a translation matrices, composed of known special functions, and $G_n(\boldsymbol{r}_1)$ depends on the incident wave. The $g(\boldsymbol{r}_1, \boldsymbol{r}_2) = \frac{p(\boldsymbol{r}_1, \boldsymbol{r}_2)}{p(\boldsymbol{r}_1)p(\boldsymbol{r}_2)}$ is the pair-correlation , and the T_n is the T-matrix which describes scattering from just one particle. If $g(\boldsymbol{r}_1, \boldsymbol{r}_2)$ and T_n were known, then the aim is use the above to solve for $\langle f_n\rangle$.

The above equation is exact, with no approximations. It is similar to Dyson's equation, which is typically used by the physics community.

1.1 Statistical assumptions

To solve (3) it is typical to make some assumption about $g(\boldsymbol{r}_1, \boldsymbol{r}_2)$, and how $\langle f_{n'}\rangle(\boldsymbol{r}_2, \boldsymbol{r}_1)$ is related to $\langle f_{n'}\rangle(\boldsymbol{r}_2)$. The simplest assumptions are

$$g(\boldsymbol{r}_2; \boldsymbol{r}_1) \approx \begin{cases} 1 & \text{for } |\boldsymbol{r}_1 - \boldsymbol{r}_2| \geq a_{12}, \\ 0 & \text{for } |\boldsymbol{r}_1 - \boldsymbol{r}_2| < a_{12}, \end{cases} \tag{4}$$

and $\langle f_{n'}\rangle(\boldsymbol{r}_2, \boldsymbol{r}_1) \approx \langle f_{n'}\rangle(\boldsymbol{r}_2)$ for $|\boldsymbol{r}_1 - \boldsymbol{r}_2| \geq a_{12}$, which are called *hole correction* and the *Quasi Crystalline Approximation*. There are many different models for $g(\boldsymbol{r}_2; \boldsymbol{r}_1)$ that represent clumped materials, or even particles on a lattice. For particles distributed randomly, according to a uniform probability density, a more accurate modal is called the Percus-Yevick pair-correlation.

We will discuss validating these assumptions, and how these lead to analytic solutions below.

2 Effective waves

A key development has been to show that (3), together with the statistical assumptions above, leads to two simpler equations

$$\langle f_n\rangle(\boldsymbol{r}_1) = \sum_{n'} \int_{\partial\mathcal{B}} W_{nn'}(\boldsymbol{r}_2)\langle f_{n'}\rangle(\boldsymbol{r}_2 + \boldsymbol{r}_1)\mathrm{d}\boldsymbol{r}_2$$

$$G_n(\boldsymbol{r}_1) = \sum_{n'} \int_{\partial\mathcal{R}} B_{nn'}(\boldsymbol{r}_1 - \boldsymbol{r}_2)\langle f_{n'}\rangle(\boldsymbol{r}_2)\mathrm{d}\boldsymbol{r}_2$$

where $\mathcal{B}$ is a small ball depending only on the particle geometry, and $W_{nn'}$ and $B_{nn'}$ are known special functions. The first equation we call *the ensemble wave equation*, as it does not depend on the incident wave, or the geometry of the whole material $\mathcal{R}$, and can specify completely the modes of $\langle f_n\rangle(\boldsymbol{r}_1)$. The second equation we call the *ensemble boundary conditions*, as it depends on the incident wave and material geometry, and is needed to specify the amplitude of the modes of $\langle f_n\rangle(\boldsymbol{r}_1)$.

With the equations above we can calculate the average scattering from a material (filled with a random particulate) of any geometry. In particular, we choose a sphere filled with particles, as this allows us to achieve something that has long been a goal: a robust and broad numerical validation of typical statistical assumptions, see Section 1.1. A sphere filled with a finite number of particles is far easier to numerically simulate. We also make use recent developments in numerical techniques to perform Monte Carlo simulations [2, 3].

For most particle volume fractions, the results are similar to Figure 2. That is, the effective waves solution is equivalent to a direct numerical solution of (3), and the heavier Monte Carlo simulations agree well when using the Percus-Yevick approximation to calculate the pair-correlation. These results give confidence that the analytic methods shown here could form the basis for quantitative sensing of particulate materials.

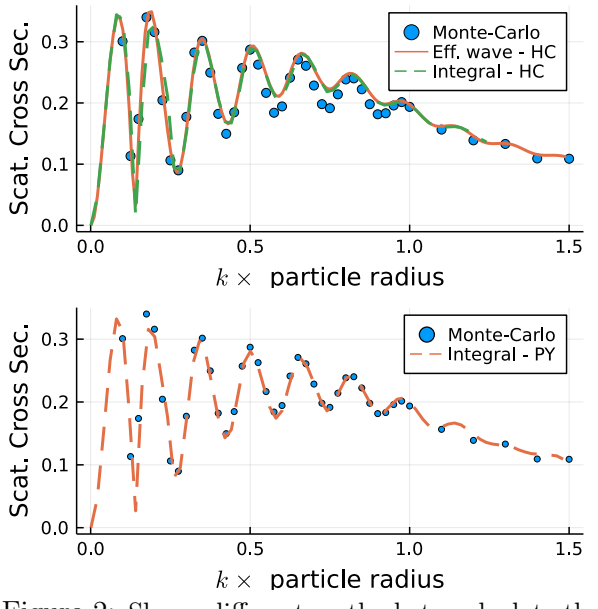

Figure 2: Shows different methods to calculate the average scattering cross section from a sphere, filled a 15% particle volume fraction, for different incident waves lengths. Monte-Carlo simulates hundreds of different particle configurations explicity. Eff. wave uses the Effective wave, and Integral uses a numerical method to solve equation (3). HC refers to using hole correction, shown in Section 1.1, where PY refers to the pair-correlation called Percus-Yevick.

References

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